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A risk assessment tool for highly energetic break-up events during the atmospheric re-entry

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Declaration

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Dated: January 9, 2017

Abstract

Most unmanned space missions end up with a destructive atmospheric re-entry. From ten to forty percent of a re-entering satellite's mass may survive re-entry and hit the Earth's surface. This has the potential to be a hazard to people, fauna, flora and produce economic damage.

The severe consequences of inaccurate predictions of the area where the debris can re-enter and land result in the need to consider all the possible causes of fragmentation. This thesis proposes and discusses the application of two Bayesian statistical models, designed to be the principles that underlie a new risk assessment tool for the modelling of the fragmentation of a spacecraft, caused by highly energetic break-up events during the atmospheric re-entry. This new tool is required to evaluate with a certain degree of uncertainty if such events can occur and, in an affirmative case, to provide the characteristics of the fragments.

Risk assessment for re-entering spacecraft is made difficult because there is very little historical information. As a consequence both the models incorporate a strategy to make the most by the judgement of atmospheric re-entry experts.

This dissertation summarises the work executed within the European Space Agency Network Partnering Initiative (reference No. 4000106747/13/NL/GLC/al).

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All models are wrong, but some are useful.

George Box

Chapter 1

Introduction

1.1 Background

Most of the unmanned space missions end up with a destructive atmospheric re-entry.

During the decay, from space to Earth, the vehicle enters into denser regions of the atmosphere at a very high velocity, exceeding speeds twenty times faster than a speeding bullet (at orbital speed, around 7.6 km/second)(www.aerospace.org, n.d.). This causes the object to be decelerated abruptly, the structure to be exposed to aerodynamic loads that can exceed ten times the acceleration of gravity and to a friction that heats up the object so that some of its components can reach their melting point or ablate. Eventually the combinations of these events cause the spacecraft to break apart by the failure of critical structural components and/or by an explosion. The former case can be defined as a low energetic break-up event, while the latter highly energetic break-up event. Unfortunately it is not easy to establish which one of these two types of events has occurred, considering how difficult is to observe and ascertain this kind of phenomena.

The resulting fragments will further travel the atmosphere and each of them can experience further fragmentation, completely demise, by melting or ablation, as long as sufficient heating and loads exist. The same happens for all the fragments generated afterwards. During the descent the surviving debris lose speed and begin to cool until they free-fall and impact the ground.

Even if they hit the Earth's surface at relatively low speed, they can still represent a hazard to people, fauna, flora and cause economic damages.

1.2 Research aims

This thesis describes a Bayesian statistical approach for the modelling of the fragmentation of a spacecraft, caused by an highly energetic break-up event during the atmospheric re-entry. It consists of two statistical models developed in order to meet the following objectives:

- Assessment of the probability for an highly energetic break-up event to occur during the atmospheric re-entry;
- Prediction of the statistical distribution of the masses of the generated fragments.

The proposed statistical models have been designed in order to be the principles that underlie a new probabilistic analysis tool for the re-entry risk assessment in case of highly energetic break-up events. Their application do not constitute a complete risk analysis, but only a component of it, as there is no work on the consequence side of risk.

The new probabilistic analysis tool is required to provide all the information that the re-entry analysis tool ASTOS (Aerospace Trajectory Optimization Software) needs to predict the propagation of the fragments generated by an highly energetic break-up event. ASTOS is currently used in the Guidance navigation and control section of the European Space Agency (ESA TEC-ECN), who proposed and supported the work behind this thesis. The implementation and integration of the proposed models into ASTOS can lead to the development of a complete risk assessment solution for highly energetic break-up event.

Specifically, the new probabilistic analysis tool must evaluate with a certain degree of uncertainty if, where, and how many times a highly energetic break-up event can occur during the atmospheric re-entry of a space vehicle and, in an affirmative case, to provide the characteristics of the generated cloud of debris. A cloud of debris is defined by all those physical features that allow to predict its propagation, its re-entering trajectory and particularly which fragments will hit the Earth and where. These physical features are: number of fragments and, for each fragment, mass, material composition, shape, area-to-mass ratio, ejection velocity, position (longitude, latitude and altitude) of the fragmentation event. The reader is referred to the book (Klinkrad, 2010) for

further information about debris propagation, re-entry prediction and on-ground risk estimation.

We propose to name this new tool ABBRA (Atmospheric Break-up Bayesian Risk Analysis). The models described in this thesis must function in a coordinated way to accomplish ABBRA's objectives:

1. Compute the probability for an highly energetic break-up event to occur, given informations about the spacecraft structure at the end-of-life (at the beginning of the de-orbiting phase) and its re-entering trajectory;
2. In case this probability is large enough, compute the number of fragments and characterize the generated fragments in terms of probability distributions;
3. Evaluate if there are fragments containing elements capable of provoking an other highly energetic break-up event and, in an affirmative case, repeat 1 and 2.

1.3 Research motivation

Many tools have been designed in order to predict how the fragmentation process occurs and much effort is still being made to improve their accuracy. It is not surprising if we think that even a small fragment coming from space could pose a threat to people and assets if it impacts the Earth's surface where it is not supposed to land.

The severe consequence of such an event results in the need to analyse all the possible re-entry cases, particularly considering that the number of re-entries, controlled and uncontrolled, will probably increase over the next few years.

A weak point of most existing re-entry analysis tools is the lack of a proper modelling of the fragmentation caused by an explosion, that can occur during the atmospheric re-entry. We faced the challenge to develop a model aimed to fill this gap.

This explains the need of a dedicated re-entry highly energetic break-up events model, able to characterize the generated fragmentation cloud in terms of statistical distributions.

The choice of a statistical approach was driven by the idea of exploiting the stochastic nature of the fragmentation process, while the Bayesian approach has been considered suitable because it allows to integrate expertise and data collection. This is a

problem where real data are scarce but physical knowledge is extensive, even if many uncertainties are involved.

1.4 Thesis contribution

This dissertation contributes to the area of Bayesian statistics applications for complex models with missing data. Specifically, it introduces:

- A model for the exploitation of the expert opinion in risk assessment;
- A model for the prediction of a fragmentation process.

The novel contribution is mainly in the application domain, or better in the use of existing stochastic models to a new situation.

Furthermore the proposed models contribute in the area of risk assessment for spacecraft re-entry:

- Introducing a new strategy never considered so far: the Bayesian approach;
- Exploiting data from real cases of fragmentation and explosions and combining them with the background knowledge.

1.5 Outline of Thesis chapters

We conclude our introduction with an outline of the content of the various chapters of this thesis.

- In *Chapter 2* the reader is introduced to the problems associated with a destructive spacecraft atmospheric re-entry and to the deterministic tools currently used to model this kind of phenomena. By underlining the limitations of these methods, we motivate the necessity of studying the development of a Bayesian statistical approach;
- *Chapter 3* summarizes the research methodology that was followed during the course of our research;
- *Chapter 4* presents the relevant literature review;

- *Chapter 5* provides an overview of the available and exploitable data and about what could be retrieved in the future. Furthermore it explains the issues related to the problem of missing data and details the expert opinion elicitation process, conducted in the European Space Research and Technology Centre (ESA-ESTEC).
- *Chapter 6* illustrates the proposed risk assessment model and an idea for the application to the evaluation of an highly energetic break-up to occur during the atmospheric re-entry. This model is defined as a Belief-network model for failure prediction and it combines the fault tree analysis and an elicitation process that is inspired by the multi criteria decision making method, called Analytic Hierarchy Process. It is a model calibrated by an integration of expert opinion with sparse data.
- *Chapter 7* describes the proposed Bayesian fragmentation model with missing data. It is a procedure for the construction and the inference of a distribution over the partitions of the unit interval, generated by a partially random fragmentation process.
- *Chapter 8* concludes the thesis with several remarks of future work.
- The *Appendices A,B,C,D* provide an overview of the applied statistical topics:
 - The Bayesian approach and the sampling methods exploited for the inference;
 - The Fault tree analysis used as framework of the proposed risk assessment model;
 - The Expert opinion with particular attention to the Analytic Hierarchy Process applied for the expert opinion elicitation in the risk assessment model;
 - The stick breaking process which inspired the fragmentation model.
- Example of expert surveys and a timeline of the whole project are reported *Appendix E* and *Appendix F* .

Chapter 2

Research description and objectives

2.1 Introduction

In this chapter, the reader is introduced to the problems associated with a destructive spacecraft atmospheric re-entry. After a description of what is a destructive re-entry and what are the connected issues, we provide an overview of the deterministic tools currently used to model this kind of phenomena. Then we underline the limitations of these methods in order to motivate the necessity of studying the development of a statistical approach, that is the research question of this thesis. Finally, we explain why the Bayesian approach is relevant for this problem.

2.2 The destructive spacecraft re-entry

Whenever possible, spacecraft ¹ should perform a safe re-entry, or where appropriate manoeuvred into a graveyard orbit (above 2000Km), at the end of their operational phases.

This is recommended by the Inter-Agency Space Debris Coordination Committee (IADC) Mitigation Guidelines (IADC Coordination Committee, 2007) and it is necessary to limit the interferences with objects in operation. Similarly, Space agencies and the United Nations developed regulations to reduce lifetime of space vehicles and then to mitigate collision risk (e.g. Klinkrad (2003), UNCOPUOS (2007), UN (2002)). For instance, In Europe, on a cooperative basis amongst the interested national space

¹A vehicle designed for travel or operation in space beyond the Earth's atmosphere or in orbit around the Earth. We call it spaceship or space vehicle too.

agencies, the European Code of Conduct for Space Debris Mitigation (ASI, BNSC, CNES, DLR, ESA, 2004) has been compiled and formally adopted. ESA defined specific requirements on space debris mitigation (ESA, 2008*b*) applicable to all ESA space systems orbiting the Earth or re-entering the Earth's atmosphere.

First, we are going to provide an overview of the re-entry disposal mechanisms, the spacecraft fragmentation process and the associated risk, explaining what can differ in the outcome between a low energetic and a highly energetic break-up event.

Furthermore we present an example of vehicle which performed safe re-entries and whose re-entries has been the subject of many risk assessment studies concerning the probability of explosion: the Automated Transfer Vehicle.

2.2.1 Re-entry disposal mechanisms

The atmospheric re-entry can be uncontrolled (natural decay) or controlled.

The artificial satellites ², orbiting around the Earth, would continue to orbit forever if gravity were the only force acting on it, but it is not. There exist other forces acting on the satellite to perturb it away from the nominal orbit: the luni-solar attraction, the perturbation due to the non-spherical geopotential ³, the solar radiation pressure and obviously the atmospheric drag.

The atmospheric drag acts in the opposite direction of motion and it is a non-conservative, energy dissipating perturbation. This is the major cause of a natural decay. The atmospheric drag is due to the frequent collisions between the spaceship and the surrounding air molecules, for this reason it increases with the density and the atmospheric density increases as the altitude decreases. Hence the dissipating action is greater at lower altitudes. For this reason, objects orbiting in the Low Earth Orbit ⁴, or simply LEO (hundreds of kilometres in altitude), may decay naturally by atmospheric drag within weeks, months, or years depending on the object and its altitude, while objects at higher altitudes may remain in orbit for hundreds or thousands of years. The consequent energy reduction of the satellite causes the orbit to get smaller, leading to further increases in drag. Eventually, the altitude of the orbit becomes so small that

²A man-made object put into orbit around a celestial body

³The Earth has not a spherically symmetric mass distribution. Indeed, the Earth has a bulge at the equator, a slight pear shape, and flattening at the poles.

⁴LEO orbits are usually the place of earth science, observation, monitoring and communications missions.

the satellite re-enters the atmosphere. This disposal method leads to a random fashion re-entry and then to a large uncertainty about where on Earth the object will actually land. A 10-minute error in the prediction of the re-entry time is enough to obtain 3000 miles of uncertainty in the impact point Patera and Ailor (1998).

On the other hand, we talk about controlled re-entry when a propulsive capability is used to steer the spacecraft towards the re-entry more quickly and to target it to a specific safe landing area, under supervision. This disposal method requires more attention in the planning, execution and follow through, in particular if we consider that a spacecraft due to re-entry is normally near to its end-of-life.

The reader is referred to Gallais (2007) and Tewari (2007) for a more detailed comprehension of the atmospheric re-entry of spacecraft.

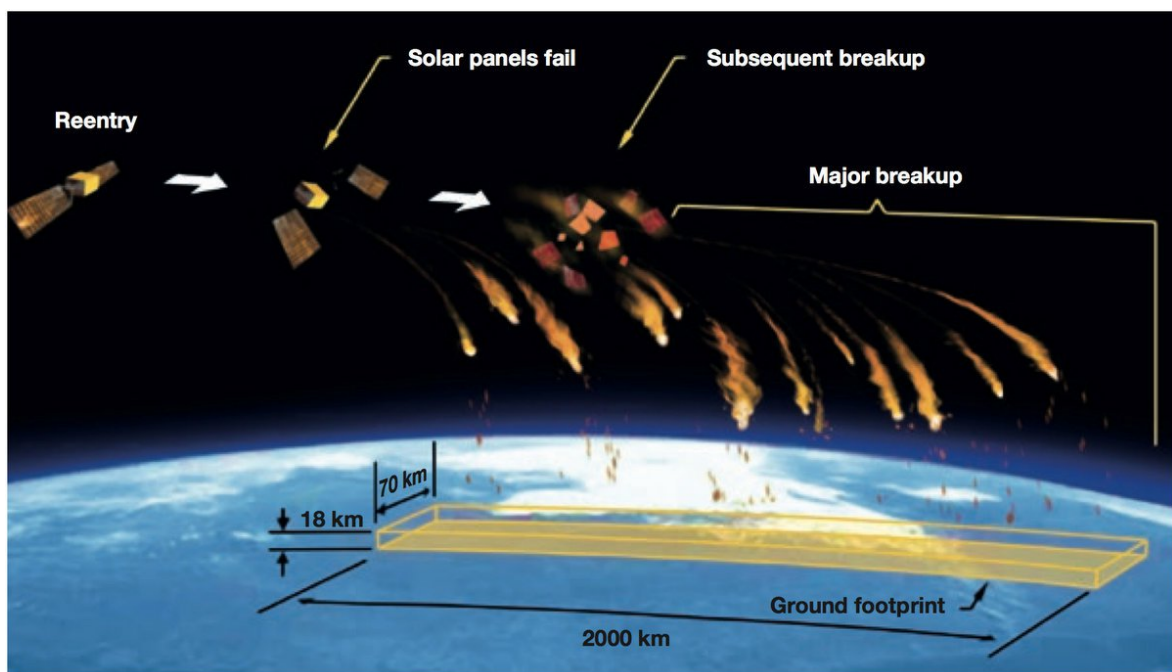


Fig. 2.1: The stages of the spacecraft break-up during the atmospheric re-entry. Credits: Space Safety magazine IAASS

2.2.2 Spacecraft re-entry fragmentation and risk

As already mentioned in 1.1, during the decay, the space vehicle experiences severe heating and loads that cause its fragmentation.

During the descent, the first components that get detached from the main body and break into fragments are usually the solar panels, the antennas and other protruding



Fig. 2.2: On the left: tank recovered in Texas in 2003. This object fell from the disintegrating Space Shuttle Columbia. Photograph: Steve Liss/Corbis. Source: The Guardian UK. On the right: debris of decaying satellite found about 150 kilometres outside of Cape Town in April 2000. Photograph: Enver Essop/EPA. Source: The Guardian UK.

elements. This is followed by one or more major break-up events, that generally involves all the structure and that occurs at an altitude between seventy and ninety kilometres. The level of energy released by these major break-up events depends on the causes: there are circumstances where explosions can be triggered and in this case an higher level of energy will be released. In this thesis we use the expressions highly energetic break-up event and low energetic break-up events to distinguish respectively the break-up due to an explosion from the failure of the supporting structure due to the effects of the aerodynamic loads.

The resulting fragments will follow trajectories based on the state vector at the separation and their own ballistic coefficients⁵. They can suffer further fragmentation and generate smaller debris or completely demise, by melting or ablation. The same happens for the new debris as long as sufficient heating and loads exist Patera and Ailor (1998). Some of them can survive, lose speed and begin to cool until they free-fall and impact the ground.

Fortunately no casualties or injuries have been reported from components of re-entering spacecraft until now: based on the available reports, it seems that only one person has been struck-but not injured-by a lightweight fragment of a re-entering satellite in Oklahoma in 1997. If a spacecraft is to be disposed of by re-entry into the atmosphere, debris that survives to reach the surface of the Earth should not pose an undue

⁵The ballistic coefficient is defined as the ratio $\frac{M}{C_d A}$ where M is the mass of the object, C_d is the drag coefficient and A the cross-sectional area.

risk to people or property. Limiting the amount of surviving debris and confining the debris to uninhabited regions, such as broad ocean areas, may accomplish this. The reader can get a clear idea of the hazards associated with the spacecraft re-entry from the examples of recovered debris showed in Figures 2.2, 2.3.

Sophisticated simulations (Anselmo and Pardini (2005), Rochelle et al. (1999), Fritsche et al. (2000)) and the analysis of retrieved spacecraft debris (Sgobba et al., 2013) suggest that about 10-40 per cent of a spacecraft mass may survive the re-entry (Klinkrad (2010), Ailor et al. (2005)).

First of all, the actual percentage changes with the re-entering vehicle features (materials, mass, size, shape). Moreover it depends on the steepness of the re-entry trajectory and the energy released during the break-up. For this reason it is fundamental to predict which kind of break-up event occurs, if low energetic or highly energetic.

The probability of survival for a specific component is mainly determined by the materials used in its construction, the size and its position. For example, magnesium and aluminium structures tend to fail at an altitude of approximately 78 km (Sgobba et al., 2013), while components made of materials with high melting temperatures, such as stainless steel, titanium, and glass, often survive and reach the ground. The larger debris with moderate melting temperatures have higher chances of survival, because they can radiate a greater amount of heat, taking advantage of their large surface areas. When a component is shielded by other resistant components or contained within the body of the vehicle and then protected by surrounding structure, it may survive even if it is made of a low melting temperature material (Sgobba et al., 2013).

The surviving debris ground footprint is typically 1000-2000 km long. Generally, the cross track dispersion of the potentially hazardous fragments is less than a few tens of kilometers, but smaller debris may be found farther because of the wind (Anselmo and Pardini, 2013).

In order to minimize the safety risk of the space flight projects, it is fundamental to identify the hazardous conditions and accident scenarios as well as the probabilistic assessment of their consequences (Opiela and Matney, 2004). In order to assess the damage caused by these surviving objects, with steadily increasing numbers of space objects and increase of possible candidates for ground impact, it is crucial to have a tool able to predict the mass of impacting fragments, their features, their re-entry



Fig. 2.3: Space debris, belonging to a Russian Zenit-3 rocket, recovered In March 2011, in Colorado. Source: Aircraft-Info.net

trajectory and finally the area where they will hit the Earth.

2.2.3 The Automated Transfer Vehicle reentry: study case

The Automated Transfer vehicles are good examples of spacecraft which performed safe re-entries subject to the risk of explosion.

ATV overview

The Automated Transfer Vehicle (ATV) was an indispensable ISS (International Space Station) supply spaceship, developed by the European Space Agency and European Industry. By delivering experimental equipment, propellants and goods for the permanent crew, it provided for years the European contribution to the Space Station operating costs (ESA, 2008*a*).

From 2008 to 2015, the ATV delivered up to 7.7 tonnes of cargo to the ISS, which is located 400 km above the Earth. Furthermore it had the task to lift the ISS to a higher orbital altitude in order to compensate the altitude loss of the station due to atmospheric drag. Each ATV remained attached as a pressurised and integral part of the Station for about half a year, before performing a controlled destructive re-entry into the Earth's atmosphere, with on board up to 6.4 tonnes of material and general waste no longer necessary on the Station.

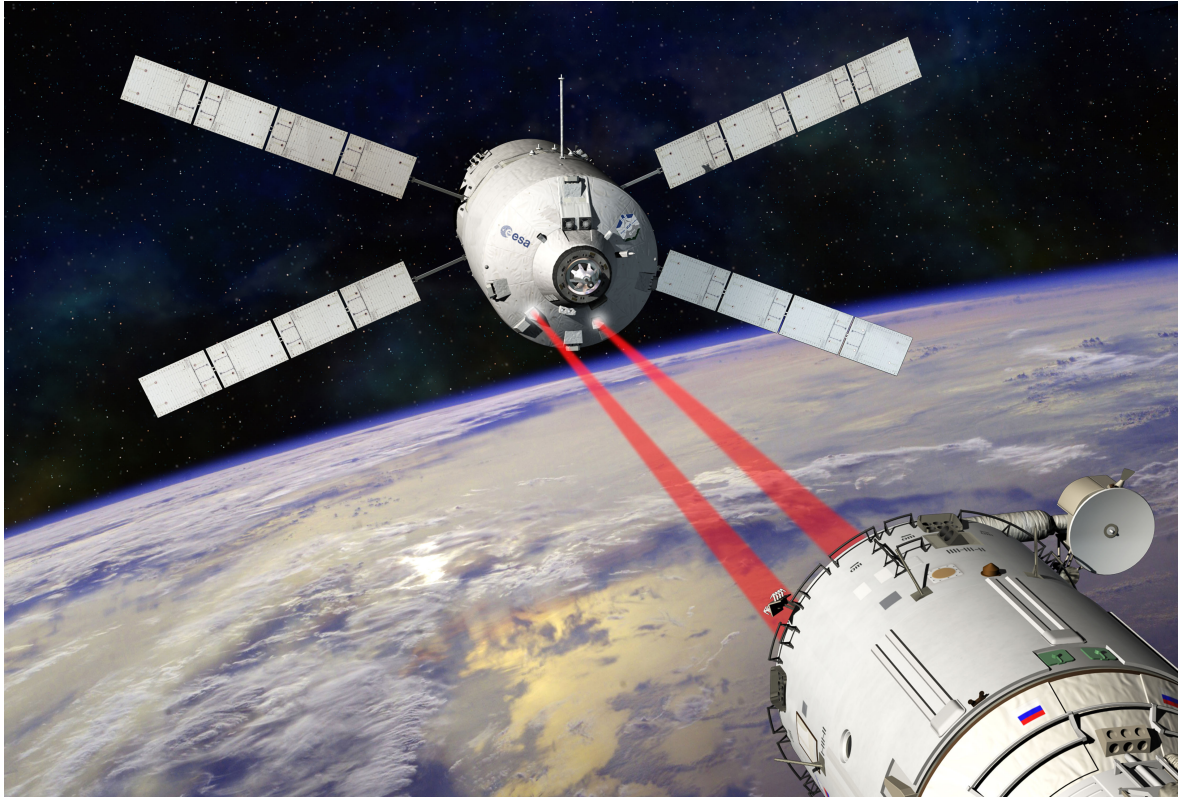


Fig. 2.4: Artist's impression showing ATV-5 docking with ISS. Credits: ESA Space in images

Five ATVs, ATV-1 Jules Verne, ATV-2 Johannes Kepler, ATV-3 Edoardo Amaldi, ATV-4 Albert Einstein, and ATV-5 Georges Lemaitre were launched, with the first launched in March 2008 and the last one in 2014 and all of them performed a successful controlled re-entry.

The main body of ATV was a cylinder, 10.3 metres long and up to 4.5 metres in diameter (ESA, 2008a). As the reader can see in the figure 2.7, X-shaped metallic blue solar arrays extended outward from the main body.

Inside, it was constituted of two elements. The first one was the spacecraft sub-assembly (SCS) equipped with propulsion (propulsion tanks and thrusters) and avionics bays (batteries, gyroscopes, and harness). The second part was the integrated cargo carrier, containing the equipped external bay (water and gas tanks, web structure) and the equipped pressurized module (containers, cargo, and the attitude control thrusters). The material list of which the subsystem of ATV 1 Jules Verne was made contains about 100 different collection types: from Titanium to Aluminum, from Beryllium, to carbon fiber, etc.

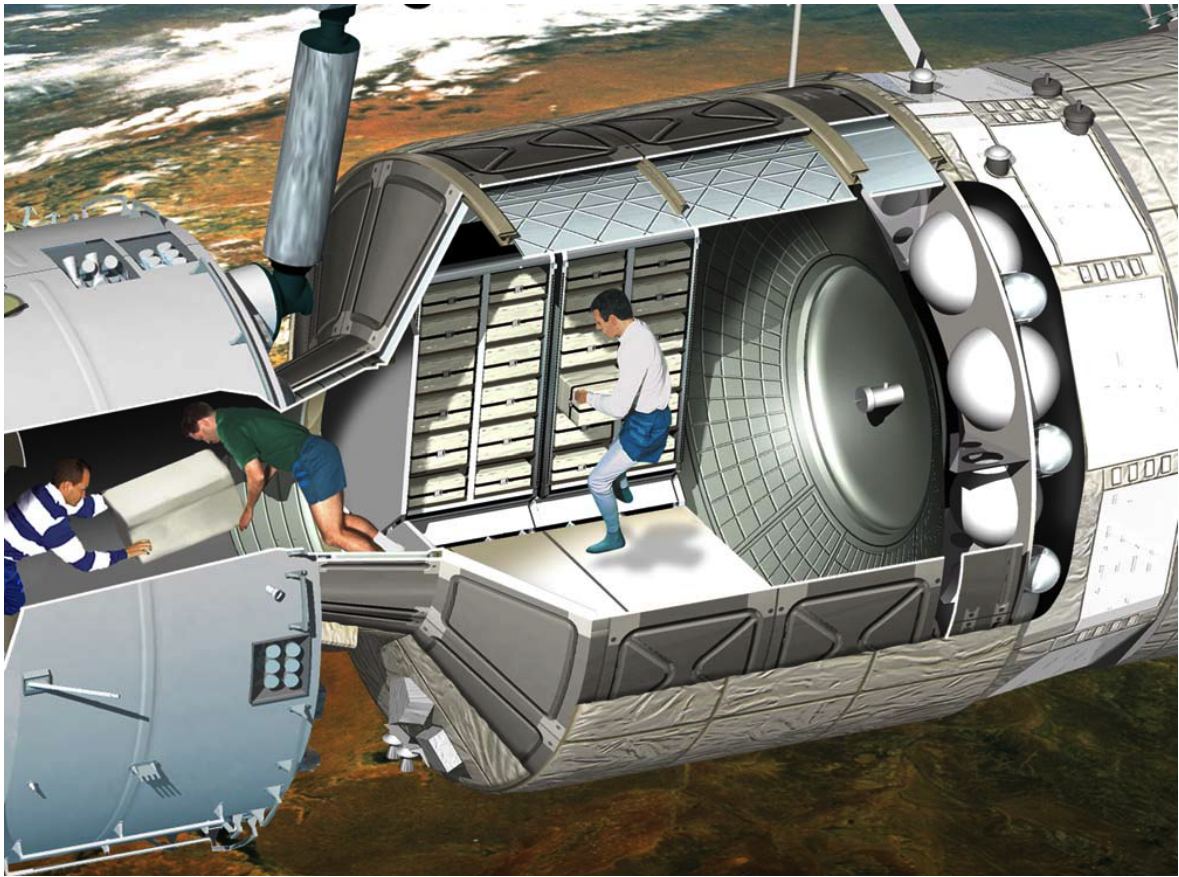


Fig. 2.5: Artist's impression of the ATV Cargo Carrier attached to the ISS. Credits: ESA Space in images

ATV re-entry

ATV was intentionally designed for controlled re-entry (as the Japanese ISS cargo HTV). The manoeuvre plan is detailed in (Labourdet et al., 2008). After the undocking from the ISS, thrusters were planned to use their remaining fuel to de-orbit the spacecraft and then to initiate a safe controlled destructive re-entry into the SPOUA (South Pacific Uninhabited Area), a predefined uninhabited South Pacific area.

The planning of a safe controlled re-entry mission, compliant with the current requirements established to reduce orbital lifetime for satellites, requires a significant amount of work in terms of predictive studies. Many analysis have been conducted for ATVs, in order to forecast the impact area of the surviving fragments, taking into account all the possible perturbations: altitude of fragmentation, de-orbit manoeuvre accuracy, atmospheric drag, debris behaviour, meteorological effect and, as already

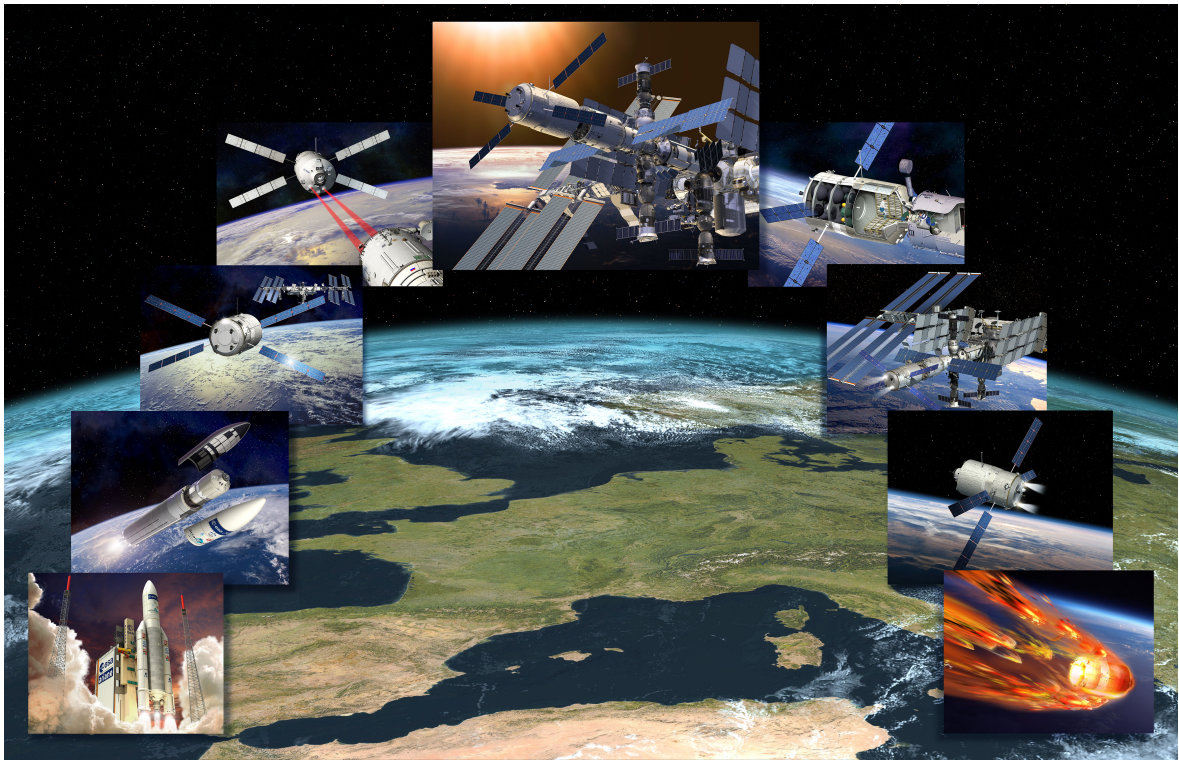


Fig. 2.6: ATV-5 mission scenario. Credits: ESA Space in images



ISS017E015496

Fig. 2.7: ATV seen from the station. Credits: ESA Space in images

mentioned, explosion potentials.

Scientists considered various circumstances, which could create an explosion environment, e.g. the ignition of residual hypergolic propellants upon exposure to the hot and reactive flow environment or tank bursting (Schmehl et al. (2005), Fritsche et al. (2005*a*)). A detailed analysis of the re-entry is reported in (Koppenwallner, Fritsche, Lips, Martin, Francillout and De Pasquale (2005), Fritsche et al. (2001)).

Some ATV cargo vehicles hosted a device called Reentry Breakup Recorder (Weaver and Ailor, 2012) (REBR), designed to gather data about temperature, acceleration, rotation rate, internal pressure and to transmit them to Earth during the break-up (Tosney and Cheng, 2015). REBR was not designed to survive re-entry, but the communications transmitter was encased in a spherical ceramic heat shield to withstand the high temperature, then send images before impacting the ocean. Unfortunately in most cases data could not be retrieved:

- In ATV-2 REBR failed;
- In ATV-3 REBR functioned nominally and data was probably transmitted during the break-up;
- In ATV-5 REBR failed. It is interesting to note that the also the Japanese i-Ball camera (JAXA, 2007) was planned to fly with ATV-5, but unfortunately it was lost in the Antares rocket explosion in October 2014.

In 2008, ATV-1 was observed via a dedicated airborne re-entry observation campaign (see for more details Chapter 5). ATV-4 was only observed from the International Space Station. Scientists worked for more than a year to organize a new airborne observation campaign for ATV-5, the final one. In order to record the break-up under better conditions, a modified re-entry profile was planned, at a shallower angle than usual. Unfortunately a battery failure in one of the freighter's four power chains cropped up few weeks before the planned re-entry date: this event led the ESA officials to decide to go for a standard steep profile and the observation campaign to be cancelled.



Fig. 2.8: Artist's impression of the ATV burning up in Earth's atmosphere at the end of its mission. Credits: ESA/D.Ducros

2.3 Re-entry analysis tools overview

The models developed in order to predict how a spacecraft shatters into pieces into the atmosphere during its re-entry to Earth, usually called re-entry analysis tools, simulate the physics of re-entry, taking into account the trajectory, atmosphere, aerodynamics, aero-thermodynamics, and thermal/ablation aspects. They are deterministic models and they forecast and analyse the fragmentation triggered by events like the excess of a critical temperature or a certain percentage of melted material.

These models vary considerably in their modelling approach and the accuracy level they can provide. They can be classified under two main categories (Wu et al., 2011):

- Object oriented codes;
- Spacecraft oriented codes.

2.3.1 Object-oriented code and Spacecraft-oriented code

Object-oriented methods assume that at a certain altitude (usually in the range 75-85 Km) the spacecraft is decomposed into its individual elements. The entry body is treated as a set of elementary geometric shape objects covered by one or more containers: upon melting of one of these the internal objects are released. The parent body trajectory is run until the assumed break-up altitude, then for each critical element of the decomposed spacecraft a destructive re-entry analysis is performed.

This approach simplifies significantly the geometric spacecraft definition and all the re-entry analysis, taking into consideration only the critical parts and neglecting the complete spacecraft assembly. Thus the computational time of the entire analysis and the difficulties of the preparatory work are strongly reduced, but clearly some incompleteness may occur, e.g. the effect of the protection of internal spacecraft parts by the outer shells is totally ignored.

Examples of object oriented codes are:

- NASA Object Re-entry Survival Analysis Tool (ORSAT (Dobarco-Otero et al., 2005));
- SESAM and SERAM (Spacecraft Entry Survival Analysis Module and Spacecraft Entry Risk Analysis Module), included in ESA Debris Risk Assessment and Mitigation Analysis (DRAMA (Martin, 2005));
- DARS (Debris Analysis for Re-entering Spacecraft) and RAM (Risk Analysis Module), included in ESA ASTOS (The Aerospace Trajectory Optimization Software (Weikert et al., 2013), (Ortega et al., 2008));
- DEBRISK Omalý and Spel (2012).

Spacecraft-oriented codes model the entire spacecraft as a single entity. Geometries are not simplified approximations, but are complex representations based on the actual spacecraft design. Flow-fields around the spacecraft are calculated to determine accurate aerodynamic and thermal characteristics. Fragmentation events are based on simulated melting and mechanical demise rather than a single event at a pre-determined altitude. They analyse the re-entry of a complete spacecraft with its complete dynamics and the objects are continuously separated from the parent body. In contrast to the

object-oriented tools each modelled part has a certain position, instead of just assuming that it is placed somewhere inside the container. SCARAB (Spacecraft Atmospheric Re-entry Aero-thermal Break-up) is currently the only known spacecraft oriented code.

SCARAB development started in 1995 with a European Space Operation Center (ESOC) contract awarded to HTG (Hyperschall Technologie Göttingen) with Institute of Theoretical and Applied Mechanics (ITAM, Russia), Grupo de Mecanica del Vuelo (GMV, Spain) and Fluid Gravity Engineering (FGE, United Kingdom) (Koppenwallner, Fritsche, Lips and Klinkrad (2005)). SCARAB is capable of modelling tank explosions.

Finally SAM (Spacecraft Aerothermal Module) is recently developed tool that lies between both the categories, object-oriented and spacecraft-oriented, as described in (Merrifield et al. (2014), Beck J. (2014)).

These re-entry analysis tools provide very good results, with different level of accuracy, in the case of lowly energetic break-up events, due to aerodynamic forces, but all of them lack a proper modelling for the cases of highly energetic break-up (e.g. high-speed atmospheric explosion). A good comparison of the commonly used re-entry analysis tools is detailed in Lips and Fritsche (2005).

2.3.2 Strategies and assumptions

Break-up altitude

In the object-oriented method the altitudes of the break-up events are fixed and user defined, while in SCARAB they are computed by analysing the actual acting mechanical and thermal loads. Modelling the spacecraft with secondary containers, multiple break-up events can also be considered, as in ORSAT and in DARS models. DARS allows the user to define additional break-up altitudes.

It is fundamental to note that at the moment SCARAB is the only tool including a method for the assessment of the break-up altitude.

The upper margin for the ground risk will strongly depend on the assumed break-up altitude. The ground risk will increase with decreasing break-up altitude. When the assumption that the individual destructive re-entry of the spacecraft parts only starts at a fixed break-up altitude (which is usually unknown a priori), implies that the heating at a higher altitude of initial parent object is ignored and consequently

each child object is exposed with the same starting temperature.

Material properties

All material properties in DARS and in SESAM are assumed to be temperature independent. SCARAB and ORSAT take into account the emissivity as temperature dependent property. ORSAT considers also the oxidation heating. The oxidation process produces heat which is absorbed by the surface wall of the object. The amount of the transferred heat is based on the chemical heating efficiency factor, which is a property included in ORSAT database. In addition to the most common materials used for spacecraft, the newest versions of SCARAB database includes also liquid or gaseous tank contents, non metallic ceramics, glasses or plastics, and orthotropic, multi layered composites. Liquid and gaseous tank contents have been modelled as virtual solids. Various assumptions have been made (Lips et al., 2004):

- Tank contents are assumed as fixed and do not slosh around in the tank;
- The melting temperature is set to very high values in order to ensure that no melting occurs;
- The density results from the volume of the tank and the mass of the content and it is assumed as constant until a possible tank bursting event;
- Strength and elasticity are both zero, because a virtual solid cannot take any forces;
- Thermal properties like heat capacity and thermal conductivity must be determined for the mean operating pressure of the tank.

Plastics (also in composite form like carbon fiber reinforced plastic, CFRP) are very problematic materials: they do not melt at high temperature, but they are destroyed in a combination of sublimation, oxidation, and other types of chemical reactions or decompositions at molecular level.

Thermal and aero-thermal analysis

For thermal analysis object oriented tools use the lumped mass method for all object types, therefore an object is assumed to demise once the total cumulative heat load

reaches the material heat of ablation. These models are not able to predict partial melting of objects. If an object does not totally melt away, it will survive to the ground in its entirety. Consequently the computed casualty area for a surviving object could be larger than if layers were enabled to melt away during re-entry as in the heat conduction model. It's right to point out that the lumped mass method can be a valid approach for objects too thin to be modelled accurately with many layers. SCARAB uses a 2-dimension heat conduction model.

2.3.3 Discussion

Computational time

Given the lowest number of simplifications SCARAB is the slowest tool among those described. A simple run could take even many days. In other re-entry tools there are no appreciable differences with regard to the computational time: it depends on the number of fragments and for each fragment a run could take seconds or minutes.

Uncertainties

In all the re-entry analysis there are always some variables that are not exactly known. The following can be considered causes of errors:

- Atmosphere model deficiency: questionable assumptions are required in the characterization of the applied pressure load in space and time (Field Jr and Grigoriu, 2006);
- Uncertainties in solar and geomagnetic activity forecast;
- Unknown spacecraft attitude and attitude evolution;
- Poor data on the mass and geometry of the spacecraft;
- Errors in the initial orbit state.

Sensitivity analysis

A careful analysis of likely parametric variations in the initial conditions at re-entry is needful for a scrupulous risk evaluation of impacting debris. Studies showed that it

could be stated that the risk probability of an impact increases by as much 100%, even if there is only a 10% variation in the orbital parameters (Tewari, 2009). Particularly with regard to the unknown initial conditions for uncontrolled re-entering spacecraft, this could make questionable the use of deterministic approaches.

2.3.4 Modelling of spacecraft explosion during the re-entry

Due to the lack of alternatives, a model developed for explosions happening in orbit is embedded in some re-entry analysis tools (SCARAB (Fritsche et al., 2005*b*) and ASTOS), in order to predict the risk generated by high-speed atmospheric explosions. This model is called NASA Standard Break-up model (also known with the name EVOLVE Johnson et al. (2001)). Developed in the late 1990s and continuously upgraded over the years, NASA Standard Break-up model is a statistical model based on the observations of in-orbit explosions event. It is an empirical model derived by fitting distribution functions to observed fragments characteristics (area-to-mass ratio, size and ejection velocity). Although it provides accurate results for on-orbit explosions (Fritsche et al., 2005*b*), its application to spacecraft re-entry showed some limitations.

For in-orbit explosions, the objectives pursued with a predictive analysis of the fragmentation are different from the atmospheric re-entry break-up, because the threatening scenario to consider is different. For ground risk the fragments that can survive the re-entry are the major concern, usually the bigger ones, while in the orbital debris environment even the smaller fragments can cause accidents. Besides the conditions and the events that can trigger an explosion change between the orbital and sub-orbital altitudes and with the travelling speed.

The NASA Standard Break-up model does not provide any information about the shape and material of the fragments, information useful for the prediction of the re-entering trajectory. The explosion is considered as a complete and unique disintegration of the spacecraft and it neglects the possibility that more than one explosion can occur or that a large section of the vehicle may keep its integrity.

In 2008, Fritsche B, Koppenwallner G., Lips T., from HTG (Hyperschall Technologie Göttingen), proposed and discussed in (Fritsche et al., 2005*b*) an idea for the combination of the deterministic re-entry analysis tool SCARAB with the probabilistic fragmentation model NASA Standard Break-up model and a method for the evaluation

of the probability for an explosion to occur during the re-entry, based on deterministic simulations. Furthermore they provided a list of events that can create an environment favourable for explosions and criteria to consider for the occurrence of these critical events.

In 2009, the fractal fragmentation method was presented during the Australian Space Science Conference (Bryce et al., 2009) as a new model for both explosion and aerodynamic break-up during the re-entry. The new concept that underlies this method is the visualization of the spacecraft break-up as an iterative fragmentation that exhibits a repeating pattern, similarly to the fractals. This model distinguishes different kinds of break-up depending on a energy level scale.

2.4 Research question and motivation for a statistical approach

The research described in this dissertation is aimed to answer the following question: which statistical models can be proposed for the prediction of the occurrence of an highly energetic break-up event during the atmospheric re-entry and the related fragmentation process? How can be this problem solved with a statistical approach?

The chance that some components of a spacecraft, after a destructive re-entry, survive and hit the ground is not negligible. Accurate simulations and predictions of the impact point and its associated uncertainty range are essential during the planning of a re-entry mission. As mentioned in the previous section, the deterministic re-entry analysis tools currently used for this purpose show some limitations and need further developments.

In deterministic models, the output of the model is fully determined by the parameter values and the initial conditions. The behaviour of a spacecraft during the break-up, especially when an highly energetic break-up occurs, is organized but very difficult to predict, given the large number of involved parameters and uncertainties. Note that a spacecraft during the re-entry is usually outside its standard operating conditions. We are considering a phenomenon entirely deterministic, but whose regulating functions are not completely known and they cannot be recovered by observations. The uncertainty that arises because of the necessity to resolve the system inside a model is

given by two different factors: first of all the model uncertainty, due to the unknown error between what actually happens and what the model is able to describe, next the parameter uncertainty, given by the difficulties in specify a priori the values of the parameters that most closely match the real process. Uncertainty is exactly the key property of the proposed problem that makes a statistical approach more suitable.

Statistical models possess some inherent randomness: the outcome are random variables that can take value on a set of possible different values, each with an associated probability. The notion of unknown is reduced to the notion of random. Given the evident complexity of the considered system and the limitations in specifying all the values of the parameters, it would seem appropriate to find a strategy able to learn from historical observations.

Statistical modelling provides an interpretation of the past realizations of a random phenomenon, based on its outcomes, and the means to predict the future realizations of a similar nature. The values of the parameters that define the outcome distributions are inferred by data. Historical observations are the input of statistical models, while deterministic approaches exploit historical observations only to validate the model predictions.

Lastly a statistical approach, including uncertainties in its outcomes, can be more efficient than the deterministic one, in terms of computational time.

2.5 Motivation for the Bayesian choice

The Bayesian paradigm is essentially a probabilistic view of the world which says that all uncertainty should only be described by probability and its calculus, and that probability is personal or subjective. (Singpurwalla, 2006).

Observations are meaningless when they do not come as a support of a referential model. Philosophers agreed that knowledge is built merging experiments with a priori representation of the world (Robert, 2007). For instance Kant said *although knowledge starts with experimenting, it does not follow that knowledge is entirely derived from experimenting*, meaning that experiments create knowledge only after a confrontation with a pre-defined model. The Bayesian approach stems exactly from this principle: the inference of the parameters is given by a combination of a priori (background in-

formation) and post priori (observations) knowledge (the reader is reminded to the Appendix A for further details about the Bayesian approach). The background information is exploited in order to formulate a subjective choice of a prior distribution of the parameters, as the result of an interaction between individual perceptions and exterior reality. In this way, Bayesians introduced a subjective idea of probability that nullifies the sentence *we know nothing before observing* and admits the possibility of considering the probability of not repeatable events.

The choice of proposing a Bayesian approach to tackle the problem of the spacecraft break-up during the atmospheric re-entry is motivated by the lack of observations and not reproducibility that characterize this kind of events. The attainable knowledge regarding the behaviour of a spacecraft during its atmospheric re-entry is incomplete and limited. Very few sparse historical data are available. Indeed, the current used deterministic re-entry analysis tools lack of information for model validation, given the limited ability to simulate re-entry conditions in ground-based tests, limited recovered debris and in-situ observations. Furthermore atmospheric re-entries are not repeatable events. Spacecraft are usually quite different, because designed for different missions, and even a slight variation in the trajectory can change significantly the encountered conditions. Very rare situations, as the multi-satellite missions, could be source of historical data describing similar realizations of the same system.

Expert opinion plays an important role in Bayesian strategies and we planned to rely on it since from the beginning of this project. Expert opinion is information provided by people who have a good knowledge and experience of the field under study, therefore it is a good source of prior knowledge (more details about expert opinion elicitation and analysis are available in Appendix 7.6). Lack of real data can be filled by expert opinion, even if finding the best elicitation strategy can be a great challenge. For this reason, this research included a study on what the sources of such information are and how to quantify that information in an appropriate manner.

Another important aspect that makes the Bayesian approach suitable in this context is its flexibility in being updated in light of new data and new information. Hopefully a more detailed background knowledge of the phenomenon will arise in the future, as well as new observations.

Chapter 3

Research methodology and results

3.1 Introduction

We now progress to summarize the research methodology that was followed during the course of our research and then to illustrate the main concept of the proposed methods. Furthermore we provide an introduction to the Bayesian approach for the reader who is not familiar with it.

3.2 Research methodology

We divided the project in two stages: exploratory data analysis, statistical modelling and implementation. In the first stage, our foremost aim was to become familiar with the data that is available, as that guided, in the next stage, the development of the models.

First of all, we delved into the available background knowledge in order to understand the phenomenon subject of our studies. This analysis included the strategies currently used in the re-entry analysis tools, a general comprehension of the atmospheric re-entry, orbital dynamics and the physics of the break-up process and a survey of the availability of real data and what is difficult to predict during the break-up.

In Section 2.3 we thoroughly examine the most notable re-entry analysis tools, highlighting the limitations of the deterministic approach and the lack of a proper modelling of highly energetic break-up events.

During this stage we had the preliminary meetings with the experts, in order to get

familiar with the problem and the elicitation process. The procedure of expert opinion elicitation is detailed in Section 5.3. It is quite common to rely on expert opinion when other kinds of data are scarce, too costly or difficult to be collected or even unavailable. In order to be able to understand the issues associate with the elicitation process, a reading of the seminal texts was required. These are presented in the literature review in Section 4.4.

The fundamental result of this stage was the severe scarcity of exploitable data that we could use to calibrate the models. After the accomplishment of this phase, regrettably it became clear that data from ground-based tests of elements capable of provoking an explosion and flight-data were not accessible and it was agreed to not rely on results of deterministic simulations. The only approachable source of real data, which is not complete, was the in-situ observation of the destructive re-entry of ATV 1 Jules Verne, described in Section 5.2. This outcome was pivotal in the final choices we made during the statistical modelling stage, as well as the idea that, regarding the future, hopefully more and more observations will be available over time, with an increasingly interest in this context.

As indicated in the Introduction (Section 1.2), the risk assessment for highly energetic break-up events during the atmospheric re-entry can be decomposed in two problems: the assessment of the probability for them to occur and then the prediction of the statistical distribution of the masses of the generated fragments. The first one was framed as a reliability (or risk assessment) problem with missing data, while the second one as a problem of statistical inference of a partially random fragmentation process (a fragmentation process partly dependent on stochastic factors and partly dependent on deterministic factors) with missing data, both in a Bayesian perspective. The contribution of this phase is in the statistical application domain: our major goal was to select the most suitable existing statistical models and apply them to a new situation of complex modelling. In order to be able to devise novel approaches, the reading of the literature reported in Section 4.3 and Section 4.5 was crucial.

For both the problems, we addressed the issues concerning the data fusion and update, that is how to combine expert opinion and data in a coherent manner, how to maximize its value and how to improve the model in light of new data.

Particularly in the solution of the first problem (detailed in Chapter 6), we pursued

three main objectives: figuring out how to assess prior probabilities from experts opinion, how to adjust the elicitation to reflect a new set of re-entry conditions without re-doing the elicitation and finally how to update these probabilities in light of new information. The literature review of Section 4.4.1 provides the interested reader an adequate motivation for the techniques we decided to integrate.

For the second problem, we aimed to devise a strategy that could take into account the different behaviour of the different materials during the break-up events, the data that could be retrieved in the future by analysing in-situ observations and the awareness that only a portion of the fragments survives the re-entry and can be found in circumstances such that it can be observed. Furthermore the development of the second model was driven by the idea of implementing something that can be easily tailored for each re-entering spacecraft event, easily adjusted to changing datasets and, again, improved as the comprehension of the re-entry improves. For this reason we contrived some constraints that the interested reader will understand better reading the Chapter 7. The chance of having matters surrounding the implementation of the statistical inference in a practical amount of time (e.g. convergence and robustness) is typical with models adhering to the Bayesian paradigm and our approach, particularly for the second problem, did not make exception. The used computational methods are detailed in the Appendix A.

3.3 Introduction to the Bayesian approach

The Bayesian inference consists in the computation of the distribution of the parameter θ after taking into account the observed data \mathbf{X} , or conditional on \mathbf{X} . This distribution $p(\theta|\mathbf{X})$ is called the *posterior distribution* and it represents the *post-belief*.

Given the *Bayes' theorem*, which is the foundation of the Bayesian inference, as the name suggests, the *posterior distribution* is determined by

$$p(\theta|\mathbf{X}) = \frac{P(\mathbf{X}|\theta)p(\theta)}{\int P(\mathbf{X}|\theta)p(\theta)d\theta} \quad (3.1)$$

from which follows that the posterior distribution is proportional to the *likelihood function* multiplied by the *prior distribution*:

$$p(\theta|\mathbf{X}) \propto P(\mathbf{X}|\theta)p(\theta) \quad (3.2)$$

The *probability* of the evidence given the parameter $P(\mathbf{X}|\theta)$, rewritten in proper order:

$$\mathcal{L}(\theta|\mathbf{X}) = P(\mathbf{X}|\theta) \quad (3.3)$$

is called *likelihood function* $\mathcal{L}(\theta|\mathbf{X})$. The *likelihood* of θ , given evidence \mathbf{X} , is equal to the *probability* of the evidence (or observed outcomes) given θ . This function synthesizes formally the inverting concept of Statistics. Indeed it is a function of the parameter θ , which is *unknown* and depends on the evidence \mathbf{X} . *Probability* characterizes possible future outcomes given a fixed value of the parameter before data, while the *likelihood* is a function of the parameter for a given outcome (or evidence), that is after data are available. Note that we are using capital P to highlight that the *likelihood function* is equal to a *probability* and it is not a density probability function as the posterior and the prior distribution: the evidence \mathbf{X} is given and it is not a random variable.

The *prior distribution* $p(\theta)$ is defined as the distribution of the parameters before data are observed and it represents the *initial subjective belief*. The selection of the prior distribution depends on the background knowledge and it is a very delicate problem. It is the key to Bayesian inference. The more information is available the more effective will be its choice and the more reliable is the inference. The prior distribution allows the incorporation of an expert's experience into a statistical model.

The revolutionary introduction of Bayesian statistics consists in assigning a probability distribution to both causes (evidence) and effects (parameters) or, in other words, in assigning to the parameters the role of random variables. The *posterior distribution* incorporates the information on the parameter θ contained in the observation \mathbf{X} and the *initial subjective belief*.

3.4 Overview of the proposed models

We present in this section the statistical model we proposed, starting from the reasons that drove our choices. The first model is for the assessment of the probability for a highly energetic break-up event to occur, while the second one is for the prediction of the probability distribution of the masses of the generated fragments.

3.4.1 The Belief-network model for failure prediction

After the accomplishment of the first stage of this project, finalized to the comprehension of the problem and the exploration of the available knowledge, we summed up that the required statistical approach would have had to take into consideration the following:

1. The spacecraft break-up during the re-entry can be described as a complex system subject to a failure or an undesired event, whose realization can be observed more times over time, under similar external conditions;
2. The scenario of a highly energetic break-up event can be considered as the result of the occurrence and combination of the failure of specific components;
3. An accurate analysis of an in-situ observation can provide information about the events that triggered a highly energetic break-up event: spectroscopic systems with high bandwidth in wavelength resolution and coverage (Loehle S, Marynowsky T, Zander F, 2014). For instance fuel release can be analysed through spectroscopy. Unfortunately due the inherent difficulties in observing this kind of events, this information can be missed;
4. Experts can provide subjective judgements about the occurrence of a specific failure event, based on a priori analysis, simulations of the re-entry and ground-tests when available;
5. The differences of the vehicle characteristics and of re-entry conditions can affect the result;
6. Regarding the future, more observations can be available over time.

Given this frame of the problem, we proceeded with the formulation of a reliability model combining a fault tree analysis and an elicitation process inspired by a multi criteria decision making, called Analytic Hierarchy Process. These methods are described in the Appendices B and C, while Chapter 6 is entirely dedicated to show the details of the novel model, called Belief-network model for failure prediction.

This model, that adheres to the Bayesian paradigm, can be summarized in the following steps:

1. Resolution of the highly energetic break-up event into its causes (as showed in Section 6.13) through the construction of a Fault tree: identification of the basic (or elementary) and intermediate events that can lead to the highly energetic break-up event and their logic inter-relationship.

The fault tree analysis is a technique for the reconstruction of all the possible ways that can lead to the occurrence of a given and undesired event. The fault tree itself is a qualitative representation of the problem, that can be evaluated qualitatively. We chose to use this technique as model framework, because appropriate to describe the complex scenario of a highly energetic break-up event. Under assumption of independence, the probability for a highly energetic break-up event to occur can be assessed by the qualitative evaluation of the probabilities for the basic events to occur. The model is then parameterised by the elementary event probabilities only and, following the Bayesian approach, these parameters take the role of random variables.

2. Prior elicitation, by expert opinion, of basic events probabilities in a nominal case.

Given the lack of data, it is crucial to rely on the expert opinion for prior elicitation. The meetings with the experts and the large relevant literature shoved us to propose an elicitation method, based on pairwise comparisons, inspired by the Analytic Hierarchy Process and suitably tailored to this problem. In the awareness that each re-entry is different from the other and that, currently, there is only one accessible observation, we decided to discuss everything with respect to a nominal re-entry and spacecraft type.

3. Likelihood computation in a nominal case. We decided to exploit the logic of the fault tree to derive the likelihood of not-observed events, when feasible, in order to integrate the incompleteness of data.

4. For each upcoming re-entry:

- Expert opinion elicitation of the relative risk of occurrence for all the basic events;
- Evaluation of the likelihoods of observed and not-observed events;

- Weighting of the likelihood accordingly with the results of the expert opinion elicitation phase;
- Evaluation and weighting of the probabilities for the basic events to occur, through the Bayesian approach and accordingly with the results of the expert opinion elicitation phase;
- Assessment of the probability for a highly energetic break-up, following the fault tree logic.

The goal of the weighting strategy is the incorporation of the opinion of the experts, who are invited to take into account the differences of the boundary conditions with respect to the nominal profile (e.g. characteristics of the vehicle and re-entry conditions).

3.4.2 The Fragmentation model

The first stage of the project led us to the conclusions that the statistical approach to propose would have had to comply the following:

1. The raw data sources are recordings of the break-up process. In order to make this data exploitable, an accurate, time-consuming and expensive analysis is required.
2. The physical features required to predict the entry trajectory of a fragment generated after a break-up event are: mass, material composition, shape, area-to-mass ratio, ejection velocity, position of its generation. The ballistic coefficient provides a relationship between area-to-mass ratio, shape and material composition. Ideally all these features could be derived by an analysis of the observations and then predicted for future re-entries through a Bayesian approach, even if the observations are not complete.
3. Due to many complications in observing such a kind of event and in analysing the results of the observation, the idea of collecting complete data is not conceivable;
4. Observations are not missing completely at random. Experts can justify the missing observation, considering the technical details of the instrumentations used to record the event (e.g. pixel resolution, field of view, wavelength coverage,

frame rate, eventual saturation of images), observations conditions (e.g. relative position of the aircraft) and entry characteristics;

5. Spectroscopy could identify the material of the fragments and from which component of the spacecraft it comes from, but the way how to make this possible is still under investigation. Due to the overlapping of fragments in the field of view, it would be very complicated to identify the material of a single fragment. Unfortunately spectroscopic data coming from ATV-1 re-entry does not provide any exploitable information about the materials and origin of fragments, due to this issue.

Observation campaigns could be planned such that spectroscopic instruments are dedicated to species of interest. For instance spectroscopy UV-NIR has been proposed for the identification of metallic structures (Loehle S, Marynowsky T, Zander F, 2014). Furthermore, painting of components of the space vehicle could be useful for the debris identification (Loehle S, Marynowsky T, Zander F, 2014).

6. It is feasible to follow the evolution of the fragments over time, assumed that they remain in the same field of view. Anyway our focus is in the fragments that survive the highly energetic break-up event;
7. The unique exploitable set of data for this thesis is a list of masses of sixteen fragments, that is a result of the data analysis carried out after the ATV-1 observation campaign.
8. Experts can provide subjective judgements, based on a priori analysis and simulations.
9. The probability of survival for a specific component is mainly determined by the materials used in its construction, the area-to-mass ratio, shape and its position in the vehicle;
10. We can assume exhaustive the following list of materials to be considered:
 - Ti6A14V;
 - stainless steel 316L;
 - aluminum alloy 7075;

- silicon carbide;
 - carbon fiber/epoxy Cfrp;
11. The total mass of the spacecraft before the break-up event can be assumed known;
 12. We can assume negligible the effects of low energetic break-up events on the fragments generated after a highly energetic break-up event;
 13. The fragmentation of a spacecraft can be modelled as a partition of the unit interval. The preliminary partition that we need to consider is between demised masses, not observed masses and survived masses;

Looking at the problem from a Bayesian statistical point of view and given this setting of the problem, we started the model devising process from the only tangible set of data, a list of masses, and then we decided to focus on the prediction of the masses of the fragments, rather than on other features. We proceeded with the development of a method for the construction of a distribution over the partitions of the unit interval, inspired by the stick breaking process, and a combination of sampling methods for the Bayesian inference of its parameters, given sparse observations. The stick breaking process and the used sampling methods are described in the Appendices D and A, while Chapter 7 is entirely dedicated to show the details of the novel model, called Fragmentation model.

The decision of providing a method for the construction of a tailored distribution, following the idea of the stick breaking process, derives from the necessity to leave the model a large flexibility in the application and future updates. The form of the resulting distribution depends on specific constraints that can reflect the background knowledge of what we aim to predict.

The spacecraft could be considered as the set of different elements and for each of them a different distribution could be built. In order to make the inference of the parameters of the various distributions, these different elements must depend on the available data. It may be an abstract subdivision (e.g. by material) or a concrete subdivision (by location). As the reader will understand better reading the details and the examples of the model in Chapter 7, the distribution is constructed in a step by step fashion: this could reproduce concretely the evolution of the fragmentation or

represent an abstract process leading to the final outcomes. In the awareness that it will be more likely to have data of the generated fragments rather than data about how they are generated, we think that the abstract lead is more suitable.

Chapter 4

Literature review

4.1 Introduction

The project presented in this dissertation combined the application of various statistical topics:

- The Fault tree analysis used as framework of the proposed risk assessment model;
- The Expert opinion elicitation with particular attention to the paired comparisons elicitation approach, applied in the risk assessment model;
- The stick breaking process which inspired the fragmentation model.

The interested reader can find an overview of these subjects in the Appendices B, C, D. In order to be able to write knowledgeably and to work with them, a reading of the relevant literature was required. This is presented and discussed in this Chapter.

4.2 Statistical inference and Bayesian approach

The reader interested in statistical inference can refer to the excellent book of Casella and Berger (2002) or the rigorous reference of Cox (2006). For a concise course we can recommend Wasserman (2003). An interesting book about the history of statistics is Stigler (1986). Finally a valuable text for a good introduction of theory of probability, random processes is Grimmett and Stirzaker (2001).

4.2.1 Statistical inference with missing data

We recommend the book Little and Rubin (2014) and the publication Chen et al. (2008) for a complete overview of the methodologies applied for handling missing data problems and a survey of the literature.

4.2.2 The Bayesian approach

For a comprehensive study of the Bayesian approach, including the theory about the selection of the prior distribution, we can suggest the reading of Robert (2007), which inspired this introduction to the Bayesian approach, or Howson and Urbach (2006). Furthermore we recommend the reading of Lindley (1961) for an accurate justification of the use of the prior distribution or the book De Finetti (1990) whose author is one of the pioneers of the Bayesian school.

4.3 Risk assessment and Fault tree analysis

Risk assessment is performed on phenomena whose complete knowledge is missing: this makes the treatment of uncertainties of the main issues in this context. The paper Paté-Cornell (1996) analyses extensively the theme of uncertainty in risk analysis, defining and illustrating six different levels of treatment. After a clarification of the differences between epistemic and aleatory uncertainties, a categorization already highlighted by many authors (e.g. Hacking (2006), Chernoff and Moses (2012)), this paper underlines and motivates the need for expert opinion in measuring the epistemic uncertainty. The mutability in observable populations creates aleatory uncertainties, while epistemic uncertainties derive from the incompleteness of the achievable knowledge. Frequentist methods provide the tool to tackle the first ones, while the latter requires the support of the experts experience that can be incorporated in the statistical analysis only through the Bayesian approach. Furthermore three classical approaches for gathering expert opinion for risk assessment are discussed by Paté-Cornell (1996) and an application to seismic hazard analysis, that can be transferred to other domains, is described. We will come back to talk about this subject in the Section 4.4, that is fully dedicated to introduce what the expert opinion is.

Fault tree analysis is a widely used method in reliability and safety analysis since

1960, as reported in Lee et al. (1985). The reading of this paper is highly recommended to the reader interested in a literature survey of all the fault tree analysis methods.

4.3.1 Further reading

In addition to the paper already cited above, we provide in this Section some recommendations for further reading.

For a complete overview of reliability and risk in a Bayesian perspective the book Singpurwalla (2006) is highly recommended. Barlow et al. (1975) is a seminal paper about reliability and fault tree analysis: this paper is a collection of the main contributions of the Professor Z. W. Birnbaum, who is one of the founder of Reliability theory.

Finally the reader is referred to Vesely et al. (1981) for a tutorial about the fault tree analysis.

4.3.2 Space applications

An appropriate reference for Fault tree methodology with aerospace applications is presented in Vesely et al. (2002), which is readily available on line.

In 2009 NASA released the handbook Kelly et al. (2009) to provide engineers and scientists the Bayesian foundation of reliability methods in space activities.

An example of probabilistic risk assessment in the space field is published in the paper Vesely (2004), where the analysis performed for the NASA Space Shuttle is described.

4.4 Expert opinion elicitation

Missing data is a common problem in risk analyses (see also Bedford and Cooke (2001a)), so it should not be surprising if Bayesian risk analysts have largely and successfully relied on subjective experts opinion for years.

A complete overview of the different available elicitation methods is provided by Cooke (1991). Garthwaite et al. (2005) is a fundamental paper about statistical methods for eliciting probability distributions: it is mainly a review of the state of art of

what makes an elicitation successful and the related obstacles (heuristics and biases), with particular remarks on the elicitation of group opinions.

Finally it is worth mentioning the paper (Lindley and Singpurwalla, 1986), that illustrates a procedure for the use of expert opinion in fault tree analysis.

The model for risk assessment described in this thesis, in Chapter 6, proposes the use of a paired comparisons elicitation method. The next section is dedicated to a literature review of this class of expert opinion elicitation methods.

4.4.1 Paired comparisons elicitation approaches

The extensive application of paired comparison elicitation approaches in the reliability engineering and system safety domain is justified by the observation that experts feel more comfortable making paired comparisons rather than providing a direct estimate of a quantity of interest. We decided to rely on this approach mainly for its simplicity, given that pairwise comparisons do not require the experts have a knowledge of the probability theory.

The law of comparative judgement was introduced by the pioneer Thurstone (1927) with applications in the measurement of psychophysical stimuli. Popular pairwise comparisons elicitation method are the Bradley-Terry method (see Bradley and Terry (1952) and Cooke (1991) for a excellent examination of the method) and the Analytical Hierarchy Process, developed by Saaty ((Saaty, 1980)). Both these techniques involve the definition of contributing factors (or covariates), representing the criteria with respect to which the experts is asked to compare the alternatives. The Analytic Hierarchy Process is described in the Appendix C.

The first formulation of the pairwise comparisons method as a Bayesian statistical problem was developed by Pulkkinen in 1994 in Pulkkinen (1994). This paper contains a theoretical exposition of an aggregation method of the expert elicitation paired comparisons, adhering to the Bayesian paradigm. Basically, the expert opinion is exploited for the updating of the prior distribution of a random vector of variables through a Bayesian framework. The experts are asked to compare all pairs of variables and to define for each pairs which variable they believe has a bigger value. Their belief is described by a binary indicator variable and the collection of the indicator variables form the evidence building the likelihood.

An interesting conjugate Bayesian analysis, using paired comparison to elicit expert judgements is illustrated in Szwed et al. (2006). It proposes a novel methodology for the quantification of accident probability, in case of rare events, and particularly an application to a risk analysis of the Washington State ferry system, that is the largest passenger ferry system in the U.S. This is a risk assessment model where less than three relevant accidents had been recorded. This study is aimed to assess the distribution of an accident probability defined by a vector of contributing factors describing the system state. Experts are asked to compare each time two different system states and it is assumed that the expert responses are not based on overlapping information. This research is further developed in Merrick and Van Dorp (2006), where full distributional information about the risk of collision between a ferry and another vessel is calculated with a method combining Bayesian estimation techniques and a pairwise comparison approach for the evaluation of the uncertainty of expert judgements.

With regard to the elicitation of subjective probabilities through pairwise comparisons, we recommend the reading of the paper Budescu et al. (2016) where the authors show with two experiments that the results obtained by collecting ratio estimates are more precise than by asking direct estimates. They conclude stating that this method, developed for decision making problems, can result appropriate, with minor adaptations, to the prior elicitation problems, very common in the Bayesian statistics methods for risk analysis. Finally, this paper provides an accurate and interesting literature review about the discussions raised by the introduction of this new elicitation approach versus the more traditional methods.

An example of application of pairwise comparison as method for expert opinion elicitation in risk assessment is presented in Mazzuchi et al. (2008). The goal of this research is to develop a risk assessment model, based on expert opinion, for the assessment of the risk of wire failure. This work deals with a problem similar to that for which we propose the risk assessment model in Chapter 6: there is a system where the failure probability depends on an overwhelming number of variables and the available historical data are sparse. The authors propose an idea for the inference, based on the integration of data with background knowledge. The support of this model is a time to failure probability density function derived by the Proportional Hazard model (a method largely applied in reliability engineering and proposed by Cox (1972)). The

failure rate estimates necessary for the inference of the parameters of the failure probability density are inferred by the results of pairwise comparisons elicited on a selected set of failure environments. It is worth mentioning that the application of the procedure demands that a reasonable amount of historical data at least for one of these environments: this is a requirement that would not make this model applicable to the assessment of the probability to occur during the atmospheric re-entry. As the reader will understand better reading Chapter 6, there are two other analogies with our problem: the first is that the use of expert opinion is completely new for the arena of the involved experts and it may take time to be accepted and tailored, while the latter is that a background knowledge in different fields of expertise is required.

The use of the Analytic Hierarchy Process is proposed in Cagno et al. (2000*b*) as elicitation method of the expert opinion for a risk assessment model aimed to evaluate the propensity of different sections of low-pressure cast-iron pipelines used in metropolitan gas distributions networks, in order to manage their replacement policy. This is another example of application where expert opinion is needed to redeem the lack of historical data on failures. Furthermore this is another situation where the considered failure depends on the combination of many factors. When the consequences under analysis are those generated by the combination of factors and not by single factors, the differentiation of the effects generated by each single factor turns out to be anti-productive. Authors reported that, during the interviews, experts confirmed the validity of the choice of a pairwise comparison method for this kind of problem, because, in this way, they could formulate the required evaluations considering the interactions between the factors. The procedure for the collection of the expert opinion is accurately detailed in the paper, from the definition of the sample to interview, the division in groups depending on different expertises, to the encountered problems and the consistency check. A prior density function for the failure rate of each class of pipeline is estimated by a combination of the weights, results of the application of the AHP with the eigenvalue method, and a scale factor, depending on historical data. The paper also details how to change the approach to improve the robustness of the method and the reliability of the results. The experts are allowed to answer with intervals rather than a single-point value, introducing confidence intervals in the weights assessment. Then a class of prior distributions is elicited, that is a common situation

in the robust Bayesian inference (Berger (1990), (Cagno et al., 2000a)). Finally, a comparison of the results with a frequentist analysis showed that the use of Bayesian approach is more convenient and reliable in these situations. The success of this work is claimed by the decision of the gas company management to use it.

An example of combined use of the AHP with Fault tree analysis is the work proposed in Vrijling (2009) for the risk assessment of petroleum pipelines. In this case, the Analytic Hierarchy process is exploited with its original purpose, that is as ranking methodology and not as a prior elicitation method. The overall objective of this work is a risk based pipeline selection, that is the selection of the most reliable pipeline between the three considered (oil and gas pipelines respectively located in Escravos, Warri and Benin in Nigeria) as case study. Authors used the software Web-Hipre software (Mustajoki and Hamalainen, 2000) for the hierarchical decomposition of the problem: the hierarchical tree is given by the goal (risk based pipeline selection), criteria (failure factors) and subcriteria(sub division of failure factors). The AHP is used to rank the failure criteria (or in other words the events that can lead to a pipeline failure), in order to establish which ones are more likely to cause the failure, and the reliability of the considered pipelines. The fault tree analysis is applied to assess the failure probability of a petroleum pipeline. This is given by the sum of the failure probabilities due to the considered criteria. Given the probability of failure of one of the failure criteria, the failure probability of the pipeline can be computed using the AHP weights. For each criterion, the fault tree provides a qualitative reconstruction of all the possible events that can cause its failure and then allows the assessment of its probability of failure. The geometric mean approach is applied for the weights.

A very interesting overview of AHP applications is reported in Forman and Gass (2001). They are divided by the following fields of application: choice, prioritization/evaluation, resource allocation, benchmarking, quality management, public policy, health care, strategic planning. Other examples of applications for decision making, in different fields, e.g. agriculture, oil and gas and public sector are: Qureshi and Harrison (2003), Dey et al. (2004), Partovi et al. (1990).

4.4.2 Further reading

In addition to the paper already cited above, we provide in this Section some recommendations for further reading.

For a practical guide to the expert opinion elicitation and analysis, consult the book Meyer and Booker (2001).

The reader is referred to Teknomo (2014) for a tutorial that explains AHP in a very simple way and to the book Saaty and Vargas (2012) for a comprehensive study.

4.4.3 Space applications

It is worth mentioning in this thesis two applications related to space activities (Forman and Gass, 2001) :

- The AHP has been applied to select a propulsion system for the Lunar Lander Moreland and Sanders (1993) by NASA's Lyndon B. Johnson Space Center;
- The computer-aided systems engineering tool set (CASETS) environment, developed by the Rockwell International's space systems division, relies on AHP for criteria weighting, utility functions and sensitivity analysis. This tool has been applied to the development of new space launch vehicles, surveillance satellites, and SDI architectural studies.

4.5 Statistical modelling of fragmentation

The fragmentation is a phenomenon investigated in many fields, because concerning various natural and man-made systems. This explains why numerous , e.g. empirical, deterministic, statistical etc. (Elek and Jaramaz, 2008), have been studied in order to describe and characterize the outcome of a fragmentation process: number, size, shape, mass, ejection velocity and spatial distribution of fragments. Particularly and for obvious reasons, military applications gave a significant boost to this field.

The second chapter of the book Grady (2007) as well as the paper Elek and Jaramaz (2008) provide a good summary of the state of art of geometric fragmentation statistics for shells and bombs (e.g. Mott's and Grady-Kipp's approaches (Grady and Kipp,

1985) (Mott and Linfoot, 1943), the models based on Voronoi diagrams, the Lineau distribution of random fractures (Lineau, 1936)).

A large literature is also available for the statistical modelling of fragmentation of solids (Sil'vestrov, 2004).

For a complete reading about Dirichlet and related distribution, that we used in the proposed fragmentation model, we recommend the book Ng et al. (2011).

Finally it is worth mentioning Kiselev (1997) where a numerical model for the fragmentation of exploding tanks is proposed and an inherent literature review is reported.

Chapter 5

Data

5.1 Introduction

”Statistics is the science of learning from data” (Davidian and Louis, 2012) and lack of data is the biggest issue in the development of a statistical model for spacecraft break-up. Indeed, the design of the two statistical models described in Chapter 6 and Chapter 7 was driven by the scarce availability of data.

In the 70s NASA launched a series of spacecraft just for the purpose of investigating the consequences of the spacecraft break-up during the atmospheric re-entry. After that, the research on destructive re-entry was quiet for almost forty years until 2008, when an airborne observation campaign was arranged for the re-entry of the first Automated Transfer Vehicle (ATV 1). This observation campaign was organized and funded by ESA and NASA, under the coordination of the SETI institute. All the details about this observation campaign are reported in the website atv.seti.org (2009) and many papers have been published about it (e.g. Blasco et al. (2011), Snively et al. (2011a), Jenniskens and Hatton (2008), Esa et al. (2009)). Afterwards, a second airborne observation campaign was organized for the re-entry of the Hayabusa Sample Return Capsule in 2010 (hayabusa.seti.org (2010)).

The work behind this thesis can be divided in two main phases: the first and preliminary one was dedicated to the collection of information and the latter to the statistical modelling. This chapter is dedicated to summarize the process followed during the first phase and its results. An exploratory data analysis has been carried out in order to identify what could be managed as a resource, what could be learnt

and the feasible assumptions.

Before starting to devise which kind of statistical methodologies could be applied in order to solve the problem proposed by the European Space Agency, we focussed on the investigation and selection of:

- What is available;
- What can be required;
- What is exploitable;
- What is helpful;
- What can be useful in the future;
- What we expect to be retrieved in the future.

It was agreed with the European Space Agency to rely only on real data and especially on what is currently available and reliable, in terms of typology and quantity. Simulated data coming from deterministic tools could be used in the future only for comparisons or testing purposes. Devising a statistical model capable of employing real data was an important requirement. In order to accomplish it, we had access to all the reports of the data analysis carried out after the ATV 1 airborne observation campaign, but unfortunately very few data resulted to be exploitable.

After an overview of the outcome of the ATV 1 observation campaign, which is the unique source of real data, the process followed to query the experts is reported.

5.2 ATV 1 Observation campaign

The unique source of real data in this context are the observation campaigns, ranging from airborne, ship- and ground-based. These kinds of missions are aimed at gaining a better understanding of the destructive process of the spacecraft, to validate the existing modelling scenarios and re-entry analysis tools and, as consequence, to improve decision making process for the design of safer space missions. This section is dedicated to introducing the outcome of the Automated Transfer Vehicle Jules Verne observation campaign. For the sake of completeness we start with a brief description of the Automated Transfer Vehicle.

5.2.1 Overview of objectives and results

The ATV-1 observation campaign was a multi-instrument aircraft campaign performed using two aircraft equipped with a suite of optical instruments, capable of covering a wide dynamic, temporal and spatial resolution range: advanced video systems and spectroscopic instruments covering various wavelengths (near-UV, visible and nearIR). The aircraft were the NASA DC-8 and a commercially available Gulfstream V.

Data gathering and data analysis were driven by the following objectives (Lips et al., 2011):

- Characterization of the fragmentation and break-up events, including the altitude when they occurred, the typology of breaking-up (lowly or highly energetic) and identification of the causes;
- Reconstruction of the fragments trajectories;
- Characterization of the fragments, consisting in material and source identification;
- Estimation of number and size distribution of the fragments.

The fulfilment of these tasks requires a cross analysis of raw visual and spectroscopic data. For example the trajectories can be reconstructed through frame by frame tracking from the video recordings and 3D triangulation, while the material composition of the fragments can be identified analysing the raw spectroscopic data. Tracking the fragments can help in locating the location of the break-up event. On the other hand, spectra immediately after a fragmentation event can individuate which spacecraft components are immediately exposed to the entry heating and therefore help in understanding the break-up nature and location. It is easy to imagine that, after an explosion, the nearby parts of the spacecraft vaporize producing spikes of emission in the spectra: if analysed, these spike of emission can suggest the location of the explosion source. Finally, another example of information that can be inferred by imaging data, is the releasing of fuel: this event can be highlighted by specific signatures in the spectra.

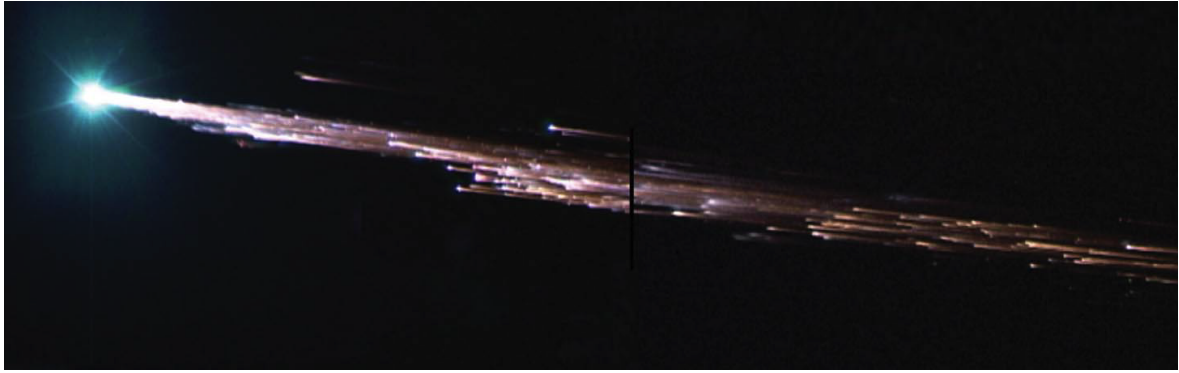


Fig. 5.1: Antoine Bavandi, ESA/ESTEC, obtained these still frames with a Sony 3CCD camcorder, owned by Mike Taylor of Utah State University. This picture is a good example of raw data. Composite: Peter Jenniskens (Snively et al., 2011*b*). Source: atv.seti.org

Data analysis proved that many fragmentation events occurred, in particular two explosions with a gap of 35 seconds and the first one was triggered by the MMH propellant (an hypergolic propellant).

Potentially many data could be collected by this multi-instruments airborne observation campaign, but unfortunately there were also several difficulties and hurdles involved, which lead to not complete observations. Issues occurred in both data collection and data analysis. This should not surprise the reader, since this was a pioneer observation campaign.

The encountered problems are associated with:

- Calibration issues;
- Field of view issues;
- Tracking issues;
- Timing issues;
- Saturation issues;
- Reflections issues and then detection of fake particles;
- Data archiving issues;
- Limited funding for data analysis.

Unfortunately, for the purposes of this thesis, only the masses of sixteen fragments were exploitable, the rest lacked for reliable data. These masses are definitely the most important data available for this project and, as the reader will see in Chapter 7, we used them to test the fitting of the Fragmentation model.

5.3 Experts knowledge

Expert opinion provided a significant contribution to the work carried out for this thesis. First of all, we interviewed experts, familiar with the spacecraft system and the atmospheric re-entry, with the aim of understanding the proposed problem. The devising process of the proposed models and the proposed ideas for their application was based on this preliminary collected information. Then we relied again on the expert opinion for the construction of the framework in the Belief-network model for failure prediction (Chapter 6) and obviously for the prior elicitation.

The preliminary phase consisted in interviewing experts, in order to get a general comprehension of the atmospheric re-entry and to state:

- The availability of exploitable information and data (including laboratory experiments);
- The most suitable strategy to elicit information and how to formulate the surveys;
- The feasible assumptions;
- The constraints to keep in consideration, e.g. the feasible ranges of the fragments characteristics;
- The right choice of the models parameters and the involved uncertainties;

and, subsequently, to identify:

- The items capable of provoking an explosion;
- The events that can lead to an explosion;
- The relevant external conditions affecting the fragmentation process.

Several meetings have been arranged in different areas of expertise:

- Guidance, navigation and control;
- Propulsion;
- Materials;
- Structure;
- Heating;
- Energy storage and power;
- Observation campaigns;
- Deterministic re-entry analysis tools;
- Experimental studies about spacecraft design for demise.

As the reader will read in the description of the belief-network model (Chapter 6), we proposed to rely on the expert opinion for the elicitation of the *tendency-to-occur* weight and quotient, with the objective of eliciting a prior distribution for the nominal case and to integrate the experts point of view in the predictions for the upcoming realizations of the system. We proposed to ask experts to compare pairwise the tendency to occur of the fault tree events, divided by groups. The procedure of the expert opinion elicitation experiment is described in Section 6.15. Some examples of interviews, which we addressed to experts in ESA, are reported in the Appendix E.

We have also asked them to provide critical insights for the enhancement of the surveys itself, since we are aware that the list of considered events cannot be considered exhaustive. The most remarkable feedback was that there are dependency relationship between the events that create difficulties in providing a pairwise judgement and that it is unusual to provide a subjective guess in such extreme conditions. This response was not completely unexpected considering that, in this field, the choice of relying on expert opinion for statistical modelling is an innovative way of dealing with uncertainties and, consequently, a new way of thinking.

The collected expert opinion was also integrated with information coming from various reports and papers made available by ESA (e.g. ESA Space Debris Mitigation Working group (2015), Rex et al. (1999), Walker et al. (2001), Klinkrad et al. (2004), Kiselev (1997), Lloyd (1998)).

Chapter 6

Belief-network model for failure prediction

6.1 Introduction

In this chapter we introduce a belief-network model for failure prediction, calibrated by a combination of expert opinion and sparse data. This involves a new approach for the integration of expert opinion in the dependability analysis of a complex critical system.

This methodology combines the fault tree analysis (see Section B.3) and an elicitation process that is inspired by the multi criteria decision making, called Analytic Hierarchy Process (described in Section C.3). A joint application of these two methods has already been proposed in Vrijling (2009) for the risk assessment of petroleum pipelines (see Section 4.4.1), but in a completely different way.

6.2 The research question

The development of this risk assessment model was driven by the need to answer the following research question: *What is the probability that a given spacecraft explodes during its return journey from space to Earth?*

This problem can be viewed as a failure model where the failure is an highly energetic break-up of the spacecraft.

A common spacecraft during the atmospheric re-entry is beyond design-basis, which

means that we are considering the failure of a system under conditions not considered during its design.

We recognize this system as a complex system. The spacecraft itself, under standard operating conditions, is a complex system, since it is composed of many subsystems interacting with each other. The explosion of a spacecraft is the result of the combination and overlapping of many factors concerning the spacecraft subsystems, the re-entering trajectory and the surrounding conditions.

Generally speaking, the attainable knowledge is incomplete: unfortunately the understanding of re-entry of space vehicle is still limited. Very few sparse historical data are available and probably this constraint will not change significantly in the future. This is a context where collecting data, even sparse, is very complicated and expensive.

For all the above mentioned reasons, this problem requires the development of a risk assessment model relying on a combination of expert opinion and sparse data and that can be easily updated as knowledge increases.

Atmospheric re-entries are not repeatable events. Spacecraft are usually quite different, because they are designed for different missions, and even a slight variation in the trajectory can change significantly the encountered conditions. Very rare situations, such as the multi-satellite missions (e.g. ATV, Sentinel, Galileo), could be a source of historical data describing similar realizations of the same system.

This model is required to take into account that there may be large variations in conditions surrounding the system and in the system itself. For this reason, as the reader will understand better later, we propose to perform the expert opinion elicitation process before each realization and discussing everything with respect to a nominal case.

6.3 Summary of results and contribution

This is a Bayesian model for the exploitation of the expert opinion in risk assessment, specially developed for the highly energetic break-up events of spacecraft during the atmospheric re-entry.

We performed simulations of the model with synthetic data, in order to assess the model, and the obtained results are consistent with the expectations. We believe that

the illustrated procedure can be potentially useful for the assessment of the probability for a spacecraft to explode, even if we recognize that it still needs to be properly tested and refined, to assess whether the results make sense from a physical point of view. It is important to highlight that this is a new way of thinking about for the arena of the involved experts.

6.4 De Finetti justification

The prior elicitation method proposed in this chapter is inspired by the De Finetti's *operational subjective* conception of probability. The personalistic or subjective theory, as explained in Booker and Singpurwalla (2001), states that “probability is a degree of belief of a given person at a given time”. This idea claims that an objective probability does not exist and nullifies the sentence *we know nothing before observing*. Indeed the subjective idea of probability admits the possibility of considering the probability of not repeatable events. Prior elicitation methods through expert opinion provide a method for the quantification of the intensity of this degree of belief.

This concept was developed and exposed by the statistician Bruno De Finetti, one of the pioneer of Bayesian statistics (de Finetti (1930), De Finetti et al. (1974), Nau (2001), Walter (2001))

6.5 Notation and definitions

This section is to introduce the notation to the reader and explain its usage.

Let τ be a fault tree diagram, built by a set of gates, events and edges (see Section B.3).

Let τ be divided by layers (or levels) $i = 0, 1, \dots, L$, depending on the distance from the base layer. Layer 0 or base layer is the furthest layer from the top event layer, 1 is the next furthest, etc. Layer i corresponds to the layer that is i layers away from the furthest layer from the top event (briefly TE). The last layer L is the layer connected to the top event through one gate.

We denote every single event of the fault tree with the notation E_{ij} , where the

index i is the layer, while $j = 1, \dots$ indicates the position of the event in the i -th layer, as shown in Figure 6.1.

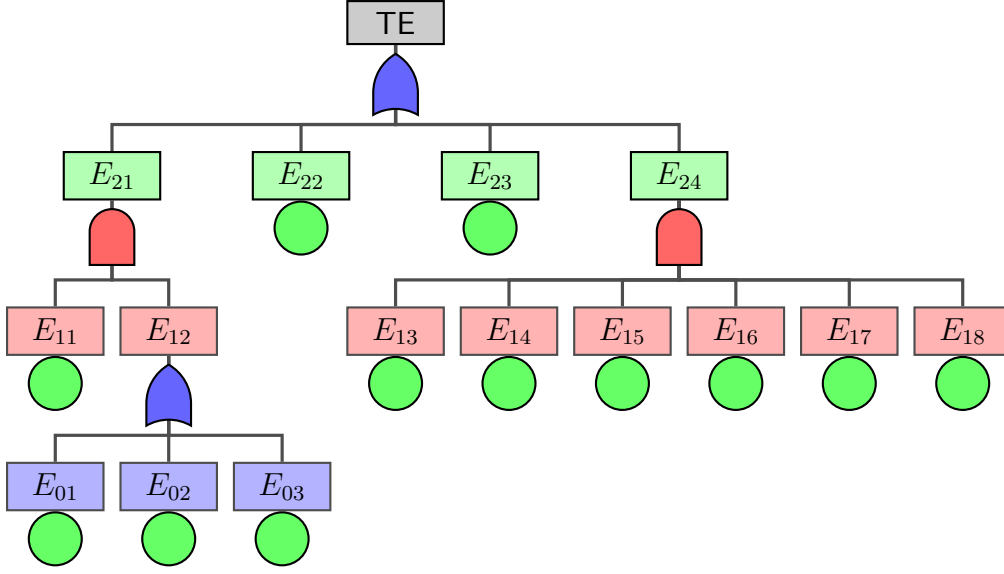


Fig. 6.1: Example of fault tree with layers $i = 0, 1, 2$. Following the proposed notation the events of the base layer are indicated with E_{0j} with $j = 1, \dots, 3$, the events of the next layer with E_{1j} with $j = 1, \dots, 8$ and finally the events of the layer connected to the TE with E_{2j} with $j = 1, \dots, 4$. In this case, following the logic of the fault tree, $P(TE = 1) = 1 - \prod_{j=1}^4 (1 - \theta_{2j})$.

Let θ_{ij} be the probability for the E_{ij} event to occur.

$$P(E_{ij} \text{ occurs}) = P(E_{ij} = 1) = \theta_{ij} \quad \theta_{ij} \in [0, 1] \quad (6.1)$$

$E_{(i-1)j}$ is a *parent* of E_{ij} and E_{ij} is a *child* of $E_{(i-1)j}$ if the occurrence of E_{ij} depends on $E_{(i-1)j}$ through a gate. $E_{(i-1)j}$ and $E_{(i-1)z}$ are *conjugates* if they have the same child E_{ij} . The events that do not have parents are called *parentless*, or *basic*, or *elementary*, or *primary* events. All the remaining events, but the top event, are called *intermediate* events.

Let Φ be the set of the events that build up the fault tree :

$$\Phi = \{E_{ij} : E_{ij} \text{ is an event of the fault tree } \tau\} \quad (6.2)$$

Let Ψ be the set of the basic events of the fault tree :

$$\Psi = \{E_{ij} : E_{ij} \text{ is a basic event}\} \quad (6.3)$$

Let ϵ_{i-1} be the set of the events to consider for the likelihood up to level $i - 1$

$$\epsilon_{i-1} = \{E_{kj} | k \leq i - 1\} \quad (6.4)$$

We introduce an indicator variable $I_{ij} \in \{0, 1\}$ such that:

$$I_{ij} = \begin{cases} 1 & \text{If the event } E_{ij} \text{ is observed} \\ 0 & \text{Otherwise} \end{cases} \quad (6.5)$$

An observation is defined by the following set:

$$\begin{cases} E_{ij} \in \{0, 1\} \\ I_{ij} \in \{0, 1\} \\ \forall i, j : E_{ij} \in \Phi = \{E_{ij} : E_{ij} \text{ is an event of the fault tree } \tau\} \end{cases} \quad (6.6)$$

Note that the expression that the event E_{ij} is observed does not mean that the E_{ij} is observed to occur, as common in risk analysis. The event E_{ij} is observed when $I_{ij} = 1$ and it is observed to occur when $I_{ij} = 1$ and $E_{ij} = 1$.

We denote the *nominal* case as observation $k = 0$, while the *non-nominal* cases with $k = 1, \dots, K$.

Finally we recall two well known probability distributions, that we are going to use in the model:

Definition 6.5.1 *Beta distribution*

A random variable $\theta \in (0, 1)$ is said to have a Beta distribution if its probability density function is given by

$$p(\theta | \alpha, \beta) = \frac{\theta^{\alpha-1} (1 - \theta)^{\beta-1}}{\mathbf{B}(\alpha, \beta)}, \quad 0 \leq \theta \leq 1 \quad (6.7)$$

where $\alpha, \beta > 0$ are the shape parameters. The normalizing constant $\mathbf{B}(\cdot)$ is the Beta function, which can be expressed in terms of the Gamma function

$$\mathbf{B}(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)} \quad \alpha, \beta > 0 \quad (6.8)$$

Definition 6.5.2 *Bernoulli distribution*

A random variable γ which takes value 1 with success probability θ and value 0 with failure probability $1 - \theta$ is said to have a Bernoulli distribution if its probability mass function is given by:

$$f(\gamma; \theta) = \theta^\gamma (1 - \theta)^{1-\gamma} \quad \text{for } \gamma \in \{0, 1\} \quad (6.9)$$

The Bernoulli distribution is a special case of the Binomial distribution with $n = 1$.

6.6 The statistical model

Let us assume that we have a complex system subject to a failure or an undesired event, whose realization can be observed more times over time, under similar external conditions. We propose a procedure for the assessment of the probability for this undesired event to occur during an upcoming realization, relying on expert knowledge and sparse past observations.

The proposed procedure can be divided in the following stages:

1. *Stage 1.* Construction of the model framework;
2. *Stage 2.* Elicitation;
3. *Stage 3.* Prediction;
4. *Stage 4.* Updating with data.

6.7 The construction of the model framework

The first phase is the modelling phase. The model needs to be tailored to the considered system and the undesired event through the following steps:

- Thorough comprehension of the system: establishment of the system boundary conditions and the external factors affecting the system;
- Resolution of the undesired event into its causes through the construction of a Fault tree (as explained in Section B.3): identification of the basic and intermediate events that can lead to the undesired event and their logic inter-relationships (Vesely et al., 1981). The *top event* of the fault tree is the undesired event;
- Selection of a nominal profile for the realization of the system under study (observation $k = 0$). The more information is available about the nominal profile the more accurate is the analysis.

6.8 Expert opinion elicitation

We propose to rely on expert opinion for two objectives:

- To assess the prior on the probabilities θ_{ij} for each elementary event to occur;
- To complement the available sparse observations.

With these purposes in mind, we suggest to elicit two target estimates by expert opinion for each elementary events $E_{ij} \in \Psi$:

- The *tendency-to-occur* weight w_{ij} .

Definition 6.8.1 *Tendency-to-occur weight*

We define the *tendency-to-occur* weight w_{ij} , with $0 < w_{ij} \leq 1 \forall i, j : E_{ij} \in \Psi$ as a subjective measure of the *tendency-to-occur* of the basic event E_{ij} .

This is similar to what is proposed in Cagno et al. (2000b).

- The *tendency-to-occur* quotient $q_{ij}^{(k)}$ for each observation $k \geq 1$.

Definition 6.8.2 *Tendency-to-occur quotient*

We define the *tendency-to-occur* quotient $q_{ij}^{(k)}$, with $0 < q_{ij}^{(k)} \leq 9 \forall i, j : E_{ij} \in \Psi, \forall k = 1, \dots, K$, as a subjective measure of how much the basic event E_{ij} is more or less likely to occur in the k -th realization of the system with respect to the $(k - 1)$ -th.

6.8.1 Elicitation of the tendency-to-occur weight

We propose to elicit the tendency-to-occur weight without explicitly asking for estimates, but applying a pairwise comparison methodology inspired by the Analytic Hierarchy Process described in Section C.3.3. We decided to use this method mainly for its simplicity, given that pairwise comparisons do not require the experts have a knowledge of the probability theory.

We consider the basic events E_{ij} and we group in such that every event belonging to the same group leads to the same intermediate or top event. Rather than asking experts to quantify the probability for a single event to occur, which may be very

difficult to assess, we suggest to ask them to compare pairwise every single event with the others belonging to the same group. In other words, we invite experts to specify, based on their knowledge and experience, if the occurrence of an event is

- equally or
- moderately more or
- strongly more or
- very strongly more
- absolutely more

probable than the occurrence of each of the other events of the same set.

Finally their opinion about the occurrence of the basic event E_{ij} can be mapped to the weight w_{ij} , following the AHP methodology detailed by the items 2, 3, 4 in Section C.3.3 and the Saaty's table (see Table C.1).

6.8.2 Elicitation of the tendency-to-occur quotient

Again we propose to elicit the tendency-to-occur quotient following the pairwise comparison methodology, but comparing the occurrence of the same event with respect to different realizations of the system.

Precisely, experts are asked to compare the probability of occurrence of the event E_{ij} during the k -th realization and the probability of occurrence of the same event E_{ij} during the $k - 1$ realization, for each basic event $E_{ij} \in \Psi$. They should analyse the upcoming $k + 1$ realization of the system and specify if the occurrence of an event is

- equally or
- moderately more or
- strongly more or
- very strongly more
- absolutely more

probable than the occurrence of the same event in the previous k -th realization. Then the number of judgements is equal to the number of the basic events. Their linguistic opinion can be translated into a correction coefficient q following again Saaty's table (see Table C.1).

If $q_{ij}^{(k)} > 1$ the event E_{ij} is more likely to occur in the k -th realization than in the $(k - 1)$ -th.

6.9 Risk probability prediction

The probability for the top event to occur $P(TE = 1 | \theta_{ij} \forall i, j : E_{ij} \in \Psi)$ is assessed by a quantitative evaluation of the fault tree, assuming that all the events are independent. Following the propagation of the probabilities layer by layer and taking into account the Boolean logic of the gates, it is parameterized in terms of the probabilities θ_{ij} of the primary events in Ψ .

First of all, given the events of layer L connected to the top event through a gate, we can distinguish two cases:

- If they are connected to the top event through an AND gate:

$$P(TE = 1 | \theta_{Lj} \forall j) = \prod_j \theta_{Lj} \quad (6.10)$$

- If they are connected to the top event through an OR gate:

$$P(TE = 1 | \theta_{Lj} \forall j) = 1 - \prod_j (1 - \theta_{Lj}) \quad (6.11)$$

where the complement rule of probability is applied.

The probabilities θ_{Lj} can be defined in terms of the probabilities $\theta_{(L-1)j}$ when E_{Lj} is not an elementary event, following the Boolean logic of the gates. Similarly the probabilities $\theta_{(L-1)j}$ can be defined in terms of the probabilities $\theta_{(L-2)j}$, if $E_{(L-1)j}$ has parents, until we get $P(TE = 1 | \theta_{ij} \forall i, j : E_{ij} \in \Psi)$, where Ψ is the set of the elementary events. Given Ω_{ij} , the set of the parents of E_{ij} ,

- If E_{ij} is at the output of an OR gate

$$\theta_{ij} = \prod_{\forall j: E_{(i-1)j} \in \Omega_{ij}} \theta_{(i-1)j} \quad (6.12)$$

- If E_{ij} is at the output of an AND gate

$$\theta_{ij} = 1 - \prod_{\forall j: E_{(i-1)j} \in \Omega_{ij}} (1 - \theta_{(i-1)j}) \quad (6.13)$$

6.10 The nominal case

6.10.1 Risk probability prediction based on prior beliefs

Prior elicitation

We propose to elicit Beta prior distributions for the probabilities for the elementary events to occur $p(\theta_{ij}|\alpha_{ij}, \beta_{ij}) \forall i, j : E_{ij} \in \Psi$ in the nominal-case. We show in this paragraph how to derive these distributions from the *tendency-to-occur* weights w_{ij} collected from the expert opinion as explained in 6.8. Given the Beta density

$$p(\theta_{ij}|\alpha_{ij}, \beta_{ij}) = \frac{\theta_{ij}^{\alpha_{ij}-1} (1 - \theta_{ij})^{\beta_{ij}-1}}{\mathbf{B}(\alpha_{ij}, \beta_{ij})}, \quad (6.14)$$

then elicitation is to arrive to values of α_{ij} and β_{ij} of the Beta distribution for θ_{ij} .

For each primary event we have a weight w_{ij} coming from the experts' pairwise comparisons. The primary events are grouped in such a way as every event belonging to the same group leads to the same intermediate or top event.

For each group z , we assume that the probability θ_{ij} for the event E_{ij} to occur is proportional to the weight $\theta_{ij} = w_{ij} / W_z$ for some common normalising factor W_z , with $W_z \geq \max w_{ij}$ so that $0 \leq \theta_{ij} \leq 1, \forall i, j : E_{ij} \in \Psi$.

We can ask the expert if there is one of the events that he or she is most confident about knowing the probability of, say event E_{ij}^* . Then we ask for a range of values of θ_{ij}^* , say $\theta_L \leq \theta_{ij}^* \leq \theta_U$. Finally we fit a beta distribution to this range, by matching the range to mean ± 2 standard deviations.

Since $\theta_{ij}^* = w_{ij}^* / W_z$, the range $\theta_L \leq \theta_{ij}^* \leq \theta_U$ gives us a range

$$\theta_L \leq \frac{w_{ij}^*}{W_z} \leq \theta_U \quad (6.15)$$

and then

$$\frac{\theta_L}{w_{ij}^*} \leq \frac{1}{W_z} \leq \frac{\theta_U}{w_{ij}^*} \quad (6.16)$$

Thus for any other $\theta_{ij} = w_{ij}/W_z$, we have a range

$$\frac{w_{ij}}{w_{ij}^*}\theta_L \leq \theta_{ij} \leq \min \left\{ 1, \frac{w_{ij}}{w_{ij}^*}\theta_U \right\} \quad (6.17)$$

For each θ_{ij} we can map this range to a beta prior distribution $p(\theta_{ij}|\alpha_{ij}, \beta_{ij})$ for θ_{ij} (by matching the range to mean ± 2 standard deviations) with parameters α_{ij} and β_{ij} . Note that mapping the ranges to beta distributions, there is no need to determine the normalizing factor W_z . It was introduced in order to derive and show the relationship between the range expressed for θ_{ij}^* and the range of a generic θ_{ij} , given the respective weights, which are evaluated by the geometric mean approach (as explained in C.3.4).

Sampling θ_{ij} from the prior distribution $p(\theta_{ij}|\alpha_{ij}, \beta_{ij})$ for all the elementary events $E_{ij} \in \Psi$, we can compute the prior distributions for higher events up the tree, using the gate algebra, and then sample a value from the prior distribution of the probability of the top event $P(TE = 1|\theta_{ij}\forall i, j : E_{ij} \in \Psi)$, based on prior beliefs, following the explanation in Section 6.9.

6.10.2 The likelihood

From a particular realization of the system we can collect the following sparse data:

- If the top event occurred, did not occur or was unobserved;
- Similarly for any intermediate event;
- Similarly for any elementary event.

We explain in this section how to derive the total likelihood function for the inference of the probabilities θ_{ij} for the basic events to occur, given the observation of the nominal case.

We have a two stage procedure for determining the likelihood:

1. *Logical deduction step.* Work up the fault tree from bottom to the top event and logically deduce from the tree structure if any unobserved events must have occurred or not;
2. *Likelihood evaluation step.* Work up the fault tree from bottom to the top event and evaluate the likelihood term for each observed node in the tree.

First we discuss some examples and then we provide a general formulation of the likelihood function.

Example 1 Let us consider a critical system with the fault tree illustrated in Figure 6.2.

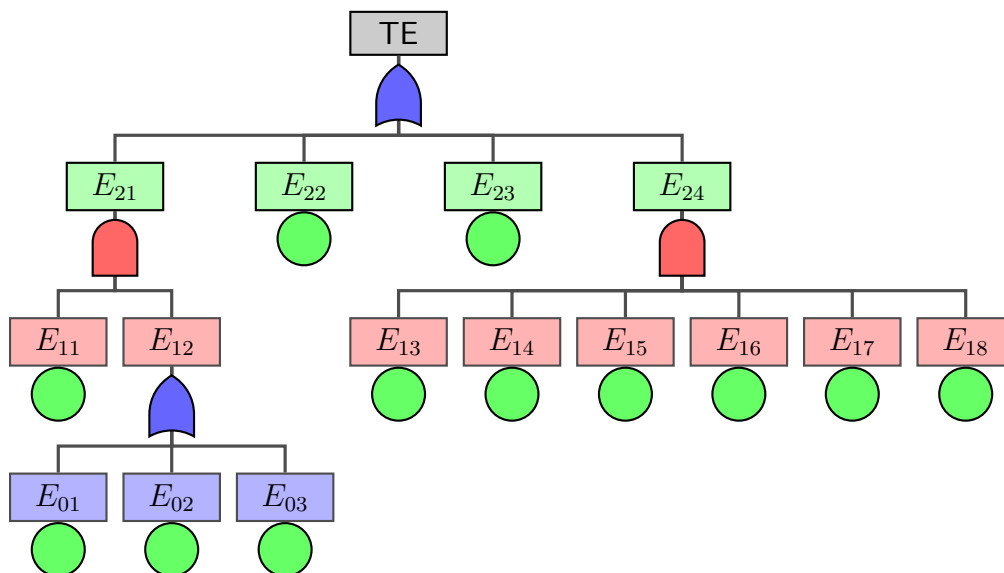


Fig. 6.2: Fault tree representation of the system to analyse in the Example 1. Note that the basic events are indicated with green circles.

Assume we have the following nominal-case observation:

$$\begin{cases} I_{21}, I_{22}, I_{24}, I_{11} = 1 \\ E_{21}, E_{24}, E_{11} = 1 \\ E_{22} = 0 \end{cases} \quad (6.18)$$

This can be visualized in Figure 6.3.

Working up the fault tree to the top event we can logically deduce what follows, for some of the unobserved events:

- The events $E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}$ must have occurred, since their child E_{24} is observed to have occurred and it is at the output of an AND gate;
- The event E_{12} must have occurred, since its child E_{21} is observed to have occurred and it is at the output of an AND gate;

- E_{01}, E_{02}, E_{03} are connected to the intermediate event through an OR gate and
- we observed that $E_{12} = 1$;
- $E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}$ are connected to the intermediate event through an AND gate and
- we observed that $E_{24} = 1$.

we can conclude that at least one of the events E_{01}, E_{02}, E_{03} (the parents of E_{12}) occurred and that all the events $E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}$ occurred. It follows that:

$$P(E_{12} = 1 | \theta_{01}, \theta_{02}, \theta_{03}) = [1 - \prod_{j=1}^3 (1 - \theta_{0j})] \quad (6.20)$$

$$P(E_{24} = 1 | \theta_{13}, \theta_{14}, \theta_{15}, \theta_{16}, \theta_{17}, \theta_{18}) = \prod_{j=3}^8 \theta_{1j} \quad (6.21)$$

Let Ψ be the set of the basic events in τ

$$\Psi = \{E_{ij} : E_{ij} \text{ is a basic event in } \tau\} \quad (6.22)$$

Finally we can evaluate the total likelihood for this nominal-case observation:

$$P(obs. | \theta_{ij} \forall i, j : E_{ij} \in \Psi) = \prod_{\forall i, j : E_{ij} \in \Xi} \theta_{ij}^{E_{ij}} (1 - \theta_{ij})^{1 - E_{ij}} \times \quad (6.23)$$

$$\times \left[1 - \prod_{j=1}^3 (1 - \theta_{0j}) \right] \prod_{j=3}^8 \theta_{1j} \quad (6.24)$$

or using the indicator variable $I_{ij} \in \{0, 1\}$:

$$P(obs. | \theta_{ij} \forall i, j : E_{ij} \in \Psi) = \prod_{\forall i, j : E_{ij} \in \Psi} [\theta_{ij}^{E_{ij}} (1 - \theta_{ij})^{1 - E_{ij}}]^{I_{ij}} \times \quad (6.25)$$

$$\times \left[1 - \prod_{j=1}^3 (1 - \theta_{0j}) \right] \prod_{j=3}^8 \theta_{1j} \quad (6.26)$$

Example 2 We consider now a different nominal-case observation of the critical system illustrated by the fault tree in Figure 6.2.

As shown in Figure 6.4, let us assume we have the following observation:

$$\begin{cases} I_{21}, I_{22}, I_{24}, I_{11}, I_{12}, I_{13}, I_{14}, I_{15}, I_{16}, I_{17}, I_{18}, I_{03} = 1 \\ TE, E_{21}, E_{24}, E_{11}, E_{12}, E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18} = 1 \\ E_{22}, E_{03} = 0 \end{cases} \quad (6.27)$$

In this case we observed $E_{03} = 0$.

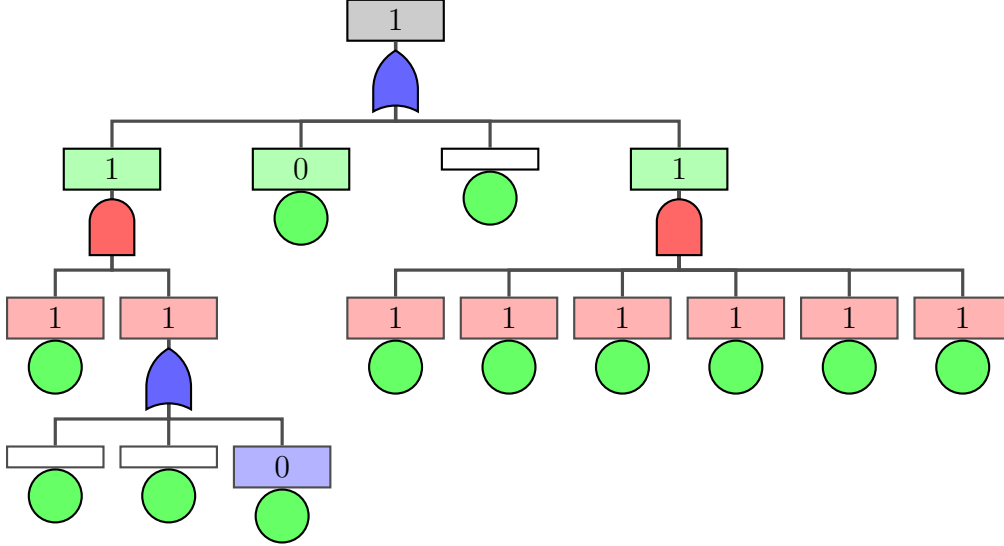


Fig. 6.4: Example of a nominal-case observation of the system represented in Figure 6.2. The white rectangles represent the unobserved events, while the coloured ones represent the observed events. The observed events with 1 are the events observed to occur, while the 0 indicates that the event did not occur.

We want to calculate again the total likelihood of the basic events.

It is given by the contribution of

1. The observed basic events :

$$\Xi = \{E_{22}, E_{11}, E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}, E_{03}\}$$

Each of them contribute to the total likelihood with a factor

$$\begin{cases} \theta_{ij} & \text{if } E_{ij} = 1 \\ 1 - \theta_{ij} & \text{if } E_{ij} = 0 \end{cases} \quad (6.28)$$

2. The unobserved basic events whose occurrence affects the occurrence of the observed intermediate event through AND/OR gates:

$$E_{01}, E_{02} \text{ whose child } E_{12} \text{ is observed}$$

Since

- E_{01}, E_{02}, E_{03} are connected to the intermediate event through an OR gate and
- we observed that $E_{12} = 1$,
- we observed that $E_{03} = 0$

we can conclude that at least one of the events E_{01}, E_{02} occurred. It follows that:

$$P(E_{12} = 1, E_{03} = 0 | \theta_{01}, \theta_{02}, \theta_{03}) = \left[1 - \prod_{j=1}^2 (1 - \theta_{0j}) \right] (1 - \theta_{03}) \quad (6.29)$$

Note that θ_{03} is already contributing to the total likelihood as an observed basic event.

Then the total likelihood is given by

$$P(obs. | \theta_{ij} \forall i, j : E_{ij} \in \Psi) = \prod_{\forall i, j : E_{ij} \in \Xi} \theta_{ij}^{E_{ij}} (1 - \theta_{ij})^{1 - E_{ij}} \times \quad (6.30)$$

$$\times \frac{P(E_{12} = 1 | \theta_{01}, \theta_{02}, \theta_{03})}{(1 - \theta_{03})} \quad (6.31)$$

$$= \prod_{\forall i, j : E_{ij} \in \Xi} \theta_{ij}^{E_{ij}} (1 - \theta_{ij})^{1 - E_{ij}} \times \quad (6.32)$$

$$\times \left[1 - \prod_{j=1}^2 (1 - \theta_{0j}) \right] \times 1 \quad (6.33)$$

$$(6.34)$$

In this case, note that the intermediate event E_{24} contributes with a factor 1 to the likelihood because:

- we observed E_{24} to occur;
- we observed all its parents to occur;
- the parents are connected to the intermediate event E_{24} through and AND gate.

Example 3 Lastly we examine the following observation of the critical system, represented by the fault tree in Figure 6.2.

$$\begin{cases} I_{21}, I_{22}, I_{24}, I_{11}, I_{12}, I_{13}, I_{14}, I_{15}, I_{16}, I_{17}, I_{18}, I_{03}, E_{03} = 1 \\ TE, E_{21}, E_{24}, E_{11}, E_{12}, E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18} = 1 \\ E_{22} = 0 \end{cases} \quad (6.35)$$

Similarly to the Example 2 we observed E_{03} , but this time as an occurring event $E_{03} = 1$.

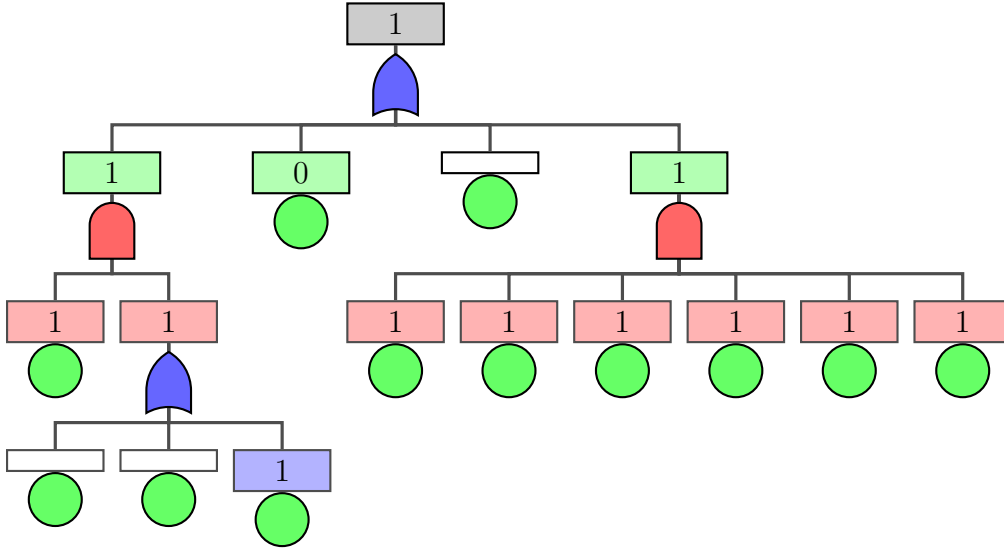


Fig. 6.5: Example of a nominal-case observation of the system represented in Figure 6.2. The white rectangles represent the unobserved events, while the coloured ones represent the observed events. The observed events with 1 are the events observed to occur, while the 0 indicates that the event did not occur.

In this case the total likelihood is given just by the contribution of

1. The observed basic events :

$$\Xi = \{E_{22}, E_{11}, E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}, E_{03}\}$$

Each of them contribute to the total likelihood with a factor

$$\begin{cases} \theta_{ij} & \text{if } E_{ij} = 1 \\ 1 - \theta_{ij} & \text{if } E_{ij} = 0 \end{cases} \quad (6.36)$$

Since

- E_{01}, E_{02}, E_{03} are connected to the intermediate event through an OR gate and
- we observed that $E_{12} = 1$,
- we observed that $E_{03} = 1$

we cannot say anything about the occurrence of E_{01} , E_{02} . Indeed, if we consider all the possible cases, we have that:

$$P(E_{12} = 1 | \theta_{01}, \theta_{02}, \theta_{03}) = \theta_{03} \quad (6.37)$$

where θ_{03} appears already at point 1.

Then the total likelihood is reduced to:

$$P(\text{obs.} | \theta_{ij} \forall i, j : E_{ij} \in \Psi) = \prod_{\forall i, j : E_{ij} \in \Xi} \theta_{ij}^{E_{ij}} (1 - \theta_{ij})^{1 - E_{ij}} \quad (6.38)$$

Likelihood evaluation step - General nominal-case

We can now formulate the total likelihood of the primary (or basic or parentless) events $P(\text{obs.} | \theta_{ij} \forall i, j : E_{ij} \in \Psi)$ for a general nominal-case observation. The total likelihood is expressed in terms of the probabilities for the basic events to occur $\theta_{ij} : E_{ij}$ is a basic event, either observed or unobserved, but its computation depends on all the observed events, either intermediate or basic.

We call \mathcal{L}_{ij} the contribution term to the total likelihood of the event E_{ij} . It depends on the lower layers $i = 0, \dots, j - 1$ of the fault tree τ .

Given:

$$\begin{cases} E_{ij} \in \{0, 1\} \\ I_{ij} \in \{0, 1\} \\ \forall i, j : E_{ij} \in \Phi = \{E_{ij} : E_{ij} \text{ is an event of the fault tree } \tau\} \end{cases} \quad (6.39)$$

Defining

$$\epsilon_{i-1} = \{E_{kj} | k \leq i - 1\} \quad (6.40)$$

as the set of the events (observed or not) to consider for the likelihood up to level $i - 1$, the total likelihood function can be expressed with the product:

$$\begin{aligned} P(\text{obs.} | \theta_{ij} \forall i, j : E_{ij} \in \Psi) &= \prod_{\forall i, j : E_{ij} \in \Phi} \mathcal{L}_{ij} & (6.41) \\ &= \prod_{\forall i, j : E_{ij} \in \Phi} \left[P(E_{ij} = 1 | \epsilon_{i-1})^{E_{ij}} P(E_{ij} = 0 | \epsilon_{i-1})^{1 - E_{ij}} \right]^{I_{ij}} \end{aligned}$$

where \mathcal{L}_{ij} is given by a Bernoulli likelihood if the event E_{ij} is observed ($I_{ij} = 1$).

We distinguish two scenarios:

1. If E_{ij} is a parentless event, the probability for E_{ij} to occur is not conditioned on any other event:

$$P(E_{ij} = 1|\epsilon_{i-1}) = P(E_{ij} = 1) \text{ or similarly } P(E_{ij} = 0|\epsilon_{i-1}) = P(E_{ij} = 0) \quad (6.42)$$

Then the contribution term to the total likelihood (or in this case simply the likelihood) is given by the Bernoulli likelihood:

$$\mathcal{L}_{ij} = [\theta_{ij}^{E_{ij}} (1 - \theta_{ij})^{1-E_{ij}}]^{I_{ij}} \quad \forall i, j : E_{ij} \text{ is a basic event} \quad (6.43)$$

2. If E_{ij} is an observed intermediate event, $P(E_{ij} = 1|\epsilon_{i-1})$ or $P(E_{ij} = 0|\epsilon_{i-1})$, and then its contribution to the total likelihood, can be computed applying recursively the algorithms explained in the next section.

Likelihood contribution of an observed intermediate event

Let E_{ij} be an observed intermediate event and let Ω_{ij} be the set of the parents of E_{ij} . The flow diagrams in Figures 6.7 and 6.7, in the next two pages, show how to calculate the term \mathcal{L}_{ij} for E_{ij} .

We distinguish two cases with respect to the relationship to the parent events:

1. If E_{ij} is at the output of an AND gate;
2. If E_{ij} is at the output of an OR gate.

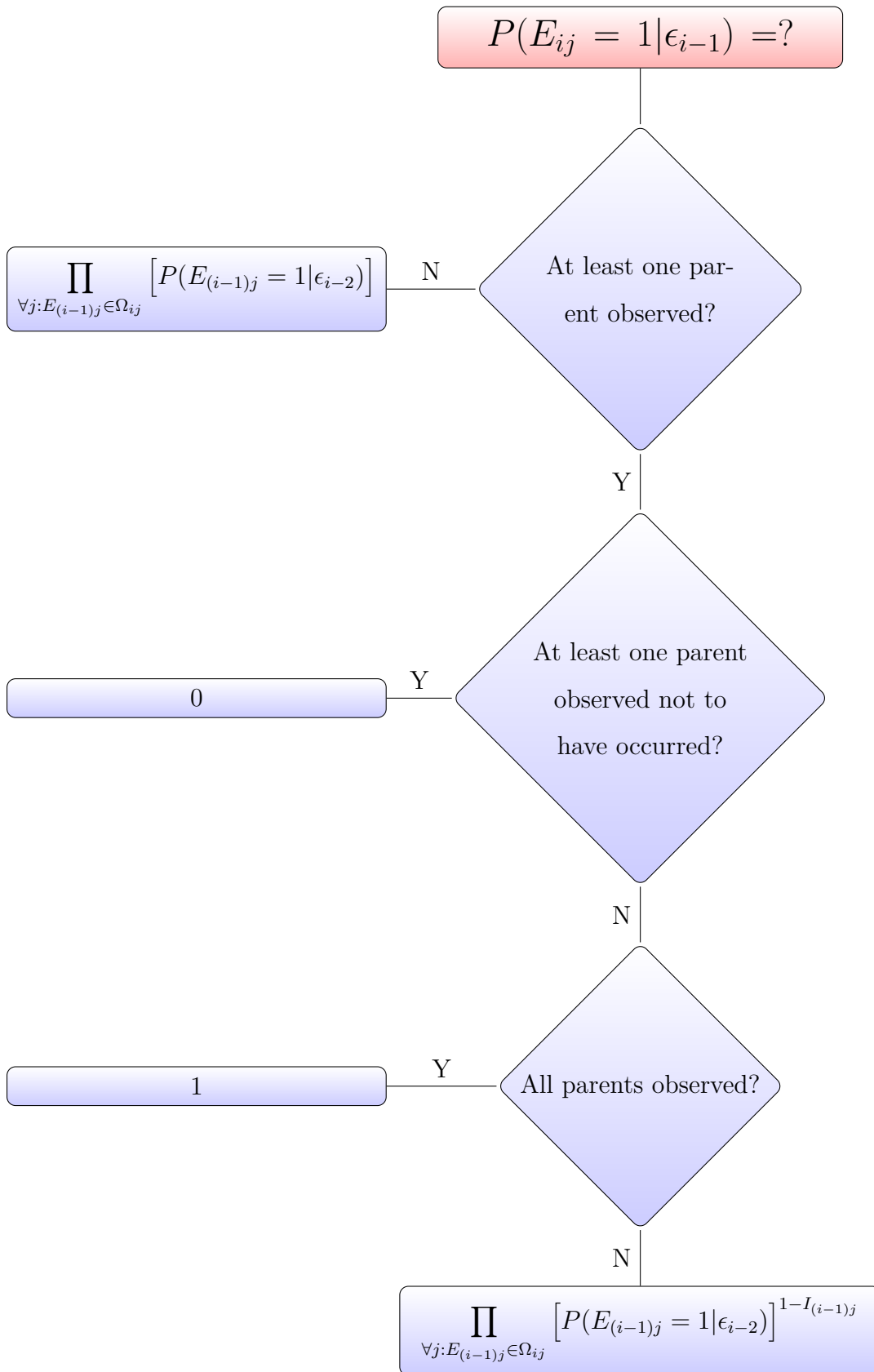


Fig. 6.6: Relationship to parent events: AND gate. This algorithm shows the evaluation of \mathcal{L}_{ij} for the intermediate event E_{ij} at the output of an AND gate.

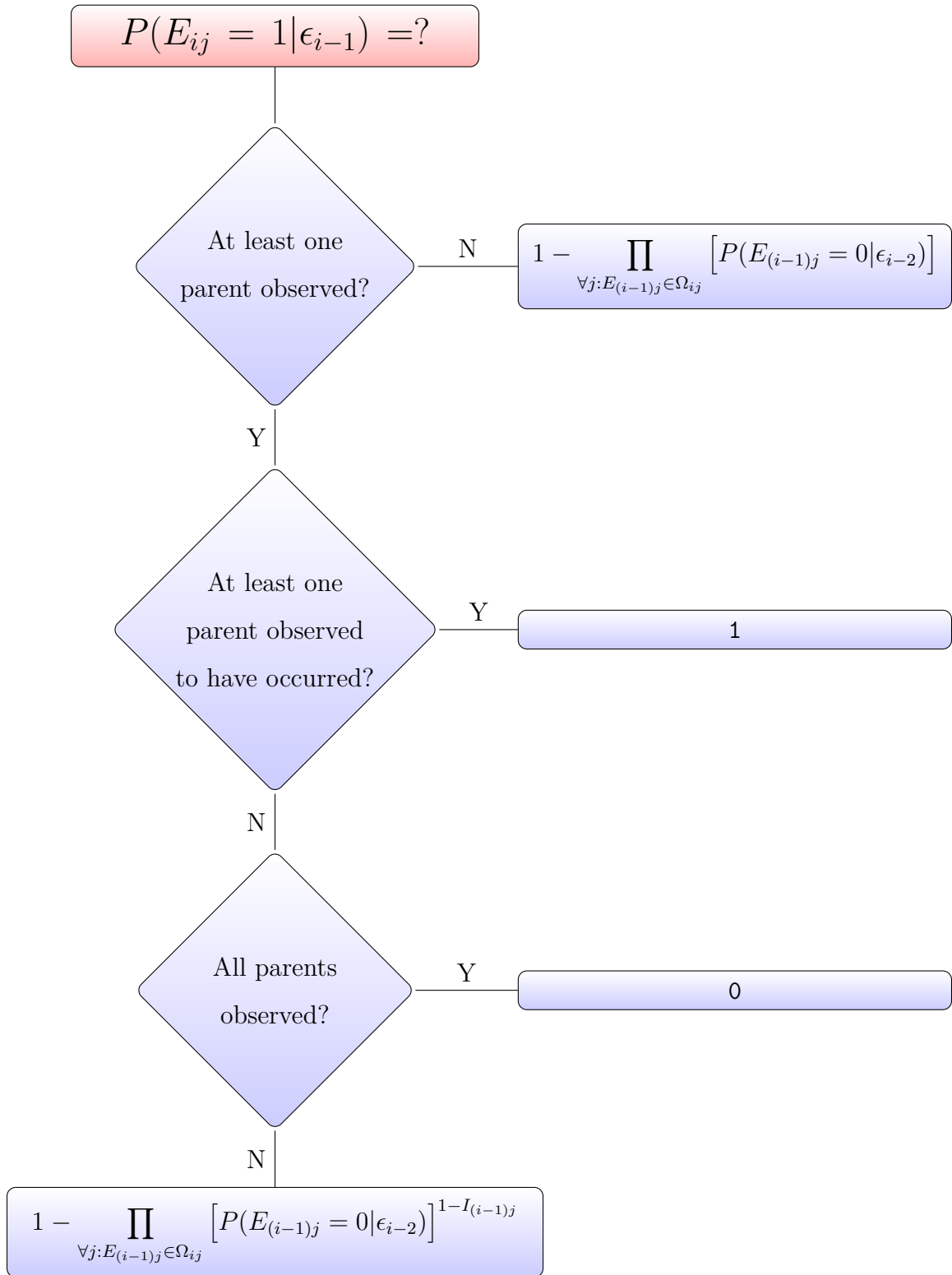


Fig. 6.7: Relationship to parent events: OR gate. This algorithm shows the evaluation of \mathcal{L}_{ij} for the intermediate event E_{ij} at the output of an OR gate.

Finally from these flow diagrams we can derive the expressions:

- for an AND gate:

$$\begin{aligned}
P(E_{ij} = 1 | \epsilon_{i-1}) &= \prod_{\forall j: E_{(i-1)j} \neq 0 \in \Omega} \left[P(E_{(i-1)j} = 1 | \epsilon_{i-2}) \right]^{1-I_{(i-1)j}} \\
&\cdot \prod_{\forall j: E_{(i-1)j} = 0 \in \Omega} \left[P(E_{(i-1)j} = 1 | \epsilon_{i-2}) \right] \quad (6.44)
\end{aligned}$$

$$\begin{aligned}
P(E_{ij} = 0 | \epsilon_{i-1}) &= 1 - P(E_{ij} = 1 | \epsilon_{i-1}) = \\
&= 1 - \prod_{\forall j: E_{(i-1)j} \neq 0 \in \Omega} \left[P(E_{(i-1)j} = 1 | \epsilon_{i-2}) \right]^{1-I_{(i-1)j}} \\
&\cdot \prod_{\forall j: E_{(i-1)j} = 0 \in \Omega} \left[P(E_{(i-1)j} = 1 | \epsilon_{i-2}) \right] \quad (6.45)
\end{aligned}$$

- and for an OR gate:

$$\begin{aligned}
P(E_{ij} = 1 | \epsilon_{i-1}) &= 1 - \prod_{\forall j: E_{(i-1)j} \neq 1 \in \Omega} \left[P(E_{(i-1)j} = 0 | \epsilon_{i-2}) \right]^{1-I_{(i-1)j}} \\
&\cdot \prod_{\forall j: E_{(i-1)j} = 1 \in \Omega} \left[P(E_{(i-1)j} = 0 | \epsilon_{i-2}) \right] \quad (6.46)
\end{aligned}$$

$$\begin{aligned}
P(E_{ij} = 0 | \epsilon_{i-1}) &= 1 - P(E_{ij} = 1 | \epsilon_{i-1}) = \\
&= \prod_{\forall j: E_{(i-1)j} \neq 1 \in \Omega} \left[P(E_{(i-1)j} = 0 | \epsilon_{i-2}) \right]^{1-I_{(i-1)j}} \\
&\cdot \prod_{\forall j: E_{(i-1)j} = 1 \in \Omega} \left[P(E_{(i-1)j} = 0 | \epsilon_{i-2}) \right] \cdot \quad (6.47)
\end{aligned}$$

Example 4 We consider the critical system represented in Figure 6.8.

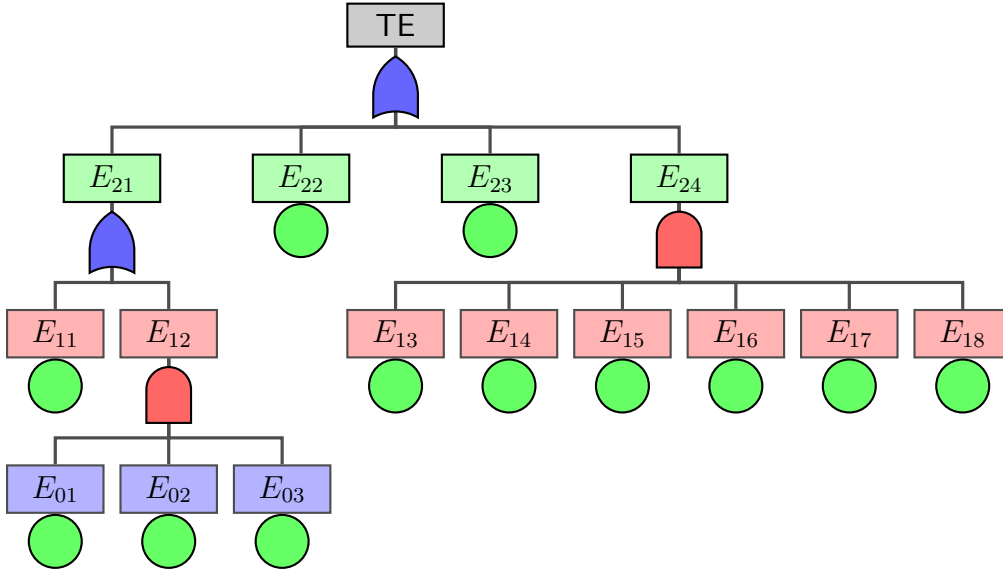


Fig. 6.8: Fault tree representation of a critical system.

Assume we have the following nominal-case observation:

$$\begin{cases} I_{21}, I_{24}, I_{13}, I_{14}, I_{15}, I_{16}, I_{17}, I_{18} = 1 \\ TE, E_{21}, E_{24}, E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18} = 1 \end{cases} \quad (6.48)$$

We can visualize it in Figure 6.9.

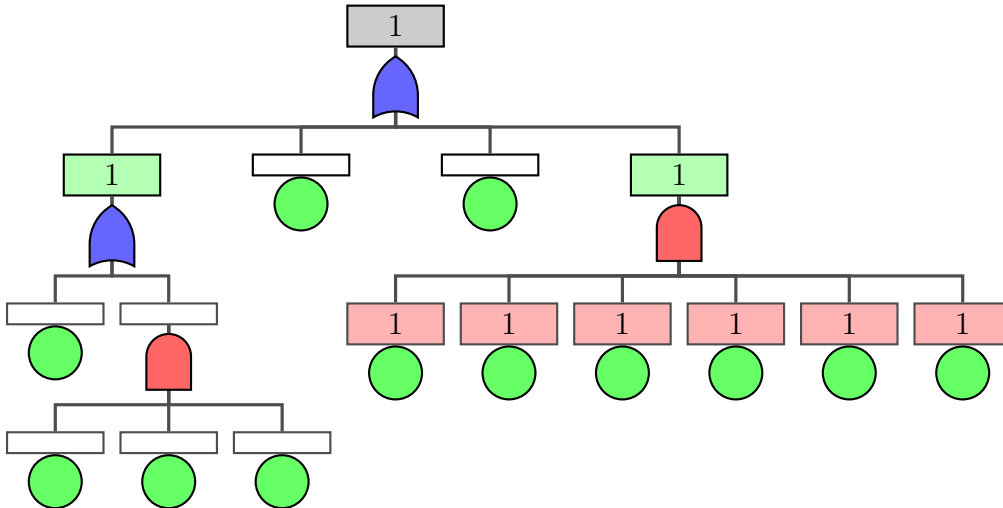


Fig. 6.9: Example of a nominal-case observation of the system represented in Figure 6.8. The white rectangles represent the unobserved events, while the coloured ones represent the observed events. The observed events with 1 are the events observed to occur.

1. Each of the observed basic events

$$\Xi = \{E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}\}$$

contributes to the total likelihood with the factor expressed in 6.43:

$$\mathcal{L}_{ij} = \left[\theta_{ij}^{E_{ij}} (1 - \theta_{ij})^{1-E_{ij}} \right]^{I_{ij}} \quad \forall (i, j) \in \{(1, 3), (1, 4), (1, 5), (1, 6), (1, 7), (1, 8)\} \quad (6.49)$$

2. The likelihood contribution term of the observed intermediate event E_{21} can be computed applying, first of all, the formula 6.46, since E_{21} is at the output of an OR gate:

$$\begin{aligned} \mathcal{L}_{21} = P(E_{21} = 1 | \epsilon_1) &= 1 - \left[P(E_{11} = 0 | \epsilon_0) \right] \left[P(E_{12} = 0 | \epsilon_0) \right] \\ &= 1 - \left[P(E_{11} = 0) \right] \left[P(E_{12} = 0 | \epsilon_0) \right] \end{aligned} \quad (6.50)$$

Then since E_{11} is a parentless event:

$$\mathcal{L}_{21} = 1 - [1 - \theta_{11}] \left[P(E_{12} = 0 | \epsilon_0) \right] \quad (6.51)$$

Finally applying the formula 6.45, since E_{12} is at the output of an AND gate:

$$\mathcal{L}_{21} = 1 - [1 - \theta_{11}] [1 - \theta_{01}\theta_{02}\theta_{03}] \quad (6.52)$$

In conclusion, the total likelihood of the basic events is given by:

$$\begin{aligned} P(obs.0 | \theta_{ij} \forall i, j : E_{ij} \in \Psi) &= \mathcal{L}_{21} \prod_{j=3}^8 \mathcal{L}_{1j} \quad (6.53) \\ &= [1 - (1 - \theta_{11})(1 - \theta_{01}\theta_{02}\theta_{03})] \prod_{j=3}^8 \theta_{1j}. \end{aligned}$$

6.10.3 Risk probability prediction based on posterior distributions

Given the prior distributions in 6.14 and the total likelihood in 6.41 for the primary events in the nominal case, the formulation of the joint posterior probability follows straightforwardly from Bayes rule:

$$p(\theta_{ij} \forall i, j : E_{ij} \in \Psi | obs.0) \propto P(obs. 0 | \theta_{ij} \forall i, j : E_{ij} \in \Psi) \prod_{\forall i, j : E_{ij} \in \Psi} p(\theta_{ij} | \alpha_{ij}, \beta_{ij}) \quad (6.54)$$

Samples of θ_{ij} can be generated from 6.54 to assess the probability for the top event to occur based on the joint posterior distribution, in the nominal-case. Except for the lucky cases when the likelihood is binomial and then the posterior beta-binomial ¹, the samples can be generated by importance sampling (or MCMC for high dimensional situations).

Importance sampling

Posterior samples can be generated by importance sampling.

1. Consider for each θ_{ij} the Beta prior distribution $p(\theta_{ij}|\alpha_{ij}, \beta_{ij})$ as proposal distribution;
2. Draw from the prior distributions $p(\theta_{ij}|\alpha_{ij}, \beta_{ij}) \forall i, j : E_{ij} \in \Psi$ N samples:

$$\hat{\boldsymbol{\theta}}^{(1)} = \{\theta_{ij}^{(1)} \forall i, j : E_{ij} \in \Psi\} \quad (6.55)$$

$$\vdots \quad (6.56)$$

$$\vdots \quad (6.57)$$

$$\hat{\boldsymbol{\theta}}^{(N)} = \{\theta_{ij}^{(N)} \forall i, j : E_{ij} \in \Psi\} \quad (6.58)$$

$$(6.59)$$

3. For each sample $\hat{\boldsymbol{\theta}}^{(n)}$, calculate the *importance weight* r_η from the likelihood

$$r_\eta = P(obs.0|\hat{\boldsymbol{\theta}}^{(n)}) \quad (6.60)$$

4. Finally draw M samples

$$\bar{\boldsymbol{\theta}}^1 = \{\theta_{ij}^{(1)} \forall i, j : E_{ij} \in \Psi\} \quad (6.61)$$

$$\vdots \quad (6.62)$$

$$\vdots \quad (6.63)$$

$$\bar{\boldsymbol{\theta}}^M = \{\theta_{ij}^{(M)} \forall i, j : E_{ij} \in \Psi\} \quad (6.64)$$

$$(6.65)$$

with probability

$$\frac{r_\eta}{\sum_{j=1}^N r_j} \quad (6.66)$$

¹Since the beta prior is the conjugate prior of the binomial distribution.

For further details about this sampling method the reader is addressed to Section A.2.2.

6.11 The non-nominal cases

Assume we can observe $K + 1$ realizations of the system under study, including the nominal profile. Note that each realization can be observed only once, because they are not repeatable. We use k to refer a variable to the k -th realization or observation.

6.11.1 Risk probability prediction based on prior beliefs

The probability for the top event to occur during the upcoming k -th realization of the system (before observing it) is expressed in terms of the samples $\{\theta_{ij}^{(k-1)} \forall i, j : E_{ij} \in \Psi\}$ sampled by the joint posterior distribution of the $k-1$ -th observation $p(\theta_{ij} \forall i, j : E_{ij} \in \Psi | \text{obs. } 0, \dots, k-1)$.

In order to integrate the outcome of the expert opinion into the failure probability assessment, these samples are raised to the power of $(q_{ij}^{(k)})^{-1}$, where $(q_{ij}^{(k)})$ is the *tendency-to-occur* quotient, defined in 6.8.2. If $q_{ij}^{(k)} > 1$ the expert opinion suggests that the event E_{ij} is more likely to occur in the k -th realization than in the $(k-1)$ -th.

The proposed weighting strategy reproduces this opinion considering that

$$\theta_{ij}^{\frac{1}{q}} > \theta_{ij} \quad \text{if } q > 1 \quad (6.67)$$

since θ_{ij} is a probability and hence $0 \leq \theta_{ij} \leq 1$.

Then, the probability for the top event to occur for the k -th realization, based on prior beliefs, is given by the expressions 6.10 and 6.11 (see Section 6.9), in terms of the basic events θ_{ij} , but with θ_{ij} replaced by $(\theta_{ij}^{(k-1)})^{\frac{1}{q_{ij}^{(k)}}}$.

- If the events of the last layer L are connected to the top event through an AND gate:

$$P(TE = 1) = \prod_j (\theta_{ij} | (\theta_{ij}^{(k-1)})^{\frac{1}{q_{ij}^{(k)}}} \forall i, j : E_{ij} \in \Psi) \quad (6.68)$$

- If the events of the last layer L are connected to the top event through an OR gate:

$$P(TE = 1) = 1 - \prod_j (1 - \theta_{ij} | (\theta_{ij}^{(k-1)})^{\frac{1}{q_{ij}^{(k)}}} \forall i, j : E_{ij} \in \Psi) \quad (6.69)$$

6.11.2 The likelihood

For each observation k we define a total weighted likelihood given by:

$$P(\text{obs. } 0, \dots, k | \theta_{ij} \forall i, j : E_{ij} \in \Psi) = \prod_{z=0}^k P(\text{obs. } z | \theta_{ij}^{(q_{ij}^{(z)})^{-1}} \forall i, j : E_{ij} \in \Psi) \quad (6.70)$$

where

- $q_{ij}^{(z)}$ is again the *tendency-to-occur* quotient, defined in 6.8.2;
- $P(\text{obs. } z | \theta_{ij}^{(q_{ij}^{(z)})^{-1}} \forall i, j : E_{ij} \in \Psi)$ is the likelihood of the z -th observation computed as explained for the nominal case in Section 6.10.2, but in terms of the probabilities θ_{ij} weighted by the *tendency-to-occur* quotient.

The intuition behind the idea of weighting the probability θ_{ij} for the basic event E_{ij} to occur in the k observation with the *tendency-to-occur* quotient $q_{ij}^{(k)}$ is that seeing E_{ij} happen is like it happening q_{ij} times under the conditions of the k observation. It can be considered a reinforcement to the likelihood based on expert opinion.

6.11.3 Risk probability prediction based on posterior distributions

After observing the k -th realization of the system, the joint posterior probability distribution can be updated from $p(\theta_{ij} \forall i, j : E_{ij} \in \Phi | \text{obs. } 0, \dots, k-1)$ to $p(\theta_{ij} \forall i, j : E_{ij} \in \Phi | \text{obs. } 0, \dots, k)$, given the prior distributions elicited for the nominal profile and the total weighted likelihood:

$$p(\theta_{ij} \forall i, j | \text{obs. } 0, \dots, k) \propto P(\text{obs. } 0, \dots, k | \theta_{ij} \forall i, j : E_{ij} \in \Psi) \prod_{(\forall i, j : E_{ij} \in \Psi)} p(\theta_{ij} | \alpha_{ij}, \beta_{ij}) \quad (6.71)$$

Then the probability for the top event to occur during the k -th realization, based on posterior distribution, can be evaluated sampling from 6.71 and applying 6.68 or 6.69.

6.12 The entire procedure

The proposed model can be summarized in the following steps:

1. Construct fault tree;
2. Prior elicitation of elementary event probabilities in nominal case $k = 0$;
3. For each realization $k = 1, \dots, K$:

- (a) Elicit by expert opinion the *tendency-to-occur* quotient

$$q_{ij}^{(k)} \quad \forall i, j : E_{ij} \in \Psi$$

;

- (b) By Importance sampling, generate the vector of samples of

$$\{\theta_{ij}^{(k)} \quad \forall i, j : E_{ij} \in \Psi\}$$

from the current joint posterior

$$p(\theta_{ij} \quad \forall i, j : E_{ij} \in \Psi | \text{obs. } 0, \dots, k-1)$$

.

These samples and the quotients $q_{ij}^{(k)}$ can be used to assess the probability of occurrence of the top event for the k -th realization;

- (c) Observe data for k -th realization;
- (d) Update the joint posterior probability distribution from

$$p(\theta_{ij} \quad \forall i, j : E_{ij} \in \Phi | \text{obs. } 0, \dots, k-1)$$

to

$$p(\theta_{ij} \quad \forall i, j : E_{ij} \in \Phi | \text{obs. } 0, \dots, k)$$

, given:

- The product of the prior distributions elicited for the nominal profile:

$$p(\theta_{ij} \quad \forall i, j : E_{ij} \in \Psi) = \prod_{(\forall i, j : E_{ij} \in \Psi)} p(\theta_{ij} | \alpha_{ij}, \beta_{ij}), \quad (6.72)$$

since they are assumed to be independent.

- The entire weighted likelihood:

$$P(\text{obs. } 0, \dots, k | \theta_{ij} \quad \forall i, j : E_{ij} \in \Psi) = \quad (6.73)$$

$$= \prod_{z=1}^k P(\text{obs. } z | \theta_{ij}^{(q_{ij}^{(z)})^{-1}} \quad \forall i, j : E_{ij} \in \Psi) \quad (6.74)$$

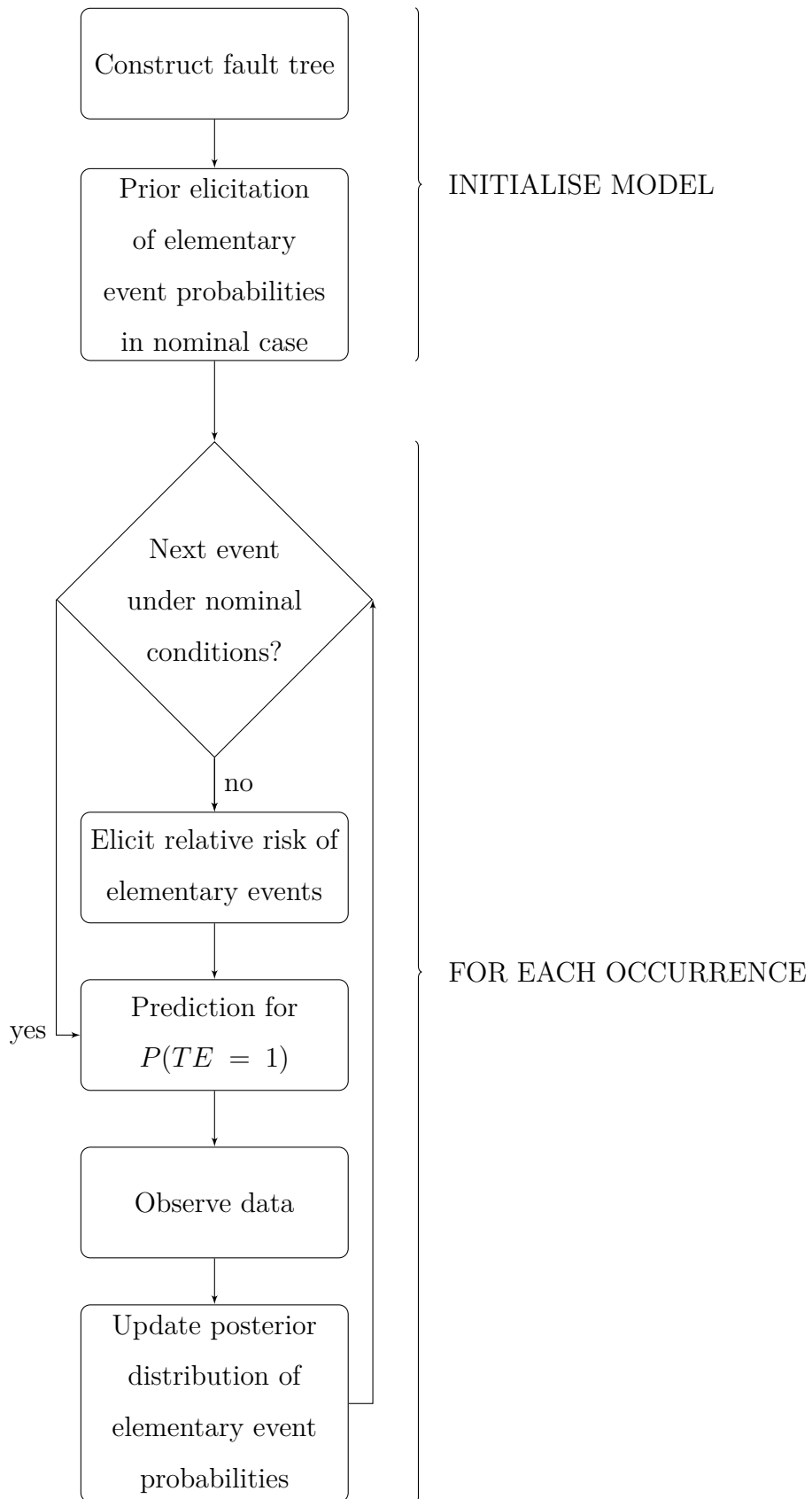


Fig. 6.10: The entire procedure.

6.13 Application proposal

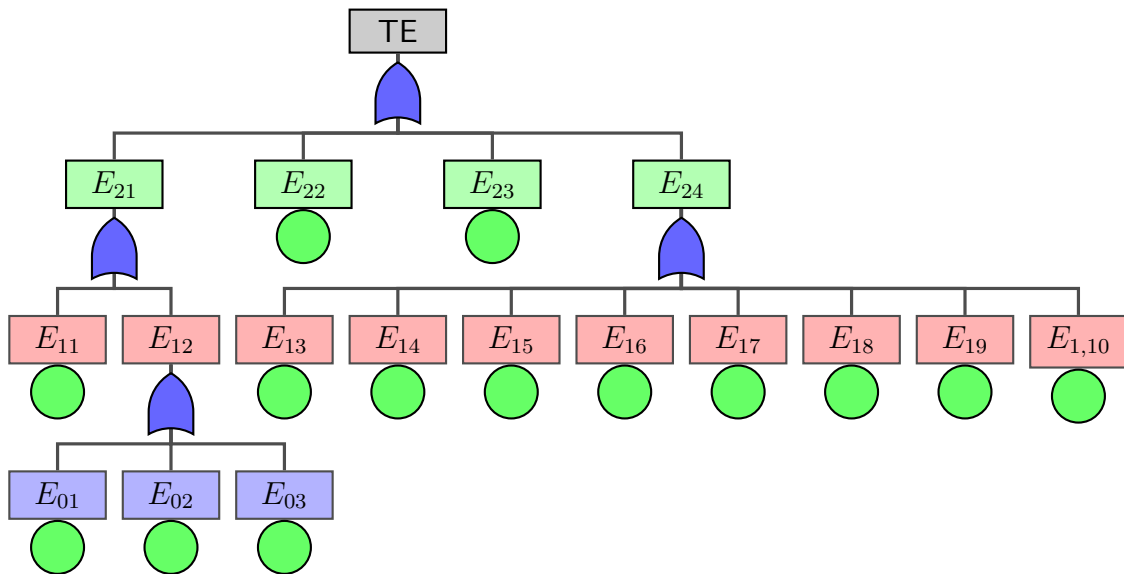


Fig. 6.11

The model proposed and detailed in this chapter has been developed for the assessment of the probability for an explosion to occur during the atmospheric re-entry of a spacecraft. Through discussion with experts working in the European Space Research and Technology Centre and the reading of the ESA Space Debris Mitigation Compliance Verification Guidelines (ESA Space Debris Mitigation Working group, 2015), the ATV1 re-entry analysis reported in (Boutamine et al., 2007),(G. Koppenwallner, B. Fritsche, T. Lips, T. Martin, L.Francillout, 2005) and (Schmehl, 2004) and a review of the state of art (see Fritsche et al. (2005*b*), Mirzaei (2008), Chrostowski et al. (2010), Breu et al. (2008)), we constructed the fault tree in Figure 6.11, whose events are divided in the following groups:

- Outcome: Explosion of the spacecraft (TE)
 - E_{21} Chemical reaction propellant+air;
 - E_{22} Burst of a pressure vessel;
 - E_{23} Chemical reaction between hypergolic propellants;
 - E_{24} Burst of a battery cell.
- Outcome: E_{21} Chemical reaction propellant+air

- E_{11} Sudden release of propellant (due to Burst of a pressure vessel E_{22});
 - E_{12} Slow release of propellant.
- Outcome: E_{12} Slow release of propellant
 - E_{01} Valve leakage;
 - E_{02} Tank destruction;
 - E_{03} Pipe rupture.
- Outcome: E_{24} Burst of a battery
 - E_{13} Chemical reactions;
 - E_{14} Overpressure;
 - E_{15} Short circuit;
 - E_{16} Corrosion;
 - E_{17} Overcharge;
 - E_{18} Overdischarge;
 - E_{19} Overtemperature;
 - $E_{1,10}$ Cell degradation.

Since the event E_{11} is equivalent to the event E_{22} and there are only OR gates, the fault tree could be simplified as follows:

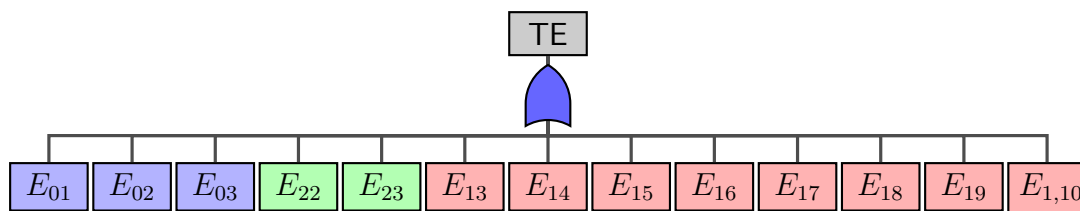


Fig. 6.12

6.13.1 Some useful definitions

For the understanding of the events that build the fault tree we report some useful definitions:

- **Explosion** is an extremely fast and high pressure increase, which may either occur inside a vessel or in the free atmosphere without enclosure. It has a large destructive action.
- **Burst of a pressure vessel:** caused by overpressure $P > P_{burst}$ and weakening of the structure (material degradation due to high temperatures). During the bursting process the vessel usually tears along lines of weakness. Therefore only few fragments are generated.
- **Leakage** Leakage may be caused during re-entry by heated valves or fuel line joints. We may assume that at elevated temperatures the fuel lines and valves will lose their sealing capacity and thus after a certain heating phase of the vehicle a leak flow of propellant will exist.
- **Hypergolic propellants:** these propellants spontaneously ignite when they come into contact with each other.

6.14 Worked example

In this section we present the results of a simulation of the model with the fault tree proposed in 6.11.

Basic events: $\Psi = \{E_{22}, E_{23}, E_{11} = E_{22}, E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}, E_{19}, E_{1,10}, E_{01}, E_{02}, E_{03}\}$. Intermediate events: E_{21}, E_{24}, E_{12} .

All the events are grouped as follows for the prior elicitation:

- Group A: $E_{21}, E_{22}, E_{23}, E_{24}$.
- Group B: E_{01}, E_{02}, E_{03} .
- Group C: $E_{13}, E_{14}, E_{15}, E_{16}, E_{17}, E_{18}, E_{19}, E_{1,10}$.

6.14.1 Prior elicitation for the nominal case

Let us assume we collected the following AHP matrices (see the Section C.3.3) by expert opinion:

$$A = \begin{pmatrix} 1 & 5 & 7 & 7 \\ \frac{1}{5} & 1 & 5 & 1 \\ \frac{1}{7} & \frac{1}{5} & 1 & 1 \\ \frac{1}{7} & 1 & 1 & 1 \end{pmatrix} \quad (6.75)$$

$$B = \begin{pmatrix} 1 & 3 & 1 \\ \frac{1}{3} & 1 & \frac{1}{3} \\ 1 & 3 & 1 \end{pmatrix} \quad C = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \quad (6.76)$$

The consistency ratios (see equations C.5 and C.4 in Section C.3.3) show that the consistency property holds for all the groups (since they are less than 0.1):

$$CR_A = 0.1 \quad CR_B \ll 0.1 \quad CR_C = 0$$

We assume the expert is more confident about the event E_{02} and that he provided a range of values for θ_{02} . Following the procedure in 6.10.1 we can fit the expert opinion to beta prior distributions with the shape parameters reported in Table 6.1.

6.14.2 Observations

The occurrence of the events could be derived by analysing the outcome of an observation campaign. For instance fuel release could be analysed through spectroscopy.

We assume to have the following synthetic data:

- Nominal case

$$\begin{cases} E_{03} = 1 \\ I_{03} = 1 \\ I_{ij} = 0 \quad \forall (ij) \neq (03) \end{cases} \quad (6.77)$$

Event	Weight	Range	Nominal Beta shapes (α, β)
E_{01}	$w_{01} = 0.09$	(0.01, 0.04)	(10.81, 421.52)
E_{02}	$w_{02} = 0.09$	(0.01, 0.04)	(10.81, 421.52)
E_{03}	$w_{03} = 0.82$	(0.09, 0.36)	(8.39, 28.88)
E_{22}	$w_{22} = 0.05$	(0.005, 0.021)	(10.95, 826.01)
E_{23}	$w_{23} = 0.46$	(0.05, 0.201)	(9.59, 66.54)
E_{13}	$w_{13} = 0.125$	(0.014, 0.055)	(10.69, 300.43)
E_{14}	$w_{14} = 0.125$	(0.014, 0.055)	(10.69, 300.43)
E_{15}	$w_{15} = 0.125$	(0.014, 0.055)	(10.69, 300.43)
E_{16}	$w_{16} = 0.125$	(0.014, 0.055)	(10.69, 300.43)
E_{17}	$w_{17} = 0.125$	(0.014, 0.055)	(10.69, 300.43)
E_{18}	$w_{18} = 0.125$	(0.014, 0.055)	(10.69, 300.43)
E_{19}	$w_{19} = 0.125$	(0.014, 0.055)	(10.69, 300.43)
$E_{1,10}$	$w_{1,10} = 0.125$	(0.014, 0.055)	(10.69, 300.43)

Table 6.1: This table summarizes the results of the nominal prior elicitation step. The AHP weights are computed by the geometric mean method explained in C.3.4. From the weights and the range of values of θ_{02} we derived a range of values for the probabilities of all the other basic events and then mapped the elicited weights to the beta prior distributions.

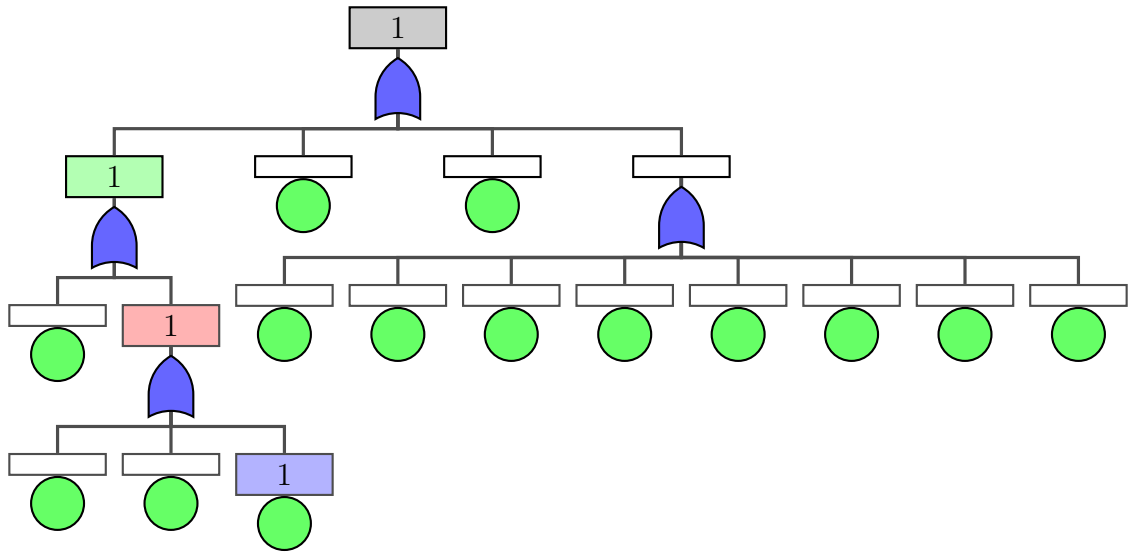


Fig. 6.13: Graphical representation of the nominal observation, including the logical reduction step.

- First observation

$$\left\{ \begin{array}{l} E_{12} = 1 \\ I_{12} = 1 \\ I_{ij} = 0 \quad \forall (ij) \neq (12) \\ q_{01}^{(1)} = q_{02}^{(1)} = q_{03}^{(1)} = 3 \\ q_{ij}^{(1)} = 1 \quad \forall (ij) \forall (ij) : i \neq 0 \end{array} \right. \quad (6.78)$$

- Second observation

$$\left\{ \begin{array}{l} E_{12} = 1 \\ I_{12} = 1 \\ I_{ij} = 0 \quad \forall (ij) \neq (12) \\ q_{01}^{(2)} = q_{02}^{(2)} = q_{03}^{(2)} = 1/5 \\ q_{ij}^{(2)} = 1 \quad \forall (ij) : i \neq 0 \end{array} \right. \quad (6.79)$$

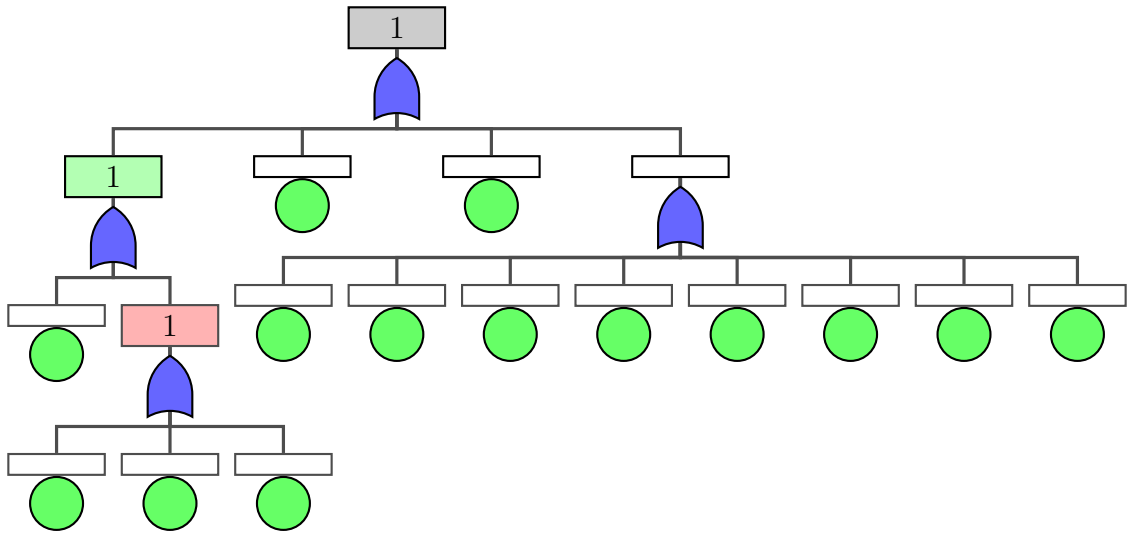


Fig. 6.14: Graphical representation of the first and the second observations, including the logical reduction step.

- Third observation

$$\begin{cases} E_{12} = 0 \\ I_{12} = 1 \\ I_{ij} = 0 \quad \forall (ij) \neq (12) \\ q_{16}^{(3)} = q_{18}^{(3)} = 7 \\ q_{ij}^{(3)} = 1 \quad \forall (ij) \notin \{(18)(16)\} \end{cases} \quad (6.80)$$

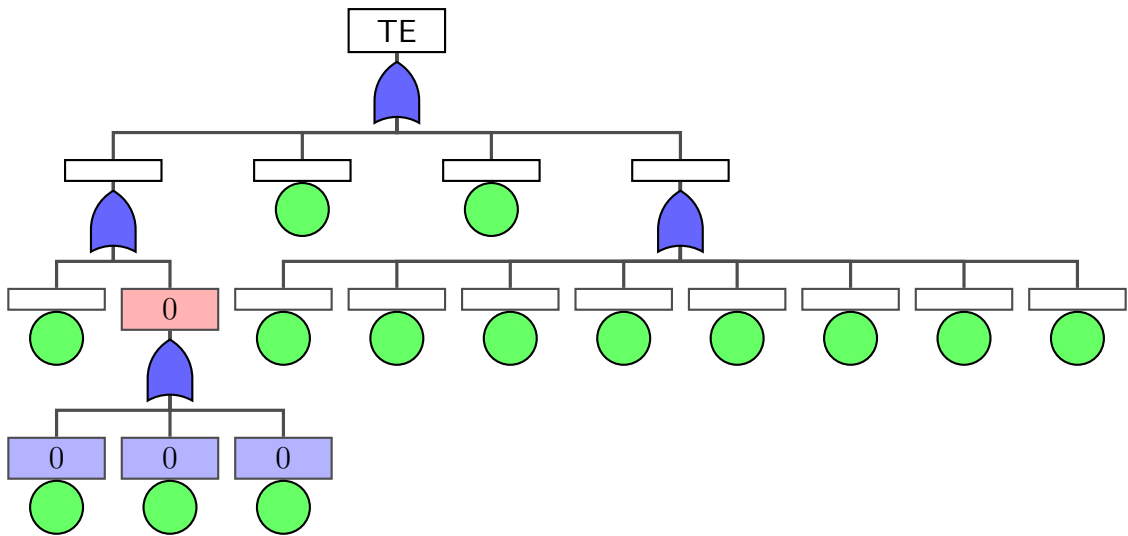


Fig. 6.15: Graphical representation of the third observation, including the logical reduction step.

Event			
E_{01}	$q_{01}^{(1)} = 3$	$q_{01}^{(2)} = 1/5$	$q_{01}^{(3)} = 1$
E_{02}	$q_{02}^{(1)} = 3$	$q_{02}^{(2)} = 1/5$	$q_{02}^{(3)} = 1$
E_{03}	$q_{03}^{(1)} = 3$	$q_{03}^{(2)} = 1/5$	$q_{03}^{(3)} = 1$
E_{22}	$q_{22}^{(1)} = 1$	$q_{22}^{(2)} = 1$	$q_{22}^{(3)} = 1$
E_{23}	$q_{23}^{(1)} = 1$	$q_{23}^{(2)} = 1$	$q_{23}^{(3)} = 1$
E_{13}	$q_{13}^{(1)} = 1$	$q_{13}^{(2)} = 1$	$q_{13}^{(3)} = 1$
E_{14}	$q_{14}^{(1)} = 1$	$q_{14}^{(2)} = 1$	$q_{14}^{(3)} = 1$
E_{15}	$q_{15}^{(1)} = 1$	$q_{15}^{(2)} = 1$	$q_{15}^{(3)} = 1$
E_{16}	$q_{16}^{(1)} = 1$	$q_{16}^{(2)} = 1$	$q_{16}^{(3)} = 7$
E_{17}	$q_{17}^{(1)} = 1$	$q_{17}^{(2)} = 1$	$q_{17}^{(3)} = 1$
E_{18}	$q_{18}^{(1)} = 1$	$q_{18}^{(2)} = 1$	$q_{18}^{(3)} = 7$
E_{19}	$q_{19}^{(1)} = 1$	$q_{19}^{(2)} = 1$	$q_{19}^{(3)} = 1$
$E_{1,10}$	$q_{1,10}^{(1)} = 1$	$q_{1,10}^{(2)} = 1$	$q_{1,10}^{(3)} = 1$

Table 6.2: This table summarizes the *tendency to occur* quotients elicited by expert opinion for all the basic events.

6.14.3 Risk assessment

Risk probability prediction based on the nominal case posterior

$$P(TE = 1) = \prod_{\forall i,j: E_{ij} \in \Psi} (1 - \theta_{ij}) \quad (6.81)$$

where θ_{ij} can be sampled by the posterior

$$p(\theta_{ij} \forall i, j : E_{ij} \in \Psi | obs.0) = \theta_{03} \prod_{\forall i,j: E_{ij} \in \Psi} p(\theta_{ij} | \alpha_{ij}, \beta_{ij}) \quad (6.82)$$

Risk probability prediction based on the posterior of the 1st observation

$$P(TE = 1) = \prod_{\forall i,j: E_{ij} \in \Psi} (1 - \theta_{ij}) \prod_{j=1}^3 (1 - \theta_{0j}^{\frac{1}{3}}) \quad (6.83)$$

where θ_{ij} can be sampled by the posterior

$$p(\theta_{ij} \forall i, j : E_{ij} \in \Psi | obs.0, 1) = \left(1 - \prod_{j=1}^3 (1 - \theta_{0j}^{\frac{1}{3}})\right) \theta_{03} \prod_{\forall E_{ij} \in \Psi} p(\theta_{ij} | \alpha_{ij}, \beta_{ij}) \quad (6.84)$$

Risk probability prediction based on the posterior of the 2nd observation

$$P(TE = 1) = \prod_{\forall i,j: E_{ij} \in \Psi, i \neq 0} (1 - \theta_{ij}) \prod_{j=1}^3 (1 - \theta_{0j}^5) \quad (6.85)$$

where θ_{ij} can be sampled by the posterior

$$\begin{aligned} p(\theta_{ij} \forall i, j : E_{ij} \in \Psi | obs.0, 1, 2) &= \\ &= \left(1 - \prod_{j=1}^3 (1 - \theta_{0j}^5)\right) \left(1 - \prod_{j=1}^3 (1 - \theta_{0j}^{\frac{1}{3}})\right) \theta_{03} \prod_{\forall E_{ij} \in \Psi} p(\theta_{ij} | \alpha_{ij} \beta_{ij}) \end{aligned} \quad (6.86)$$

Risk probability prediction based on the posterior of the 3rd observation

$$P(TE = 1) = \prod_{\forall i,j: E_{ij} \in \Psi} (1 - \theta_{ij}) \quad (6.87)$$

where θ_{ij} can be sampled by the posterior

$$\begin{aligned} p(\theta_{ij} \forall i, j : E_{ij} \in \Psi | obs.0, 1, 2, 3) &= \\ &= \prod_{j=1}^3 (1 - \theta_{0j}) \left(1 - \prod_{j=1}^3 (1 - \theta_{0j}^5)\right) \left(1 - \prod_{j=1}^3 (1 - \theta_{0j}^{\frac{1}{3}})\right) \theta_{03} \prod_{\forall E_{ij} \in \Psi} p(\theta_{ij} | \alpha_{ij} \beta_{ij}) \end{aligned} \quad (6.88)$$

6.14.4 Results

We report in this section four plots showing the results of the worked example, based on simulated data.

The first plot shows a comparison of the pdfs of the probability for the top event (explosion) to occur for the nominal case, after the first, the second and the third observation. The goal of this plot is to show how the elicited tendency-to-occur quotients affect the results of the risk probability predictions. For example we can see how the probability for an explosion to occur increase when the experts say that two basic events are very strongly more probable to occur ($q_{16}^{(3)} = q_{18}^{(3)} = 7$) in the third observation than during the second one. This exactly what we can expect, considering that in this worked example, all the basic events can lead to an explosion.

The next plots have a similar goal, but for the probability of occurrence of the single events.

It is fundamental to note that the obtained results do not match the physical process, as well as the simulated tendency-to-occur quotients. In fact we are aware that the probabilities should be relatively small in a risk analysis situation.

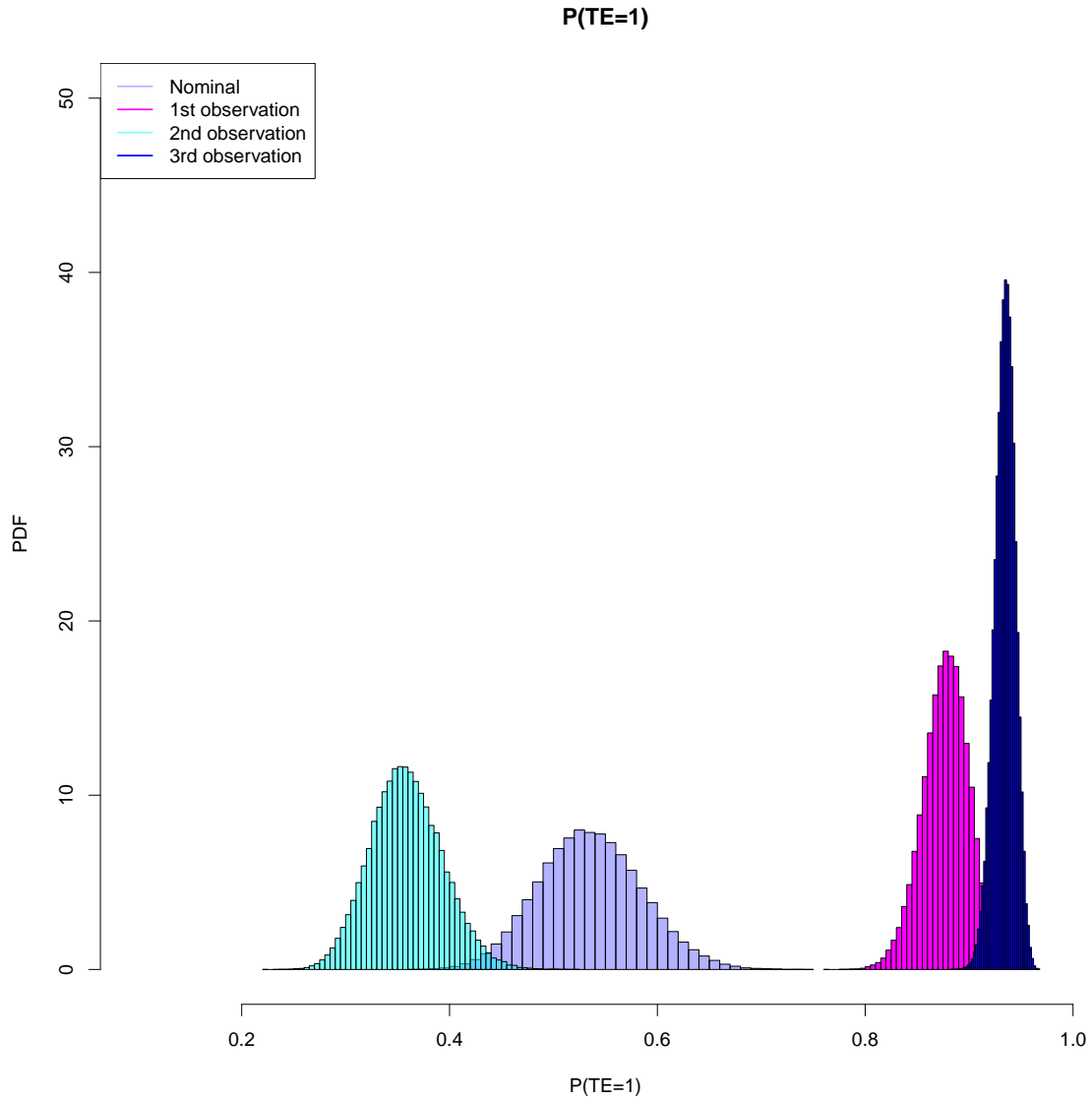


Fig. 6.16: Comparison of the pdfs of the probability for an explosion to occur assessed relying on data and expert opinion respectively for the nominal case, after the first, second and third observation. The shifting of the pdfs seems to reflect the collected values of the *tendency-to-occur* quotients: $q_{01}^{(1)} = q_{02}^{(1)} = q_{03}^{(1)} = 3$, $q_{01}^{(2)} = q_{02}^{(2)} = q_{03}^{(2)} = 1/5$, $q_{16}^{(3)} = q_{18}^{(3)} = 7$. Relying on the available observations, it can be deduced that the explosion occurred during the nominal case, the first and the second observations. Nothing can be stated about the third one.

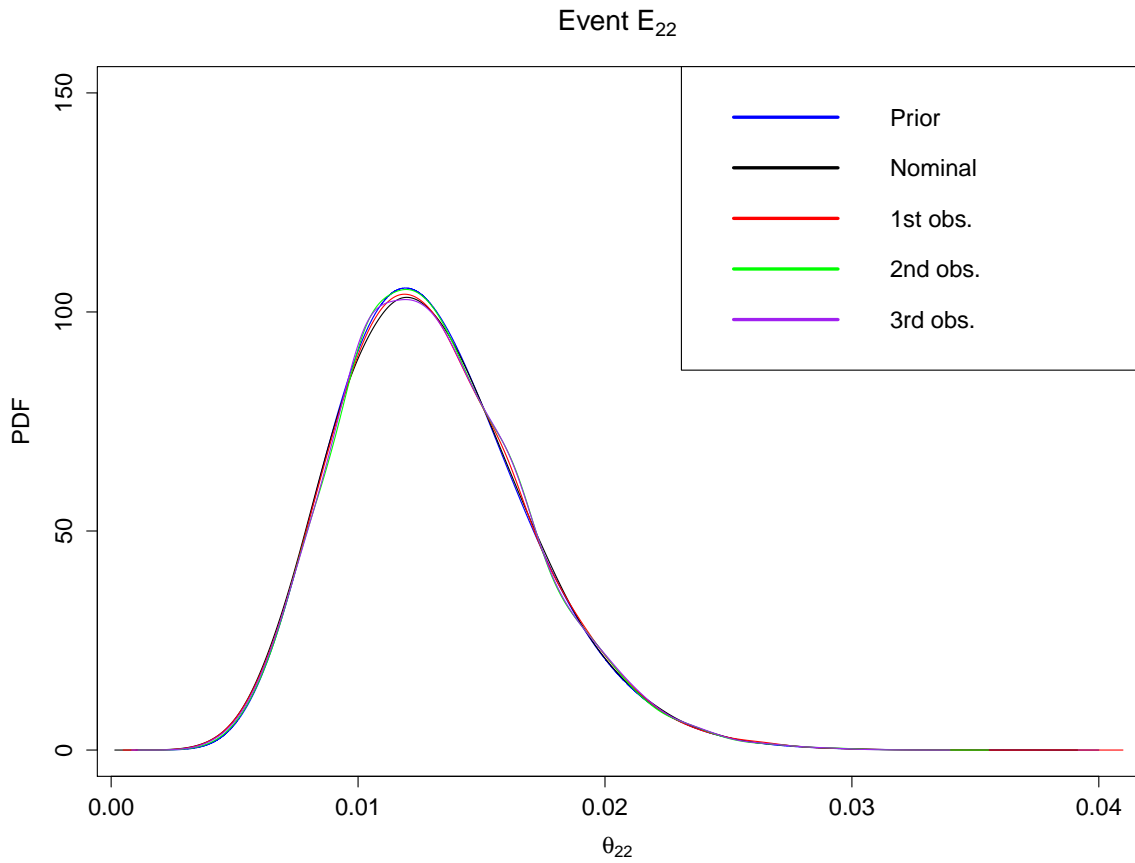


Fig. 6.17: Comparison between the probability density functions of the probability θ_{22} for the event E_{22} to occur: the blue curve is the prior elicited by expert opinion for the nominal case, the black one is the posterior of the nominal case, the red one, the green one and the violet one are respectively posterior of the first, the second and the third observation. The event E_{22} is the burst of a pressure vessel. According to the synthetic data it has never been observed to occur and the *tendency-to-occur* quotient $q_{22}^{(k)} = 1 \forall k = 1, 2, 3$.

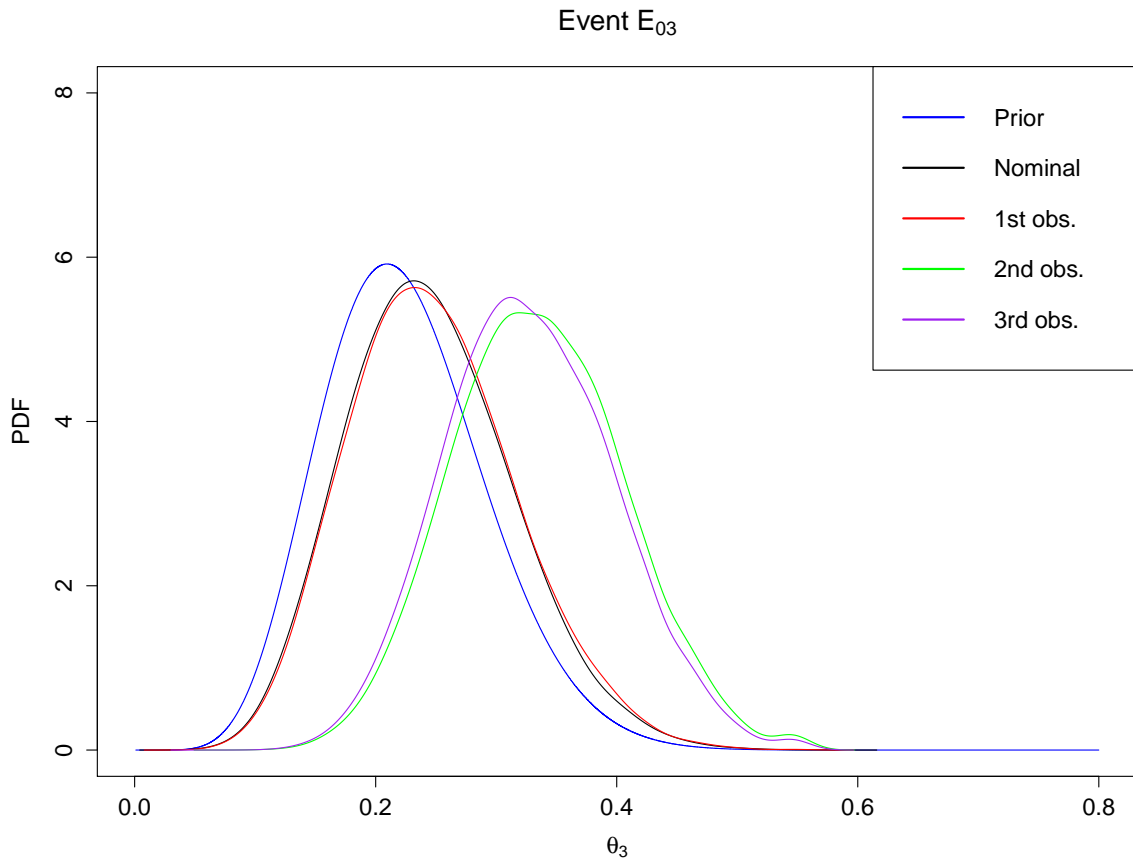


Fig. 6.18: Comparison between the probability density functions of θ_{03} : the blue curve is the prior elicited by expert opinion for the nominal case, the black one is the posterior of the nominal case, the red one, the green one and the violet one are respectively the posterior of the first, the second and the third observation. The event E_{03} is the Pipe rupture. According to the synthetic data it was observed to occur in the nominal case, his father E_{12} was observed to occur during the first and the second observation and observed not to occur during the third observation. The relationship with its father is an OR gate. We assumed the experts provided the following values for the *tendency-to-occur* quotient: $q_{03}^{(1)} = 3, q_{03}^{(2)} = 1/5, q_{03}^{(3)} = 1$. We can observe from the plot a shifting towards right of the global maximum point with respect to the prior belief and this is consistent with the observed data. As consequence of the fact that the event was observed not to occur. The abscissa of the maximum of the posterior evaluated after the third observation is slightly lower than the abscissa of the maximum of the posterior evaluated after the second observation.

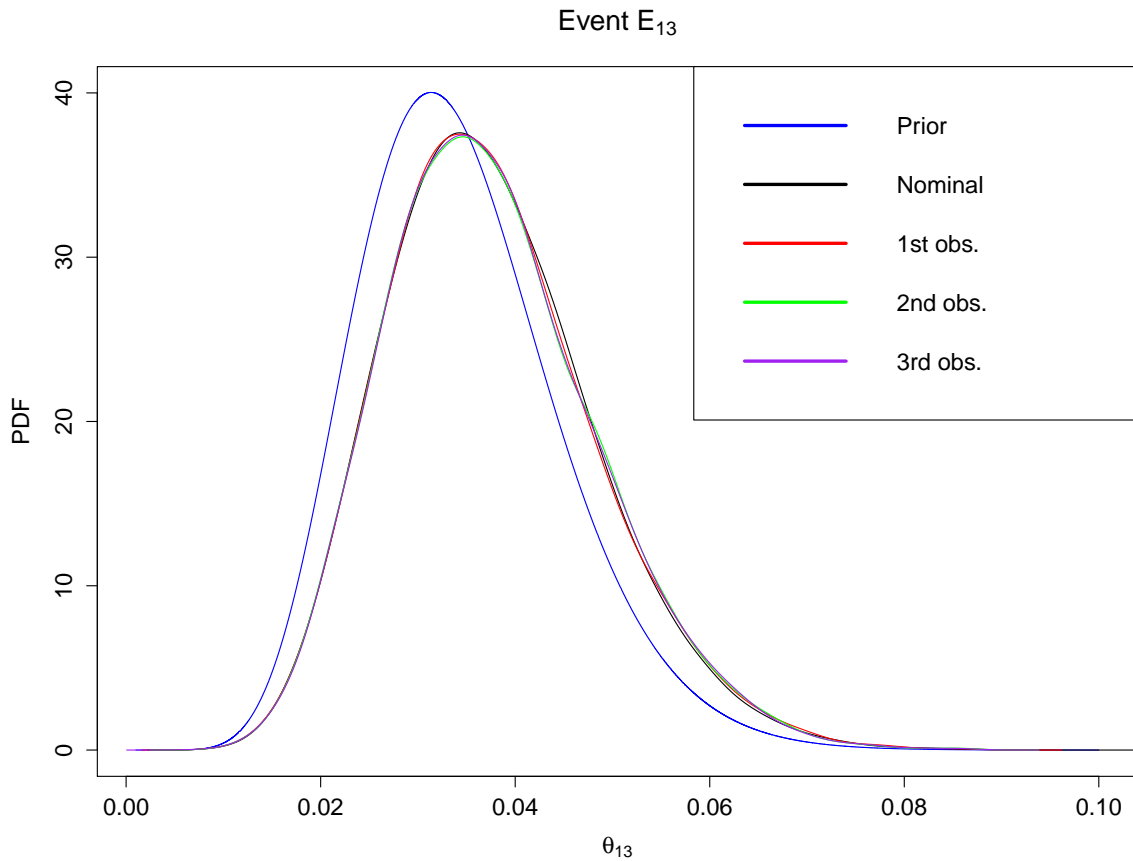


Fig. 6.19: Comparison between the probability density functions of θ_{13} : the blue curve is the prior elicited by expert opinion for the nominal case, the black one is the posterior of the nominal case, the red one, the green one and the violet one are respectively posterior of the first, the second and the third observation. The event E_{13} is the Chemical reaction (inside batteries). According to the synthetic data it has been observed to occur only in the nominal case and the *tendency-to-occur* quotient $q_{13}^{(k)} = 1 \forall k = 1, 2, 3$. Indeed we can observe that the posterior of the nominal case is different from the prior, but there is no any significant difference between the nominal posterior and the posterior of the next observations.

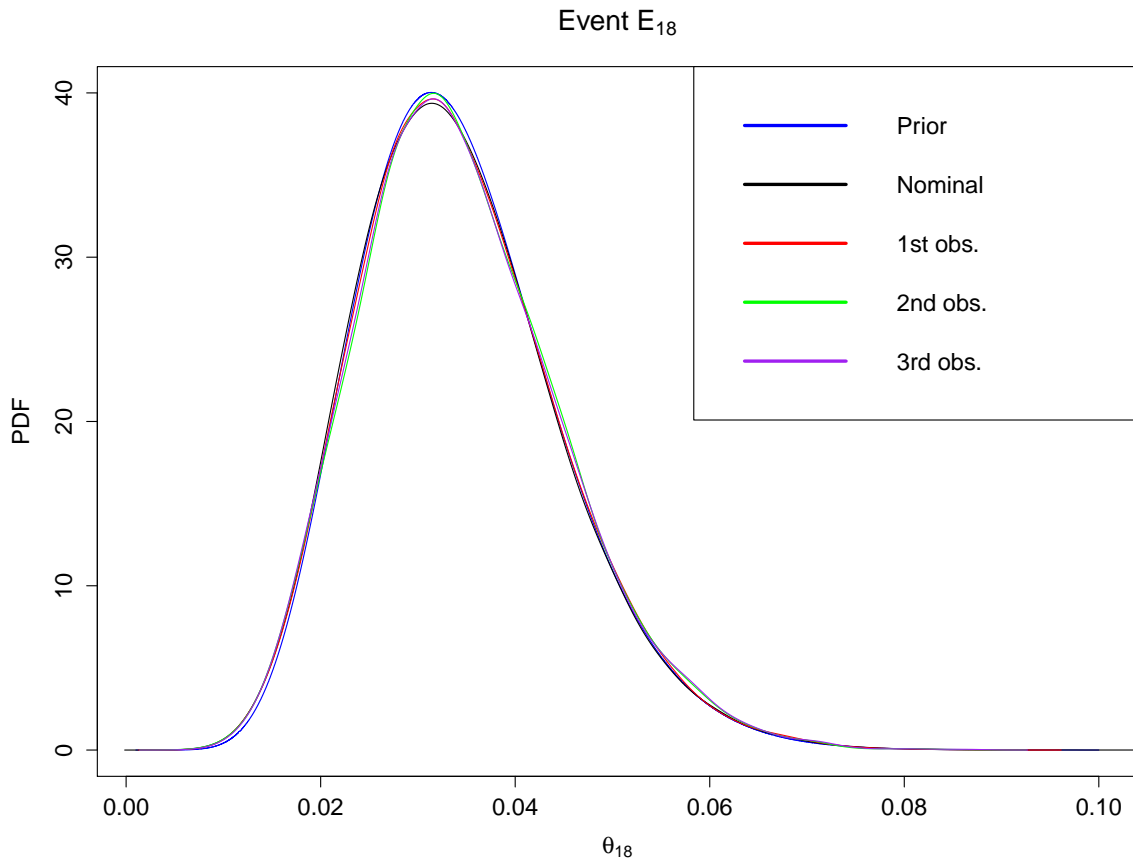


Fig. 6.20: Comparison between the probability density functions of θ_{18} : the blue curve is the prior elicited by expert opinion for the nominal case, the black one is the posterior of the nominal case, the red one, the green one and the violet one are respectively posterior of the first, the second and the third observation. The event E_{18} is Over-discharge (for batteries). According to the synthetic data it has never been observed to occur and the *tendency-to-occur* quotient $q_{18}^{(k)} = 1$ $k = 1, 2$ and $q_{18}^{(3)} = 7$ $k = 1, 2$. As result of the evidence, we cannot observe any significant change in the pdf of θ_{18} .

6.15 Expert opinion collection experiment

We illustrate in this section the steps of the proposed expert judgement gathering experiment.

As the reader can see from Section 6.13, the basic events that build the fault tree are divided in three different groups:

1. In the first group we placed the events that can lead to the burst of a battery;

2. In the second group we placed the events that can lead to the slow release of propellant;
3. In the third group we placed the events that can lead to a chemical reaction between propellant and air.

Then we propose to formulate three different surveys, one for each group, and to administer each of them to a different group of experts, selected by the relevance of expertise.

Each survey contains two sections: one with the goal of gathering the expert judgement for the elicitation of and one for the elicitation of tendency-to-occur weights for a nominal re-entry and one for the elicitation of the tendency-to-occur quotients for future re-entries.

We propose to consider as nominal re-entry the re-entry of ATV 1 because at the moment this is the re-entry on which we have more information.

We can now list the steps to follow:

1. Select the experts for each group:
 - Experts from the ESA division of Energy storage and power for the first group;
 - Experts from the ESA division of Propulsion, Propellants, Structure for the second and the third group.
2. Formulate the questionnaires.
 - (a) Create the setting under which we aim the survey to be answered:
 - Collect the available relevant information about the spacecraft and the re-entries. This set of information is different for each survey. Examples are:
 - Re-entering trajectories;
 - Predictions about the altitude of the explosion;
 - Results of the observation campaign for the nominal re-entry.
 - Collect the available information about the conditions of the batteries, for the first group, and of the propulsion system, for the second and the third group, at the EOL (end-of-life). Examples are:

- Batteries: type of batteries, age of the spacecraft, protection mechanism, predictions about temperature and pressure of the batteries at the EOL (end-of-life)
- Propulsion system: filling percentage, thickness of wall tanks after material degradation,

The setting under which the questionnaire needs to be answered is specified because the analysis is intended to be limited to specific re-entries.

- (b) Invite the expert to consider one event for each group he is more confident about and to provide a minimum and a maximum number of times in which that event can occur out of 10 re-entries similar to the nominal one.
- (c) Formulate the pairwise comparison questions and invite the experts to follow the Saaty's scale.
- (d) Add an explanation of the linguistic Saaty's scale.
- (e) Add invitations to provide critical insights for the enhancement of the surveys and the procedure.

3. Perform a consistency test as explained in Section C.3.3.

The experts were interviewed by email and individually. It could be more advantageous to interview them face by face and in groups, in order to allow them to communicate with each other about the answers. Some examples of interviews, which we addressed to experts in ESA, are reported in the Appendix E.

Chapter 7

Fragmentation model

7.1 Introduction

In this chapter we introduce a model for the construction of a distribution over the partitions of the unit interval, generated by a partially random fragmentation process. A partially random fragmentation process is a fragmentation process partly dependent on stochastic factors and partly dependent on deterministic factors. Inference for the parameters of this model, given incomplete observations, is developed.

7.2 The research question

Re-entering from space to Earth, spacecraft shatter into pieces that can either burn as they encounter friction with the atmosphere along their descent, or fall to the ground.

The development of this fragmentation model was driven by the need to answer the following research question: *What is the probability distribution of the masses of the fragments generated when a given spacecraft explodes during its return journey from space to Earth? How can we infer its parameters given the few exploitable real data? Which percentage demises? How can we exploit what we know about the spacecraft structure and its materials?*

Again we are tackling the challenge to model a unrepeatable event, with missing data and where the background knowledge is incomplete, but needs to be exploited as prior belief.

The only way to gather observations to populate this model (with real data) is

via airborne observation campaigns and unfortunately not many of them have been arranged so far. As we will explain in more detail in Chapter 5, we could consult the outcome of only one observation campaign: the campaign organized in 2008 to observe the re-entry of the Automated Transfer Vehicle 1 (ATV1). In future years, optimistically, there will be more opportunities to gather data for the fine-tuning of the model.

Due to many complications in observing such a kind of event and in analysing the results of the observations, the idea of collecting complete data is not conceivable (see Chapter 5 for further details). It follows that incomplete observations is an inherent issue of this research question.

Finally the resolution of this problem requires a flexible model:

- That can be easily updated as the understanding of the re-entry improves;
- That can be easily tailored for each re-entering spacecraft event;
- That can be easily adjusted to changing datasets.

7.3 Summary of results and contribution

This is a Bayesian model for the fragmentation specially developed for the modelling of the distribution of the masses of the fragments generated after a highly energetic break-up event. We decided to develop a model with a flexible structure in order to make it applicable in different ways to the physical problem, depending on the attainable knowledge.

Due to the lack of a reasonable amount of observations we performed simulations of the model with synthetic data, to validate the inference process. We created a sample distribution applying the model itself, then we generated data from this distribution and we made them randomly incomplete. Finally we used this set of data to verify if the model produces an accurate inference of the parameters of the sample distribution. These simulations showed problems in the convergence that could be solved in future work.

7.4 The statistical model

The first sub-section describes a method for the construction of a distribution over the partitions of the unit interval, while the second one is dedicated to the inference strategy.

7.4.1 Construction of the distribution

The distribution is constructed with the aim of building a model that is both reasonable for the fragmentation process and tractable enough for inference.

Alternative stick breaking process

We propose an extension of the stick breaking process, (introduced in Section D.3), as an alternative method for the construction of a distribution over infinite partitions of the unit interval.

Borrowing notation from Ghahramani et al. (2010), let $\epsilon = (\epsilon_1, \dots, \epsilon_K)$, denote a length- K sequence of positive integers, i.e., $\epsilon_k \in \mathbb{N}^+$. $\epsilon = \emptyset$ indicates the zero-length string and $|\epsilon|$ the length of ϵ 's sequence. We denote with $\epsilon\epsilon_i$ the sequence that results from appending $\epsilon_i = i, i \in \mathbb{N}^+$ onto the end of the sequence ϵ . These strings index the pieces in which the string is divided. We define a variation of the stick breaking process as follows:

1. We take the stick a_\emptyset with length $\pi_\emptyset = 1$. We randomly break it into n_\emptyset pieces, with proportions

$$\nu_1, \nu_2, \dots, \nu_{n_\emptyset-1}, \left(1 - \sum_{i=1}^{n_\emptyset-1} \nu_i\right)$$

We call these pieces $a_1, a_2, \dots, a_{n_\emptyset}$ with lengths $(\pi_1 = \nu_1, \pi_2 = \nu_2 \dots)$.

2. We select some of the n_\emptyset pieces and we keep the remaining ones. We randomly break each selected piece a_j with proportions

$$\nu_{j1}, \nu_{j2} \dots \nu_{j(n_j-1)}, \left(1 - \sum_{i=1}^{n_j-1} \nu_{ji}\right)$$

Then each selected a_j is broken into n_j parts of lengths $(\pi_{j1} = \nu_{j1}\nu_j, \pi_{j2} = \nu_{j2}\nu_j, \dots)$.

3. Again we apply the same process for some of the a_{jl} pieces with $j = 1 \dots n_\emptyset$ and $l = 1 \dots n_j$. Then each selected a_{jl} is partitioned into n_{jl} parts of lengths $(\pi_{\epsilon\epsilon_1} = \nu_{\epsilon\epsilon_1}\nu_\epsilon, \pi_{\epsilon\epsilon_2} = \nu_{\epsilon\epsilon_2}\nu_\epsilon, \dots)$ with $\epsilon = (j, l)$.
4. We can continue this process to randomly partition the stick.

We can see the proportions ν_ϵ as Dirichlet distributed random variables. The Dirichlet distribution, defined in Section D.2, is the multivariate generalization of the Beta distribution.

If the proportions $\{\nu_\epsilon\}$ are Dirichlet distributed, the lengths $\{\pi_\epsilon\}$ are also Dirichlet distributed. This is due to the decimation property, defined in Section D.2.

It is proved that this property can be generalized with

$$(\tau_1, \dots, \tau_m) \sim Dir(\alpha_1\beta_1, \dots, \alpha_1\beta_m)$$

and $\sum_{i=1}^m \beta_i = 1$ and even to the more general case where many x_i s are split into different fractions.

We can define the parameter vector α as the product $A\gamma$ of a scalar concentration parameter A and a vector base measure $\gamma = (\gamma_1, \dots, \gamma_n)$ where $\sum_{i=1}^n \gamma_i = 1$.

Example 5 For example we consider $n_\emptyset = 3$, $n_1 = 2$ and $n_2 = 4$, as depicted below in Figure 7.1.

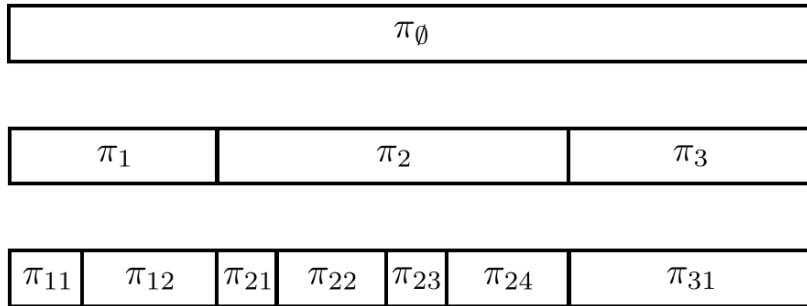


Fig. 7.1: Representation of the proposed alternative stick breaking process.

The stick a_\emptyset is divided into three pieces a_1, a_2, a_3 , whose lengths are Dirichlet distributed

$$(\pi_1 = \nu_1, \pi_2 = \nu_2, \pi_3 = \nu_3) \sim Dir(A(\gamma_1, \gamma_2, \gamma_3))$$

Next a_1 is split into two pieces a_{11}, a_{12} and a_2 into four pieces $a_{21}, a_{22}, a_{23}, a_{24}$. The unit interval is so partitioned into seven parts. It follows from the decimation property that the lengths $(\pi_{11}, \pi_{12}, \pi_{21}, \pi_{22}, \pi_{23}, \pi_{24}, \pi_{31})$ are again Dirichlet distributed $Dir(A(\gamma_1\gamma_{11}, \gamma_1\gamma_{12}, \gamma_2\gamma_{21}, \gamma_2\gamma_{22}, \gamma_2\gamma_{23}, \gamma_2\gamma_{24}, \gamma_3))$. If

$$\pi_{11} = \nu_1\nu_{11}, \pi_{12} = \nu_1\nu_{12},$$

then

$$(\nu_{11}, \nu_{12}) \sim Dir(A\gamma_1(\gamma_{11}, \gamma_{12})),$$

and

$$\pi_{2i} = \nu_2\nu_{2i} \quad i = 1, \dots, 4$$

$$(\nu_{21}, \nu_{22}, \nu_{23}, \nu_{24}) \sim Dir(A\gamma_2(\gamma_{21}, \gamma_{22}, \gamma_{23}, \gamma_{24}))$$

where $\gamma_{11} + \gamma_{12} = 1$ and $\gamma_{21} + \gamma_{22} + \gamma_{23} + \gamma_{24} = 1$.

The corresponding tree-structure

Let τ be a rooted oriented tree, that is a directed acyclic graph where all the edges are directed away from a particular vertex, called the root. Let τ_w be a weighted tree, whose underlying graph is τ and whose edges labels, called weights, are assigned. We call τ the tree-structure of τ_w .

The weighted rooted oriented tree τ_w provides a representation of the breaking process, when it complies with the following characteristics:

- The root stands for the length π_\emptyset of the stick.
- Every node (or vertex) represents the length π_ϵ of a chunk of the stick and the string ϵ identifies the node. The length of the sequence $|\epsilon|$ is the depth of the node ϵ , being the depth of a node the length of the path to the root. The root has depth zero.

- The node ϵ has children $\epsilon\epsilon_i : \epsilon_i \in \{1, 2, \dots, d_\epsilon\}$. The number of children of the node ϵ is the out-degree d_ϵ . The children of ϵ represent the lengths $\pi_{\epsilon\epsilon_i} : \epsilon_i \in \{1, 2, \dots, d_\epsilon\}$.
- The leaves, i.e. the nodes with out-degree zero, represent the lengths of the surviving pieces.
- Every edge connecting ϵ to $\epsilon\epsilon_i$ is weighted with the splitting proportion $\nu_{\epsilon\epsilon_i}$. Therefore the length π_ϵ is given by the product between the weights of the edges that belong to the shortest path from ϵ to the root.

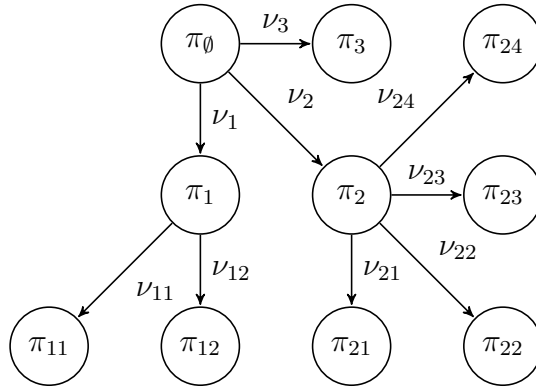


Fig. 7.2: Tree structure of the example described in Example 5 and depicted in Figure 7.1.

The same tree structure τ can represent the associated vector base measure γ . The number of elements of the vector base measure is equal to the number of leaves.

In this case, the edge connecting ϵ to $\epsilon\epsilon_i$ is weighted with $\gamma_{\epsilon\epsilon_i}$.

Therefore the corresponding element of the parameter vector α to the leaf ϵ is given by the product between A and the weights of the edges that belong to the shortest path from ϵ to the root.

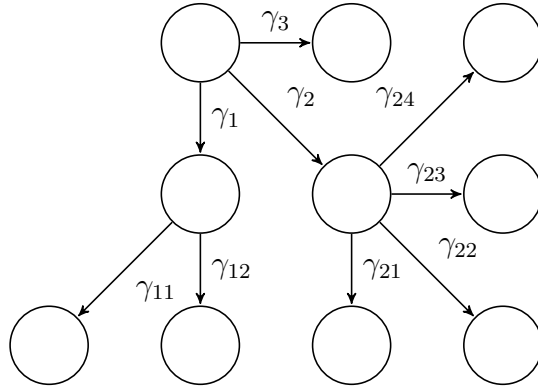


Fig. 7.3: Tree structure of the vector base measure of the Dirichlet distribution of the example described in 5 and illustrated in Figure 7.1.

The splitting proportions vector

Given the weighted oriented tree τ_w with out-degree d_{max} , being the out-degree (or branching factor) of an oriented tree the maximum out-degree of any of its nodes and the out-degree of a node the number of its children, we introduce a vector called the splitting proportions vector $\boldsymbol{\mu} = (\mu_1, \dots, \mu_{d_{max}})$ such that $\sum_{i=1}^{d_{max}} \mu_i = 1$.

The edges of the tree $\tau_w = f(\tau, \boldsymbol{\mu})$ directed away from node ϵ are weighted with the elements of the partition of this vector $(\mu_1, \dots, \mu_{d_\epsilon-1}, 1 - \sum_{i=1}^{d_\epsilon-1} \mu_i)$ where d_ϵ is the out-degree of the node ϵ , as shown in the next Figure 7.4.

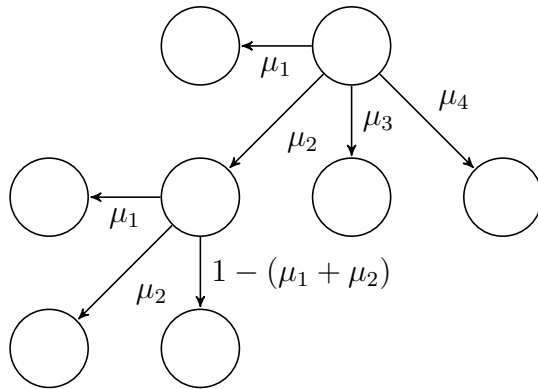


Fig. 7.4: Example of a tree weighted by the elements of the splitting proportions vector $\boldsymbol{\mu}$.

The vector base measure $\boldsymbol{\gamma}$ can be defined in terms of the structure of the tree τ and the splitting proportions vector $\boldsymbol{\mu}$. For instance, the vector base measure represented by the weighted tree in Figure 7.4 is $\boldsymbol{\gamma} = (\mu_1, \mu_2\mu_1, \mu_2^2, \mu_2(1 - (\mu_1 + \mu_2)), \mu_3, \mu_4)$.

The function $\alpha = f(A, \boldsymbol{\mu}, \tau)$

Given the above definition of the splitting proportions vector and the tree-structure analogy the constructed distribution is a Dirichlet distribution with parameter α , where α is a function of the scalar concentration parameter A , the splitting proportions vector $\boldsymbol{\mu}$, the tree structure τ and the tree structure is a graphical representation of the fragmentation process. Note that the scalar concentration parameter A is introduced in the model in order to scale the parameter of the Dirichlet distribution to avoid possible computational issues with small values.

The function $f(A, \boldsymbol{\mu}, \tau)$ summarizes the proposed method for the construction of the distribution and it will be largely used in the rest of the chapter, for the explanation of the inference method.

This function relates each element α_i of the vector α to a leaf ϵ of the weighted oriented tree τ_w and therefore to the linear combination of the elements of the vector $\boldsymbol{\mu}$ that weigh the edges belonging to the shortest path from ϵ to the root. Using this representation of α , we do not need to explicitly state the vector base measure $\boldsymbol{\gamma}$, whose cardinality is n as the cardinality of α . Note that the cardinality of $\boldsymbol{\mu}$ is fixed and it does not vary with n , therefore this representation can result advantageous when n is large.

We can consider again the example showed in Figure 7.4. Given the illustrated weighted oriented tree τ_w , we have:

$$\boldsymbol{\alpha} = f(A, \boldsymbol{\mu}, \tau) = A(\mu_1, \mu_2\mu_1, \mu_2^2, \mu_2(1 - (\mu_1 + \mu_2)), \mu_3, \mu_4) \quad (7.1)$$

7.4.2 Inference for the Fragmentation model

Introduction

We propose a method for the Bayesian inference of the parameters of the proposed Dirichlet distribution: $Dir(\boldsymbol{\alpha} = f(A, \boldsymbol{\mu}, \tau))$ which is function of A , $\boldsymbol{\mu}$ and the tree structure τ .

We consider k realizations of a random variable

$$\boldsymbol{x} \in \Delta_n := \left\{ \boldsymbol{x} \in \mathbb{R}^n : \sum_i x_i = 1, x_i \geq 0 \right\}$$

:

$$\begin{aligned}\mathbf{x}_1 &= \{x_{11}, \dots, x_{n_11}\} \\ \mathbf{x}_2 &= \{x_{12}, \dots, x_{n_22}\} \\ &\vdots \\ \mathbf{x}_k &= \{x_{1k}, \dots, x_{n_kk}\}\end{aligned}$$

and its partitions into

- Observable data $\mathbf{y}_j = \{y_{1j}, \dots, y_{s_jj}\}$;
- Not observable (or missing) data $\mathbf{z}_j = \{z_{1j}, \dots, z_{(n_j-s_j)j}\}$, with $j = 1, \dots, k$.

The random variable \mathbf{x} is Dirichlet distributed $\mathbf{x} \sim Dir(\boldsymbol{\alpha} = \{\alpha_1, \dots, \alpha_k\})$ with parameter $\boldsymbol{\alpha} = f(A\boldsymbol{\mu}, \tau)$ function of

- The splitting proportions vector $\boldsymbol{\mu}$ (see Section 7.4.1);
- The tree structure τ (see Section 7.4.1).

We propose an algorithm for the inference of the parameter $\boldsymbol{\alpha}$, given the observable data $\mathbf{y}_1, \dots, \mathbf{y}_k$.

The complete data posterior density, from which we wish to sample $\boldsymbol{\alpha}$, is:

$$p(\boldsymbol{\alpha}|\mathbf{x}_1, \dots, \mathbf{x}_k) \propto \prod_{j=1}^k \left\{ \left(\frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^n x_{ij}^{\alpha_i-1} \right) \right\} p(\boldsymbol{\alpha}) \quad (7.2)$$

Unfortunately we are not able to evaluate the complete likelihood due to the missing data and so we do not know the form of the observed data posterior density $p(\boldsymbol{\alpha}|\mathbf{y}_1, \dots, \mathbf{y}_k)$. The solution is to find the way to complete our observations.

For ease of notation, we consider $n_j = n$ constant and known $\forall j = 1, \dots, k$, being n_j the length of the j -th realization.

For each observation $j = 1, \dots, k$ the length of observed data s_j can be considered as the number of successes in a sequence of n trials, each of which yields success with probability p_{obs} . We consider each element x_{ij} observed with a certain probability p_{obs} .

The vector \mathbf{s} includes all the elements $s_j \forall j = 1, \dots, k$.

The indicator variable

We need to introduce an auxiliary variable that we are going to call indicator variable r_j for each observation j .

In order to explain what it is and the reason why we need it, we come back to the analogy with the tree structure.

The random variable \mathbf{x} takes the outcomes of the alternative stick breaking process 7.4.1 and its realization can be represented by the leaves of a tree, as illustrated in Figure 7.5.

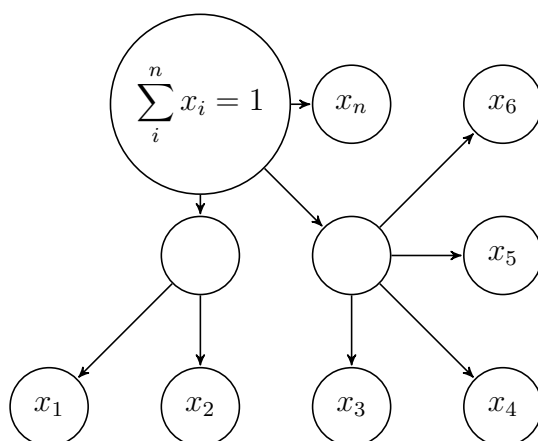


Fig. 7.5: Realization of the random variable \mathbf{x} .

The observable data \mathbf{y}_j are the observable fractions of this outcomes. Each \mathbf{y}_j is a subset of a partition of the unit interval.

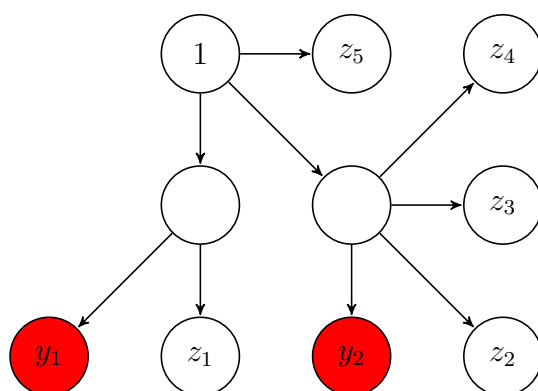


Fig. 7.6: The realization \mathbf{x}_j of the random variable \mathbf{x} is partitioned into observable data $\mathbf{y}_j = \{y_{1j}, y_{2j}\}$ and missing data $\mathbf{z}_j = \{z_{1j}, \dots, z_{5j}\}$.

As we observe only some leaves, we do not know anything about the tree structure

of the realization \mathbf{x}_j , except the total number of leaves n . We do not know which position in the tree is occupied by the observable leaves either.

The observable data set $\mathbf{y}_j = \{y_{1j}, y_{2j}\}$, illustrated by the next figure:

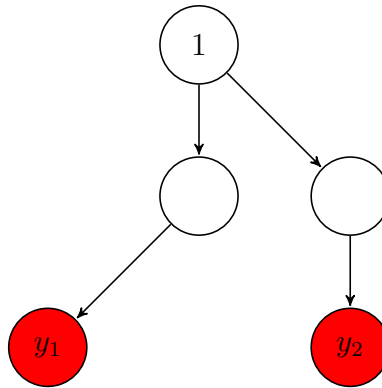


Fig. 7.7: Representation of the observable data set $\mathbf{y}_j = \{y_{1j}, y_{2j}\}$.

can be the observable fraction of different trees. Given the same observable data set, we can have different tree-structures, as represented in the following figures:

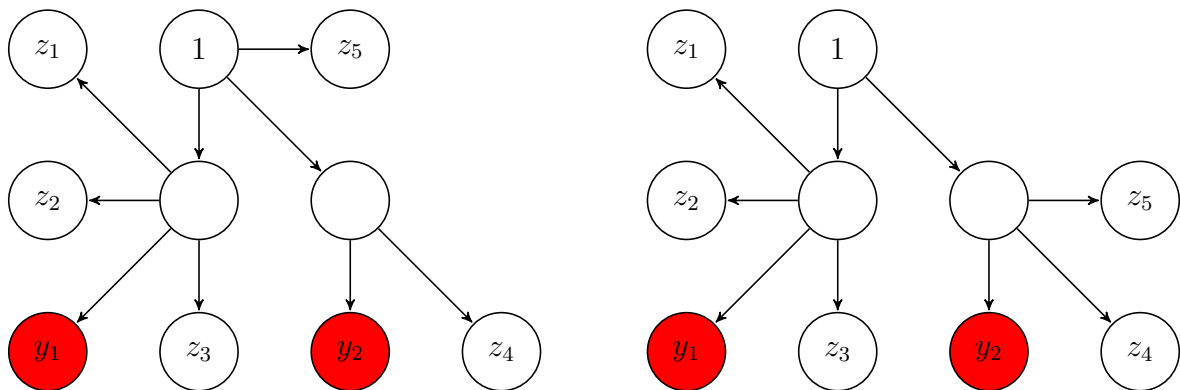


Fig. 7.8: These examples show how an observable data set can be placed into a tree-structure.

Furthermore, even if the tree structure is fixed, the observable leaves can occupy different positions, as illustrated in the next figures:

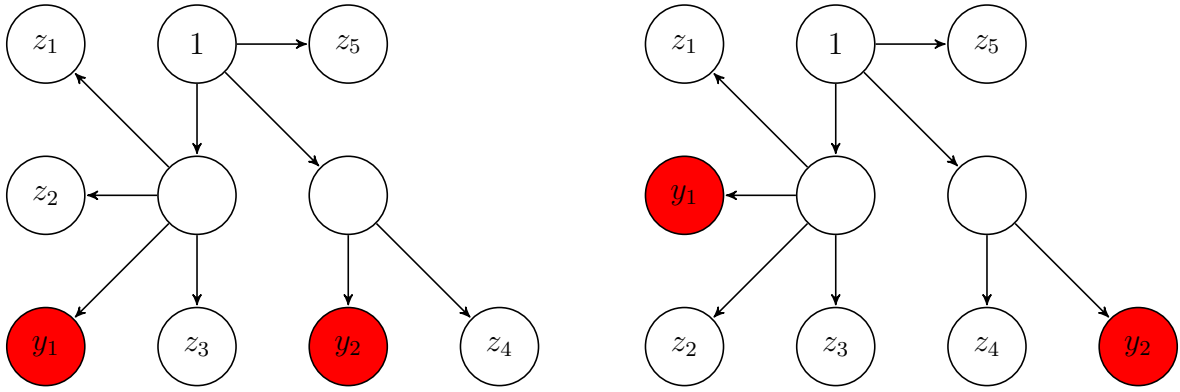


Fig. 7.9: These examples show how an observable data set can be placed into a tree-structure.

When we consider the random variable \mathbf{x} Dirichlet distributed with parameter $\boldsymbol{\alpha} = f(A\boldsymbol{\mu}, \tau)$, we state a correspondence between the position occupied in the tree τ by the element x_i and its value, as already explained in the previous section. Therefore the available observations cannot be completed without defining the position of the missing data.

For this reason, we introduce an indicator variable $r_{ij} \in \{0, 1\}$ such that $\mathbf{y}_j = \{x_{ij} | r_{ij} = 1\}$ and that $\mathbf{z}_j = \{x_{ij} | r_{ij} = 0\}$. r_{ij} indicates if the element $x_{ij} \in \mathbf{x}_j$ belongs to \mathbf{y}_j or \mathbf{z}_j or in other words if it is an observable variable or not. The indicator variable is illustrated in Figure 7.10.

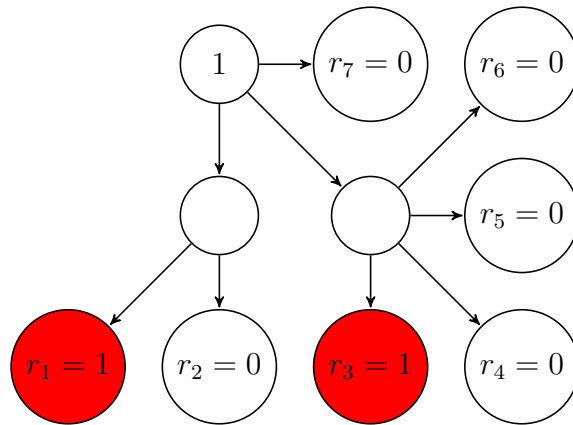


Fig. 7.10: Representation of the indicator variable.

Full model

We are now ready to define the main goal. We aim to sample the missing data \mathbf{z} and the Dirichlet parameter $\boldsymbol{\alpha} = f(A\boldsymbol{\mu}, \tau)$, given the observed data, from the joint

posterior distribution:

$$p(\mathbf{z} = (\mathbf{z}_1, \dots, \mathbf{z}_k), \mathbf{r} = (\mathbf{r}_1, \dots, \mathbf{r}_k), A\boldsymbol{\mu}, \tau | \mathbf{y} = (\mathbf{y}_1, \dots, \mathbf{y}_k), \mathbf{s}, n) \quad (7.3)$$

where:

- $\sum_i r_{ij} = s_j$ is given $\forall j = 1, \dots, k$;
- The scalar concentration parameter A is known;
- The length of $\boldsymbol{\mu}$ is a priori defined.

We propose the following Gibbs sampler (see Section A.3.2) to sample from this posterior distribution:

1. *Initialization.* Start with some initial state for the Markov chain, defining a starting value for the splitting proportions vector $\boldsymbol{\mu}^{(0)}$, the tree structure $\tau^{(0)}$, the indicator variable $\mathbf{r}^{(0)}$.
 - Generate the splitting proportions vector $\boldsymbol{\mu}^{(0)}$ from a Dirichlet distribution, giving known the scalar concentration parameter A ;
 - Generate the tree structure $\tau^{(0)}$, simulating it uniformly from all the possible tree with n leaves and maximum out-degree d_{max} . Note that d_{max} is equal to the length of the splitting proportions vector;
 - Given $\tau^{(0)}$ and $\boldsymbol{\mu}^{(0)}$, derive the correspondent weighted tree and extract the related Dirichlet parameter vector $\boldsymbol{\alpha}^{(0)}$;
 - The indicator variable $\mathbf{r}^{(0)}$ can be simulated uniformly from all the possible $\binom{n}{s_j}$ configurations. Note that there are $\binom{n}{s_j}$ ways to choose the s_j observed items, disregarding their order, from n elements.
2. For each iteration, given the current state $(\boldsymbol{\mu}^{(n)}, \tau^{(n)}, \mathbf{r}^{(n)})$:
 - (a) For each observation $j = 1, \dots, k$ sample the missing values \mathbf{z}_j from the distribution of \mathbf{z}_j conditioned on the values of the remaining variables:

$$\mathbf{z}_j \sim p(\mathbf{z}_j | \mathbf{r}_j, A\boldsymbol{\mu}, \tau, \mathbf{y}_j, \mathbf{s}, n) \quad (7.4)$$

$$\propto Dir(\mathbf{x}_j | \boldsymbol{\alpha}(A\boldsymbol{\mu}, \tau)) = \frac{1}{B(\boldsymbol{\alpha})} \left(\prod_{i:r_{ij}=1} y_{ij}^{\alpha_i-1} \prod_{i:r_{ij}=0} z_{ij}^{\alpha_i-1} \right) \quad (7.5)$$

Each \mathbf{z}_j can be sampled independently.

This is equivalent to draw a vector \mathbf{z}_j of $n - s_j$ elements Dirichlet distributed with parameter $\boldsymbol{\alpha} = \{\alpha_i = f(A\boldsymbol{\mu}, \tau) | r_{ij} = 0\}$ on $(0, 1 - \sum_i y_{ij})$. By adding the sampled vector \mathbf{z}_j to the observed data \mathbf{y}_j , we get the Dirichlet distributed augmented data $\mathbf{x}_j = (\mathbf{y}_j, \mathbf{z}_j)$ that sum to 1.

This step replaces the application of a data augmentation algorithm (see Section A.3.3).

- (b) For each observation $j = 1, \dots, k$ sample the indicator variable \mathbf{r}_j from the distribution of \mathbf{r}_j conditioned on the values of the remaining variables:

$$\mathbf{r}_j \sim p(\mathbf{r}_j | \mathbf{x}_j = (\mathbf{y}_j, \mathbf{z}_j), A\boldsymbol{\mu}, \tau, \mathbf{s}, n, p_{obs}) = p(\mathbf{r}_j | \mathbf{s}, n) \quad (7.6)$$

We propose a Metropolis-Hastings algorithm (A.3.1) to obtain it.

Metropolis-Hastings algorithm for the inference of the indicator variable

- Generate a candidate $\mathbf{r}_j^{(*)}$, simulating it uniformly. The proposal distribution is simply $q(\mathbf{r}_j^{(*)} | \mathbf{r}_j^{(\eta)}) = \frac{1}{\binom{n}{s_j}}$ and the same in the opposite direction $q(\mathbf{r}_j^{(\eta)} | \mathbf{r}_j^{(*)}) = \frac{1}{\binom{n}{s_j}}$;
- Reassign the position of the observed items (between the leaves), based on $\mathbf{r}_j^{(*)}$;
- Calculate the acceptance probability:

$$\begin{aligned} a(\mathbf{r}_j^{(*)} | \mathbf{r}_j^{(\eta)}) &= \frac{Dir(\mathbf{x}_j = (\mathbf{y}_j, \mathbf{z}_j) | \mathbf{r}_j^{(*)}, \boldsymbol{\alpha})}{Dir(\mathbf{x}_j = (\mathbf{y}_j, \mathbf{z}_j) | \mathbf{r}_j^{(\eta)}, \boldsymbol{\alpha})} \times \frac{q(\mathbf{r}_j^{(\eta)} | \mathbf{r}_j^{(*)})}{q(\mathbf{r}_j^{(*)} | \mathbf{r}_j^{(\eta)})} \quad (7.7) \\ &= \frac{\left(\prod_{i:r_{ij}^{(*)}=1} y_{ij}^{\alpha_i-1} \prod_{i:r_{ij}^{(*)}=0} z_{ij}^{\alpha_i-1} \right)}{\left(\prod_{i:r_{ij}^{(\eta)}=1} y_{ij}^{\alpha_i-1} \prod_{i:r_{ij}^{(\eta)}=0} z_{ij}^{\alpha_i-1} \right)} \quad (7.8) \end{aligned}$$

As explained in Section A.3.1, the acceptance probability is given by the product of the probability ratio between the proposed state and the current state and the ratio of the proposal distributions in two

directions. The ratio of the proposal distributions is obviously 1 in this case;

- Accept the new sample assigning

$$\mathbf{r}_j^{(\eta+1)} = \mathbf{r}_j^*$$

with probability

$$a(\mathbf{r}_j^* | \mathbf{r}_j^{(\eta)}).$$

When the indicator variable $\mathbf{r}_j \forall j$ is uniformly sampled, we are assuming that all the elements $x_{ij} \in \mathbf{x}_j \forall j$ have the same probability of being observed. This assumption is not suitable for all the applications.

- (c) Sample the splitting proportions vector $\boldsymbol{\mu}$ from the distribution of $\boldsymbol{\mu}$ conditioned on the values of the remaining variables:

$$A\boldsymbol{\mu} \sim p(A\boldsymbol{\mu} | \mathbf{x}_j, \mathbf{r}_j, \tau, \mathbf{s}, n) \quad (7.9)$$

We propose again a Metropolis-Hastings algorithm (see Section A.3.1).

Metropolis-Hastings algorithm for the inference of the splitting proportions vector

- Generate a candidate $\boldsymbol{\mu}^{(*)}$ from the proposal distribution $q(\boldsymbol{\mu}^{(*)} | \boldsymbol{\mu}^{(\eta)})$

$$\boldsymbol{\mu}^{(*)} \sim Dir(\boldsymbol{\mu}^{(\eta)}); \quad (7.10)$$

- Update the weights of the tree $\tau^{(\eta)}$ based on $\boldsymbol{\mu}^{(*)}$;
- Extract the related candidate $\boldsymbol{\alpha}^{(*)}$;
- Calculate the acceptance probability:

$$a(\boldsymbol{\mu}^{(*)}, \boldsymbol{\mu}^{(\eta)}) = \frac{\prod_{j=1}^k \left(\frac{1}{B(\boldsymbol{\alpha}^{(*)})} \prod_{i=1}^n x_{ij}^{\alpha_i^{(*)}-1} \right) \left(\frac{1}{B(\boldsymbol{\mu}^{(\eta)})} \prod_{i=1}^d (\mu_i^{(*)})^{\mu_i^{(\eta)}-1} \right)}{\prod_{j=1}^k \left(\frac{1}{B(\boldsymbol{\alpha}^{(\eta)})} \prod_{i=1}^n x_{ij}^{\alpha_i^{(\eta)}-1} \right) \left(\frac{1}{B(\boldsymbol{\mu}^{(*)})} \prod_{i=1}^d (\mu_i^{(\eta)})^{\mu_i^{(*)}-1} \right)}; \quad (7.11)$$

- Accept the new candidate

$$\boldsymbol{\mu}^{(\eta+1)} = \boldsymbol{\mu}^{(*)}$$

with probability

$$p(\boldsymbol{\mu}^{(*)}, \boldsymbol{\mu}^{(\eta)})$$

or keep the previous one

$$\boldsymbol{\mu}^{(\eta+1)} = \boldsymbol{\mu}^{(\eta)}$$

with probability

$$1 - p(\boldsymbol{\mu}^{(*)}, \boldsymbol{\mu}^{(\eta)});$$

- Update the weighted tree given $\boldsymbol{\mu}^{(\eta+1)}$;
- Extract the related candidate $\boldsymbol{\alpha}^{(\eta+1)*}$.

(d) Sample the tree structure τ from the distribution of τ conditioned on the values of the remaining variables:

$$\tau \sim p(\tau | A\boldsymbol{\mu}, \mathbf{x}_j, \mathbf{r}_j, \mathbf{s}, n) \quad (7.12)$$

We propose again a Metropolis-Hastings algorithm (see Section A.3.1).

Metropolis-Hastings algorithm for the inference of the tree structure

- Given the proposal distribution $q(\tau(n)^{(*)} | \tau(n)^{(\eta)})$, generate a candidate for the tree structure $\tau(n)^{(*)}$, moving one leaf from a father node to another:

$$q(\tau(n)^{(*)} | \tau(n)^{(\eta)}) = \frac{1}{n \times n_{fathers}} \quad (7.13)$$

where $n_{fathers}$ is the number of available nodes where the leaf can be appended:

$$n_{fathers} = n. \text{ feasible fathers in } \tau(n)^{(*)};$$

- Build a tree $\tau(n)^{(*)} = \tau(n)^{(\eta)}$ with the same structure of $\tau(n)^{(\eta)}$;
 - Select one leaf in $\tau(n)^{(\eta)}$ and delete the correspondent leaf in $\tau(n)^{(*)}$;
 - Select a feasible new father node in $\tau(n)^{(\eta)}$ where the selected leaf can be appended;
 - Append a new leaf to the selected father in $\tau(n)^{(*)}$.
- Update the weights of the proposed tree $\tau(n)^{(*)}$ based on $\boldsymbol{\mu}^{(\eta+1)}$;

- Extract the related candidate $\boldsymbol{\alpha}^{(*)}$;
- Calculate the acceptance probability $p\left(\tau(n)^{(*)}, \tau(n)^{(\eta)}\right)$

$$= \frac{\prod_{j=1}^k \left(\frac{1}{B(\boldsymbol{\alpha}^{(*)})} \prod_{i=1}^n x_{ij}^{\alpha_i^{(*)}-1} \right) \left(\frac{1}{n \times n_{fathers}} \right)}{\prod_{j=1}^k \left(\frac{1}{B(\boldsymbol{\alpha}^{(\eta)})} \prod_{i=1}^n x_{ij}^{\alpha_i^{(\eta)}-1} \right) \left(\frac{1}{n \times n_{fathers}} \right)} \quad (7.14)$$

$$= \frac{\prod_{j=1}^k \left(\frac{1}{B(\boldsymbol{\alpha}^{(*)})} \prod_{i=1}^n x_{ij}^{\alpha_i^{(*)}-1} \right) (n \times n_{fathers})}{\prod_{j=1}^k \left(\frac{1}{B(\boldsymbol{\alpha}^{(\eta)})} \prod_{i=1}^n x_{ij}^{\alpha_i^{(\eta)}-1} \right) (n \times n_{fathers})} \quad (7.15)$$

where $n_{fathers} = n$. feasible fathers in $\tau(n)^{(*)}$;

- Accept the new candidate

$$\tau(n)^{(\eta+1)} = \tau(n)^{(*)}$$

with probability

$$p\left(\tau(n)^{(*)}, \tau(n)^{(\eta)}\right)$$

or keep the previous one

$$\tau(n)^{(\eta+1)} = \tau(n)^{(\eta)}$$

with probability

$$1 - p\left(\tau(n)^{(*)}, \tau(n)^{(\eta)}\right);$$

- Update the weights of the new tree structure $t(n)^{\tau+1}$ based on $\boldsymbol{\mu}^{(\eta+1)}$;
- Extract the related sample $\boldsymbol{\alpha}^{(\eta+1)}$;

On the necessity of the assumption over the number of leaves n

We stated at the beginning of this section that n is considered constant and known. Accordingly we believe that all the complete observations have the same length and that we know it a priori. If we relax this assumption, the inference algorithm needs to be changed and it gets definitely more complicated, since n defines the length of all the following vectors:

- the Dirichlet parameter $\boldsymbol{\alpha}$;

- the indicator variable $r_j \forall j$;
- the missing variables $z_j \forall j$.

Furthermore the tree structure τ is dependent on n , since n is the number of leaves. It could be interesting to try to solve this issue applying the Reversible-jump Markov chain Monte Carlo (Green, 1995).

7.5 How to control the model

As stated at the beginning of this chapter, this model aims to model a fragmentation process that also depends on known deterministic factors. When we have some background information about how the fragmentation happens and we want our model to reflect this knowledge, we can control the model setting up constraint on the splitting proportions vector μ and in particular on the tree-structure τ .

7.5.1 How to constrain the tree-structure

As we have already shown, the tree-structure is simply a representation of the proposed alternative stick breaking process. Precisely, the tree-structure displays, step by step, in how many pieces the stick is broken.

The advantage of the tree-structure as a graphical tool is that it can be easily simulated and modified through the adjacency matrix. The adjacency matrix is a square matrix Σ such that its element σ_{ij} is one if the node i is connected by an edge to the node j and zero where there is no edge. In case of a weighted tree, the weight of the edge connection i to j replaces the number one. The tree-structure τ is a variable inferred by data, but setting up some constraint on its samples ensures a control on the model. This is a way of merging coherently the different sources of data that are available: the observed data and the background knowledge coming from expert opinion.

First of all, assuming that the number of fragments n is known, as in our model, we are considering only the trees with n leaves. There may be situations where it can be convenient to define a priori even the height ¹ of the tree, its maximum out-

¹The height of a node is the number of edges on the longest path between that node and a leaf. The height of a tree is the height of its root node.

degree or other properties. Note that the height of the tree is the number of steps in the alternative stick breaking process and the maximum out-degree is the maximum number in which a fragment can be divided.

The tree-structure, together with the associated alternative stick breaking process, can be used as a reproduction of the fragmentation history or simply a nuisance variable if what counts is the final outcome of the fragmentation process.

Let us proceed with some clarifying examples.

Note that all the depicted solutions are aimed to keep small the number of elements of μ and then to limit the number of parameters to be inferred. Bear in mind that the cardinality of μ is equal to the maximum out-degree of the oriented tree.

Example 6 Let us consider, for example, a fragmentation process where we expect as outcome two larger pieces and many small pieces, as showed below.



This example can be modelled as the outcome of the following alternative stick breaking process and its related tree-structure (Figure 7.11).

π_0										
π_1	π_2	π_3								
π_{11}	π_{21}	π_{31}			π_{32}			π_{33}		
π_{111}	π_{211}	π_{311}	π_{312}	π_{313}	π_{321}	π_{322}	π_{323}	π_{331}	π_{332}	π_{333}

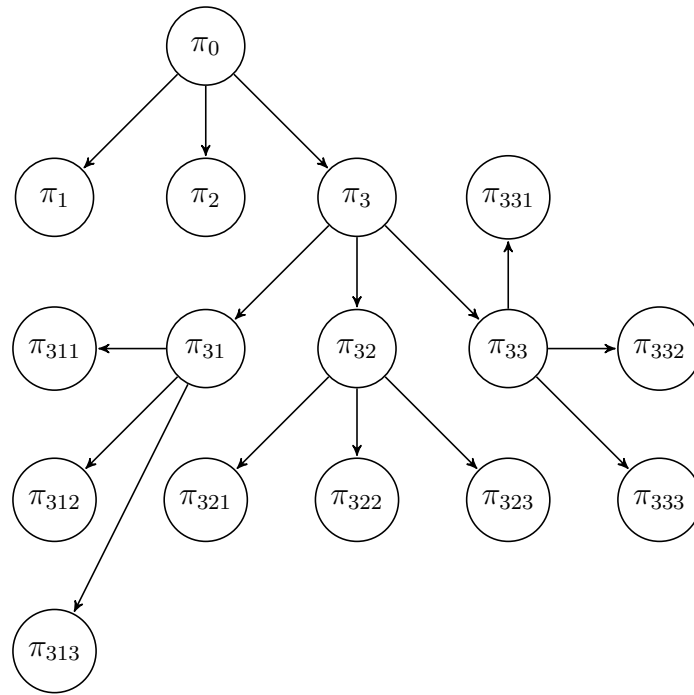


Fig. 7.11: Tree-structure.

Example 7 The tree structure can also be taken as a track of the fragmentation history. Each level of the tree can be considered a fragmentation event. Let us consider, again for example, a fragmentation process that consists in the detachment of pieces from the main body step by step.

This case can be modelled with the alternative stick breaking process depicted in Figure 7.12. The red nodes represent the main body. This kind of tree are known in literature as *caterpillar* tree, that is a tree in which all vertices are within distance ² 1 of a central path subgraph.

π_0						
π_1	π_2					π_3
π_{11}	π_{21}	π_{22}			π_{23}	π_{31}
π_{111}	π_{211}	π_{221}	π_{222}	π_{223}	π_{231}	π_{311}

²in terms of number of edges.

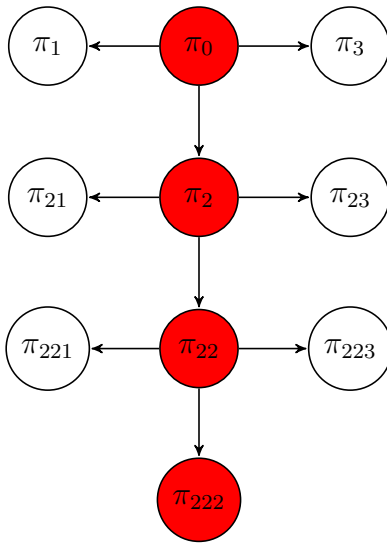


Fig. 7.12: Tree-structure.

Example 8 Another interesting example is a small variant of the previous one. Let us assume that we expect a fragmentation process that consists mainly in the detachment of pieces from the main body step by step and that one of the generated pieces will fragment again (this can be called a secondary fragmentation event).

The red nodes represent the main body, while the piece that is going to break up again is depicted in green. Note that the height of the tree is 3 and there are 3 breaking steps in the stick breaking process. Likewise the main body is subject to 3 fragmentation events (primary fragmentation events). This variety of tree is known in literature as *lobster* tree, that is a tree in which all the vertices are within distance 2 of a central path.

π_0							
π_1	π_2					π_3	
π_{11}	π_{21}	π_{22}			π_{23}	π_{31}	π_{32}
π_{111}	π_{211}	π_{221}	π_{222}	π_{223}	π_{231}	π_{311}	π_{321}

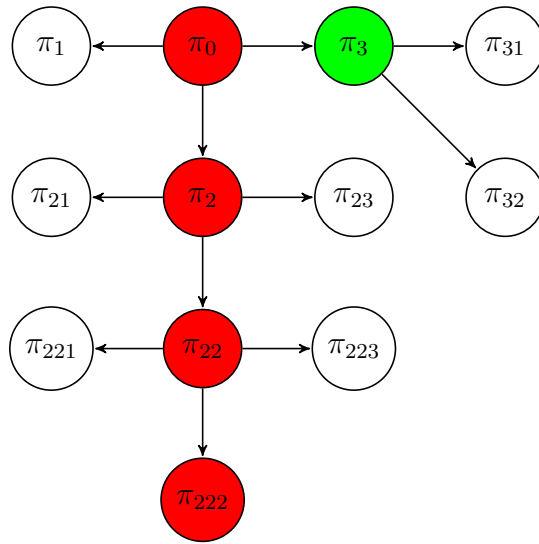


Fig. 7.13: Tree-structure.

Example 9 Lastly let us consider a case where our expectations about the outcome of the breaking process are very limited and we can guess simply that we can get many bits of completely different size. One modelling proposal is showed in Figure 7.14.

π_0					
π_1		π_2	π_3		
π_{11}	π_{12}	π_{21}	π_{31}	π_{32}	π_{33}

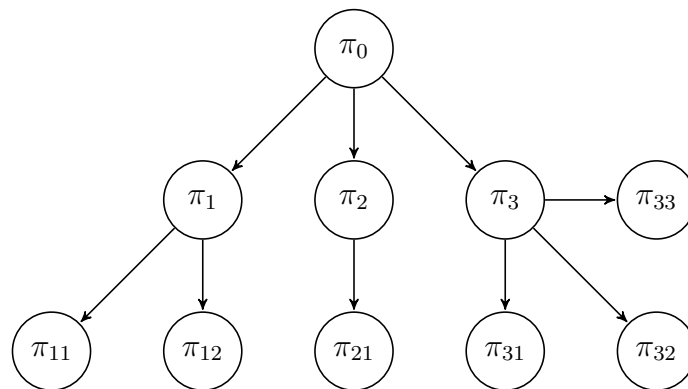


Fig. 7.14: Tree-structure.

The tree-structure for simulating purposes

We simulated *lobster* and *caterpillar* tree structures. As already defined in Examples 7 and 8:

- The *caterpillar* tree is a tree in which all vertices are within distance 1 of a central path;
- The *lobster* tree is a tree in which all vertices are within distance 2 of a central path.

The nodes or leaves with distance 1 of the central path stands for the outcome of a *primary* fragmentation, while the leaves with distance 2 stand for the result of a *secondary* fragmentation.

We present here the algorithm we developed for simulating purposes.

The tree has the following user input:

- n_l number of leaves;
- h height of the tree, that is the number of edges of the central path ($h > 2$);
- deg_1 = maximum out-degree of the nodes of the central path;
- deg_2 = maximum out-degree of the nodes within distance 1 of the central path.

1. Generate the central path. Create a path graph as illustrated in Figure 7.15 of a number of nodes equal to the height of the tree (4 in this case).

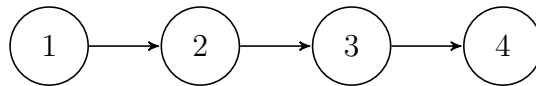


Fig. 7.15: Central path.

2. Append the leaves to the central path to create a *caterpillar* tree-structure.
 - If $n_l < (h(deg_1 - 1) + 1)$ stop. The tree has number of nodes = $n_l + h$;
 - Otherwise create a *lobster* tree structure with n_l leaves and the maximum number of nodes with the maximum out-degree (deg_1 in case of nodes belonging to the central path and deg_2 for the nodes with distance 1 from the central path), following the next steps:
 - Evaluate n_2 the number of nodes with distance 1 from the central path with the maximum out-degree deg_2 :

$$\lfloor (n_l - h(deg_1 - 1) - 1) / (deg_2 - 1) \rfloor ;$$

- Evaluate n_2^* the number of nodes with distance 1 from the central path with a number of children lower than the maximum out-degree deg_2 :

$$\text{mod } [(n_l - h(deg_1 - 1) - 1)/(deg_2 - 1)]$$

If $n_2^* = 1$ then $n_2^* = n_2^* + 1$;

- Append new leaves such that the number of nodes is equal to:

$$(h(deg_1 - 1) + 1) + h + n_2 deg_2 + n_2^*.$$

Note that deg_1 and deg_2 must be taken into account in the evaluation of $n_{fathers}$ when applying the Metropolis-Hastings algorithm for the inference of the tree-structure.

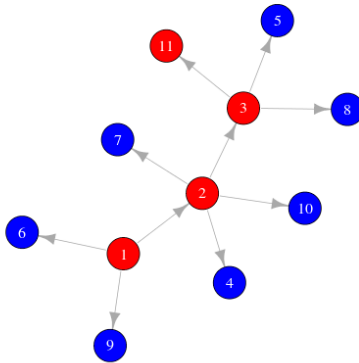


Fig. 7.16: Example of caterpillar tree-structure generated in R, using the package `igraph`, $h = 3$, $deg_1 = 4$, $deg - 2 = 4$, $n_l = 8$. This case is limited to primary fragmentations.

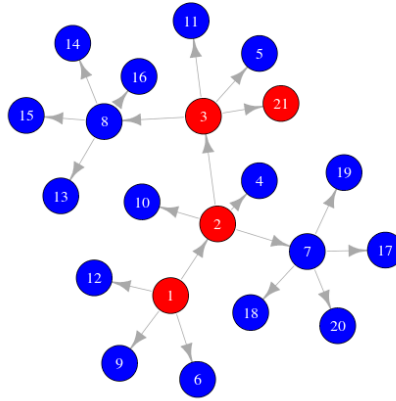


Fig. 7.17: Example of lobster tree-structure generated in R, using the package `igraph`, with $h = 3$, $deg_1 = 4$, $deg - 2 = 4$, $n_l = 16$. This is a case with primary and secondary fragmentations.

7.5.2 Notes about the splitting proportions vector

The splitting proportions vector $\boldsymbol{\mu}$ defines in which proportions each node is divided.

When there is no prior knowledge favouring one component over another, the symmetric Dirichlet distribution is a good candidate distribution for its sampling. The symmetric Dirichlet distribution is a Dirichlet distribution where all of the elements making up the parameter vector $\boldsymbol{\alpha} = \{\alpha_1, \alpha_2, \dots\}$ have the same value $\alpha_i = \alpha_j \forall i, j$. When $\alpha_i = 1 \forall i$, the symmetric Dirichlet distribution is equivalent to a uniform distribution over all points in its support and it takes the name of flat Dirichlet distribution.

On the necessity of the scalar concentration parameter A

We introduce a scalar concentration parameter in order to control the variance of the outcome and to avoid computational issues with too small values.

7.6 Model selection

As we have already highlighted at the end of Section 7.4.2, we decided to assume known and constant the size n of the complete observation $\boldsymbol{x}_j \forall j$. This assumption

can affect the quality of the inference results, especially in those applications where this hypothesis is very far from reality (e.g. the fragmentation of a spacecraft). In order to offset this limitation, we propose to perform a model selection varying the value of n , with the Bayesian information criterion.

The Bayesian information criterion or Schwarz criterion (briefly BIC), published for the first time in Schwarz et al. (1978), is computed as follows:

$$-2 \cdot \ln \hat{\mathcal{L}} + k \cdot \ln(n) \quad (7.16)$$

where

- $\hat{\mathcal{L}}$ is the maximized value of the likelihood function of the model: for our model it is equal to the maximum value of $P(\mathbf{x}|\boldsymbol{\alpha}, \mathbf{z})$;
- k is the number of the elements to be estimated: in this case k is given by the sum of the number of missing data and the length of the parameter $\boldsymbol{\alpha}$

$$k = n + |\mathbf{z}|;$$

- n is the sample size: in this case it is the length of the parameter $\boldsymbol{\alpha}$, the parameter that we aim to estimate. Note that n is also the size of a complete observation.

The best model is the model with the lowest value of the BIC.

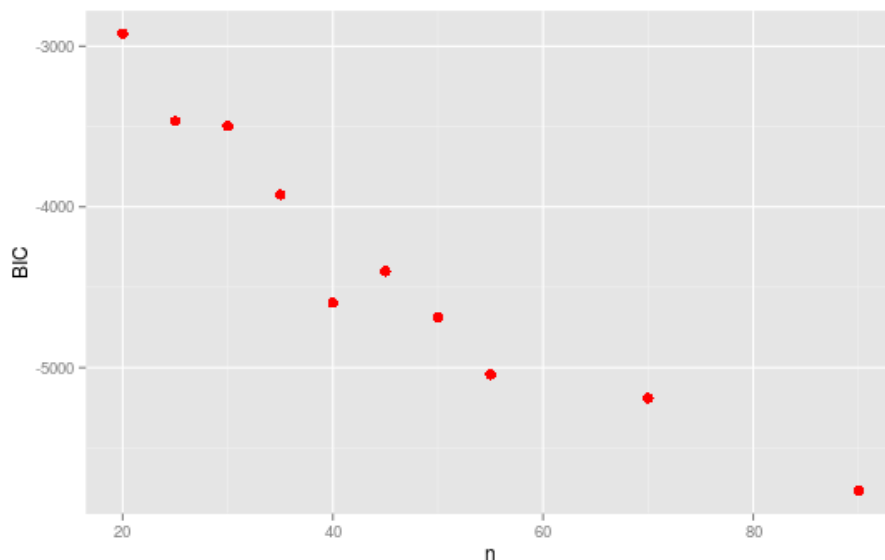


Fig. 7.18: Bayesian information criterion for different values of the sample size n ($n = 20, n = 25, n = 30, n = 35, n = 40, n = 45, n = 50, n = 55, n = 70, n = 90$), evaluated with the available real observation (see Chapter 5).

7.7 Model fitting

7.7.1 How to model the spacecraft break-up

In this section we want to describe an idea for the application of the proposed model to the fragmentation process of a spacecraft caused by a highly energetic break-up event, during the atmospheric re-entry.

As detailed in Section 2.2, the spacecraft undergoes a series of break-up events, during the decay, such as shedding of solar arrays, external sensors and other low energetic break-up events, well before an explosive event is likely to happen. The reader will remember that at the beginning of this thesis, in Section 1.1, we introduced the definition highly energetic break-up event to denote the explosion events and to distinguish them from the low energetic break up events that always happen, during the decay, because of the action of the aero forces.

We want to make clear that the application here proposed has been thought for the modelling of the distribution of the fragments generated by the destructive action of an highly energetic break-up event, given the assumption that it could be possible to isolate data concerning this type of event.

We consider the masses of the generated fragments as random variables and we assume they are Dirichlet distributed, exactly as we did for the lengths of the pieces of the stick. We want to fit the model to data coming from the observations of the re-entries where an explosion occurred. The objective is the inference of the parameters of their distribution by merging coherently the different sources of data that are available: the observed data and the background knowledge coming from expert opinion.

This is an approach for learning from past observations in order to create a tool for the prediction of how a vehicle will break-up in upcoming re-entries, under specific hypothesis and conditions. Unfortunately real data are very scarce in this context and physical knowledge involves many uncertainties, but optimistically more and more observations will be available over time.

The model is structured in a flexible manner on purpose, such that it can be easily updated as more information is collected. The strategy that can be followed to adjust the proposed method to this problem is strictly depending on the availability of data. It follows the description of an idea for this application.

7.7.2 The idea

We divide the total mass of the vehicle before starting the fragmentation process by material and we consider known an estimate of the total mass M for each material. Then we assume that the masses of the fragments are distributed with a different Dirichlet distribution depending on the material they are made of. Although the assumption that every fragment is made of a unique material is clearly unrealistic, this hypothesis is reasonable and convenient since the probability of survival for a specific component is mainly determined by the material used in its construction. For example, it is well known that components made of materials with high melting temperatures, such as stainless steel, titanium, and glass, often survive, while pieces made of aluminium, which has a low melting temperature, do not survive re-entry. A nice challenge in this project would be the investigation of a method allowing the prediction of the non-uniform material composition of the fragments, but the available data does not make this feasible at the moment.

It is more reasonable to suppose that we have k observations of the masses of the fragments made of a specific material, available from the spectroscopic analysis of highly energetic break-up events that have occurred during past re-entries. These observations include only the masses of the visible and surviving fragments, or simply the observed masses. It does not include:

- The masses of the surviving fragments that cannot be observed. We denote them as not-observed or missing masses;
 - The masses of the fragments that melt in the atmosphere before being observed.
- We call their sum the demised mass.

Let s_j be the number of observed masses for the $j = 1, \dots, k$ observation. A set of complete data \mathbf{X} is a set that include for each observation j the observed masses, the missing masses and the demised mass (m_1, \dots, m_{n_j}) . The sum of the masses included in a complete observation is equal to the mass M . For consistency with the proposed stick breaking method, we take the normalized masses

$$\left(\frac{m_1}{M}, \dots, \frac{m_{n_j}}{M} \right) \quad \text{such that} \quad \sum_{i=1}^{n_j} \frac{m_i}{M} = 1.$$

Let \mathbf{Y} be the set which includes the observed masses and the demised mass, with $\mathbf{Y} \subseteq \mathbf{X}$, while $\mathbf{X} \setminus \mathbf{Y}$ is the set of missing masses.

We set up some constraints to the tree-structure τ and to the splitting proportions vector $\boldsymbol{\mu}$ as follows:

1. The maximum out-degree d_{max} and the height of the tree, which is the number of edges on the longest downward path between the root and a leaf, are a priori defined. Their choice depends on the expert opinion regarding the expected variance of the masses.
2. The element $\mu_{d_{max}}$ of the splitting proportions vector $\boldsymbol{\mu}$ is equal to the ratio between the demised mass and the total mass M . It appears only in the element of the vector base measure $\boldsymbol{\gamma}$ corresponding to one child of the root. Thus this node is a leaf and it represents the parameter corresponding to the demised mass. As a consequence the prior distribution for $\mu_{d_{max}}$ is different depending on the material, since different materials have a different probability of surviving the re-entry. Eventually the root is the only node with the maximum out-degree.

7.8 Model assessment

We performed simulations of the model with synthetic data, to validate the inference process. We created a sample distribution applying the model itself, then we generated data from this distribution and we made them not complete. Finally we used this set of data to verify if the model produces an accurate inference of the parameters of the sample distribution.

7.8.1 MCMC convergence with synthetic data

In this simulation we used the same user input (see Section 7.5.1) for the building of the tree-structure to generate the synthetic data and to make the inference. We generated complete data and then we made them not complete with $p_{obs} = 0.5$

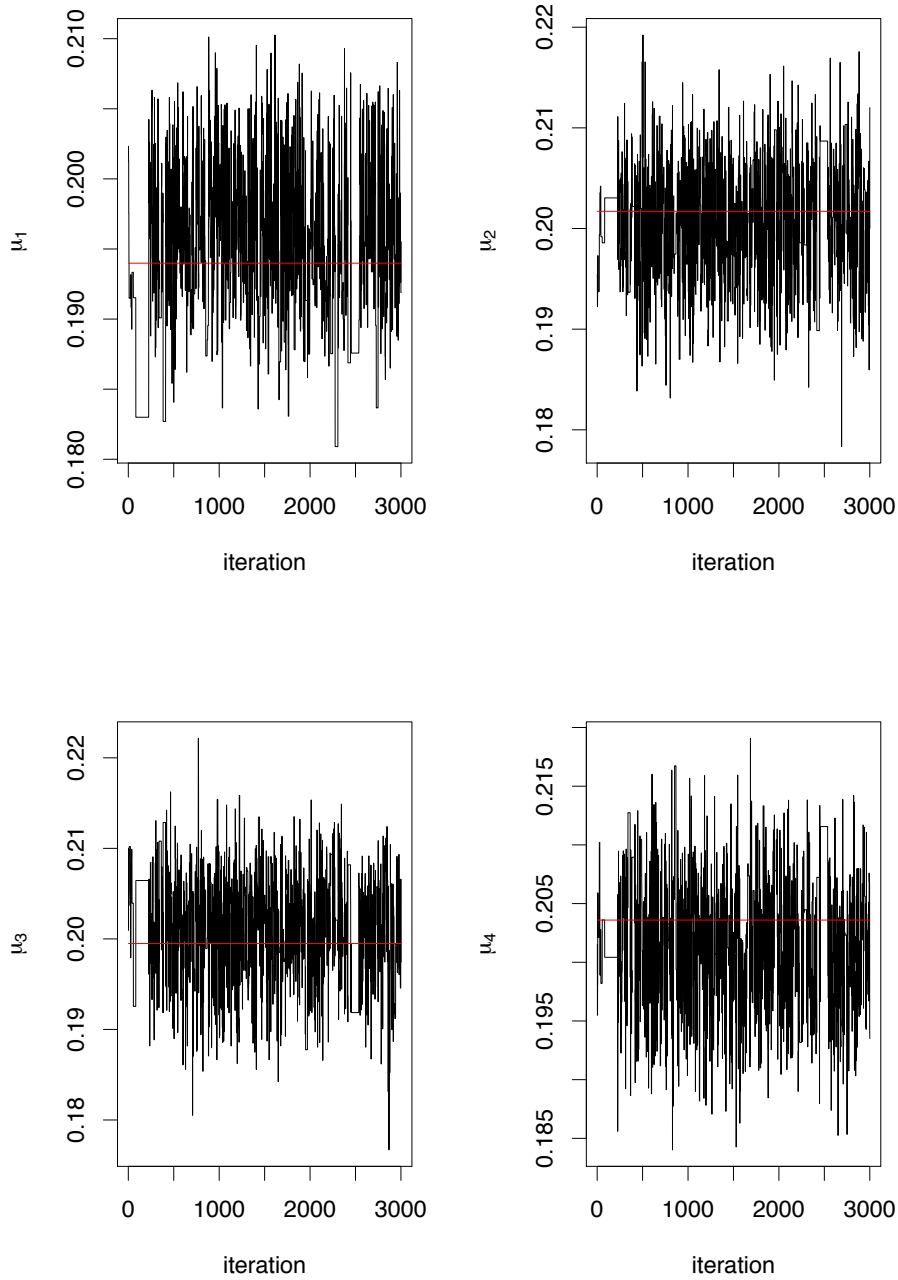


Fig. 7.19: Traceplot of $\boldsymbol{\mu} = \left\{ \mu_1, \mu_2, \mu_3, \mu_4, 1 - \sum_{i=1}^4 \mu_i \right\}$. Simulation data: number of leaves $n = 15$, height of the tree $h = 4$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 5$, number of observations $k = 2$, scalar concentration parameter $A = 1000$, lengths of the observations $\mathbf{s} = \{8, 5\}$. The initial value of $\boldsymbol{\mu}$ is generated by a flat Dirichlet distribution. True values are indicated in red.

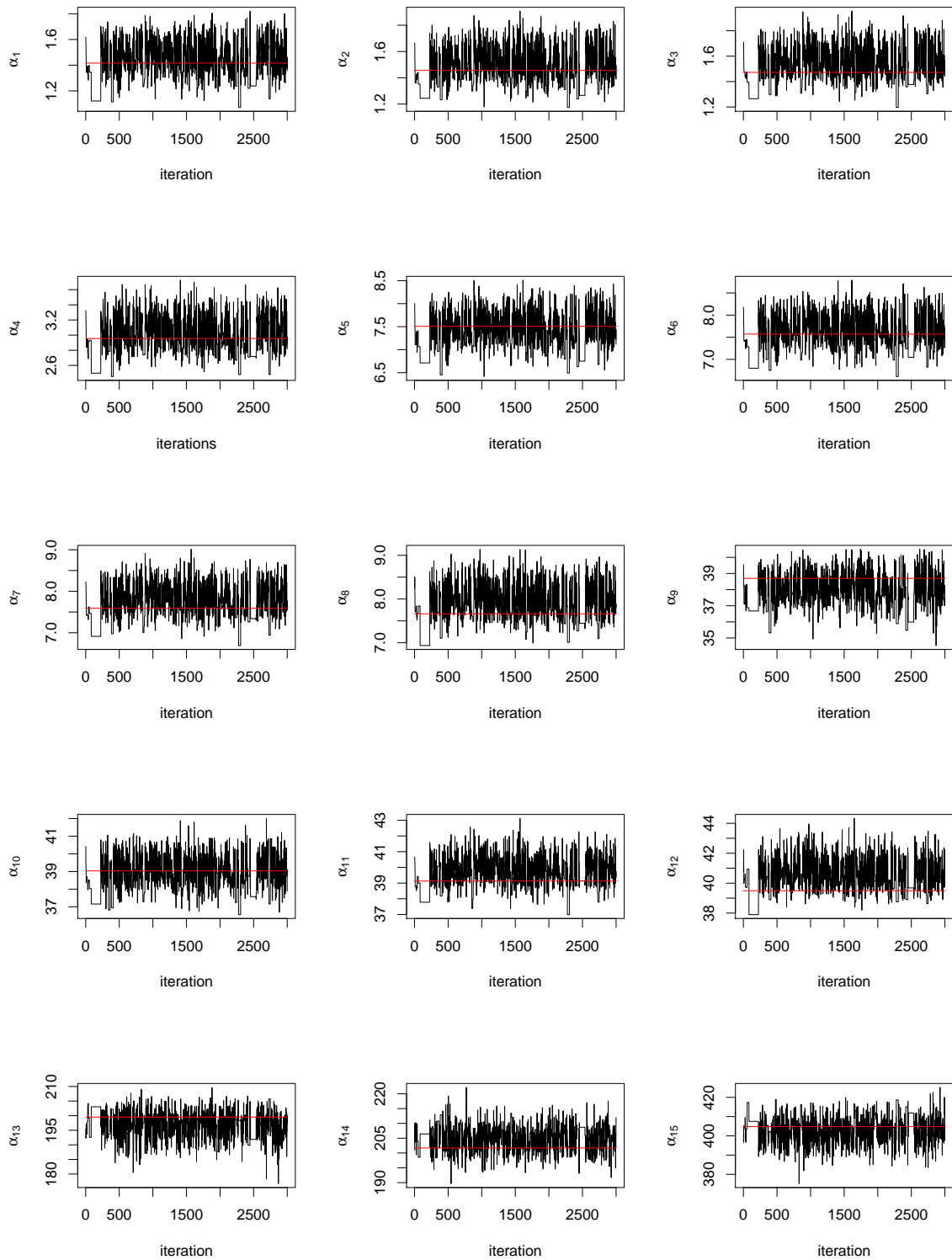


Fig. 7.20: Traceplot of $\alpha = \{\alpha_1, \dots, \alpha_{15}\}$. Simulation data: number of leaves $n = 15$, height of the tree $h = 4$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 5$, number of observations $k = 2$, scalar concentration parameter $A = 1000$, lengths of the observations $s = \{8, 5\}$. True values are indicated in red.

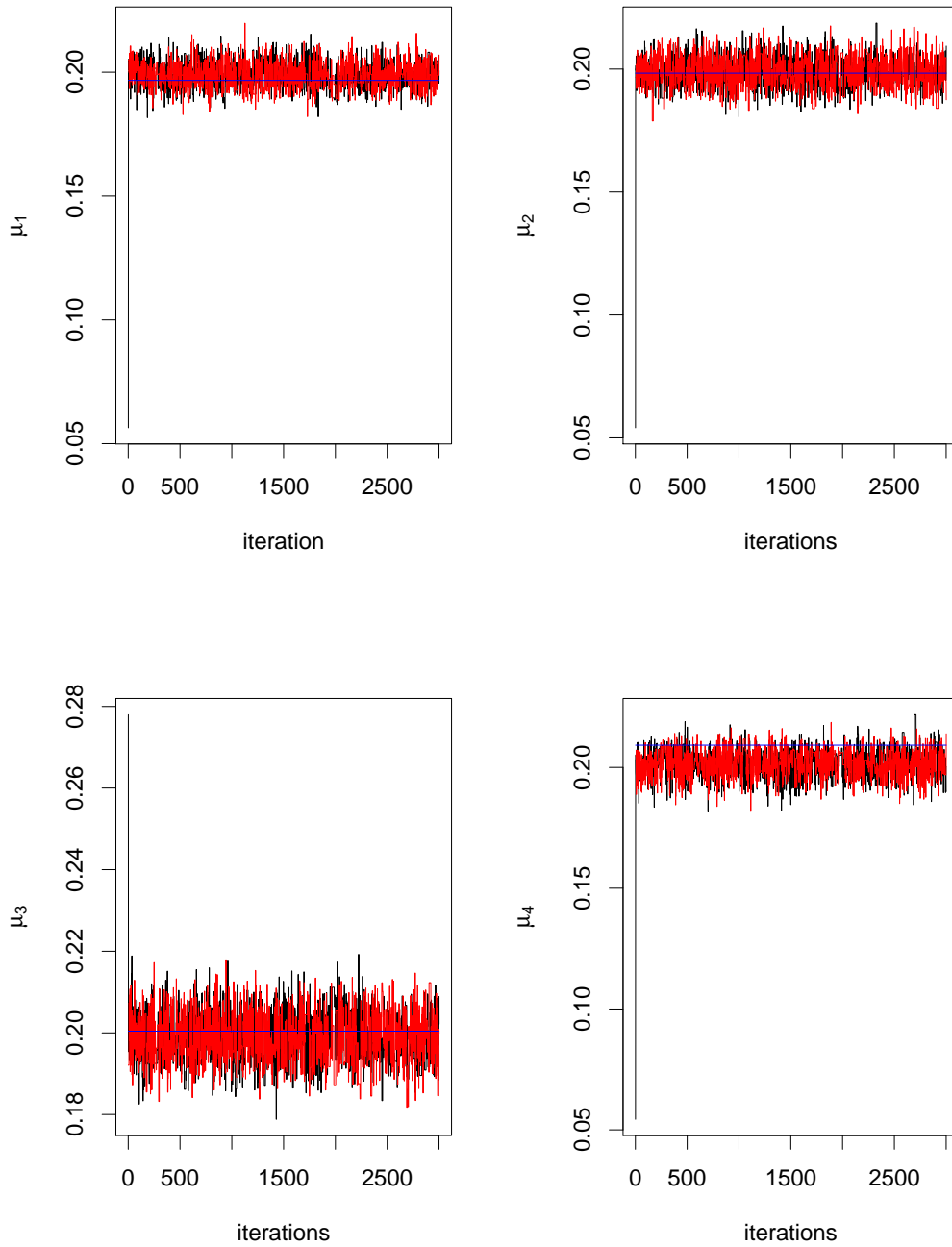


Fig. 7.21: Comparison of traceplots of $\boldsymbol{\mu} = \left\{ \mu_1, \mu_2, \mu_3, \mu_4, 1 - \sum_{i=1}^4 \mu_i \right\}$ with different initial values. Simulation data: number of leaves $n = 15$, height of the tree $h = 4$, maximum out-degree of the nodes of the central path $deg_1 = 5$, number of observations $k = 2$, scalar concentration parameter $A = 1000$. The initial value of the black traceplot is generated by a flat Dirichlet distribution, while the red one by a Dirichlet distribution with parameter $\boldsymbol{\alpha} = A\{1, 1, 5, 1, 1\}$. True values are indicated in blue.

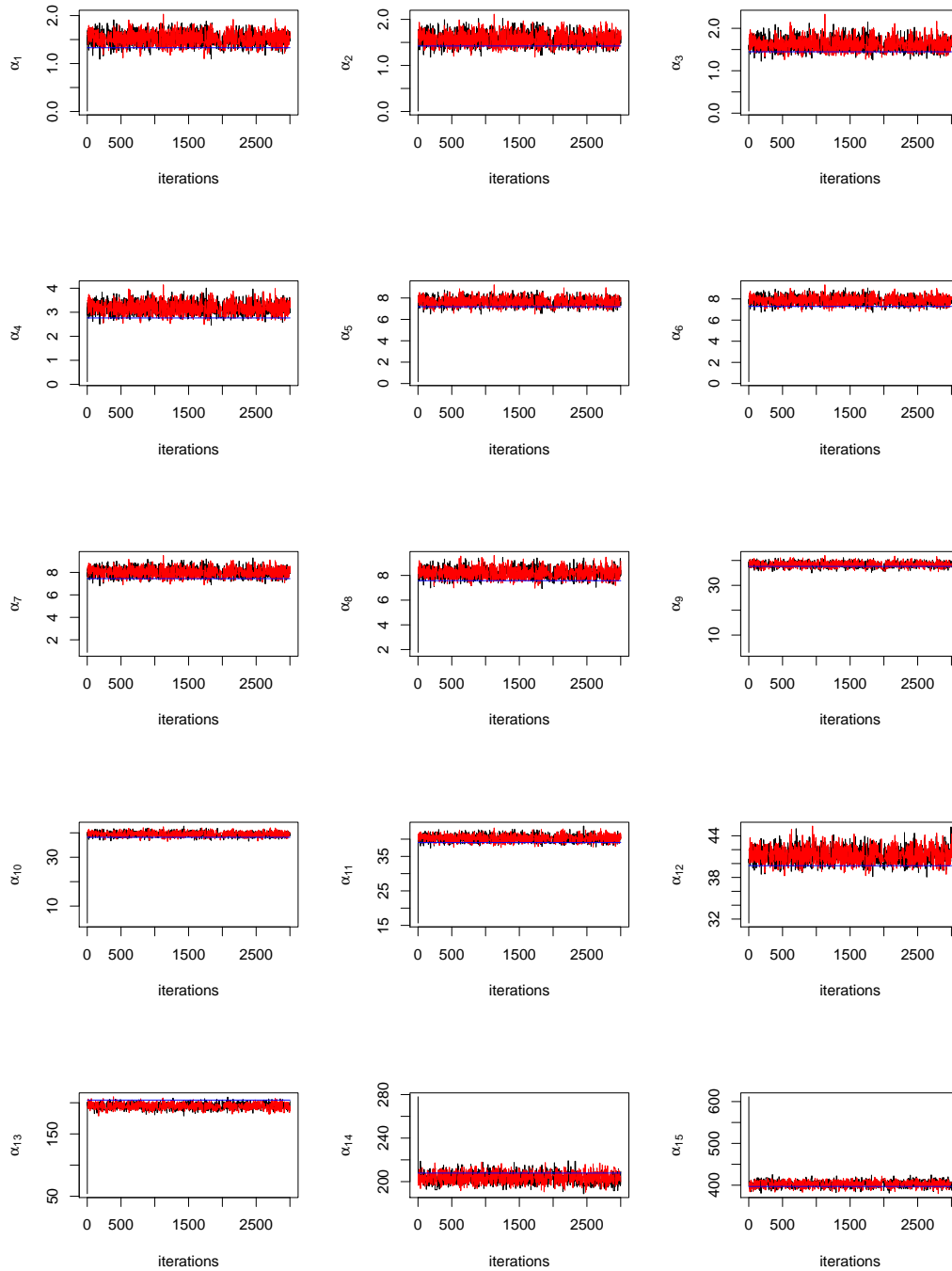


Fig. 7.22: Traceplot of $\alpha = \{\alpha_1, \dots, \alpha_{15}\}$. Simulation data: number of leaves $n = 15$, height of the tree $h = 4$, maximum out-degree of the nodes of the central path $deg_1 = 5$, number of observations $k = 2$, scalar concentration parameter $A = 1000$, lengths of the observations $\mathbf{s} = \{10, 3\}$. We can see in black the traceplot of $\alpha = f(\boldsymbol{\mu}, \tau)$ where the initial value of $\boldsymbol{\mu}$ is generated by a flat Dirichlet distribution and in red the traceplot of $\alpha = f(\boldsymbol{\mu}, \tau)$ where the initial value of $\boldsymbol{\mu}$ is generated by a Dirichlet distribution with parameter $\alpha = A\{1, 2, 5, 2, 1\}$. True values are indicated in blue.

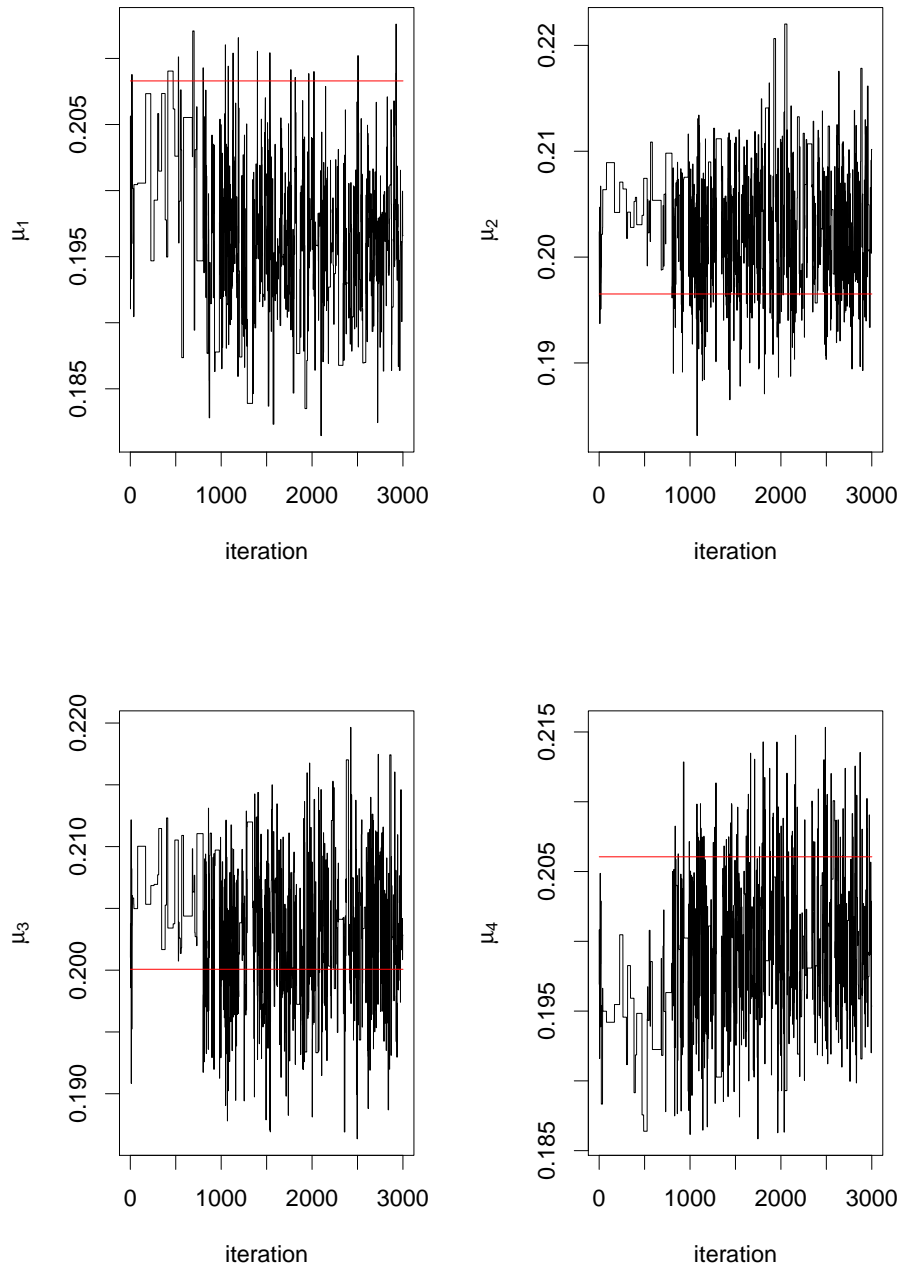


Fig. 7.23: Traceplot of $\boldsymbol{\mu} = \left\{ \mu_1, \mu_2, \mu_3, \mu_4, 1 - \sum_{i=1}^4 \mu_i \right\}$. Simulation data: number of leaves $n = 15$, height of the tree $h = 4$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 5$, number of observations $k = 8$, scalar concentration parameter $A = 1000$, lengths of the observations $\mathbf{s} = \{5, 7, 6, 5, 7, 7, 8, 7\}$. The initial value of $\boldsymbol{\mu}$ is generated by a flat Dirichlet distribution. True values are indicated in red.

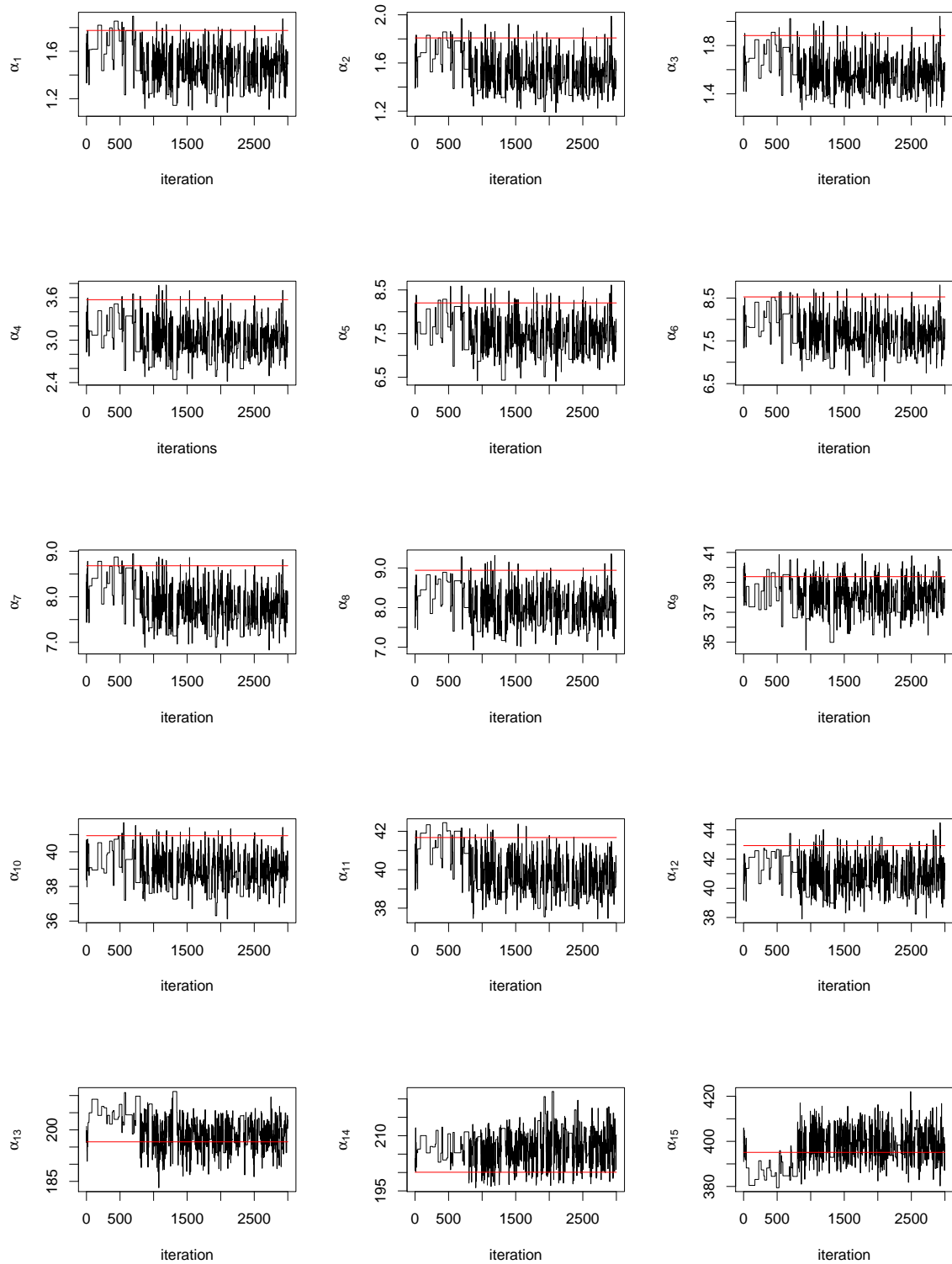


Fig. 7.24: Traceplot of $\alpha = \{\alpha_1, \dots, \alpha_{15}\}$. Simulation data: number of leaves $n = 15$, height of the tree $h = 4$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 5$, number of observations $k = 8$, scalar concentration parameter $A = 1000$, lengths of the observations $\mathbf{s} = \{5, 7, 6, 5, 7, 7, 8, 7\}$. The true values are indicated in red.

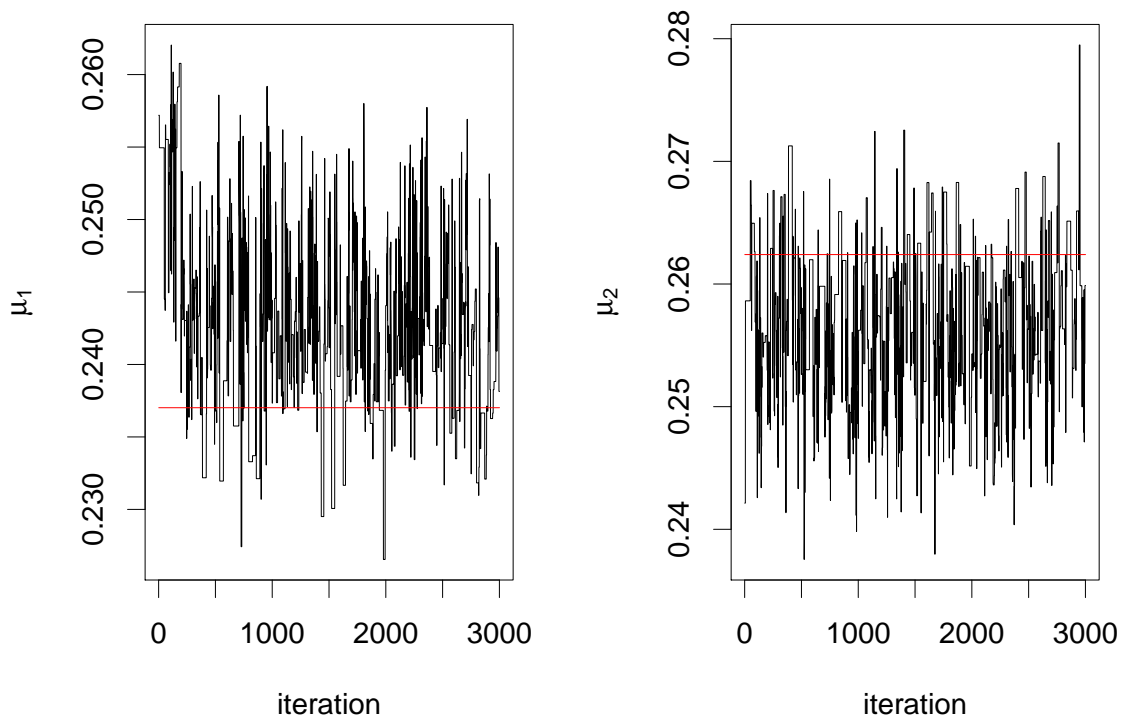


Fig. 7.25: Traceplot of $\boldsymbol{\mu} = \left\{ \mu_1, \mu_2, 1 - \sum_{i=1}^2 \mu_i \right\}$. Simulation data: number of leaves $n = 15$, height of the tree $h = 7$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 4$, number of observations $k = 2$, scalar concentration parameter $A = 1000$. The initial value of $\boldsymbol{\mu}$ is generated by a flat Dirichlet distribution. True values are indicated in red.

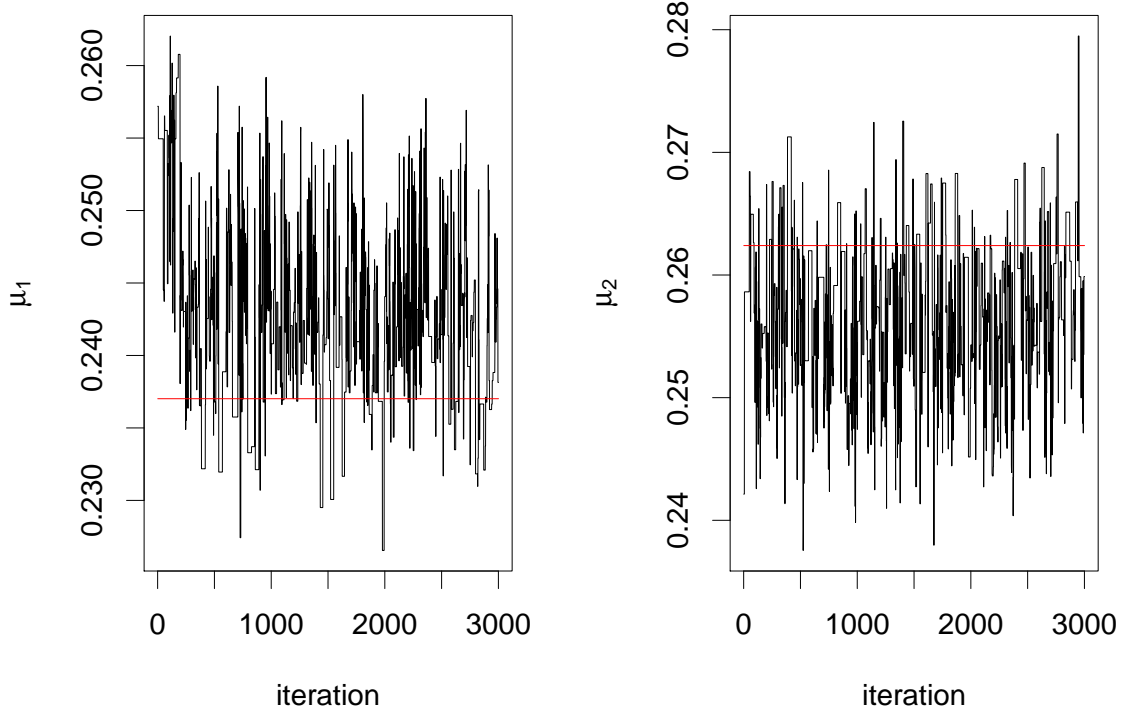


Fig. 7.26: Traceplot of $\boldsymbol{\mu} = \left\{ \mu_1, \mu_2, 1 - \sum_{i=1}^2 \mu_i \right\}$. Simulation data: number of leaves $n = 15$, height of the tree $h = 7$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 4$, number of observations $k = 8$, scalar concentration parameter $A = 1000$. The initial value of $\boldsymbol{\mu}$ is generated by a flat Dirichlet distribution. True values are indicated in red.

7.8.2 Prediction of future realizations with synthetic data

The posterior predictive distribution is defined as the distribution of unobserved observations (prediction) given the observed data. Let be $\tilde{\boldsymbol{x}}$ the prediction of the random variable $\boldsymbol{x} \sim Dir(\boldsymbol{\alpha}(A\boldsymbol{\mu}, \tau))$. The posterior predictive distribution $p(\tilde{\boldsymbol{x}}|\text{data}, \tau)$ is computed marginalising over the splitting proportions vector $\boldsymbol{\mu}$

$$p(\tilde{\boldsymbol{x}}|\text{data}, \tau) = \int_{\forall \boldsymbol{\mu}} p(\boldsymbol{x}|\boldsymbol{\alpha}(A\boldsymbol{\mu}, \tau))p(\boldsymbol{\mu}|\text{data})d\boldsymbol{\mu} \quad (7.17)$$

$$= \mathbb{E}(p(\boldsymbol{x}|\boldsymbol{\alpha}(A\boldsymbol{\mu}, \tau))) \quad \text{wrt } p(\boldsymbol{\mu}|\text{data}) \quad (7.18)$$

$$\approx \frac{1}{M} \sum_{m=1}^M p(\boldsymbol{x}|\boldsymbol{\alpha}(A\boldsymbol{\mu}^{(m)}, \tau)) \quad (7.19)$$

where $\mu^{(1)}, \dots, \mu^{(M)}$ are the M MCMC samples of μ

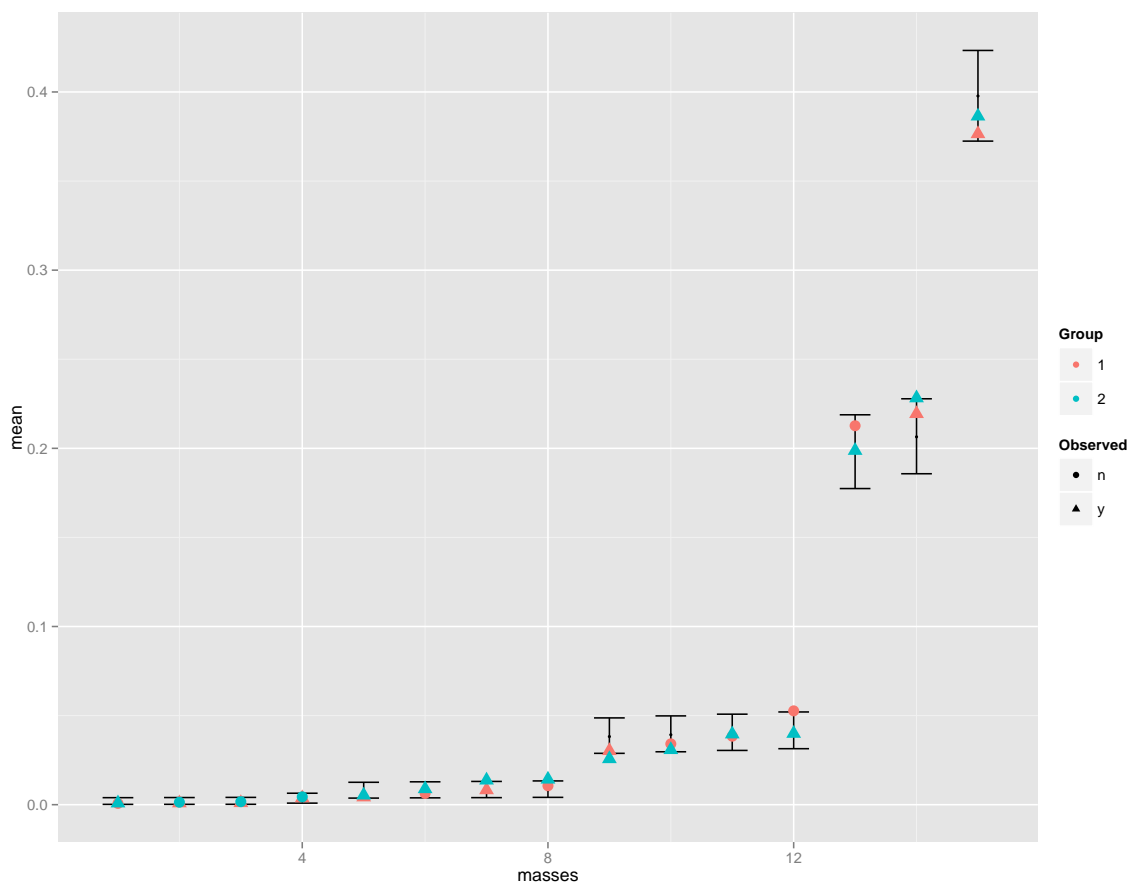


Fig. 7.27: Prediction of masses. Comparison between the expected values and data. We can see in black the expected values of the elements of the partition of the unit interval with a 90% confidence interval. The groups 1 and 2 in pink and light blue represent the complete data. The complete data include the observed data drawn with a triangle and the inferred missing data drawn with a circle. Simulation data: number of leaves $n = 15$, height of the tree $h = 4$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 5$, number of observations $k = 2$, scalar concentration parameter $A = 1000$.

7.8.3 MCMC convergence with real data

We show in this section the results of simulations carried out with the only available set of real observation, coming from the data analysis of the ATV1 re-entry observation campaign (see Chapter 5 for further details).

Prediction of future realizations with real data

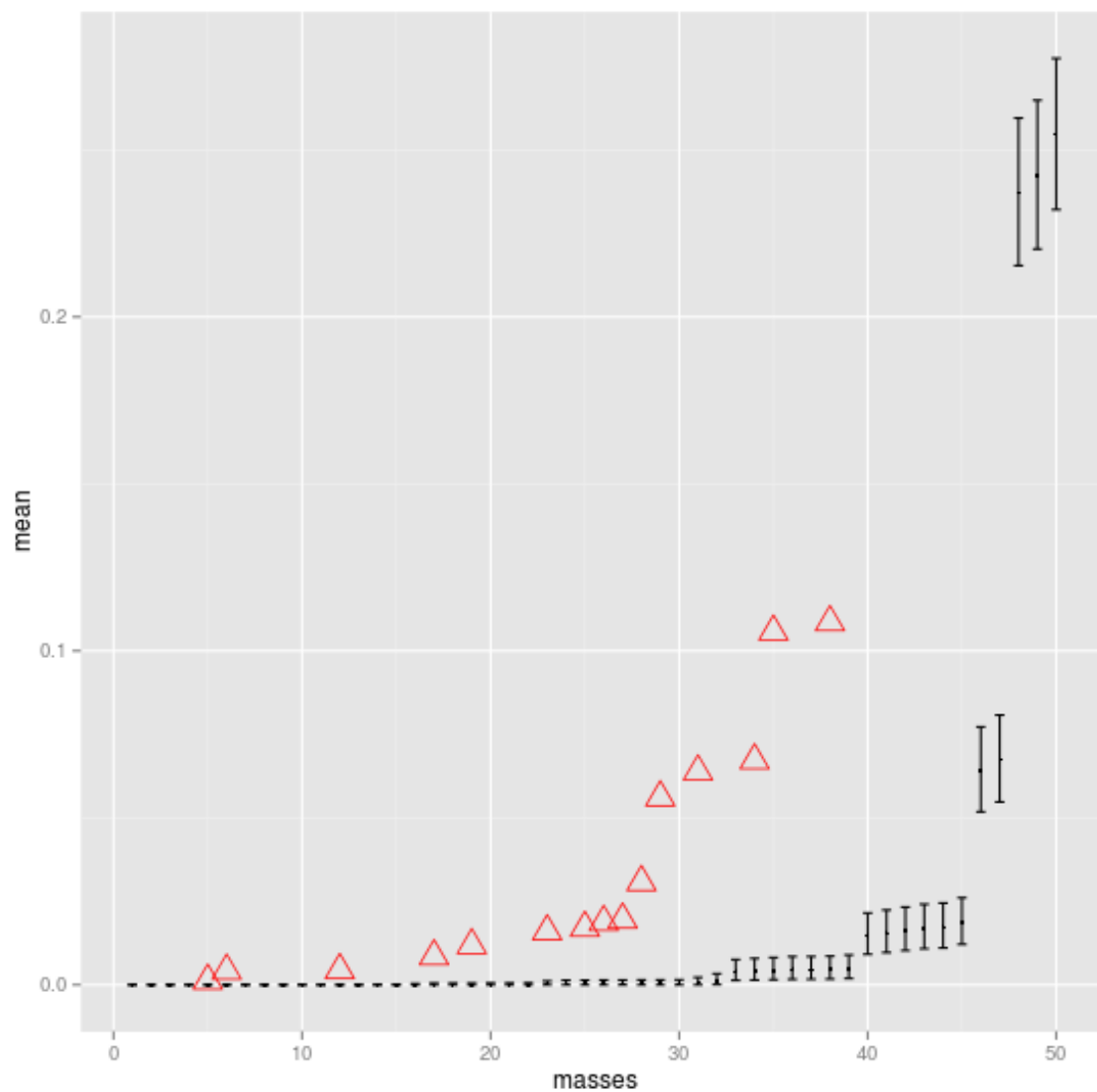


Fig. 7.28: Comparison between the expected values and data. We can see in black the expected values of the elements of the partition of the unit interval with a 90% confidence interval. The triangles represent the observed data and their position is given by the outcome value of the indicator variable. Simulation data: number of leaves $n = 50$, height of the tree $h = 10$, lobster tree with maximum out-degree of the nodes of the central path $deg_1 = 4$, maximum out-degree of the nodes within distance 1 of the central path $deg_2 = 4$, number of observations $k = 1$, scalar concentration parameter $A = 1000$.

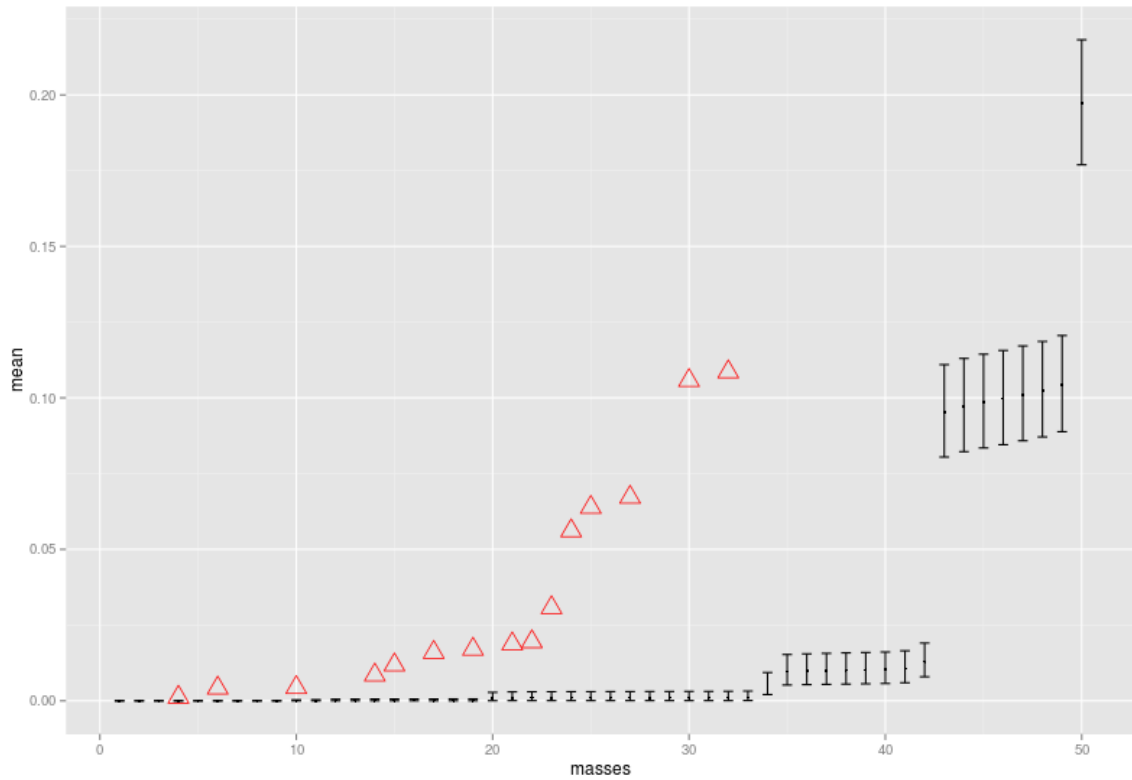


Fig. 7.29: Comparison between the expected values and data. We can see in black the expected values of the elements of the partition of the unit interval with a 90% confidence interval. The triangles represent the observed data and their position is given by the outcome value of the indicator variable. Simulation data: number of leaves $n = 50$, height of the tree $h = 4$, lobster tree with maximum out-degree of the nodes of the central path $deg_1 = 10$, maximum out-degree of the nodes within distance 1 of the central path $deg_2 = 5$, number of observations $k = 1$, scalar concentration parameter $A = 1000$.

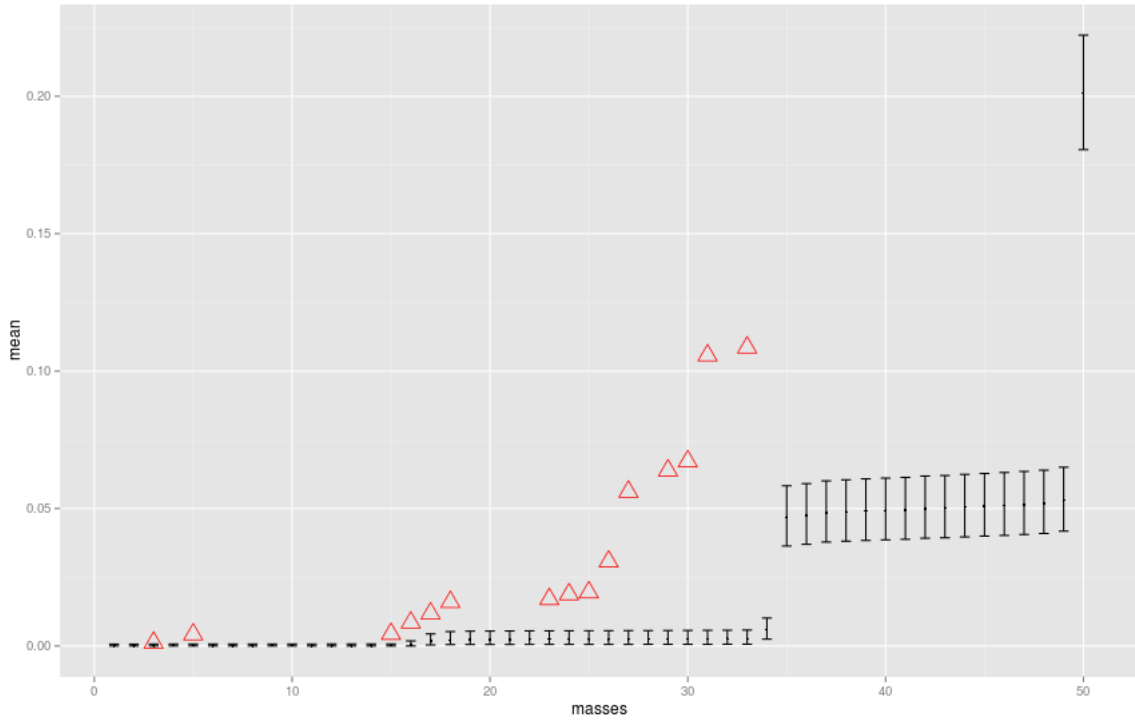


Fig. 7.30: Comparison between the expected values and data. We can see in black the expected values of the elements of the partition of the unit interval with a 90% confidence interval. The triangles represent the observed data and their position is given by the outcome value of the indicator variable. Simulation data: number of leaves $n = 50$, height of the tree $h = 3$, caterpillar tree with maximum out-degree of the nodes of the central path $deg_1 = 20$, number of observations $k = 1$, scalar concentration parameter $A = 1000$.

7.8.4 Discussion

The reliability of the results (expected values) is connected with the choice of the constraints of the tree structure, as explained in Section 7.5. These parameters define the variance of the outcomes of the proposed alternative stick breaking process.

The simulations that we carried out using real data, whose results are showed in Figures 7.28, 7.29 and 7.30, demonstrate that the model did not behave well in the inference of the Dirichlet parameter α . We need to make clear that these simulations are not supported by a suitable choice of the tree-structure, due to the lack of knowledge. We could not rely on any prior information about the materials of the observed masses and how they could be grouped in a tree structure representation. As we can

see from the plots, the expected values do not match with the real data.

The obtained results confirm the relationship between the predictions and the selected tree-structure, which plays the role of model framework. Regarding this issue, it would be interesting to investigate a strategy for devising the most appropriate tree structure from expert judgements, as well as the prior of the splitting proportions vector.

Chapter 8

Discussion, recommendations and conclusions

8.1 Summary

In this thesis, we have proposed two Bayesian statistical models:

- A belief-network model for failure prediction and especially a new approach for the integration of expert opinion elicitation, based on pairwise comparisons, in the dependability analysis of a complex critical system;
- A fragmentation model, that is a model for the construction of a distribution over the partitions of the unit interval, generated by a partially random fragmentation process, and especially a strategy for the inference of its parameters, given incomplete observations.

This study serves as the technology concept formulation phase in the development of a new risk assessment tool for highly energetic break-up events of a spacecraft during the atmospheric re-entry.

The proposed belief-network model can be applied for the assessment of the probability for an highly energetic break-up to occur, while the proposed fragmentation model provides a strategy for the evaluation of the distribution of the masses of the generated fragments. The application of both the models requires a tailored expert opinion and sparse observations.

8.2 Discussion and Limitations

8.2.1 Belief-network model for failure prediction

The most significant drawback we met in the devising of this model was the lack of historical data coming from in-situ observations or on-ground experiments and the incompleteness of the background knowledge. Much effort has been devoted in the research of exploitable data, but with very poor results. For this reason, we have decided to develop a model based on expert elicitation and we focussed in the investigation of a strategy that would make this process as simple as possible for experts. We believe that the illustrated procedure can be potentially useful for the assessment of the probability for a spacecraft to explode, even if we recognize that it still needs to be properly tested and refined. It is important to highlight that this is a new way of thinking for the involved experts.

Let us point out that expert opinion can provide accurate results when integrated with real data, but it cannot be considered adequate by itself.

8.2.2 Fragmentation model

The simulations performed with synthetic data (some of them are reported at the end of the Chapter 7) showed problems in the convergence of the full model, especially with the increasing of the number of observations. This is a very common issue in Markov chain Monte Carlo (MCMC) applications, due to the fact that the likelihood gets narrower.

Furthermore we noticed that the mixing behaviour of the MCMC samples of the tree-structure is very poor. This limitation affects the result of the inference of the tree-structure representing the distribution of the masses of the fragments. Again this is a common issue, occurring when the local alteration proposed at each iteration is not efficient. In our case it consists in the shift of a leaf from a father node to another. We recommend to the interested reader the paper Pratola (2016), where the mixing problem of the Bayesian regression trees is well explained and a novel mechanism for efficient sampling is proposed.

8.3 Looking forward

To date both the models have been simulated relying on synthetic data and on the outcomes processed after the Automated Transfer Vehicle Jules Verne re-entry observation campaign. Optimistically there will be more opportunities to gather data for the fine-tuning of the model. The extra data that will be available the better the model will match the real physical process. As already mentioned, the proposed models have frameworks that can be adjusted to suit changing data sets and new information. Real data would allow also for the validation of the models.

It would be also interesting to assess the trade off between the cost/effort to collect data versus the amount of information that is provided to the model.

Finally the following list summarize the concrete points for the next steps of the research, concerning both the models:

- Perform simulations with synthetic data in order to assess the minimum amount of data needed in an observation campaign to be able to create a database for the model such that it can produce results with minimum confidence: verify how the posterior is sensitive to the number of observations;
- Run simulations with synthetic data in order to assess the convergence of the models to the right answer and its reliability, varying the initial conditions, and verify in which circumstances the uncertainty is reduced;
- Keep collecting expert opinion following the proposed approach, in order to calibrate the models for the physical problem researched;
- Create a front-end interface to run the model and to make it user-friendly. After the development of an user interface, the models could be embedded in the re-entry analysis tool ASTOS (Aerospace Trajectory Optimization Software).

We focus on the single models in the next paragraphs.

8.3.1 Belief-network model for failure prediction

We aim to embed both the models in a new risk assessment tool for highly energetic break-up events of a spacecraft during the atmospheric re-entry, whose target users are

experts of the different spacecraft subsystems. The next step is to convert the proposed methodologies to a proof-of-concept tool and evaluate it.

As already noted, an extensive investigation of the sensitivity of the results to the initial conditions is crucial. For instance, for the accomplishment of this goal, we propose to perform the following simulation:

- Specify values for the probabilities of the elementary events to occur and call them *true values*;
- Sample sparse observations of the occurrence of the elementary events from these probabilities for a bunch of realizations of the system (or re-entry events);
- Run the model, assuming known the outcome of the pairwise comparisons, and verify if the posterior distribution of the elementary events converges to the *true values* and how this result changes, varying the number of considered realizations of the system and the sparseness of the observations.

The fault tree analysis deserves some comments. We considered only a very basic fault tree, limited to *and* and *or* gates, but we believe this analysis could be easily extended to more general and complicated situations, with a larger variety of gates. With the increasing of the complexity of the fault tree it will be necessary to consider a minimal cut sets rearrangement (Vesely et al., 1981) of the tree in order to perform an efficient quantitative evaluation. The minimal cut sets representation avoids the double counting of any basic event that appears in different parts of the fault tree, keeping unchanged the logic interrelationships of the events .

Furthermore, broadening the analysis, It would be interesting to consider the conversion of the tree to a binary decision diagram as illustrated in Reay and Andrews (2002), again for the enhancement of the computation of the top event probability.

Lastly, in its application to the re-entry problem, since we are aware that the proposed set of events is a simplified version of the reality, we propose to investigate which other events should be considered and how their dependence relationship can be handled.

Regarding the elicitation method, it is missing a strategy to calibrate properly the answers coming from the different group of experts. The effects of the subjectivity of expert opinion have been neglected so far. It could easily happen that one group

provides very optimistic answers and another one very pessimistic ones: this would easily cause biased results.

As we explained in Chapter 6, experts responses to paired comparisons are aggregated by taking geometric mean of their response and mapped to beta prior distributions. We defined this method as a method inspired by the Analytic Hierarchy Process (AHP). It would be interesting to investigate the possibility of identifying contributing factors or covariates, defining various states of the system. This would allow the application of the Bradley-Terry approach or a full AHP method (see Section 4.4.1 for further details).

Furthermore, future work concerning the belief-network model for failure prediction, involves the development of a web based tool to enable expert elicitation of the probabilities associated with the Bayesian inference. This tool would allow automating the enhancement of the model reliability as the background knowledge improves.

Finally, we propose to explore the use of the software for structured expert judgments, developed by TU Delft Risk Analysis department (Cooke (2008), Goulet et al. (2009)) and to exploit the available literature on pairwise comparisons better.

8.3.2 Fragmentation model

Future work, concerning the fragmentation model, could be aimed to relax the unrealistic assumptions.

We assumed that every fragment has the same probability of being observed and then we sampled uniformly the indicator variable. This assumption, which does not reflect the reality, could be relaxed using the Poisson binomial distribution, that is the discrete probability distribution of a sum of independent Bernoulli trials that are not necessarily identically distributed. To facilitate the analysis, we assumed missing observations completely at random (for further details about the classification of missing data, the reader is invited to read the Section A.1.1), considering the probability of observing an item independent of the value of the item itself. We propose to investigate further the attributes of the missing data and then to adapt the analysis. Certainly the outcome of an observation campaign includes censored observations, that could be treated in a different way from the missing data completely at random. Examples of censored observations might be fragments that are not observable because of their size

or simply because they are outside the field of view.

As already noted in Section 7.4.2, the number of leaves of the tree (and then the number of generated fragments) is assumed constant and known. It would be interesting to add this parameter to the parameters to be inferred, by integrating the reversible-jump Markov chain Monte Carlo in the full model. The points where the spacecraft break-up and hence a prior prediction of the amount of actual fractures could be identifiable and connected with the released energy.

The reliability of the results is associated with the choice of the constraints of the tree structure. These parameters define the variance of the outcomes of the proposed alternative stick breaking process. It would be interesting to investigate a strategy for devising the best kind of tree structure from the background knowledge and for updating this strategy as new observations become available. For example, if we observe some characteristics of a fragment, how can we use this information to improve the predictions on the tree-structure?

We remind the reader that the tree structure can represent the tracking of the fragmentation history and that setting-up constraints on the tree-structure allows the user to control the model. The application of this model could be extended also to the fragmentation events preceding the highly energetic break-up. Indeed the same strategy could be applied also to the whole fragmentation of the spacecraft, including the low energetic break-up events, if fitted with the appropriate data.

A sensitivity analysis could be performed in order to find the best proposal distributions.

Finally attention should be paid to the convergence issues of the MCMC algorithms.

8.3.3 How ESA can benefit from this research

We recognize that both the models are at second level of technology readiness, according to the ISO standard 16290:2013, used by ESA to define the Technology Readiness Levels (TRLs): basic principles are observed, practical applications can be invented. Applications are speculative, simulations and examples are limited to analytic studies.

The simulations that we performed are confined at an abstract level and they do not relate explicitly to the physical problem. They showed results consistent with the expectations in the sense that their reliability is connected with the choices made by

the user to control the model (or the expert opinion). This thesis is accompanied by a commented code that allows to run simulations of the proposed models.

The next technology readiness level to pursue is: analytical and experimental critical function and/or characteristic proof-of-concept. This includes laboratory studies to physically validate the analytical predictions. Due to the lack of data in the proposed problem, this objective could be pursued better applying the models to a similar problem but with a larger availability of data.

8.4 Conclusions and potential application fields

The main goal of this thesis was to face the challenge to make statistical predictions in a context where real data are very scarce and the events under study are not repeatable under the same conditions. The planning of future in-situ airborne observation campaigns is critical for gathering data for this kind of problem. The required accuracy of data could be reached only maximizing the spatial resolution and spectroscopic possibilities.

Missing data is a recurrent problem in space activities. When designing a space mission, decision makers are often asked to make inference relying on sparse observed data. Most of the space missions are made of unique and not repeatable events or events not easy to observe. The drive towards exploration, cost constraints and the need to constantly test new technologies, which are typical factors in this field, do not allow to wait for a good amount of historical data to rely on. For this reason, we expect that the Bayesian models here proposed, and especially the expert opinion elicitation method, can be applied, with minor modifications, also to other reliability and risk assessment problems in the same field, where a treatment and quantification of the uncertainty is crucial.

The closest alternative application could be the launch vehicles upper stage re-entry survivability analysis, in the cases when a controlled re-entry is performed after the spacecraft delivery. Unlike in the past, this could become soon a trend in the launcher business Heinrich et al. (2015). Examples are the launcher Arianespace, which recently performed a controlled re-entry on SOYUZ-ST after delivering Sentinel-1, the European launch vehicle VEGA (Vettore Europeo di Generazione Avanzata), developed

within a European Programme promoted by ESA Heinrich et al. (2015) and H-IIB launch vehicle, designed by the Japan Aerospace Exploration Agency (JAXA) in collaboration with Mitsubishi Heavy Industries. The design of missions, for which this new generation of launchers provides launch services, needs to take into account the estimation of the upper stage fragmentation after orbital injections, in order to comply with the requirements on space debris mitigation, likewise re-entering spacecraft. A good relevant reference is Battie et al. (2012), where the reader can find the re-entry survivability analysis performed for the VEGA liquid propellant upper module, called AVUM (Attitude Vernier Upper Module).

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Appendix A

Statistical inference and sampling methods

A.1 Statistical inference and the Bayesian approach

A.1.1 Statistical inference

Let us assume we have a random phenomenon generating data. Given this data, what can we say about this random phenomenon? This is the basic question that statistical inference aims to answer (Wasserman, 2003). Inference is the process of deducing properties or parameters of an underlying distribution by data analysis.

Statistical modelling provides an interpretation of the past realizations of a random phenomenon, based on its outcomes, and the means to predict the future realizations of a similar nature (Robert, 2007). It exploits the probabilistic modelling as support, but the purpose of the statistical modelling is fundamentally an inversion purpose with respect to the probabilistic modelling. When observing a random phenomenon described by a probability distribution depending on a parameter θ , statistical methods indicate the strategy to infer the parameter θ , while the probabilistic modelling aims to forecast the future outcomes conditioned on the parameter θ . This is the reason why, at the end of the eighteenth century, Statistics was often called *Inverse Probability* (Stigler, 1986).

Statistics is divided into two different school of thoughts: the *frequentist* (or the *classical*) and the *Bayesian*. Frequentists interpret the probability as the relative fre-

quency of the event happening in an infinite population of repeatable trials. Hence the probability only exists for repeatable events. The parameter θ is considered an *unknown* with a fixed value and the inference result depends exclusively on data. Conversely, as we will explain in more detail in the next section, for Bayesians the probability is a *degree of belief*. In real world we are often faced with events that are not repeatable, Notwithstanding the event cannot be repeated, Bayesians can still compute its probability of occurring, combining experience and observations and applying a probability distribution for that event.

Missing and censored data

One of the most common issues in statistical inference is the occurrence of missing data. Missing data can seriously affect the reliability of the results, leading to biased estimates of parameters or loss of information. A datapoint is missing when no value is recorded for a variable in an observation. Differently, when the observed value of some variable is partially known we have a censored data point. We consider for example a bathroom scale measuring up 100 kg and an individual whose weight is 120 kg. The information that we can get weighting the considered individual with this scale is a censored information: we could only know that his weight is lower than 100 kg.

According to Rubin's classification (Rubin, 1976), missing data can be distinguished in

- MCAR (completely at random) when the probability of missing data on a variable X is unrelated to other measured variables and to the values of X itself. Missingness is completely unsystematic and the observed data can be thought of as a random subsample of the hypothetically complete data;
- MAR (at random) when the missingness is systematic, that is the propensity for missing data is correlated with other study-related variables in the analysis, but not with the hypothetical values that would have resulted had the data been complete;
- MNAR (not at random) when the probability of missing data is systematically related to the hypothetical values that are missing.

A realistic scenario of the re-entry break-up events needs to take account of the occurrence of missing and, even more frequently, censored observations (Stern, 2003). For instance, there might be fragments that are not observable because of their size or simply because they are outside the field of view: these could be one example where data could be considered missing completely at random data and one example of censored data. Another censored information can be due to the fact that observations are usually taken overnight: it is easier to observe burning fragments but cold fragments can be missed.

To facilitate the analysis, in the development of the Fragmentation model (Chapter 7), we assume missing observation completely at random, considering the probability of observing an item independent of the value of the item itself. This is a common assumption in real world problems, which could be relaxed in future work (Marlin et al. (2005), Stubbendick and Ibrahim (2006)), after having carried out a proper classification of data with missing and/or censored attributes. Different data attributes should be handled in a different way.

A.1.2 The Bayesian approach

Bayesian inference consists in the computation of the distribution of the parameter θ after taking into account the observed data \mathbf{X} , or conditional on \mathbf{X} . This distribution $p(\theta|\mathbf{X})$ is called the *posterior distribution* and it represents the *post-belief*.

Given *Bayes' theorem*, which is the foundation of the Bayesian inference, as the name suggests, the *posterior distribution* is determined by

$$p(\theta|\mathbf{X}) = \frac{P(\mathbf{X}|\theta)p(\theta)}{\int P(\mathbf{X}|\theta)p(\theta)d\theta} \quad (\text{A.1})$$

from which it follows that the posterior distribution is proportional to the *likelihood function* multiplied by the *prior distribution*:

$$p(\theta|\mathbf{X}) \propto P(\mathbf{X}|\theta)p(\theta). \quad (\text{A.2})$$

The *probability* of the evidence given the parameter $P(\mathbf{X}|\theta)$, rewritten in proper order:

$$\mathcal{L}(\theta|\mathbf{X}) = P(\mathbf{X}|\theta) \quad (\text{A.3})$$

is called *likelihood function* $\mathcal{L}(\theta|\mathbf{X})$. The *likelihood* of θ , given evidence \mathbf{X} , is equal to the *probability* of the evidence (or observed outcomes) given θ . This function synthesizes

formally the inverting concept of Statistics. Indeed it is a function of the parameter θ , which is *unknown* and depends on the evidence \mathbf{X} . *Probability* characterizes possible future outcomes given a fixed value of the parameter before data, while the *likelihood* is a function of the parameter for a given outcome (or evidence), that is after data are available. Note that we are using capital P to highlight that the *likelihood function* is equal to a *probability* and it is not a density probability function as the posterior and the prior distribution: the evidence \mathbf{X} is given and it is not a random variable.

The *prior distribution* $p(\theta)$ is defined as the distribution of the parameters before data are observed and it represents the *initial subjective belief*. The selection of the prior distribution depends on the background knowledge and it is a very delicate problem. It is the key to Bayesian inference. The more information is available the more effective will be its choice and the more reliable is the inference. The prior distribution allows the incorporation of an expert's experience into a statistical model.

The revolutionary introduction of Bayesian statistics consists in assigning a probability distribution to both causes (evidence) and effects (parameters) or, in other words, in assigning to the parameters the role of random variables. The *posterior distribution* incorporates the information on the parameter θ contained in the observation \mathbf{X} and the *initial subjective belief*.

Despite the fact that the Bayesian approach was introduced in the 18th century, its real world application was limited and conditioned by computational difficulties, especially by the necessity to integrate over the whole of parameter space.

The advancement of sampling methods, along with the strengthening of computers capacity, in terms of speed and memory, boosted the practical use of Bayesian statistics, particularly from the last decade of 20th century. Details about these sampling methods are provided in the next sections.

A.2 Monte Carlo methods

The project described in this thesis required an extensive use of the approximate inference methods based on numerical sampling, also known as Monte Carlo techniques. For this reason the reader can find here a section devoted to explain how they work.

The Monte Carlo method is one of the most dominant inference methods in Bayesian

statistics. Their use is justified by two theorems: the *strong law of large numbers* and the *central limit theorem* (Grimmett and Stirzaker, 2001).

The driving question is: given a probability distribution π , how do we simulate a random object with distribution π ?

A.2.1 Rejection sampling

This method is also commonly called the acceptance-rejection method or accept-reject algorithm.

The driving question in this section is: given a relatively complex univariate distribution π , how do we simulate a random object with distribution π ?

We wish to sample from a distribution $\pi(\mathbf{z})$, but we know that sampling directly from it is difficult.

Then we consider a distribution $\tilde{\pi}(\mathbf{z})$ that we can easily evaluate for any given value of \mathbf{z} , such that $\forall \mathbf{z} \in \mathcal{Z}$

$$\pi(\mathbf{z}) = \frac{1}{K} \tilde{\pi}(\mathbf{z}) \tag{A.4}$$

where K is a normalizing constant.

We take a proposal distribution $q(\mathbf{z})$, from which we can readily draw samples, and a constant k such that $\forall \mathbf{z}$

$$kq(\mathbf{z}) \geq \tilde{\pi}(\mathbf{z}). \tag{A.5}$$

Algorithm A.1 shows the step to follow for the application of the rejection method.

Note that scaling the function π by a constant $\tilde{\pi} = K\pi$ has no effect on the sampled x -position, than the accepted sample valued z_0 can be considered a realization of π , which is the normalized version of $\tilde{\pi}$.

This is a useful method for one or two dimensions problems, but it suffers from the “curse of dimensionality”, because the accept probability decreases exponentially as a function of the number of dimensions. It becomes increasingly difficult to identify a proposal distribution that yields a reasonable proportion of accepted parts. For this reason we are going to introduce other methods for sampling in higher dimensional space.

Algorithm A.1 Rejection method

1. Generate a number z_0 (an x -position) from the proposal distribution $q(z)$;
2. Generate a number u_0 from the uniform distribution over $[0, kq(z_0)]$, that is equivalent to sample uniformly along the vertical line from the selected x -position up to the curve of the proposal distribution scaled by k ;
3. Check if that the last generated value is greater than the value of the desired distribution $\tilde{\pi}$ along this line

$$u_0 > \tilde{\pi}(z_0)$$

- if this holds, reject the sampled values and return to step (1);
 - if not, accept the sampled value z_0 as a realization of $\tilde{\pi}$.
-

A.2.2 Importance sampling

Let us consider the problem of approximating the expectation of some function $f(\mathbf{z})$ with respect to a probability distribution $\pi(\mathbf{z})$ of the form:

$$\mathbb{E}|f| = \int f(\mathbf{z})\pi(\mathbf{z})d\mathbf{z} \tag{A.6}$$

where the integral is replaced by a infinite summation in the case of discrete variables.

This could be solved applying the general idea behind the sampling methods, that is by drawing independently a set of samples $\mathbf{z}^{(i)}$ with $i = 1, \dots, M$ from the distribution $\pi(\mathbf{z})$ and compute the finite sum:

$$\hat{f} = \frac{1}{M} \sum_{i=1}^M f(\mathbf{z}^{(i)}) \tag{A.7}$$

as long as we are able to generate the samples $\mathbf{z}^{(i)}$.

The importance sampling method (Geweke, 1989) provides a strategy to compute the expectation directly, without drawing samples from the distribution $\pi(\mathbf{z})$ itself.

Then the driving question in this section is: how can we approximate the expectation in A.6 when it is analytically intractable and when we cannot draw samples directly from the probability distribution $\pi(\mathbf{z})$, but we can evaluate $\pi(\mathbf{z})$ for any given value of \mathbf{z} ?

Given a proposal distribution $q(\mathbf{z})$, from which we can readily draw samples $\mathbf{z}^{(i)}$

with $i = 1, \dots, M$, the expectation can be written as follows¹:

$$\mathbb{E}[f] = \int f(\mathbf{z})\pi(\mathbf{z})d\mathbf{z} \quad (\text{A.8})$$

$$= \int f(\mathbf{z})\frac{\pi(\mathbf{z})}{q(\mathbf{z})}q(\mathbf{z})d\mathbf{z} \quad (\text{A.9})$$

$$\simeq \frac{1}{M} \sum_{i=1}^M \frac{\pi(\mathbf{z}^{(i)})}{q(\mathbf{z}^{(i)})} f(\mathbf{z}^{(i)}). \quad (\text{A.10})$$

where the ratio $r_i = \pi(\mathbf{z}^{(i)})/q(\mathbf{z}^{(i)})$ is defined *importance weight* and it is aimed to remove the bias introduced by sampling from the wrong distribution.

Let us assume that the distribution $\pi(\mathbf{z})$ can only be evaluated up to a normalization constant, so that $\pi(\mathbf{z}) = \tilde{\pi}(\mathbf{z})/Z_\pi$ where $\tilde{\pi}(\mathbf{z})$ is easy to compute and the constant Z_π is unknown. In a similar manner $q(\mathbf{z}) = \tilde{q}(\mathbf{z})/Z_q$. As a result we have:

$$\mathbb{E}[f] = \int f(\mathbf{z})\pi(\mathbf{z})d\mathbf{z} \quad (\text{A.11})$$

$$= \frac{Z_q}{Z_\pi} \int f(\mathbf{z})\frac{\tilde{\pi}(\mathbf{z})}{\tilde{q}(\mathbf{z})}q(\mathbf{z})d\mathbf{z} \quad (\text{A.12})$$

$$\simeq \frac{Z_q}{Z_\pi} \frac{1}{M} \sum_{i=1}^M \tilde{r}_i f(\mathbf{z}^{(i)}). \quad (\text{A.13})$$

where $\tilde{r}_i = \tilde{\pi}(\mathbf{z}^{(i)})/\tilde{q}(\mathbf{z}^{(i)})$. Since $\int \pi(\mathbf{z})d\mathbf{z} = 1$, the ratio Z_π/Z_q is equal to:

$$\frac{Z_\pi}{Z_q} = \frac{1}{Z_q} \int \tilde{\pi}(\mathbf{z})d\mathbf{z} = \int \frac{\tilde{\pi}(\mathbf{z})}{\tilde{q}(\mathbf{z})}q(\mathbf{z})d\mathbf{z} \quad (\text{A.14})$$

$$\simeq \frac{1}{M} \sum_{i=1}^M \tilde{r}_i. \quad (\text{A.15})$$

It follows forthwith:

$$\mathbb{E}[f] \simeq \sum_{i=1}^M w_i f(\mathbf{z}^{(i)}) \quad (\text{A.16})$$

where w_i is the *normalized importance weight*:

$$w_i = \frac{\tilde{r}_i}{\sum_m \tilde{r}_m} = \frac{\tilde{\pi}(\mathbf{z}^{(i)})/q(\mathbf{z}^{(i)})}{\sum_m \tilde{\pi}(\mathbf{z}^{(m)})/q(\mathbf{z}^{(m)})}. \quad (\text{A.17})$$

Algorithm A.2 summarizes the step of the importance sampling.

¹the sign \simeq stands for *asymptotically equal to*

Algorithm A.2 Importance sampling

1. Generate n iid samples $\mathbf{z}^{(i)}$ from the proposal distribution $q(\mathbf{z})$
 2. Define the *importance weight* and normalize it.
 3. Approximate the target expectation by A.16
-

A.3 Markov chain Monte Carlo methods

The rejection sampling and importance sampling methods, above detailed, have a limited application in high dimensionality spaces. We introduce in this section the Markov chain Monte Carlo methods, that, on the contrary, suit them well.

The Markov chain Monte Carlo (MCMC) methods, originally published by physicists in the 1950's, provided a large contribution in 1990's to the development of the Bayesian statistics area. These methods provided a computational tool to tackle the hard computational issues concerning the application of the Bayesian approach. The reader is referred to the excellent book Häggström (2002) for the theoretical basis of these methods and the explanation of why they are powerful approximation tools.

A.3.1 Metropolis-Hastings

The driving question of this section is: given a relatively complex multivariate distribution π , how do we simulate a random object with distribution π ?

In 1953 Metropolis developed a MCMC scheme (Metropolis et al., 1953) to solve this issue and later, in 1970, Hastings (Hastings, 1970) added flexibility to it, introducing the well known Metropolis-Hastings algorithm. The aim of the Metropolis-Hastings algorithm is the generation of a Markov process that asymptotically reaches a unique stationary distribution $p(\mathbf{z})$ such that $p(\mathbf{z}) = \pi(\mathbf{z})$.

We choose again a proposal distribution $q(\mathbf{z})$ from which we can easily draw a sequence of random samples $\mathbf{z}^{(1)}, \mathbf{z}^{(2)}, \mathbf{z}^{(3)}, \dots$ in order to create a Markov chain. The proposal distribution is indicated in the form $q(\mathbf{z}^{(\tau)}|\mathbf{z}^{(\tau-1)})$ to show that we want to simulate from it a sample $\mathbf{z}^{(\tau)}$ given the previous sample value $\mathbf{z}^{(\tau-1)}$.

In the basic Metropolis algorithm, the proposal distribution needs to be symmetric,

that is

$$q(\mathbf{z}_A|\mathbf{z}_B) = q(\mathbf{z}_B|\mathbf{z}_A) \quad \forall \mathbf{z}_A, \mathbf{z}_B \quad (\text{A.18})$$

but this constraint is relaxed in the Metropolis-Hastings version. This the point where Hastings added flexibility to the scheme.

As with the rejection sampling method, we consider a distribution $\tilde{\pi}(\mathbf{z})$ that we can easily evaluate for any given value of \mathbf{z} , such that $\forall \mathbf{z} \in \mathcal{Z}$

$$\pi(\mathbf{z}) = \frac{1}{K} \tilde{\pi}(\mathbf{z}) \quad (\text{A.19})$$

where K is a normalizing constant.

We are now ready to follow the next step by step instructions to apply the Metropolis-Hastings algorithm, that is the most generalized version:

Algorithm A.3 Metropolis-Hastings

1. Initialization. Choose an arbitrary point $\mathbf{z}^{(0)}$ as initial candidate;
2. For each iteration τ , given the current state $\mathbf{z}^{(\tau)}$:
 - Generate a candidate \mathbf{z}^* from the proposal distribution $q(\mathbf{z}^*|\mathbf{z}^{(\tau)})$;
 - Calculate the acceptance probability. $\alpha(\mathbf{z}^*, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{\pi}(\mathbf{z}^*)q(\mathbf{z}^{(\tau)}|\mathbf{z}^*)}{\tilde{\pi}(\mathbf{z}^{(\tau)})q(\mathbf{z}^*|\mathbf{z}^{(\tau)})}\right)$

where

– $\frac{\tilde{\pi}(\mathbf{z}^*)q(\mathbf{z}^{(\tau)}|\mathbf{z}^*)}{\tilde{\pi}(\mathbf{z}^{(\tau)})q(\mathbf{z}^*|\mathbf{z}^{(\tau)})}$ is called acceptance ratio;

– $\frac{\tilde{\pi}(\mathbf{z}^*)}{\tilde{\pi}(\mathbf{z}^{(\tau)})}$

is the probability (e.g. Bayesian posterior) ratio between the proposed state and the current state;

– $\frac{q(\mathbf{z}^{(\tau)}|\mathbf{z}^*)}{q(\mathbf{z}^*|\mathbf{z}^{(\tau)})}$ is the ratio of the proposal distribution in two directions (from the current state to the proposed state and vice versa);²

Note that the evaluation of the acceptance ratio doesn't require the knowledge of the normalizing constant K in A.19 and that $\frac{\pi(\mathbf{z}^*)}{\pi(\mathbf{z}^{(\tau)})} = \frac{\tilde{\pi}(\mathbf{z}^*)}{\tilde{\pi}(\mathbf{z}^{(\tau)})}$.

- Accept the new sample assigning $\mathbf{z}^{(\tau+1)} = \mathbf{z}^*$ with probability $\alpha(\mathbf{z}^*, \mathbf{z}^{(\tau)})$.
-

The accepted samples represent a sample form the desired distribution π . This model gets better results if the proposal density matches the shape of the target distribution.

A.3.2 Gibbs sampler

Gibbs sampling (so named by Geman and Geman (1984), but published some years earlier by Ripley (1979)), is another simple Markov chain Monte Carlo algorithm that applies to a multivariate distribution. Suppose we want to sample $\mathbf{z} = \{z_1, \dots, z_n\}$ from the distribution $\pi(z_1, \dots, z_n)$. Gibbs sampler proceeds as follows:

Algorithm A.4 Gibbs sampler

1. *Initialization.* Start with some initial state for the Markov chain $\mathbf{z}^{(0)}$;
2. For each iteration $\tau = 1, \dots, K$, given the current state $\mathbf{z}^{(\tau)}$:
 - Sample $z_1^{(\tau+1)}$ from the distribution of z_1 conditioned on the values of the remaining variables at the state τ

$$z_1^{(\tau+1)} \sim \pi(z_1 | z_2^{(\tau)}, \dots, z_n^{(\tau)})$$

- Sample $z_2^{(\tau+1)}$ from the distribution of z_2 conditioned on the values of the remaining variables

$$z_2^{(\tau+1)} \sim \pi(z_2 | z_1^{(\tau+1)}, z_3^{(\tau)}, \dots, z_n^{(\tau)})$$

⋮

- Sample $z_j^{(\tau+1)}$ from the distribution of z_j conditioned on the values of the remaining variables

$$z_j^{(\tau+1)} \sim \pi(z_j | z_1^{(\tau+1)}, \dots, z_{j-1}^{(\tau+1)}, z_{j+1}^{(\tau)}, \dots, z_n^{(\tau)})$$

⋮

- Sample $z_n^{(\tau+1)}$ from the distribution of z_n conditioned on the values of the remaining variables at the state $\tau + 1$

$$z_n^{(\tau+1)} \sim \pi(z_n | z_1^{(\tau+1)}, \dots, z_{n-1}^{(\tau+1)})$$

.

Clearly this algorithm is applicable when the conditional distribution of each variable is known and easy to sample from, or at least easier than the joint distribution $\pi(z)$.

A.3.3 Data augmentation algorithm

The driving question of this section is: how can we deal with missing data problems? How can we sample from a posterior distribution when we know that the available data set are not complete? If the available data are not complete we are not able to write the complete likelihood.

We consider a parametric model $p(\mathbf{Y}, \mathbf{Z}|\theta)$ and we suppose we want to sample from the observed posterior density $p(\theta|\mathbf{Y})$ given the observed data \mathbf{Y} . We call complete (or augmented) data set the set of data given by:

- The observed data \mathbf{Y} and
- The unobserved data \mathbf{Z} (also called latent or missing).

The data augmentation algorithm provides a strategy to improve the inference based on the entire posterior distribution $p(\theta|\mathbf{Y}, \mathbf{Z})$, even if only the observed data are available. The idea behind this method consists in the augmentation of the observed data \mathbf{Y} by adding the latent data \mathbf{Z} , then it suits the cases where the augmented data can be easily generated.

The observed posterior density $p(\theta|\mathbf{Y})$, given the observed data \mathbf{Y} , is related to the predictive density in the Posterior Identity:

$$p(\theta|\mathbf{Y}) = \int_{\mathbf{H}} p(\theta|\mathbf{Z}, \mathbf{Y})p(\mathbf{Z}|\mathbf{Y})dZ \quad (\text{A.20})$$

where

- \mathbf{H} denotes the sample space for the unobserved data \mathbf{Z} ;
- $p(\theta|\mathbf{Z}, \mathbf{Y})$ denotes the conditional density of θ given the augmented data $\mathbf{X} = (\mathbf{Z}, \mathbf{Y})$ or simply the complete-data parameter posterior;
- $p(\mathbf{Z}|\mathbf{Y})$ denotes the predictive density of the unobserved data \mathbf{Z} given \mathbf{Y} , that can be expressed in terms on the desired posterior density in the Predictive

Identity:

$$p(\mathbf{Z}|\mathbf{Y}) = \int_{\Theta} p(\mathbf{Z}|\theta, \mathbf{Y})p(\theta|\mathbf{Y})d\theta \quad (\text{A.21})$$

where Θ denotes the parameter space.

Hence, replacing the Predictive Identity into the Posterior Identity and interchanging the order of integration, $p(\theta|\mathbf{Y})$ satisfies the integral equation:

$$p(\theta|\mathbf{Y}) = g(\theta) = \int K(\theta, \phi)g(\phi)d\phi \quad (\text{A.22})$$

where

$$K(\theta, \phi) = \int p(\theta|\mathbf{Z}, \mathbf{Y})p(\mathbf{Z}|\phi, \mathbf{Y})d\mathbf{Z} \quad (\text{A.23})$$

and $g(\phi) = p(\phi|\mathbf{Y})$.

Note that

$$p(\theta|\mathbf{Y}) = \int_{\mathbf{H}} p(\theta|\mathbf{Z}, \mathbf{Y})p(\mathbf{Z}|\mathbf{Y})d\mathbf{Z} \quad (\text{A.24})$$

$$= \int_{\mathbf{H}} p(\theta|\mathbf{Z}, \mathbf{Y}) \left(\int_{\Theta} p(\mathbf{Z}|\phi, \mathbf{Y})p(\phi|\mathbf{Y})d\phi \right) d\mathbf{Z} \quad (\text{A.25})$$

$$= \int_{\mathbf{H}} \int_{\Theta} p(\theta|\mathbf{Z}, \mathbf{Y})p(\mathbf{Z}|\phi, \mathbf{Y})p(\phi|\mathbf{Y})d\phi d\mathbf{Z} \quad (\text{A.26})$$

where we applied A.21 denoting with ϕ the parameter (rather than θ), in order to keep the term $p(\theta|\mathbf{Z}, \mathbf{Y})$ out from the integration over the parameter space and show the identity in A.22.

This suggests that A.22 can be solved by successive substitutions, starting with any initial candidate $g_0(\theta)$, but integrating out the unobserved variables \mathbf{Z} . In other words, it can be solved iteratively calculating

$$g_{i+1}(\theta) = (Tg_i)(\theta) \quad (\text{A.27})$$

where

$$Tf(\theta) = \int K(\theta, \phi)f(\phi)d\phi. \quad (\text{A.28})$$

Tanner and Wong proposed this Monte Carlo method called *data augmentation*, to perform the integration. This method consists in the iteration of two steps, motivated by the Posterior Identity.

The steps are respectively defined as

- I-step (imputation step), where one generates multiple values (indeed imputations) of \mathbf{Z} from the predictive distribution $p(\mathbf{Z}|\mathbf{Y})$;

- and P-step (posterior step), where the average of $p(\theta|\mathbf{Y}, \mathbf{Z})$ is computed over the imputations.

In the next page, Algorithm A.5 summarizes the step of the data augmentation method.

Algorithm A.5 Data augmentation

Given the current approximation g_i to $p(\theta|\mathbf{Y})$:

1. *I-step.* Generate a sample z^1, \dots, z^m of size m from the current approximation to the predictive density $p(\mathbf{Z}|\mathbf{Y})$. This can be accomplished applying the Method of Composition to the Predictive Identity;
 - (a) Sample θ_i^* from the current approximation $g_i(\theta)$;
 - (b) Generate the sample z^1, \dots, z^m from $p(\mathbf{Z}|\phi, \mathbf{Y})$ where $\phi = \theta_i^*$ is the value obtained in (a);
2. *P-step.* Use this sample to update the approximation to $p(\theta|\mathbf{Y})$ as the average of $p(\theta|z^{(i)}, \mathbf{Y})$

$$g_{i+1}(\theta) = m^{-1} \sum_{i=1}^m p(\theta|z^{(i)}, \mathbf{y}). \quad (\text{A.29})$$

Appendix B

Fault tree analysis

B.1 Introduction

In this appendix, after a brief introduction to the concept of risk assessment, we describe the fault tree analysis. This explanation will be useful for the understanding of the *Belief-network model for failure prediction* proposed in Chapter 6.

B.2 Risk assessment

Risk assessment or analysis consists in answering the following three questions:

- What can go wrong?
- How can it happen?
- What are the consequences?

This *risk triplet* was introduced and discussed by Kaplan and Garrick (1981).

Risk management and policy decisions rely on risk assessment, before the consequences of the threatening phenomenon are fully understood, in order to select the proper risk reduction measures within cost-effectiveness constraints (Paté-Cornell, 1996).

B.3 The Fault tree analysis

Fault tree analysis is a technique for the reconstruction of all the possible ways that can lead to the occurrence of a given and undesired event. The undesired event is resolved into its causes through the structure of a logic diagram, called a fault tree and represented in Figure B.1. For these reasons it can be defined as a deductive failure analysis and a backward looking analysis method.

The fault tree itself is a qualitative representation of the problem, that can be evaluated qualitatively. It graphically portrays all the various combinations of faults that can cause the undesired event.

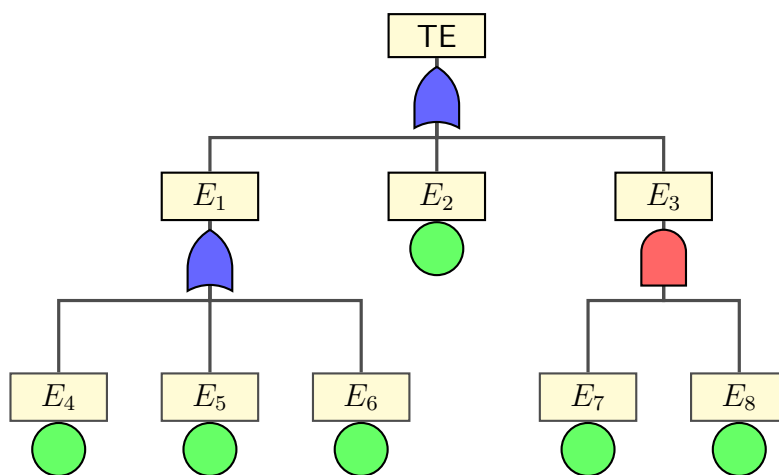


Fig. B.1: Fault tree.

The undesired event, that is usually a failure of the system, is called the top event (briefly TE), because it constitutes the top event in the diagram (see Figure B.1). A fault tree is tailored to its top event. As described in the handbook Vesely et al. (1981), the fault tree is made of different symbols that represent gates and events. The most commonly used are represented in Tables B.1 and B.2. We can distinguish the primary events, or basic events and the intermediate events. The primary events are the events that are not further developed on the fault tree, while the intermediate events are found at the output of a gate. Each gate is connected to an output event and more input events. The gates represent the relationship between the events and define the occurrence of the output event, or in other words it establishes if the output event occurs, given the occurrence of the input events.

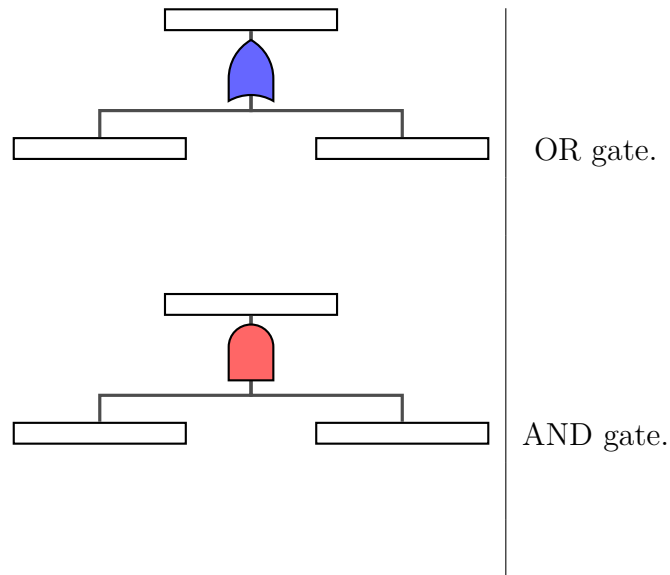


Table B.1: Gate symbols. OR gate = the output occurs if at least one of the inputs occur. AND gate = the output occurs if all of the inputs occur.

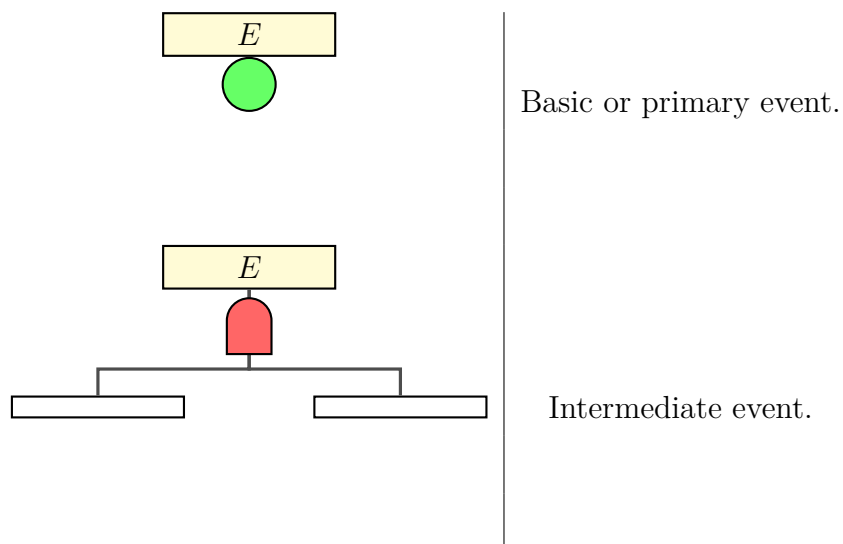


Table B.2: Event symbols. Basic or primary event = an event not further developed. Intermediate event = An event that occurs because of the events acting through a logic gate.

The fault tree analysis consists of two main steps:

1. Identification and classification of the events causing the undesired event and the connections that they hold between them, or logic interrelationships;
2. Construction of the fault tree.

Appendix C

Expert opinion

C.1 Introduction

Expert opinion plays an important role in the risk assessment model proposed in this thesis. In this appendix, the reader can find an introduction of this technique and the structure of the elicitation process. Then a multi criteria decision making tool, called Analytic Hierarchy process, is presented in its theoretical and applicative perspectives. The elicitation method developed for the assessment of the probability for a spacecraft to occur during the atmospheric re-entry, explained in Chapter 6, is inspired by this multi criteria decision making tool.

C.2 Expert opinion elicitation and analysis

C.2.1 Expert opinion

Expert opinion or *expert judgement* is data that is provided by people who have a good knowledge and experience of the field under study.

It is quite common to rely on expert opinion when other kinds of data (e.g. observations, measurements, simulations) are scarce, too costly or difficult to be collected or even unavailable. For instance experts can give estimates, based on their experience, on poorly understood phenomena, to integrate or interpret available data, to determine what is currently known, what is not known and what is worth investigating (Ouchi et al. (2004), Cooke and Goossens (2000), Bedford and Cooke (2001*b*)). One easy

example is when the expert is asked to express their opinion on the distribution of a random variable by the median and a symmetric interval around it.

Experts are a data source largely exploited in technical fields such as risk analysis, reliability engineering and science.

C.2.2 Elicitation and analysis

Elicitation is the process of data-gathering when the experts are the data-source.

The expression *expert opinion elicitation* refers to a set of specially designed methods of verbal or written communication. There is a vast theory about this subject, but we do not mean to explain it here. However, for a better understanding of the work behind this thesis, it is important to introduce the main steps to follow to structure the elicitation process:

- Identifying the needed information;
- Formulating the questions, taking into account that their phrasing can affect the expert and his answers;
- Selecting the experts;
- Designing and tailoring the elicitation to fit the experts and the way they think, considering the human tendency toward bias (well documented in literature, e.g. Schwarz and Vaughn (2002), Tversky and Kahneman (1974), Einhorn (1972), Morgan and Keith (1995));
- Eliciting and documenting expert opinion (answers and/or ancillary information);
- Analysing the results and assessing if they are valid data;
- Exploit them to refine the whole elicitation process when necessary;
- Combining expert judgements coming from various sources.

The person conducting the study can easily meet the following obstacles:

- The experts refrain from expressing a judgement under uncertainty;
- There is no agreement between the experts;

- The questions do not appear clear to the experts.

Experts knowledge improves as new information becomes available and consequently the expert opinion can and should legitimately change over time.

Data gathered by the expert opinion needs to be translated in quantitative terms, in order to make them exploitable. Expert opinion data have a multivariate nature and unfortunately there are no standard rules to analyse all of them. There exist a large literature of methods whose applications vary depending upon the design of the elicitation and upon the objective of the analysis. For the purposes of this study, we propose to rely on pairwise comparison methods to elicit expert opinion (Yager (1979), Torgerson (1958), Gulliksen (1959), Saaty (1977)).

In the next section C.3 we present the Analytic Hierarchy Process, a decision analytical tool also known as Saaty's method (Saaty, 1980), which inspired the elicitation technique applied in the risk assessment model proposed in Chapter 6.

C.3 Analytic Hierarchy Process

The Analytic Hierarchy Process, well known with the acronym AHP, is a multi criteria decision making method based on pairwise comparisons. It was developed by Thomas Saaty (Saaty, 1980), while he was directing research projects in the US Arms Control and Disarmament Agency. It is a method designed for the *resolution of choice problems in a multi-criteria environment* (Forman and Gass, 2001), but it has been widely applied in other fields too, as forecasting or resource allocations, over the years.

The AHP first structures the problem as a hierarchy. Next the decision maker provides paired comparisons of the alternatives. Finally the AHP converts these estimates to numerical values (weights or priorities or merits) and uses them to assign a score to each alternative. Some small inconsistency is taken into account because expert opinions are not always consistent.

The advantages that make this method appealing for use in expert opinion problems are:

- It is easy to use;
- It easily monitors the consistency of experts answers;

- It easily quantifies qualitative evaluations.

The idea supporting this method is that most individuals find it psychologically easier to formulate pairwise relative judgements than ranking directly n events (Budescu et al., 2016).

As in many other decision making approaches, the rank reversal can occur when applying the Analytic Hierarchy process. This means that the relative rankings of two alternatives could be reversed when an alternative is added or deleted, impairing the reliability of the results. The interested reader can find a comprehensive literature review about this topic in Wang and Luo (2009). The issue of rank reversal raised many discussions in the world of multi criteria decision making and especially concerning the Analytic Hierarchy process. The pioneer of this debate is Belton and Gear (1983).

Another important disadvantage in the application of the Analytic Hierarchy process is that the number of comparisons increases obviously with the number of events. For this reason, an accurate selection of a reasonable set of events to be compared (Budescu et al. (2016)) is strictly necessary.

C.3.1 Multi criteria decision making

When we select the best alternative from a set of available *alternatives* (or choices), and our selection is based on multiple *criteria* (or factors, objectives), we are solving a multi criteria decision making problem.

Suppose we fancy a pizza: pizza is our *goal*. Then we probably go to a pizza place and we read the menu. In order to satisfy our wish we need to make a choice among the available *alternatives*, which might be: margherita, capricciosa, pepperoni, veggie and four cheese. The best choice for us is dependent on our personal *criteria* (i.e. toppings, price, a strong or weak appetite, personal tastes, allergies). This means that, before starting to eat, we need to face an easy multi criteria decision making problem or briefly a MCDM problem.

The Analytic Hierarchy Process is one of the numerous MCDM methods.

C.3.2 Theoretical foundation - Principles and axioms

The AHP is based on three basic principles:

- *Decomposition*;
- *Comparative judgements*;
- *Hierarchic composition or synthesis of priorities*.

A human's way of thinking resolves complex problems partitioning it in smaller problems. The AHP emulates this behaviour through the *decomposition principle*: the complexity is structured into a hierarchy of clusters, subclusters, subsubclusters and so on.

The *principle of comparative judgement* is the key for the measurement. It is applied to formulate pairwise comparisons of all combinations of elements in a cluster with respect to the parent of the cluster. The pairwise comparisons provide the local priorities of the single elements forming the cluster with respect to their parent.

Finally the *hierarchic composition or synthesis of priorities* principle allows the AHP to produce global priorities throughout the hierarchy, for representing the overall outcome.

Furthermore, the AHP is based on the following four axioms (Saaty (1986)).

Definition C.3.1 *Reciprocal axiom.* The reciprocal axiom states that if $P_C(A, B)$ is a paired comparison of elements A and B with respect to their parent element C , representing how many times more the element A possesses a property than does element B , then $P_C(A, B) = 1/P_C(B, A)$. For example, if A is 5 times larger than B , then B is one-fifth as large as A .

Definition C.3.2 *Homogeneity axiom.* The homogeneity axiom states that the elements being compared should not differ by too much in the property being compared.

Definition C.3.3 *Synthesis axiom.* The synthesis axiom states that judgements about or the priorities of the elements in a hierarchy do not depend on lower level elements.

Definition C.3.4 *Expectation axiom.* The expectation axiom states that individuals who have reasons for their beliefs should make sure that their ideas are adequately represented for the outcome to match these expectations.

The last axiom, also known as the fourth axiom, was introduced later than the others by Saaty, in response to some academic debates (see Section 4.4.1).

C.3.3 The AHP - Step by step

The analytical process of the AHP can be explained in the following steps:

1. *Hierarchical decomposition of the decision.* The decision problem is structured as a hierarchy of clusters: goal, criteria, sub-criteria and alternatives. Breaking the problem down into its component is the most creative and important part of the decision-making process. Figure C.1 shows a generic hierarchic structure. In order to fulfill the *homogeneity axiom*, the elements need to be grouped in such a way as to make comparisons feasible.

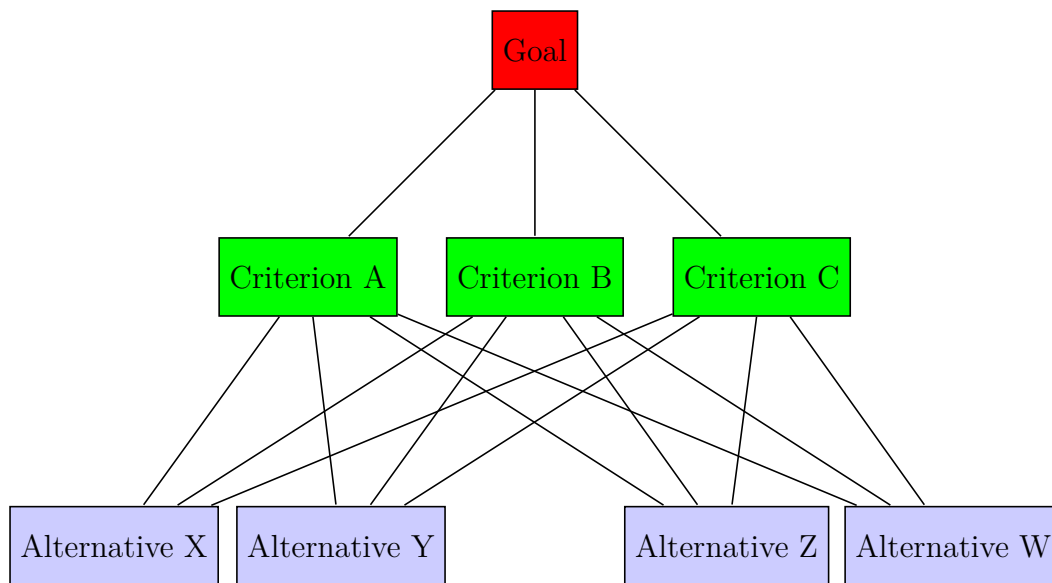


Fig. C.1: This figure shows an example of the AHP hierarchical structure. There are 3 levels: the root or level 0 represents the goal, the level 1 the criteria and the level 2 the alternative choices. Other levels of sub criteria and sub sub criteria could be added. The lines show the relationships between the criteria, the alternatives and the goal. The comparison matrix of level 1 has size 3 by 3, because it contains the pairwise comparisons of the 3 criteria with respect to the goal. Since each alternative is connected to each criterion and there are 3 criteria for 4 alternatives, the comparison matrices at level 2 are 3 and their size is 4 by 4. Hence the alternatives are pair-wise compared with respect to each criterion.

2. *Data collection through pairwise comparisons.* Let us explain with an easy example what a paired comparison is. When we have two pizzas, a pepperoni and a four cheese, and we wonder which one we like better than the other, and how

much we like it, we are carrying out a paired comparison. We can express our preference using a relative scale to measure how much we prefer one compared to the other: equal, marginally favours, strongly favours, very strong favours, extremely favours.

Data are collected from experts (or decision makers) following the hierarchic structure. Experts are asked to compare pairwise every single element with the elements belonging to the same cluster and rate their comparisons. It seems more appropriate to ask experts to provide their judgements in a linguistic shape rather than asking directly a quantitative evaluation. Next the linguistic judgement can be translated in a numerical grade. The fundamental scale originally proposed by Saaty is reported in Table C.1.

As stated by the *reciprocal axiom* if the alternative X is extremely more important than Y, with respect to the criterion A, and is rated at 9, then the alternative Y must be extremely less important than X and is valued at $\frac{1}{9}$.

Decision makers carry out two types of pairwise comparisons in the AHP: the first one is between pairs of factors, while the second one is between pairs of choices. It is important to note that the comparisons are made with respect to the contribution of the lower-level items to the upper-level one, according to the *synthesis axiom*.

Table C.1: Saaty's scale.

Option	Numerical value(s)
Equal	1
Marginally strong	3
Strong	5
Very strong	7
Extremely strong	9
Intermediate values	2,4,6,8

3. *Pairwise matrix.* The pairwise comparisons of a cluster of n elements are arranged in a square matrix \mathbf{Q} of size n by n . The comparison of the item i with the item j results in a grade in the (i, j) position of the matrix and its reciprocal in the

position (j, i) . It clearly follows that the matrix has ones on the main diagonal as the $i - th$ element is compared with itself. Then the number of the required pairwise judgements is $n(n-1)/2$. For example the factor in the i th row is better than the factor in the j th column if the value of element (i, j) is greater than 1; otherwise the factor in the j th column is better than in the i th row. It is suggested to compare no more than nine elements at a time, within the same matrix (Saaty, 1980).

4. *Weights assessment - Eigenvector method.* There are various methods for deriving the weights of the n elements w_1, \dots, w_n from the matrix of pairwise comparisons ($\mathbf{Q} = [q_{ij}]$). The eigenvector method, here illustrated, was initially proposed by Gulliksen (1959) and they refined by Saaty and colleagues (Saaty and Vargas (1980), Saaty (1980)).

The pairwise comparison matrix can be expressed in terms of the weights $\mathbf{w} = \{w_1, \dots, w_n\}$. We assume that $\sum_{i=1}^n w_i = 1$.

$$\mathbf{Q} = \begin{pmatrix} q_{11} & q_{12} & \cdots & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & \cdots & q_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ q_{n1} & q_{n2} & \cdots & \cdots & q_{nn} \end{pmatrix} = \begin{pmatrix} 1 & \frac{w_1}{w_2} & \frac{w_1}{w_3} & \cdots & \frac{w_1}{w_n} \\ \frac{w_2}{w_1} & 1 & \frac{w_2}{w_3} & \cdots & \frac{w_2}{w_n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{w_n}{w_1} & \frac{w_n}{w_2} & \frac{w_n}{w_3} & \cdots & 1 \end{pmatrix} \quad (\text{C.1})$$

Note that

$$q_{ij} = \frac{w_i}{w_j} = \frac{w_i}{w_k} \frac{w_k}{w_j} = w_{ik} w_{kj} \quad (\text{C.2})$$

When this condition C.2 holds, the matrix \mathbf{Q} is termed consistent. Given the ratios $q_{ij} = \frac{w_i}{w_j}$, we can compute the weights $\mathbf{w} = \{w_1, \dots, w_n\}$ by solving for \mathbf{w} the equivalence $\mathbf{Q}\mathbf{w} = n\mathbf{w}$:

$$\begin{pmatrix} 1 & \frac{w_1}{w_2} & \frac{w_1}{w_3} & \cdots & \frac{w_1}{w_n} \\ \frac{w_2}{w_1} & 1 & \frac{w_2}{w_3} & \cdots & \frac{w_2}{w_n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{w_n}{w_1} & \frac{w_n}{w_2} & \frac{w_n}{w_3} & \cdots & 1 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} nw_1 \\ nw_2 \\ \vdots \\ nw_n \end{pmatrix}. \quad (\text{C.3})$$

It is easy to recognize that this is an eigenvalue problem. It can be proved that \mathbf{w} is the normalized right eigenvector of \mathbf{Q} corresponding to the maximum eigenvalue λ_{max} ¹. The maximal eigenvalue is $\lambda_{max} = n$, if C.2 holds.

5. *Consistency check.* AHP tolerates and monitor human judgements inconsistency. In most cases, in the matrix \mathbf{Q} of the pairwise comparisons the consistency property does not hold and this can be checked by computing the consistency index CI

$$CI = \frac{\lambda_{max} - n}{n - 1}. \quad (C.4)$$

This index provides a measure of consistency of experts evaluations. The closer λ_{max} is to n , the more consistent the expert opinion.

Saaty proposed to use this index by comparing it with a random consistency index RI . He randomly generated 500 reciprocal matrices (Teknomo, 2014) using the Saaty's scale and computed the average random consistency index RI for different values of n , as showed in Table C.2.

Table C.2: Random consistency index

n	1	2	3	4	5	6	7	8	9	10
RI	0	0	0.58	0.9	1.12	1.24	1.32	1.41	1.45	1.49

Then he defined the consistency ratio CR and he suggested it should be less than 0.1

$$CR = \frac{CI}{RI}. \quad (C.5)$$

6. *Synthesis.* After carrying out the pairwise comparisons in each cluster, the results must be aggregated to get a global rating for each alternative.

C.3.4 Weights assessment - Geometric mean approach

The eigenvector method was criticised by Crawford and Williams (1985) because it is not invariant under transposition (the left eigenvector is not the reciprocal of the right eigenvector). Crawford and Williams (1985) proposed an alternative method, even

¹Perron-Frobenius theorem asserts that a real square matrix with positive entries has a unique largest real eigenvalue.

easier to apply, called the geometric mean approach. The weights are computed by the normalized geometric means of the rows of the pairwise comparisons matrix \mathbf{Q} :

$$w_i = \frac{m_i}{\sum_{i=1}^n m_i} \quad \forall i = 1, \dots, n \quad (\text{C.6})$$

where the geometric mean m_i is equal to:

$$m_i = \left(\prod_{j=1}^n q_{ij} \right)^{\frac{1}{n}}. \quad (\text{C.7})$$

Budescu et al. (1986) compared the geometric mean approach with the eigenvalue method and drew the conclusion that the results are very similar. In some circumstances, the rank order is better preserved relying on the geometric mean. This approach is used in the expert elicitation method proposed in Chapter 6.

Appendix D

The stick breaking process

D.1 Introduction

The stick breaking process inspired the way we proposed to construct the distribution for the modelling of the fragmentation process, detailed in Chapter 7.

The stick breaking process is one of the views of the Dirichlet process. For this reason, we start this appendix defining the Dirichlet distribution and the Dirichlet process, then we explain what the stick breaking process is, for a better understanding of the proposed Fragmentation model.

D.2 Dirichlet process

The Dirichlet distribution of order n is defined over the space of an n -dimensional simplex

$$\Delta_n := \left\{ \mathbf{x} \in \mathbb{R}^n : \sum_i x_i = 1, x_i \geq 0 \right\}$$

The distribution is parametrised by n positive parameters $\{\alpha_i\}_{i=1}^n (\alpha_i > 0)$. These parameters control the variance of the random variables x_i .

Definition D.2.1 *Dirichlet distribution (Zhang, 2008)*

A random variable $\mathbf{x} \in \Delta_n$ is said to have a Dirichlet distribution if its probability density function is given by:

$$p(x_1, \dots, x_n) = \frac{1}{B(\boldsymbol{\alpha})} \prod_{i=1}^n x_i^{\alpha_i - 1}$$

and it is denoted as $\mathbf{x} \sim \text{Dir}(\alpha_1, \dots, \alpha_n)$ or simply $\mathbf{x} \sim \text{Dir}(\boldsymbol{\alpha})$. The normalizing constant is the multinomial Beta function, which can be expressed in terms of the Gamma function

$$B(\boldsymbol{\alpha}) = \frac{\prod_{i=1}^n \Gamma(\alpha_i)}{\Gamma(\sum_{i=1}^n \alpha_i)} \quad \boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n) \quad (\text{D.1})$$

If $(x_1, \dots, x_n) \sim \text{Dir}(\alpha_1, \dots, \alpha_n)$, then the expected value is defined

$$\mathbb{E}[(x_1, \dots, x_n)] = \left(\frac{\alpha_1}{s}, \dots, \frac{\alpha_n}{s} \right). \quad s := \sum_i \alpha_i$$

The Dirichlet distribution can be seen as a *distribution over distributions*, because the vector of values that it generates are a probability vector e.g. all values non negative and sum to 1.

An important, and crucial for us, property of this distribution is the decimation property.

Proposition D.2.1 *Decimation property* If $(x_1, \dots, x_n) \sim \text{Dir}(\alpha_1, \dots, \alpha_n)$ and $(\tau_1, \tau_2) \sim \text{Dir}(\alpha_1\beta_1, \alpha_1\beta_2)$ where $\beta_1 + \beta_2 = 1$, then

$$(x_1\tau_1, x_1\tau_2, \dots, x_n) \sim \text{Dir}(\alpha_1\beta_1, \alpha_1\beta_2, \dots, \alpha_n)$$

The Beta distribution is a special case of the Dirichlet distribution in two dimensions.

Definition D.2.2 *Beta distribution*

A random variable $\theta \in (0, 1)$ is said to have a Beta distribution if its probability density function is given by

$$p(\theta|\alpha, \beta) = \frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\mathbf{B}(\alpha, \beta)}, \quad 0 \leq \theta \leq 1 \quad (\text{D.2})$$

where $\alpha, \beta > 0$ are the shape parameters. The normalizing constant $\mathbf{B}(\cdot)$ is the Beta function, which can be expressed in terms of the Gamma function

$$\mathbf{B}(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)} \quad \alpha, \beta > 0 \quad (\text{D.3})$$

The Dirichlet process can be considered as the infinite-dimensional generalization of the Dirichlet distribution. Similarly to the Dirichlet distribution, it is also a *distribution over distributions* or, in other words, its domain is a set of probability distributions. The Dirichlet process $DP(\alpha, G_0)$ is parameterized by the concentration parameter α

and the base distribution G_0 . The random probability measure G with the same support of G_0 is the Dirichlet process distributed $G \sim DP(\alpha, G_0)$.

The Dirichlet process provided a significant contribution to the development of the Bayesian nonparametric methods, when introduced by Ferguson (1973). Then Sethuraman (1994) proposed a method for its construction and showed formally the relationship with the Dirichlet process. This method, called stick breaking method, is detailed in the next section.

D.3 The stick breaking construction

Suppose we have a stick of length 1. The so-called stick breaking process, introduced by Sethuraman (1994), is defined as follows:

1. We randomly break the stick into two parts, one left and one right, with proportions ν_1 and $1 - \nu_1$. We keep the left part of length $\pi_1 = \nu_1$.
2. We then take the right part of length $1 - \nu_1$. We randomly break it into two parts, one left and one right, with proportions ν_2 and $1 - \nu_2$. Again we keep the left part of length $\pi_2 = (1 - \nu_1)\nu_2$.
3. We then take the right part of length $(1 - \nu_1)(1 - \nu_2)$. We apply the same process with proportions ν_3 and $1 - \nu_3$. Then we have three left pieces of lengths $\pi_1 = \nu_1$, $\pi_2 = (1 - \nu_1)\nu_2$, $\pi_3 = (1 - \nu_1)(1 - \nu_2)\nu_3$.
4. We can continue this process to randomly partition the stick in pieces of lengths (π_1, π_2, \dots)

By the decimation property, we can see that the proportions (π_1, \dots, π_n) are random variables with a Dirichlet distribution for any finite number of breaks, if the distribution of each ν_i is beta.

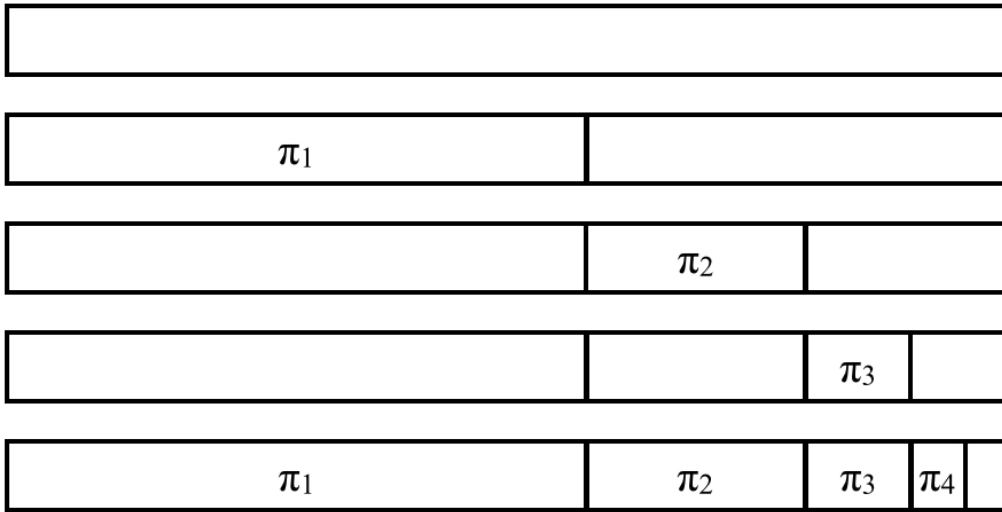


Fig. D.1: Representation of the first four steps of the Sethuraman stick breaking process.

Then this process, shown in figure D.1, can be formalized in the definition of the Griffiths-Engen-McCloskey (GEM) distribution (Pitman, 2002):

Definition D.3.1 For $0 \leq a < 1$ and $b > -a$, suppose that independent random variables ν_k are such that ν_k has Beta($1 - a, b + ka$) distribution.

Let

$$\pi_i = \nu_i \prod_{i'=1}^{i-1} (1 - \nu_{i'})$$

define the GEM distribution with parameters a, b , to be the resultant distribution of (π_1, π_2, \dots) .

The stick breaking process is the construction of a distribution over infinite partitions of the unit interval.

Appendix E

Expert Surveys based on pairwise comparisons

E.1 Burst of a battery

Assume you are analysing the causes of the fragmentation/explosion of a spacecraft during the atmospheric re-entry and in particular if the explosion of a battery can be considered the triggering event.

Information you have about the spacecraft:

- There are Nichel-Cadmium batteries
- Age of the spacecraft
- Protection mechanism

Information you have about the re-entry:

- Trajectory
- Altitude of the explosion
- Results from an observation campaign

Information (or forecasts) you have about the conditions of the battery before the re-entry:

- Temperature

- Pressure

We consider the events in E.1 that can lead to the explosion of a battery during the atmospheric re-entry. Assume there are 10 re-entries exactly like that one you are analysing:

- What is the minimum number of times do you think each of the 1-8 events could occur?
- What is the maximum number of times do you think each of the 1-8 events could occur?
- Could you please answer this question at least for one of them?

		/10	/10
1	Cell degradation		
2	Exothermal chemical reactions		
3	Short-circuit		
4	Overcharge		
5	Over discharge		
6	Over pressure		
7	Corrosion		
8	Over temperature		

Table E.1

Please compare each of the pairs of events listed below by answering the following question:

Was event A more likely to occur than event B?

Please mark them with an index from 1 to 9 following Table E.2.

Index	Meaning
1	A and B were equally probable
3	A was moderately more probable than B
5	A was strongly more probable than B
7	A was very strong more probable than B
9	A was absolutely more probable than B
2,4,6,8	Intermediate values

Table E.2

Event A	Event B	Index
Cell degradation	Exothermal chemical reactions	X
Exothermal chemical reactions		
short-circuit	Exothermal chemical reactions	
overcharge	Exothermal chemical reactions	
overdischarge	Exothermal chemical reactions	
overpressure	Exothermal chemical reactions	
corrosion	Exothermal chemical reactions	
over temperature	Exothermal chemical reactions	

Table E.3

Event A	Event B	Index
Cell degradation	Short-circuit	X
Exothermal chemical reactions	Short-circuit	
short-circuit		
overcharge	Short-circuit	
overdischarge	Short-circuit	
overpressure	Short-circuit	
corrosion	Short-circuit	
over temperature	Short-circuit	

Table E.4

Event A	Event B	Index
Cell degradation	Short-circuit	X
Exothermal chemical reactions	Short-circuit	
short-circuit		
overcharge	Short-circuit	
overdischarge	Short-circuit	
overpressure	Short-circuit	
corrosion	Short-circuit	
over temperature	Short-circuit	

Table E.5

Event A	Event B	Index
Cell degradation	Overcharge	X
Exothermal chemical reactions	Overcharge	
Short-circuit	Overcharge	
Overcharge		
Overdischarge	Overcharge	
Overpressure	Overcharge	
Corrosion	Overcharge	
Over temperature	Overcharge	

Table E.6

Event A	Event B	Index
Cell degradation	Overdischarge	X
Exothermal chemical reactions	Overdischarge	
Short-circuit	Overdischarge	
Overcharge	Overdischarge	
Overdischarge		
Overpressure	Overdischarge	
Corrosion	Overdischarge	
Over temperature	Overdischarge	

Table E.7

Event A	Event B	Index
Cell degradation	Overpressure	X
Exothermal chemical reactions	Overpressure	
Short-circuit	Overpressure	
Overcharge	Overpressure	
Overdischarge	Overpressure	
Overpressure		
Corrosion	Overpressure	
Over temperature	Overpressure	

Table E.8

Event A	Event B	Index
Cell degradation	Corrosion	
Exothermal chemical reactions	Corrosion	
Short-circuit	Corrosion	
Overcharge	Corrosion	
Overdischarge	Corrosion	
Overpressure	Corrosion	
Corrosion		X
Over temperature	Corrosion	

Table E.9

Event A	Event B	Index
Cell degradation	Over temperature	
Exothermal chemical reactions	Over temperature	
Short-circuit	Over temperature	
Overcharge	Over temperature	
Overdischarge	Over temperature	
Overpressure	Over temperature	
Corrosion	Over temperature	
Over temperature		X

Table E.10

Please consider now the hypothetical upcoming re-entry of a spacecraft with similar characteristics.

Please suppose I ask you to answer the following question for each event listed in Table E.12, by expressing an index from 1 to 9 as described in Table E.11:

Is this event more likely to occur in the re-entry B than in the re-entry A?

Index	Meaning
1	This event is equally probable to occur in both the re-entries A and B
3	This event is moderately more probable to occur in re-entry B
5	This event is strongly more probable to occur in re-entry B
7	This event is very strong more probable to occur in re-entry B
9	This event is absolutely more probable to occur in re-entry B
2,4,6,8	Intermediate values

Table E.11

Re-entry A	Re-entry B	Index
Cell degradation	Cell degradation	
Exothermic chemical reactions	Exothermic chemical reaction	
Short-circuit	Short-circuit	
Overcharge	Overcharge	
Overdischarge	Overdischarge	
Overpressure	Overpressure	
Corrosion	Corrosion	
Over temperature	Over temperature	

Table E.12

- Which characteristics do you need to know about the upcoming re-entry?
- Could you please answer these questions comparing the re-entry of ATV1 with the re-entry of ATV5?
- Would you add other triggering events to the list?
- Would you need other informations about the environment conditions? If yes, which ones?
- And about the spacecraft?
- Is there something you want to propose to improve this survey?

E.2 Chemical reaction propellant + air

Assume you are analysing the causes of the fragmentation/explosion of a spacecraft during the atmospheric re-entry and in particular if the *Chemical reaction propellant + air* can be considered the triggering event.

Information you have about the spacecraft:

- Architecture of chemical propulsion system
- Reliability tests of the valves (if available)
- Location of the valves
- Material of the membrane which separates oxidizer and fuel tanks
- Thermal conductivity from spacecraft structure to the tanks
- Material of the wall tanks (titanium, carbon fiber wrapped, steel)
- Shape of the tanks (spherical or cylindrical with domes)
- Location and mounting direction of the tanks
- Maximum Expected Operating Pressure of tanks
- Age of spacecraft

Information you have about the re-entry:

- Trajectory
- Predictions about the altitude of the explosion with uncertainty range
- Predictions about temperature and external pressure at that altitude
- Deterministic simulations of the spacecraft fragmentation before the altitude where the explosion is expected to occur
- Results from an observation campaign

Information (or forecasts) you have about the conditions of the propulsion system at EOL (End of Life):

- Filling percentage
- Thickness of wall tanks (after material degradation)

We consider the events in Table E.13 that can lead to the *Chemical reaction propellant + air* during the atmospheric re-entry:

Assume there are 10 re-entries exactly like that one you are analysing:

- What is the minimum number of times do you think each of the 1-2 events could occur?
- What is the maximum number of times do you think each of the 1-2 events could occur?
- Could you please answer this question at least for one of them?

		/10	/10
1	Sudden release of propellant (caused by: burst of a pressure vessel)		
2	Slow release of propellant (caused by: valve leakage or tank destruction or pipe rupture)		

Table E.13

Please compare each of the pairs of events listed below by answering the following question:

Was event A more likely to occur than event B?

Please mark them with an index from 1 to 9 following Table E.14.

Index	Meaning
1	A and B were equally probable
3	A was moderately more probable than B
5	A was strongly more probable than B
7	A was very strong more probable than B
9	A was absolutely more probable than B
2,4,6,8	Intermediate values

Table E.14

Event A	Event B	Index
Sudden release of propellant	Slow release of propellant	

Table E.15

Please consider now the hypothetical upcoming re-entry of a spacecraft with similar characteristics.

Please suppose I ask you to answer the following question for each event listed in Table E.17, by expressing an index from 1 to 9 as described in Table E.16:

Is this event more likely to occur in the re-entry B than in the re-entry A?

Index	Meaning
1	This event is equally probable to occur in both the re-entries A and B
3	This event is moderately more probable to occur in re-entry B
5	This event is strongly more probable to occur in re-entry B
7	This event is very strong more probable to occur in re-entry B
9	This event is absolutely more probable to occur in re-entry B
2,4,6,8	Intermediate values

Table E.16

Re-entry A	Re-entry B	Index
Sudden release of propellant	Sudden release of propellant	
Slow release of propellant	Slow release of propellant	

Table E.17

- Which characteristics do you need to know about the upcoming re-entry?
- Could you please answer these questions comparing the re-entry of ATV1 with the re-entry of ATV5? If not, could you please answer these questions comparing the re-entries of two spacecraft you worked for?
- Do you know if there are deterministic simulations that could help you in providing these (subjective) judgements?

- Would you add other triggering events to the list?
- Would you need other informations about the environment conditions? If yes, which ones?
- And about the spacecraft?
- Is there something you want to propose to improve this survey?

E.3 List of Interviewed experts divided by topics

- Guidance, Navigation and Control: Irene Huertas;
- Propulsion: Christopher Hunter, Luca Ferracina;
- Propellants: Nick Goody;
- Materials: Tommaso Ghidini;
- Structure: Gerben Sinnema, Tiziana Cardone, Roger Walker;
- Thermal: Silvio Dolce, Giovanni Chirulli, Heiko Ritter;
- Energy storage and power: Evelyne Simon, Francois Bausier;
- ATV-1 Re-entry campaign: Stephan Loehle, Maite Trujillo ,Neil Murray, Claudio Damasio, Mark Beks;
- Deterministic re-entry analysis tools: Sergio Ventura;
- Experimental studies about spacecraft design for demise: Francois Bausier.

Appendix F

PhD and NPI Timeline

F.1 Summary of the coursework and preparatory phase

F.1.1 First year

The study plan of the first year consisted in the following modules:

- A Research Methods course for 5 ECTS (European credit transfer system)
- 4 full-time 1-week courses in Statistics through the APTS 2012 (Academy for PhD Training in Statistics) programme in the UK
- 2 2-semester modules in Statistical Inference and Applied Linear Statistical Models for 20 ECTS
- A parallel computing course
- Summer school Alpbach 2012 - Exploration of the Giant planets and their systems

The research methods and APTS courses included assignments and exams.

The research method course was aimed to develop an awareness of the nature of scientific research and the methodologies applicable to PhD research in Computer Science and Statistics, plus written and oral communication skills.

The Academy for PhD Training in Statistics is a collaboration between major UK and Irish statistics research groups to organise courses for first-year PhD students in statistics and applied probability nationally.

It follows a description of the content of the APTS 2012 modules:

- Week 1 - From January 9th to January 13th 2012 - Cambridge

Statistical Computing

Topics:

- Finite-precision arithmetic; related types of error and stability.
- Numerical linear algebra (with statistical applications): basic computational efficiency, Choleski, QR, stability (e.g. Normal/Choleski vs QR for LS), eigen and singular value decompositions. Standard libraries.
- Optimization: Newton-type methods; other deterministic methods; stochastic methods; using methods effectively in practice; what to use when.
- Differentiation and integration by computer: finite differencing; automatic differentiation; quadrature methods; stochastic integration.
- Basics of stochastic simulation.
- Other types of problem (e.g. sorting and matching); the pervasiveness of efficiency and stability issues.

Statistical Inference

Topics:

- Role of formal inference, nature of probability, frequentist and Bayesian approaches.
- Role of sufficiency; role of Neyman-Pearson theory; relation between significance tests and confidence limits.
- Maximum likelihood and associated issues; properties in 'standard' situations, and in some more difficult cases.
- Exponential-family models.
- Other approaches (e.g., estimating equations, pseudo-likelihoods).

- Week 2 - From April 16th to April 20th 2012 - Nottingham

Statistical Modelling

Topics:

- Missing data and latent variables.
- Principles and practice of model selection.
- Random-effects/hierarchical/mixed models.
- Semi parametric models and smoothing.
- The role of conditional independence in modelling. Introduction to graphical models.

Statistical Asymptotics

Topics:

- Multivariate central limit theorem, (a gentle introduction to) the continuous mapping theorem, the delta method.
 - Stochastic asymptotic expansion.
 - Likelihood asymptotics (including asymptotic properties of MLEs).
 - Asymptotic normality of posterior distributions (parametric case).
 - Laplace’s approximation (univariate and multivariate).
 - Introduction to Edgeworth expansions and saddlepoint density approximations (via tilting).
 - Saddlepoint approximations to tail probabilities.
- Week 3 - From July 2nd to July 6th 2012 - Warwick

Applied Stochastic Processes

Topics:

- Reversibility of Markov chains in both discrete and continuous time, computation of equilibrium distributions for such chains, application to important examples.
- Discrete time martingales, examples, application, super- martingales, sub- martingales.
- Stopping times, statements and applications of optional stopping theorem, martingale convergence theorem.

- Recurrence and rates of convergence for Markov chains, application to important examples.
- Statements and applications of Foster-Lyapunov criteria, viewed using the language of martingales.
- Statistical applications and relevance.

Computer Intensive Statistics

Topics:

- Overview of simulation-based inference; Monte Carlo testing.
 - Basic theory of bootstrap methods; practical considerations; limitations.
 - Basic theory of MCMC; types of MCMC samplers; assessment of convergence/mixing; other practical considerations; case studies.
 - Strategies for dealing with large datasets: use of database management systems, multipass algorithms, subsampling, distributed computing. A case study, e.g. generalized linear models.
- Week 4 - From September 3rd to September 7th - Glasgow

Spatial and Longitudinal Data Analysis

Topics:

- Introduction: motivating examples; the fundamental problem- analysing dependent data.
- Longitudinal data: linear Gaussian models; conditional and marginal models; why longitudinal and time series data are not the same thing.
- Continuous spatial variation: stationary Gaussian processes; variogram estimation; likelihood-based estimation; spatial prediction.
- Discrete spatial variation: Markov random field models.
- Spatial point patterns: exploratory analysis; Cox processes and the link to continuous spatial variation; pairwise interaction processes and the link to discrete spatial variation.

- Spatio-temporal modelling: spatial time series; spatio-temporal point processes.
- Conclusion: review of available software (as preparation for mini- project); connections-spatial and longitudinal data analysis as two sides of the same coin.

Nonparametric Smoothing

Topics:

- Kernel and spline approaches to smoothing.
- Determination of degree of smoothing (bandwidth, penalty, effective degrees of freedom).
- Density estimation.
- Nonparametric regression.
- Applications, e.g., covariate measurement error, generalized additive models.

F.1.2 Second year

During the second year the candidate attended the EPSRC/RSS (Engineering and Physical Science Research Council/Royal Statistical Society) Graduate Training Programme 2013/14 from the 22nd July to 26th July 2013 in the School of Mathematics and Statistics, Newcastle University. This training programme is aimed at PhD students in their second year and consists in two intensive course modules concerning Highly Structured Stochastic Systems:

- Bayesian Computation with INLA (Integrated nested Laplace approximation).

INLA is a new approach to statistical inference for latent Gaussian Markov random field (GMRF), a good alternative to MCMC methods. The Gaussian Markov random fields are multivariate Gaussian random variables having a Markov property described by an undirected graph. A Markov random field is similar to a Bayesian network in its representation of dependencies; the differences being that Bayesian networks are directed and acyclic, whereas Markov networks are undirected and may be cyclic. For instance it can be applied to image processing.

- Graphical Models for High Dimensional Data (undirected graphs and directed acyclic graphs)

F.2 Important dates

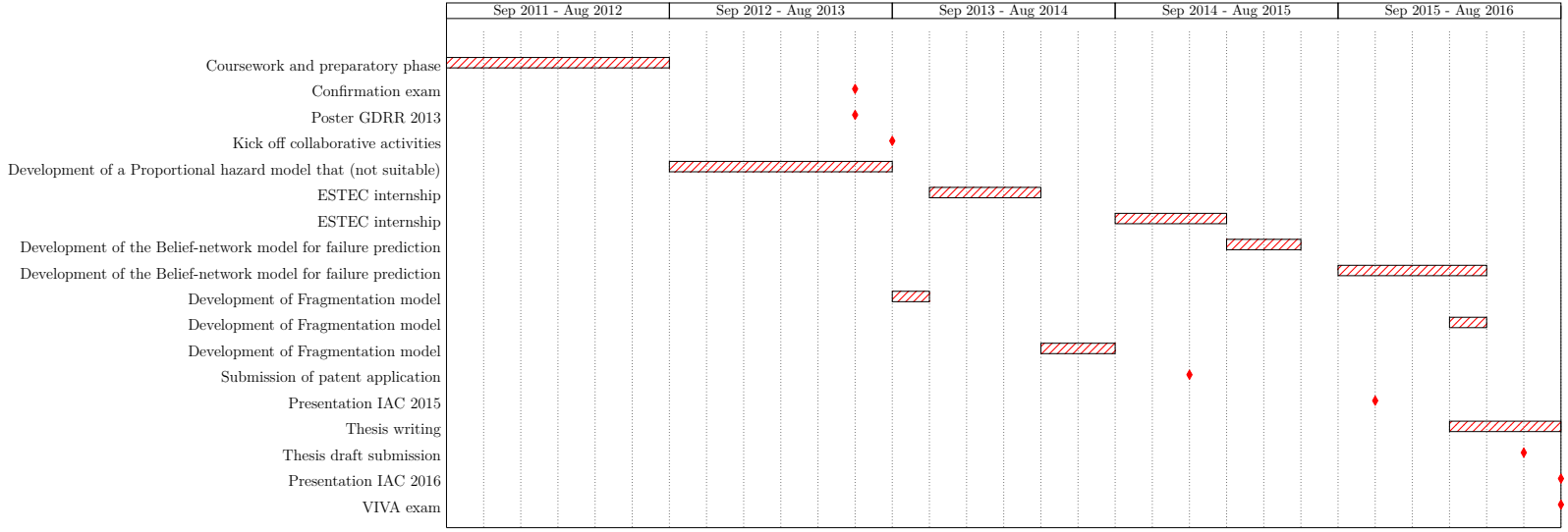
- Confirmation exam: 27th June 2013
- The NPI contract was signed on 18th July 2013
- Kick off collaborative activities: 6th August 2013
- ESTEC internship: 15th October 2013 - 30th April 2014
- ESTEC internship: 1st September 2014 - 28 February 2015
- VIVA exam: 10th October 2016

F.3 Conferences

- Participation at CASI (Conference on Applied Statistics in Ireland) 2012
- Participation at GDRR (Symposium on Games and Decisions in Reliability and Risk) 2013
- Participation at ATV 5 Instrumentation and Requirements for Re-entry Observation Campaign Workshop
- Participation at 7th IAASS (International Association for the Advancement of Space Safety) Conference *Space Safety is No Accident*
- Presentation at International Astronautical Congress 2015
- Presentation at International Astronautical Congress 2016

F.4 Other Summer Schools

- International Space University Space Studies Program 2015 (June-August 2015)
- Data assimilation from Earth observation Summer School 2016



Appendix G

Code Manual

G.1 Introduction

This appendix provides the instructions to run the code developed in order to get the results reported in this thesis.

G.2 Getting Started

- Download and install R from <https://www.r-project.org>. R is a free software environment for statistical computing and graphics. It compiles and runs on a wide variety of UNIX platforms, Windows and MacOS.
- Set the working directory to ("...path to.../NPI activity Stochastic Modelling of Atmospheric Re-entry Highly Energetic Break-up Events - Code"): *Misc* → *Change working directory....*
- Install the following packages and their dependencies:
 - `igraph`;
 - `MASS`;
 - `MCMCpack`;
 - `Rlab`;
 - `psych`.

Package and Data → *Package installer* Tick the option *Install dependencies*.

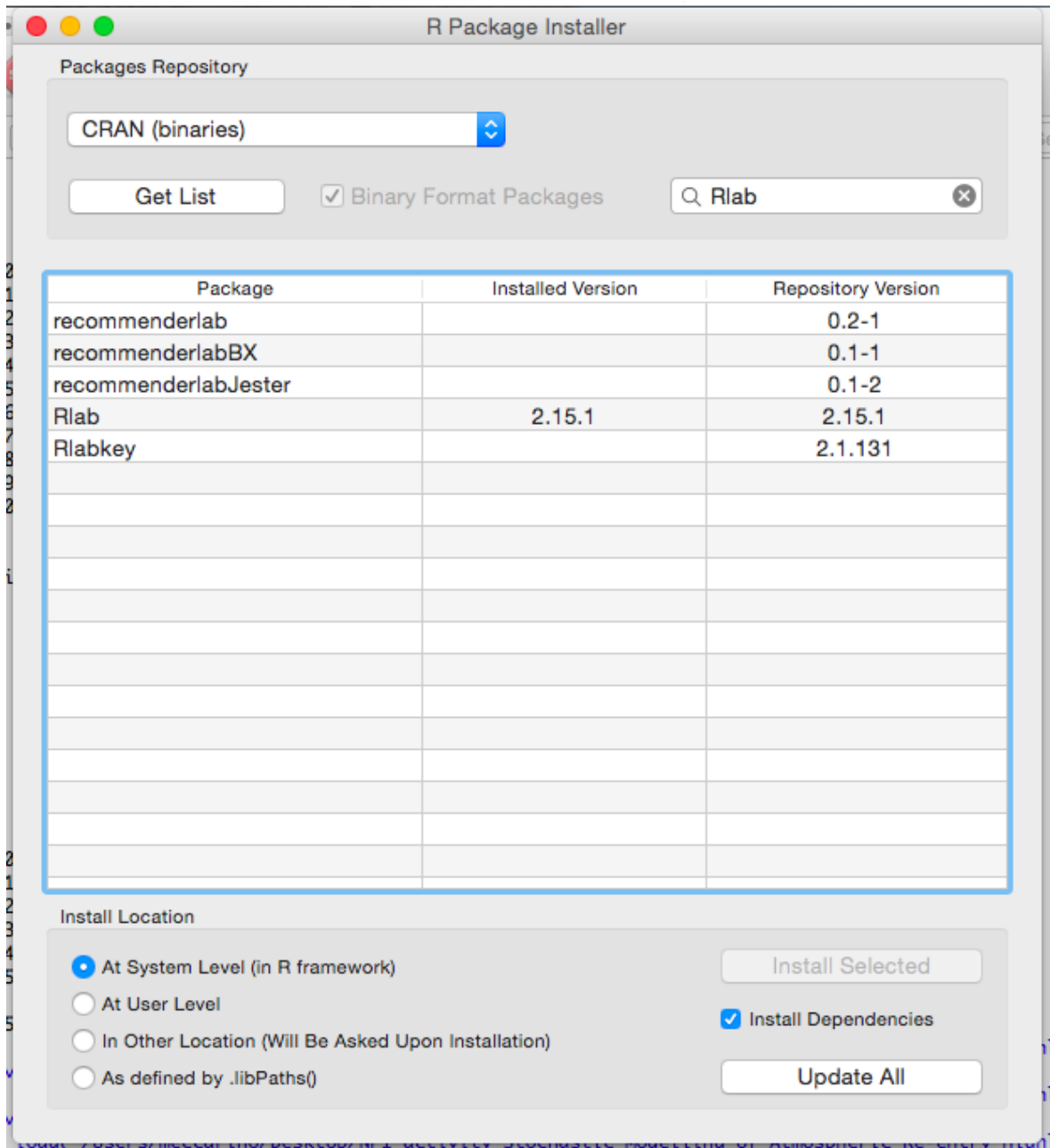


Fig. G.1: Package installer

G.3 Fragmentation model

Files:

- Fragmentation model main.R;
- Tree-structure generator.R;

- Generate synthetic data.R;
- Gibbs sampler for the inference.R;
- Masses prediction.R;
- Test of fragmentation model with real data.R.

Instructions:

- Run *Fragmentation model main.R* selecting it from *File* → *Source file....*

Output:

- Expected values of the masses of fragments and related confidence interval, given synthetic data.

Remarks:

- User inputs can be modified at the beginning of the routine *Fragmentation model main.R*;
- The average execution time of this routine is 4 minutes;
- The routine *Test of fragmentation model with real data.R* provides the expected values of the masses of fragments and related confidence interval, given the set of real data coming from the ATV 1 re-entry observation campaign.

G.4 Belief-network model for failure prediction

File:

- AHP model main.R

Instructions:

- Run *AHP model main.R* selecting it from *File* → *Source file....*

Output:

- Generate the plot *Failureprobabilities.pdf*, depicting the probabilities for the failure to occur in a sequence of events, given pairwise comparisons from experts and observations.

Remarks:

- Experts judgements can be modified at the beginning of the routine.

G.5 Next steps

The concrete points for the improvement of these routines are:

- Improve the usability of the code;
- Make the code usable for a more generic case, solving the computational issues.
- Improve the code efficiency.