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Fabian Antonio Stamm

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Delft University of Technology
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Fabian Antonio Stamm

September 4, 2017

Department of Geoscience & Engineering	·	Delft University of Technology
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Delft University of Technology

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IDEA LEAGUE
JOINT MASTER'S IN APPLIED GEOPHYSICS

Delft University of Technology, The Netherlands
ETH Zürich, Switzerland
RWTH Aachen, Germany

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Abstract

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First of all I want to thank all the people who have participated in this project .. Remember, often more people have (in some way) contributed to your final thesis than you would initially think of....

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Acronyms

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Chapter 1

Introduction

- mention developments in geological modeling
- economic significance of geological modeling: examples of application in petroleum, mining, aquifers, CCS, etc.
- Bayesian analysis developments
- decision-making in for such economic scenarios and projects which involve geosciences
- classical approach (decision trees) vs. Bayesian approach, expression of decision-maker's interests in continuous loss functions
- influence of uncertainty and work done by Wellmann DeLaVarga

Chapter 2

Methods

The methods utilized in this work are presented in the following chapter. Bayesian analysis and decision theory are introduced. Focus is laid on Bayesian inference, estimation of uncertain values and the use of loss functions in this context. These methods are incorporated in computational modeling of structural geological settings by programming in a python 3 environment. Central tools for model construction and conduction of the statistical evaluation are GeMpy and PyMC 2 in particular. These are also presented in this chapter.

2-1 Bayesian analysis and decision theory

As implied by the name, the problems and reasoning behind decision-making are examined in the field of decision theory ([Berger, 2013](#)). Such decision problems are commonly influenced by parameters that are uncertain. In statistical decision theory, available statistical knowledge is used to gain information on the nature of these uncertainties. (Such uncertain parameters can be considered as numerical quantities.) In order to find the best decision to a problem, it is possible to combine sample information with other aspects such as the possible consequences of decision-making and the availability of prior information on our uncertainties. Decision consequences are expressed as gains in economic decision theory and as losses, which equal negative gains, in statistics. Prior information might be given for example based on experience from previous similar problems or from expert knowledge (see Batvold and Begg). The approach of utilizing priors is known as Bayesian analysis, which is explained in the following ([Berger, 2013](#)). (It goes well with decision theory.)

2-1-1 Basic elements

First, some basic elements are to be defined. The unknown (uncertain) quantity influencing decision-making is usually denominated as the state of nature θ ([Berger, 2013](#)). Given statistical information on θ in the form of probability distributions, θ is called the parameter.

Decisions are also referred to as actions a . The outcome of statistical tests in form of information or statistical evidence is denoted as X . Loss is defined as $L(\theta, a)$, so $L(\theta_1, a_1)$ is the actual loss incurred when action a_1 is taken while the true state of nature is θ_1 (Berger, 2013). Loss, expected loss and loss functions are explained in detail further below.

2-1-2 Bayesian inference

Bayesian inference is most importantly characterized by its preservation of uncertainty, in contrast to standard statistical inference (Davidson-Pilon, 2015). Probability is seen as a measure of belief for an event to occur. It has been argued by Davidson-Pilon (2015) that this Bayesian approach is intuitive and inherent in the natural human perspective. These beliefs can be assigned to individuals (Davidson-Pilon, 2015). Thus, different and even contradicting beliefs about the probability of an event might be held by different individuals, based on variations and disparities in the information available to each one individual (Davidson-Pilon, 2015).

The initial belief or guess about an event A can be denoted as $P(A)$ (Davidson-Pilon, 2015). This is used as the so-called prior probability on which Bayesian updating is based. The beliefs about the occurrence of an event are revalued in the presence of additional information, i.e. the observation of new evidence X . These observations are included as likelihoods $P(X|A)$. This process of updating results in a posterior probability $P(A|X)$ (Davidson-Pilon, 2015). It is important to note that the prior is not simply discarded but re-weighted by Bayesian updating. It was also pointed out by Davidson-Pilon (2015) that by utilizing an uncertain prior, the potential for wrongfulness of the initial guess is already included. This means that Bayesian updating is about reducing uncertainty in a belief and reaching a guess that is less wrong (Davidson-Pilon, 2015). Bayesian updating is defined by and conducted via the following equation, called the Bayes' Theorem:

$$P(A|X) = \frac{P(X|A)P(A)}{P(X)} \propto P(X|A)P(A) \quad (2-1)$$

-Law of Large Numbers!

2-1-3 Estimation

The resulting posterior distribution can be used to acquire point estimates for the true state of nature θ . Common and simple examples for such estimators are the mode (i.e. the generalized maximum likelihood estimate), the mean and the median of a distribution (Berger, 2013). The presentation of a point estimate should usually come with a measure for its estimation error. According to Berger (2013), the posterior variance is most commonly used as an indication for estimate accuracy. However, it is argued by Davidson-Pilon (2015) that by using pure accuracy metrics, while this technique is objective, it ignores the original intention of conducting the statistical inference in cases, in which payoffs of decisions are valued more than their accuracies. A more appropriate approach can be seen in the introduction of loss and the use of loss functions (Davidson-Pilon, 2015).

2-1-4 Expected loss and loss functions

Loss is a statistical measure of how bad an estimate is, i.e. how much is lost by making a certain decision. Gains are considered by statisticians as negative losses (Davidson-Pilon, 2015). The magnitude of an estimate's loss is defined by a loss function, which is a function of the estimate of the parameter and the true value of the parameter (Davidson-Pilon, 2015):

$$L(\theta, \hat{\theta}) = f(\theta, \hat{\theta}) \quad (2-2)$$

So, "how bad" a current estimate is, depends on the way a loss function weighs accuracy errors and returns respective losses. Two standard loss functions are the absolute-error and the squared-error loss function. Both are simple to understand and commonly used (Davidson-Pilon, 2015).

As implied by its name, the absolute-error loss function returns loss as the absolute error, i.e. the difference between the estimate and the true parameter (Davidson-Pilon, 2015):

$$L(\theta, \hat{\theta}) = |\theta - \hat{\theta}| \quad (2-3)$$

Accordingly, losses increasing linearly with the distance to the true value are returned for respective estimates. This means that all differences between relative errors are weighed equally, no matter whether they are found in the realm of relatively small or relatively large errors (Hennig and Kutlukaya, 2007).

Using the squared-error loss function returns losses that increase quadratically with distance of the estimator to the true parameter value (Davidson-Pilon, 2015):

$$L(\theta, \hat{\theta}) = |\theta - \hat{\theta}|^2 \quad (2-4)$$

This exponential growth of loss also means that large errors are weighed much stronger than small errors. This might come with over-valuation of distant outliers and misrepresentation of magnitudes in distance. Regarding this, the absolute-error loss function can be seen as more robust (Davidson-Pilon, 2015).

Both of these standard loss functions are symmetric and can be described as objectively aiming at a high precision in estimating the true parameter value. Davidson-Pilon (2015) and Hennig and Kutlukaya (2007) propose that it might be useful to move away from these type of objective loss functions to the design of customized loss functions that specifically reflect an individual's (i.e. the decision maker's) objectives, preferences and outcomes. Hennig and Kutlukaya (2007) argue that choosing and designing a loss function involves the translation of informal aims and interests into mathematical terms. This process naturally implies the integration of subjective decisions and subjective elements. According to Hennig and Kutlukaya (2007), this is not necessarily unfavorable or "less objective", as it may better reflect an expert's perspective on the situation and contribute to a productive scientific discussion. The standard loss functions defined above are symmetric, but can easily be adapted to be asymmetric, for example by weighing errors on the negative side stronger than those on the positive side. Preference over estimates larger than the true value (i.e. overestimation) is thus incorporated in an uncomplicated way (Davidson-Pilon, 2015; Hennig and Kutlukaya,

2007). Much more complicated designs of loss functions are possible, depending on purpose, objective and application (Davidson-Pilon, 2015). Some case-specific loss functions are designed in the following chapters of this work.

The presence of uncertainty during decision making implies that the true parameter is unknown and thus the truly incurred loss $L(\theta, a)$ cannot be known at the time of making the decision (Berger, 2013; Davidson-Pilon, 2015). The Bayesian perspective considers unknown parameters as random variables and samples that are drawn from the posterior distribution as possible realizations of the unknown parameter, i.e. all possible true values are represented by this distribution (Davidson-Pilon, 2015). A suitable alternative to the actual loss is to consider a decision's expected loss and to make a decision that is optimal in relation to this expected loss (Berger, 2013).

Given a posterior distribution $P(\theta|X)$, the expected loss of choosing an estimate $\hat{\theta}$ over the true parameter θ (after evidence X has been observed) is defined by the function below (Davidson-Pilon, 2015):

$$l(\hat{\theta}) = E_{\theta}[L(\theta, \hat{\theta})] \quad (2-5)$$

The expectation symbol E is subscripted with θ , by which it is indicated that θ is the respective unknown variable. This expected loss as defined above, is also referred to as the risk of estimate $\hat{\theta}$ (Davidson-Pilon, 2015).

By the Law of Large Numbers, the expected loss of $\hat{\theta}$ can be approximated drawing a large sample size N from the posterior distribution, respectively applying a loss function L and averaging of the number of samples (Davidson-Pilon, 2015):

$$\frac{1}{N} \sum_{i=1}^N L(\theta_i, \hat{\theta}) \approx E_{\theta}[L(\theta, \hat{\theta})] = l(\hat{\theta}) \quad (2-6)$$

Minimization of a loss function returns a Bayesian point estimate known as Bayes action $\delta^P(X)$, which is the estimate, action or decision with the least expected loss according to the loss function (Berger, 2013). For a unimodal and symmetric absolute-error loss function, the Bayes action is simply the median of the posterior distribution, while squared-error loss it is the mean (Davidson-Pilon, 2015; Berger, 2013). The MAP (maximum a posteriori) estimate is the minimizing solution for the posterior using zero-one loss (Davidson-Pilon, 2015). The possibility of more than one minimum also implies that several Bayes actions can exist for one problem (Berger, 2013).

Davidson-Pilon (2015) implemented different risk affinities by simply introducing a risk parameter into the loss function. By using different values for this parameter, it can be represented how comfortable an individual is with being wrong and furthermore which "side of wrong" is preferred by this decision maker (Davidson-Pilon, 2015). This approach to expressing risk-affinities is used the design of loss functions in this work.

2-2 Application in structural geological modeling

In this work, these methods of Bayesian analysis and decision theory are applied in the field of geological structural modeling. The fundamental approach follows closely the research

conducted by [de la Varga and Wellmann \(2016\)](#) and builds upon their findings.

According to them, structural geological modeling can be regarded as a forward problem and the elements of Bayesian inference can be specified in this context as follows:

1. **Mathematical forward model (M):** The connections between parameters θ and observed data y are defined in this mathematical model. ...
2. **Model parameters (θ):** These model-defining parameters, such as the position or dip of layers and faults in geological settings, can be deterministic or stochastic. In the latter case, they are uncertain parameters to which a probability distribution is assigned.
3. **Observed data (y):** This is any type of additional information that can be related to the forward modeling results and might possibly be used to reduce uncertainty. Such data can be gained by measurements and observations, for example by core sampling, well-log analysis or seismic acquisition.
4. **Likelihood functions ($p(y|\theta)$):** Links between the previous parameters θ and the additional data y are established by these functions in way that they reflect the likelihood of the parameter states given the observations ([de la Varga and Wellmann, 2016](#)).

A fundamental sequence of the inference process was proposed by [Gelman et al. \(2014\)](#), adapted by [de la Varga and Wellmann \(2016\)](#) and is subsequently adjusted for the application in this work as follows:

1. **Setting up a full probability model:** A multi-dimensional joint probability space is to be generated, taking into account the probability distributions of every model parameter θ . (- here, this not only results in the creation of geological models, but is subsequently also coupled with algorithms which deduct economic realizations from these models.)
2. **Conditioning on observed data:** Subsequently, an appropriate posterior distribution $p(\theta|y)$ is to be calculated by conditioning the parameters θ on the observed data y given the likelihood $p(y|\theta)$. This is the step of Bayesian updating of the belief about the parameter uncertainty given new information. In a chosen model (M), this is achieved by linking parameters and data through deterministic operations which are additionally compared to the likelihood functions. It is pointed out by [de la Varga and Wellmann \(2016\)](#) that any combination of parameter-observation connections is allowed, i.e. not all parameters need to be necessarily connected to all observed data. After all conditional probabilities have been set up, the Bayes Theorem (Equation 2-1) is applied to attain the posterior. However, due to the multi-dimensionality given in geological problems, the use of Markov chain Monte Carlo methods is advised to achieve this as described in Section 2-2-1 below.
3. **Evaluation of the posterior model:** Depending on the aim of the study, a post-processing analysis can be conducted accordingly. [de la Varga and Wellmann \(2016\)](#) focused on the examination of the posterior distributions of the parameters θ and the generated models, particularly regarding information entropy within the model space.

In this work, the geological models are assigned an economic meaning by declaring them potential petroleum reservoirs and introducing customized loss functions to reflect the economic interest of decision makers in developing respective resource extraction projects (see Section 2-1-4). Shifts in Bayes actions are considered a measure for the influence of Bayesian inference on decision-making and the significance of additional observations for different decision makers.

2-2-1 Markov chain Monte Carlo sampling (MCMC)

Despite the apparent simplicity of the Bayes Theorem, a direct analytical calculation and exact inference of the posterior distribution $P(A|X)$ is rarely possible in non-idealized cases, due to intractability in multi-dimensional spaces (Hoffman and Gelman, 2014; de la Varga and Wellmann, 2016). Thereby arises the necessity to resort to methods of statistical inference approximation. Markov chain Monte Carlo (MCMC) sampling has proven to be a generally applicable and reliable method for exploring multi-dimensional parameter spaces in an intelligent way (Hoffman and Gelman, 2014; Davidson-Pilon, 2015). Gilks (2005) has emphasized the significance of MCMC for the application of Bayesian statistics.

In the ordinary Monte Carlo approach, random independent samples are drawn from a target distribution in order to approximate its shape (Gilks, 2005; de la Varga and Wellmann, 2016). High-dimensional parameter spaces as found in Bayesian applications lead to complex shapes and often make independent sampling infeasible (Gilks, 2005). This can be solved by extending the Monte Carlo principle with a Markov chain, in which every sample iteration of the parameter $\theta^{(t+1)}$ is dependent uniquely on the previous value $\theta^{(t)}$ (Gilks, 2005; de la Varga and Wellmann, 2016).

The general principle of MCMC can be described as follows: Drawing representative samples from an target distribution of unknown shape is based on the conduction of a so-called random walk on the parameter distribution space. T sampling steps are to be performed. The first sampling location is chosen at random. With each subsequent step, a new sampling location is proposed. The new sample value is then related to the previous step. According to a weight defined by the scaled up candidate density of the value, the proposed step is then accepted or rejected. In the case of acceptance, the value is added to the sample trace and the process is continued from the current location. In the case of rejection, sampling is reverted to the previous accepted step (Schaaf, 2017; de la Varga and Wellmann, 2016). The intention behind this concept it to achieve convergence of the sampling algorithm towards areas of high probability (Davidson-Pilon, 2015).

Variations in the way of how new sample steps are proposed and in the acceptance-rejection condition result in different single MCMC sampling methods (Schaaf, 2017; de la Varga and Wellmann, 2016). Various algorithms for random MCMC walks have been developed for over more than six decades and advancements have still been made in recent years. Common examples for such algorithms are the Metropolis-Hastings samplers as devised by Metropolis et al. (1953) and generalized by Hastings (1970). The Gibbs sampler (Geman and Geman, 1984) is another well-known method. For the purpose of this work, an adaptive Metropolis-Hastings sampler is used.

In Metropolis-Hastings methods, each sampling step at iteration t is determined by a candidate probability distribution $q(\theta, \theta')$, from which a proposed sample θ' is drawn (de la Varga and Wellmann, 2016). The acceptance-rejection condition is defined by the acceptance ratio

$a(\theta', \theta)$:

$$a(\theta', \theta) = \frac{p(\theta')p(y|\theta')}{p(\theta)p(y|\theta)} \quad (2-7)$$

To ensure a thorough exploration of the probability space, the transition to higher probability densities should not be enforced in every case but selectively. This is assured by relating the acceptance ratio from Equation 2-7 to a random value u from a Uniform distribution $U(0, 1)$ as follows:

$$\theta^{(t+1)} = \begin{cases} \theta' & \text{if } a(\theta', \theta) > U(0, 1) \\ \theta^t & \text{otherwise} \end{cases} \quad (2-8)$$

Thereby, the algorithm assigns high probabilities to high-density points and low probabilities to low-density points, so that the chain state is moved accordingly (de la Varga and Wellmann, 2016).

Metropolis methods are furthermore defined by the step size scale factor that is chosen. While large steps are good for exploration of the space and mixture in the chain, acceptance rates are low. Small steps have better acceptance rates, but lead to slower exploration and convergence of the algorithm (de la Varga and Wellmann, 2016).

The Adaptive Metropolis (AM) by Haario et al. (2001) is used in this work. It adapts the traditional Metropolis-Hastings by incorporating the ability of continuous step size tuning during convergence, by taking into account the full information saved along the process. This is achieved by generating a covariance matrix that is updated every iteration. The adaptive nature of the process enables fast convergence for non-linear distributions while maintaining ergodicity Haario et al. (2001); de la Varga and Wellmann (2016). Its suitability for multi-dimensional distribution spaces make it an excellent method for dealing with complex models such as the structural geological models in this work (Schaaf, 2017)

2-2-2 Structural geological forward modeling

Performing forward modeling in the context of structural geology requires the use of a suitable modeling step. Additionally, for the application in a probabilistic setting, the method should enable fully automatic reconstruction of the model, when parameters are changed. The application in this work follows the example of de la Varga and Wellmann (2016) and relies on the use of implicit interpolation for geological modeling, a method developed and elaborated by Lajaunie et al. (1997) and Calcagno et al. (2008).

This implicit method relies on the interpolation of a potential field scalar function $T(\vec{x})$ of any point (\vec{x}) in a 3D space, and thus reflects the geometry of geological structures (Calcagno et al., 2008). Modeling $T(\vec{x})$ is achieved by cokriging that regards two forms of data: (i) contact points on geological interfaces through increments of the potential field $T(\vec{x}) - T(\vec{x}')$ and (ii) orientation data as gradients, i.e. partial derivatives of the potential field $\delta T(\vec{x})/\delta u_\beta$ in each direction u (Calcagno et al., 2008). The respective estimator is defined as follows:

$$T(\vec{x}) - T(\vec{x}_0) = \sum_{\alpha=1}^M \mu_\alpha (T\vec{x}_\alpha - T(\vec{x}'_\alpha)) + \sum_{\beta=1}^N \nu_\beta \frac{\delta T}{\delta u_\beta}(\vec{x}_\beta), \quad (2-9)$$

where \vec{x}_0 is an arbitrary origin, M and N are the total number of data points and partial derivatives respectively, and their relative contributions are weighed by the factors μ_α and ν_β . Furthermore, T is assumed to be a random function defined by polynomial drift and a stationary covariance $K(h)$ (Calcagno et al., 2008). The use of a cubic covariance model is suggested by Calcagno et al. (2008), based on the results from studies conducted by Aug (2004) and Chilès et al. (2004).

Resulting potential fields can be used to describe geological interfaces as iso-surfaces in any

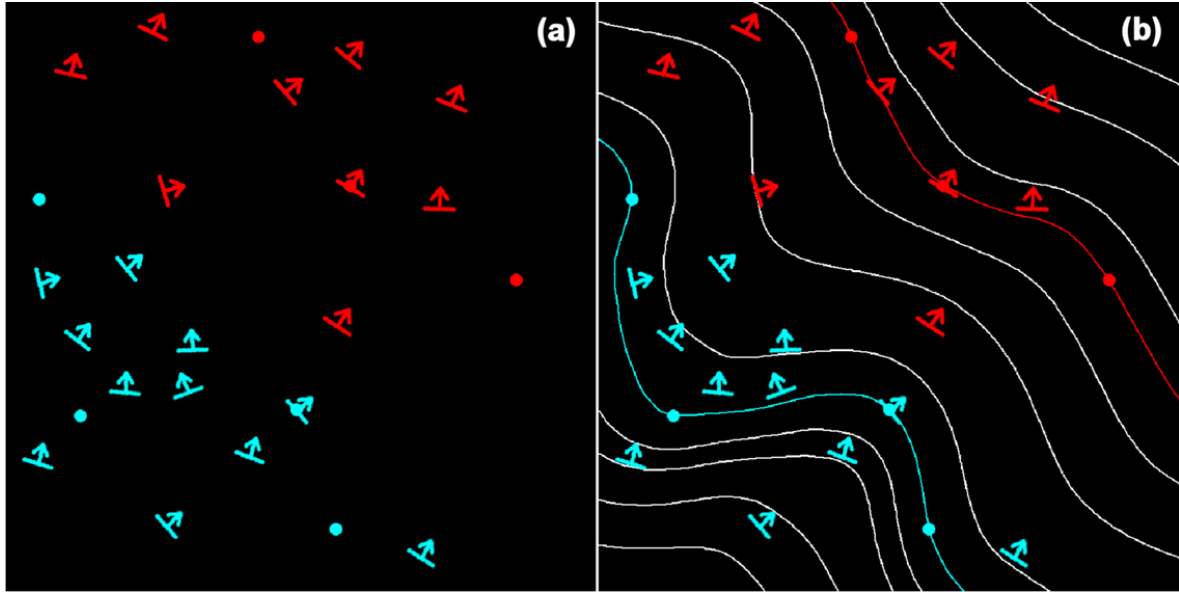


Figure 2-1: woo a potential field! from Calcagno et al. (2008)

kind of 3D geometry (Calcagno et al., 2008). Fault geometries can be interpolated analogously. These can be infinite in the 3D space, interrelated in a fault network or finite. To account for the effect of faults on geological layers, discontinuous potential fields are created by applying discontinuous drift functions in the cokriging system. Additionally, geological rules allow for the representation of several types of interactions between sets of geological layers (Calcagno et al., 2008).

It is pointed out by Calcagno et al. (2008), that this method is particularly appropriate for cases in which knowledge about the geology is only given a sparse locations and is thus applicable for a wide variety of typical problem in geological settings. Its suitability for this work is furthermore emphasized by the possibility to modify the topology-defining geological pile to achieve different geometric realizations without altering the data. The model can thus be updated in the face of new data or interpretations (Calcagno et al., 2008).

2-2-3 Implementing Bayesian analysis numerically with Python and PyMC

Bayesian analysis can be conducted using probabilistic programming (Salvatier et al., 2016). For doing this, the programming language of choice in this work is Python. The merits of Python have been pointed out by Behnel et al. (2010); Salvatier et al. (2016); Langtangen (2008). Development is facilitated by an expressive but concise and clean syntax that is easy to learn. Python is dynamic, compatible with multiple platforms and offers good support

for numerical computing. Integration of other scientific libraries and extension via C, C++, Fortran or Cython is easily possible (Behnel et al., 2010; Salvatier et al., 2016; Langtangen, 2008). Python is thus a straightforward tool for the implementation of central components of Bayesian analysis, such as custom statistical distributions and samplers (Salvatier et al., 2016).

In probabilistic programming, programming variables are used as components to build probabilistic models (Davidson-Pilon, 2015).

The numerical implementation of Bayesian analysis is further aided by the use of the Python library PyMC3, which was developed for conducting Bayesian inference and prediction problems in an open-source probabilistic programming framework (Davidson-Pilon, 2015; Salvatier et al., 2016). Different model fitting techniques are provided in PyMC3, such as the *maximum a posteriori* (MAP) method and several *Monte Carlo Markov Chain* (MCMC) sampling methods (Salvatier et al., 2016). Name examples for state-of-the-art samplers included. Salvatier et al. (2016) point out that the development of PyMC3 continuing, as the inclusion of further tools is planned for future updates.

2-2-4 Reservoir Volumetric Calculation

Chapter 3

One-dimensional reservoir case

For simple understanding and working out the application of the methods, first, an abstract one-dimensional reservoir case is presented in this chapter. The underlying model and basic approach are inherited from [de la Varga and Wellmann \(2016\)](#). Parameters were adapted to more appropriately represent a reasonable geological petroleum system, consisting of a reservoir with overlying seal in the subsurface. In doing this, a certain economic significance is ascribed to the model and further relevant questions can be derived. Regarding the petroleum sector, the problem of interest is most commonly one of estimating the volume of resources or monetary value contained in an oil or gas reservoir. Limiting the model to only one dimension and a small number of uncertain parameters allows for a relatively straightforward and simplified approach to assessing an abstract type of value for a reservoir and designing a respective loss function for value estimation. A step by step derivation of such as case follows below.

3-1 Constructing the one-dimensional model

[de la Varga and Wellmann \(2016\)](#) constructed a simple geological model using three uncertain positions in vertical one-dimensional space, marking hypothetical boundaries of layers in a subsurface column. The location probabilities for these points are defined by sampling from normal distributions. Standard deviations of these distributions increase with depth, representing an increase in uncertainty. For an approximate representation of a petroleum system, the distribution means were set to depths of 2000 m (seal top), 2050 m (reservoir top) and 2200 m (reservoir bottom). These points confine two layers in the middle, from which the upper one can be labeled as seal and the lower one as reservoir. The resulting model with its possible layer boundary locations is illustrated in Figure 3-1.

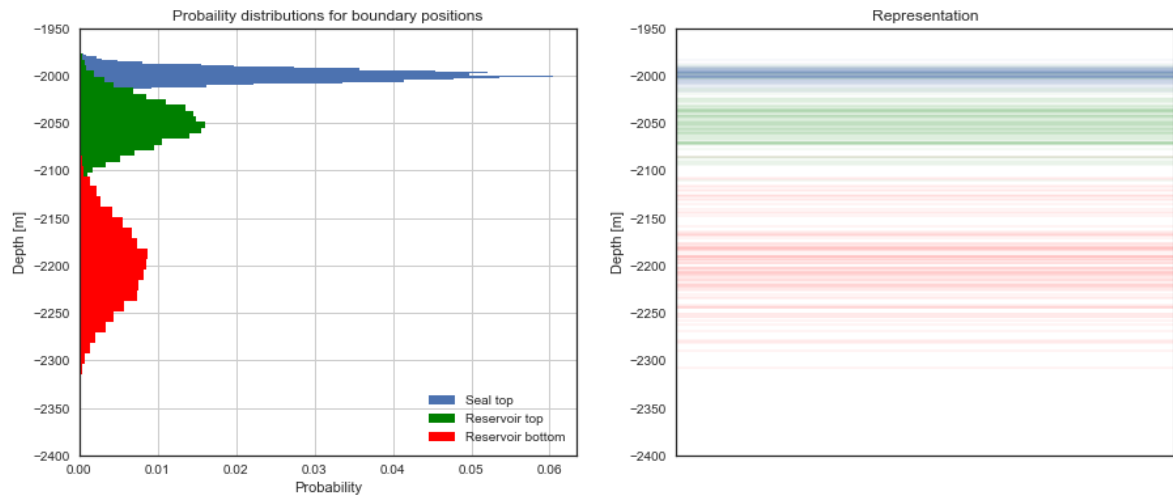


Figure 3-1: Probability distributions for positions of layer boundaries in the subsurface and a respective representation using lines.

3-2 Assessing reservoir quality using scores

The next step is to find a way to assess the quality of the reservoir from a petroleum industry perspective in such a simplified model. What can be deduced from the distributions of layer boundary locations, is the thickness of the seal and the reservoir, as well as the depth of both, again as probability distributions. To assess the reservoir quality in an abstract way, it can be assigned a score. This score is made dependent on the three uncertain parameters (1) reservoir thickness, (2) reservoir top depth and (3) seal thickness (see Figure 3-2).

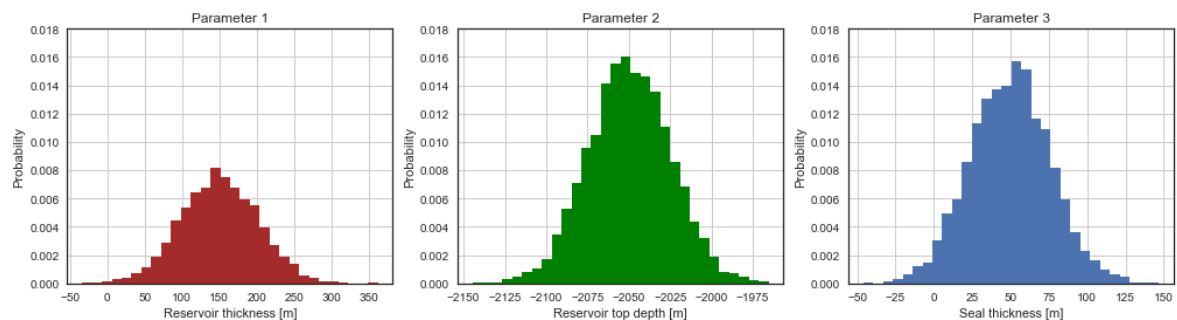


Figure 3-2: Probability distributions for the three parameters used for modeling reservoir score.

3-2-1 Two parameters scoring

Assuming that reservoir thickness is a simplified indicator for the extractable oil or gas and thus value in place, a gain in score can be correlated with increase in thickness. Here, two score points are assigned to one meter of thickness. Increasing costs of drilling are indicated by increasing depth of the reservoir top. Consequently, one negative score point is ascribed to every meter in depth. Samples from the probability distributions of these two parameters

are drawn to model the true score of the reservoir (depth scores are subtracted from reservoir thickness scores). For the data used here, it can be seen in Figure 3-3-A, that the results of modeling with only these two parameters, are represented by an approximately normal distribution. The score is negative in about 17% of the cases. Mean and median are about the same.

3-2-2 Three parameters scoring

Next, influence by the third parameter seal thickness is included. Score points are not added or subtracted by this parameter directly. Instead, a threshold for seal reliability is defined beforehand. Here it is set at 20 m thickness. If the seal thickness falls below this threshold, it is assumed that the seal fails completely and thus all the potential value (positive score) of the reservoir is lost, while costs of depth (negative score) remain. Thus, a condition to check whether the seal is reliable is now included in the model. Results are visualized in Figure 3-3-B. The main distribution is not changed significantly, except for a striking peak of probability at the possibility of a score of -2000. Furthermore, mean and median have been shifted to lower values and are now found further apart.

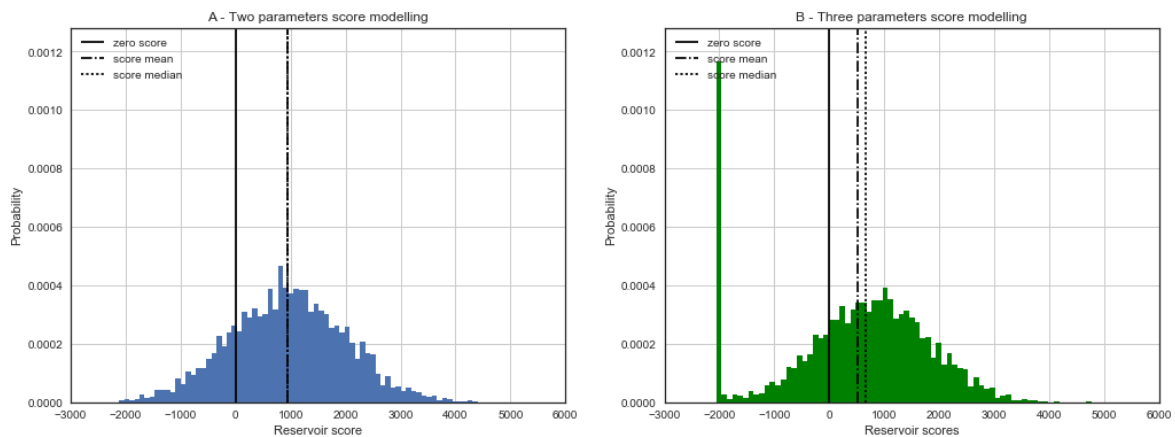


Figure 3-3: Posterior probability distributions from modeling scores using two (A) and three parameters (B).

3-3 Designing a case-specific loss function

Now that a distribution of reservoir score probabilities has been modeled, a loss function for estimation of the true score value can be developed.

3-3-1 Testing standard loss functions

Some standard loss function were presented in chapter 2-1-4. For this case, the absolute-error loss and the squared-error loss function were considered as starting points, to design a more case-specific loss function. Calculating the expected loss for estimates ranging from -3000 to 6000 based on these two standard loss function results in the graphs depicted in Figure 3-4.

It can be observed that the median of the distribution coincides with the minimum of the absolute-error and the mean with the minimum of the squared-error expected loss.

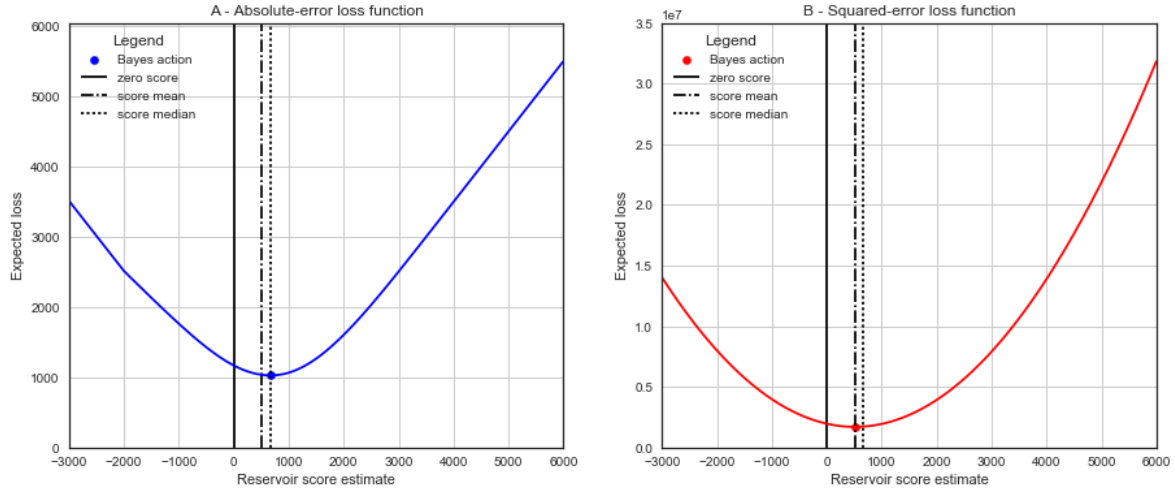


Figure 3-4: Expected loss based on the standard absolute-error (A) and squared-error (B) loss functions applied on the probability distribution resulting from 3-2 and for estimates ranging from -3000 to 6000.

3-3-2 Adaptions for loss function customization

These standard loss functions provide objectively good estimators minimizing expected loss. Due to their symmetric properties, both will always give the median or mean of the underlying distribution as minimizing estimator respectively. However, assigning an economic notion to our model and assuming the case of an actor or decision maker in any field, naturally necessitates the consideration of preferences, interests and the overall subjective perspective such an individual or for example a company might have. Further constraints, properties and factors can also be specific to the field, industry or generally to the problem at hand. Consequently, the design of a more specific non-standard and possibly asymmetric loss function might be required, so that an adapted Bayesian estimator can be found. One that includes subjective aspects and difference in weighting of particular gains or losses, arising from an actor's inherent preferences and the environment in which the actor has to estimate or make a decision. In the face of several uncertain parameters, a perfectly true estimate is virtually unattainable. However, an attempt can be made, to design a customized loss function that returns a Bayesian estimator involving the least bad consequences for an individual in a specific environment. Regarding the petroleum system case modeled above, such an attempt is made and explained step by step in the following.

For the purpose of estimation, it makes sense that one of the standard loss functions is chosen as a basis and a customized loss function is developed from there. The absolute-error loss seems most appropriate for this case of petroleum reservoir quality estimation. As stated above, the reservoir score is an abstract and simplified way to reflect a value contained in the reservoir. Ideally, an actor would like to know the exact true score, so that investments or resources can be allocated appropriately, in order to acquire economic gains. This allocation

is the decision to be made or action to be taken. Deviations from the unknown true score in the form of over- and underestimation bring about an error and loss accordingly. In this case, there is no reason for loss to increase exponentially with distance from the true value. It is assumed that investments increase linearly with linear growth in the value of the resource. For this reason, the absolute-error loss function is favored over the squared-error loss function in this case. Some customization steps are taken below, based on mostly logical case-specific assumptions.

1. Step I: The standard symmetrical absolute-error loss function is chosen as a starting point for further customization steps:

$$L(\theta, \hat{\theta}) = |\theta - \hat{\theta}| \quad (3-1)$$

2. Step II: Considering the development of a petroleum reservoir, it can be assumed that over-investing is worse than under-investing. Overestimating the size of a reservoir might for example lead to the installation of equipment or facilities that are actually redundant or unnecessary. This would come with additional unrecoverable expenditures. Consequences from underestimating, however, may presumably be easier to resolve. Additional equipment can often be installed later on. Hence, overestimation is weighted stronger in our loss function by multiplying the error with an overestimation factor a ($= 1.25$):

$$L(\theta, \hat{\theta}) = |(\theta - \hat{\theta})| * a \quad (3-2)$$

3. Step III: The worst case for any project would be that its development is set into motion, expecting a gain, only to discover later that the value in the reservoir does not cover the costs of realizing the project, resulting in an overall loss. A petroleum system might also turn out to be a complete failure, containing no value at all, although the actor's estimate indicated the opposite. Here, this is referred to as a worst case or fatal overestimation. A positive score is estimated, but the true score is zero or negative. This is worse than the "normal" non-fatal overestimation, where both values are positive and a net gain is still achieved, which is only smaller than the best possible gain of expecting the true score. Fatal overestimation is included in the loss function by using another weighting factor b ($= 2$) that replaces a :

$$L(\theta, \hat{\theta}) = |(\theta - \hat{\theta})| * b \quad (3-3)$$

(In other words: Worst case or fatal overestimation is twice as bad as simple underestimation.)

4. Step IV: A worst case or fatal underestimation can also be derived from the idea of estimating a zero or negative score, when the true score is actually positive. This is assumed to be worse than non-fatal overestimation, but clearly better than fatal overestimation. No already owned resources are wasted, it is only the potential value that is lost, i.e. opportunity costs that arise from completely discarding a reservoir with a potential gain equal to the positive true score. Fatal underestimation is weighted using a third factor c :

$$L(\theta, \hat{\theta}) = |(\theta - \hat{\theta})| * c \quad (3-4)$$

Combining these adaption steps and the conditions defined in them, results in the following customized loss function:

$$L(\theta, \hat{\theta}) = \begin{cases} |\theta - \hat{\theta}|, & \text{for } 0 < \hat{\theta} < \theta \\ |\theta - \hat{\theta}| * a, & \text{for } 0 < \theta < \hat{\theta} \\ |\theta - \hat{\theta}| * b, & \text{for } \theta \leq 0 < \hat{\theta} \\ |\theta - \hat{\theta}| * c, & \text{for } \hat{\theta} \leq 0 < \theta \end{cases}, \text{ with } a, b, c \in \mathbb{Q} \quad (3-5)$$

Realizations of the four adaption steps are depicted in the plots in Figure 3-5. It is important to note that the weighting factors defined above can take basically any numerical values but should be chosen in a way that they appropriately represent the framework conditions of the problem. Here, for example, it is assumed that normal overestimation is 25% ($a = 1.25$), fatal overestimation 100% ($b = 2$) and fatal underestimation 50% ($c = 1.5$) worse than normal underestimation.

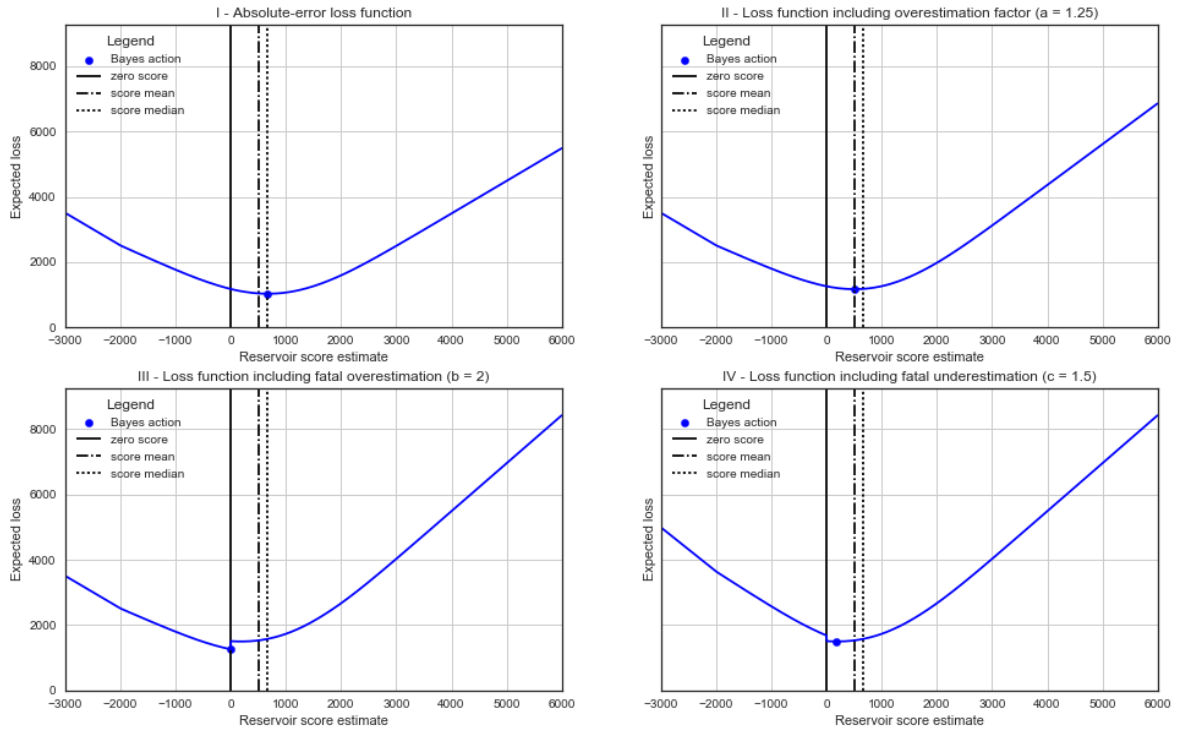


Figure 3-5: The single steps of customizing the loss function are depicted in plots I - IV.

In Figure 3-5 it can be observed, that assigning a stronger weight on overestimation (plot II) steepens the curve on the right hand side and shifts the minimum to the left, i.e. to a lower estimate. Using $a = 1.25$, the Bayes action changes from the median, to a value close to the mean of the distribution. The shift and steepening are significantly reinforced by the introduction of fatal overestimation (plot III). With $b = 2$, the Bayes action drops to the zero

score estimate. It can also be noted, that by defining a condition dependent on the algebraic sign of the values, according to which only losses for positive estimates are multiplied by b , a distinct jump appears at the zero score boundary. Due to a similar condition, the same effect is observed on the negative side of estimate values, where the curve has also been steepened, after including fatal underestimation (plot IV). This comes with a shift of the minimum towards positive values. It is also to be noted that with every customization step, the overall expected loss is increased.

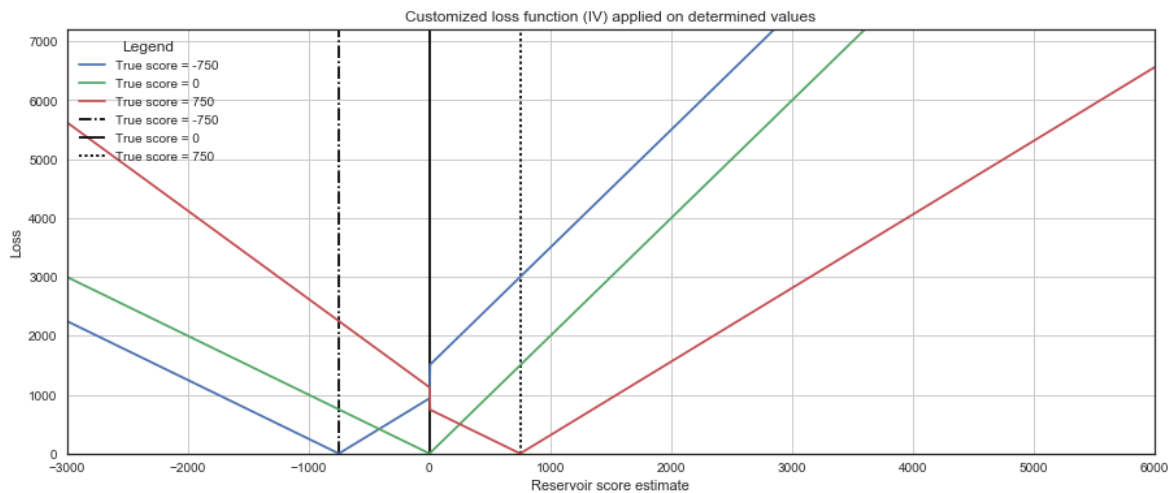


Figure 3-6: Loss based on the customized loss function (IV) for determined true scores of -750, 0 and 750.

The implementation of this customized loss function (IV) using single determined values for the true score is plotted in Figure 3-6. This helps to clarify the way real losses result for each guess, relative to given true score values. The expected loss is acquired by arithmetically averaging such loss realizations based on the true score probability distribution by using formula 2-6.

It has to be emphasized that this is just one possible proposal for loss function customization. There exists not one perfect design for such a case. Slight to strong changes can already be implemented by simply varying the values of the weighting factors a , b and c . Fundamentally different loss functions can also be based on a significantly different mathematical structure. Loss functions are customized regarding the problem environment and according to the subjective needs and objectives of an actor. Thus, they are mostly defined by the actor expressing his perspective. Changes in the individual's perception and viewpoint might lead to further customization needs even later on. (Especially considering individual persons as actors, psychological aspects may play a significant role.)

(Estimate or prediction? True value only known if a "yes"-action (development) is taken.)

3-3-3 Including different risk-affinities in the loss function

One can assume that several actors in one sector or decision environment may have the same general loss function, but different affinities concerning risks. This might be based for example

on the different psychological factors or economic philosophies followed by companies. It might also be based on budgets and options such actors have available. An intuitive example is the comparison of a small and a large company. A certain false estimate or error might have a significantly stronger impact on a company which has a generally lower market share and only few projects, than on a larger company which might possess a higher financial flexibility and for which one project is only one of many development options in a portfolio.

In the following, the loss function is further adapted to consider different risk-affinities of several actors. Representing risk behavior in a loss function can also be done in different ways and regarding different types of risks. Here, bidding lower is considered the cautious, risk-averse option, as smaller losses can be expected from underestimating. Guessing higher is deemed riskier. Losses from overestimation are greater. However, bidding correctly on a higher value, will also return a greater gain. It is assumed that risk-friendly actors care less about fatal underestimation, i.e. they will rather develop a project than discard it. In the loss function, risk is simply included using a risk factor r which alters the weighting factors a , b and c respectively:

$$L(\theta, \hat{\theta}) = \begin{cases} |\theta - \hat{\theta}|, & \text{for } 0 < \hat{\theta} < \theta \\ |\theta - \hat{\theta}| * (a * r), & \text{for } 0 < \theta < \hat{\theta} \\ |\theta - \hat{\theta}| * (b * r), & \text{for } \theta \leq 0 < \hat{\theta} \\ |\theta - \hat{\theta}| * (c * (r^{-0.5})), & \text{for } \hat{\theta} \leq 0 < \theta \end{cases}, \text{ with } a, b, c, r \in \mathbb{Q} \quad (3-6)$$

According to this, for $r = 1$ the risk-neutral loss function is returned, since a , b and c are not altered. For $r < 1$, the weight on overestimating is reduced and increased for fatal underestimation. This represents a more risk-friendly actor that is willing to bid on a higher estimate to attain a greater gain. For $r > 1$, the overestimation weight is increased, the underestimation weight decreased in the loss function and respectively more risk-averse actors are prompted to bid on lower estimates.

The factor r can take basically any positive values. However, since risk-neutrality is expressed by $r = 1$, values $0 < r < 2$ are considered to be the most appropriate choices to represent both sides of risk-affinity equally.

Implementing it as a factor r leads to different steepnesses of the plotted curves depicting loss and expected loss. The effect on the latter is visualized in Figure 3-7, where 0.5, 0.75, 1, 1.25 and 1.5 were chosen as values for r . It can be observed that the minima for expected loss, i.e. the Bayesian estimators for differently risk-affine actors, are located at different estimates. Mean and median are clearly surpassed by the best estimate of the most risk-friendly actor ($r = 0.5$), while for the most risk-averse actors ($r = 0.5$ and $r = 0.75$), the Bayes action equals a zero score estimate (and thus the decision to take on action). In Figure 3-7 it can also be recognized that the expected loss is generally lower for risk-friendlier actors (on the side of positive estimates).

3-4 Updating the model with additional information in the form of thickness likelihoods

de la Varga and Wellmann (2016) made use of Bayesian inference to reduce the uncertainty

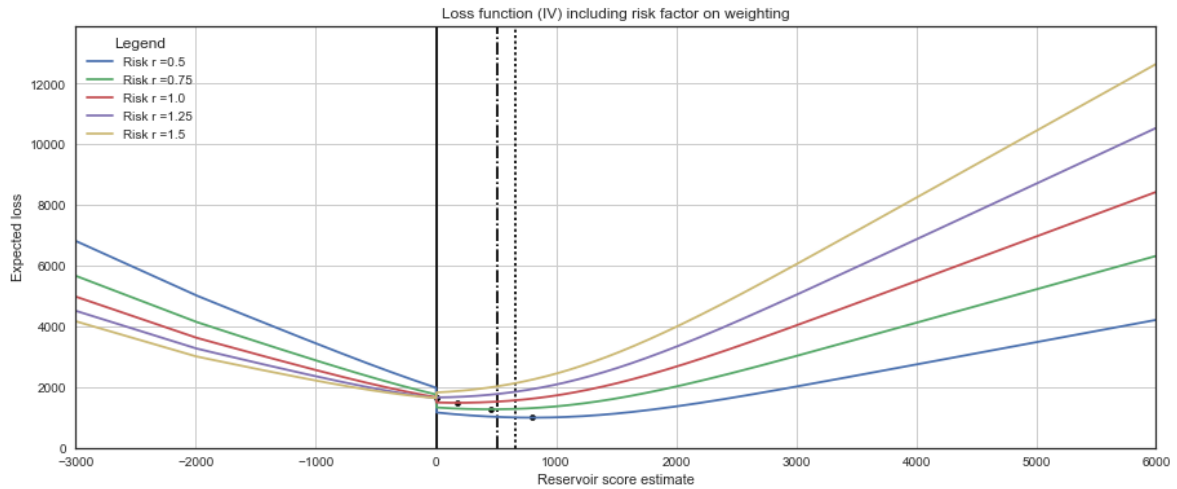


Figure 3-7: Plotting of expected loss realizations after including the risk factor r in the loss function (IV) for actors with risk-affinities ranging from risk-averse ($r = 0.5$ and 0.75), over risk-neutral ($r = 1$), to risk-friendly ($r = 1.25$ and $r = 1.5$).

in this type of one-dimensional model. The same is conducted here in the following.

The probability distributions for the location of the layer boundaries are treated as priors. Now it is assumed that new observations have been made, providing additional information on the likelihoods of the thicknesses of the two layers. Likelihood functions for reservoir and seal thicknesses are introduced in the form of normal distributions, defined by means and standard deviations. These parameters vary according to nature of the observations made. Using the principle of Bayesian inference as explained in chapter 2, the model is updated and new posterior distributions for our true reservoir score are attained.

- VOI Quantification ???

Different examples with different sets of likelihoods are conducted in the following, so that various possible results can be compared. Each take the layer boundaries defined in section 3-1 about model construction as priors and use Bayesian inference with data defined below for each example.

3-4-1 Updating example I: Moderately reinforcing information

In this first case, a normal distribution with a mean of 25 m and a standard deviation of 20 m is chosen to reflect the likelihood of the seal thickness. For the reservoir, a normal distribution with a mean of 180 m and a standard deviation of 60 m is chosen. Using these likelihoods to update the one-dimensional model, the uncertainty in the posterior probability distributions for the positions of layer boundaries in depth is reduced (see Figure 3-8).

Modeling the reservoir score is conducted as above, now based on these new distributions. In Figure 3-9 A it can be recognized that the bulk of the distribution was shifted to the positive side of scores, while the peak at - 2000 was raised. The probability of scores between - 2000 and 0 decreased significantly, i.e. the true score is most likely either positive or - 2000 if it is negative.

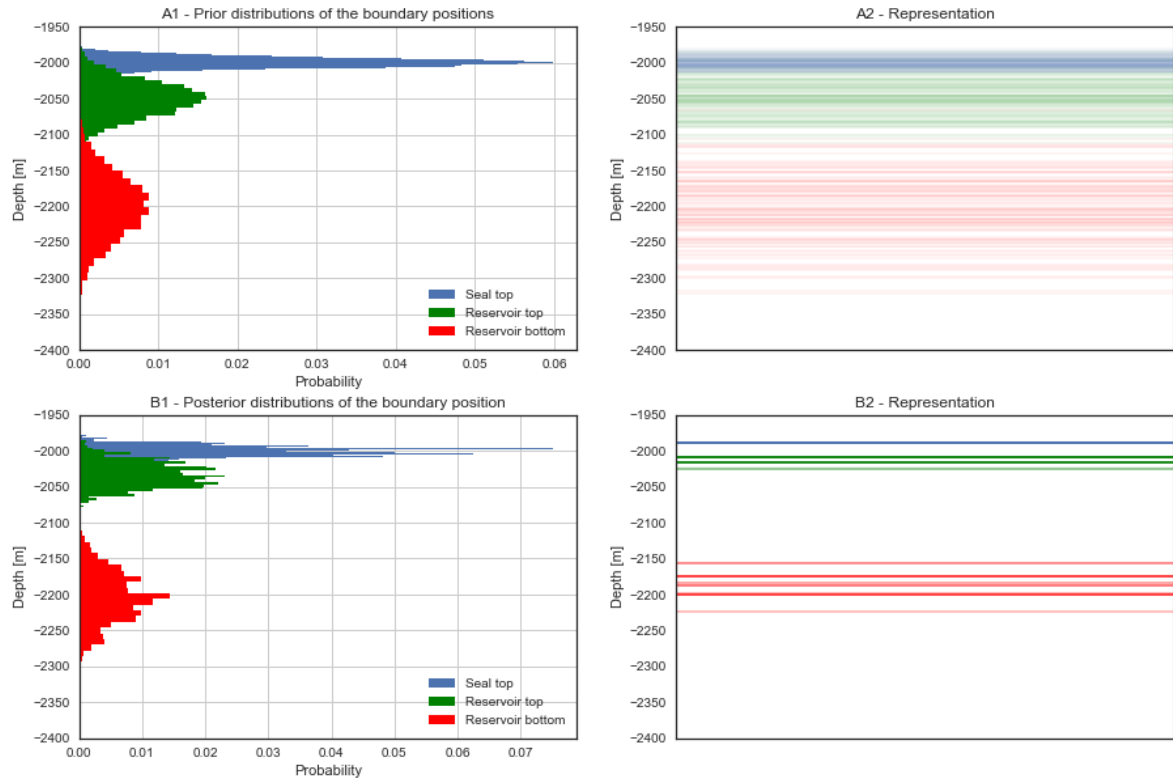


Figure 3-8: Prior (A1) and posterior distributions (A2) of the layer boundary positions in depth and respective representations (A2, B2).

The customized loss function (IV) is now applied on this updated distribution of the reservoir score. This is visualized in Figure 3-9 in which the expected losses are compared before (B1) and after (B2) uncertainty reduction. It is observable, that by adding information about layer thickness likelihoods, Bayes actions are shifted relative to the nature of the information. In this case, the added data generally reinforces the likelihoods of the reservoir to be significantly thick. Information on the seal, however, based on a normal distribution around 25 m thickness, leaves uncertainty about the reliability of the seal, as the safety threshold is defined as 20 m.

Increased certainty about the reservoir thickness is sufficient to shift Bayes actions to higher estimates for all actors, but the most risk-averse one. These shifts are quantified in Table 3-2. According to these numbers, the risk-neutral actor's estimate is increased the most. Expected losses decreased for the risk-neutral and the two risk-friendlier individuals. It is clear that the expected loss was reduced the most for the risk-friendliest actor and it increased most significantly for the most risk-averse actor.

3-4-2 Updating example II: Likely reliable seal

In this second case, the reservoir thickness likelihood is defined in the same way as before. For the seal, a mean of 50 m with a standard deviation of 20 m is chosen, favoring the likelihood of a reliable seal relative to the threshold of 20 m thickness. This results in the score distribution depicted in Figure 3-10. The bulk of the distribution is narrowed on the

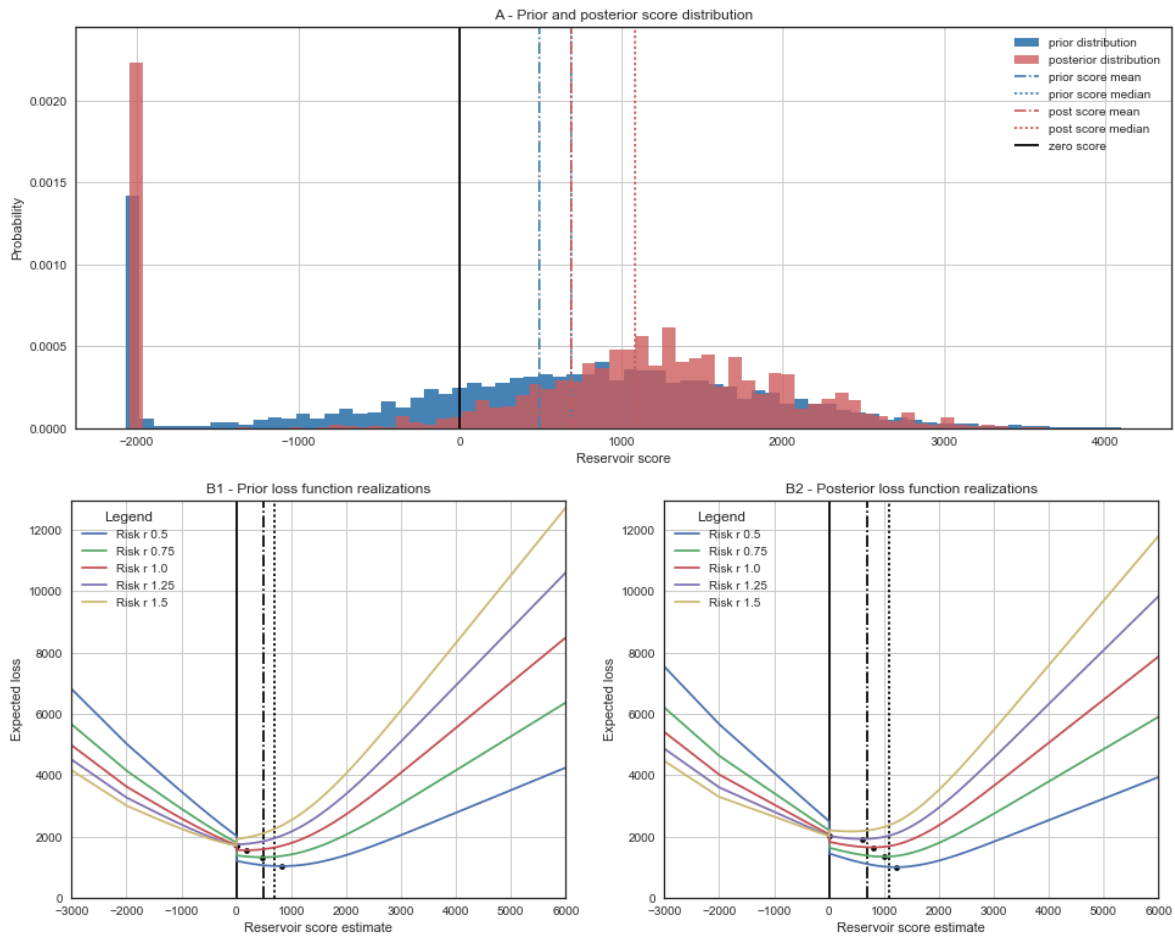


Figure 3-9: Reservoir score distributions (A) and change in the realizations of expected loss for several risk parameters (B1, B2) before and after Bayesian updating based on likelihoods defined as follows: Seal thickness mean = 25 m, std = 20 m. Reservoir thickness mean = 180 m, std = 60 m.

positive side of estimates. Mean and median are clearly shifted to higher values as well. The "seal failure" peak at -2000 is significantly decreased.

Applying the loss function on this new score distribution results in the realizations of expected loss illustrated in Figure 3-10. Bayes actions are shifted clearly to higher estimates and expected losses of these minima are significantly reduced for all actors. This is quantified in Table 3-2. According to these values, the risk-neutral to risk-averse individuals seem to profit the most.

3-4-3 Updating example III: Safe seal but likely subpar reservoir thickness

In this third example, seal safety is ensured by using a mean of 70 m with a standard deviation of 10 m for the seal thickness likelihood. However, the new observations are assumed to provide information about the reservoir that makes it likely to be thinner as expected. Reservoir thickness likelihood is assigned a mean of 100 m and a standard deviation of 40 m.

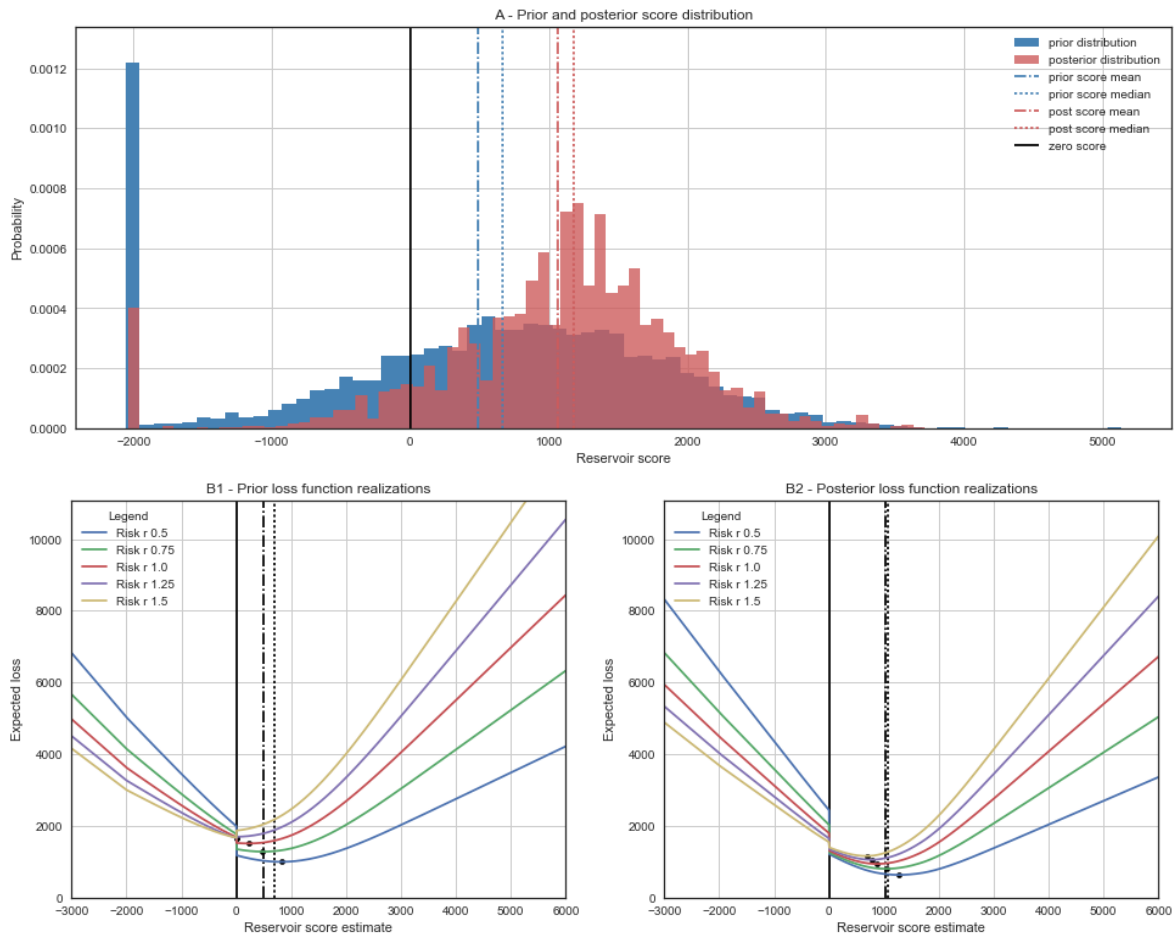


Figure 3-10: Reservoir score distributions (A) and change in the realizations of expected loss for several risk parameters (B1, B2) before and after Bayesian updating based on likelihoods defined as follows: Seal thickness mean = 50 m, std = 20 m. Reservoir thickness mean = 180 m, std = 60 m.

The subsequent score distribution is depicted in Figure 3-11. It can be seen that while the whole distribution is narrowed, it also is shifted to the left, to lower and negative estimates. Mean and median are almost the same. As seal reliability is practically guaranteed, the peak at -2000 m vanishes.

Based on this probability distribution of the reservoir score, Bayes actions are shifted to lower estimates for all actors (see Figure 3-11). In fact, also but the most risk-friendly individual ($r = 0.5$) find their Bayesian estimator to be zero now, i.e. project development is deemed to be too risky to them. Furthermore, the spread of expected loss values around the minima for all actors is diminished (the expected loss values of the Bayes actions are now much closer to each other).

Quantified changes in the position and the values of the Bayes actions are comparable to the results in example II (there is no shift for risk-averse actors, as they already found their best estimates to be zero). Most notable is the large reduction of expected loss in general (see Table 3-2).

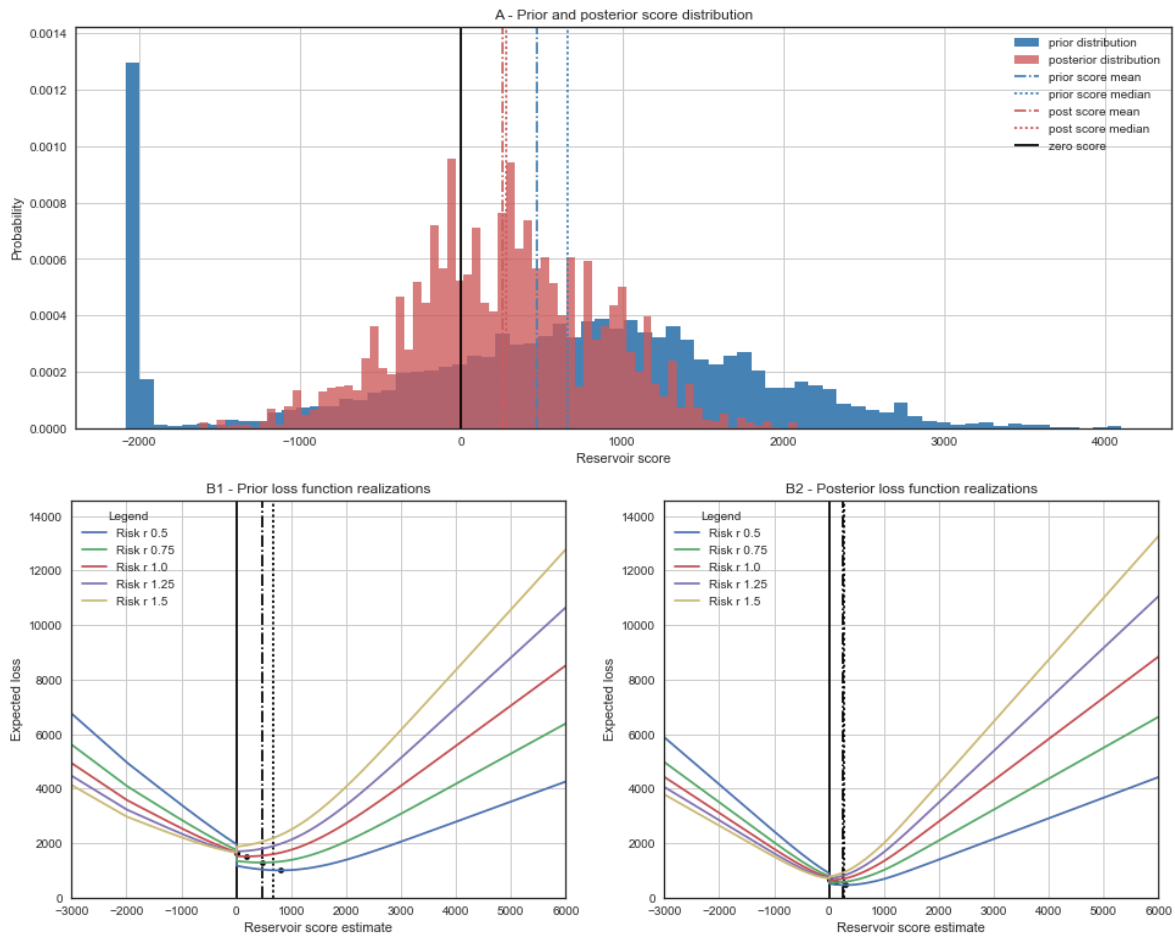


Figure 3-11: Reservoir score distributions (A) and change in the realizations of expected loss for several risk parameters (B1, B2) before and after Bayesian updating based on likelihoods defined as follows: Seal thickness mean = 70 m, std = 10 m. Reservoir thickness mean = 100 m, std = 40 m.

3-5 General case results

-abstract case: easy model construction and straightforward design of a loss function making basic assumptions and taking relative values that can simply be exchanged

-so representative in a "relative" way, mostly appropriate to illustrate principles and benefits of the methodology

-decision making/ estimation is defined by the design of the loss function which includes framework parameters which depend on the problem environment (e.g. market, technical constraints, etc.)

-similar actors but different behaviors concerning risk: different decisions but same general loss function path (just different minima of EL)

-additional information changes decision (BA) and EL

	Example I		Example II		Example III	
r	Δ BA	Δ EL	Δ BA	Δ EL	Δ BA	Δ EL
0.50	+ 553.67	- 105.49	+ 522.95	- 436.26	- 498.98	- 538.08
0.75	+ 673.40	- 81.67	+ 697.73	- 551.92	- 346.16	- 717.83
1.00	+ 750.05	- 33.56	+ 855.57	- 631.92	- 176.13	- 872.02
1.25	+ 713.19	+ 75.71	+ 912.43	- 647.10	- 0.00	- 946.04
1.50	+ 0.00	+ 282.64	+ 819.26	- 545.96	- 0.00	- 951.57

Table 3-1: Changes in Bayes action (BA) and minimal expected loss (EL) for Bayesian updating examples I, II and III and respective actors with risk parameters r .

Risk factor r	Shift in Bayes action	Change in expected loss
0.50	- 498.98	- 538.08
0.75	- 346.16	- 717.83
1.00	- 176.13	- 872.02
1.25	- 0.00	- 946.04
1.50	- 0.00	- 951.57

Table 3-2: Bla

-magnitude of change varies not only with the nature of the information (magnitude of uncertainty reduction) but also with the risk parameter

-some actors might benefit more from some specific additional information than others

-quantifiable value of information??

Chapter 4

Three-dimensional reservoir case

- concept of 1D case in chapter 3 transferred to a 3D case of a structural geological model
- same again here: relatively simple model including some important typical geological and structural features and giving it an economic meaning - alternating layers of sandstones and shales, so typical reservoir and seal formations - structurally defined by a tilted dome-formation (folding along in the direction of two perpendicular axes) which is displaced by a standard normal fault - these features are arranged in a way, that they result in the formation of a trap, defined by the anticlinal features and the fault, as well as enabled by the presence of a reservoir rock - considering a petroleum production industry perspective, actors/ decision makers would be interested in the evaluation of value this potential reservoir - "traditionally", this is represented by volumetric calculations or estimations of the recoverable reserves
- here: maximum volume of entrapment and subsequently, relative or hypothetical volumes of recoverable reserve can be calculated (for each model realization) - (later: numbers from example case are taken, to achieve estimations of the NPV for a development project realization) - looking at this structural model, not only the calculated volume can be taken into account, but also risk factors, such as fault permeability seal safety (and capacity?), possible juxtapositions and leaks

- as in the 1D case, uncertainties are introduced for a number of parameters in the model, in a way that they affect the resulting maximum volume of the trap (and following also the recoverable reserves) - again, a specific loss function is designed and applied on the results from numerous iterations of the constructed uncertain model, thus resembling the different value estimations/predictions or decisions different actors might make - (to bring this Bayesian method of using loss functions closer to the traditional application of deterministic decision-making in decision-trees, the continuous estimation space of the reservoir value (volume) is combined with the assumption, that the estimated value is linked to a consequent investment into a determined project development size. thus, the continuous approach is used to make the decision in a deterministic decision-making space.))

- later on, the effect of adding information (in the form of likelihoods) is examined, particularly by looking at the changes in decision-making after applying this Bayesian updating and uncertainty has been reduced

- in the following, the construction and design of this model is described

4-1 Constructing the three-dimensional structural geological model

- base of the structural geological model is a 3Dcubic space (block) with 2000 m size in X, Y and Z x3 - place layer positional points in three lines, resembling three hypothetical seismic lines as base information -

4-2 Identifying trap structures in the geological model

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Appendix A

The back of the thesis

A-1 An appendix section

A-1-1 An appendix subsection with C++ Listing

```
// 1
// C++ Listing Test
//
#include <stdio.h>
for(int i=0;i<10;i++)
{
    cout << "Ok\n";
}
6
```

A-1-2 A Matlab Listing

```
%
% Comment
%
n=10;
for i=1:n
    disp('Ok');
end
5
```

Appendix B

Yet another appendix

B-1 Another test section

Ok, all is well.

