

Hierarchical Bayesian Modelling and Posterior
Inference Applied to an Atmospheric
Limb-Sounder Measuring Ozone



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Abstract

In this thesis, we develop a hierarchical Bayesian model based on the radiative transfer equation for an idealised atmospheric limb-sounder targeting ozone, as described in [43]. To ensure effective measurements, we briefly assess the informativity of different measurement approaches via a singular value decomposition of the forward model and adapt the data collection accordingly. Following [17], we utilise the marginal and then conditional scheme to provide posterior distributions of hyper-parameters and ozone profiles, and compare with a regularisation approach. After approximating the non-linear forward model with an affine map, we extend our hierarchical Bayesian framework and the marginal and then conditional scheme to jointly infer posterior ozone, pressure and temperature.

The main contribution of this work is the application of tensor-trains to approximate high-dimensional posterior probability distributions [8, 11]. This enables us to generate samples from the target distribution with far fewer function evaluations compared to the t-walk sampling algorithm [6]. Tensor-train methods require a predefined grid and a “normalisation constant” so that function outputs are within computer precision, but once defined, they reduce the function evaluations per independent sample significantly. Another advantage of the tensor-train format is that marginal probability distributions, useful for characterisation of integrals via quadrature, can be calculated at a low computational cost, without any sampling. To further improve tensor-train methods, we suggest future work should focus on lowering tensor ranks, calculating “normalisation constants” to avoid numerical issues and reducing correlation structures between parameters automatically, all of which we currently have to do by exploratory analysis. Additionally, choosing accurate interpolation schemes between grid points is crucial to improving the effectiveness of the approximation.

Our results show that a hierarchical Bayesian approach, which quantifies posterior mean and variance of the parameter (ozone), provides more information than a regularisation approach at comparable computational time. In regions where the signal strength is low and the data is noise-dominated, we can not recover ozone structures from the ground truth. When including pressure and temperature describing hyper-parameters within our hierarchical Bayesian model, we find a strong correlation between ozone and pressure, whereas the model and data are uninformative about temperature. For future work, we recommend developing a more physically informed parametrised model for ozone within the atmosphere, incorporating atmospheric chemistry and other important processes.

Contents

List of Abbreviations	xi
1 Introduction	1
1.1 Motivation	1
1.2 Research Gap and Contribution	2
1.3 Thesis Structure	3
2 Theoretical and Technical Background	5
2.1 Hierarchical Bayesian Inference	5
2.1.1 Marginal and then Conditional Method	8
2.2 Sample-Based Estimates via Markov Chain Monte-Carlo Methods	10
2.3 Numerical Function Approximation – Tensor-Train (TT)	11
2.3.1 Marginal Functions	13
2.3.2 Sampling from a TT Approximation	16
2.3.3 Error of the TT Approximation	18
2.4 Regularisation Approach	20
3 The Forward Model	23
3.1 Radiative Transfer Equation	24
3.2 Simulate Data Based on a Ground Truth	25
3.2.1 Understanding the Forward Model	27
4 Linear Bayesian vs. Regularisation – Ozone	37
4.1 Hierarchical Bayesian Framework	37
4.1.1 Prior Modelling	39
4.2 Posterior Distribution	40
4.2.1 Marginal Posterior	40
4.2.2 Full Conditional Posterior	46
4.3 Solution by Regularisation	50
5 Affine Approximation of the Non-Linear Model	53
5.1 Finding an Affine Map	54
5.2 Marginal and Full Conditional Posterior – Ozone	56

6 Joint Retrieval of Ozone, Pressure and Temperature	59
6.1 Hierarchical Bayesian Framework	59
6.1.1 Prior Modelling	61
6.2 Posterior Distribution	65
6.2.1 Marginal Posterior – Pressure and Temperature	66
6.2.2 Full Conditional Posterior – Ozone	81
7 Summary and Outlook	83
7.1 Regularisation Solution vs. Hierarchical Bayesian Approach	83
7.2 Sampling Methods vs. TT Approximation	84
7.3 Atmospheric Physics	85
References	87
Appendices	
A Theoretical and Technical Background	93
A.1 Correlation Structure	93
A.2 Monte-Carlo Error and Integrated Autocorrelation Time	94
A.3 Python Code	96
B Additional Figures	99
B.1 Ozone	100
B.1.1 Ozone Prior	100
B.1.2 Integrated Autocorrelation Time	101
B.1.3 Eigenvectors of Full Conditional Posterior Precision Matrix	104
B.2 Pressure and Temperature	106
B.2.1 Priors	106
B.2.2 Integrated Autocorrelation Time	108

List of Abbreviations

CDF	Cumulative Distribution Function
DAG	Directed Acyclic Graph
HITRAN	High Resolution Transmission
IACT	Integrated Autocorrelation Time
IRT	Inverse Rosenblatt Transform
L	Linear
MCMC	Markov Chain Monte-Carlo
MH	Metropolis–Hastings
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MLS	Microwave Limb Sounder
MTC	Marginal and then Conditional
MWG	Metropolis within Gibbs
NASA	National Aeronautics and Space Administration
PDF	Probability Density Function
RMS	Root Mean Square
RTE	Radiative Transfer Equation
RTO	Randomise then Optimise
SIRT	Squared Inverse Rosenblatt Transform
STD	Standard Deviation
SVD	Singular Value Decomposition
TT	Tensor-Train
VMR	Volume Mixing Ratio

1

Introduction

Here we briefly describe the standard currently used to retrieve atmospheric trace gas concentrations, e.g. ozone concentration, from limb-sounding measurements and what motivates us to employ a hierarchical Bayesian framework to address this inverse problem. We explain how our approach contributes to and improves upon existing methods. Lastly, we provide the reader with the thesis structure.

1.1 Motivation

Presently, the only operating ozone limb sounder is the Microwave Limb Sounder (MLS) on NASA’s Aura satellite. This satellite is gradually drifting away from its orbit and scheduled to be phased out by 2026 [13]. A group led by Harald Schwefel has proposed an alternative approach to fill this observational gap using a much smaller platform such as a 6U CubeSat (roughly 30cm × 15cm × 10cm) [62]. The proposed system includes a disk-shaped resonator targeting a narrow frequency band and converting the thermal radiation emitted by ozone molecules from the terahertz region to the optical domain [58, 54]. This frequency conversion offers a cost-effective and energy-efficient solution as it avoids the need for large, energy-hungry cooling devices that are traditionally required to capture terahertz signals. Instead, signal acquisition in the optical domain can be implemented by using compact, cheap, and low-power photonic technologies.

Currently, the inverse problem to retrieve any trace gas from limb-sounding data is approached by the atmospheric physics community using optimisation and regularisation techniques developed in the 1970s [47, 34]. These methods focus on finding the “best fit to data but not the best fit to parameters” [59]. Instead, we employ a hierarchically structured Bayesian framework to provide a distribution of ozone profiles, which represents

multiple possible solutions according to some given data. This probabilistic approach allows us to determine meaningful estimates and uncertainties of parameters.

1.2 Research Gap and Contribution

As already mentioned, currently the MLS retrieval algorithm [33] is based on the “optimal estimation” method from [47]. This approach provides a point estimate by fitting parameters to some data and iteratively minimising a squared residual norm, penalised against a chosen regularisation. However, this does not provide comprehensive information about the parameters’ underlying correlation structures can lead to unphysical results, e.g. negative ozone concentration values [53], and biased solutions where the bias is then removed based on empirical decisions [35, 21]. Errors are provided by a local derivative of the forward map at the optimal solution, which is inherently highly sensitive to that specific point in the parameter space. Furthermore, these regularisation methods condition on external point estimates of other parameters such as temperature or pressure [33].

In Bayesian modelling all unknown parameters are treated as random variables [29]. Further, a hierarchically ordered model incorporates unknown hyper-parameters, which for example, control the noise of the data and the smoothness of the ozone profile. Therefore, it is able to model conditional dependencies between parameters and hyper-parameters. For some given data, the posterior probability distribution of this hierarchical Bayesian framework provides a range of feasible unbiased solutions and hence true errors. Livesey et al. [33] report “unexpected spectrally correlated noise” on the MLS Aura, so here is another real reason why one should include noise in the model.

In this thesis the marginal and then conditional (MTC) method [17] is utilised and a hierarchical Bayesian model based on the radiative transfer equation (RTE) is developed to provide posterior distributions of ozone as well as temperature and pressure profiles. First, we neglect the non-linearity of the RTE and employ a linear-Gaussian hierarchical Bayesian model. Since the RTE is weakly non-linear we use the results based on the linearised RTE to find an affine map that approximates the non-linear forward model. This appears to be another novelty in the field of atmospheric remote sensing. Lastly, the hierarchical Bayesian framework is extended to include pressure and temperature. The MTC scheme is a relatively new method within the Bayesian community, and we are the first, to the best of our knowledge, to apply it to a forward model based on the RTE and to jointly provide posterior ozone, pressure, and temperature profiles.

Instead of using sampling algorithms to characterise the posterior probability distribution of the hierarchical Bayesian model we approximate this distribution directly utilising the tensor-train (TT) format [8]. This allows us to generate independent samples from a

TT approximation via a scheme similar to the inverse Rosenblatt transform (IRT) [11] with far fewer function evaluations compared to conventional samplers. Further, in the TT format one can calculate marginal probability distributions of each hyper-parameter and evaluate integrals via quadrature without any sampling.

1.3 Thesis Structure

In Chapter 2, we give a brief overview of the key methods used, along with references for further reading. Chapter 3 introduces the simplified forward model based on the RTE. Here we test several measurement cases and assess the information content using a singular value decomposition (SVD) to understand the forward model and determine the most effective measurement method. Based on those results and a ground truth, we simulate noisy data for an idealised limb sounder within a simplified atmosphere. Then in Chapter 4, a linear-Gaussian hierarchical Bayesian model, neglecting absorption in the RTE, is constructed. We discuss some prior modelling choices, apply the MTC scheme and compare posterior ozone profiles and a regularisation approach to a ground truth ozone profile. Using those results we find an affine map in Chapter 5 to approximate the non-linear forward model. In Chapter 6, based on the affine map the previously built hierarchical Bayesian model is extended to include hyper-parameters corresponding to pressure and temperature. Again, we touch on some prior modelling choices and use the MTC method to provide joint estimates of posterior ozone, pressure and temperature profiles. Additionally, some important aspects for improving the effectiveness and stability of TT approximations are highlighted. Lastly, in Chapter 7 we summarise and discuss our results and provide an outlook for future work. All programming and analysis in this thesis are done in Python, and the reported computation times are taken on a MacBook Pro from 2019 with a 2.4 GHz quad-core Intel i5 processor.

2

Theoretical and Technical Background

This Chapter introduces the hierarchical Bayesian approach to inverse problems, along with key concepts of Markov Chain Monte Carlo (MCMC) methods and tensor-train (TT) approximations for high-dimensional probability distributions. We keep it as general as possible. Specific sampling algorithms are not introduced here, as they are specifically tailored towards the structure of the forward model and the particular problem. Therefore, they will be presented in detail when applied.

2.1 Hierarchical Bayesian Inference

Assume we observe some data

$$\mathbf{y} = \mathbf{A}(\mathbf{x}) + \boldsymbol{\eta}, \quad (2.1)$$

based on a forward model $\mathbf{A}(\mathbf{x})$, which may be non-linear, an unknown parameter vector \mathbf{x} and some additive random noise $\boldsymbol{\eta}$.

Naturally, due to the noise, the observation process in Eq. 2.1 is a random process. Hence, in Bayesian modelling, the aim is to determine a probability distribution over the parameter \mathbf{x} given some data \mathbf{y} . Further, a hierarchical Bayesian model incorporates (auxiliary) hyper-parameters $\boldsymbol{\theta}$. Within a Bayesian approach all unknown hyper-parameters and parameters are treated as random variables [29, Chapter 3].

According to Bayes' theorem, the joint posterior distribution over the parameters \mathbf{x} and the hyper-parameter $\boldsymbol{\theta}$ is given as

$$\pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}) = \frac{\pi(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta})\pi(\mathbf{x}, \boldsymbol{\theta})}{\pi(\mathbf{y})} \propto \pi(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta})\pi(\mathbf{x}, \boldsymbol{\theta}), \quad (2.2)$$

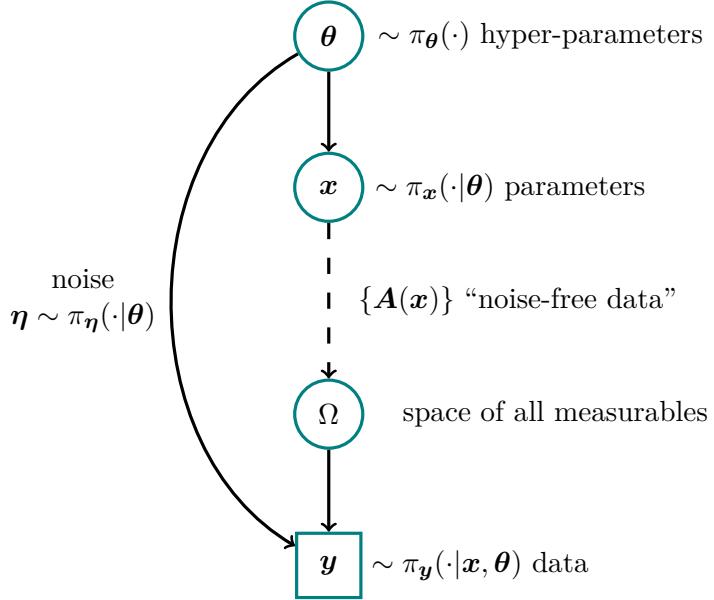


Figure 2.1: A directed acyclic graph (DAG) for an inverse problem visualises statistical dependencies as solid line arrows and deterministic dependencies as dotted arrows. The hyper-parameters θ are distributed as (\sim) the hyper-prior distribution $\pi(\theta)$. The prior distribution $\pi_x(\cdot|\theta)$ for the parameter x and the noise $\eta \sim \pi_\eta(\cdot|\theta)$ are statistically dependent on some of those hyper-parameters. Then a parameter $x \sim \pi_x(\cdot|\theta)$ is deterministically mapped onto the space of all measurable $\Omega = A(x)$ through the forward model. From the space of all measurable noise-free data we observe (square box) a data set $y = A(x) + \eta$ with some additive random noise, which determines the likelihood function $\pi(y|x, \theta)$.

with finite and non-zero $\pi(y)$. The likelihood function $\pi(y|x, \theta)$ is defined by the nature of the noise and the noise-free data $A(x)$, which we read as the distribution over y conditioned on x and θ . Here θ may describe multiple hyper-parameters. The hyper-parameters can e.g., model the noise vector $\eta \sim \pi_\eta(\cdot|\theta)$, where \sim reads as “is distributed as”, and account for physical properties or functional dependencies of x , such as the smoothness of x . Because unknown parameters are treated as random variables the joint prior distribution is introduced as $\pi(x, \theta) = \pi(x|\theta)\pi(\theta)$ with the parameter prior distribution $\pi(x|\theta)$ and the hyper-prior distribution $\pi(\theta)$. Choosing these prior distributions is ultimately a modeller’s choice and is crucial, as those shall be as uninformative as possible for regions in hyper-parameter and parameter space where the data is informative. If the data is uninformative, the prior distributions can be informative and may represent a rather restrictive range of (physically) feasible hyper-parameters and parameters.

Fig. 2.1 visualises the conditional dependencies between hyper-parameters and parameters as well as how distributions progress through to an observation (square box) using a directed acyclic graph (DAG). We plot statistical dependencies as solid arrows and deterministic dependencies as dotted arrows.

Usually, the objective is to calculate the expectation of a function $h(\mathbf{x})$, which is defined as

$$\mathbb{E}_{\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}}[h(\mathbf{x})] = \underbrace{\int \int h(\mathbf{x}) \pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}) d\mathbf{x} d\boldsymbol{\theta}}_{\bar{h}}. \quad (2.3)$$

If it is a high-dimensional integral and computationally not feasible to solve we approximate

$$\mathbb{E}_{\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}}[h(\mathbf{x})] \approx \underbrace{\frac{1}{N} \sum_{k=1}^N h(\mathbf{x}^{(k)})}_{\bar{h}_N}, \quad (2.4)$$

with an the unbiased sample-based Monte-Carlo estimate [45] for large enough N (law of large numbers [36, Chapter 17]). Here the posterior samples $\{\mathbf{x}^{(k)}, \boldsymbol{\theta}^{(k)}\} \sim \pi_{\mathbf{x}, \boldsymbol{\theta}}(\cdot | \mathbf{y})$, for $k = 1, \dots, N$, form a sample set $\mathcal{M} = \{(\mathbf{x}, \boldsymbol{\theta})^{(1)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(N)}\}$. The central limit theorem states that the sample mean $\bar{h}_N^{(i)}$ of independent sample sets $\mathcal{M}^{(i)} \sim \pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y})$, for $i = 1, \dots, n$, converges to be normally distributed, so that

$$\sqrt{n}(\bar{h}_N^{(i)} - \bar{h}) \xrightarrow{\mathcal{D}} \mathcal{N}(0, \sigma^2) [22], \quad (2.5)$$

and if $\sigma^2 < \infty$ the Monte-Carlo error $\bar{h}_N^{(i)} - \bar{h}$ is bounded. In practice, the Monte-Carlo error from a sample set $\mathcal{M}^{(i)}$ is approximated as

$$(\sigma^{(i)})^2 = \text{Var}(\mathbb{E}_{\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}}[h(\mathbf{x})]) \approx \frac{\text{Var}(h(\mathbf{x}))}{N} \left(1 + 2 \underbrace{\sum_{t=1}^W \frac{\Gamma(t)}{\Gamma(0)}}_{:= \tau_{\text{int}}} \right) = \text{Var}(h(\mathbf{x})) \frac{\tau_{\text{int}}}{N}, \quad (2.6)$$

where we have to take into account that the samples generated by any system or algorithm are correlated. We define the integrated autocorrelation time (IACT) τ_{int} as in [17] which is a common definition in statistics. This is twice the value of the IACT in [70, pp. 103-105] and [68, 28], as commonly defined within the physics community. Here the autocorrelation coefficient $\Gamma(t) \propto \exp\{-|t|/\tau\} \rightarrow 0$ for $t \rightarrow \infty$ at lag t decays exponentially and $\Gamma(0) = \text{Var}(h(\mathbf{x}))$. Choosing the summation window W is crucial because it has to be large compared to the decay time τ , but for too large t the autocorrelation coefficient $\Gamma(t)$ is noise-dominated. U. Wolff [68] (and the Python implementation by D. Hesse [28]) provide a way to not only calculate the IACT safely but also to quantify the errors of the estimated IACT.

The IACT provides a good estimate of the number of steps the sampling algorithm needs to take to produce one independent sample. According to the IACT, the effective sample size is defined as τ_{int}/N . We point out that for uncorrelated samples $\tau_{\text{int}} = 1$ the error $(\sigma^{(i)})^2$ is a typical Monte-Carlo estimate. See Appendix A.2 and [57, 68, 70] for a more detailed derivation.

2.1.1 Marginal and then Conditional Method

Quickly generating a representative sample set from the posterior distribution often presents a significant challenge. This is mainly due to the strong correlations that usually exist between the parameters and hyper-parameters, as discussed by Rue and Held in [49] and illustrated in Appendix A.1. Depending on the problem and the available model it is beneficial to factorise the joint posterior distribution

$$\pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}) = \pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y}) \pi(\boldsymbol{\theta} | \mathbf{y}) \quad (2.7)$$

into the full conditional posterior $\pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})$ over the latent field \mathbf{x} and the marginal posterior $\pi(\boldsymbol{\theta} | \mathbf{y})$ over hyper-parameter $\boldsymbol{\theta}$. This approach, known as the MTC method, is particularly advantageous when $\mathbf{x} \in \mathbb{R}^n$ is high-dimensional, while $\boldsymbol{\theta}$ is low-dimensional and the evaluation of the marginal posterior

$$\pi(\boldsymbol{\theta} | \mathbf{y}) = \frac{\pi(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta}) \pi(\mathbf{x} | \boldsymbol{\theta}) \pi(\boldsymbol{\theta})}{\pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y}) \pi(\mathbf{y})} \propto \frac{\pi(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta}) \pi(\mathbf{x} | \boldsymbol{\theta}) \pi(\boldsymbol{\theta})}{\pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})} \quad (2.8)$$

as in [17, Lemma 2] is relatively cheap.

Applying the law of total expectation [5], Eq. (2.3) becomes

$$\mathbb{E}_{\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}}[h(\mathbf{x})] = \int \int h(\mathbf{x}) \pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y}) d\mathbf{x} \pi(\boldsymbol{\theta} | \mathbf{y}) d\boldsymbol{\theta} \quad (2.9)$$

$$= \int \mathbb{E}_{\mathbf{x} | \boldsymbol{\theta}, \mathbf{y}}[h(\mathbf{x})] \pi(\boldsymbol{\theta} | \mathbf{y}) d\boldsymbol{\theta} \quad (2.10)$$

$$= \mathbb{E}_{\boldsymbol{\theta} | \mathbf{y}} \left[\mathbb{E}_{\mathbf{x} | \boldsymbol{\theta}, \mathbf{y}}[h(\mathbf{x})] \right]. \quad (2.11)$$

In the case of a linear-Gaussian hierarchical Bayesian model, both the marginal distribution $\pi(\boldsymbol{\theta} | \mathbf{y})$ and the inner expectation $\mathbb{E}_{\mathbf{x} | \boldsymbol{\theta}, \mathbf{y}}[h(\mathbf{x})]$ are well defined (see next subsection). If the integral in Eq. 2.10 is expensive to calculate, we use sample-based methods to produce a Markov chain $\{(\mathbf{x}, \boldsymbol{\theta})^{(1)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(N)}\} \sim \pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y})$ and sample from $\pi(\boldsymbol{\theta} | \mathbf{y})$ first and then draw samples from the full conditional posterior $\pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})$ (see Sec. 6.2.2).

Linear-Gaussian hierarchical Bayesian model

In case of normally distributed noise $\boldsymbol{\eta} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}(\boldsymbol{\theta}))$ with zero mean and covariance $\boldsymbol{\Sigma}(\boldsymbol{\theta})$ and a linear forward model matrix \mathbf{A} Eq. 2.1 simplifies to

$$\mathbf{y} = \mathbf{Ax} + \boldsymbol{\eta}. \quad (2.12)$$

Then we can obtain the marginal and full conditional posterior distribution explicitly. Our hierarchical linear-Gaussian Bayesian model is defined as

$$\mathbf{y} | \mathbf{x}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{Ax}, \boldsymbol{\Sigma}(\boldsymbol{\theta})) \quad (2.13a)$$

$$\mathbf{x} | \boldsymbol{\theta} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{Q}(\boldsymbol{\theta})^{-1}) \quad (2.13b)$$

$$\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta}), \quad (2.13c)$$

with a Gaussian likelihood function $\pi(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta})$, a normally distributed prior $\pi(\mathbf{x}|\boldsymbol{\theta})$, with prior mean $\boldsymbol{\mu}$ and prior precision $\mathbf{Q}(\boldsymbol{\theta})$, and a hyper-prior distribution $\pi(\boldsymbol{\theta})$. For the derivation of the marginal posterior and the full conditional posterior distribution, consider the joint multivariate Gaussian distribution

$$\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \sim \mathcal{N} \left[\begin{pmatrix} \boldsymbol{\mu} \\ \mathbf{A}\boldsymbol{\mu} \end{pmatrix}, \begin{pmatrix} \mathbf{Q}(\boldsymbol{\theta}) + \mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1} \mathbf{A} & -\mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1} \\ \Sigma(\boldsymbol{\theta})^{-1} \mathbf{A} & \Sigma(\boldsymbol{\theta})^{-1} \end{pmatrix}^{-1} \right], \quad (2.14)$$

with the joint precision matrix as in [56] (see also [49, 17]). Immediately¹, the full conditional posterior distribution can be formulated as

$$\mathbf{x}|\boldsymbol{\theta}, \mathbf{y} \sim \mathcal{N} \left(\underbrace{\boldsymbol{\mu} + (\mathbf{Q}(\boldsymbol{\theta}) + \mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1} \mathbf{A})^{-1} \mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu})}_{\boldsymbol{\mu}_{\mathbf{x}|\boldsymbol{\theta}, \mathbf{y}}}, \underbrace{(\mathbf{Q}(\boldsymbol{\theta}) + \mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1} \mathbf{A})^{-1}}_{\Sigma_{\mathbf{x}|\boldsymbol{\theta}, \mathbf{y}}} \right). \quad (2.15)$$

Then the marginal posterior distribution over the hyper-parameters in Eq. 2.8 is derived as

$$\begin{aligned} \pi(\boldsymbol{\theta}|\mathbf{y}) \propto & \sqrt{\frac{\det(\Sigma(\boldsymbol{\theta})^{-1}) \det(\mathbf{Q}(\boldsymbol{\theta}))}{\det(\mathbf{Q}(\boldsymbol{\theta}) + \mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1} \mathbf{A})}} \exp \left\{ -\frac{1}{2} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu})^T \right. \\ & \left. [\Sigma(\boldsymbol{\theta})^{-1} - \Sigma(\boldsymbol{\theta})^{-1} \mathbf{A} (\mathbf{Q}(\boldsymbol{\theta}) + \mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1} \mathbf{A})^{-1} \mathbf{A}^T \Sigma(\boldsymbol{\theta})^{-1}] (\mathbf{y} - \mathbf{A}\boldsymbol{\mu}) \right\} \pi(\boldsymbol{\theta}), \end{aligned} \quad (2.16)$$

where, as noted by Fox and Norton [17], the parameter \mathbf{x} cancels. Having the marginal posterior distribution $\pi(\boldsymbol{\theta}|\mathbf{y})$ (independent of \mathbf{x}) available breaks up the correlation structure between \mathbf{x} and $\boldsymbol{\theta}$ and makes the MTC approach very efficient [17] (see Appendix A.1). Within this scheme, we evaluate the marginal posterior first and then either condition on hyper-parameters to draw full conditional posterior samples $\mathbf{x} \sim \pi(\mathbf{x}|\boldsymbol{\theta}, \mathbf{y})$ (see Sec. 6.2.2) or evaluate the posterior mean

$$\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}} = \int \boldsymbol{\mu}_{\mathbf{x}|\boldsymbol{\theta}, \mathbf{y}} \pi(\boldsymbol{\theta}|\mathbf{y}) d\boldsymbol{\theta} \quad (2.17)$$

and the posterior covariance matrix

$$\Sigma_{\mathbf{x}|\mathbf{y}} = \int \Sigma_{\mathbf{x}|\boldsymbol{\theta}, \mathbf{y}} \pi(\boldsymbol{\theta}|\mathbf{y}) d\boldsymbol{\theta} \quad (2.18)$$

of $\pi(\mathbf{x}|\mathbf{y})$ by some quadrature rule.

¹Assume $\begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \sim \mathcal{N} \left[\begin{pmatrix} \boldsymbol{\mu}_{\mathbf{x}} \\ \boldsymbol{\mu}_{\mathbf{y}} \end{pmatrix}, \begin{pmatrix} \mathbf{Q}_{\mathbf{xx}} & \mathbf{Q}_{\mathbf{xy}} \\ \mathbf{Q}_{\mathbf{yx}} & \mathbf{Q}_{\mathbf{yy}} \end{pmatrix} \right]$, then $\mathbf{x}|\mathbf{y} \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbf{x}} - \mathbf{Q}_{\mathbf{xx}}^{-1} \mathbf{Q}_{\mathbf{xy}} (\mathbf{y} - \boldsymbol{\mu}_{\mathbf{y}}), \mathbf{Q}_{\mathbf{xx}}^{-1})$.

2.2 Sample-Based Estimates via Markov Chain Monte-Carlo Methods

One may use Markov chain Monte-Carlo (MCMC) methods to calculate sample-based estimates of $\mathbb{E}_{\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}}[h(\mathbf{x})]$ as in Eq. 2.4. Within the MTC scheme we draw samples $\{\boldsymbol{\theta}^{(1)}, \dots, \boldsymbol{\theta}^{(k)}, \dots, \boldsymbol{\theta}^{(N)}\} \sim \pi(\boldsymbol{\theta} | \mathbf{y})$ from the marginal posterior first and then characterise the full conditional posterior $\pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})$. In doing so we generate a Markov chain $\mathcal{M} = \{\boldsymbol{\theta}^{(1)}, \dots, \boldsymbol{\theta}^{(k)}, \dots, \boldsymbol{\theta}^{(N)}\}$ where every new sample $\boldsymbol{\theta}^{(k)}$ is proposed according to a random proposal $\boldsymbol{\theta}^{(k)} \sim q(\cdot | \boldsymbol{\theta}^{(k-1)})$ and only affected by the previous one $\boldsymbol{\theta}^{(k-1)}$. For large enough N , this chain of random variables can be used to calculate Monte-Carlo estimates, where ergodicity of the Markov chain \mathcal{M} is a sufficient criterion to do so [59, 45].

The ergodicity theorem in [59] states that, if a Markov chain \mathcal{M} is aperiodic, irreducible, and reversible, then it converges to a unique stationary equilibrium distribution. In other words, the chain can reach any state from any other state (irreducibility), is not stuck in periodic cycles (aperiodicity), and satisfies the detailed balance condition [59] (reversibility). Then the samples in that chain $\mathcal{M} \sim \pi(\boldsymbol{\theta} | \mathbf{y})$ are samples from the desired target distribution. In practice, one can inspect the trace $\pi(\boldsymbol{\theta}^{(k)} | \mathbf{y})$ for $k = N_{\text{burn-in}}, \dots, N$ after a “burn-in” period $N_{\text{burn-in}}$ and visually assess if the chain is consistent with ergodicity. The “burn-in” period $N_{\text{burn-in}}$ removes initialisation bias. The specific sampling methods in this thesis possess proven ergodic properties, and we therefore provide the reader with corresponding literature for further details when the methods are introduced.

If the instance $\boldsymbol{\theta}^{(k)}$ of an ergodic Markov chain represents an independent sample of the marginal posterior $\pi(\boldsymbol{\theta} | \mathbf{y})$ and $\mathbf{x}^{(k)}$ is a sample from the full conditional posterior $\pi(\mathbf{x} | \boldsymbol{\theta}^{(k)}, \mathbf{y})$ e.g., as in Sec. 6.2.2, then the resulting sample $(\mathbf{x}^{(k)}, \boldsymbol{\theta}^{(k)})$ is an independent sample from the joint posterior $\pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y})$ [17, 63]. Repeating this procedure gives the chain $\{(\mathbf{x}, \boldsymbol{\theta})^{(1)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(k)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(N)}\} \sim \pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y})$ of independent samples from the joint posterior.

2.3 Numerical Function Approximation – Tensor-Train (TT)

Instead of relying on sampling-based methods to explore an unnormalised density function $\pi(\mathbf{x})$, which in our case will be the marginal posterior distribution over the hyper-parameters, we can approximate this function using a tensor-train (TT) approximation. The TT approximation $\tilde{\pi}(\mathbf{x}) \approx \pi(\mathbf{x})$, where $\mathbf{x} \in \mathbb{R}^d$, on a d -dimensional grid requires far fewer function evaluations compared to conventional sampling methods. In the following, we describe how to compute a normalised marginal probability density function (PDF) $f_{X_k}(x_k)$, for an $x_k \in \mathbf{x}$ and $k = 1, \dots, d$, from a target function $\pi(\mathbf{x})$ approximated in TT format. Further, a scheme similar to the inverse Rosenblatt transform (IRT) in [11] is introduced to generate samples from $\pi(\mathbf{x})$. In doing so, we follow the notation and procedure introduced by Cui and Dolgov [8].

As in [8], the parameter space is defined as the product space $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2 \times \dots \times \mathcal{X}_d$ with $x_k \in \mathcal{X}_k \subseteq \mathbb{R}$. The marginal PDF for the k -th component is then given by

$$f_{X_k}(x_k) = \frac{1}{z} \int_{\mathcal{X}_1} \dots \int_{\mathcal{X}_{k-1}} \int_{\mathcal{X}_{k+1}} \dots \int_{\mathcal{X}_d} \lambda(\mathbf{x}) \pi(\mathbf{x}) \, dx_1 \dots dx_{k-1} \, dx_{k+1} \dots dx_d, \quad (2.19)$$

where we integrate over all dimensions except the k -th, and z is a normalisation constant. Cui and Dolgov [8] refer to $\lambda(x)$ as the “product-form Lebesgue-measurable weighting function”, which can be useful for quadrature rules [9], and define it as

$$\lambda(\mathcal{X}) = \prod_{i=1}^d \lambda_i(\mathcal{X}_i), \quad \text{where } \lambda_i(\mathcal{X}_i) = \int_{\mathcal{X}_i} \lambda_i(x_i) \, dx_i. \quad (2.20)$$

The approximation of a function in the TT format requires a predefine d -dimensional discrete univariate grid over the parameter space \mathcal{X} with n grid points in each direction. For a fixed grid point $\mathbf{x} = (x_1, \dots, x_d)$, $\pi(\mathbf{x})$ is approximated by

$$\tilde{\pi}(\mathbf{x}) = \tilde{\pi}_1(x_1)\tilde{\pi}_2(x_2) \dots \tilde{\pi}_d(x_d),$$

which is a sequence of matrix multiplications with $\tilde{\pi}_k(x_k) \in \mathbb{R}^{r_{k-1} \times r_k}$. A TT core $\tilde{\pi}_k \in \mathbb{R}^{r_{k-1} \times n \times r_k}$ has ranks r_{k-1} and r_k , which connect the core to its respective neighbouring dimensions. The outer ranks of a TT are $r_0 = r_d = 1$. Then, a discrete parameter space \mathcal{X} is approximated by $\pi(\mathcal{X}) \approx \tilde{\pi}_1 \tilde{\pi}_2 \dots \tilde{\pi}_d$ with $2nr + (d-2)nr^2$ evaluation points for fixed ranks $r = r_{k-1} = r_k$, as illustrated in Figure 2.2, instead of n^d function evaluations. In the TT format the integral in Eq. 2.19 can be calculated at a low computational cost and the marginal PDF

$$\begin{aligned} f_{X_k}(x_k) &\approx \frac{1}{z} \left| \left(\int_{\mathcal{X}_1} \lambda_1(x_1) \tilde{\pi}_1(x_1) \, dx_1 \right) \dots \left(\int_{\mathcal{X}_{k-1}} \lambda_{k-1}(x_{k-1}) \tilde{\pi}_{k-1}(x_{k-1}) \, dx_{k-1} \right) \right. \\ &\quad \left. \lambda_k(x_k) \tilde{\pi}_k(x_k) \right. \\ &\quad \left(\int_{\mathcal{X}_{k+1}} \lambda_{k+1}(x_{k+1}) \tilde{\pi}_{k+1}(x_{k+1}) \, dx_{k+1} \right) \dots \left(\int_{\mathcal{X}_d} \lambda_d(x_d) \tilde{\pi}_d(x_d) \, dx_d \right) \right| \end{aligned} \quad (2.21)$$

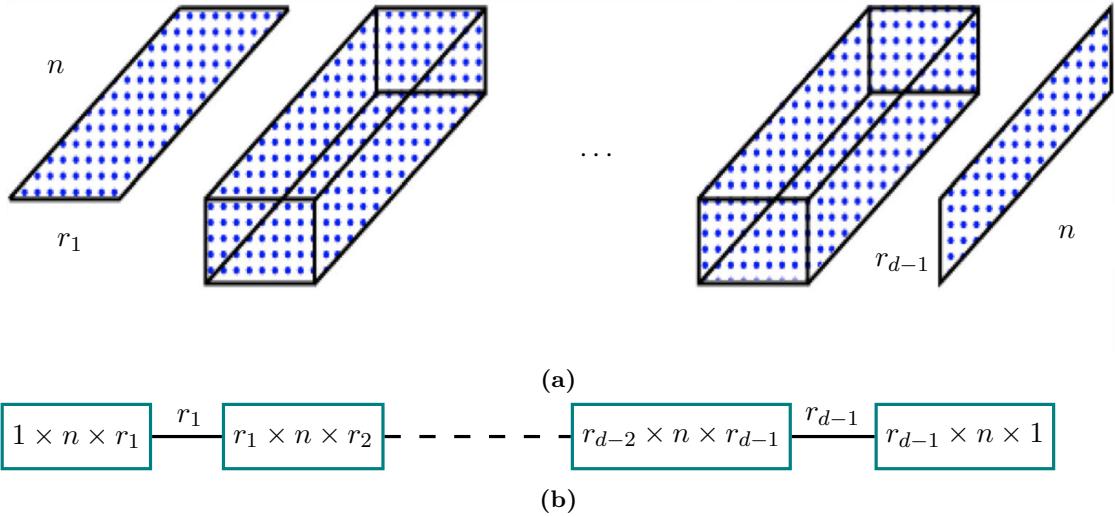


Figure 2.2: Here the TT cores are visualised as a train of two- and three-dimensional matrices. Each core has a length n , corresponding to the number of grid points in each dimension, and the cores are connected through ranks r_k . More specifically, a core $\tilde{\pi}_k$ has dimensions $r_{k-1} \times n \times r_k$, with outer ranks $r_0 = r_d = 1$. Using the TT format enables us to represent a d -dimensional grid with only $2nr + (d - 2)nr^2$ evaluation points instead of n^d grid points. Figure (a) is adapted from [20].

is computed by integrating over all TT cores except the k -th core π_k , as in [11], and normalised by the constant z [8].

In practice, TT approximations may suffer from numerical instability. In particular when the target function is non-negative the TT approximation can have negative values in regions where true function values are very small. One way to ensure non-negativity is to square the target function, hence [8] approximate the square root of the target function and define the approximation as [8, Eq. 18]

$$\sqrt{\pi(\mathbf{x})} \approx \tilde{g}(\mathbf{x}) = \mathbf{G}_1(x_1), \dots, \mathbf{G}_k(x_k), \dots, \mathbf{G}_d(x_d). \quad (2.22)$$

Here, each TT core is given by [8, Eq. 21]

$$G_k^{(\alpha_{k-1}, \alpha_k)}(x_k) = \sum_{i=1}^{n_k} \phi_k^{(i)}(x_k) \mathbf{A}_k[\alpha_{k-1}, i, \alpha_k], \quad k = 1, \dots, d, \quad , \quad (2.23)$$

where $\mathbf{A}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ is the k -th coefficient tensor and $\{\phi_k^{(i)}(x_k)\}_{i=1}^{n_k}$ are the basis functions corresponding to the k -th coordinate. The unnormalised density function is approximated as in [8, Eq. 19] so that

$$\pi(\mathbf{x}) \approx \xi + \tilde{g}(\mathbf{x})^2 \quad (2.24)$$

with a small additive constant $\xi > 0$ to ensure positivity. This maintains that the cumulative distribution functions (CDFs) are monotonically increasing. The CDFs are

needed to draw samples from $\tilde{\pi}(\mathbf{x})$ (see Sec. 2.3.2). The constant ξ is chosen according to the ratio of the Lebesgue weighted L2-norm error and the Lebesgue weighting (see Eq. 2.20 and [8, Eq. 35]) such that

$$0 \leq \xi \leq \frac{1}{\lambda(\mathcal{X})} \|\tilde{g} - \sqrt{\pi}\|_{L^2_\lambda(\mathcal{X})}^2. \quad (2.25)$$

This leads to the normalised PDF [8, Eq. 19]

$$f_X(\mathbf{x}) \approx \frac{1}{z} \left(\lambda(\mathbf{x}) \xi + \lambda(\mathbf{x}) \tilde{g}(\mathbf{x})^2 \right), \quad (2.26)$$

with the normalisation constant $z = \int_{\mathcal{X}} f_X(\mathbf{x}) d\mathbf{x}$. Given the tensor train approximation of $\sqrt{\pi}$, the marginal PDF $f_{X_k}(x_k)$ can be expressed as

$$\begin{aligned} f_{X_k}(x_k) &\approx \frac{1}{z} \left(\xi \prod_{i=1}^{k-1} \lambda_i(\mathcal{X}_i) \prod_{i=k+1}^d \lambda_i(\mathcal{X}_i) \right. \\ &\quad + \left(\int_{\mathcal{X}_1} \lambda_1(x_1) \mathbf{G}_1^2(x_1) dx_1 \right) \cdots \left(\int_{\mathcal{X}_{k-1}} \lambda_{k-1}(x_{k-1}) \mathbf{G}_{k-1}^2(x_{k-1}) dx_{k-1} \right) \\ &\quad \lambda_k(x_k) \mathbf{G}_k^2(x_k) \\ &\quad \left. \left(\int_{\mathcal{X}_{k+1}} \lambda_{k+1}(x_{k+1}) \mathbf{G}_{k+1}^2(x_{k+1}) dx_{k+1} \right) \cdots \left(\int_{\mathcal{X}_d} \lambda_d(x_d) \mathbf{G}_d^2(x_d) dx_d \right) \right). \end{aligned} \quad (2.27)$$

2.3.1 Marginal Functions

The marginal functions $f_{X_k}(x_k)$ of the PDF $f_X(\mathbf{x})$ are computed by a procedure to which Cui and Dolgov [8] refer to as backward marginalisation, see Prop. 2, and to which we add the forward marginalisation, see Prop. 1. This is similar to the left and right orthogonalisation of TT cores [38, 37]. The backward marginalisation provides the coefficient matrices \mathbf{B}_k , while the forward marginalisation gives the coefficient matrices $\mathbf{R}_{\text{pre},k}$. These matrices enable the efficient evaluation of marginal functions since they are formed by integration over the parameter space either left or right of the k -th dimension, as in [8]. In doing so, the mass matrix $\mathbf{M}_k \in \mathbb{R}^{n_k \times n_k}$ is defined as in [8, Eq. 22]

$$\mathbf{M}_k[i, j] = \int_{\mathcal{X}_k} \phi_k^{(i)}(x_k) \phi_k^{(j)}(x_k) \lambda(x_k) dx_k, \quad i, j = 1, \dots, n_k, , \quad (2.28)$$

where $\{\phi_k^{(i)}(x_k)\}_{i=1}^{n_k}$ denotes the set of basis functions for the k -th coordinate. The proposition used to compute \mathbf{B}_k , stated in Prop. 1, is adapted directly from [8].

After computing the coefficient tensors $\mathbf{R}_{\text{pre},k-1}$ as in Prop. 2 and \mathbf{B}_k from Prop. 1, the marginal PDF of k -th dimension can be expressed as

$$f_{X_k}(x_k) \approx \frac{1}{z} \left(\xi \prod_{i=1}^{k-1} \lambda_i(X_i) \prod_{i=k+1}^d \lambda_i(X_i) + \sum_{l_{k-1}=1}^{r_{k-1}} \sum_{l_k=1}^{r_k} \left(\sum_{i=1}^n \phi_k^{(i)}(x_k) \mathbf{D}_k[l_{k-1}, i, l_k] \right)^2 \right) \lambda_k(x_k), \quad (2.29)$$

where $\mathbf{D}_k \in \mathbb{R}^{r_{k-1} \times n \times r_k}$ and given as

$$\mathbf{D}_k[l_{k-1}, i, l_k] = \sum_{\alpha_{k-1}=1}^{r_{k-1}} \mathbf{R}_{\text{pre}, k-1}[l_{k-1}, \alpha_{k-1}] \mathbf{B}_k[\alpha_{k-1}, i, l_k], \quad (2.30)$$

with $\mathbf{R}_{\text{pre}, k-1} \in \mathbb{R}^{r_{k-1} \times r_{k-1}}$ and $\mathbf{B}_k \in \mathbb{R}^{r_{k-1} \times n \times r_k}$.

For the first dimension, $f_{X_1}(x_1)$ can be expressed as [8, Eq. 30]

$$f_{X_1}(x_1) \approx \frac{1}{z} \left(\xi \prod_{i=2}^d \lambda_i(\mathcal{X}_i) + \sum_{l_1=1}^{r_1} \left(\sum_{i=1}^n \phi_1^{(i)}(x_1) \mathbf{D}_1[i, l_1] \right)^2 \right) \lambda_1(x_1), \quad (2.31)$$

where $\mathbf{D}_1[i, l_1] = \mathbf{B}_1[\alpha_0, i, l_1]$ and $\alpha_0 = 1$, and similarly in the last dimension

$$f_{X_d}(x_d) \approx \frac{1}{z} \left(\xi \prod_{i=1}^{d-1} \lambda_i(\mathcal{X}_i) + \sum_{l_{d-1}=1}^{r_{d-1}} \left(\sum_{i=1}^n \phi_d^{(i)}(x_d) \mathbf{D}_d[l_{d-1}, i] \right)^2 \right) \lambda_d(x_d), \quad (2.32)$$

where $\mathbf{D}_d[l_{d-1}, i] = \mathbf{B}_{\text{pre}, d}[l_{d-1}, i, \alpha_{d+1}]$ and $\alpha_{d+1} = 1$. In practice, we calculate z numerically within the process of computing the marginal PDFs so that $\sum f_{X_k}(x_k) = 1$ and for Cartesian basis the mass matrix becomes $\mathbf{M}_k = \text{diag}(\lambda_k(\mathcal{X}_k))$ with $\lambda(x) = 1$.

Proposition 1 (Backward Marginalisation as in [8]): Starting with the last coordinate $k = d$, we set $\mathbf{B}_d = \mathbf{A}_d$. The following procedure can be used to obtain the coefficient tensor $\mathbf{B}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$, which is needed for defining the marginal function $f_{X_k}(x_k)$ or to draw samples from $\tilde{\pi}(\mathbf{x})$ via the squared IRT scheme (see Alg. Box 1):

1. Use the Cholesky decomposition of the mass matrix, $\mathbf{L}_k \mathbf{L}_k^\top = \mathbf{M}_k \in \mathbb{R}^{n_k \times n_k}$, to construct a tensor $\mathbf{C}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ [8, Eq. 27]:

$$\mathbf{C}_k[\alpha_{k-1}, \tau, l_k] = \sum_{i=1}^{n_k} \mathbf{B}_k[\alpha_{k-1}, i, l_k] \mathbf{L}_k[i, \tau]. \quad (2.33)$$

2. Unfold \mathbf{C}_k along the first coordinate and compute the thin QR decomposition, so that $\mathbf{C}_k^{(R)} \in \mathbb{R}^{r_{k-1} \times (n_k r_k)}$ [8, Eq. 28]:

$$\mathbf{Q}_k \mathbf{R}_k = (\mathbf{C}_k^{(R)})^\top. \quad (2.34)$$

3. Compute the new coefficient tensor [8, Eq. 29]:

$$\mathbf{B}_{k-1}[\alpha_{k-2}, i, l_{k-1}] = \sum_{\alpha_{k-1}=1}^{r_{k-1}} \mathbf{A}_{k-1}[\alpha_{k-2}, i, \alpha_{k-1}] \mathbf{R}_k[l_{k-1}, \alpha_{k-1}]. \quad (2.35)$$

Proposition 2 (Forward Marginalisation): Starting with the first coordinate $k = 1$, we set $\mathbf{B}_{\text{pre},1} = \mathbf{A}_1$. The following procedure can be used to obtain $\mathbf{R}_{\text{pre},k-1} \in \mathbb{R}^{r_{k-1} \times r_{k-1}}$ for defining the marginal function $f_{X_k}(x_k)$:

1. Use the Cholesky decomposition of the mass matrix, $\mathbf{L}_k \mathbf{L}_k^\top = \mathbf{M}_k \in \mathbb{R}^{n_k \times n_k}$, to construct a tensor $\mathbf{C}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$:

$$\mathbf{C}_{\text{pre},k}[\alpha_{k-1}, \tau, l_k] = \sum_{i=1}^{n_k} \mathbf{L}_k[i, \tau] \mathbf{B}_{\text{pre},k}[\alpha_{k-1}, i, l_k]. \quad (2.36)$$

2. Unfold $\mathbf{C}_{\text{pre},k}$ along the first coordinate and compute the thin QR decomposition, so that $\mathbf{C}_{\text{pre},k}^{(R)} \in \mathbb{R}^{(r_{k-1} n_k) \times r_k}$:

$$\mathbf{Q}_{\text{pre},k} \mathbf{R}_{\text{pre},k} = (\mathbf{C}_{\text{pre},k}^{(R)}). \quad (2.37)$$

3. Compute the new coefficient tensor $\mathbf{B}_{\text{pre},k+1} \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$:

$$\mathbf{B}_{\text{pre},k+1}[l_{k+1}, i, \alpha_{k+1}] = \sum_{\alpha_k=1}^{r_k} \mathbf{R}_{\text{pre},k}[l_{k+1}, \alpha_k] \mathbf{A}_{k+1}[\alpha_k, i, \alpha_{k+1}]. \quad (2.38)$$

2.3.2 Sampling from a TT Approximation

Instead of evaluating marginal functions for quadrature, the inverse Rosenblatt transform (IRT) provides a scheme to draw samples from an approximated function in the TT format [11]. The idea is that a target function can be represented as the sequence $f_X(\mathbf{x}) = f_{X_1}(x_1)f_{X_2|X_1}(x_2|x_1)\cdots f_{X_k|X_{<k}}(x_k|x_{k-1},\dots,x_1)$. Within the IRT scheme samples are iteratively drawn from each $f_{X_k|X_{<k}}(x_k|x_{k-1},\dots,x_1)$ conditioned on the previous left $k-1$ samples and marginalised over the right $k+1$ dimensions, for $k=2,\dots,d-1$. Since the square root of the target function is approximated, Cui and Dolgov [8] call that the squared inverse Rosenblatt transform (SIRT).

Algorithm 1: Squared Inverse Rosenblatt Transform (SIRT)

```

1: Input: seeds  $\{\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(N)}\} \sim \mathcal{U}(0, 1)^d$  and  $\mathbf{B}_1, \dots, \mathbf{B}_d$  from Prop. 1.
2: for  $s = 1, \dots, N$  do
3:   for  $k = 1, \dots, d$  do
4:     Compute normalised PDF  $f_{X_k|X_{<k}}(x_k|x_{k-1}^{(s)}, \dots, x_1^{(s)})$  as in Eq. 2.40.
5:     Compute cumulative distribution function  $F_{X_k|X_{<k}}(x_k)$  as in Eq. 2.39.
6:     Project sample  $x_k^{(s)} = F_{X_k|X_{<k}}^{-1}(u_k^{(s)})$ .
7:     Interpolate  $\mathbf{G}_k(x_k^{(s)})$  as in Eq. 2.41.
8:     Update  $\mathbf{G}_{\leq k}(x_{\leq k}^{(s)}) = \mathbf{G}_{<k}(x_{<k}^{(s)})\mathbf{G}_k(x_k^{(s)})$ .
9:   end for
10: end for
11: Output: samples  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\}$  with  $\mathbf{x}^{(s)} \in \mathbb{R}^d$ , for  $s = 1, \dots, N$ .
```

Given the backward marginal coefficient tensors $\mathbf{B}_1, \dots, \mathbf{B}_d$ as in Prop. 1 and N uniformly distributed seeds $\{\mathbf{u}^{(1)}, \dots, \mathbf{u}^{(N)}\} \sim \mathcal{U}(0, 1)^d$, where each $\mathbf{u}^{(s)}$ is d -dimensional for $s = 1, \dots, N$, the first marginal $f_{X_1}(x_1)$ is calculated as in Eq. 2.31 and normalised with $z = \int_{\mathcal{X}_1} f_{X_1}(x_1) dx_1$. Next, the CDF $F_{X_1}(x_k) = \int_{-\infty}^{x_k} f_{X_1}(\hat{x}_1) d\hat{x}_1$ is formed, which for the general case is given as [8, Eq. 17]:

$$F_{X_k|X_{<k}}(x_k) = \int_{-\infty}^{x_k} f_{X_k|X_{<k}}(\hat{x}_k|x_{k-1}, \dots, x_1) d\hat{x}_k ; \quad (2.39)$$

Then the seed $u_k^{(s)}$ is projected onto the parameter space to generate the sample $x_k^{(s)} = F_{X_k|X_{<k}}^{-1}(u_k^{(s)})$. For $k = 2, \dots, d$ the general “conditional marginal” is given as [8, Eq. 31]:

$$\begin{aligned} f_{X_k|X_{<k}}(x_k|x_{k-1}^{(s)}, \dots, x_1^{(s)}) &\approx \frac{1}{z} \left(\xi \prod_{i=k+1}^d \lambda_i(X_i) + \right. \\ &\quad \left. \sum_{l_k=1}^{r_k} \left(\sum_{i=1}^n \phi_k^{(i)}(x_k^{(s)}) \left(\sum_{\alpha_{k-1}=1}^{r_{k-1}} \mathbf{G}_{<k}^{(\alpha_{k-1})}(x_{<k}^{(s)}) \mathbf{B}_k[\alpha_{k-1}, i, l_k] \right) \right)^2 \right) \lambda_k(x_k) , \end{aligned} \quad (2.40)$$

where we marginalise over the dimensions $k+1, \dots, d$ via \mathbf{B}_k and condition on the previous $k-1$ samples through the product $\mathbf{G}_k(x_k^{(s)}) \in \mathbb{R}^{1 \times r_{k-1}}$. Function values between grid points i and $i+1$ are approximated with a piecewise polynomial interpolation

$$\mathbf{G}_k(x_k^{(s)}) \approx \frac{x_k^{(s)} - x_k^{(i)}}{x_k^{(i+1)} - x_k^{(i)}} \mathbf{G}_k(x_k^{(i+1)}) + \frac{x_k^{(i+1)} - x_k^{(s)}}{x_k^{(i+1)} - x_k^{(i)}} \mathbf{G}_k(x_k^{(i)}), \quad (2.41)$$

for $x_k^{(i)} \leq x_k^{(s)} \leq x_k^{(i+1)}$, as in [11] for the next ‘‘conditional marginal’’.

The procedure is repeated for each $u_k^{(s)} \in \mathbf{u}^{(s)}$ to produce the samples $\mathbf{x}^{(s)} \sim f_X(\mathbf{x})$, as summarised in Alg. Box 1.

Metropolis–Hastings – correction step

Since the samples by the SIRT scheme are generated from an approximation, it is sensible to correct those using a Metropolis–Hastings (MH) importance step as in [11].

Algorithm 2: MH correction step

```

1: Input: samples  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N+1)}\}$ , where each  $\mathbf{x}^{(s)} \in \mathbb{R}^d$  for  $s = 1, \dots, N+1$ .
2: for  $s = 1, \dots, N-1$  do
3:   Compute MH ratio  $\frac{w^{(s+1)}}{w^{(s)}} = \frac{\pi(\mathbf{x}^{(s+1)})}{\pi(\mathbf{x}^{(s)})} \frac{f_X(\mathbf{x}^{(s)})}{f_X(\mathbf{x}^{(s+1)})}$ .
4:   Compute acceptance probability  $\alpha = \min(w^{(s+1)}/w^{(s)}, 1)$ .
5:   Draw  $u \sim \mathcal{U}(0, 1)$ .
6:   if  $\alpha \geq u$  then
7:     Accept and set  $\mathbf{x}_{\text{MH}}^{(s+1)} = \mathbf{x}^{(s+1)}$ .
8:   else
9:     Reject and keep  $\mathbf{x}_{\text{MH}}^{(s+1)} = \mathbf{x}^{(s)}$ .
10:  end if
11: end for
12: Output: corrected sample chain  $\{\mathbf{x}_{\text{MH}}^{(1)}, \dots, \mathbf{x}_{\text{MH}}^{(N)}\}$ , where each  $\mathbf{x}_{\text{MH}}^{(s)} \in \mathbb{R}^d$  for  $s = 1, \dots, N$ .
```

In doing so, we compute the acceptance probability $\alpha = \min(w^{(s+1)}/w^{(s)}, 1)$, where

$$w(\mathbf{x}) = \frac{\pi(\mathbf{x})}{f_X(\mathbf{x})} = \frac{\pi(\mathbf{x})}{\xi + \tilde{g}(\mathbf{x})^2} \quad (2.42)$$

is the importance ratio. Note the normalising constants in the ratio $w^{(s+1)}/w^{(s)}$ cancel. In practice, the importance ratio is calculated in the log-space so that $\log f_X(\mathbf{x}) = \log f_{X_1}(x_1) + \log f_{X_2|X_1}(x_2|x_1) + \dots + \log f_{X_k|X_{<k}}(x_k|x_{k-1}, \dots, x_1)$ (see Eq. 2.40). We refer to this as the SIRT-MH scheme, which provides the corrected chain $\{\mathbf{x}_{\text{MH}}^{(1)}, \dots, \mathbf{x}_{\text{MH}}^{(N)}\} \sim \pi(\mathbf{x})$.

2.3.3 Error of the TT Approximation

A straightforward way to assess an average error of a TT approximation is to calculate the relative root mean squared (RMS) error

$$\left(\frac{\int_{\mathcal{X}} (\pi(\mathbf{x}) - (\xi + \tilde{g}(\mathbf{x})^2))^2 \lambda(\mathbf{x}) d\mathbf{x}}{\int_{\mathcal{X}} \pi(\mathbf{x})^2 \lambda(\mathbf{x}) d\mathbf{x}} \right)^{1/2} = \frac{\|\pi(\mathbf{x}) - (\xi + \tilde{g}(\mathbf{x})^2)\|_{L^2_\lambda(\mathcal{X})}}{\|\pi(\mathbf{x})\|_{L^2_\lambda(\mathcal{X})}}. \quad (2.43)$$

The RMS is approximated by

$$\left(\frac{1}{N} \sum_{i=1}^N \left(\pi(\mathbf{x}^{(i)}) - (\xi + \tilde{g}(\mathbf{x}^{(i)})^2) \right)^2 \lambda(\mathbf{x}^{(i)}) \right)^{1/2} \approx \left(\int_{\mathcal{X}} (\pi(\mathbf{x}) - (\xi + \tilde{g}(\mathbf{x})^2))^2 \lambda(\mathbf{x}) d\mathbf{x} \right)^{1/2} \quad (2.44)$$

and similarly $\int_{\mathcal{X}} \pi(\mathbf{x})^2 \lambda(\mathbf{x}) d\mathbf{x}$.

Absolute error bound

If large errors occur in regions with low probability, the RMS is sensitive to those, whereas the Wasserstein distance weighs differences according to their respective probability values.

The Wasserstein distance is the infimum over all couplings between two probability distributions with respect to some distance measure. The Kantorovich-Rubinstein duality, as in [60, 1], says that the 1-Wasserstein distance is equal to the supremum of differences in expectations over all 1-Lipschitz functions h between two probability distributions. So the 1-Wasserstein distance provides an upper absolute error bound and is defined as

$$W_1(\pi, \tilde{\pi}) = \inf_{\nu \in \Pi(\pi, \tilde{\pi})} \int_{\mathcal{X} \times \mathcal{X}} c_{\mathcal{X}}(\mathbf{x}, \tilde{\mathbf{x}}) \nu(\mathbf{x}, \tilde{\mathbf{x}}) d\mathbf{x} d\tilde{\mathbf{x}}, \quad (2.45)$$

where ν couples \mathbf{x} and $\tilde{\mathbf{x}}$ so that the integral over the distance $c_{\mathcal{X}}(\mathbf{x}, \tilde{\mathbf{x}})$ weighted by the probability measures π and $\tilde{\pi}$ is the greatest lower bound of all integrals with respect to ν in the set of all couplings $\Pi(\pi, \tilde{\pi})$. Often ν is the transport plan, where $c_{\mathcal{X}}(\mathbf{x}, \tilde{\mathbf{x}})$ is the (ground) cost function, and $\nu(\mathbf{x}, \tilde{\mathbf{x}})$ is related to the mass which has to be transported and the 1-Wasserstein distance is the earth mover distance. On the other hand (Kantorovich-Rubinstein duality), the 1-Wasserstein distance

$$W_1(\pi, \tilde{\pi}) = \sup_{h(\mathbf{x}); c_{\mathcal{Y}}(h(\mathbf{x}), h(\tilde{\mathbf{x}})) \leq c_{\mathcal{X}}(\mathbf{x}, \tilde{\mathbf{x}})} \left\{ \int_{\mathcal{X}} h(\mathbf{x}) d\pi(\mathbf{x}) - \int_{\mathcal{X}} h(\tilde{\mathbf{x}}) d\tilde{\pi}(\tilde{\mathbf{x}}) \right\} \quad (2.46)$$

$$= \sup_{h(\mathbf{x}); c_{\mathcal{Y}}(h(\mathbf{x}), h(\tilde{\mathbf{x}})) \leq c_{\mathcal{X}}(\mathbf{x}, \tilde{\mathbf{x}})} \left\{ \mathbb{E}_{\mathbf{x} \sim \pi}[h(\mathbf{x})] - \mathbb{E}_{\tilde{\mathbf{x}} \sim \tilde{\pi}}[h(\tilde{\mathbf{x}})] \right\}. \quad (2.47)$$

is the lowest upper bound of differences in expectations over all 1-Lipschitz function $h(\mathbf{x}) : \mathcal{X} \rightarrow \mathcal{Y}$ in between the two distributions π and $\tilde{\pi}$, with the distance measure $c_{\mathcal{X}}$ on the set \mathcal{X} forming the metric space $(\mathcal{X}, c_{\mathcal{X}})$ and similarly the metric space $(\mathcal{Y}, c_{\mathcal{Y}})$.

For two sample sets $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\} \sim \pi$ and $\{\tilde{\mathbf{x}}^{(1)}, \dots, \tilde{\mathbf{x}}^{(M)}\} \sim \tilde{\pi}$ the calculation of the Wasserstein distance becomes an optimisation problem. That is to find the best coupling of samples weighted by their distribution value according to an appropriate distance measure [15], which we set to $c_{\mathcal{X}}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} - \tilde{\mathbf{x}}\|_{L^2}$. More specifically,

$$W_1(\pi, \tilde{\pi}) = \min_{\nu \in \Pi(\pi, \tilde{\pi})} \sum_{j=1}^M \sum_{i=1}^N \nu_{ij} \|\mathbf{x}^{(i)} - \tilde{\mathbf{x}}^{(j)}\|_{L^2}, \quad (2.48)$$

where the transport plan $\nu \in \mathbb{R}_{\geq 0}^{N \times M}$ defines the coupling $\nu_{ij} \in \nu$ as $\nu_{ij} := \pi(\mathbf{x}^{(i)})\tilde{\pi}(\tilde{\mathbf{x}}^{(j)})$ similar to [15, Eq. 3.166]. Additionally it is required that $\sum_{i=1}^N \pi(\mathbf{x}^{(i)}) = \sum_{j=1}^M \tilde{\pi}(\tilde{\mathbf{x}}^{(j)}) = 1$. This gives us an upper bound of the absolute error between the expected value of any 1-Lipschitz function h .

2.4 Regularisation Approach

The currently most used method to analyse data in atmospheric physics is regularisation-based. Since we want to show that Bayesian methods provide more information than regularisation at a similar computational cost, the chosen regularisation approach is the closest equivalent to the linear-Gaussian Bayesian framework [17] in Sec. 4.1.

For a linear forward model matrix \mathbf{A} , data \mathbf{y} and a regularisation operator \mathbf{T} , the regularisation approach provides one solution \mathbf{x} that minimises both the data misfit norm

$$\|\mathbf{Ax} - \mathbf{y}\|_{L^2} \quad (2.49)$$

and a regularisation norm

$$\|\mathbf{T}\mathbf{x}\|_{L^2}. \quad (2.50)$$

For a fixed regularisation parameter $\lambda > 0$, the regularised solution as in [25, 17, 59] is given by \mathbf{x}_λ that minimises the weighted sum

$$\mathbf{x}_\lambda = \arg \min_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{y}\|_{L^2}^2 + \lambda \|\mathbf{T}\mathbf{x}\|_{L^2}^2, \quad (2.51)$$

which can be calculated by taking the derivative with respect to \mathbf{x} :

$$\nabla_{\mathbf{x}} \left\{ (\mathbf{Ax} - \mathbf{y})^T (\mathbf{Ax} - \mathbf{y}) + \lambda \mathbf{x}^T \mathbf{T}^T \mathbf{T} \mathbf{x} \right\} = 0 \quad (2.52)$$

$$\iff \nabla_{\mathbf{x}} \left\{ \mathbf{y}^T \mathbf{y} + \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - 2 \mathbf{y}^T \mathbf{A} \mathbf{x} + \lambda \mathbf{x}^T \mathbf{T}^T \mathbf{T} \mathbf{x} \right\} = 0 \quad (2.53)$$

$$\iff 2 \mathbf{A}^T \mathbf{A} \mathbf{x} - 2 \mathbf{A}^T \mathbf{y} + 2 \lambda \mathbf{T}^T \mathbf{T} \mathbf{x} = 0. \quad (2.54)$$

Eq. 2.54 yields the regularised solution

$$\mathbf{x}_\lambda = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L})^{-1} \mathbf{A}^T \mathbf{y}, \quad (2.55)$$

where we define $\mathbf{L} := \mathbf{T}^T \mathbf{T}$. Typically, \mathbf{L} represents a discrete matrix approximation of a differential operator [59]. For example

$$\mathbf{T} = \frac{1}{h} \begin{bmatrix} -1 & 1 & & & \\ 0 & -1 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & -1 & 1 \\ & & & 0 & -1 \end{bmatrix}, \quad (2.56)$$

is the first order forward difference operator with equal spacing h as in [59] that approximates the first derivative. Then

$$\mathbf{T}^T \mathbf{T} = \frac{1}{h^2} \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix}, \quad (2.57)$$

is a discrete approximation to the second derivative with Neumann boundary conditions [66].

If λ is large, then the effect of the data on the solution \mathbf{x}_λ is small and dominated by the regulariser, resulting in an under-fitted \mathbf{x}_λ . For example, if the regulariser imposes smoothness, the solutions will be overly smooth and not sensitive to structures from the data. If λ is small, the solution \mathbf{x}_λ will be dominated by the data misfit norm. Then \mathbf{x}_λ is sensitive to noise, resulting in an over-fitted solution inheriting the structure of the noise. We refer to [26] and [59] for a more comprehensive analysis on the effects of the regularisation parameter on the solution e.g., due to small singular values of the forward model.

In practice, \mathbf{x}_λ is computed for a range of λ -values and the data misfit norm versus the regularisation norm is plotted in log-space to form an L-curve (see Fig. 4.8). Based on the trade-off between the data misfit and the regularisation norm, the regularised estimate corresponds to the point of maximum curvature of the L-curve [27].

Alternatively one can introduce a Lagrangian $\mathcal{L}(\mathbf{x}, \lambda) := \|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{L^2}^2 + \lambda \mathbf{x}^T \mathbf{L}\mathbf{x}$ similar to [32], where λ is a Lagrange multiplier. For a given λ , a solution \mathbf{x}_λ that minimises $\mathcal{L}(\mathbf{x}, \lambda)$ is usually obtained by finding the minimum of $\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{L^2}^2$ with respect to the constant constrained $\mathbf{x}^T \mathbf{L}\mathbf{x} = c$ [51, Fig. 2.13]. This is equivalent to $\mathbf{x}_\lambda = \arg \min_{\mathbf{x}} \mathbf{x}^T \mathbf{L}\mathbf{x}$ subject to a constant constrain $\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{L^2}^2 = c$ (see [17, fn. 6]). So every solution \mathbf{x}_λ is extremely regularised for a given data misfit and the L-curve presents a lower boundary to an open set of high-dimensional posterior samples [65]. Hence, every sample of the high-dimensional posterior, which represents a feasible solution given the data, lies above the L-Curve, is less regularised and has a higher $\mathbf{x}^T \mathbf{L}\mathbf{x}$ value.

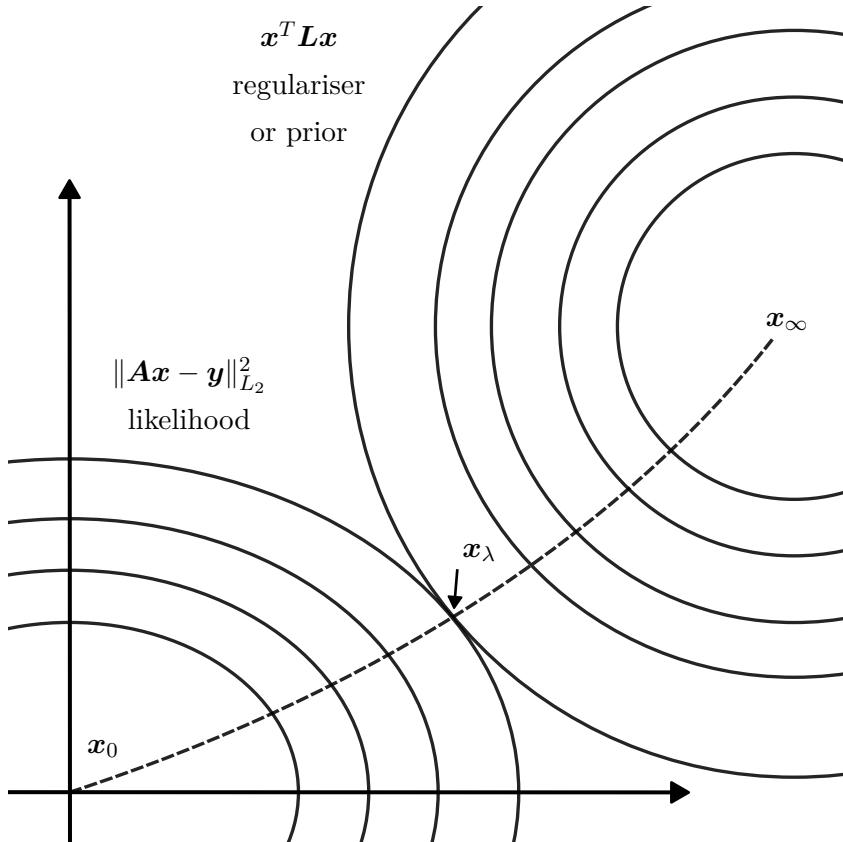


Figure 2.3: This Figure is not to scale and directly inspired by [19]. One regularisation solution \mathbf{x}_λ is obtained by following a contour line $\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{L^2}^2 = c$ until $\mathbf{x}^T \mathbf{L} \mathbf{x}$ is minimised. λ is the regularisation parameter or Lagrange multiplier and ranges from 0 to ∞ . In the centre of the likelihood contours a solution \mathbf{x}_0 unaffected by the regulariser is obtained, whereas the solution \mathbf{x}_∞ is determined a-priori.

3

The Forward Model

In this Chapter, we present the forward model to which we apply our entire methodology. A singular value analysis for different measurement scenarios is conducted to understand the forward model and to determine a sensible way to measure ozone. We follow the Michelson interferometer for passive atmospheric sounding (MIPAS) handbook [43] and simulate data according to an idealised cloud-free atmosphere in local thermodynamic equilibrium, assuming a measurement instrument with infinite spectral resolution and no pointing errors. This is a simplified forward model, and no other instrument-specific details such as sensor area or antenna response are inculded because they are not available to us.

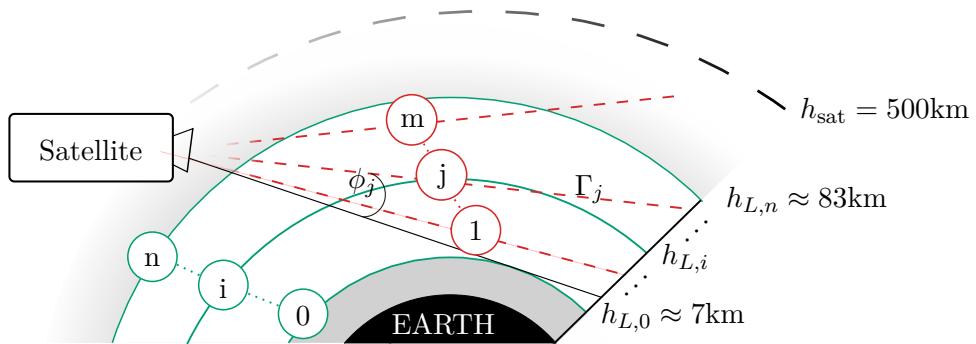


Figure 3.1: Schematic of measurement and analysis geometry, not to scale. The stationary satellite, at a constant height h_{sat} above Earth, takes m measurements along its line-of-sight defined by the line Γ_j . Each measurement has a pointing angle ϕ_j and a tangent height $h_{\ell,j}$, $j = 1, 2, \dots, m$ defined as the closest distance of Γ_j to the Earth's surface. Between $h_{L,0} \approx 7\text{km}$ and $h_{L,n} \approx 83\text{km}$, the atmosphere is discretised into n layers as illustrated by the solid green lines.

3.1 Radiative Transfer Equation

A satellite at a constant height h_{sat} points through the atmosphere (limb-sounding) and measures thermal radiation of gas molecules along its straight line of sight Γ_j , see Figure 3.1. One measurement of the thermal radiation of one specific molecule, in our case ozone, denoted by the ozone volume mixing ratio (VMR) $x(r)$ at distance r from the satellite, at the wave number ν , is given by the path integral

$$y_j = \int_{\Gamma_j} B(\nu, T) k(\nu, T) \frac{p(T)}{k_B T(r)} x(r) \tau(r) dr + \eta_j \quad (3.1)$$

$$\tau(r) = \exp \left\{ - \int_{r_{\text{obs}}}^r k(\nu, T) \frac{p(T)}{k_B T(r')} x(r') dr' \right\}, \quad (3.2)$$

which is the radiative transfer equation (RTE) [43]. For more information on the processes within the atmosphere for ozone, we refer to [31]. We define a tangent height h_{ℓ_j} and Γ_j for each $j = 1, 2, \dots, m$, so that the data vector $\mathbf{y} \in \mathbb{R}^m$ including some additive noise η_j . Additionally, the pointing angle $0 \leq \phi_j < \phi_{\max}$ is defined so that if $\phi = 0$ arc sec the satellite points at $h_{L,0}$ and for a pointing angle ϕ_{\max} at $h_{L,n}$. Within the atmosphere, the number density $p(T)/(k_B T(r))$ of molecules is dependent on the pressure $p(T)$, the temperature $T(r)$, and the Boltzmann constant k_B . The factor $\tau(r) \leq 1$ accounts for re-absorption of the radiation along the line-of-sight, which makes the RTE non-linear. The absorption constant

$$k(\nu, T) = L(\nu, T_{\text{ref}}) \frac{Q(T_{\text{ref}})}{Q(T)} \frac{\exp \{-c_2 E''/T\}}{\exp \{-c_2 E''/T_{\text{ref}}\}} \frac{1 - \exp \{-c_2 \nu/T\}}{1 - \exp \{-c_2 \nu/T_{\text{ref}}\}} \quad (3.3)$$

is dependent on the line intensity $L(\nu, T_{\text{ref}})$ at reference temperature $T_{\text{ref}} = 296K$, the lower-state energy E'' in cm^{-1} of the targeted transition and the second radiation constant $c_2 := hc/k_B \approx 1.44\text{cmK}$ as in the HITRAN database [23], with Planck's constant h and speed of light c . It is assumed that the measurement device has a negligible frequency window. That is why we neglect line broadening around ν for the calculations of $L(\nu, T_{\text{ref}})$. This would normally be modelled as the convolution of the normalised Lorentz profile (collisional/pressure broadening) and the normalised Doppler profile (thermal broadening) [43]. Additionally, we target one specific molecule and calculate $k(\nu, T)$ accordingly, which usually would involve summing the individual absorption constants for multiple radiating molecules weighted by their respective VMR [43]. The total internal partition function is given as

$$Q(T) = g' \exp \left\{ -\frac{c_2 E'}{T} \right\} + g'' \exp \left\{ -\frac{c_2 E''}{T} \right\}, \quad (3.4)$$

with the statistical weight g'' for the lower and g' for the upper energy state (also called the degeneracy factors) accounting for the molecule's non-rotational and rotational energy

states (see [55]), and the upper state energy $E' = E'' + \nu$. Under the assumption of local thermodynamic equilibrium (LTE), the black body radiation acts as a source function

$$B(\nu, T) = \frac{2hc^2\nu^3}{\exp\left\{\frac{c_2\nu}{T}\right\} - 1}. \quad (3.5)$$

For fundamentals on the RTE, we recommend [50, Chapter 1], and for a more comprehensive model, we refer to [42].

3.2 Simulate Data Based on a Ground Truth

One measurement is calculated according to the integrals in Eq. 3.1 and Eq. 3.2. In doing so, we discretise the atmosphere in n layers and define height values $h_{L,i-1} < h_{L,i}$ with respect to the surface of the Earth, for $i = 1, \dots, n$. The i -th layer is defined by two spheres around the centre of the Earth with radii $r_0 + h_{L,i-1}$ and $r_0 + h_{L,i}$, where r_0 is the Earth's radius. Then the ozone VMR $\mathbf{x} = \{x_1, x_2, \dots, x_n\} \in \mathbb{R}^n$, pressure $\mathbf{p} = \{p_1, p_2, \dots, p_n\} \in \mathbb{R}^n$ and temperature $\mathbf{T} = \{T_1, T_2, \dots, T_n\} \in \mathbb{R}^n$, as well as all other height dependent parameters, are discretised profiles with constant values between the heights $h_{L,i-1} \leq h < h_{L,i}$. Above $h_{L,n}$ and below $h_{L,0}$, the ozone VMR is set to zero, so no signal can be obtained. We evaluate the integral in Eq. (3.1) for one noise-free measurement $A_j(\mathbf{p}, \mathbf{T}, \mathbf{x})$, using the trapezoidal rule. Here, each entry A_j of $\mathbf{A}(\mathbf{p}, \mathbf{T}, \mathbf{x}) \in \mathbb{R}^m$ includes multiple evaluations of the integral in Eq. 3.2 to calculate the absorption $\tau(r)$. The data vector

$$\mathbf{y} = \mathbf{A}(\mathbf{x}) + \boldsymbol{\eta} \quad (3.6)$$

includes an additive noise vector $\boldsymbol{\eta} \in \mathbb{R}^m$. For brevity the non-linear forward model is defined as $\mathbf{A}(\mathbf{x}) := \mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T}) \in \mathbb{R}^m$. Similarly, $\mathbf{A}_L \in \mathbb{R}^{m \times n}$ denotes the linear forward model matrix and neglects absorption (e.g., set $\tau = 1$ in Eq. (3.2)) and enables matrix-vector multiplication $\mathbf{A}_L \mathbf{x}$ to compute noise-free linear data. Further, we classify the inverse problem as a weakly non-linear inverse problem, because neglecting the absorption changes the measurements only slightly (about 1%, see Chapter 5).

As the ground truth for our methodology, we consider an ozone profile at distinct pressure values generated from some data [53] of the MLS on the Aura satellite within the Antarctic region. This ozone profile has a peak in the middle atmosphere and a second peak at higher altitudes, see Fig. 4.5, which seems to be a typical nighttime profile [31].

We recursively relate pressure p to geometric height h with the hydrostatic equilibrium equation

$$\frac{dp}{p} = \frac{-gM}{R^*T} dh, \quad (3.7)$$

subscript i	geometric height $h_{T,i}$ in km	gradient a_i
0	0	-6.5
1	11	0
2	20.1	1
3	32.2	2.8
4	47.4	0
5	51.4	-2.8
6	71.8	-2

Table 3.1: Definition of height depending temperature gradients.

starting with the mean sea level pressure 1013.25hPa and temperature $T_0 = 288.15\text{K}$ [61]. The acceleration due to gravity is

$$g = g_0 \left(\frac{r_0}{r_0 + h} \right), \quad (3.8)$$

where the polar radius of the Earth is $r_0 \approx 6356\text{ km}$, the gravitation at sea level is $g_0 \approx 9.81\text{m/s}^2$, $R^* = 8.31432 \times 10^{-3}\text{Nm/kmol/K}$ and the mean molecular weight of the air is $M = 28.97\text{kg/kmol}$ [61]. This holds up to a geometric height of 86km, where we ignore a 0.04% non-linear change in M from 80km to 86km.

Following [61] we form the temperature function

$$T(h) = \begin{cases} T_0 & , h = 0 \\ T_0 + a_0 h & , 0 \leq h < h_{T,1} \\ T_0 + a_0 h_{T,1} & , h_{T,1} \leq h < h_{T,2} \\ T_0 + a_0 h_{T,1} + a_1 (h_{T,2} - h_{T,1}) + a_2 (h - h_{T,2}) & , h_{T,2} \leq h < h_{T,3} \\ T_0 + a_0 h_{T,1} + a_1 (h_{T,2} - h_{T,1}) \\ + a_2 (h_{T,3} - h_{T,2}) + a_3 (h - h_{T,3}) & , h_{T,3} \leq h < h_{T,4} \\ T_0 + a_0 h_{T,1} + a_1 (h_{T,2} - h_{T,1}) \\ + a_2 (h_{T,3} - h_{T,2}) + a_3 (h_{T,4} - h_{T,3}) + a_4 (h - h_{T,4}) & , h_{T,4} \leq h < h_{T,5} \\ T_0 + a_0 h_{T,1} + a_1 (h_{T,2} - h_{T,1}) \\ + a_2 (h_{T,3} - h_{T,2}) + a_3 (h_{T,4} - h_{T,3}) + a_4 (h_{T,5} - h_{T,4}) \\ + a_5 (h - h_{T,5}) & , h_{T,5} \leq h < h_{T,6} \\ T_0 + a_0 h_{T,1} + a_1 (h_{T,2} - h_{T,1}) \\ + a_2 (h_{T,3} - h_{T,2}) + a_3 (h_{T,4} - h_{T,3}) + a_4 (h_{T,5} - h_{T,4}) \\ + a_5 (h_{T,6} - h_{T,5}) + a_6 (h - h_{T,6}) & , h_{T,6} \leq h \lesssim 86 \end{cases} \quad (3.9)$$

with gradient and height values provided by [61] (see Tab. 3.1) which acts as the ground truth temperature profile (see Fig. 6.2).

In this thesis, we define an atmosphere between $h_{L,1} = 6.9\text{km}$ and $h_{L,n} = 83.3\text{km}$ with $n = 45$ equidistant layers and a satellite at a fixed height of $h_{\text{sat}} = 500\text{km}$ (see Fig. 3.1). The height value $h_{L,i}$ for each layer $i = 1, \dots, n$ is defined by the pressure values from the ground truth ozone profile [53] and the hydrostatic equilibrium equation, see Eq. 3.7. We target ozone at a frequency of 235.71GHz, which lies within the region where the MLS observes ozone [35, 67]. The corresponding wave number is $\nu = 7.86\text{cm}^{-1}$. The absorption constant $k(\nu, T)$ is calculated as in Eq. 3.2, following the high resolution transmission (HITRAN) database [23]. The HITRAN database provides the line intensity $L(\nu, T_{\text{ref}})$ for the isotopologue $^{16}\text{O}_3$ with the AFGL Code 666. To compute a data vector $\mathbf{y} = \mathbf{A}(\mathbf{x}) + \boldsymbol{\eta}$ independent and identically-distributed Gaussian noise $\boldsymbol{\eta} \sim \mathcal{N}(0, \gamma^{-1} \mathbf{I})$ is added so that the signal-to-noise ratio (SNR) is approximately 150 (see Eq. 3.11). This is similar to [21], where a signal with a maximal spectral intensity of around 100K and a noise range of 0.4 to 1.6K is reported. Note that the methods used in this thesis will work with different SNRs or other frequencies.

3.2.1 Understanding the Forward Model

Before computing a data vector we test different measurement strategies and asses the information provided by the forward model via a singular value decomposition (SVD). An SVD of the forward model matrix provides a quick and intuitive way of assessing if the data collection is effective. More specifically, the behaviour of the singular values tells us how much information is passed through the forward model and how the measurement strategy affects that information. The SVD of the linear forward model matrix $\mathbf{A}_L \in \mathbb{R}^{m \times n}$ is given as

$$\mathbf{A}_L = \sum_{j=1}^r \mathbf{u}_j \sigma_j \mathbf{v}_j^T = \mathbf{U} \boldsymbol{\Sigma} \mathbf{V}^T \quad (3.10)$$

with $r = \min\{m, n\}$. Our main objective is to measure ozone \mathbf{x} , so this forward model \mathbf{A}_L includes temperature and pressure. The pressure is dominant, see Fig. 6.4, decreases exponentially in height and affects the information passed through the model. If the pressure is high, the signal is large. If the pressure is low, the signal is low, and the data tends to be noise-dominated.

The SVD of the forward model \mathbf{A}_L provides information on how the right singular vectors \mathbf{v}_i act on the parameter \mathbf{x} , because a noise-free measurement vector is given as $\mathbf{A}_L \mathbf{x}$. The singular values σ_j , ordered in size from the largest σ_1 to the smallest σ_r , weigh that information from the right singular vectors to the left singular vectors \mathbf{u}_j . The left singular vectors project $\sigma_j \mathbf{v}_j^T \mathbf{x}$ onto the data space. For a large singular value the forward model is informative about parameter structures represented by the

corresponding right singular vector. For a small singular value the forward model is uninformative about parameter structures represented by the corresponding right singular vector. Further, we define the SNR as

$$\text{SNR} := \frac{\max(y)}{\text{STD noise}} = \frac{\text{peak signal}}{\text{RMS noise}} \quad (3.11)$$

where STD is the standard deviation. Based on the assumption that the largest singular value $\sigma_1 \approx \max(y)$, then most of the information transmitted through the forward model corresponds to the singular values $\sigma_j \gtrsim \max(y)/\text{SNR}$ [18]. For very small singular values $\sigma_j \ll \sigma_1/\text{SNR}$ below the RMS noise level or the noise STD, an effective rank $r_{\text{eff}} \leq r$ is introduced and the data space spanned by $\{\mathbf{u}_{r_{\text{eff}}+1}, \dots, \mathbf{u}_r\}$ is noise-dominated. We say a forward model matrix is informative if it has a large effective rank and the singular values decrease gradually. If the effective rank is small and the singular values decrease quickly, we classify this forward model as uninformative.

For large singular values above the SNR the associated data space is hardly influenced by the noise. Therefore, reconstructions in the parameter space spanned by the respective right singular vectors are expected to be close to the ground truth. For singular values around the SNR the noise is starting to influence the data space. Hence, reconstructions in the parameter space spanned by the corresponding right singular vectors are expected to have increasing uncertainties. Reconstructed parameter values in the parameter space spanned by $\{\mathbf{v}_{r_{\text{eff}}+1}, \dots, \mathbf{v}_r\}$ (e.g. in Fig. 3.6) are expected to have large errors and to be determined by the prior because they relate to very small singular values. See [59] for a more comprehensive analysis.

For five different measurement strategies the tangent heights according to the pointing angles are plotted in Fig. 3.2. The measurement test cases are:

- **Case 1** includes 42 measurements between heights of $\approx 7\text{km}$ and $\approx 83\text{km}$ with pointing angles

$$\phi_j = \left(\frac{-1}{1.25^{j-1}} + 1 \right) \phi_{\max}, \quad \text{for } j = 1, \dots, 42.$$

- **Case 2** includes 42 measurements between heights of $\approx 7\text{km}$ and $\approx 83\text{km}$ with pointing angles

$$\phi_j = \frac{1.25^{j-1}}{1.25^{m-1}} 0.99 \phi_{\max}, \quad \text{for } j = 1, \dots, 42.$$

- **Case 3** includes 42 measurements between heights of $\approx 7\text{km}$ and $\approx 83\text{km}$ with pointing accuracy 150arc sec and pointing angles

$$\phi_j = (j - 1) 150 \text{arc sec}, \quad \text{for } j = 1, \dots, 42.$$

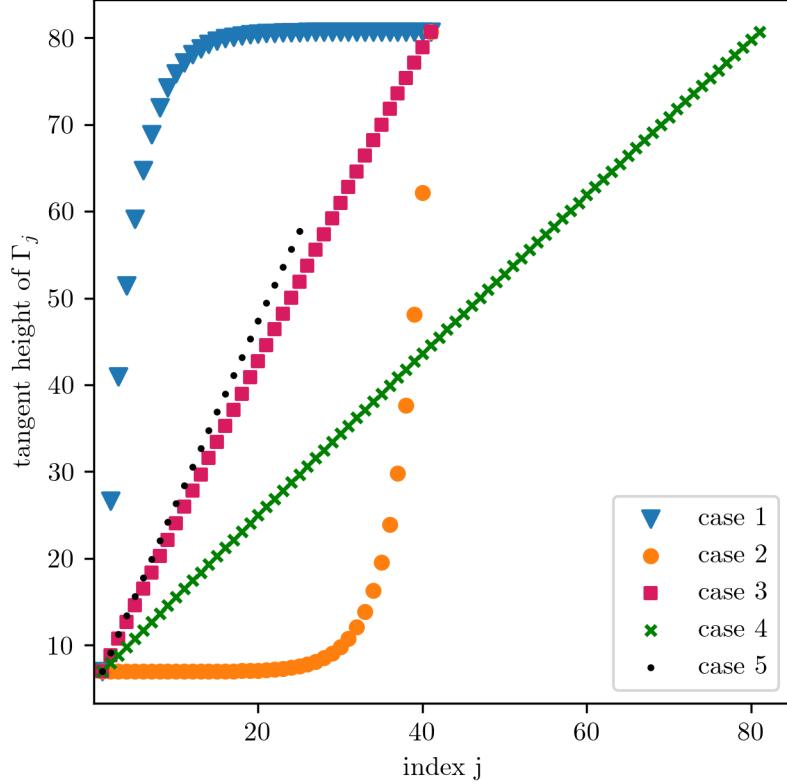


Figure 3.2: Tangent heights for five different sequences of measurements.

- **Case 4** includes 83 measurements between heights of $\approx 7\text{km}$ and $\approx 83\text{km}$ with pointing accuracy 77.5arc sec and pointing angles

$$\phi_j = (j - 1)77.5\text{arc sec}, \quad \text{for } j = 1, \dots, 83.$$

- **Case 5** includes 30 measurements between heights of $\approx 7\text{km}$ and $\approx 68\text{km}$ with pointing accuracy 175arc sec and pointing angles

$$\phi_j = (j - 1)175\text{arc sec}, \quad \text{for } j = 1, \dots, 30.$$

Case 1 collects more data in low signal regions at high altitudes. Case 2 collects more data in high signal regions at low altitudes. Case 3, case 4, and case 5 measure at equidistantly spaced pointing angles with different pointing accuracies. The pointing accuracy determines how well the satellite can point in a certain direction and so the spacing of tangent heights in the atmosphere for a satellite at h_{sat} . Case 1, 2, 3, and 4 measure in between heights $h_{L,1} = 6.9\text{km}$ and $h_{L,n} = 83.3\text{km}$, whereas case 5 does not collect measurements in high altitude regions. The pointing accuracy for case 3 in Fig. 3.2 of 150arc sec was given to us by the Canberra Space team of the University of New South

Wales [14]. Case 4 has half the pointing accuracy of case 3, and case 5 has a slightly larger pointing accuracy than case 3. We visually assess the effective rank and how the singular values behave to determine which of the test cases is most effective. More specifically, if the singular values decay fast and only a few singular values lie above an SNR of 150, the forward map is rather uninformative. If the singular values decay slowly and many singular values lie above an SNR of 150, we classify the forward map as informative.

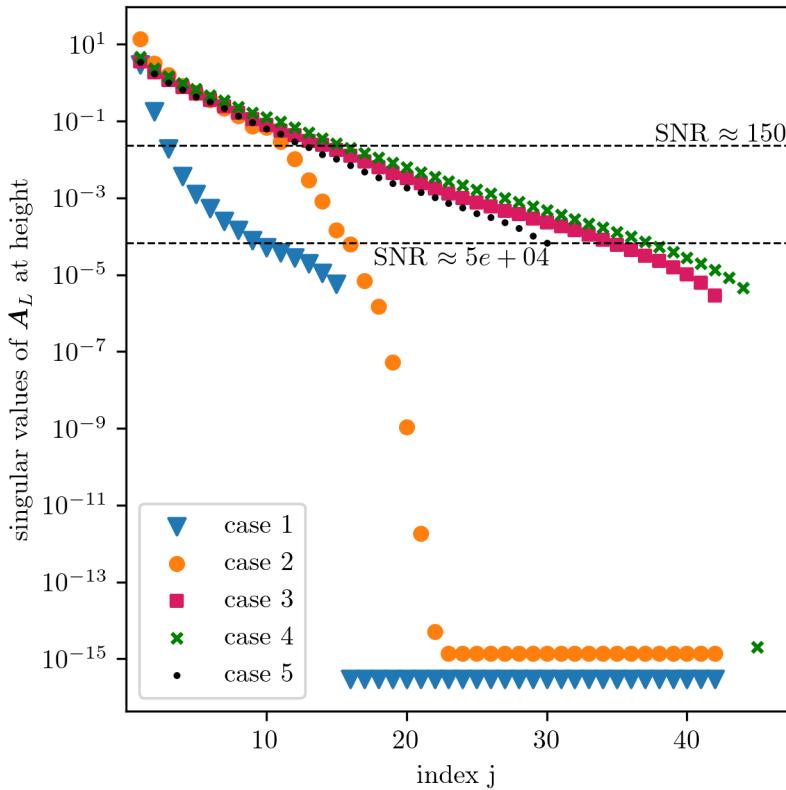


Figure 3.3: Singular values of the forward model matrix for different sequences of measurements. The corresponding tangent heights of the test cases are plotted in Fig. 3.2. The dotted vertical line marks an SNR according to σ_1 of measurement case 5.

In Fig. 3.3, we plot the singular values for each of the measurement cases. The dotted lines in Fig. 3.3 correspond to an SNR of roughly 150 with respect to the largest singular value of case 5 and an SNR according to the lowest singular value of case 5, which would be required to reconstruct all information provided by the forward model. The largest singular value of case 5 is similar to the largest singular values of case 1, 3, and 4, so the dotted line for an SNR of ≈ 150 is indicative for those cases as well. Fig. 3.3 shows that case 2 has the largest singular value of all cases but its singular values decrease faster than the singular values of cases 3, 4, and 5 especially below the SNR of 150. Additionally, case 2 has a smaller effective rank than cases 3, 4, and 5. The singular values of case 1 are decreasing most rapidly compared to all other cases. Case 1 has

the largest number of singular values below an SNR of 150 and the smallest effective rank. We conclude that neither case 1 nor case 2 is effective.

Cases 3, 4, and 5 with equidistantly spaced pointing angles have similar effective ranks and the singular values do not decrease as quickly compared to case 1 and case 2. Case 4 measures almost twice as much compared to case 3 but does not provide much more information, which would justify the engineering effort required to achieve such pointing accuracy. The slightly larger pointing accuracy in case 5 compared to case 3 provides similar information. The last 5 to 10 singular values of case 3 are so small that the information will be lost due to the noise. That is why without losing too much crucial information above the SNR of 150 case 5 measures only up to a height of $\approx 68\text{km}$ instead of $\approx 83\text{km}$ where the data is noise-dominated. Note, that if one wanted to obtain all information provided by the forward model, an SNR of roughly 10^4 is required.

In principle, this shows that it does matter how one measures, but the forward model does not provide more information by measuring more in regions where the information content is low or high. The test cases show that an efficient measurement strategy may consist of equidistantly spaced pointing angles and does stop measuring when the singular values are too low. Consequently, we proceed with case 5. Next, the right singular vectors of the forward model will be assessed to see to which parameter structures within the atmosphere our model is sensitive to.

The parameter space of \mathbf{A}_L spanned by the first 10 right singular vectors, corresponding to the 10 largest singular values in Fig. 3.3, is plotted in Fig. 3.4. These right singular vectors represent parameter structures in the lower atmospheric regions. So we can assume that, given some data, we will be able to provide good reconstructions of the parameter in lower altitudes up to $\approx 30\text{km}$. The right singular vectors in Fig. 3.5 correspond to the singular values σ_j for $j = 11, \dots, 20$ around the SNR of 150 (see Fig. 3.3). This is roughly where the noise starts to dominate the data. The parameter space spanned by those right singular vectors represents parameter values in the middle atmosphere. Consequently, we expect an increasing uncertainty of reconstructed parameter values at heights between $\approx 20\text{km}$ and $\approx 50\text{km}$. The right singular vectors in Fig. 3.6 corresponding to the smallest 10 singular values span structures in parameter space at higher altitudes, and the associated data space is noise-dominated. That is why we will not be able to reconstruct parameter values from the ground truth above $\approx 50\text{km}$. More specifically, the retrieved parameter values at higher altitudes will have large uncertainties and will be determined by the prior or, in the case of a regularisation approach, by the regulariser [59].

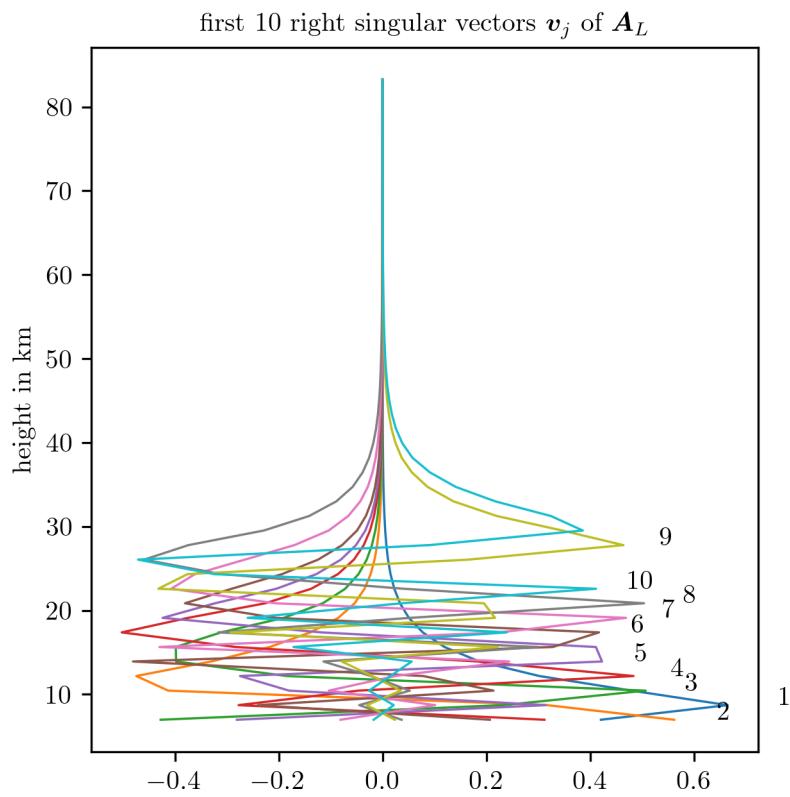


Figure 3.4: First 10 right singular vectors of the forward model matrix \mathbf{A}_L for measurements case 5 in Fig. 3.2. These singular vectors correspond to high singular values of the forward model in Fig. 3.3.

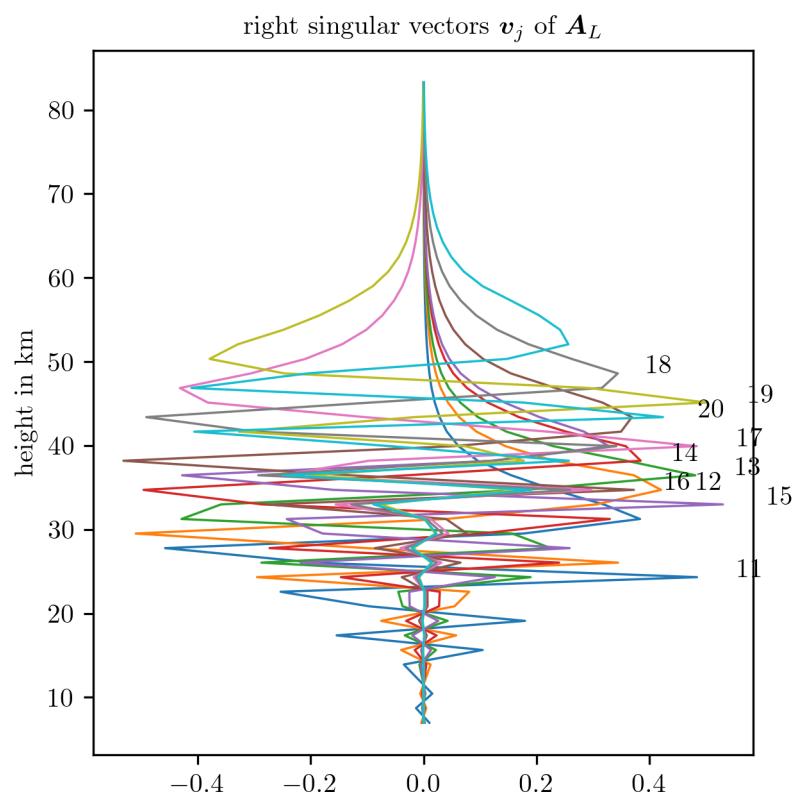


Figure 3.5: Right singular vectors with index $j = 11, \dots, 200$ of the forward model matrix A_L for measurements case 5 in Fig. 3.2. These singular vectors correspond to singular values in Fig. 3.3, where the noise level is similar to the data.

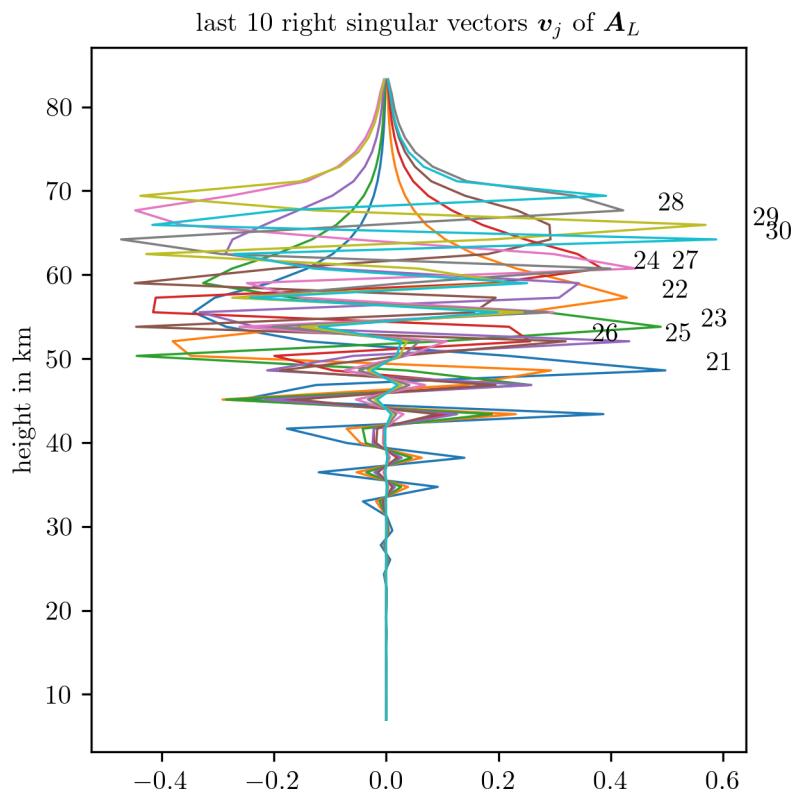


Figure 3.6: Last 10 right singular vectors of the forward model matrix \mathbf{A}_L for measurements case 5 in Fig. 3.2. These singular vectors correspond to small singular values of the forward model in Fig. 3.3, where the data is noise-dominated.

Finally, the data vector $\mathbf{y} = \mathbf{A}(\mathbf{x}) + \boldsymbol{\eta}$ is computed according the RTE (see Eq. 3.1 and Eq. 3.2) and the froward model is determined by the data collection strategy of case 5, with $m = 30$ measurements between $\approx 7\text{km}$ and $\approx 68\text{km}$ and a satellite pointing accuracy of 175arc sec (see in Fig. 3.2). As already mentioned, we set the SNR to 150 and plot the data in Fig. 3.7, which is noise-dominated in higher altitudes. Given the data, we aim to determine the posterior distributions over ozone \mathbf{x} , pressure \mathbf{p} and temperature \mathbf{T} .

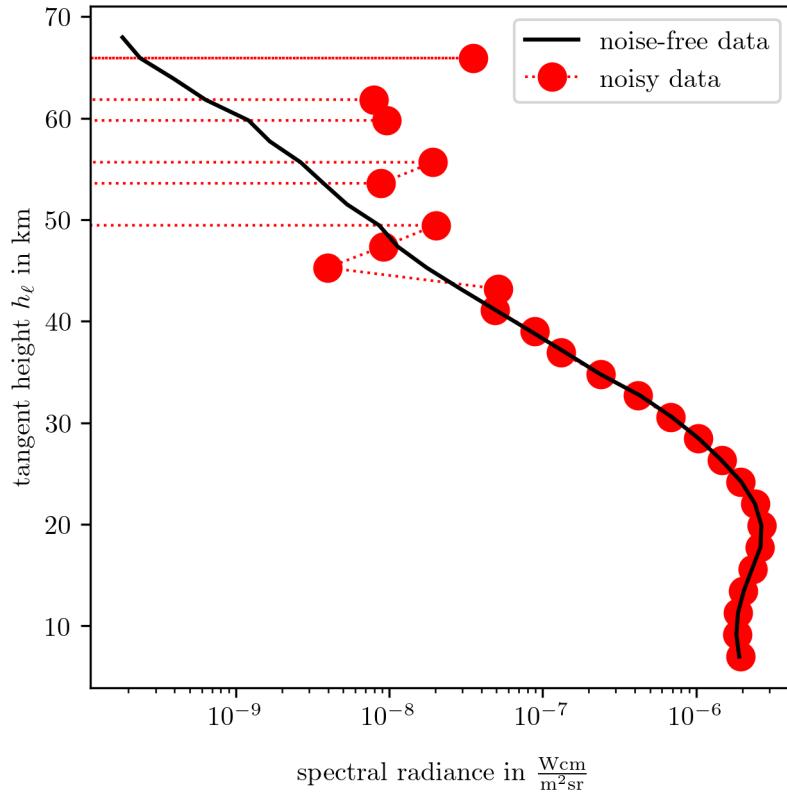


Figure 3.7: Logarithmic plot of data points at different tangent height. Note that negative values are not plotted, and noise is dominating at higher altitudes.

4

Linear Bayesian vs. Regularisation – Ozone

In this Chapter, we guide the reader through the process of setting up a hierarchical Bayesian framework, establishing a choice of prior distributions, and using a DAG to visualise conditional dependencies between hyper-parameters and parameters. Applying the MTC scheme the marginal and then full conditional posterior distributions are explicitly formulated. Here this inverse problem is treated as a linear inverse problem by neglecting the absorption term in the RTE (see Eq. 3.1). A Metropolis within Gibbs sampler and a TT approximation are utilised to characterise the marginal posterior. Then the mean and the covariance matrix of the posterior distribution for ozone are calculated and compared to a regularisation approach.

4.1 Hierarchical Bayesian Framework

In this section, we set up the hierarchically-ordered linear-Gaussian Bayesian framework to determine the ozone posterior distribution, conditioned on ground truth temperature and pressure. For now the forward model matrix is defined as $\mathbf{A} := \mathbf{A}_L$ and the distributions that define the hierarchical Bayesian model are:

$$\mathbf{y}|\mathbf{x}, \gamma, \delta \sim \mathcal{N}(\mathbf{A}\mathbf{x}, \gamma^{-1}\mathbf{I}) \quad (4.1a)$$

$$\mathbf{x}|\delta \sim \mathcal{N}(\mathbf{0}, (\delta\mathbf{L})^{-1}) \quad (4.1b)$$

$$\delta \sim \Gamma(\alpha_\delta, \beta_\delta) \quad (4.1c)$$

$$\gamma \sim \Gamma(\alpha_\gamma, \beta_\gamma). \quad (4.1d)$$

Assuming Gaussian noise $\boldsymbol{\eta} \sim \mathcal{N}(0, \gamma^{-1}\mathbf{I})$, the likelihood function is a normal distribution with mean \mathbf{Ax} and covariance matrix $\gamma^{-1}\mathbf{I}$. We define a normal prior-distribution $\pi(\mathbf{x}|\delta)$

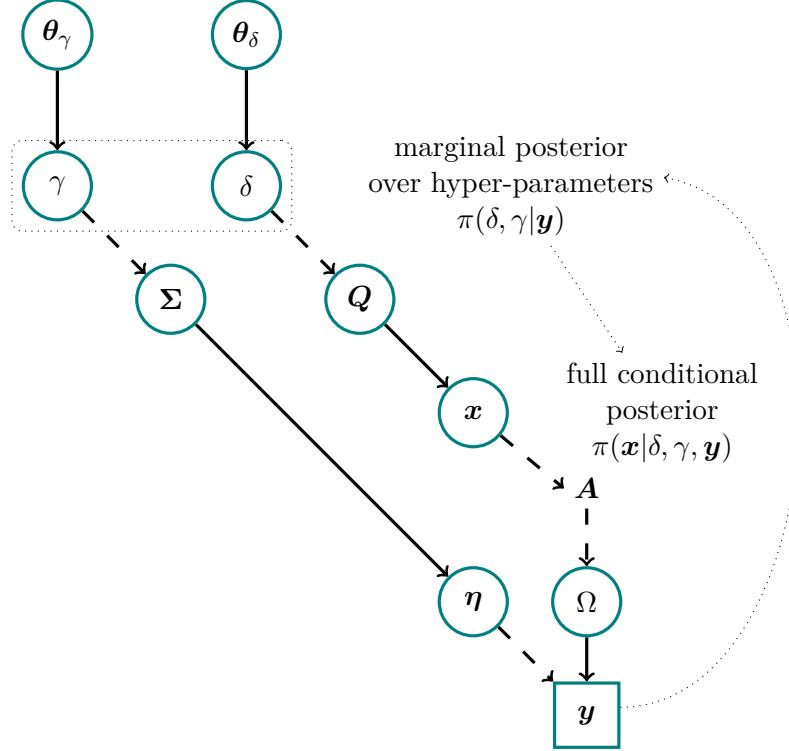


Figure 4.1: DAG for visualisation of hierarchical modelling and measuring process of ozone, including the MTC scheme. The hyper-parameter γ deterministically (dotted line) sets the noise covariance $\Sigma = \gamma^{-1} \mathbf{I}$ and hence the random (solid line) noise vector $\boldsymbol{\eta} \sim \mathcal{N}(0, \gamma^{-1} \mathbf{I})$. The hyper-parameter δ determines (dotted line) the prior precision matrix $\mathbf{Q} = \delta \mathbf{L}$ for the normally distributed (solid line) prior $\mathbf{x} | \delta \sim \mathcal{N}(0, \delta \mathbf{L})$, where \mathbf{L} is a graph Laplacian, see Eq. 4.2. The hyper-prior distributions (solid line) $\pi(\delta, \gamma)$ are defined by θ_γ and θ_δ . Through a linear forward model \mathbf{A} , we generate a space of all measurable noise-free data \mathbf{Ax} from which we randomly observe a data set \mathbf{y} including some added noise $\boldsymbol{\eta}$. Within the MTC scheme, we evaluate the marginal posterior over the hyper-parameters $\pi(\gamma, \delta | \mathbf{y})$ first and then the full conditional posterior $\pi(\mathbf{x} | \delta, \gamma, \mathbf{y})$. This breaks the correlation structure of \mathbf{x} and δ and γ , and allows us to evaluate the marginal posterior independent of \mathbf{x} .

with zero mean and precision matrix $\delta \mathbf{L}$, where δ is a smoothness hyper-parameter and \mathbf{L} is a discrete approximation to the second derivate operator (see Eq. 4.2). Here the hyper-prior distributions $\pi(\delta)$ and $\pi(\gamma)$ are Gamma distributions with shape α and rate β .

We can visualise this hierarchical structure and the conditional dependencies between hyper-parameters and parameters through a DAG, as in Fig. 4.1. The hyper-parameter γ sets the noise covariance deterministically (dotted line), but is itself statistically (solid line) defined by the hyper-prior distribution $\pi(\gamma)$. This is a Gamma distribution, where θ_γ determines the shape and rate of $\pi(\gamma)$. Similarly θ_δ defines $\pi(\delta)$, where δ accounts for smoothness of the ozone profile and sets the prior precision $\mathbf{Q}(\delta)$. Then \mathbf{Ax} determines the space of all measurable noise-free data sets Ω through the linear forward model, from which we observe a data set \mathbf{y} including some noise $\boldsymbol{\eta}$. Given that data, we “reverse the arrows” to determine the posterior distribution $\pi(\mathbf{x}, \theta | \mathbf{y})$ over the parameter \mathbf{x} and

the hyper-parameters $\boldsymbol{\theta}$. Usually, due to underlying correlation structures between the parameter and the hyper-parameters, evaluating this posterior poses a significant challenge. The MTC scheme breaks this correlation and provides the marginal posterior $\pi(\delta, \gamma | \mathbf{y})$ first and then the full conditional posterior $\pi(\mathbf{x} | \delta, \gamma, \mathbf{y})$.

4.1.1 Prior Modelling

Completing this Bayesian framework one has to define prior distributions over the hyper-parameters and parameters. Ideally, we define the prior distributions as uninformative as possible, and include functional dependencies and physical properties.

By choosing a normally distributed prior $\pi(\mathbf{x} | \delta)$ with zero mean and no other restrictions, it is clear that our model does not take into account that ozone values cannot be negative. The precision matrix of that prior distribution is

$$\delta \mathbf{L} = \delta \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \quad (4.2)$$

which is a discrete approximation to the second derivative operator with Dirichlet boundary condition and defines a 1-dimensional Graph Laplacian as in [66, 17]. This matrix will also act as the regulariser later in Sec. 4.3. We reduce the dimension of \mathbf{x} from 45 to 34 by discarding every second ozone VMR over a height of $\approx 47\text{km}$. Doing that, while not changing \mathbf{L} effectively induces a larger correlation between points at higher altitude. The corresponding prior ozone profiles according to $\mathbf{x} \sim \mathcal{N}(0, (\delta \mathbf{L})^{-1})$ are plotted in Fig. B.1.

For δ and γ we pick relatively uninformative gamma distributions so that $\gamma \sim \mathcal{T}(\boldsymbol{\theta}_\gamma) \propto \gamma^{\alpha_\gamma - 1} \exp(-\beta_\gamma \gamma)$ and $\delta \sim \mathcal{T}(\boldsymbol{\theta}_\delta)$ with $\boldsymbol{\theta}_\gamma = \{\alpha_\gamma, \beta_\gamma\} = \{\alpha_\delta, \beta_\delta\} = \boldsymbol{\theta}_\delta = (1, 10^{-35})$ (see Fig. 5.3) similar to [17]. Because of those gamma distributions, $\pi(\gamma | \lambda, \mathbf{y}) \sim \mathcal{T}(\cdot)$ is a gamma distribution with $\lambda = \delta/\gamma$ and easy to sample from. This advantageous when using the Metropolis within Gibbs algorithm, as in Sec. 4.2.1, to sample from the marginal posterior distribution $\pi(\delta, \gamma | \mathbf{y})$.

4.2 Posterior Distribution

As explained in Sec. 2.1.1, we factorise the posterior

$$\pi(\mathbf{x}, \delta, \gamma | \mathbf{y}) \propto \pi(\mathbf{y} | \mathbf{x}, \delta, \gamma) \pi(\mathbf{x}, \delta, \gamma) \quad (4.3)$$

into

$$\pi(\mathbf{x}, \delta, \gamma | \mathbf{y}) = \pi(\mathbf{x} | \delta, \gamma, \mathbf{y}) \pi(\delta, \gamma | \mathbf{y}) \quad (4.4)$$

the marginal posterior $\pi(\delta, \gamma | \mathbf{y})$ and full conditional posterior $\pi(\mathbf{x} | \delta, \gamma, \mathbf{y})$ (see Eq. 2.7). As discussed in Sec. 2.1.1, for the linear-Gaussian case, \mathbf{x} cancels in the marginal posterior over the hyper-parameters [17]. Following the MTC scheme, we characterise the marginal posterior first and then the full conditional posterior.

4.2.1 Marginal Posterior

For the hierarchical model specified in Eq. 4.1, the marginal posterior distribution over the hyper-parameters is given by

$$\pi(\lambda, \gamma | \mathbf{y}) \propto \lambda^{n/2 + \alpha_\delta - 1} \gamma^{m/2 + \alpha_\delta + \alpha_\gamma - 1} \exp \left\{ -\frac{1}{2} g(\lambda) - \frac{\gamma}{2} f(\lambda) - \beta_\delta \lambda \gamma - \beta_\gamma \gamma \right\}, \quad (4.5)$$

with the introduced regularisation parameter $\lambda = \delta/\gamma$, and

$$f(\lambda) = \mathbf{y}^T \mathbf{y} - (\mathbf{A}^T \mathbf{y})^T (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L})^{-1} (\mathbf{A}^T \mathbf{y}), \quad (4.6a)$$

$$\text{and } g(\lambda) = \log \det(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L}). \quad (4.6b)$$

Note that when changing variables from $\delta = \lambda \gamma$ to λ the hyper-prior distribution changes to $\pi(\lambda) \propto \lambda^{\alpha_\delta - 1} \gamma^{\alpha_\delta} \exp(-\beta_\delta \lambda \gamma)$, due to $d\delta/d\lambda = \gamma$.

For each evaluation of the marginal posterior most of the computational effort lies in the calculation of $f(\lambda)$ and $g(\lambda)$. Obtaining the Cholesky decomposition $\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L} = \mathbf{C}_\lambda \mathbf{C}_\lambda^T$ via `numpy.linalg.cholesky` immediately gives $g(\lambda) = 2 \sum \log \text{diag}(\mathbf{C}_\lambda)$. Additionally this Cholesky decomposition is used to calculate $(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L})^{-1} (\mathbf{A}^T \mathbf{y})$ as in $f(\lambda)$ via the Python function `scipy.linalg.cho_solve`. In Fig. 4.2 we see that $f(\lambda)$ and $g(\lambda)$ are well behaved within the region of interest. Because of this, we approximate $\tilde{g}(\lambda) \approx g(\lambda)$ with a linear approximation in λ log-space and $f(\lambda) \approx \tilde{f}(\lambda)$ with a Taylor series around the mode λ_0 of $\pi(\lambda, \gamma | \mathbf{y})$. The Taylor series coefficient of $f(\lambda)$ is given by

$$f^{(r)}(\lambda_0) = (-1)^{r+1} (\mathbf{A}^T \mathbf{y})^T (\mathbf{B}_0^{-1} \mathbf{L})^r \mathbf{B}_0^{-1} \mathbf{A}_L^T \mathbf{y} \quad (4.7)$$

with $\mathbf{B}_0 = \mathbf{A}^T \mathbf{A} + \lambda_0 \mathbf{L}$. Usually a Taylor series includes a factor $(r!)^{-1}$, which in this case cancels [17] so that $f(\lambda)$ is approximated as

$$\tilde{f}(\lambda) = \sum_{r=0}^{\infty} f^{(r)}(\lambda_0) (\lambda - \lambda_0)^r. \quad (4.8)$$

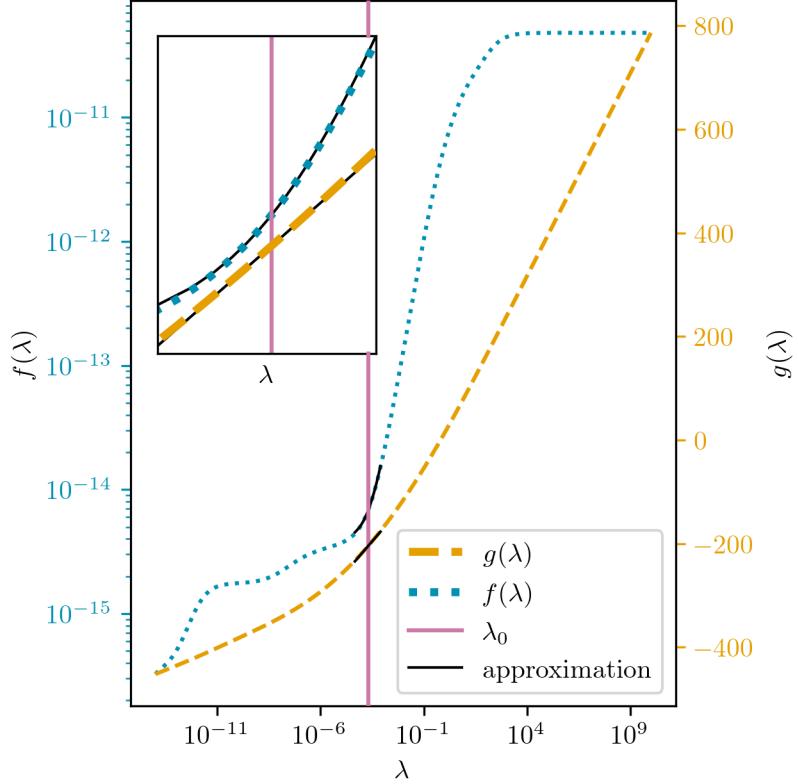


Figure 4.2: Functions $f(\lambda)$ and $g(\lambda)$ from the marginal posterior in Eq. 4.5 for a wide range of $\lambda = \delta/\gamma$. We plot the approximations (see Eq. 4.8 and Eq. 4.9) in black around the mode of the marginal posterior (vertical line) for the sampling range of λ within the MWG algorithm.

By exploratory analysis we find that the approximation

$$\tilde{g}(\lambda) = g(\lambda_0) + (\log \lambda - \log \lambda_0) \frac{g(1.25\lambda_0) - g(0.75\lambda_0)}{\log 1.25\lambda_0 - \log 0.75\lambda_0} \quad (4.9)$$

is sufficient. Note that $g(\lambda)$ can be approximated with a Taylor series as well (see [17]). We plot the function $f(\lambda)$ and $g(\lambda)$ and their approximations in Fig. 4.2 and elaborate on the approximation errors in the section below.

Error due to approximation of f and g

To assess the approximation error, we lay a 100×100 grid over the region defined by the TT grid (see Sec. 4.2.1) and compare the approximations of $f(\lambda)$, $g(\lambda)$ and $\pi(\lambda, \gamma | \mathbf{y})$ with their true function values.

Compared to a 2nd, 3-rd or 4-th order Taylor approximation, the 1-st order Taylor approximation of $f(\lambda)$ gives the smallest relative RMS error of $\approx 9\%$ for $\lambda = [10^{-5}, 8 \times 10^{-4}]$ (TT grid) and a maximum absolute error of $\approx 3 \times 10^{-16}$. Additionally, the linear approximation of $g(\lambda)$ has a relative RMS of $\approx 3\%$ and a maximum absolute error of ≈ 5 .

These errors then propagate into the marginal posterior $\pi(\lambda, \gamma | \mathbf{y})$ so that the relative RMS error is $\approx 6\%$ over the whole grid. When sampling, we evaluate the acceptance

ratio in the log-space, so we report a relative RMS error of $\approx 0.1\%$ for $\log \pi(\lambda\gamma|\mathbf{y})$. We consider this good enough.

Sample from marginal posterior – Metropolis within Gibbs

Using these approximations, a Metropolis within Gibbs (MWG) sampler summarised in Alg. Box 3 is employed to characterise $\pi(\lambda, \gamma|\mathbf{y})$ as in [17]. More specifically, we implement a Metropolis random walk on

$$\pi(\lambda|\gamma, \mathbf{y}) \propto \lambda^{n/2+\alpha_\delta-1} \exp \left\{ -\frac{1}{2}g(\lambda) - \frac{\gamma}{2}f(\lambda) - \beta_\delta \gamma \lambda \right\} \quad (4.10)$$

and do a Gibbs step on

$$\gamma|\lambda, \mathbf{y} \sim \Gamma \left(\frac{m}{2} + \alpha_\delta + \alpha_\gamma, \frac{1}{2}f(\lambda + \beta_\gamma + \beta_\delta \lambda) \right). \quad (4.11)$$

Ergodicity for this approach is proven in [46].

Algorithm 3: Metropolis within Gibbs

```

1: Initialise  $(\lambda^{(0)}, \gamma^{(0)}) = (\lambda_0, \gamma_0)$ .
2: for  $k = 0, \dots, N - 1$  do
3:   Propose  $\lambda' \sim q(\cdot|\lambda^{(k)}) = q(\lambda^{(k)}|\cdot)$ .
4:   Compute

$$\alpha(\lambda'|\lambda^{(k)}) = \min \left\{ 1, \frac{\pi(\lambda'|\gamma^{(k)}, \mathbf{y})q(\lambda^{(k)}|\lambda')}{\pi(\lambda^{(k)}|\gamma^{(k)}, \mathbf{y})q(\lambda'|\lambda^{(k)})} \right\}$$

.
5:   Draw  $u \sim \mathcal{U}(0, 1)$ .
6:   if  $\alpha \geq u$  then
7:     Accept and set  $\lambda^{(k+1)} = \lambda'$ .
8:   else
9:     Reject and keep  $\lambda^{(k+1)} = \lambda^{(k)}$ .
10:  end if
11:  Draw  $\gamma^{(k+1)} \sim \pi(\cdot|\lambda^{(k+1)}, \mathbf{y})$ .
12: end for
13: Output:  $(\lambda, \gamma)^{(0)}, \dots, (\lambda, \gamma)^{(k)}, \dots, (\lambda, \gamma)^{(N)} \sim \pi(\theta|\mathbf{y})$ .
```

The MWG algorithm starts at the initial guess $(\lambda^{(0)}, \gamma^{(0)})$ at $k = 0$. Conditioned on the previous state a new sample $\lambda' \sim q(\cdot|\lambda^{(k)})$ is proposed using a symmetric proposal distribution $q(\lambda'|\lambda^{(k)}) = q(\lambda^{(k)}|\lambda')$. This is a Metropolis step and a special case of the Metropolis–Hastings algorithm [46]. We accept and set $\lambda^{(k+1)} = \lambda'$ with the acceptance probability

$$\alpha(\lambda'|\lambda^{(k)}) = \min \left\{ 1, \frac{\pi(\lambda'|\gamma^{(k)}, \mathbf{y})q(\lambda^{(k)}|\lambda')}{\pi(\lambda^{(k)}|\gamma^{(k)}, \mathbf{y})q(\lambda'|\lambda^{(k)})} \right\}, \quad (4.12)$$

otherwise reject and keep $\lambda^{(k+1)} = \lambda^{(k)}$. In practice, we calculate the acceptance ratio in log-space, so that

$$\log \left(\frac{\pi(\lambda'|\gamma^{(k)}, \mathbf{y})}{\pi(\lambda^{(k)}|\gamma^{(k)}, \mathbf{y})} \right) = \log \pi(\lambda'|\gamma^{(k)}, \mathbf{y}) - \log \pi(\lambda^{(k)}|\gamma^{(k)}, \mathbf{y}) \quad (4.13)$$

$$= \left(\frac{n}{2} + \alpha_\delta - 1 \right) (\log \lambda' - \log \lambda^{(k)}) + \frac{1}{2} \Delta g + \frac{\gamma^{(k)}}{2} \Delta f + \beta_\delta \gamma^{(k)} \Delta \lambda, \quad (4.14)$$

where $\Delta \lambda = \lambda' - \lambda^{(k)}$ and $\Delta f \approx \tilde{f}(\lambda') - \tilde{f}(\lambda^{(k)}) = \sum f^{(r)}(\lambda_0)(\Delta \lambda')^r - (\Delta \lambda^{(k)})^r$, with $\Delta \lambda' = \lambda' - \lambda_0$ and $\Delta \lambda^{(k)} = \lambda^{(k)} - \lambda_0$. Similarly we approximate $\Delta g \approx \tilde{g}(\lambda') - \tilde{g}(\lambda^{(k)})$.

Next, a Gibbs step on $\pi(\gamma^{(k+1)}|\lambda^{(k+1)}, \mathbf{y})$ conditioned on the previously drawn $\lambda^{(k+1)}$ is performed. Gibbs sampling is again a special case of the Metropolis-Hastings algorithm with acceptance probability equal to one. Repeating this N time give us marginal posterior samples $(\lambda, \gamma)^{(1)}, \dots, (\lambda, \gamma)^{(N)} \sim \pi(\lambda, \gamma|\mathbf{y})$. To remove initialisation bias the first $N_{\text{burn-in}}$ samples are discarded.

Running the MWG sampler $f(\lambda)$ and $g(\lambda)$ are approximated around the mode (λ_0, γ_0) of $\pi(\lambda, \gamma|\mathbf{y})$ as previously described. The mode is provided by the `scipy.optimize.fmin` function, with a limit of 25 function evaluations. Initialised at the mode $(\lambda^{(0)}, \gamma^{(0)}) = (\lambda_0, \gamma_0)$ the MWG sampler takes $N = 10100$, which includes burn in period of $N_{\text{burn-in}} = 100$ steps. The standard deviation of the normal proposal distribution $\lambda' \sim \mathcal{N}(\lambda^{(k)}, \sigma_\lambda^2)$ is empirically set to $\sigma_\lambda = 0.8\lambda_0$, so that the acceptance rate is ≈ 0.5 as suggested in [44]. This takes ≈ 0.5 s and we plot in Fig. 4.4 as well as the trace of the MWG to show ergodicity. The IACTs are given by twice the value of the Python implementation of [68] provided by [28], so that $\tau_{\text{int},\gamma} \approx 4.4 \pm 0.2$ and $\tau_{\text{int},\lambda} = 10.4 \pm 1.0$. In Fig. 4.3 and Fig. B.2 the estimated autocorrelation coefficient $\Gamma(t)$ at lag t decreases exponentially, and the error of the estimated IACT at the chosen summation windows W (red line) is sufficiently small. This indicates that the chosen number of samples provides a long enough chain to obtain accurate estimates of the IACT.

TT approximation of marginal posterior

Alternatively, the square root of the marginal posterior over a predefined grid can be approximated by a TT to calculate the marginals $\pi(\gamma|\mathbf{y})$ and $\pi(\lambda|\mathbf{y})$ (see Sec. 2.3.1).

The univariate grid is defined over $\gamma = [0.8 \times 10^{15}, 1.2 \times 10^{16}]$ and $\lambda = [10^{-5}, 8 \times 10^{-4}]$ with $n = 20$ grid points (see Fig. 4.7, where we argue for the number of grid points). The “normalisation constant” is set to $c = -150$ so that the values of $\sqrt{\pi(\lambda, \gamma|\mathbf{y})} = \exp\{0.5 \log \pi(\lambda, \gamma|\mathbf{y}) + c\}$ are within computer precision. Then we initialise the `tt.cross.rectcross.rect_cross.cross` function based on the TT cross algorithm in [40, 12] from the Python package `ttpy` [39] with a random tensor. The number of

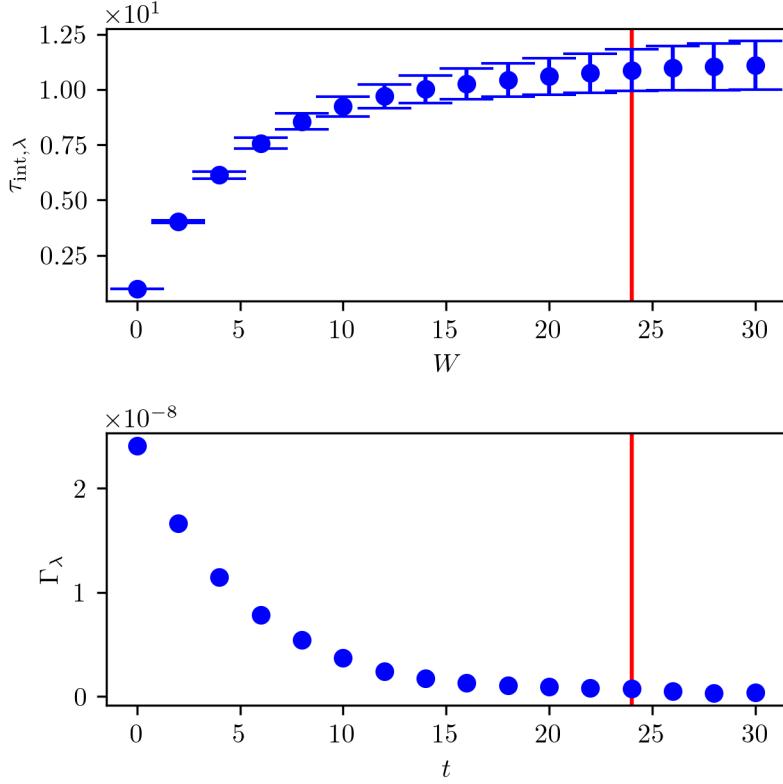


Figure 4.3: Provided by [28], the IACT $\tau_{\text{int},\lambda}$ at summation windows W as well as the estimated autocorrelation function Γ_λ at lag t of the samples $\lambda \sim \pi(\cdot|\mathbf{y})$.

ranks $r = 4$ is constant and we do one sweep with $2n_{\text{sweeps}}2nr = 400$ function evaluations and obtain a TT approximation of $\pi(\lambda, \gamma|\mathbf{y})$ in about 0.02s. Ironically, this the same number of functions evaluations to approximate a 20×20 point grid. The TT format is especially advantageous for larger grid sizes and higher-dimensional parameter spaces. To compute the marginals $\pi(\lambda|\mathbf{y})$ and $\pi(\gamma|\mathbf{y})$ the TT error is set to $\xi = 1/\lambda(\mathcal{X})$ because we observe peak values of around 10^{47} . For Cartesian basis the Mass matrix becomes $\mathbf{M}_k = \text{diag}(\lambda_k(\mathcal{X}_k))$ (see Eq. 2.28) with and $\lambda(x) = 1$. The coefficient tensor \mathbf{B} and \mathbf{R}_{pre} are calculated as in Prop. 1 and Prop. 2 (see Sec. 2.3.1).

We plot the TT approximation as a colour map on top of the obtained samples in Fig. 4.4. The relative RMS TT approximation error over the whole grid is $\approx 7\%$ and similar to the propagation error in $\pi(\lambda, \gamma|\mathbf{y})$ due to the approximations of $f(\lambda)$ and $g(\lambda)$ (see further up).

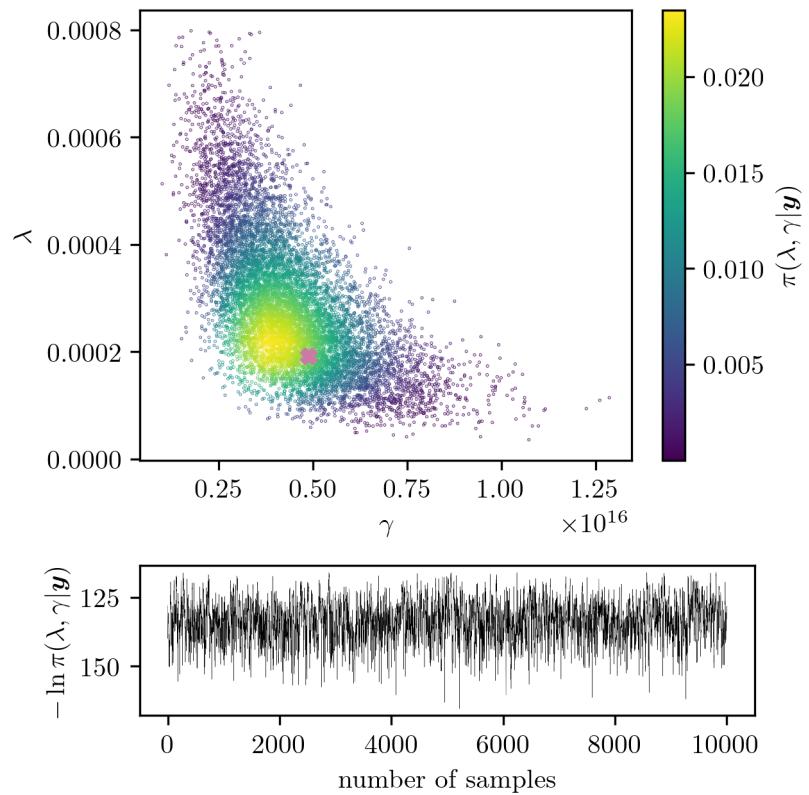


Figure 4.4: Samples from the marginal posterior colour-coded using the TT approximation of $\pi(\lambda, \gamma | \mathbf{y})$. The mode of (λ_0, γ_0) of $\pi(\lambda, \gamma | \mathbf{y})$ is marked with the pink cross. To show ergodicity, we plot the trace of the samples of the MWG algorithm.

4.2.2 Full Conditional Posterior

Finally, we can evaluate the normally distributed full conditional posterior distribution

$$\mathbf{x}|\delta, \gamma, \mathbf{y} \sim \mathcal{N}\left(\underbrace{(\mathbf{A}^T \mathbf{A} + \delta/\gamma \mathbf{L})^{-1} \mathbf{A}^T \mathbf{y}}_{\mathbf{x}_\lambda}, \underbrace{(\gamma \mathbf{A}^T \mathbf{A} + \delta \mathbf{L})^{-1}}_{\gamma \mathbf{B}_\lambda}\right), \quad (4.15)$$

as in Eq. 2.15, with $\lambda = \delta/\gamma$. In this thesis, we compute the posterior mean

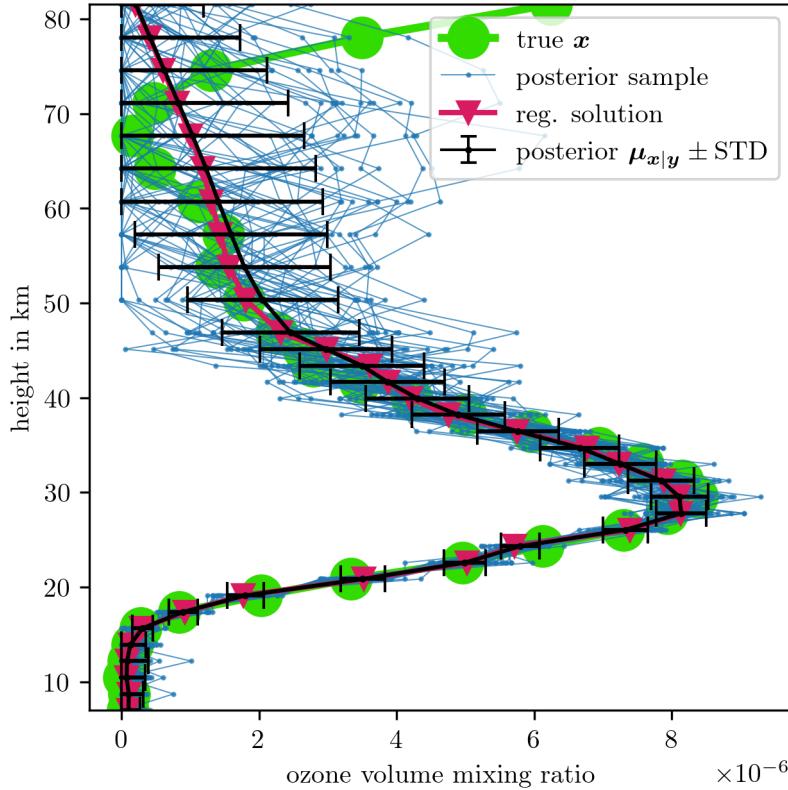


Figure 4.5: Ozone samples from the full posterior distribution $\pi(\mathbf{x}|\mathbf{y})$ after characterising posterior mean and covariance by weighted expectations over the marginal posterior $\pi(\lambda, \gamma|\mathbf{y})$ based on the linear forward map \mathbf{A}_L . We set negative ozone VMR values to zero.

$$\mu_{\mathbf{x}|\mathbf{y}} = \int \mathbf{x}_\lambda \pi(\lambda|\mathbf{y}) d\lambda \approx \sum \mathbf{x}_{\lambda_i} \pi(\lambda_i|\mathbf{y}), \quad (4.16)$$

and posterior covariance

$$\Sigma_{\mathbf{x}|\mathbf{y}} = \int \gamma^{-1} \pi(\gamma|\mathbf{y}) d\gamma \int \mathbf{B}_\lambda^{-1} \pi(\lambda|\mathbf{y}) d\lambda \approx \sum \gamma_i^{-1} \pi(\gamma_i|\mathbf{y}) \sum \mathbf{B}_{\lambda_i}^{-1} \pi(\lambda_i|\mathbf{y}) \quad (4.17)$$

of $\pi(\mathbf{x}|\mathbf{y})$ as weighted expectations over the marginal posterior $\pi(\lambda, \gamma|\mathbf{y})$ by quadrature [10, Sec. 2.1] with $\sum \pi(\lambda_i|\mathbf{y}) = \sum \pi(\gamma_i|\mathbf{y}) = 1$. The weights $\pi(\lambda_i|\mathbf{y})$ and $\pi(\gamma_i|\mathbf{y})$ are either given by the TT approximation or by the bars of the sample-based histograms. More precisely, the heights of the sample-based histogram bars act as quadrature weights,

where λ_i is defined at the centre of each bar. We use the Cholesky decomposition of $\mathbf{B}_\lambda = \mathbf{A}^T \mathbf{A} + \lambda \mathbf{L}$ to invert \mathbf{B}_λ and to calculate $\mathbf{x}_\lambda = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L})^{-1} \mathbf{A}^T \mathbf{y}$ both via `scipy.linalg.cho_solve`. It is sufficient to evaluate \mathbf{x}_λ and invert \mathbf{B}_λ 20 times to obtain mean and covariance values of $\pi(\mathbf{x}|\mathbf{y})$ within a reasonable error (see Fig. 4.7).

The posterior samples of $\pi(\mathbf{x}|\mathbf{y})$ are plotted in Fig. 4.5 with negative ozone values set to zero. The fact that we have to deal with negative ozone values is due to the poor prior choice in $\pi(\mathbf{x}|\delta)$. This indicates that one should use a different, more physically based prior or a better model for ozone in the atmosphere. Note that the posterior samples do not capture the second ozone peak at around 80km.

Finding the mode of $\pi(\lambda, \gamma|\mathbf{y})$, running the TT `cross`, calculating the marginals and the posterior mean and covariance takes 0.025s. The MWG sampler takes ≈ 0.5 s for the same results, so most computational effort lays within the sampling procedure and the time to calculate posterior mean and covariance is negligible.

If calculating the variance is too costly, see Sec. 6.2.2 where we present a feasible alternative to draw a sample from the full conditional posterior.

Eigenvalues of the full conditional posterior covariance matrix

In Fig. 4.6 the eigenvalues (ordered in size) of the precision matrix $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}} = \gamma\mathbf{A}^T\mathbf{A} + \delta\mathbf{L}$ for a random $\delta, \gamma \sim \pi(\delta, \gamma | \mathbf{y})$ are plotted and compared to the eigenvalues of the prior precision matrix $\delta\mathbf{L}$ and $\gamma\mathbf{A}^T\mathbf{A}$. We observe that the larger eigenvalues of $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}}$ are very much the same as the larger eigenvalues of $\gamma\mathbf{A}^T\mathbf{A}$. Once the eigenvalues of $\gamma\mathbf{A}^T\mathbf{A}$ are significantly smaller than the eigenvalues of $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}}$ the structure of the eigenvalues is dominated by the eigenvalues of $\delta\mathbf{L}$. The eigenvectors corresponding to the 12 largest eigenvalues of $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}}$ include ozone profile structure at lower altitudes up to 35km, where the other eigenvectors mainly represent structures above 30km (see Fig. B.5 and Fig. B.6). Note that the eigenvalues of each matrix may correspond to different eigenvectors, even if the eigenvalues are the same.

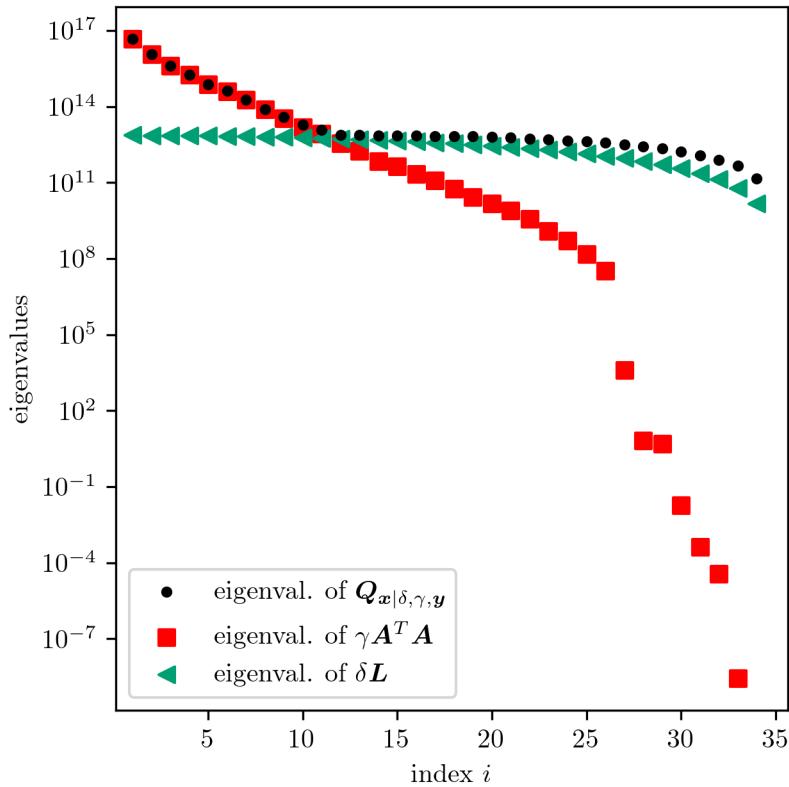


Figure 4.6: Eigenvalues of the precision matrix of $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}} = \gamma\mathbf{A}^T\mathbf{A} + \delta\mathbf{L}$ of the full conditional posterior distribution $\pi(\mathbf{x}|\delta, \gamma, \mathbf{y})$ for ozone. We see that large eigenvalues of $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}}$ are unaffected by the prior. For small eigenvalues of $\gamma\mathbf{A}^T\mathbf{A}$ the eigenvalues of $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}}$ are dominated by the structure of the eigenvalues of $\delta\mathbf{L}$.

Errors of posterior mean and covariance

In Fig. 4.7, we plot the relative RMS error for the mean $\mu_{\mathbf{x}|\mathbf{y}}$ and covariance $\Sigma_{\mathbf{x}|\mathbf{y}}$ of $\pi(\mathbf{x}|\mathbf{y})$ due to grid size or number of bins of the marginal posterior. Those results are obtained by calculating the weighted expectation over normalised histograms of $\pi(\lambda, \gamma|\mathbf{y})$, where the number of bins is increased and compared to a solution calculated from a histogram with 200 bins. The relative error behaves roughly proportional to $1/N$, and we consider a relative RMS error less than 0.5% good enough, which is easily met at 20 bins. This sets the TT grid size and the number of evaluations of \mathbf{x}_λ (posterior mean, see Eq. 4.16) and $(\gamma \mathbf{B}_\lambda)^{-1}$ (posterior covariance, see Eq. 4.17).

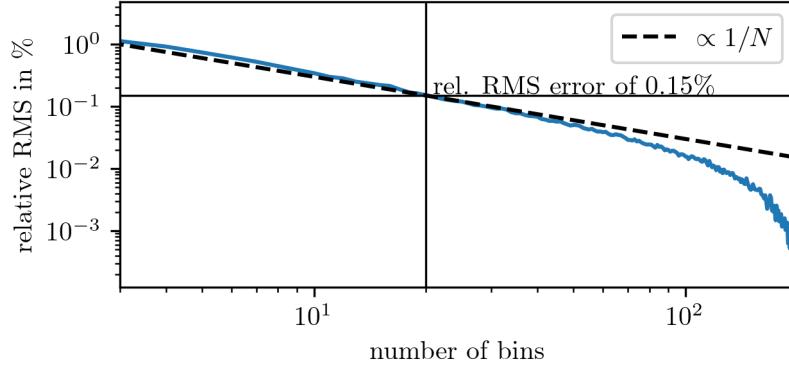


Figure 4.7: Relative RMS error of $\mu_{\mathbf{x}|\mathbf{y}}$ and covariance $\Sigma_{\mathbf{x}|\mathbf{y}}$ calculated by the weighted expectations and compared to a “ground truth” given by weighted expectations over 200 bins.

4.3 Solution by Regularisation

Since we claim that hierarchical Bayesian frameworks provide more information than regularisation methods, we compare the MTC scheme to a regularisation approach. That is why the chosen regularisation approach is the closest equivalent to the here used linear-Gaussian Bayesian framework [17].

The regularised solution is defined as in [25, 17]

$$\mathbf{x}_\lambda = \arg \min_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{y}\|_{L^2}^2 + \lambda \mathbf{x}^T \mathbf{Lx}, \quad (4.18)$$

with the regularisation parameter λ , linear forward model matrix \mathbf{A} and data \mathbf{y} . A regularised solution

$$\mathbf{x}_\lambda = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L})^{-1} \mathbf{A}^T \mathbf{y} \quad (4.19)$$

is calculated as in Sec. 2.4.

The regularised estimate is found using the L-curve method following [27]. Within this method we compute \mathbf{x}_λ , for 200 different λ values in between 10^{-8} to 10^0 and plot the regularisation norm $\sqrt{\mathbf{x}_\lambda^T \mathbf{L} \mathbf{x}_\lambda}$ against the data misfit norm $\|\mathbf{Ax}_\lambda - \mathbf{y}\|_{L^2}$ (see Figure 4.8). The regularised estimate corresponds to the “corner” of the L-curve at the point of maximum curvature provided by the kneedle algorithm [52] using the function `kneed.KneeLocator` in ≈ 0.015 s, which is slightly faster than the TT approach to obtain posterior mean and covariance. The corresponding regularisation parameter is $\lambda = 1.6 \times 10^{-4}$.

The regularised estimate in Fig. 5.4 is very similar to the posterior mean and both have a similar data misfit and regularisation norm. Neither the regularised estimate nor the posterior ozone profiles capture the second ozone peak of the ground truth at high altitudes. Note that we cannot infer the posterior mean from the regularised solutions, even if it appears to lie on the L-curve. It is pretty clear that the regularised estimate accounts for only one possible solution and does not provide uncertainties. The data misfit and regularisation norm values of the regularised estimate and the posterior mean are not similar to the corresponding values of the samples drawn from the posterior $\pi(\mathbf{x}|\mathbf{y})$ (see Fig. 4.5). All posterior samples of $\pi(\mathbf{x}|\mathbf{y})$ are less regularised and lie above the L-curve, and as already mentioned, are all feasible solutions to the data. This does make sense, if one thinks about the mean as the (smooth) average over less-smooth samples and the regularised solutions as extremely smooth ozone profiles (see Lagrangian in Sec. 2.4).

Counterintuitively, it is not possible to obtain a sample that represents the mean of a multivariate probability distribution [64, Sec. 3.1]. This is because the probability mass in a multi-dimensional space concentrates on a “shell” or “ring” away from the mean [65]. Alternatively, think about how an electron’s mean position may be inside the atom’s core but the electron can never be observed at the centre of the atom’s nucleus [24, Chapter 4] and [41, Fig. 4].

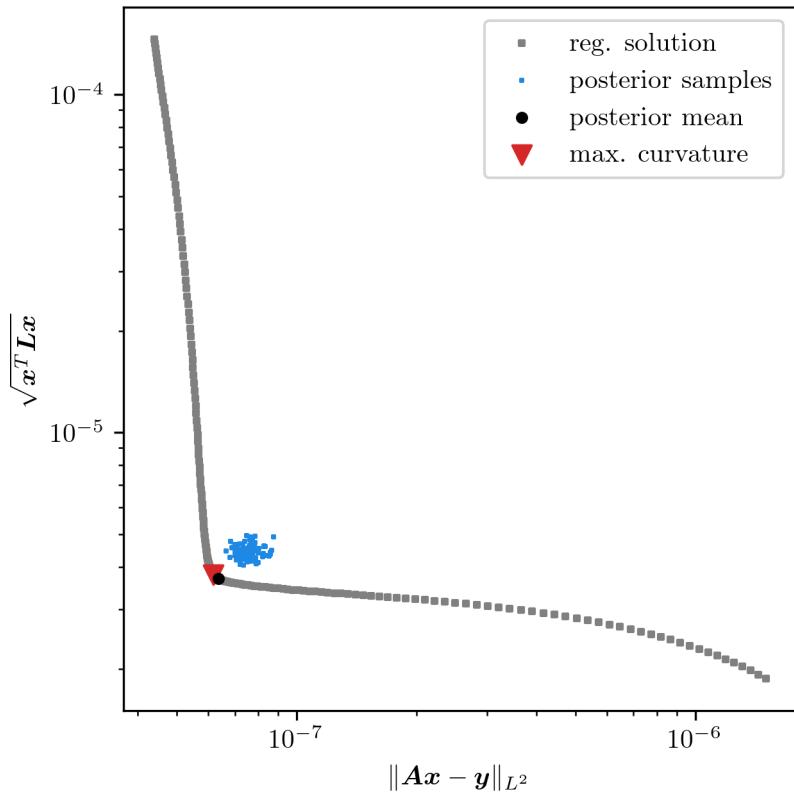


Figure 4.8: L-curve of regularisation norm $\sqrt{\mathbf{x}^T \mathbf{L} \mathbf{x}}$ against the data misfit norm $\|\mathbf{A}\mathbf{x} - \mathbf{y}\|_{L^2}$ for different λ values, where \mathbf{x}_λ is calculated as in Eq. 4.19. The best regularised estimate is located at the point of maximum curvature (pink triangle) of the L-curve. Additionally, we calculate the data misfit norm and the regularisation norm for the mean (black circle) and samples (blue squares) of the full posterior of ozone.

5

Affine Approximation of the Non-Linear Model

The forward map, introduced in Chapter 3, poses a weakly non-linear forward problem. One could tackle this non-linear inverse problem by fixing the absorption at a previously obtained parameter state and treating this as a linear inverse problem. After each parameter sample the absorption is then iteratively updated. Instead, as in Fig. 5.1 illustrated, we approximate the non-linear model using an affine map, which is a linear map with a translation e.g., $\mathbf{A}\mathbf{x} + \mathbf{b}$. An affine map $\mathbf{z} = \mathbf{A}\mathbf{x} + \mathbf{b}$ maps a Gaussian $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ onto a Gaussian $\mathbf{z} \sim \mathcal{N}(\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}^T\boldsymbol{\Sigma}\mathbf{A})$. Here we find an affine map \mathbf{M} based on the linear model \mathbf{A}_L that provides an approximation of the non-linear model $\mathbf{A}(\mathbf{x})$ for parameters \mathbf{x} near the posterior mean $\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}$.

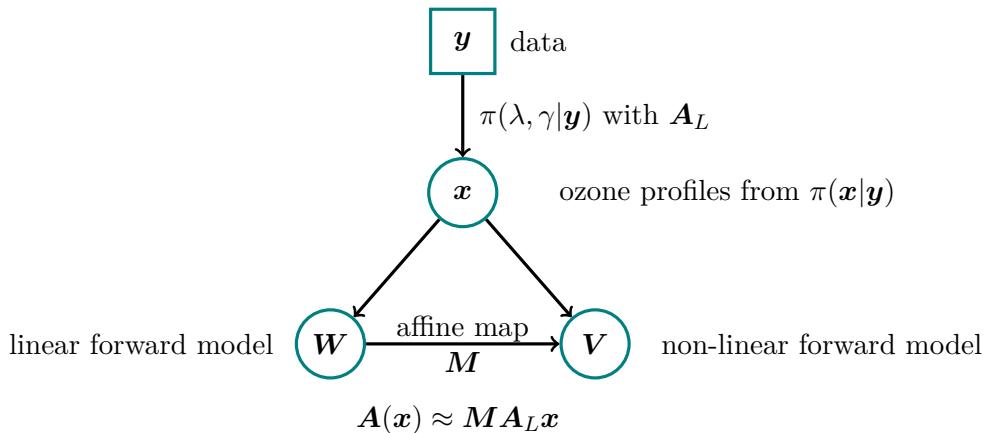


Figure 5.1: The strategy to find the affine map consists of evaluating the marginal posterior for ozone $\pi(\lambda, \gamma|\mathbf{y})$ for the linear forward model. Based on ozone samples from the posterior an affine map \mathbf{M} that approximates between noise-free linear data \mathbf{A}_L and noise-free non-linear data $\mathbf{A}(\mathbf{x})$ is calculated.

5.1 Finding an Affine Map

We find an affine map by creating the vector spaces \mathbf{W} based on the linear forward model and \mathbf{V} based on the non-linear forward model with ground truth pressure and temperature. More specifically $m - 1$ samples $\mathbf{x}^{(j)} \sim \pi(\mathbf{x}|\mathbf{y})$, for $j = 2, \dots, m$, from the posterior and the posterior mean $\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}$ generate,

$$\mathbf{W} = \begin{bmatrix} | & | & | & | \\ A_L \boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}} & A_L \mathbf{x}^{(2)} & \cdots & A_L \mathbf{x}^{(j)} & \cdots & A_L \mathbf{x}^{(m)} \\ | & | & & | & & | \end{bmatrix} \in \mathbb{R}^{m \times m}$$

and

$$\mathbf{V} = \begin{bmatrix} | & | & | & | \\ \mathbf{A}(\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}) & \mathbf{A}(\mathbf{x}^{(2)}) & \cdots & \mathbf{A}(\mathbf{x}^{(j)}) & \cdots & \mathbf{A}(\mathbf{x}^{(m)}) \\ | & | & & | & & | \end{bmatrix} = \begin{bmatrix} — & v_1 & — \\ & \vdots & \\ — & v_j & — \\ & \vdots & \\ — & v_m & — \end{bmatrix} \in \mathbb{R}^{m \times m}.$$

Then the non-linear forward model is approximated as

$$\mathbf{A}(\mathbf{x}) \approx M A_L \mathbf{x}, \quad (5.1)$$

where we solve $v_j = r_j \mathbf{W}$ for each row r_j in

$$\mathbf{V} \mathbf{W}^{-1} = \mathbf{M} = \begin{bmatrix} — & r_1 & — \\ & \vdots & \\ — & r_j & — \\ & \vdots & \\ — & r_m & — \end{bmatrix} \in \mathbb{R}^{m \times m}.$$

using the Python function `numpy.linalg.solve`. This is feasible since every noise-free measurement is independent of each other, and then every row v_j of $\mathbf{V} \in \mathbb{R}^{m \times m}$ is independent of each other as well. For an $\mathbf{x} = \boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}} + \Delta \mathbf{x}$ we rewrite Eq. 5.1 to

$$\mathbf{A}(\mathbf{x}) \approx \underbrace{M A_L \boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}}_{=A(\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}})} + \underbrace{M A_L \Delta \mathbf{x}}_{=A'(\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}) \Delta \mathbf{x}} \quad (5.2)$$

$$= \underbrace{A'(\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}) \mathbf{x}}_{A \mathbf{x}} + \underbrace{A(\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}) - A'(\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}) \boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}}_{b} \quad (5.3)$$

to show that $\mathbf{M} : A_L \mathbf{x} \rightarrow \mathbf{A}(\mathbf{x})$ is an affine map.

The relative RMS difference $\|\text{vec}(M \mathbf{W}) - \text{vec}(\mathbf{V})\|_{L^2} / \|\text{vec}(M \mathbf{W})\|_{L^2}$ between the mapped linear noise-free data and the non-linear noise-free data is approximately 0.001%. This is much smaller than the relative RMS difference between \mathbf{W} and \mathbf{V} of about 1%.

Fig. 5.2 shows the mapping for one posterior ozone sample with a relative RMS error $\approx 0.02\%$. This posterior ozone sample has not been used to create this mapping; in other words, this is an unseen event not occurring in the training data. Consequently, from here onwards, we use the approximated forward map.

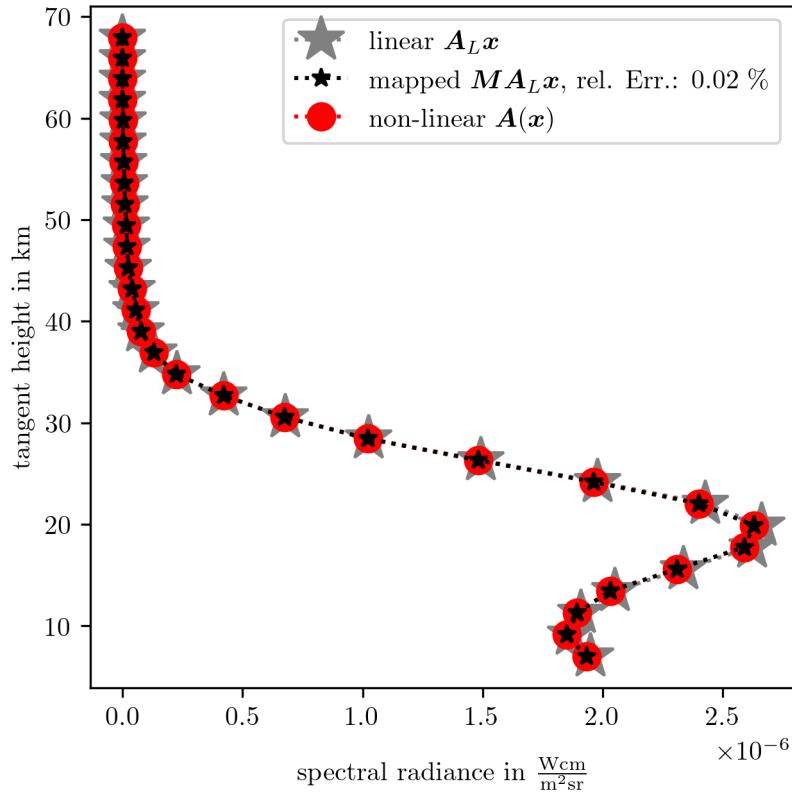


Figure 5.2: Assessment of how well the affine map \mathbf{M} approximates noise-free non-linear data $\mathbf{A}(\mathbf{x})$ (red circles) from noise-free linear data $\mathbf{A}_L\mathbf{x}$ (grey stars). The approximated noise-free data (black stars) has a relative RMS error of $\approx 0.02\%$ compared to the true non-linear noise-free data. The ozone profile \mathbf{x} to generate this noise-free data has not been used to create the affine map.

5.2 Marginal and Full Conditional Posterior – Ozone

The exact same setup and procedure as in Sec. 4.2 is used to evaluate the marginal posterior and then the full conditional posterior of ozone within a similar computational time.

The marginal posterior is defined as in Eq. 4.5, but with the approximated forward model. The MWG is initialised at the mode of $\pi(\lambda, \gamma | \mathbf{y})$, and $f(\lambda)$ and $g(\lambda)$ are approximated around the mode as in Sec. 4.2.1 (see Eq. 4.8 and Eq. 4.9). We take $N = 10000$ plus $N_{\text{burn-in}} = 100$ steps in $\approx 0.5\text{s}$. The IACTs $\tau_{\text{int},\gamma} \approx 5.2 \pm 0.3$ and $\tau_{\text{int},\lambda} = 11 \pm 1$ (see Fig. B.4 and Fig. B.3) are twice the values provided by [28] and similar to the previously calculated values (see Sec. 4.2.1). We plot the samples in Fig. 5.3 as well as the TT approximation of the marginal posterior using 400 function evaluations (same grid; same number of ranks; see Sec. 4.2.1). The relative RMS error of the TT approximation over the whole grid is similar to the relative RMS approximation error of $\pi(\lambda, \gamma | \mathbf{y})$ due to the approximations of $f(\lambda)$ and $g(\lambda)$. Both relative RMS errors are $\approx 7\%$.

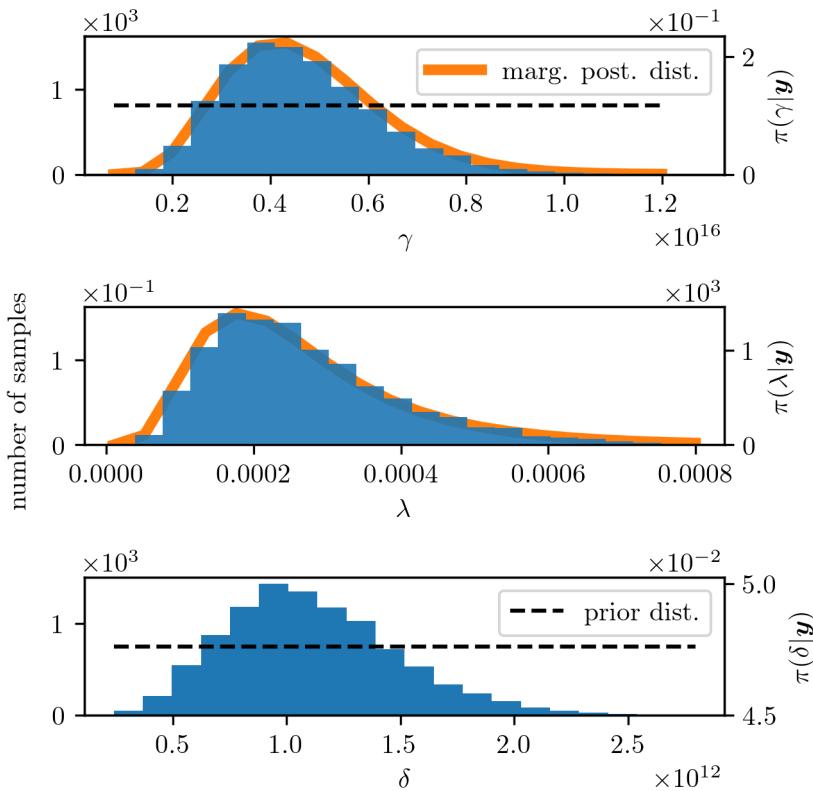


Figure 5.3: The TT approximation of the marginal posterior in orange and the samples as a histogram, as well as the prior distribution with a dotted line. We sample λ and γ using the MWG algorithm and then calculate δ for every sample of the marginal posterior.

Again, the full posterior mean $\mu_{\mathbf{x}|\mathbf{y}}$ (see Eq. 4.16) and covariance matrix $\Sigma_{\mathbf{x}|\mathbf{y}}$ (see Eq. 4.17) are calculated as weighted expectation. The resulting posterior mean and STD,

and one sample of $\pi(\mathbf{x}|\mathbf{y})$, which represents a feasible solution to this inverse problem, are plotted in Fig. 5.4. The ground truth lies within the STD around the posterior mean, except for the peak at around 80km. Compared to the previously calculated posterior mean and covariance based on the linear model \mathbf{A}_L (see Fig. 4.5), the posterior distribution based on the approximated \mathbf{MA}_L does not differ significantly. This is expected since the difference between the linear and non-linear forward map of $\approx 1\%$ is small.

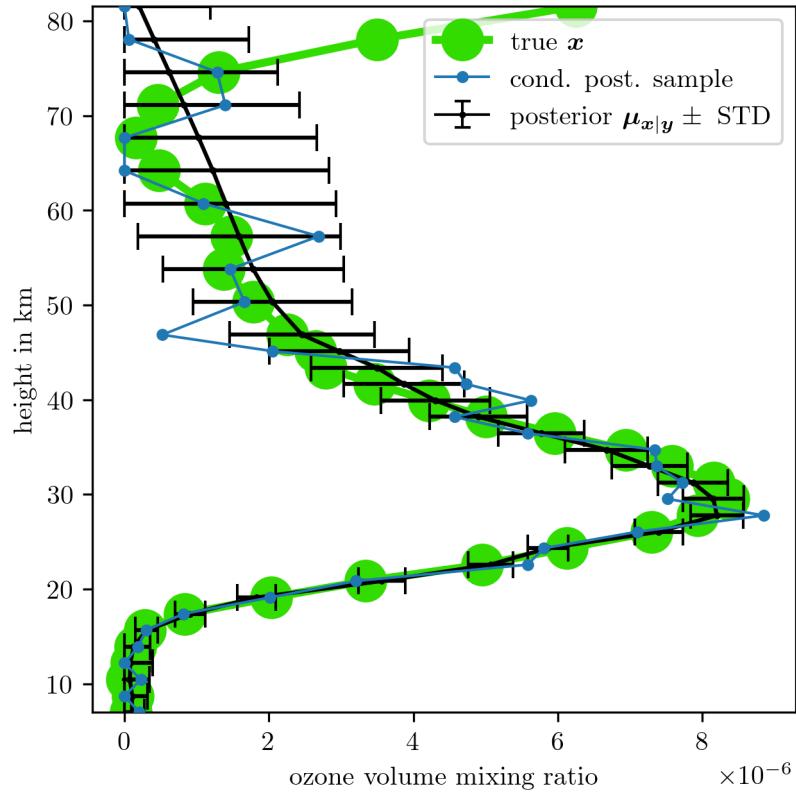


Figure 5.4: Full posterior mean and variance and one ozone sample from the full posterior. These results are based on the approximated forward model \mathbf{MA}_L .

6

Joint Retrieval of Ozone, Pressure and Temperature

Here we extend the hierarchical Bayesian model set up in Sec. 4.1 to include pressure and temperature related hyper-parameters and elaborate on some aspects of prior modelling. The MTC scheme is applied to jointly provide posterior distributions of ozone, pressure and temperature. Additionally, the reader is guided through the process of setting up an efficient TT approximation of the higher-dimensional marginal posterior.

6.1 Hierarchical Bayesian Framework

As in Sec. 4.1, the DAG in Fig. 6.1 visualises the measurement process and conditional dependencies between the parameter and the hyper-parameters. Ozone \mathbf{x} , pressure \mathbf{p} and temperature \mathbf{T} progress deterministically (dashed line) into the forward model, via $\mathbf{x} \times \mathbf{p} / \mathbf{T}$. Note that other variables in the RTE, such as the internal partition function and the black body radiation, are dependent on temperature (see Sec. 3.1). This hierarchical Bayesian framework includes the hyper-parameters p_0, b for pressure (see Eq. 6.3), $\mathbf{a}, \mathbf{h}_T, T_0$ for temperature (see Eq. 3.9), δ for ozone smoothness and γ for noise precision. Each of those hyper-parameters is described by the hyper-prior distribution $\pi(p_0, b, T_0, \mathbf{h}_T, \mathbf{a}, \delta, \gamma)$ (see Sec. 6.1.1). Through their respective prior distributions, pressure \mathbf{p} , temperature \mathbf{T} and ozone \mathbf{x} generate a space of all possible noise-free data Ω from which some data with additive normally distributed noise $\boldsymbol{\eta}$ is observed. For brevity, we define the linear forward model matrix as

$$\mathbf{A}_{\boldsymbol{\theta}} := \mathbf{M} \mathbf{A}_L(p_0, b, T_0, \mathbf{h}_T, \mathbf{a}) \quad (6.1)$$

with $\boldsymbol{\theta} := \{p_0, b, T_0, \mathbf{h}_T, \mathbf{a}\}$ accounting for the all pressure and temperature related hyper-parameters and \mathbf{M} the affine approximation from the previous Chapter.

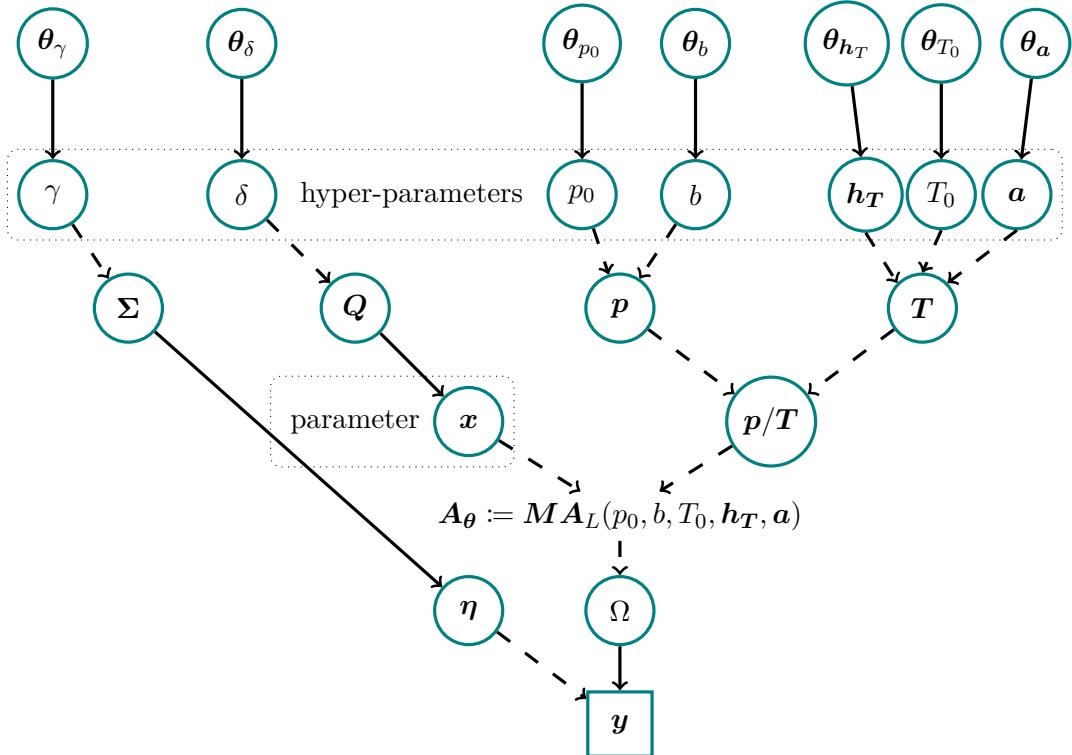


Figure 6.1: DAG of the hierarchical Bayesian model including ozone \mathbf{x} , pressure \mathbf{p} and temperature \mathbf{T} . The hyper-parameters $\mathbf{h}_T = \{h_{T,1}, h_{T,2}, h_{T,3}, h_{T,4}, h_{T,5}, h_{T,6}\}$, $\mathbf{a} = \{a_0, a_1, a_2, a_3, a_4, a_5, a_6\}$, T_0 , b and p_0 deterministically (dotted line) describe pressure through Eq. 6.3 and temperature through Eq. 3.9. In this case, the hyper-parameters $\pi(p_0, b, T_0, \mathbf{h}_T, \mathbf{a})$ are a normally distributed a-priori. That is why $\theta_{h_T}, \theta_a, \theta_{T_0}, \theta_b, \theta_{p_0}$ represent mean and variances e.g., $b \sim \mathcal{N}(\mu_b, \sigma_b^2)$ and $\theta_b = \{\mu_b, \sigma_b\}$. As previously described in Sec. 4.1, $\theta_\gamma, \theta_\delta$ determine gamma distributions e.g., $\gamma \sim \Gamma(\alpha_\gamma, \beta_\gamma)$ with $\theta_\gamma = \{\alpha_\gamma, \beta_\gamma\}$. The ozone parameter \mathbf{x} is statistically (solid line) described by the prior distribution $\mathbf{x}|\delta \sim \mathcal{N}(0, (\delta \mathbf{L})^{-1})$. Here, the hyper-parameter δ accounts for smoothness in the ozone profile and defines the precision matrix $\mathbf{Q} = \delta \mathbf{L}$, where \mathbf{L} is the graph Laplacian as in Eq. 4.2. The noise covariance $\Sigma = \gamma^{-1} \mathbf{I}$ of the random noise vector $\boldsymbol{\eta} \sim \mathcal{N}(0, \gamma^{-1} \mathbf{I})$ is defined by the hyper-parameter γ . From the space of all measurables Ω mapped through the approximated forward model $\mathbf{A}_\theta := M \mathbf{A}_L(p_0, b, T_0, \mathbf{h}_T, \mathbf{a})$, depending on the hyper-parameter $\theta := \{p_0, b, T_0, \mathbf{h}_T, \mathbf{a}\}$ a data set \mathbf{y} is randomly observed (square box) including some additive random noise $\boldsymbol{\eta}$.

The distributions of the hierarchical Bayesian framework are:

$$\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}, \delta, \gamma \sim \mathcal{N}(\mathbf{A}_{\boldsymbol{\theta}}\mathbf{x}, \gamma^{-1}\mathbf{I}) \quad (6.2a)$$

$$\mathbf{x}|\delta \sim \mathcal{N}(\mathbf{0}, (\delta \mathbf{L})^{-1}) \quad (6.2b)$$

$$\delta \sim \Gamma(\alpha_{\delta}, \beta_{\delta}) \quad (6.2c)$$

$$\gamma \sim \Gamma(\alpha_{\gamma}, \beta_{\gamma}) \quad (6.2d)$$

$$\mathbf{a} \sim \mathcal{N}(\boldsymbol{\mu}_{\mathbf{a}}, \boldsymbol{\Sigma}_{\mathbf{a}}) \quad (6.2e)$$

$$\mathbf{h}_T \sim \mathcal{N}(\boldsymbol{\mu}_T, \boldsymbol{\Sigma}_{\mathbf{h}_T}) \quad (6.2f)$$

$$T_0 \sim \mathcal{N}(\mu_{T_0}, \sigma_{T_0}) \quad (6.2g)$$

$$p_0 \sim \mathcal{N}(\mu_{p_0}, \sigma_{p_0}) \quad (6.2h)$$

$$b \sim \mathcal{N}(\mu_b, \sigma_b). \quad (6.2i)$$

Due to Gaussian noise $\pi(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}, \delta, \gamma)$ is a normally distributed likelihood function and Eq. 6.2b to Eq. 6.2i denote prior distributions. Before formulating the posterior distribution, we carefully define $\boldsymbol{\theta}_{\gamma}, \boldsymbol{\theta}_{\delta}, \boldsymbol{\theta}_{p_0}, \boldsymbol{\theta}_b, \boldsymbol{\theta}_h, \boldsymbol{\theta}_{T_0}, \boldsymbol{\theta}_{\mathbf{a}}$, the hyper-prior scales, shapes, means and variances, which are explicitly given in Tab. 6.1.

6.1.1 Prior Modelling

We observe that the pressure p in between $h_{L,0} \approx 7\text{km}$ and $h_{L,n} \approx 83\text{km}$ can be described with an exponential function

$$p(h) = \exp(-b h) p_0, \quad h_{L,0} \leq h \leq h_{L,n} \quad (6.3)$$

depending on two hyper-parameters p_0, b (see Fig. 6.3). Similarly, the temperature as described in Eq. 3.9 can be parametrised with 14 hyper-parameters $\mathbf{h}_T = \{h_{T,1}, h_{T,2}, h_{T,3}, h_{T,4}, h_{T,5}, h_{T,6}\}$, $\mathbf{a} = \{a_0, a_1, a_2, a_3, a_4, a_5, a_6\}$ and T_0 (see Fig. 6.2 and Eq. 3.9).

The hyper-prior distributions for $p_0, b, T_0, \mathbf{h}_T, \mathbf{a}$ are defined to be Gaussians, and to complete the model we have to set sensible hyper-prior variances and means. We tune the variances of $\pi(\mathbf{h}_T)$, so that the temperature profile maintains its structure and $h_{T,i} < h_{T,i+1}$, for $i = 1, \dots, 5$ (see Fig. B.7). The means of $\pi(\mathbf{h}_T)$ and $\pi(\mathbf{a})$ are set to ground truth values see Tab. 3.1 and the variances of $\pi(\mathbf{a})$ allow a wide range of prior temperature profiles. Similarly, we set the variance and mean of $\pi(T_0)$ so that it mimics a daily temperature variability of roughly 30K around the mean sea level temperature 288K [61]. These hyper-prior distributions are rather informative, because we find that the data and the model (see Fig. 6.4) are uninformative about the temperature profile. The variance of $\pi(b)$ is set to a rather large value. The variability of $\pi(p_0)$ is $\approx 80\text{hPa}$ and close

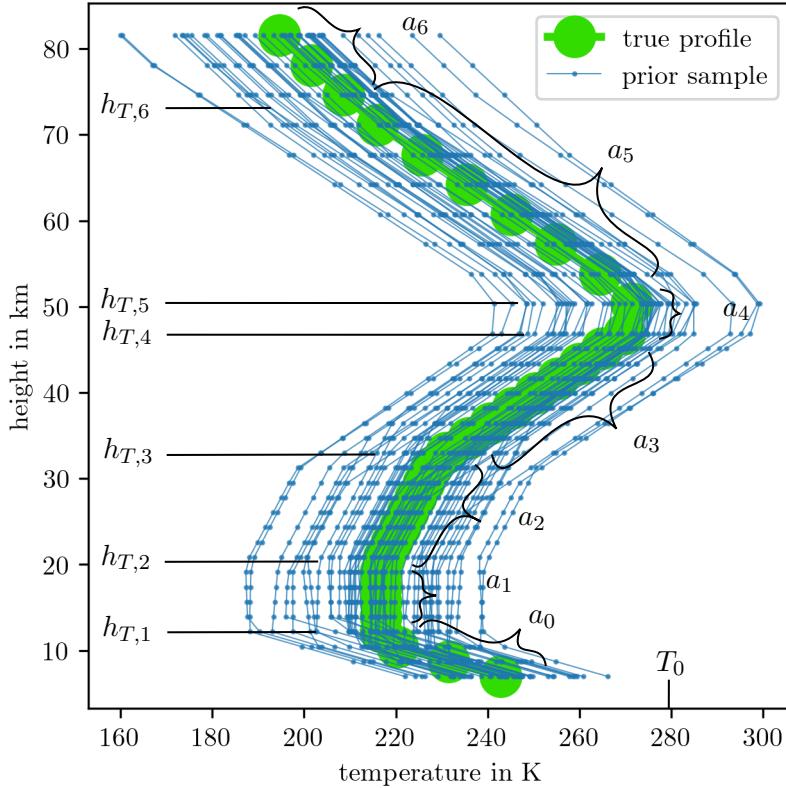


Figure 6.2: Prior samples from the hyper-prior distribution of \mathbf{h}_T , \mathbf{a} and T_0 , as defined in Tab. 6.1, where we calculate \mathbf{T} according to the function in Eq. 3.9.

to what we can observe when looking at weather data. Means for $\pi(b, p_0)$ are provided by fitting the exponential in Eq. 6.3 to ground truth pressure values via the Python function `scipy.optimize.curve_fit`. The in Sec. 4.1.1 defined Gamma distributions $\pi(\delta, \gamma)$ are not changing. See Tab. 6.1 for a summary of the hyper-prior distributions.

Prior samples of the pressure \mathbf{p} in Fig. 6.3, the temperature \mathbf{T} in Fig. 6.2, the ratio \mathbf{p}/\mathbf{T} in Fig. 6.4 and additionally prior samples of $1/\mathbf{T}$ in Fig. B.8 are plotted against their ground truth profiles. Here we already observe that \mathbf{p}/\mathbf{T} inherits the structure of the pressure function and hence the model is uninformative about the temperature.

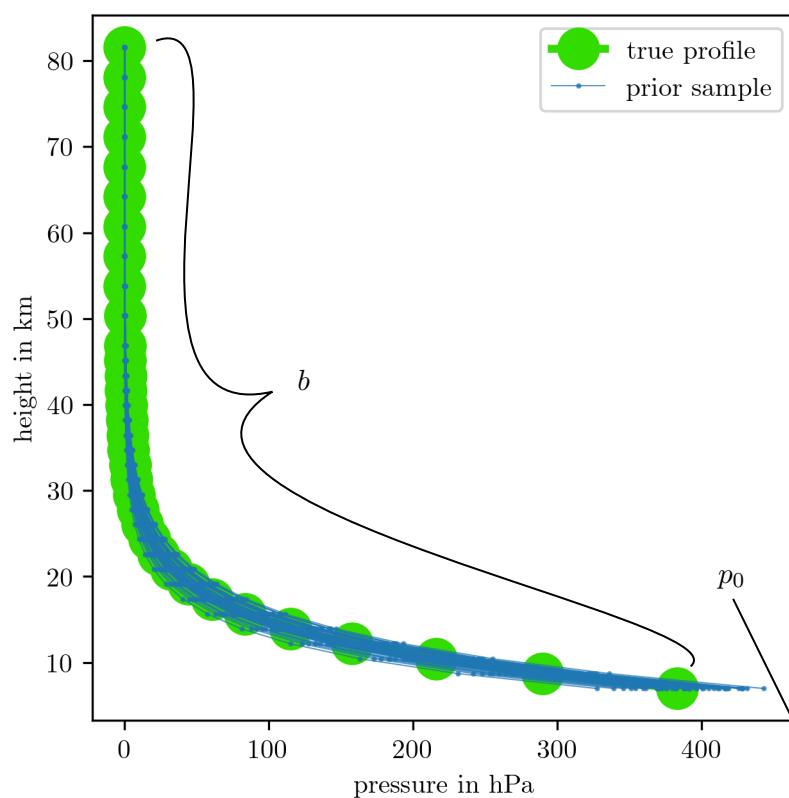


Figure 6.3: Prior samples from the hyper-prior distribution of b and p_0 as defined in Tab. 6.1, where we calculate \mathbf{p} according to the function in Eq. 6.3.

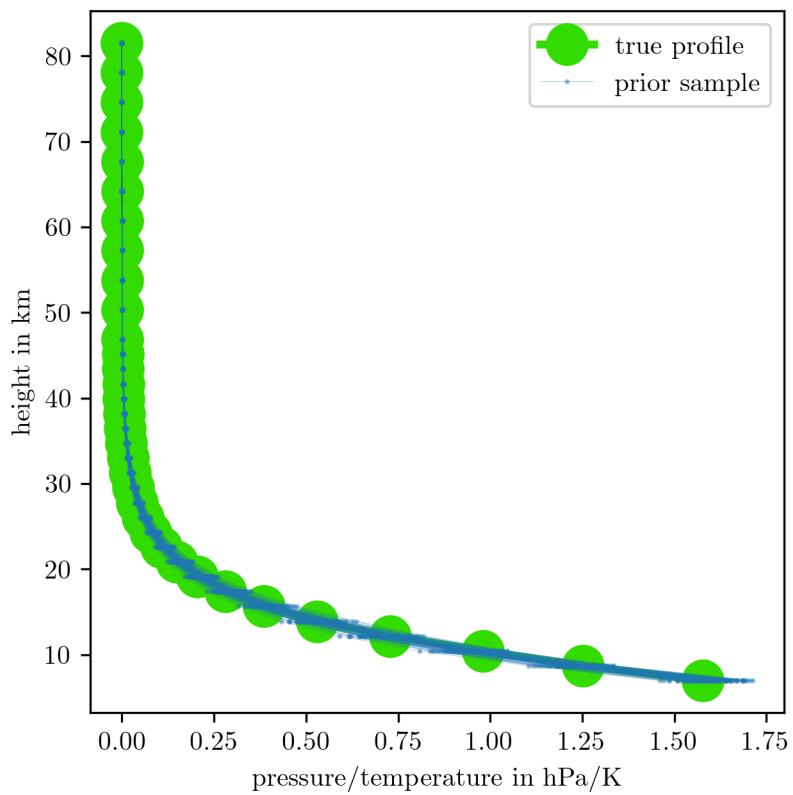


Figure 6.4: Prior samples from the hyper-prior distribution of \mathbf{h}_T , \mathbf{a} and T_0 for temperature as in Eq. 3.9 and b and p_0 for pressure as in Eq. 6.3. We plot \mathbf{p}/\mathbf{T} . The hyper-priors are defined in Tab. 6.1.

6.2 Posterior Distribution

Here the marginal and then the full conditional posterior distribution for the described Bayesian model are formulated. We either use the t-walk algorithm [6] to draw samples from $\pi(p_0, b, T_0, \mathbf{h}_T, \mathbf{a}, \lambda, \gamma | \mathbf{y})$ with $\lambda = \delta/\gamma$ or we utilise a TT approximation on a predefined grid to generate samples via the SIRT method with an MH correction step. In doing so, the reader is guided through the process of obtaining an efficient TT approximation and some key aspects are pointed out. Lastly, the RTO method is utilised to draw ozone samples from the full conditional posterior $\pi(\mathbf{x} | p_0, b, T_0, \mathbf{h}_T, \mathbf{a}, \lambda, \gamma, \mathbf{y})$. Recall that the linear forward model matrix is \mathbf{A}_{θ} is depending on the hyper-parameter defined as $\boldsymbol{\theta} := \{p_0, b, T_0, \mathbf{h}_T, \mathbf{a}\}$.

model parameters	priors	TT bounds		t-walk	
		lower	upper	τ_{int}	Context
\mathbf{x}	$\mathcal{N}(0, (\delta \mathbf{L})^{-1})$	-	-	-	\mathbf{x}
δ	$\mathcal{T}(1, 10^{-35})$	-	-	-	\mathbf{x}
γ	$\mathcal{T}(1, 10^{-35})$	8×10^{14}	1.2×10^{16}	507 ± 29	\mathbf{y}
$\lambda = \delta/\gamma$	-	1×10^{-5}	2.5×10^{-3}	979 ± 75	-
b	$\mathcal{N}(0.174, (0.01)^2)$	0.129	0.214	830 ± 60	\mathbf{p}
$h_{T,1}$	$\mathcal{N}(11, (1.5)^2)$	5.4	16.3	286 ± 13	\mathbf{T}
T_0	$\mathcal{N}(288.15, (10)^2)$	247	326	279 ± 12	\mathbf{T}
p_0	$\mathcal{N}(1311, (20)^2)$	1237	1387	279 ± 12	\mathbf{p}
$h_{T,3}$	$\mathcal{N}(32.3, (2.5)^2)$	22.9	41.7	254 ± 11	\mathbf{T}
a_1	$\mathcal{N}(0, (0.1)^2)$	-0.38	0.38	295 ± 13	\mathbf{T}
$h_{T,2}$	$\mathcal{N}(20.1, (0.7)^2)$	17.2	22.7	296 ± 13	\mathbf{T}
a_0	$\mathcal{N}(-6.5, (0.01)^2)$	-6.54	-6.47	252 ± 10	\mathbf{T}
a_2	$\mathcal{N}(1, (0.01)^2)$	0.97	1.03	267 ± 11	\mathbf{T}
a_3	$\mathcal{N}(2.8, (0.1)^2)$	2.5	3.1	267 ± 11	\mathbf{T}
$h_{T,4}$	$\mathcal{N}(47.4, (0.5)^2)$	45.5	49.3	270 ± 12	\mathbf{T}
a_4	$\mathcal{N}(0, (0.1)^2)$	-0.38	0.38	254 ± 11	\mathbf{T}
$h_{T,5}$	$\mathcal{N}(51.4, (0.5)^2)$	49.5	53.3	280 ± 12	\mathbf{T}
a_5	$\mathcal{N}(-2.8, (0.1)^2)$	-3.18	-2.43	278 ± 12	\mathbf{T}
$h_{T,6}$	$\mathcal{N}(71.8, (3)^2)$	60.5	83.1	250 ± 10	\mathbf{T}
a_6	$\mathcal{N}(-2, (0.01)^2)$	-2.04	-1.96	272 ± 12	\mathbf{T}

Table 6.1: Summary of relevant parameter and hyper-parameters bounds and statistics, ordered as in the TT format according to their correlation structure. We denote $\mathcal{N}(\mu = \text{mean}, \sigma^2 = \text{variance})$ as the Gaussian and $\mathcal{T}(\alpha = \text{scale}, \beta = \text{rate})$ as the Gamma distribution. The IACT τ_{int} from marginal posterior samples via the t-walk is twice the value provided by [69, 28].

6.2.1 Marginal Posterior – Pressure and Temperature

The marginal posterior is given as

$$\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y}) \propto \lambda^{n/2} \gamma^{m/2} \exp \left\{ -\frac{1}{2} g(\boldsymbol{\theta}, \lambda) - \frac{\gamma}{2} f(\boldsymbol{\theta}, \lambda) \right\} \pi(\boldsymbol{\theta}, \lambda, \gamma), \quad (6.4)$$

with $\lambda = \delta/\gamma$,

$$f(\boldsymbol{\theta}, \lambda) = \mathbf{y}^T \mathbf{y} - (\mathbf{A}_{\boldsymbol{\theta}}^T \mathbf{y})^T (\mathbf{A}_{\boldsymbol{\theta}}^T \mathbf{A}_{\boldsymbol{\theta}} + \lambda \mathbf{L})^{-1} (\mathbf{A}_{\boldsymbol{\theta}}^T \mathbf{y}), \quad (6.5a)$$

$$\text{and } g(\boldsymbol{\theta}, \lambda) = \log \det (\mathbf{A}_{\boldsymbol{\theta}}^T \mathbf{A}_{\boldsymbol{\theta}} + \lambda \mathbf{L}). \quad (6.5b)$$

For each evaluation of $\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})$, $\mathbf{A}_{\boldsymbol{\theta}}$ is composed as in Chapter 3, and f and g are calculated directly using the Cholesky decomposition via the Python functions `np.linalg.cholesky` and `scy.linalg.cho_solve`.

Sampling from the marginal posterior

Since the hierarchical model has 18 hyper-parameters, we utilise the t-walk algorithm by Christen and Fox [6] to sample from the marginal posterior $\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})$, because it is quick-to-implement and easy-to-use. The t-walk chooses between four different types of steps on the target distribution. It is employed as a black-box algorithm in default settings, requiring the specification of the number of samples, burn-in period, support region, and the target distribution. Convergence to the target distribution is guaranteed by the construction of this algorithm [6].

Running the t-walk [6] algorithm with the objective to generate 1000 independent samples from the marginal posterior provides a ground truth to which we compare the TT approximation. The maximum IACT provided by twice the value of [68, 28] (see Tab. 6.1 and Fig. B.9 to Fig. B.26) can be bounded by 1100. Then the t-walk takes $N = 1000 \times 1100$ steps plus a burn-in period of $N_{\text{burn-in}} = 100 \times 1100$ for 1000 independent samples. We initialise the Python implementation of the t-walk [7] around the hyper-prior mean values and the mode of $\pi(\lambda, \gamma | \mathbf{y})$ (see Sec. 4.2.1 and e.g., Fig. 4.4). For a total number of $N + N_{\text{burn-in}} = 1210000$ steps within hyper-parameter support bounds given by the iteratively defined TT grid (see Tab. 6.1) a time of ≈ 10 mins is taken. The resulting sample histograms are plotted in Fig. 6.8 to Fig. 6.12 and the trace of the samples in Fig. 6.5.

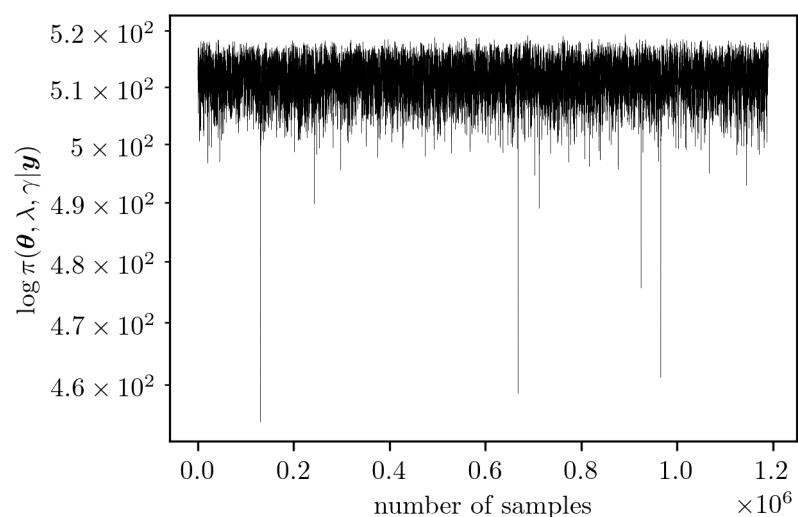


Figure 6.5: Output trace of samples from the marginal posterior distribution $\pi(\theta, \lambda, \gamma | \mathbf{y})$ via the t-walk.

TT approximation of marginal posterior

The aim now is to approximate the square root of the marginal posterior

$$\sqrt{\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})} \propto \exp\left\{0.5 \log \pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y}) + c\right\} \quad (6.6)$$

with a “normalisation constant” $c = -200$ to stay within computer precision. In doing so, we run the `tt.cross.rectcross.rect_cross.cross` function from the `ttypy` python package [39] on a grid (see Tab. 6.1) according to the results of the t-walk. When computing the marginal of each hyper-parameter as in Sec. 2.3 the maximum values of $\sqrt{\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})}$ are around 10^{27} so we set $\xi = 1/\lambda(\mathcal{X})$ with $\lambda(x) = 1$. For Cartesian basis the mass matrix becomes $\mathbf{M}_k = \text{diag}(\lambda_k(\mathcal{X}_k))$. To draw samples from the TT approximation the SIRT-MH scheme is used as introduced in Sec. 2.3.2.

Correlation structure First, we order the hyper-parameters according to their correlation structure to improve the efficiency of the TT approximation of $\sqrt{\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})}$. Specifically, the hyper-parameter space $\mathcal{X}_\gamma \times \mathcal{X}_\lambda \times \mathcal{X}_b \times \dots$ is arranged in such a way that highly correlated hyper-parameter pairs are adjacent and directly linked through their shared TT rank. For samples via the SIRT-MH, twice the value of [68, 28] provides an average IACT of $\approx 1.2 \pm 0.2$. Hence 1000 independent samples from the marginal posterior require 2000 samples via the SIRT-MH scheme. In Fig. 6.6 those 1000 samples and the Pearson correlation coefficients between hyper-parameter pairs are plotted. A coefficient close to 1 or -1 indicates strong correlation, while values near zero suggest weak or no correlation. We observe that the hyper-parameters λ and b , and λ and γ are highly correlated. Additionally, $h_{T,1}$ describing the temperature at low altitudes (strong signal) is mildly correlated to b . This is because $h_{T,1}$ influences “the smoothness” of \mathbf{p}/\mathbf{T} , which is hard to see in Fig. 6.4. Interestingly, p_0 appears largely uncorrelated with other hyper-parameters, while b is the key parameter linking pressure to ozone and temperature. Hyper-parameters describing the temperature at higher altitudes are very much uncorrelated and the IACTs of the t-walk in Tab. 6.1 agree with those results. Alternatively, one could decorrelate the hyper-parameter space e.g., via Cholesky whitening [30].

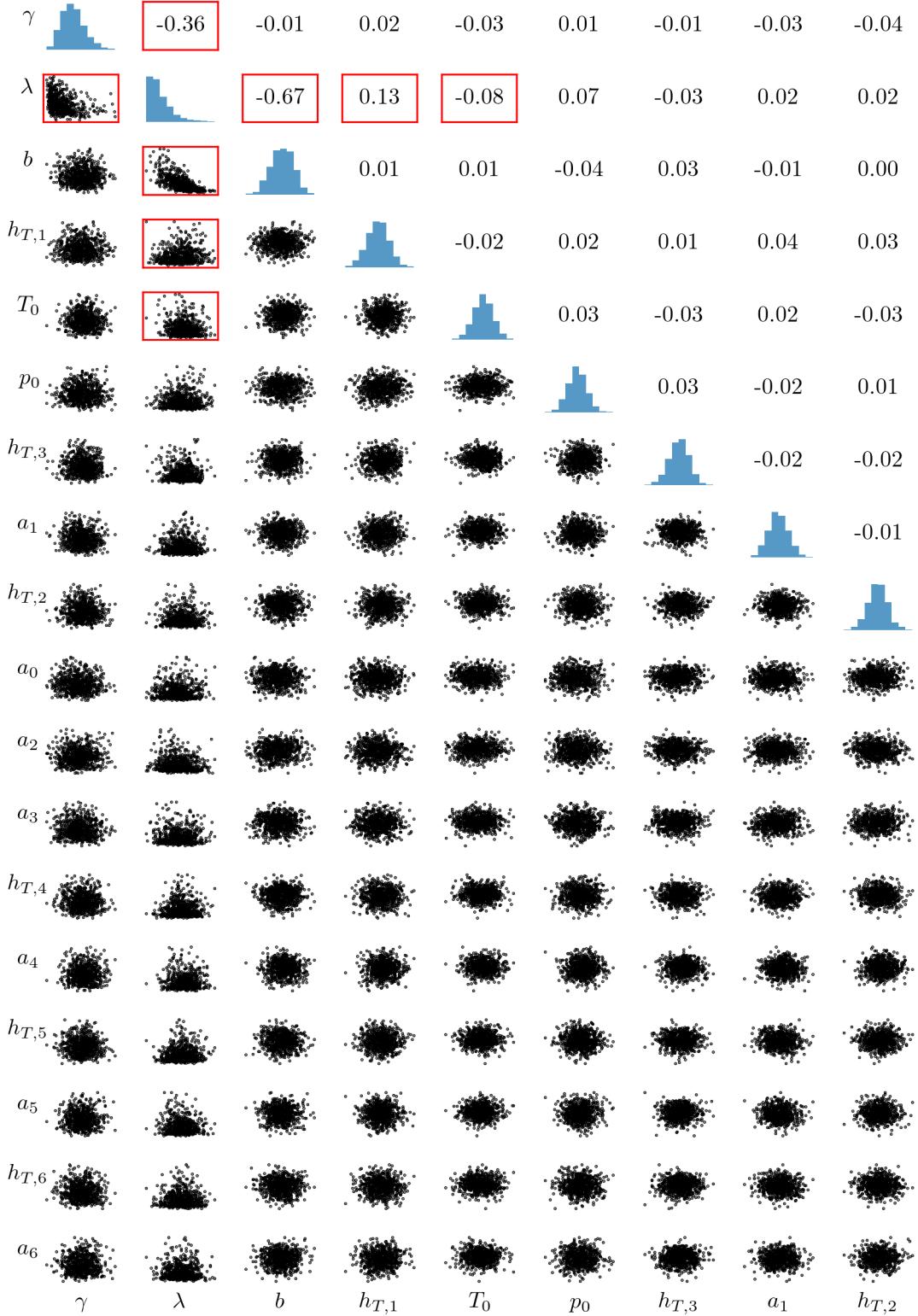
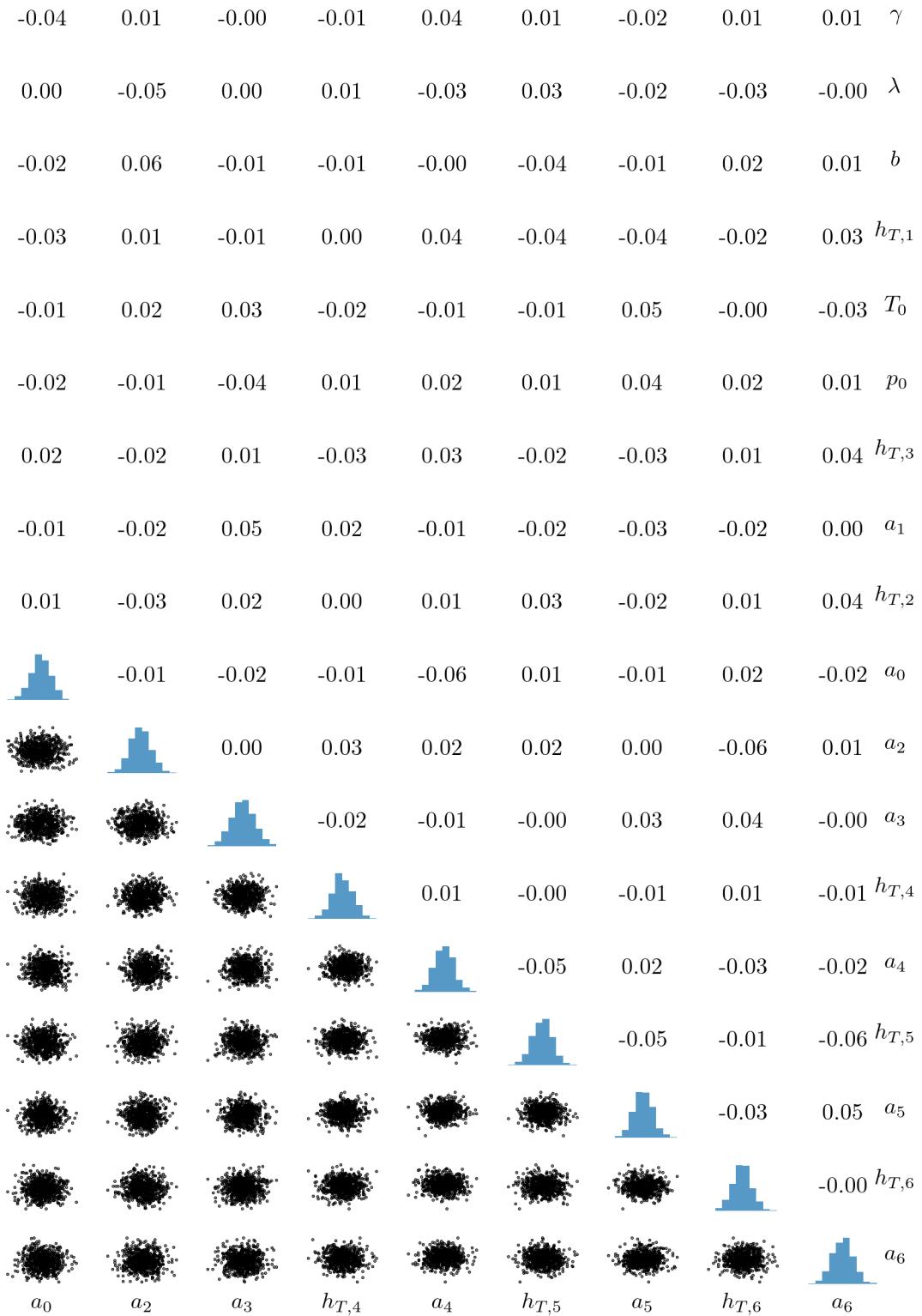


Figure 6.6: Plot of 1000 independent samples from TT approximation of $\sqrt{\pi(\theta, \lambda, \gamma | \mathbf{y})}$ via SIRT-MH scheme. We plot the Pearson correlation coefficient ranging from -1 to 1 for each hyper-parameter pair.

Correlation plot of samples from TT-approximation of $\sqrt{\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})}$ via SIRT-MH scheme.

Find optimal rank and grid size The aim is to decrease the number of function evaluations of $\sqrt{\pi(\theta, \lambda, \gamma | \mathbf{y})}$ and to determine the optimal rank and grid size without losing too much accuracy of the marginal posterior approximation. For stable and comparable results, we do five sweeps within the `tt.cross.rectcross.rect_cross.cross` Python function initialised at a random TT. The ranks between TT cores are constant. Then 1000 independent samples from the TT approximation of the marginal posterior via the SIRT-MH scheme are drawn. First, the number of grid points is set to $n = 150$ and different error measures for ranks $\{2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 20, 25, 30, 35, 50\}$ are calculated. We compare to true marginal posterior function values and 1000 independent t-walk samples to find a small but tolerable rank. Then with a fixed rank the number of grid points $\{10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 80, 90, 100\}$ is decreased until sufficient accuracy.

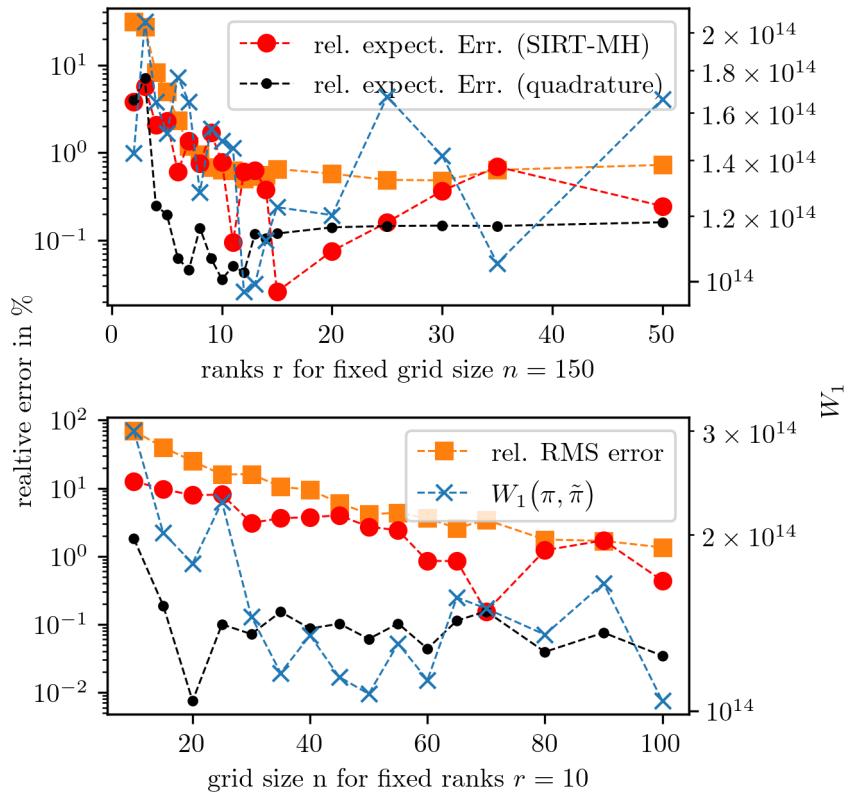


Figure 6.7: Given a TT approximation of $\sqrt{\pi(\theta, \lambda, \gamma | \mathbf{y})}$, the relative RMS error (orange squares) and the 1-Wasserstein distance (blue cross) between approximated values at sample points provided by the SIRT-MH and the true function values are calculated. The relative RMS error between the sample means provided by the t-walk and mean values for the hyper-parameters from the TT approximation is plotted (black dots). The mean values for the hyper-parameters are computed via quadrature, where the marginal functions from the TT approximation act as quadrature weights. Additionally, the relative RMS error between the sample-based mean from the SIRT-MH and the t-walk (red circles) is plotted.

One of the error measures is the 1-Wasserstein distance W_1 (blue crosses in Fig. 6.7), as in Eq. 2.48. The 1-Wasserstein distance is calculated between 1000 independent SIRT-MH samples from the TT approximation $\tilde{\pi}(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})$ weighted by their approximated values and 1000 independent t-walk samples from the true marginal posterior weighted by $\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})$. We use the Python function `SamplesLoss("sinkhorn", p=1, blur=0.05, scaling=0.8)` with default settings from the Python package `geomloss` [16] to obtain W_1 . This function provides the unbiased Sinkhorn divergence which converges towards the Wasserstein distance and can be understood as the generalised Quicksort algorithm [15]. Here $p = 1$ defines the distance measure $\|\cdot\|_{L^2}$. The blur parameter is an entropic penalty and the scaling parameter specifies the trade-off between speed ($\text{scaling} < 0.4$) and accuracy ($\text{scaling} > 0.9$) [16]. Additionally, the marginal functions of each TT approximation are used to obtain the quadrature-based means $\boldsymbol{\mu}_{\text{TT}} \in \mathbb{R}^{18}$ of each hyper-parameter by weighted expectations. Then the relative RMS difference $\|\boldsymbol{\mu}_{\text{TT}} - \boldsymbol{\mu}_{\text{t-walk}}\|_{L^2} / \|\boldsymbol{\mu}_{\text{t-walk}}\|_{L^2}$ is calculated and plotted in Fig. 6.7 (black dots). The “true sample-based means” from the t-walk are denoted as $\boldsymbol{\mu}_{\text{t-walk}}$. The relative RMS between the SIRT-MH sample-based mean $\boldsymbol{\mu}_{\text{SIRT-MH}}$ and $\boldsymbol{\mu}_{\text{t-walk}}$ is calculated and plotted in Fig. 6.7 (red circles). Further, the relative RMS error between TT approximated and true function values for 1000 independent SIRT-MH samples is calculated and plotted in Fig. 6.7 (orange squares).

All of these measures are plotted in Fig. 6.7. We observe that a rank $r = 10$ is sufficient because the error measures are relatively stable for $r \geq 10$. For a grid size $n \geq 30$ the relative differences between $\boldsymbol{\mu}_{\text{TT}}$ and $\boldsymbol{\mu}_{\text{t-walk}}$ (red circles in Fig. 6.7) and the RMS errors at the 1000 independent SIRT-MH samples (orange squares in Fig. 6.7) are around 10% and considered good enough. For an increasing number of grid points the interpolation of function values between grid points is more accurate and the sample-based relative errors decrease. This is because the chosen linear interpolation (see Eq. 2.41) is a rather rudimentary choice. The quadrature-based relative expectation error (black dots in Fig. 6.7) is almost constant for ranks $\gtrsim 7$ and grid sizes > 20 . Since the hyper-parameters have different length scales, we are only interested in the trend of the sample-based 1-Wasserstein distance (blue crosses in Fig. 6.7). The 1-Wasserstein distance is quite fluctuant but decreases with increasing ranks and stays within a similar range for grid sizes $n \geq 30$.

Based on these results the grid size is set to $n = 30$. Next, we define ranks $r = [1, 10, 10, 10, 10, 10, 5, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 1]$ between TT cores, with a maximum rank of 10. This harvests the correlation structure of $\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})$ and decreases the number of function evaluations even further. One sweep in the `tt.cross.rectcross.rect_cross.cross` initialised at a previously calculated approximation reduces the computation time to $\approx 10\text{s}$ and the number of function evaluations to 34080. For the samples drawn via the SIRT-MH scheme, the average IACT (provided by

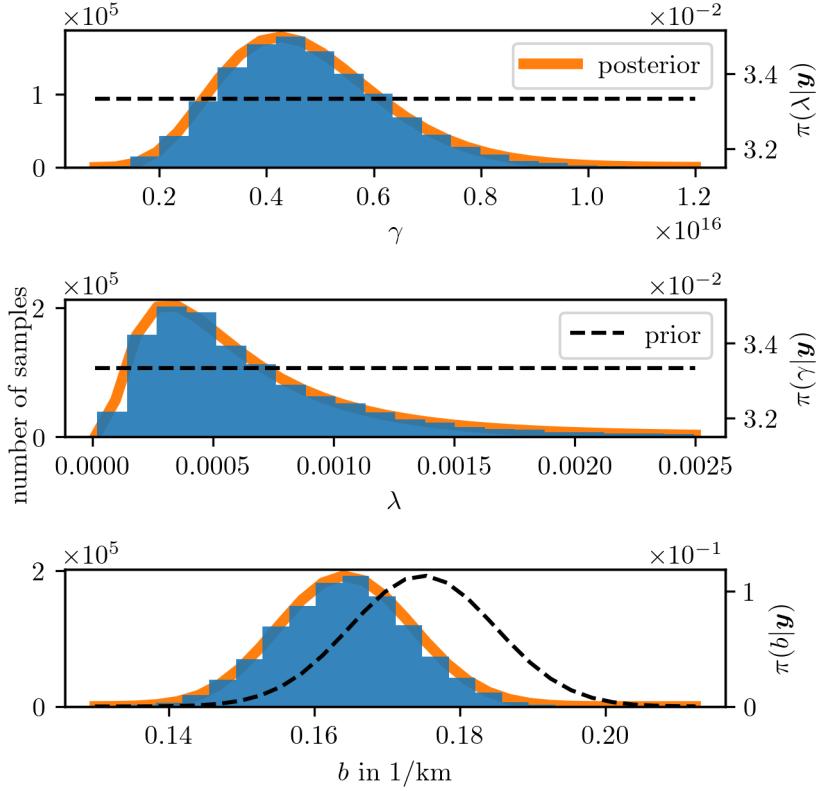


Figure 6.8: TT approximation of the marginal posterior in orange and the samples from the t-walk as a histogram, as well as the prior distribution with a dotted line.

twice the value of [68, 28]) is $\approx 1.2 \pm 0.2$. This means that once the TT approximation is available two function evaluations per independent sample are needed. To draw 1000 independent samples, including generating a TT approximation, takes ≈ 30 s, and we report a relative RMS error of $\approx 12\%$ evaluated over those 1000 independent samples. The relative RMS error over 1000 randomly chosen grid points is $\approx 1\%$ indicating that the linear interpolation causes most of the approximation error. The marginals for each hyper-parameter are plotted in Fig. 6.8 to Fig. 6.13. We observe that, besides λ and γ , only the marginal posterior of the b hyper-parameter is seriously affected by the data and has significantly changed compared to the hyper-prior distribution.

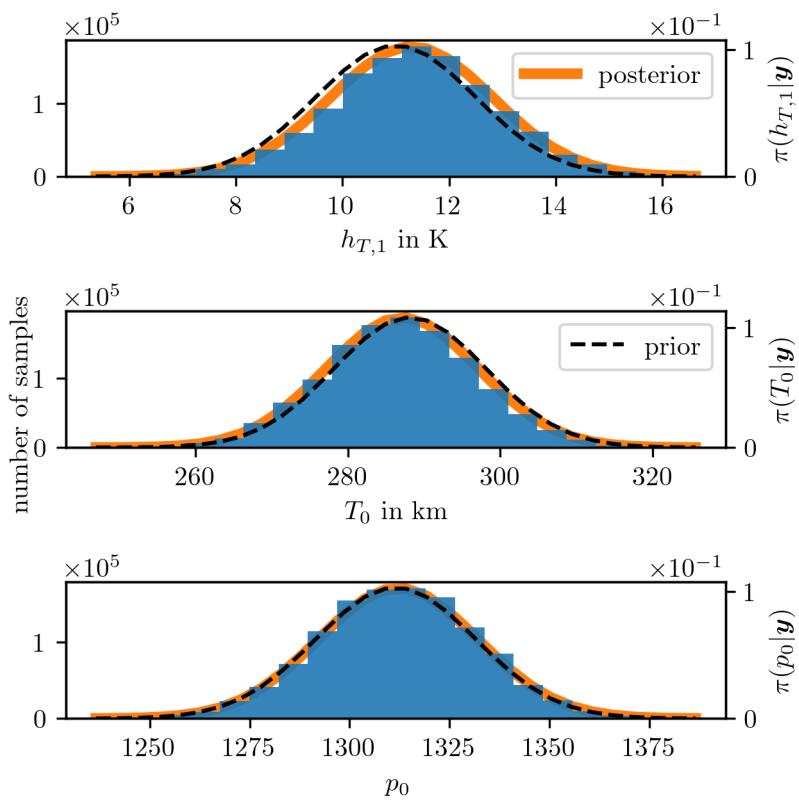


Figure 6.9: TT approximation of the marginal posterior in orange and the samples from the t-walk as a histogram, as well as the prior distribution with a dotted line.

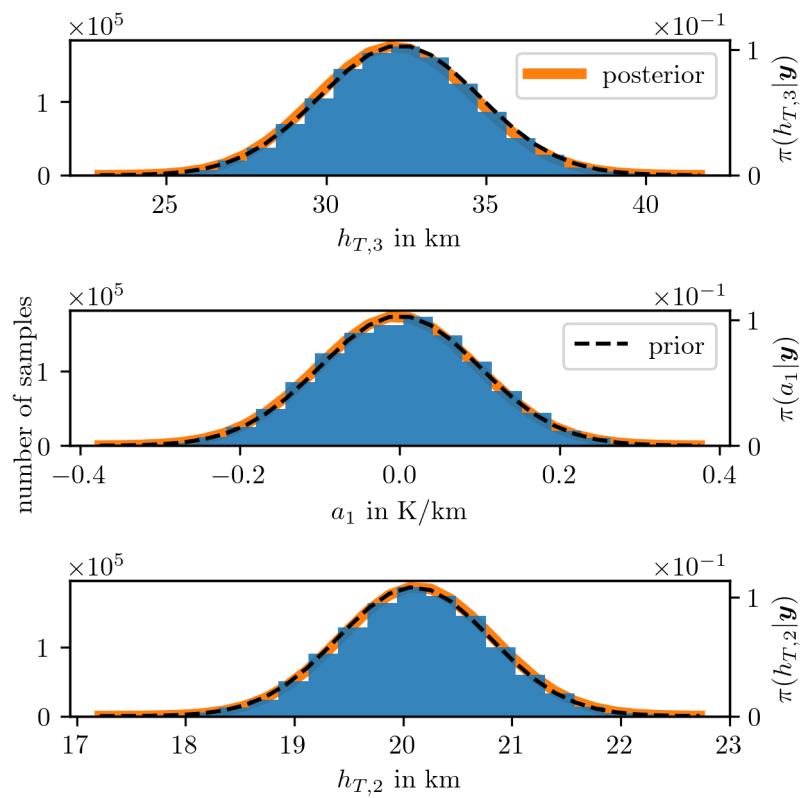


Figure 6.10: TT approximation of the marginal posterior in orange and the samples from the t-walk as a histogram, as well as the prior distribution with a dotted line.

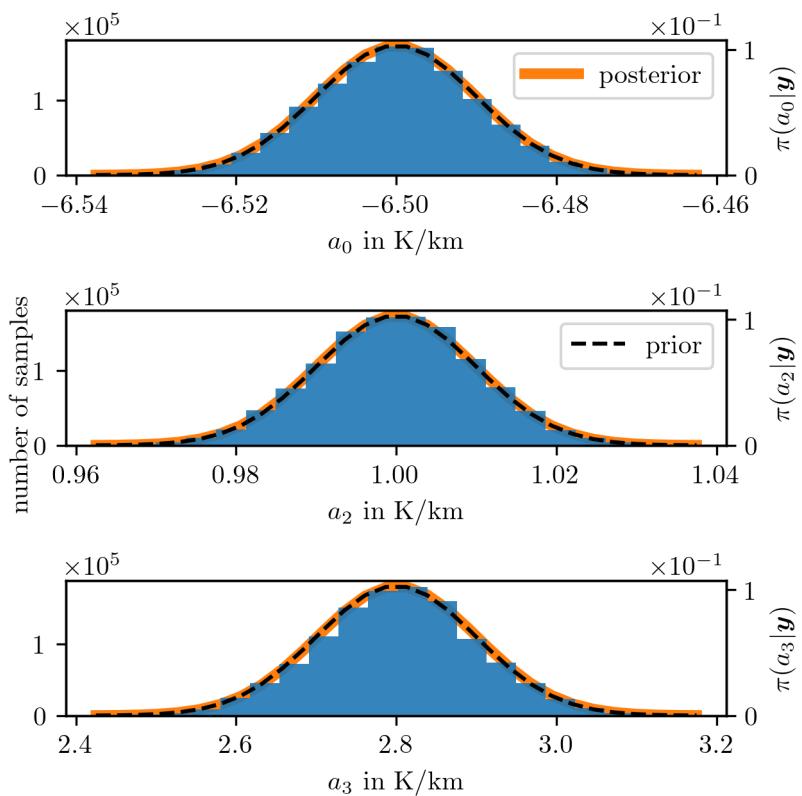


Figure 6.11: TT approximation of the marginal posterior in orange and the samples from the t-walk as a histogram, as well as the prior distribution with a dotted line.

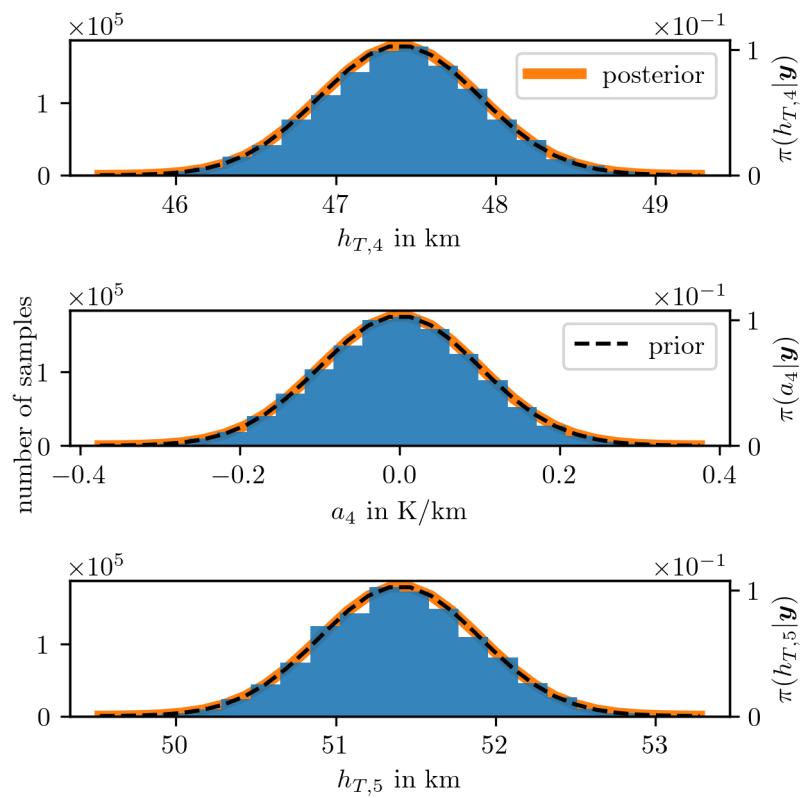


Figure 6.12: TT approximation of the marginal posterior in orange and the samples from the t-walk as a histogram, as well as the prior distribution with a dotted line.

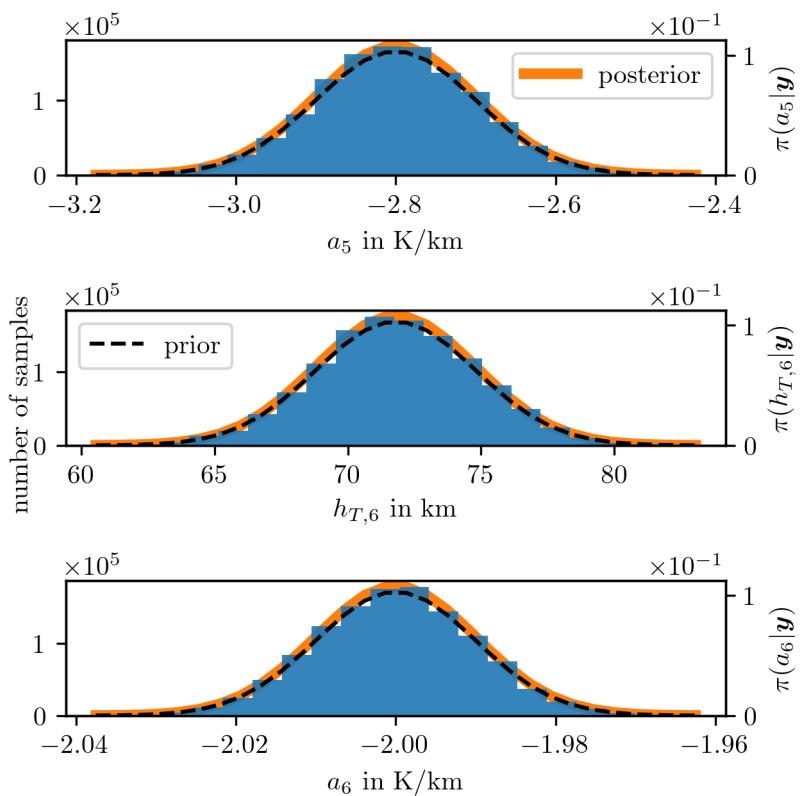


Figure 6.13: TT approximation of the marginal posterior in orange and the samples from the t-walk as a histogram, as well as the prior distribution with a dotted line.

Posterior pressure and temperature

Posterior pressure and temperature profiles are directly obtained by hyper-parameter samples from the marginal posterior $\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})$ and then calculated according to their respective function (see Eq. 3.9 and Eq. 6.3). The obtained pressure and temperature posterior profiles are plotted in Fig. 6.15 and Fig. 6.14. The posterior temperature profiles look (as expected) similar to the prior temperature profiles, whereas the pressure profile has slightly larger values compared to the ground truth. This is because the hyper-parameter b is smaller than its ground truth value (see Fig. 6.8), resulting in the posterior pressure profiles that do not exponentially decrease as fast as the ground truth pressure profile.

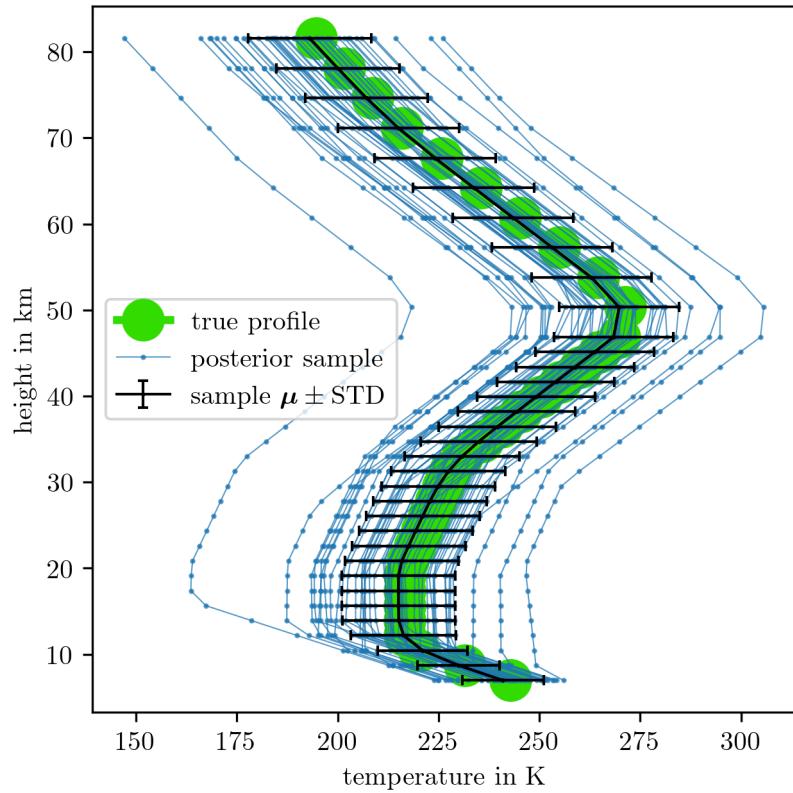


Figure 6.14: Plot of posterior temperature profiles according to Eq. 3.9 and hyper-parameter samples from the marginal posterior distribution $\pi(\boldsymbol{\theta}, \lambda, \gamma | \mathbf{y})$.

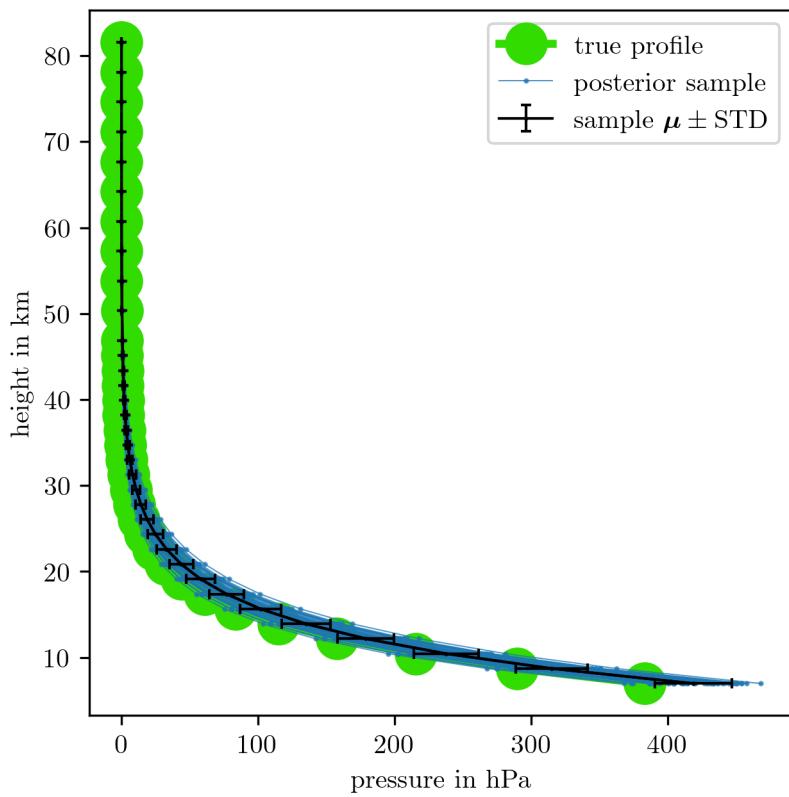


Figure 6.15: Plot of posterior pressure profiles according to Eq. 6.3 and hyper-parameter samples from the marginal posterior distribution $\pi(\theta, \lambda, \gamma | \mathbf{y})$.

6.2.2 Full Conditional Posterior – Ozone

Due to the large number of hyper-parameters calculating the posterior mean $\boldsymbol{\mu}_{\mathbf{x}|\mathbf{y}}$ and $\boldsymbol{\Sigma}_{\mathbf{x}|\mathbf{y}}$ covariance via quadrature as in Eq. 2.17 and 2.18 is computationally not feasible. If the full conditional posterior is a normal distribution, then the randomise then optimise (RTO) method provides a scheme to obtain an independent ozone sample from $\pi(\mathbf{x}|\boldsymbol{\theta}, \delta, \gamma, \mathbf{y})$ with $\delta = \lambda \gamma$. We introduce the RTO method for general case first and then draw ozone samples from $\mathbf{x}^{(k)} \sim \pi(\mathbf{x}|\boldsymbol{\theta}^{(k)}, \delta^{(k)}, \gamma^{(k)}, \mathbf{y})$ conditioned on independent marginal posterior samples $\boldsymbol{\theta}^{(k)}, \delta^{(k)}, \gamma^{(k)} \sim \pi(\boldsymbol{\theta}, \delta, \gamma|\mathbf{y})$.

Randomise then optimise

As in [2] rewrite the full conditional posterior (see Eq. 2.15) as

$$\pi(\mathbf{x}|\boldsymbol{\theta}, \delta, \gamma, \mathbf{y}) \propto \pi(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}, \gamma) \pi(\mathbf{x}|\delta) \quad (6.7)$$

$$\propto \exp\left(-\frac{1}{2}(\mathbf{A}_\theta \mathbf{x} - \mathbf{y})^T \boldsymbol{\Sigma}_\gamma^{-1} (\mathbf{A}_\theta \mathbf{x} - \mathbf{y})\right) \exp\left(-\frac{1}{2}(\boldsymbol{\mu} - \mathbf{x})^T \mathbf{Q}_\delta (\boldsymbol{\mu} - \mathbf{x})\right), \quad (6.8)$$

$$= \exp\left(-\frac{1}{2} \|\hat{\mathbf{A}}\mathbf{x} - \hat{\mathbf{y}}\|_{L^2}^2\right), \quad (6.9)$$

where

$$\hat{\mathbf{A}} := \begin{bmatrix} \boldsymbol{\Sigma}_\gamma^{-1/2} \mathbf{A}_\theta \\ \mathbf{Q}_\delta^{1/2} \end{bmatrix}, \quad \hat{\mathbf{y}} := \begin{bmatrix} \boldsymbol{\Sigma}_\gamma^{-1/2} \mathbf{y} \\ \mathbf{Q}_\delta^{1/2} \boldsymbol{\mu} \end{bmatrix}, \quad (6.10)$$

\mathbf{Q}_δ is the prior precision, $\boldsymbol{\mu}$ the prior mean and $\boldsymbol{\Sigma}_\gamma$ the noise covariance (see also [3, 4]). A sample $\mathbf{x}^{(k)}$ from the full conditional posterior $\pi(\mathbf{x}|\boldsymbol{\theta}, \delta, \gamma, \mathbf{y})$ is obtained by minimising the following equation:

$$\mathbf{x}^{(k)} = \arg \min_{\mathbf{x}} \|\hat{\mathbf{A}}\mathbf{x} - (\hat{\mathbf{y}} + \mathbf{b})\|_{L^2}^2, \quad \mathbf{b} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_m), \quad (6.11)$$

where a random perturbation \mathbf{b} is added. Similar to Section 2.4, this expression becomes

$$(\mathbf{A}_\theta^T \boldsymbol{\Sigma}_\gamma^{-1} \mathbf{A}_\theta + \mathbf{Q}_\delta) \mathbf{x}^{(k)} = \mathbf{A}_\theta^T \boldsymbol{\Sigma}_\gamma^{-1} \mathbf{y} + \mathbf{Q}_\delta \boldsymbol{\mu} + \mathbf{v}_1 + \mathbf{v}_2, \quad (6.12)$$

with $\mathbf{v}_1 \sim \mathcal{N}(\mathbf{0}, \mathbf{A}_\theta^T \boldsymbol{\Sigma}_\gamma^{-1} \mathbf{A}_\theta)$ and $\mathbf{v}_2 \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}_\delta)$, representing independent Gaussian random variables [2, 17].

Posterior ozone samples

More explicitly conditioned on an independent $\boldsymbol{\theta}^{(k)}, \lambda^{(k)}, \gamma^{(k)} \sim \pi(\boldsymbol{\theta}, \lambda, \gamma|\mathbf{y})$ and one full conditional posterior sample is given as

$$\mathbf{x}^{(k)} = \underbrace{\left(\gamma^{(k)} \mathbf{A}_{\boldsymbol{\theta}^{(k)}}^T \mathbf{A}_{\boldsymbol{\theta}^{(k)}} + \delta^{(k)} \mathbf{L} \right)^{-1}}_{\mathbf{B}^{(k)}} \left(\gamma^{(k)} \mathbf{A}_{\boldsymbol{\theta}^{(k)}}^T \mathbf{y} + \sqrt{\gamma^{(k)}} \mathbf{A}_{\boldsymbol{\theta}^{(k)}} \mathbf{v}_1 + \sqrt{\delta^{(k)}} \mathbf{L}^{1/2} \mathbf{v}_2 \right) \quad (6.13)$$

with $\mathbf{v}_1 \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_m)$, $\mathbf{v}_2 \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$, $\mathbf{Q}_\delta = \delta \mathbf{L}$, $\Sigma_\gamma^{-1} = \gamma \mathbf{I}$ and $\mathbf{L}^{1/2}$ is the Cholesky decomposition of \mathbf{L} [2]. If n is large and calculating the Cholesky decomposition of \mathbf{L} or constructing \mathbf{L} is expensive it is recommended to represent \mathbf{L} as a sum over cliques e.g., small 2×2 rank-1 matrices (see \mathbf{L} in Eq. 2.57). Then a sample $\mathbf{v}_2 \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}_\delta)$ can be obtained by drawing n random variables from $\mathcal{N}(0, 1)$ without explicitly forming \mathbf{L} [17].

The Cholesky factorisation of $\mathbf{B}^{(k)}$ and \mathbf{L} is obtained via the Python function `numpy.linalg.cholesky` and `scipy.linalg.cho_solve` is used to solve for $\mathbf{x}^{(k)}$. We plot 100 samples in Fig. 6.16 and a sample mean based on 1000 samples. The posterior ozone mean is much smaller than the ground truth, especially around the ozone peak. Compared to the posterior pressure in Fig. 6.15, which is slightly larger than the ground truth, we can conclude that pressure and ozone are highly correlated. Additionally, the individual posterior samples are more prior-dominated through larger λ values (see Fig. 6.8) and hence smoother compared to the previously calculated ozone posterior profiles. Again, we are not able to recover the second ozone peak at high altitudes.

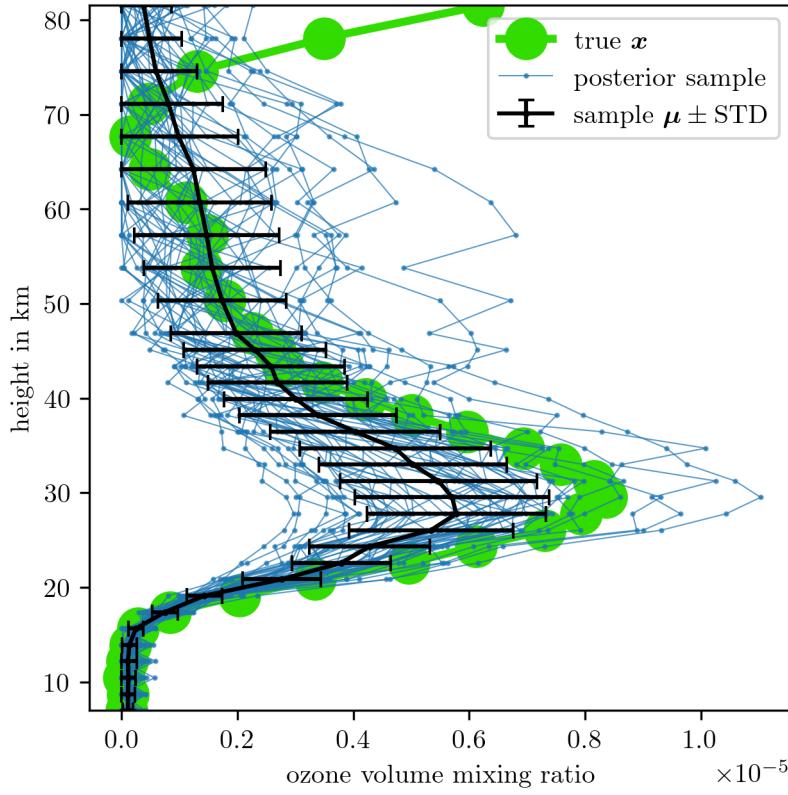


Figure 6.16: Plot of ozone samples from the full conditional posterior $\pi(\mathbf{x}|\boldsymbol{\theta}, \delta, \gamma, \mathbf{y})$ via the RTO method.

7

Summary and Outlook

In this chapter, the key results and conclusions of this work are summarised. The comparison between the Bayesian approach and the regularisation approach is made. We elaborate on the differences between sampling-based methods and the TT approximation. Lastly, our results are situated within the broader context of atmospheric modelling and the implications for the future development of an atmospheric limb sounder are discussed. An outlook for future research is provided.

7.1 Regularisation Solution vs. Hierarchical Bayesian Approach

Using a regularisation approach, 200 solves of \mathbf{x}_λ are needed to obtain one solution to this inverse problem. In contrast, the hierarchical Bayesian approach involves 25 function evaluations of the marginal posterior (to find the mode) and then 10100 samples from the approximated marginal posterior followed by 20 evaluations of \mathbf{x}_λ and \mathbf{B}_λ^{-1} to characterise the full posterior in ≈ 0.5 s. Utilising a TT approximation (including finding the mode) to compute the full posterior mean and covariance takes ≈ 0.025 s, requiring only 400 function evaluations to approximate $\pi(\lambda, \gamma | \mathbf{x})$ and is almost as fast as the regularisation approach (≈ 0.015). Regardless, either method has a runtime of much less than a second on a basic laptop.

While regularisation yields a single optimal solution (point estimate), a Bayesian framework provides a distribution of ozone profiles. This posterior distribution presents a range of feasible solutions to the inverse problem and hence true errors. Moreover, within the hierarchical Bayesian approach, we can include prior knowledge about the noise, ozone profile and many more physical processes through hyper-parameters, offering an arbitrarily flexible and informative inference framework.

7.2 Sampling Methods vs. TT Approximation

Using the TT approximation involves far fewer function evaluations of the target distribution compared to sample-based methods. The main disadvantage of TT methods is that they require a predefined grid and a “normalisation constant”, which we have to find iteratively. Relying solely on TT approximations may lead to a substantial amount of trial and error and dealing with numerical issues. Nevertheless, once properly configured, we have shown the potential and advantages of TT methods.

More specifically, the TT approximation of the 2-dimensional marginal posterior ($\approx 0.025s$) is 20 times faster than the MWG sampler ($\approx 0.5s$). Excluding the function evaluations for finding the mode of the marginal posterior, the MWG sampler takes 10100 steps while the TT approximation only needs 400 function evaluations; this is a factor of ≈ 25 . Alternatively, for low-dimensional distributions, it may be preferable to approximate integrals directly and to use existing freely available quadrature libraries and packages such as `quadpy`.

In higher dimensions, such as the 18-dimensional marginal posterior considered in this thesis, TT methods ($\approx 0.5min$) outperform samplers like the t-walk ($\approx 10min$), once a grid and normalisation constant have been defined. Although the t-walk may not be the best sampler for this specific problem and the underlying correlation structure, it is robust and easy-to-implement. To illustrate the efficiency of TT approximations, we compare the number of function evaluations per 1000 independent samples. For 1000 independent samples with a maximum IACT of 1100 and a burn-in period of 100 independent samples, the t-walk needs 1210000 function evaluations. In contrast, 34080 function evaluations are enough to approximate the marginal posterior in the TT format. Then drawing 1000 independent samples via the SIRT-MH scheme requires another 2000 function evaluations with an IACT of ≈ 1.2 . So the cost per independent sample for the t-walk is 1210 and for the TT approach is ≈ 36 function evaluations, including the burn-in period or the TT approximation via the `rect_cross.cross` Python function. Without the burn-in phase the t-walk requires around 1100 function evaluations per independent sample, while once a TT approximation is available only two function evaluations per independent sample are needed.

For future application, we suggest improving the efficiency of the TT approximation by e.g., reducing the correlation structure through a coordinate system rotation (Cholesky Whitening) or using better interpolators in between grid points to reduce the approximation error. This may be particularly important when the CDF in the SIRT scheme is not smooth due to poor approximations of the target density at previous samples. Moreover, using a different reference measure for integration as in [8], such as a Gaussian measure

instead of the current Lebesgue measure, may increase numerical stability. Currently, we have to predefine a normalisation constant and lower ranks manually, bounding the ranks automatically would be helpful (see e.g., [48]).

7.3 Atmospheric Physics

Here the results within the context of our simplified atmospheric limb-sounding model are summarised. This thesis showed that the underlying non-linear forward model can be approximated with an affine map and the linear model, making this a linear inverse problem. For future application, we wish to include more measurement device-specific hyper-parameters in the forward model. This could include e.g., uncertainty in pointing accuracy or an antenna response function.

For an SNR of ≈ 150 , Sec. 3.2.1 implicated that there is no information gain if one measures more frequently or collects more data in noise-dominated regions. An SNR of $\approx 10^4$ is needed to produce data that is informative about ozone at higher altitudes.

Fig. 6.16 and Fig. 6.15 illustrate that pressure and ozone are highly correlated. One has to consider that when conditioning on pressure estimates from other sources, a slight change in pressure does skew the ozone VMR significantly. A more restrictive prior for the pressure-related hyper-parameter b would provide a fix to that issue, but that would not be objective. By explanatory analysis, we found that data with an SNR of ≈ 1000 recovers an ozone (without a peak in higher altitudes) and pressure profile close to the ground truth. As previously mentioned in the prior analysis (see Fig. 6.4), the model as well as the data are uninformative about temperature and dominated by the exponentially decreasing pressure.

All the samples plotted in Fig. 5.4, Fig. 4.5, and Fig. 6.16 present valid solutions to the inverse problem, but consistently fail to capture the ozone peak at higher altitudes. This is due to noise-dominated data (see Fig. 3.7) and low signal strength in upper atmospheric regions, where the variability of the posterior ozone is large and primarily determined by the prior. We conclude that the main objective for future research is to develop a more accurate, potentially parametrised (prior) model, which captures physical properties and chemical processes of ozone in the atmosphere.

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Appendices

A

Theoretical and Technical Background

A.1 Correlation Structure

In the book Gaussian Markov Random Fields [49], Rue and Held demonstrate that a strong correlation between the hyper-parameter μ and the latent field \mathbf{x} can significantly slow down convergence particularly when using Gibbs samplers. They consider the hierarchical model

$$\mu \sim \mathcal{N}(0, 1) \quad (\text{A.1a})$$

$$\mathbf{x}|\mu \sim \mathcal{N}(\mu \mathbf{1}, \mathbf{Q}^{-1}), \quad (\text{A.1b})$$

and apply a Gibbs sampler based on the full conditional distributions

$$\mu^{(k)} | \mathbf{x}^{(k)} \sim \mathcal{N}\left(\frac{\mathbf{1}^T \mathbf{Q} \mathbf{x}^{(k-1)}}{1 + \mathbf{1}^T \mathbf{Q} \mathbf{1}}, \left(1 + \mathbf{1}^T \mathbf{Q} \mathbf{1}\right)^{-1}\right) \quad (\text{A.2})$$

$$\mathbf{x}^{(k)} | \mu^{(k)} \sim \mathcal{N}(\mu^{(k)} \mathbf{1}, \mathbf{Q}^{-1}). \quad (\text{A.3})$$

As illustrated in Figure A.1, when the sampler is restricted to steps only in the μ -direction (horizontal axis) or the \mathbf{x} -direction (vertical axis), it requires many iterations to adequately explore the parameter space. This inefficiency arises from the high correlation between μ and \mathbf{x} , visible in Figure A.1 as a “squeeze” of the distribution.

A solution to the slow mixing problem is to update (μ, \mathbf{x}) jointly. Since μ is one-dimensional, effectively only the marginal density of μ is needed.

$$\mu^* \sim q(\mu^* | \mu^{(k-1)}) \quad (\text{A.4})$$

$$\mathbf{x}^{(k)} | \mu^* \sim \mathcal{N}(\mu^* \mathbf{1}, \mathbf{Q}^{-1}) \quad (\text{A.5})$$

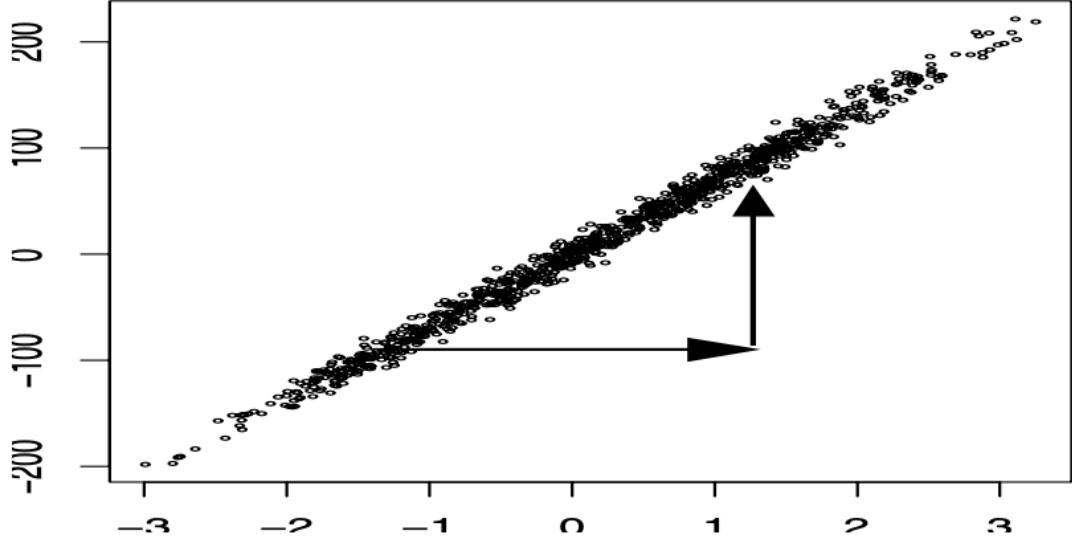


Figure A.1: The figure taken from [49, Figure 4.1 (b)] shows samples from the chain of μ (x-axis) and $\mathbf{1}^T \mathbf{Q} \mathbf{x}^{(k)}$ (y-axis) for over 1000 iterations, based on the hierarchical model in Eq. A.1, with an autoregressive process encoded in \mathbf{Q} . The algorithm updates μ and \mathbf{x} successively from their conditional distributions (see Eq. A.2 and Eq. A.3). The plot displays $(\mu^{(k)}, \mathbf{1}^T \mathbf{Q} \mathbf{x}^{(k)})$, with $\mu^{(k)}$ on the horizontal axis and $\mathbf{1}^T \mathbf{Q} \mathbf{x}^{(k)}$ on the vertical axis. The slow mixing and convergence of μ result from its strong dependence on $\mathbf{1}^T \mathbf{Q} \mathbf{x}^{(k)}$, while the sampler permits only axis-aligned (horizontal and vertical) and does not allow diagonal moves, as illustrated by the arrows.

With a simple MCMC algorithm targeting μ , one can explore the sample space efficiently and only draw a corresponding sample for \mathbf{x} from its full conditional once, for instance, the proposal μ^* has been accepted.

A.2 Monte-Carlo Error and Integrated Autocorrelation Time

To assess the error $(\sigma^{(i)})^2$ of a samples-based estimate

$$\bar{h}_N^{(i)} := \text{E}_{\mathbf{x}|\mathbf{y}}[h(\mathbf{x})] = \frac{1}{N} \sum_{k=1}^N h(\mathbf{x}^{(k)}), \quad (\text{A.6})$$

from the chain $\mathcal{M}^{(i)} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(k)}, \dots, \mathbf{x}^{(s)}, \dots, \mathbf{x}^{(N)}\} \sim \pi(\mathbf{x}|\mathbf{y})$, we ignore systematic error due to initialisation bias (burn-in period), but we have to take into account that samples produced by any system or algorithm are correlated. To derive the IACT, we follow Ulli Wolff's lecture notes [70] (or alternatively [68]).

In general, the error of a Monte-Carlo estimate is:

$$(\sigma^{(i)})^2 = \text{Var}(\bar{h}_N^{(i)}) = \text{Var}(\text{E}_{\mathbf{x}|\mathbf{y}}[h(\mathbf{x})]) = \left(\frac{1}{N} \sum_{k=1}^N h(\mathbf{x}^{(k)}) - \bar{h}_N^{(i)} \right)^2. \quad (\text{A.7})$$

Expanding this summation, we see that

$$(\sigma^{(i)})^2 = \frac{1}{N^2} \sum_{k,s=1}^N \Gamma(k-s) \quad (\text{A.8})$$

with the autocorrelation coefficient $\Gamma(k-s) = (h(\mathbf{x}^{(k)}) - \bar{h}_N^{(i)})(h(\mathbf{x}^{(s)}) - \bar{h}_N^{(i)})$. Next we rewrite

$$\sum_{k,s=1}^N \Gamma(k-s) = \text{Var}(h(\mathbf{x})) \sum_{k,s=1}^N \frac{\Gamma(k-s)}{\Gamma(0)} = \text{Var}(h(\mathbf{x})) \sum_{k,s=1}^N \rho(k-s), \quad (\text{A.9})$$

with the normalised autocorrelation coefficient $\rho(k-s) = \Gamma(k-s)/\Gamma(0)$ at lag $k-s$ and $\Gamma(0) = \text{Var}(h(\mathbf{x}))$ for $k=s$. Typically $\Gamma(t)$ decays exponentially so that, for $N \gg \tau$, $\Gamma(t) \xrightarrow{t \rightarrow \infty} \exp\{-|t|/\tau\}$ and we can approximate

$$\sum_{k,s=1}^N \rho(k-s) = N \sum_{t=-(N-1)}^{N-1} \left(1 - \frac{t}{N}\right) \rho(t) \approx N \sum_{t=-\infty}^{\infty} \rho(t), \quad (\text{A.10})$$

see [57, p. 137]. If $\tau \gg 1$

$$\sum_{t=-\infty}^{\infty} \rho(t) = 1 + 2 \sum_{t=1}^{\infty} (e^{-1/\tau})^t = 1 + 2 \frac{e^{-1/\tau}}{1 - e^{-1/\tau}} \approx 1 + 2 \frac{1 - 1/\tau}{1/\tau} = 2\tau - 1. \quad (\text{A.11})$$

Here we use the geometric power series $\sum_{n=0}^{\infty} x^n = 1/(1-x)$ and the Taylor series $e^x \approx 1+x$ for small x . In practice, the estimate for the Monte-Carlo error is:

$$(\sigma^{(i)})^2 \approx \frac{\text{Var}(h(\mathbf{x}))}{N} \sum_{t=-\infty}^{\infty} \rho(t) \approx \frac{\text{Var}(h(\mathbf{x}))}{N} \underbrace{\left(1 + 2 \sum_{t=1}^W \rho(t)\right)}_{:=\tau_{\text{int}}} = \text{Var}(h(\mathbf{x})) \frac{\tau_{\text{int}}}{N}, \quad (\text{A.12})$$

where W is the summation window and we define the IACT as twice the value as in [70, pp. 103-105]. The IACT provides a good estimate of how many steps the sampling algorithm needs to take to produce one independent sample. More specifically, the effective sample size $\frac{\tau_{\text{int}}}{N}$ gives an estimate of how efficient a sampler is.

A.3 Python Code

```

1 def MargBack(TTCore, univarGrid):
2     ''' Backward marginalisation (see Prop. 1) as in SIRT from Cui and Dolgov [8] '''
3
4     dim = len(univarGrid)
5     B = dim * [None]    # coeffTensor
6     B[-1] = TTCore[-1]
7     R = [None] * dim
8     C = [None] * dim
9
10    for k in range(dim - 1, 0, -1):
11        r_kmin1, n, r_k = np.shape(TTCore[k])
12        # Eq. 2.28, [8, Eq. 22] !! we set Lebesgue Measure to const = one
13        M = np.identity(n) * (univarGrid[k][-1] - univarGrid[k][0])  # Mass matrix
14        L = scy.linalg.cholesky(M)
15
16        # construct Tensor C Eq. 2.33, [8, Eq. 27]
17        C[k] = np.zeros((r_kmin1, n, r_k))
18        for alpha in range(0, r_kmin1):
19            for l in range(0, r_k):
20                C[k][alpha, :, l] = B[k][alpha, :, l] @ L[:, :]
21
22        # unfold along first coordinate and compute thin QR decomposition of C^T
23        # Eq. 2.34, [8, Eq. 28]
24        Q, R[k] = np.linalg.qr(C[k].reshape((r_kmin1, n * r_k)), order='C').transpose(), mode='reduced')
25
26        # compute next coefficient tensor Eq. 2.35, [8, Eq. 29]
27        r_kmin2, n, r_kmin1 = np.shape(TTCore[k - 1])
28        B[k - 1] = np.zeros(np.shape(TTCore[k - 1]))
29        for alpha_2 in range(0, r_kmin2):
30            for l_1 in range(0, r_kmin1):
31                B[k - 1][alpha_2, :, l_1] = TTCore[k - 1][alpha_2, :, :] @ R[k][l_1, :]
32
33    return B

```

Listing A.1: Python code to calculate Backward marginals, as in Prop. 1 and [8].

```

1  def MargForw(TTCore, univarGrid):
2      ''' Forward marginalisation (see Prop. 2)
3          similar to backward marginalisation as in Cui and Dolgov [8] '''
4
5      # compute pre marginal coefficients starting at dim = 1, k = 0
6      BPre = dim * [None] # coeffTensor
7      LebLam = 1 # !! Lebesgue Measure
8      BPre[0] = TTCore[0]
9      RPre = [None] * dim
10     CPre = [None] * dim
11
12     for k in range(0, dim-1):
13         r_kmin1, n, r_k = np.shape(TTCore[k])
14         # Eq. 2.28, [8, Eq. 22] !! we set Lebesgue Measure to const = one
15         M = np.identity(n) * (univarGrid[k][-1] - univarGrid[k][0]) # Mass matrix
16         L = scy.linalg.cholesky(M)
17
18         # construct Tensor C Eq. 2.36
19         CPre[k] = np.zeros((r_kmin1, n, r_k))
20         for alpha in range(0, r_kmin1):
21             for l in range(0, r_k):
22                 CPre[k][alpha, :, l] = BPre[k][alpha, :, l] @ L[:, :]
23
24         # unfold along first coordinate and compute thin QR decomposition of C
25         # Eq. 2.37
26         Q, RPre[k] = np.linalg.qr(CPre[k].reshape((r_kmin1 * n, r_k)), order='C'), mode='reduced')
27
28         # compute next coefficient tensor Eq. 2.38
29         r_k, n, r_kpls1 = np.shape(TTCore[k + 1])
30         BPre[k + 1] = np.zeros(np.shape(TTCore[k + 1]))
31         for alpha_1 in range(0, r_kpls1):
32             for l_1 in range(0, r_k):
33                 BPre[k + 1][l_1, :, alpha_1] = RPre[k][l_1, :] @ TTCore[k + 1][:, :, alpha_1]
34
35
36     return BPre
37

```

Listing A.2: Python code to calculate forward marginals, as in Prop. 2.

```

1 def SIRT(seeds, SQTT, univarGrid, BackMarg, absError):
2     ''' do squared inverse rosenblatt transform (SIRT) as in Cui et al. [8] '''
3
4     dim, numbSampl = seeds.shape
5     sampls = np.zeros(seeds.shape) # samples from approximated PDF
6     probVal = np.zeros(seeds.shape) # PDF values, for MH-correction step
7     Approx = np.zeros(seeds.shape[1]) # TT-Approx., to compare to true function
8
9     # Lebesgue measure for quadrature Eq. 2.20
10    WholeLebLam = np.zeros(dim)
11    for k in range(0, dim):
12        WholeLebLam[k] = (univarGrid[k][-1] - univarGrid[k][0])
13    lamX = np.ones(dim)
14    for k in range(1, dim):
15        lamX[k - 1] = np.prod(WholeLebLam[k:])
16
17
18    gamError = absError / np.prod(WholeLebLam) # error as in Eq. 2.25 [8, Eq. 35]
19
20    # sample from first dimension [8, Eq. 30]
21    firstMarg = gamError * lamX[0] + np.sum(BackMarg[0][0, :, :] ** 2, 1)
22    # cumulative distribution function, normalised numerically Eq. 2.39 [8, Eq. 17]
23    firstCDF = np.cumsum(firstMarg / np.sum(firstMarg))
24    # draw samples as 'inverse transform'
25    sampls[0] = np.interp(seeds[0], firstCDF, univarGrid[0])
26    probVal[0] = np.interp(sampls[0], univarGrid[0], firstMarg / np.sum(firstMarg))
27
28    # sample from other dimensions
29    for n in range(0, numbSampl):
30        # piecew. poly. interpol in first dimension Eq. 2.41 [11]
31        CurrApprCore = LinInterPolTT(SQTT[0], univarGrid[0], sampls[0][n])
32        for d in range(1, dim):
33            # marginal function, conditioned on previous samples
34            rank_min, gridSize, rank_pls = BackMarg[d].shape
35            MargDep = np.zeros((BackMarg[d].shape))
36            for r in range(0, rank_min):
37                # condition on previous samples
38                MargDep[r, :, :] = CurrApprCore[0, r] * BackMarg[d][r, :, :]
39
40            currMarg = gamError * lamX[d] + np.sum(np.sum(np.copy(MargDep), axis=0)** 2,
41                axis=1) # Eq. 2.40 [8, Eq. 31]
42
43            currCDF = np.cumsum(currMarg / np.sum(currMarg)) # Eq. 2.39 [8, Eq. 17]
44
45            # draw sample as 'inverse transform'
46            sampls[d][n] = np.interp(seeds[d][n], currCDF, univarGrid[d])
47            probVal[d][n] = np.interp(sampls[d][n], univarGrid[d],
48                currMarg / np.sum(currMarg))
49            # piecew. poly. interpol., Eq. 2.41 [11], cond. on sampl. for next PDF
50            CurrApprCore = np.copy(CurrApprCore) @ LinInterPolTT(SQTT[d], univarGrid[d],
51                sampls[d][n])
52
53            Approx[n] = gamError + CurrApprCore ** 2
54
55    return sampls, probVal, Approx

```

Listing A.3: Python code to draw samples via SIRT, as in Alg. Box 1.

B

Additional Figures

Some of the additional figures shown are repetitive and omitted from the main document; others provide details that are not necessary for understanding the main results but may be interesting and offer a more visual understanding for the curious reader.

B.1 Ozone

B.1.1 Ozone Prior

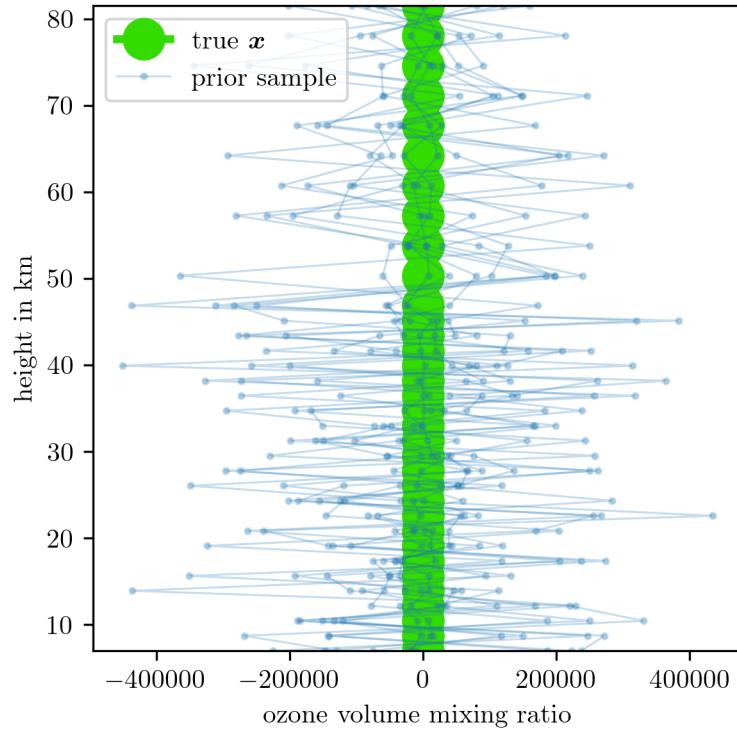


Figure B.1: We draw samples from ozone prior distribution $\mathbf{x} \sim \mathcal{N}(0, \delta \mathbf{L})$ after generating a sample from the hyper-prior distribution $\delta \sim \mathcal{T}(1, 10^{-10})$. Note that since the variance of prior samples is very large compared to the ozone volume mixing ratios, the ozone profile appears to be constant, which is not the case, see e.g., Fig. 4.5.

B.1.2 Integrated Autocorrelation Time

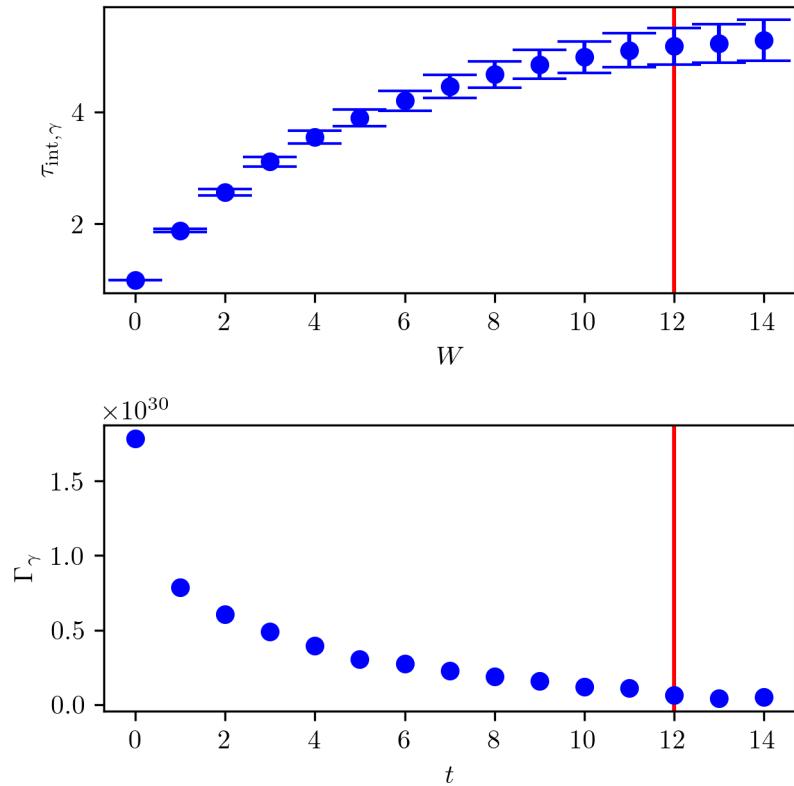


Figure B.2: Provided by [28], the IACT $\tau_{\text{int},\gamma}$ at summation windows W as well as the estimated autocorrelation function Γ_γ at lag t of the samples $\gamma \sim \pi(\cdot|\mathbf{y})$ based on the linear forward model.

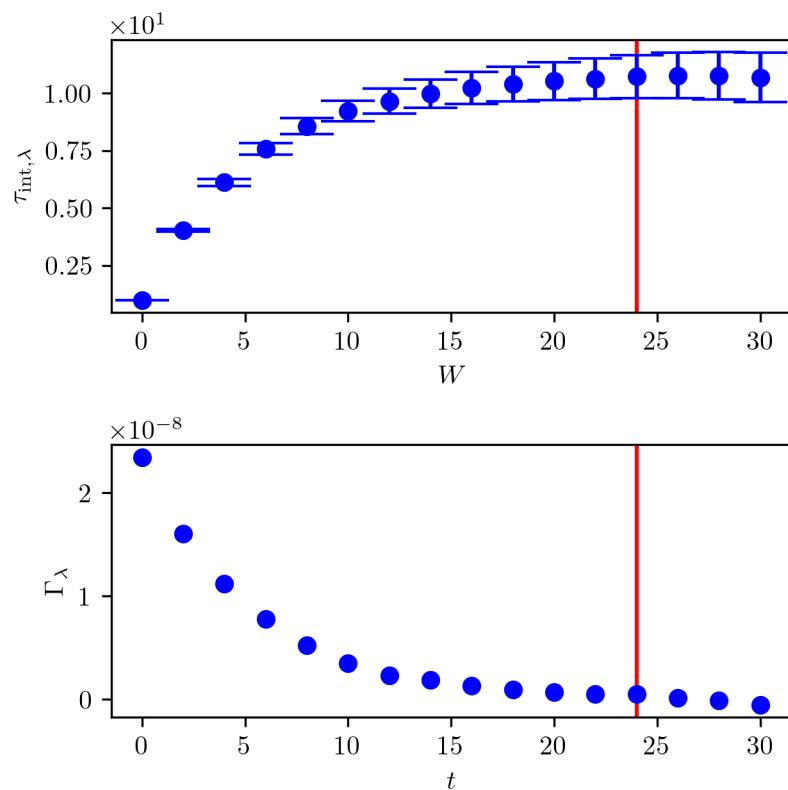


Figure B.3: Provided by [28], the IACT $\tau_{\text{int},\lambda}$ at summation windows W as well as the estimated autocorrelation function Γ_λ at lag t of the samples $\lambda \sim \pi(\cdot | \mathbf{y})$ based on the approximated forward model.

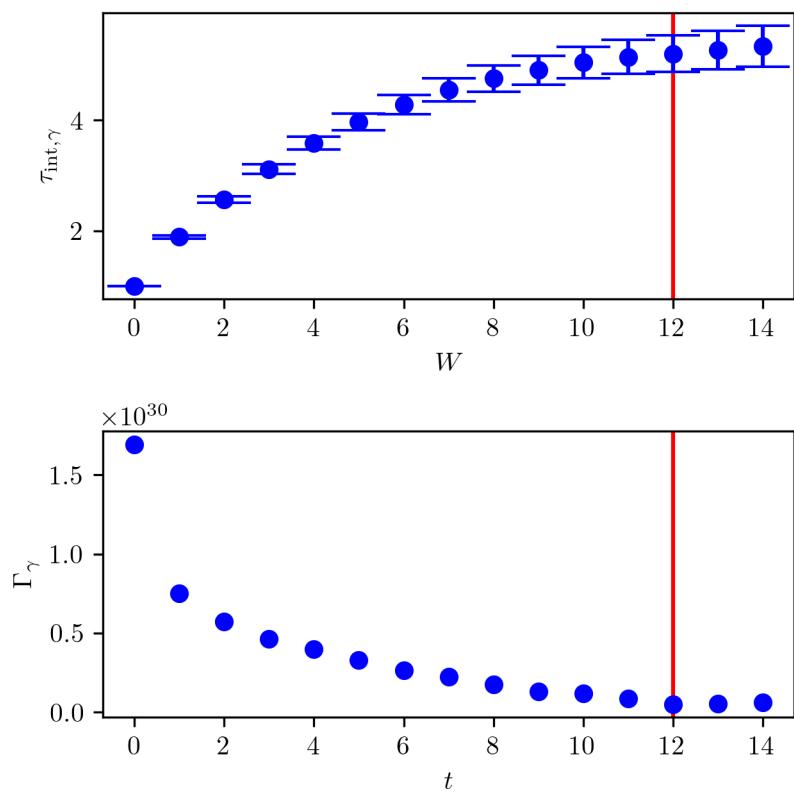


Figure B.4: Provided by [28], the IACT $\tau_{\text{int},\gamma}$ at summation windows W as well as the estimated autocorrelation function Γ_γ at lag t of the samples $\gamma \sim \pi(\cdot|\mathbf{y})$ based on the approximated forward model.

B.1.3 Eigenvectors of Full Conditional Posterior Precision Matrix

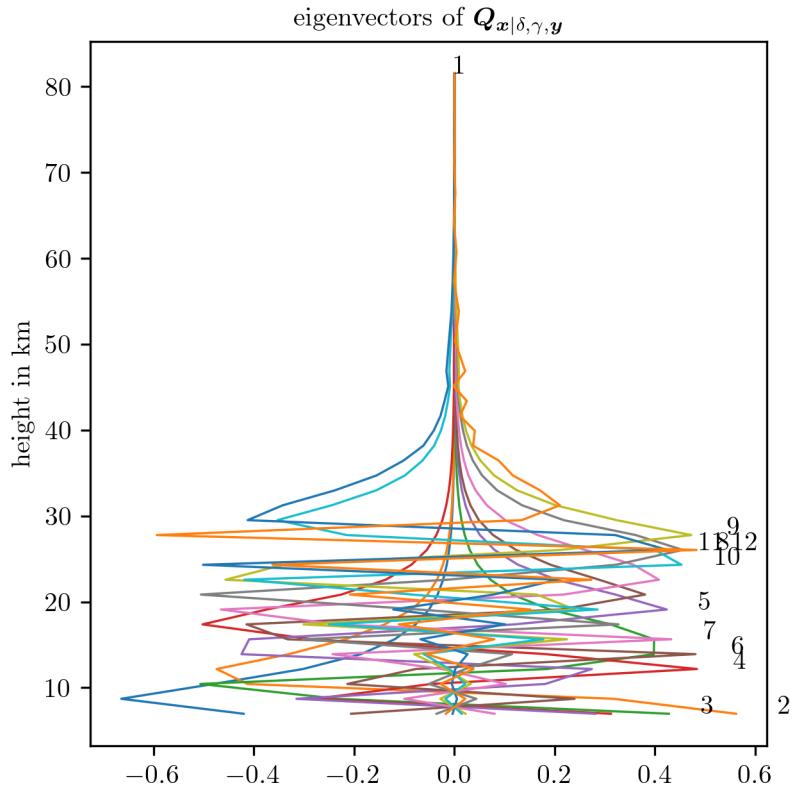


Figure B.5: First 12 eigenvectors corresponding to in size ordered eigenvalues of conditional precision matrix $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}}$. The eigenvectors span structures for heights below 35km.

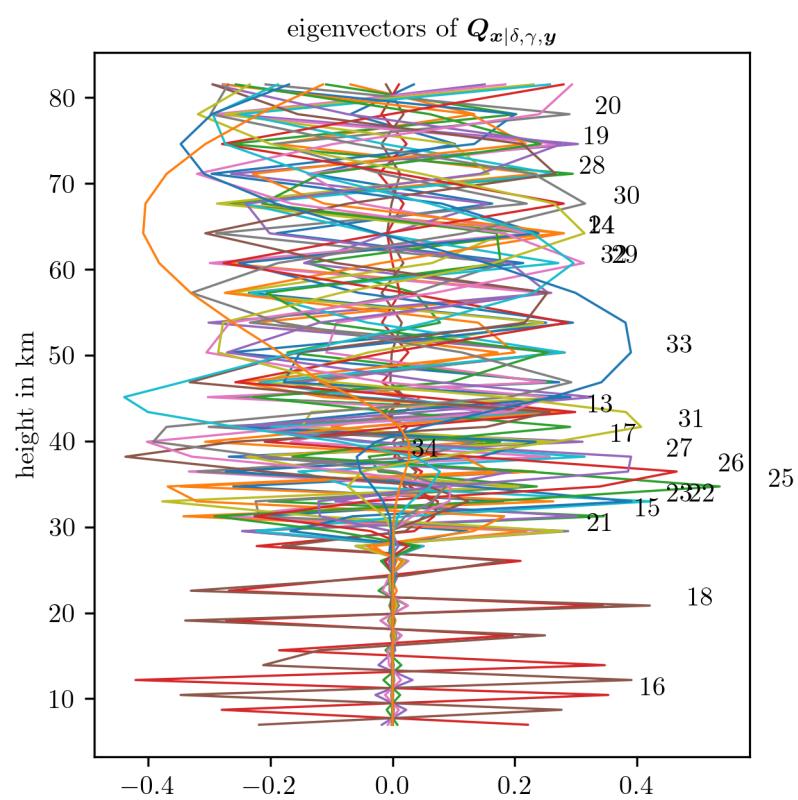


Figure B.6: Last 22 eigenvectors corresponding to in size ordered eigenvalues of conditional precision matrix $\mathbf{Q}_{\mathbf{x}|\delta,\gamma,\mathbf{y}}$. The eigenvectors represent structures mainly above 30km.

B.2 Pressure and Temperature

B.2.1 Priors

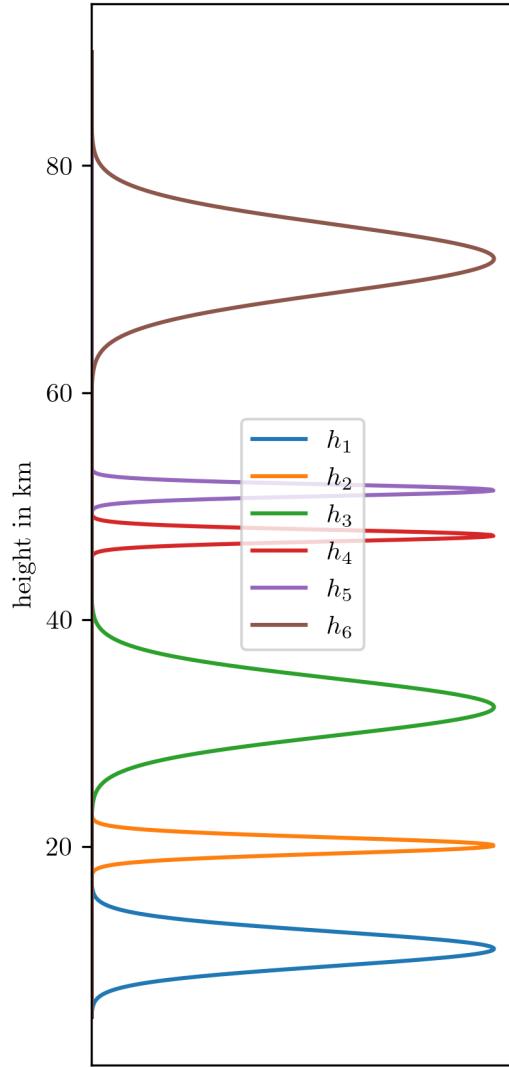


Figure B.7: Prior distributions $\pi(\mathbf{h}_T)$, which we choose so that they do not overlap and not conflict with the temperature function in Eq. 3.9.

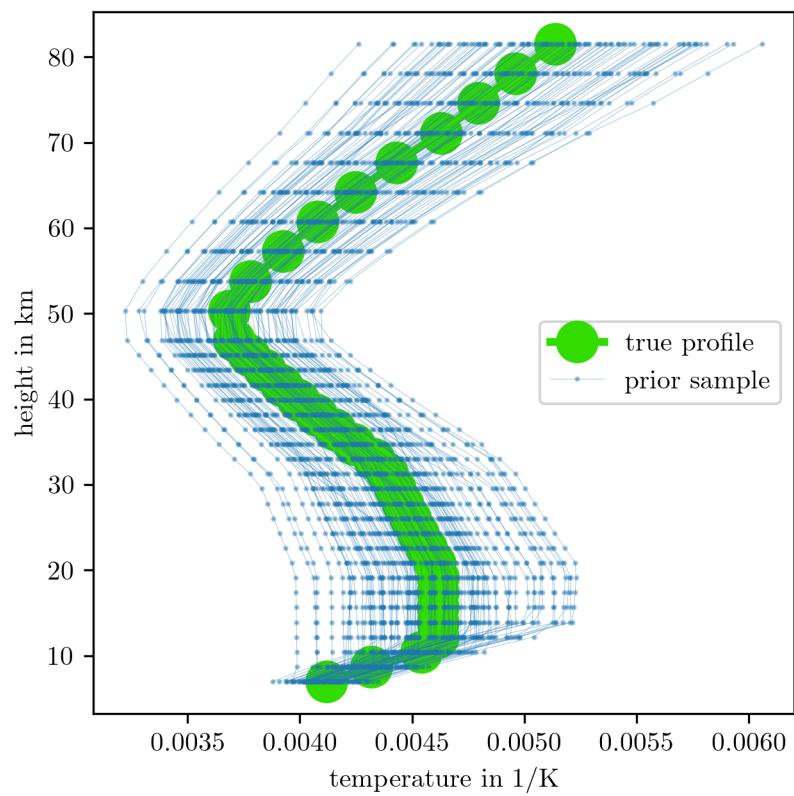


Figure B.8: Prior samples of the inverted temperature profile.

B.2.2 Integrated Autocorrelation Time

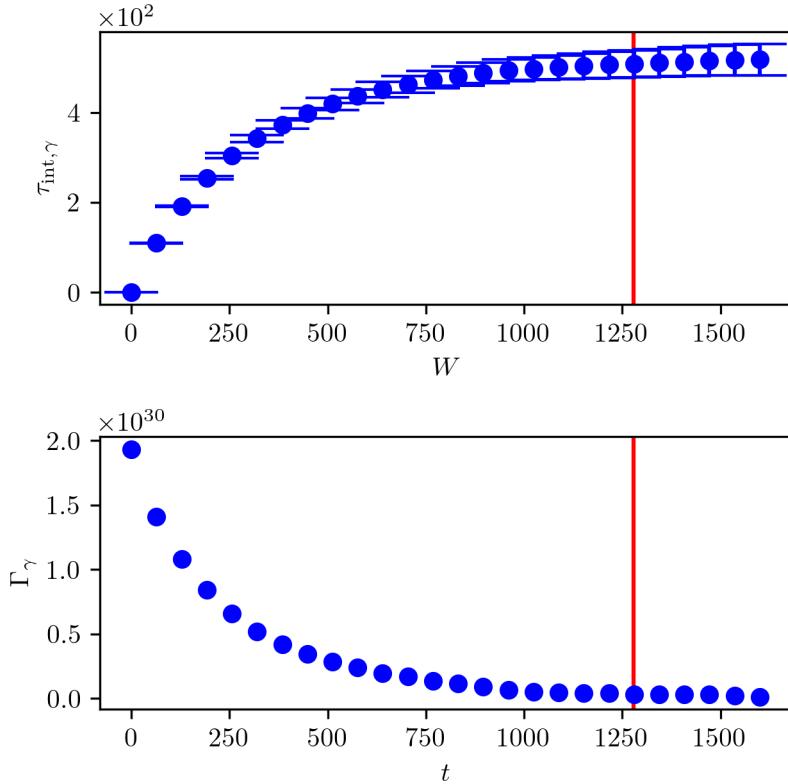


Figure B.9: Provided by [28], the IACT $\tau_{\text{int},\gamma}$ at summation windows W and the estimated autocorrelation function Γ_γ at lag t of samples $\gamma \sim \pi(\cdot|\mathbf{y})$ from the t-walk for the approximated forward model.

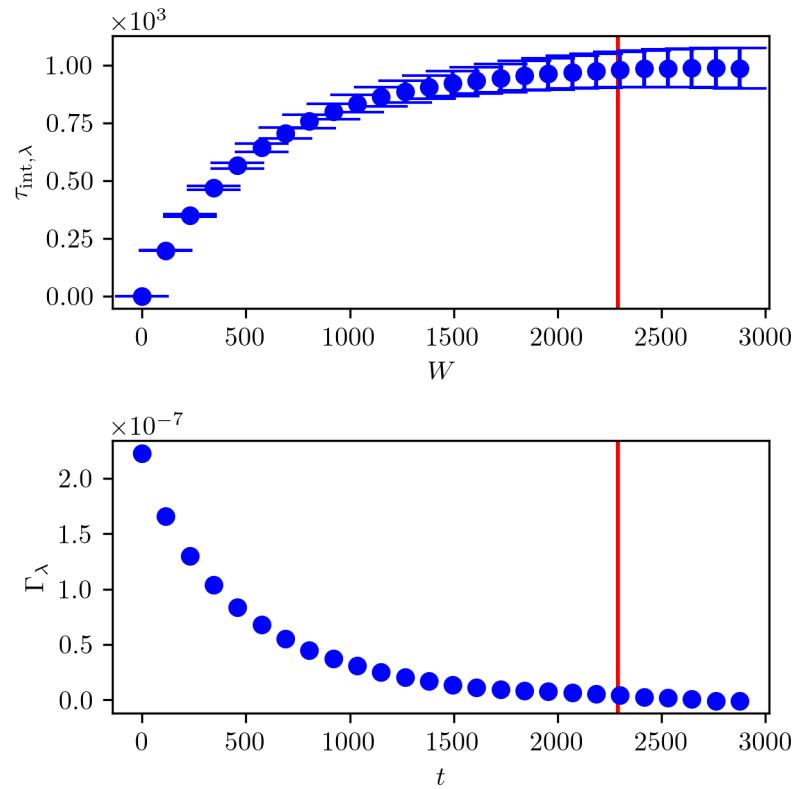


Figure B.10: Provided by [28], the IACT $\tau_{\text{int},\lambda}$ at summation windows W and the estimated autocorrelation function $\hat{\Gamma}_\lambda$ at lag t of samples $\lambda \sim \pi(\cdots | \mathbf{y})$ from the t-walkfor the approximated forward model.

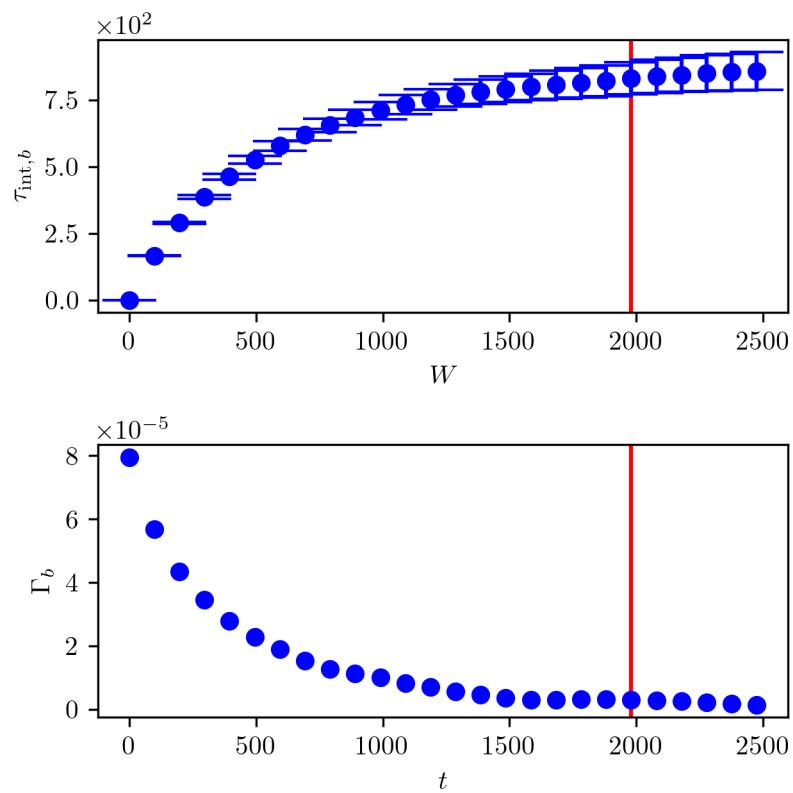


Figure B.11: Provided by [28], the IACT $\tau_{\text{int},b}$ at summation windows W and the estimated autocorrelation function Γ_b at lag t of samples $b \sim \pi(\cdot|\mathbf{y})$ from the t-walk for the approximated forward model.

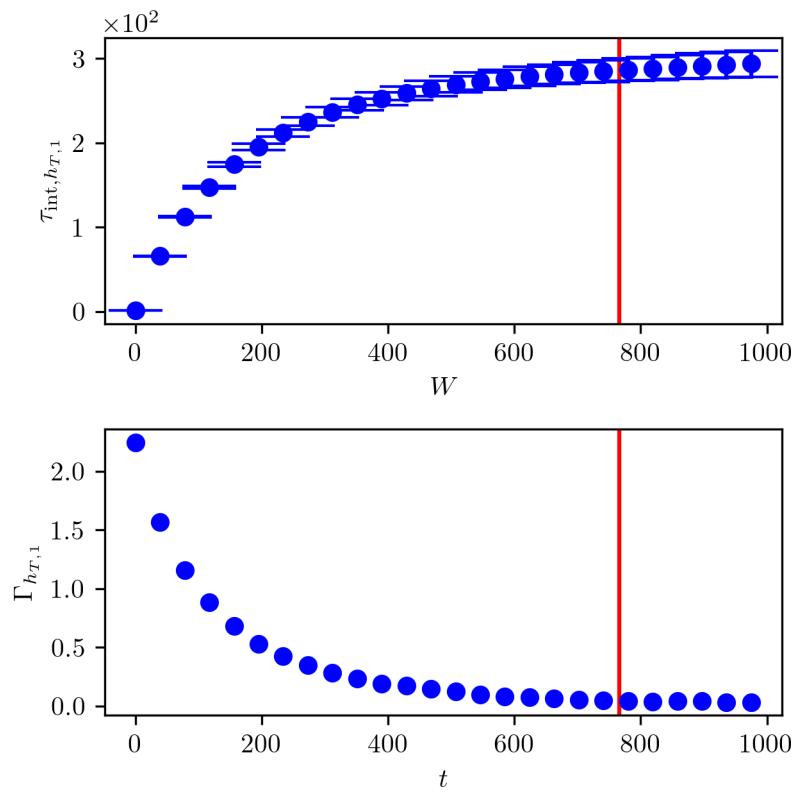


Figure B.12: Provided by [28], the IACT $\tau_{\text{int}, h_{T,1}}$ at summation windows W and the estimated autocorrelation function $\Gamma_{h_{T,1}}$ at lag t of samples $h_{T,1} \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

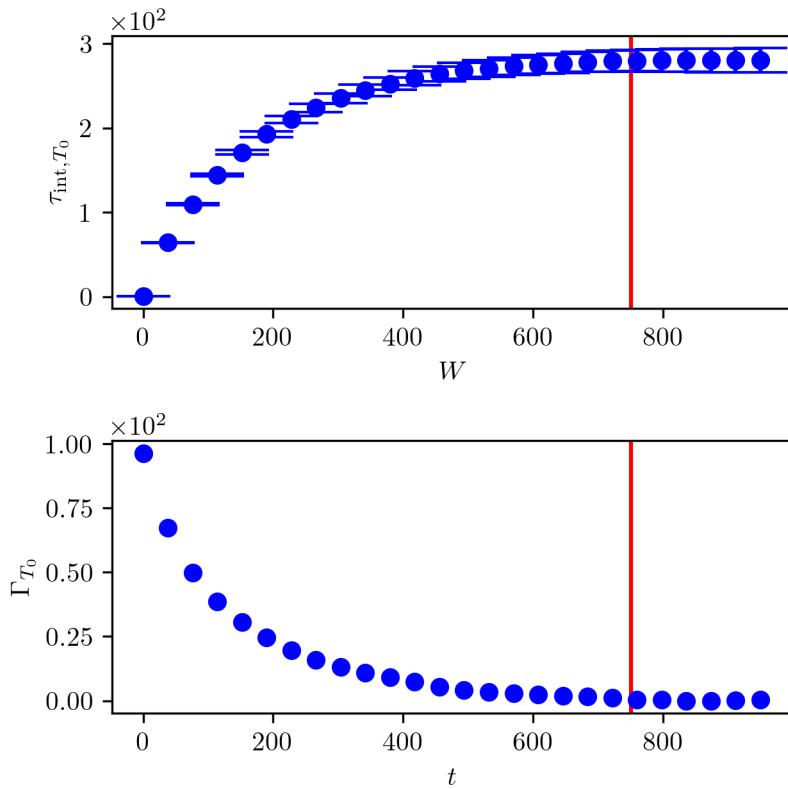


Figure B.13: Provided by [28], the IACT τ_{int, T_0} at summation windows W and the estimated autocorrelation function Γ_{T_0} at lag t of samples $T_0 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

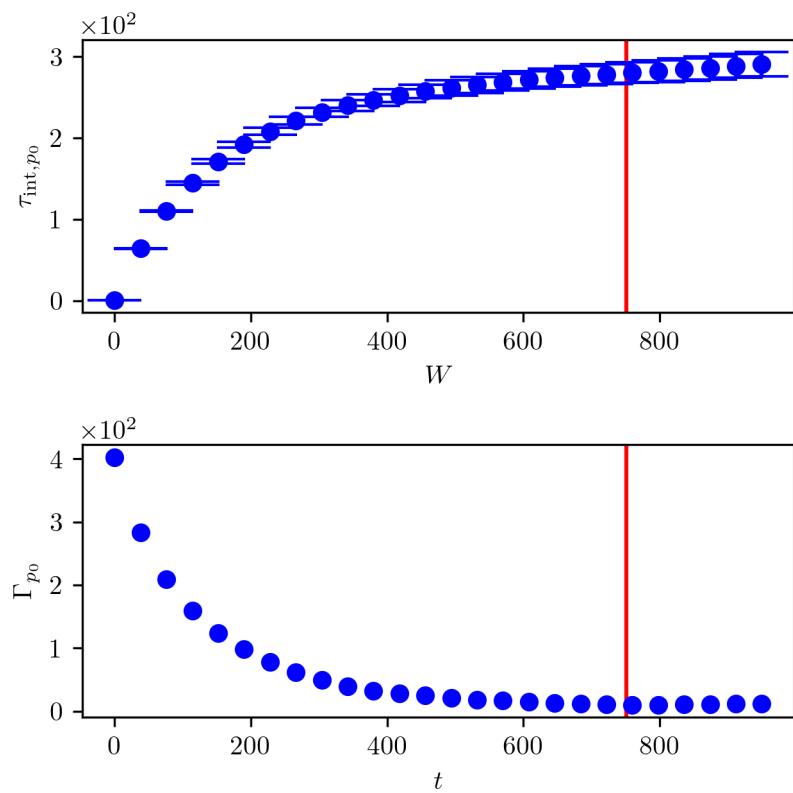


Figure B.14: Provided by [28], the IACT τ_{int,p_0} at summation windows W and the estimated autocorrelation function Γ_{p_0} at lag t of samples $p_0 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

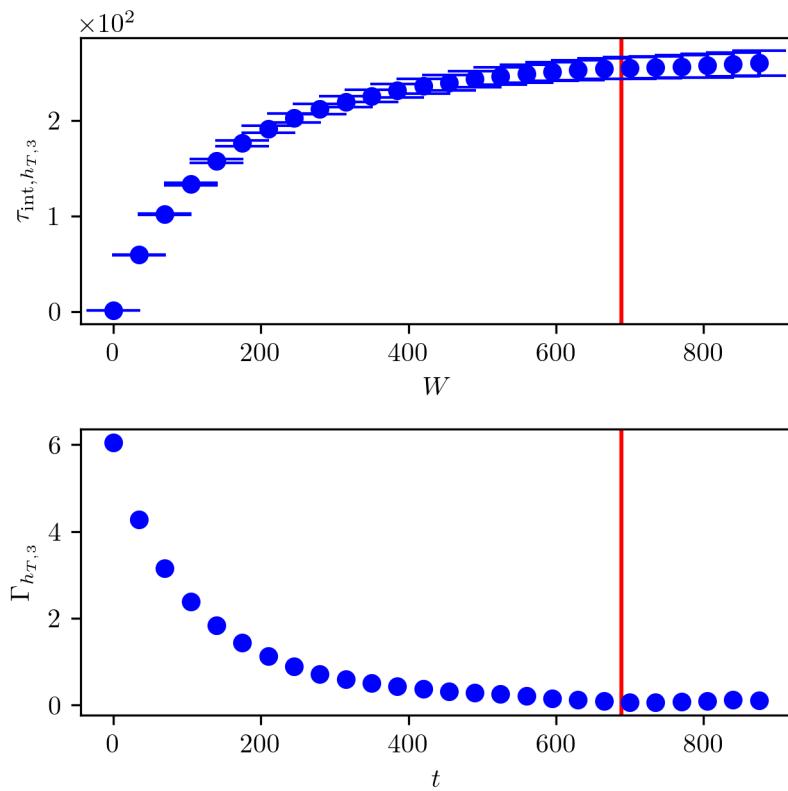


Figure B.15: Provided by [28], the IACT $\tau_{\text{int}, h_{T,3}}$ at summation windows W and the estimated autocorrelation function $\Gamma_{h_{T,3}}$ at lag t of samples $h_{T,3} \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

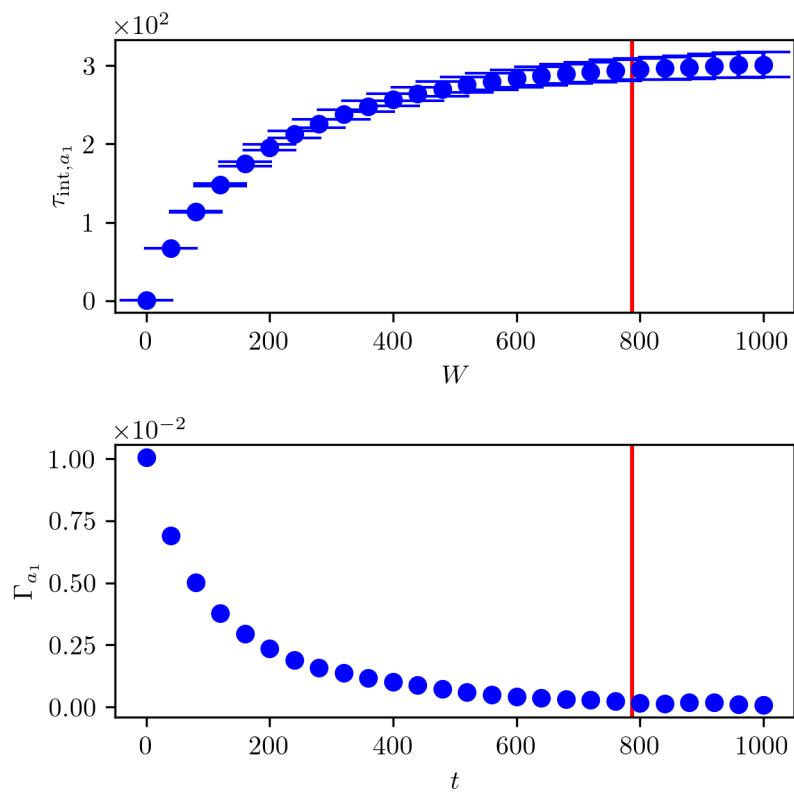


Figure B.16: Provided by [28], the IACT τ_{int,a_1} at summation windows W and the estimated autocorrelation function Γ_{a_1} at lag t of samples $a_1 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

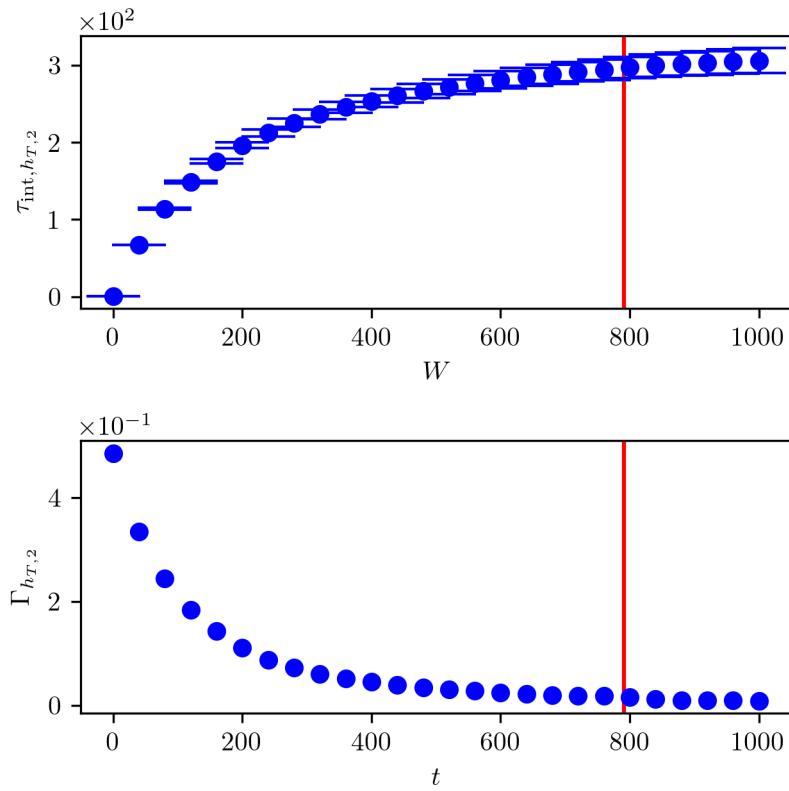


Figure B.17: Provided by [28], the IACT $\tau_{\text{int},h_{T,2}}$ at summation windows W and the estimated autocorrelation function $\Gamma_{h_{T,2}}$ at lag t of samples $h_{T,2} \sim \pi(\cdots | \mathbf{y})$ from the t-walk for the approximated forward model.

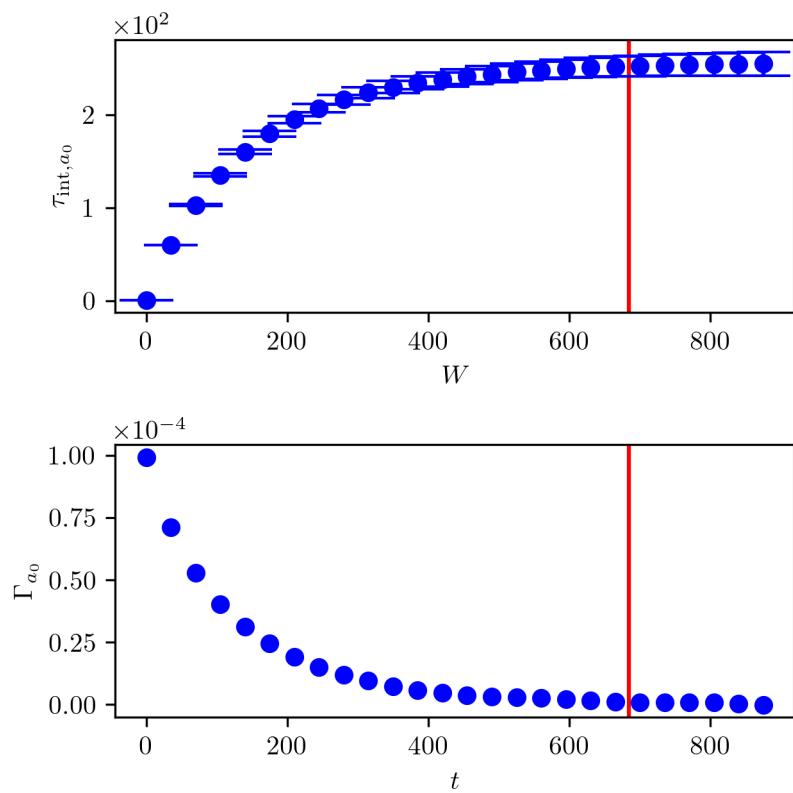


Figure B.18: Provided by [28], the IACT τ_{int,a_0} at summation windows W and the estimated autocorrelation function Γ_{a_0} at lag t of samples $a_0 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

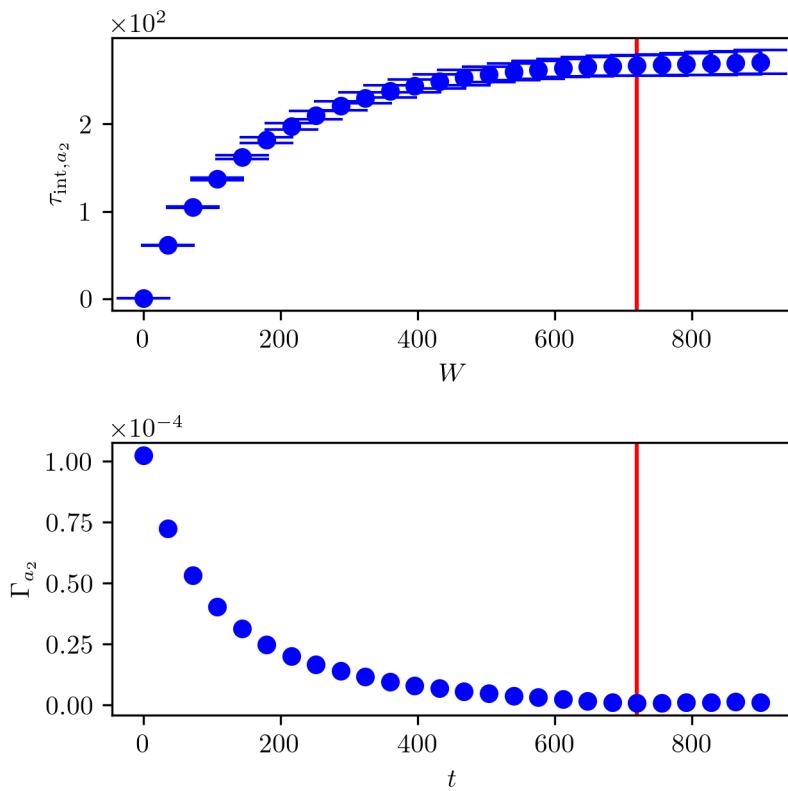


Figure B.19: Provided by [28], the IACT τ_{int,a_2} at summation windows W and the estimated autocorrelation function Γ_{a_2} at lag t of samples $a_2 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

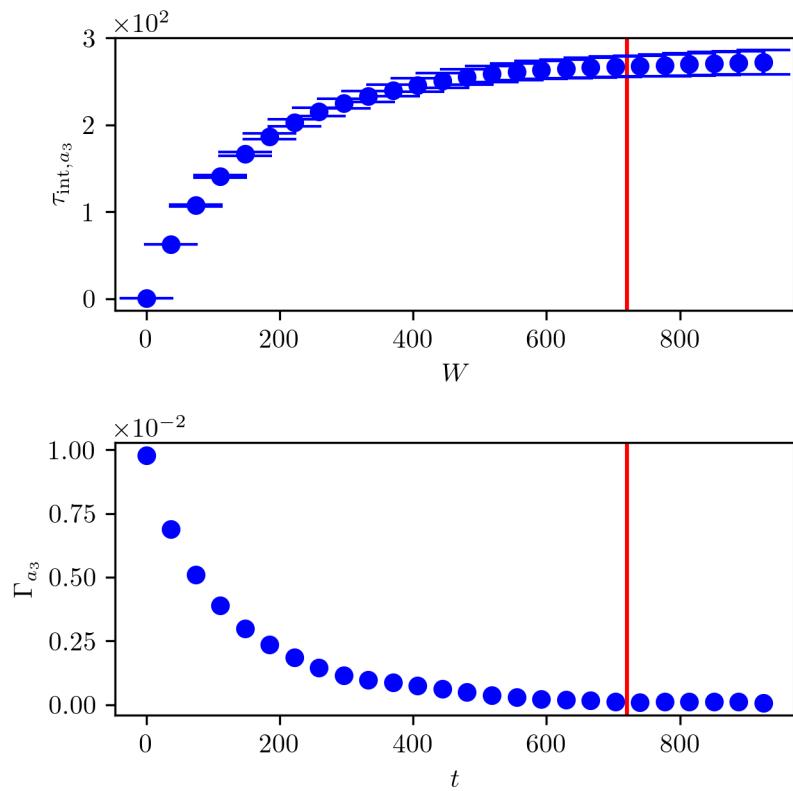


Figure B.20: Provided by [28], the IACT τ_{int,a_3} at summation windows W and the estimated autocorrelation function Γ_{a_3} at lag t of samples $a_3 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

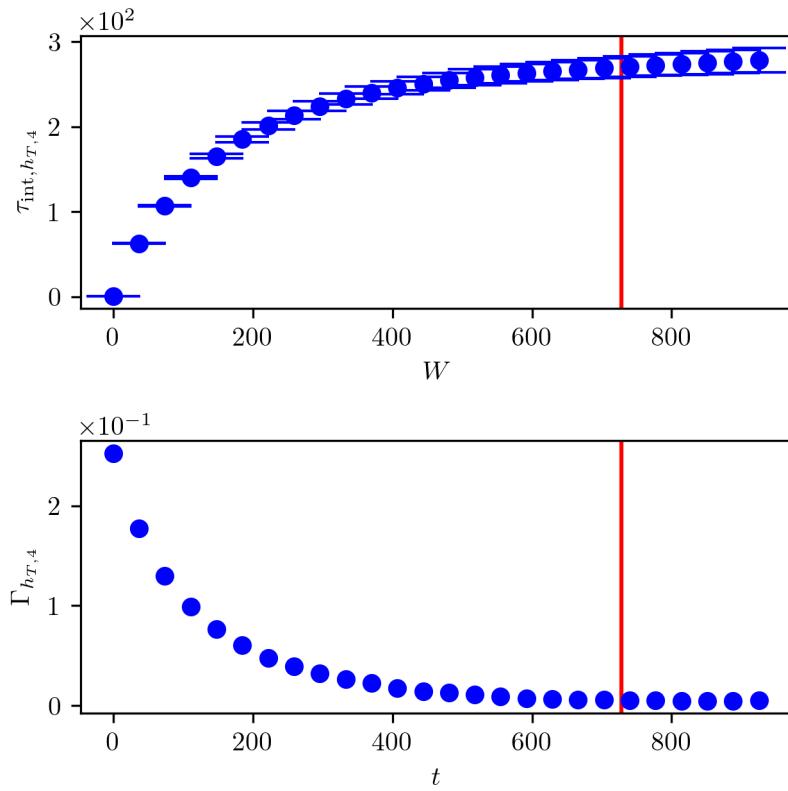


Figure B.21: Provided by [28], the IACT $\tau_{\text{int}, h_{T,4}}$ at summation windows W and the estimated autocorrelation function $\Gamma_{h_{T,4}}$ at lag t of samples $h_{T,4} \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

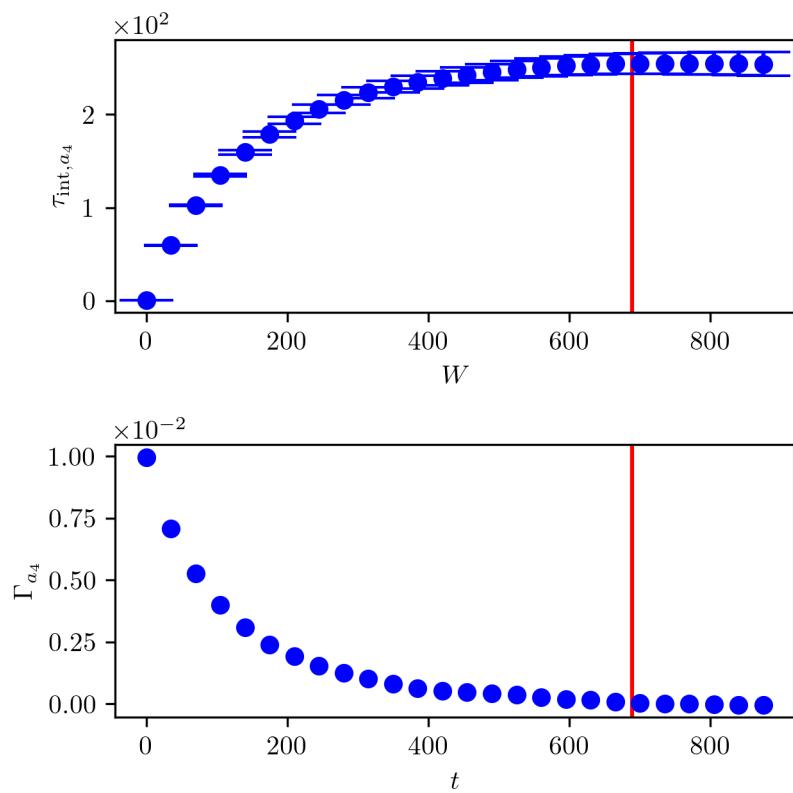


Figure B.22: Provided by [28], the IACT τ_{int,a_4} at summation windows W and the estimated autocorrelation function Γ_{a_4} at lag t of samples $a_4 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

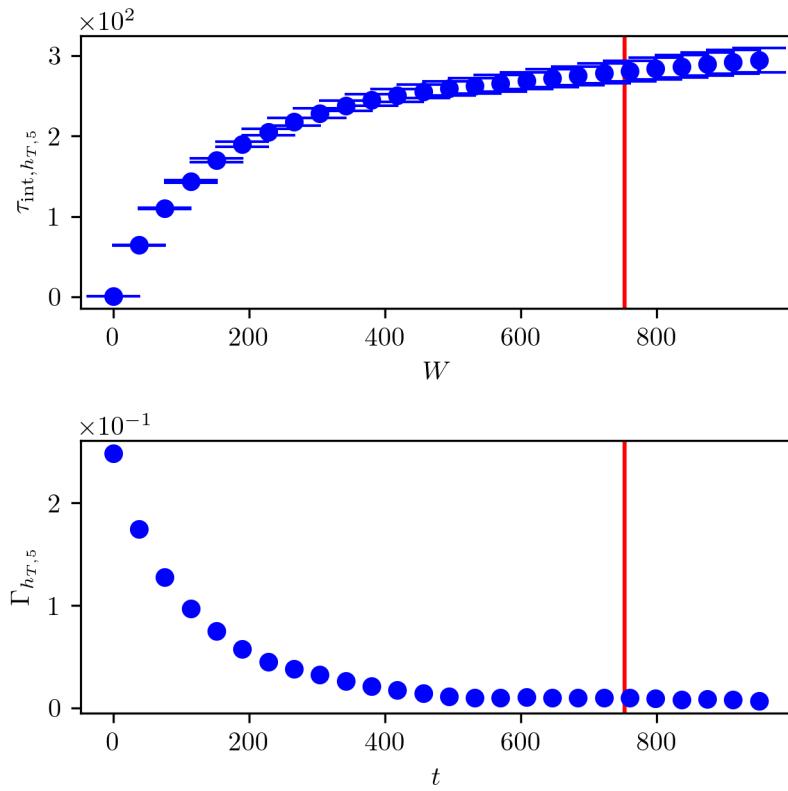


Figure B.23: Provided by [28], the IACT $\tau_{\text{int},h_{T,5}}$ at summation windows W and the estimated autocorrelation function $\Gamma_{h_{T,5}}$ at lag t of samples $h_{T,5} \sim \pi(\cdot|\mathbf{y})$ from the t-walk for the approximated forward model.

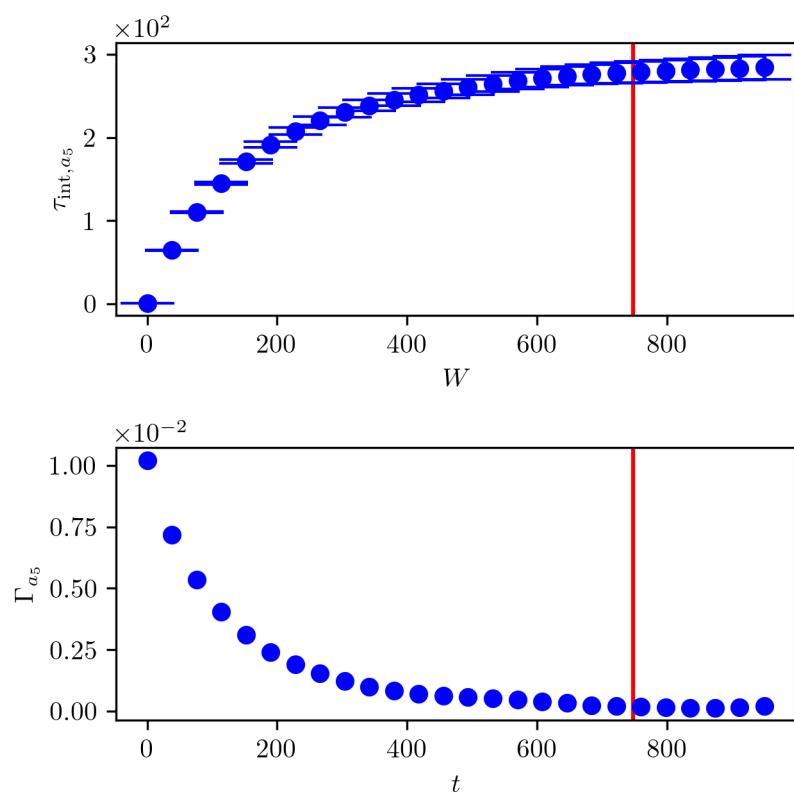


Figure B.24: Provided by [28], the IACT τ_{int,a_5} at summation windows W and the estimated autocorrelation function Γ_{a_5} at lag t of samples $a_5 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

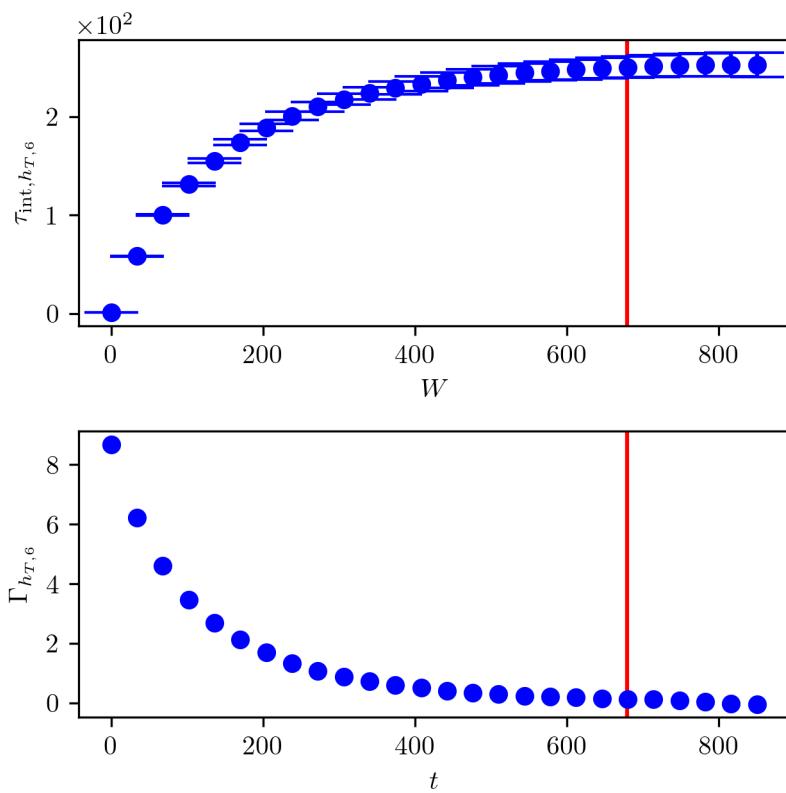


Figure B.25: Provided by [28], the IACT $\tau_{\text{int}, h_{T,6}}$ at summation windows W and the estimated autocorrelation function $\Gamma_{h_{T,6}}$ at lag t of samples $h_{T,6} \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.

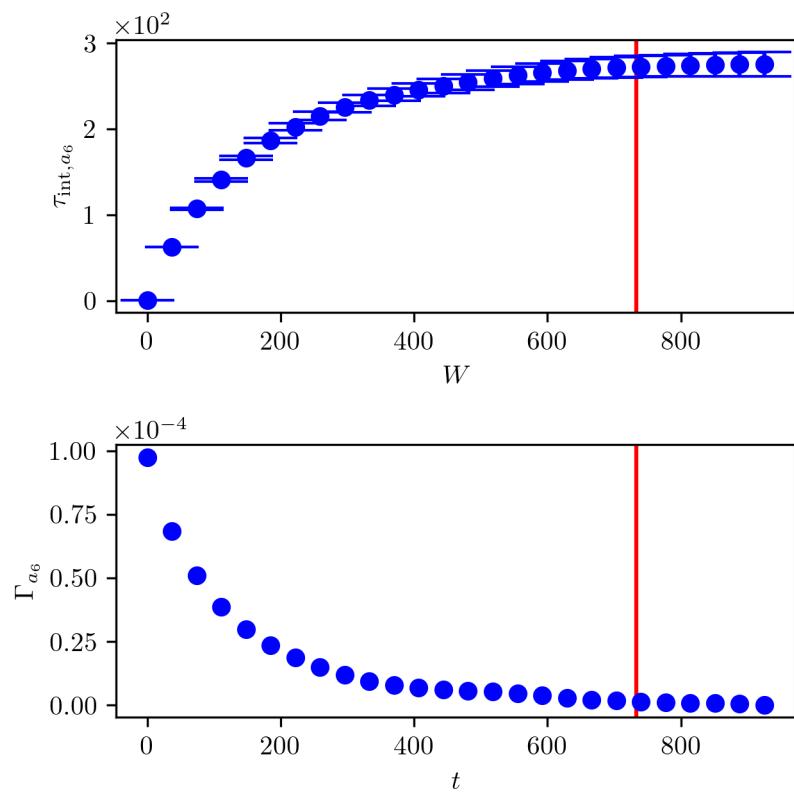


Figure B.26: Provided by [28], the IACT τ_{int,a_6} at summation windows W and the estimated autocorrelation function Γ_{a_6} at lag t of samples $a_6 \sim \pi(\cdot | \mathbf{y})$ from the t-walk for the approximated forward model.