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# 1

## Introduction

### 1.1 Motivation

- ozone coverage
- regularisation approach in atmospheric physics
- hierarchical modelling

### 1.2 What is going on?, 3 facts, What is new in this thesis?

- physical based hierarchical Bayesian model, sampling to TT approx
- RTE as an example
- non-linear to linear affine approximation

### 1.3 Thesis Outline

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# 2

## Theoretical and Technical Background

In this chapter, we provide a brief introduction to the methods used in this thesis. We keep it as general as possible, as more specific details will be presented in the results Chapter 3. We begin by introducing the forward model in Section 2.1, which we use to simulate the data. Since the forward model is weakly non-linear, we employ an affine transformation, see Section 2.2, to project the linear model onto the non-linear one, allowing us to treat the problem as a linear inverse problem. This enables the application of Bayesian inference in Section 2.3, where we formulate a hierarchical linear-Gaussian model to define and structure the posterior distribution. For comparison, we briefly present the Tikhonov regularization approach, see Section 2.4. In Section 2.5, we introduce Markov Chain Monte Carlo (MCMC) methods to sample from the posterior distribution. Finally, in Section 2.6, instead of sampling, we can approximate the posterior distribution using the tensor train (TT) format.

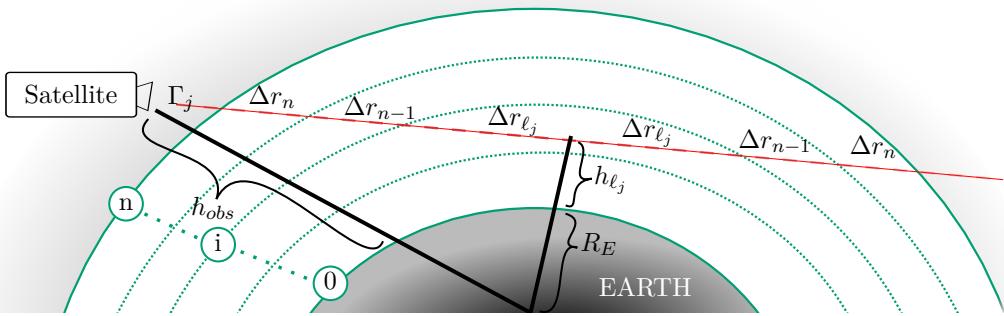
### 2.1 Forward Model

The forward model is based on a satellite measuring thermal radiation along its line of sight by pointing through the atmosphere, known as limb sounding, as shown in Figure 2.1. One measurement  $y_j$ , of a stationary satellite is the path integral through the atmosphere along the line of sight. For each measurement  $j = 1, 2, \dots, m$  of a data set, we can define a tangent height  $h_{\ell_j}$  as the shortest distance along the line of sight to the earth.

The  $j^{\text{th}}$  measurement, is modelled by the radiative transfer equation (RTE) [1]

$$y_j = \int_{\Gamma_j} B(\nu, T) k(\nu, T) \frac{p(T)}{k_B T(r)} x(r) \tau(r) dr + \eta_j \quad (2.1)$$

$$\tau(r) = \exp \left\{ - \int_{r_{\text{obs}}}^r k(\nu, T) \frac{p(T)}{k_B T(r')} x(r') dr' \right\}, \quad (2.2)$$



**Figure 2.1:** This figure illustrates a limb-sounding measurement setup, specifically how the line of sight of a satellite at altitude  $h_{\text{obs}}$  is partitioned according to a discretised atmospheric model. The atmosphere is divided into  $n$  layers, allowing the line of sight  $\Gamma_j$  to be discretised into segments  $\Delta r_i$  for  $i = \ell_j, \dots, n$ . Here,  $\ell_j \in \mathbb{N}$  denotes the index corresponding to the tangent height  $h_{\ell_j}$  relative to the Earth's radius  $R_E$ . This setup forms the basis for the numerical solution of the integral in Eq. 3.8, known as the radiative transfer equation.

where the path from the satellite along the line-of-sight of the  $j^{\text{th}}$  pointing direction is  $\Gamma_j$  and the ozone concentration at distance  $r$  from the radiometer is  $x(r)$  plus some noise  $\eta_j$ . 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  $k(\nu, T)$  for a single gas molecule at a specific wavenumber  $\nu$  is calculated according to the HITRAN database [2] and acts as a source function when multiplied with the black body radiation  $B(\nu, T)$ , given by Planck's law [3]. For fundamentals on the Radiative transfer equation we recommend [3, Chapter 1].

To enable matrix-vector multiplication, we discretise the atmosphere in  $n$  layers, where the  $i^{\text{th}}$  layer is defined by two spheres of radii  $h_{i-1} < h_i$ , for  $i = 1, \dots, n$ , with  $h_0$  and  $h_n$ . Then we can discretise the ozone, pressure and temperature profiles as a function of height, where in between the heights  $h_{i-1}$  and  $h_i$ , each of the ozone concentration  $x_i$ , the pressure  $p_i$ , the temperature  $T_i$ , as well as the thermal radiation is assumed to be constant. Above  $h_n$  and below  $h_0$ , the ozone concentration is set to zero, so no signal can be obtained. Depending on the parameter of interest, which is either the ozone volume mixing ratio  $\mathbf{x} = \{x_1, x_2, \dots, x_n\} \in \mathbb{R}^n$  or the fraction of pressure and temperature  $\mathbf{p}/\mathbf{T} = \{p_1/T_1, p_2/T_2, \dots, p_n/T_n\} \in \mathbb{R}^n$ , we can rewrite the integral in Eq. (3.8) as e.g. as a vector multiplication  $\mathbf{A}_j(\mathbf{x}, \mathbf{p}, \mathbf{T}) \mathbf{x}$  or  $\mathbf{A}_j(\mathbf{x}, \mathbf{p}, \mathbf{T}) \mathbf{p}/\mathbf{T}$ , where the non-linear absorption  $\tau(r)$  is included in  $\mathbf{A}_j(\mathbf{x}, \mathbf{p}, \mathbf{T})$ . Here, the row vector  $\mathbf{A}_j(\mathbf{x}, \mathbf{p}, \mathbf{T}) \in \mathbb{R}^n$  defines a Kernel for each measurement so that the data vector

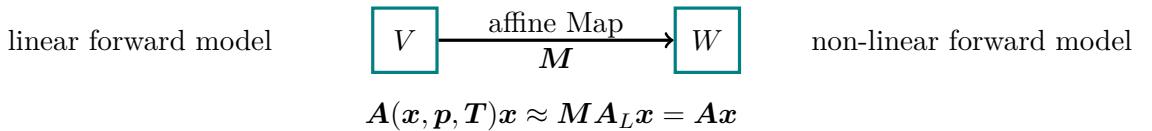
$$\mathbf{y} = \mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T}) \mathbf{x} + \boldsymbol{\eta} = \mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T}) \frac{\mathbf{p}}{\mathbf{T}} + \boldsymbol{\eta}. \quad (2.3)$$

can be written as a matrix-vector multiplication, with the matrix  $\mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T}) \in \mathbb{R}^{m \times n}$  and the noise vector  $\boldsymbol{\eta} \in \mathbb{R}^m$ . Note, for simplicity, we do not explicitly specify whether  $\mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T})$  is constructed under the assumption that  $\mathbf{x}$  or  $\mathbf{p}/\mathbf{T}$  is the parameter of interest..

Since the measurement process includes absorption  $\tau(r)$ , which reduces measurements only slightly, we classify the inverse problem as weakly non-linear. Hence, we can approximate the non-linear forward model  $\mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T})$  with a map  $\mathbf{M}$  and the linear forward model  $\mathbf{A}_L$ , so that  $\mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T}) \approx \mathbf{M}\mathbf{A}_L$ . Here,  $\mathbf{A}_{L,j}$  of matrix  $\mathbf{A}_L \in \mathbb{R}^{m \times n}$  is defined by the linear forward model, where absorption is neglected, e.g. set  $\tau = 1$  in Eq. (3.9). Then each entry in the row vector  $\mathbf{A}_{L,j}$  is either defined by  $B(\nu, T)S(\nu, T)\frac{\mathbf{p}(T)}{k_B T(r)}dr$  or  $B(\nu, T)S(\nu, T)\frac{\mathbf{x}}{k_B}dr$ , as in Eq. (3.8), depending on which parameter we focus on. This poses a linear inverse problem with the forward map defined by the matrix  $\mathbf{A} = \mathbf{M}\mathbf{A}_L$ , where  $\mathbf{M}$  is, more specifically, an affine map.

## 2.2 Affine Map

An affine map is any linear map between two vector spaces or affine spaces, where an affine space does not need to preserve a zero origin, see [4, Def. 2.3.1]. In other words, an affine map does not need to map to the origin of the associated vector space or is a linear map on vector spaces including a translation, or in the words of my supervisor, C. F., an affine map is a Taylor series of first order. For more information on affine spaces and maps, we refer to the books [4, 5]



**Figure 2.2:** This Figure shows the schematic representation of the affine map  $\mathbf{M}$ , which approximates the non-linear forward model from the linear forward model. Here,  $V$  contains values produced by the linear forward model, and  $W$  contains the corresponding values from the non-linear forward model. Both  $V$  and  $W$  are affine subspaces over the same field. The affine map  $\mathbf{M}$  projects elements from the linear forward model space  $V$  onto their counterparts in the non-linear forward model space  $W$ .

Consequently, we introduce an affine map  $\mathbf{M} : \mathbf{A}_L\mathbf{x} \rightarrow \mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T})\mathbf{x}$ , which maps the linear forward model  $\mathbf{A}_L\mathbf{x}$  onto the non-linear forward model  $\mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T})\mathbf{x}$ . Then the non-linear forward model matrix is approximated by  $\mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T}) \approx \mathbf{M}\mathbf{A}_L$ . In practise we generate two affine subspaces spaces  $V = \{\mathbf{A}(\mathbf{x}^{(1)}, \mathbf{p}, \mathbf{T}), \dots, \mathbf{A}(\mathbf{x}^{(m)}, \mathbf{p}, \mathbf{T})\}$  and  $W = \{\mathbf{A}_L\mathbf{x}^{(1)}, \dots, \mathbf{A}_L\mathbf{x}^{(m)}\}$  over the same field, with fixed  $\mathbf{p}, \mathbf{T}$  and find the mapping in between those. Here, the parameter  $\mathbf{x}$  is distributed as  $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\} \sim \pi(\mathbf{x}|\boldsymbol{\theta}, \mathbf{y})$ , where the posterior distribution  $\pi(\mathbf{x}|\boldsymbol{\theta}, \mathbf{y})$  is conditioned on the hyper-parameters  $\boldsymbol{\theta}$  and defined according to a Bayesian hierarchical model.

## 2.3 Bayesian Inference

In this section, we introduce the basics of Bayesian inference for an unknown parameter  $\boldsymbol{x}$  given observed data

$$\boldsymbol{y} = \mathbf{A}\boldsymbol{x} + \boldsymbol{\eta}, \quad (2.4)$$

based on a linear forward model  $\mathbf{A}$  and some additive noise  $\boldsymbol{\eta}$ . A more sophisticated Bayesian framework specifically applied to the previously introduced forward model and some simulated data will be developed in Section ??.

We can visualise the correlation structure between parameters as well as how distributions progress in a measurement process, using a hierarchically ordered directed acyclic graph (DAG), see Figure 2.3. Since any observational process naturally involves random noise, we include this in the DAG and classify the noise variance as a hyper-parameter within  $\boldsymbol{\theta}$  [6]. Other hyper-parameters, to which we assign a hyper-prior distribution  $\pi(\boldsymbol{\theta})$ , may influence the parameters  $\boldsymbol{x}$  either statistically (indicated by solid arrows), as in Figure 2.3, or deterministically (indicated by dashed arrows) if functional dependent on each other. Here we can incorporate prior knowledge of  $\boldsymbol{\theta}$  and the parameter  $\boldsymbol{x}$  by defining  $\pi(\boldsymbol{\theta})$  and the prior distribution  $\pi(\boldsymbol{x}|\boldsymbol{\theta})$  according to their physical properties or functional dependences. This is one of the great strength of Bayesian modelling compared to e.g. regularisation, see section 2.4. Then the parameter  $\boldsymbol{x}$  is mapped deterministically through the forward model onto the space of all measurables  $\Omega$ . From this space, we statistically observe the actual data  $\boldsymbol{y}$ , which includes random (statistical) noise as mentioned above. The distribution of the data conditioned on the hyper-parameters  $\boldsymbol{\theta}$  and the parameters  $\boldsymbol{x}$  is called the likelihood function  $\pi(\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{x})$ , which includes information about the measurement process through the forward model. Then given some observed data, we like to characterise the posterior distribution  $\pi(\boldsymbol{\theta}, \boldsymbol{x}|\boldsymbol{y})$  of the underlying parameters and hyper-parameters by reversing the arrows in Figure 2.3.

The posterior distribution, our function of interest, is defined by Bayes' theorem

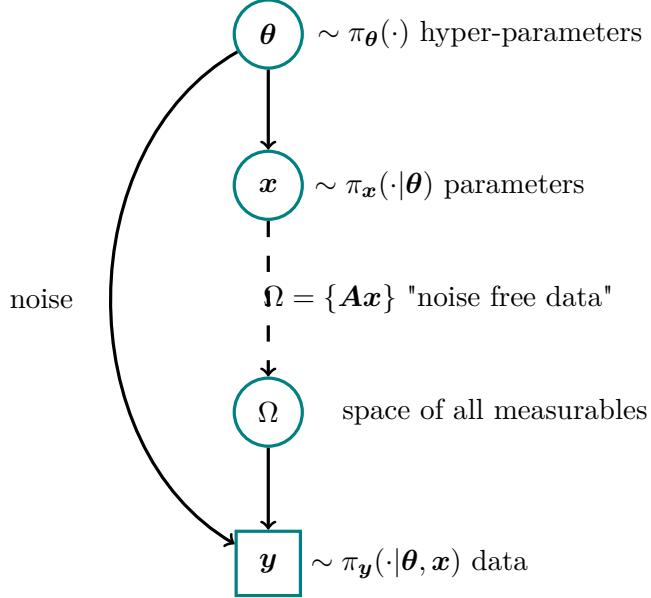
$$\pi(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}) = \frac{\pi(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})\pi(\boldsymbol{x}, \boldsymbol{\theta})}{\pi(\boldsymbol{y})}, \quad (2.5)$$

with the prior distribution  $\pi(\boldsymbol{x}, \boldsymbol{\theta}) = \pi(\boldsymbol{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})$  and the normalising constant  $\pi(\boldsymbol{y})$ . If the normalising constant is finite and non-zero we approximate the posterior distribution

$$\pi(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}) \propto \pi(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta})\pi(\boldsymbol{x}, \boldsymbol{\theta}). \quad (2.6)$$

The expectation of any a function  $h(\boldsymbol{x}_\theta)$ , where  $\boldsymbol{x}$  may depend on  $\boldsymbol{\theta}$ , is described as

$$\mathbb{E}_{\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}}[h(\boldsymbol{x}_\theta)] = \underbrace{\int \int h(\boldsymbol{x}_\theta) \pi(\boldsymbol{x}, \boldsymbol{\theta}|\boldsymbol{y}) d\boldsymbol{x} d\boldsymbol{\theta}}_{\mu_{\text{int}}}, \quad (2.7)$$



**Figure 2.3:** The directed acyclic graph (DAG) for a linear inverse problem visualises statistical dependencies as solid line arrows and deterministic dependencies as dotted arrows. The parameters  $\mathbf{x}$  have some statistical dependency of those hyper-parameters  $\boldsymbol{\theta}$ , which are distributed as  $\pi(\boldsymbol{\theta})$ . Then a parameter  $\mathbf{x} \sim \pi_{\mathbf{x}}(\cdot|\boldsymbol{\theta})$  is mapped onto the space of all measurables  $\mathbf{u} = \mathbf{Ax}$  deterministically through the linear forward model  $\mathbf{A}$ . From the space of all measurables we observe some data  $\mathbf{y} = \mathbf{Ax} + \boldsymbol{\eta}$ , statistically, so that  $\mathbf{y} \sim \pi_{\mathbf{y}}(\cdot|\boldsymbol{\theta}, \mathbf{x})$ , with naturally some random noise  $\boldsymbol{\eta} \sim \pi_{\boldsymbol{\eta}}(\cdot|\boldsymbol{\theta})$ .

which may be a high dimensional integral and computationally not feasible to solve. Therefore the unbiased [7] sample based Monte Carlo estimate

$$\mathbb{E}_{\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}}[h(\mathbf{x}_{\boldsymbol{\theta}})] \approx \underbrace{\frac{1}{N} \sum_{k=1}^N h(\mathbf{x}_{\boldsymbol{\theta}}^{(k)})}_{\boldsymbol{\mu}_{\text{samp}}}, \quad (2.8)$$

for large enough  $N$  (law of large numbers [8, Chapter 17]) is often used. Here, the 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  $\mathcal{M} = \{(\mathbf{x}, \boldsymbol{\theta})^{(1)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(N)}\}$ . Furthermore, the central limit theorem states that the samples mean  $\boldsymbol{\mu}_{\text{samp}}^{(i)}$ , of independent samples sets  $\mathcal{M}_i$  for  $i = 1, \dots, n$  of any distribution, converge in distribution to a normal distribution so that

$$\sqrt{n}(\boldsymbol{\mu}_{\text{samp}}^{(i)} - \boldsymbol{\mu}_{\text{int}}) \xrightarrow{\mathcal{D}} \mathcal{N}(0, \sigma^2)[9], \quad (2.9)$$

and if  $\sigma^2 < \infty$  the Monte Carlo error  $\boldsymbol{\mu}_{\text{samp}}^{(i)} - \boldsymbol{\mu}_{\text{int}}$  is bounded.

Generating a representative sample set from the posterior distribution presents a significant challenge. This is also due to the strong correlations that often exist between the parameters and hyper-parameters, as discussed by Rue and Held in [10] and illustrated in Appendix B. If  $\mathbf{x}$  can not be parametrised directly in terms of the hyper-parameters

$\boldsymbol{\theta}$ , i.e.,  $\mathbf{x}(\boldsymbol{\theta})$ , it is beneficial to factorise the posterior distribution as

$$\pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}) = \pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y}) \pi(\boldsymbol{\theta} | \mathbf{y}), \quad (2.10)$$

into the 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 the hyper-parameters  $\boldsymbol{\theta}$ . This approach, known as the marginal and then conditional (MTC) method, is particularly advantageous when  $\mathbf{x}$  is high-dimensional (e.g.,  $\mathbf{x} \in \mathbb{R}^n$  with  $n = 45$ ), while  $\boldsymbol{\theta}$  is low-dimensional (e.g., two-dimensional) and one can deterministically work out the marginal distribution. Applying the law of total expectation [11], Eq. (2.7) becomes

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

where, in the case of a linear-Gaussian Bayesian hierarchical model, both the marginal distribution and the inner expectation  $\mathbb{E}_{\mathbf{x}|\boldsymbol{\theta},\mathbf{y}}[h(\mathbf{x}_{\boldsymbol{\theta}})]$  are well defined.

Assuming Gaussian noise  $\boldsymbol{\eta} \sim \mathcal{N}(0, \boldsymbol{\Sigma}(\boldsymbol{\theta}))$ , we define a linear-Gaussian Bayesian hierarchical model [6]

$$\mathbf{y} | \mathbf{x}, \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{A}\mathbf{x}, \boldsymbol{\Sigma}(\boldsymbol{\theta})) \quad (2.12a)$$

$$\mathbf{x} | \boldsymbol{\theta} \sim \mathcal{N}(\boldsymbol{\mu}, \mathbf{Q}^{-1}(\boldsymbol{\theta})) \quad (2.12b)$$

$$\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta}), \quad (2.12c)$$

with a normally distributed likelihood  $\pi(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta})$  and prior distributions  $\pi(\mathbf{x} | \boldsymbol{\theta})$  and  $\pi(\boldsymbol{\theta})$ , the noise covariance matrix  $\boldsymbol{\Sigma}(\boldsymbol{\theta})$ , the prior precision matrix  $\mathbf{Q}(\boldsymbol{\theta})$  and the prior mean  $\boldsymbol{\mu}$ . This model enables efficient factorisation of the posterior distribution and application of the MTC method.

### 2.3.1 Marginal and conditional posterior distribution

For the linear-Gaussian Bayesian hierarchical model specified in Eq. 2.12, the marginal posterior distribution over the hyper-parameters is given by

$$\pi(\boldsymbol{\theta} | \mathbf{y}) = \int \pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y}) d\mathbf{x} \quad (2.13)$$

$$\propto \sqrt{\frac{\det(\boldsymbol{\Sigma}^{-1}) \det(\mathbf{Q})}{\det(\mathbf{Q} + \mathbf{A}^T \boldsymbol{\Sigma}^{-1} \mathbf{A})}} \times \exp \left[ -\frac{1}{2} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu})^T \mathbf{Q}_{\boldsymbol{\theta}|\mathbf{y}} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu}) \right] \pi(\boldsymbol{\theta}), \quad (2.14)$$

with

$$\mathbf{Q}_{\boldsymbol{\theta}|\mathbf{y}} = \boldsymbol{\Sigma}^{-1} - \boldsymbol{\Sigma}^{-1} \mathbf{A} \left( \mathbf{A}^T \boldsymbol{\Sigma}^{-1} \mathbf{A} + \mathbf{Q} \right)^{-1} \mathbf{A}^T \boldsymbol{\Sigma}^{-1}, \quad (2.15)$$

see [6, Lemma 2]. Conditioned on the hyper-parameters  $\boldsymbol{\theta}$ , we can draw samples from the normal conditional posterior distribution

$$\mathbf{x}|\boldsymbol{\theta}, \mathbf{y} \sim \mathcal{N}\left(\underbrace{\boldsymbol{\mu} + (\mathbf{A}^T \boldsymbol{\Sigma}^{-1} \mathbf{A} + \mathbf{Q})^{-1} \mathbf{A}^T \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \mathbf{A}\boldsymbol{\mu})}_{\boldsymbol{\mu}_{\mathbf{x}|\boldsymbol{\theta}, \mathbf{y}}}, \underbrace{(\mathbf{A}^T \boldsymbol{\Sigma}^{-1} \mathbf{A} + \mathbf{Q})^{-1}}_{\boldsymbol{\Sigma}_{\mathbf{x}|\mathbf{y}, \boldsymbol{\theta}}}\right), \quad (2.16)$$

using the Randomise-then-Optimise (RTO) method (see Section 2.5.2), or compute weighted expectations, as in Eq. 2.11, of the conditional mean and covariance matrix, where the weights are given by  $\pi(\boldsymbol{\theta}|\mathbf{y})$ . Note that both the noise covariance  $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\boldsymbol{\theta})$  and the prior precision matrix  $\mathbf{Q} = \mathbf{Q}(\boldsymbol{\theta})$  depend on the hyper-parameters  $\boldsymbol{\theta}$ .

## 2.4 Regularisation

Another method for obtaining a solution to the linear inverse problem in Eq. 2.4 is regularisation. In this approach, we seek a solution  $\mathbf{x}_\lambda$  that minimises both the data misfit norm and a regularisation semi-norm, as described in [6]. Here we focus on a regularisation semi-norm for the case of Tikhonov regularisation [12, 13], which is closest to a linear-Gaussian hierarchical Bayesian model, as introduced in Eq. 2.12.

Given a parameter vector  $\mathbf{x}$ , a linear forward model matrix  $\mathbf{A}$ , and data  $\mathbf{y}$ , the data misfit norm

$$\|\mathbf{y} - \mathbf{Ax}\| \quad (2.17)$$

quantifies how well the noise-free data  $\mathbf{Ax}$  matches the observed data. The regularisation semi-norm

$$\lambda \|\mathbf{T}\mathbf{x}\| \quad (2.18)$$

penalises the solution according to the regularisation operator  $\mathbf{T}$  and the regularisation parameter  $\lambda > 0$ . For a fixed  $\lambda$ , the regularised solution

$$\mathbf{x}_\lambda = \arg \min_{\mathbf{x}} \|\mathbf{y} - \mathbf{Ax}\|^2 + \lambda \|\mathbf{T}\mathbf{x}\|^2 \quad (2.19)$$

is obtained by taking the derivative with respect to  $\mathbf{x}$  of the objective function:

$$\nabla_{\mathbf{x}} \left\{ (\mathbf{y} - \mathbf{Ax})^T (\mathbf{y} - \mathbf{Ax}) + \lambda \mathbf{x}^T \mathbf{T}^T \mathbf{T} \mathbf{x} \right\} = 0 \quad (2.20)$$

$$\iff \nabla_{\mathbf{x}} \left\{ \mathbf{y}^T \mathbf{y} + \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} - 2 \mathbf{y}^T \mathbf{Ax} + \lambda \mathbf{x}^T \mathbf{T}^T \mathbf{T} \mathbf{x} \right\} = 0 \quad (2.21)$$

$$\iff 2 \mathbf{A}^T \mathbf{Ax} - 2 \mathbf{A}^T \mathbf{y} + 2 \lambda \mathbf{T}^T \mathbf{T} \mathbf{x} = 0. \quad (2.22)$$

Solving this equation yields the regularised solution

$$\mathbf{x}_\lambda = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L})^{-1} \mathbf{A}^T \mathbf{y}, \quad (2.23)$$

where we define  $\mathbf{L} := \mathbf{T}^T \mathbf{T}$ , which typically represents a discrete approximation of a derivative operator [13].

In practice,  $\mathbf{x}_\lambda$  is computed for a range of  $\lambda$ -values and evaluated based on the trade-off between the data misfit and the regularisation norm. The optimal value of  $\lambda$  is often chosen as the point of maximum curvature on the so-called L-curve [14], which we plot in Section ??.

## 2.5 Sampling Methods

In this section we present the sampling methods used in this thesis and show how these methods draw samples  $\mathcal{M} = \{(\mathbf{x}, \boldsymbol{\theta})^{(1)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(k)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(N)}\} \sim \pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y})$  from the desired target distribution, so that we can apply sample-based estimates as in Eq. 2.8. Here,  $\mathcal{M}$  denotes a Markov chain, where each new sample  $(\mathbf{x}, \boldsymbol{\theta})^{(k)}$  is only affected by the previous one,  $(\mathbf{x}, \boldsymbol{\theta})^{(k-1)}$ . Markov chain Monte Carlo (MCMC) methods generate such a chain  $\mathcal{M}$  using random (Monte Carlo) proposals  $(\mathbf{x}, \boldsymbol{\theta})^{(k)} \sim q(\cdot | (\mathbf{x}, \boldsymbol{\theta})^{(k-1)})$  according to a proposal distribution conditioned on the previous sample (Markov), where ergodicity of  $\mathcal{M}$  is a sufficient criterion for using sample-based estimates [7, 13].

The ergodicity theorem in [13] 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, if the chain can reach any state from any other state (irreducibility), is not stuck in periodic cycles (aperiodicity), and is reversible (detailed balance condition [13]), then it will converge to the desired target distribution  $\pi(\mathbf{x}, \boldsymbol{\theta} | \mathbf{y})$ . In practice, one can inspect the trace  $\pi(\mathbf{x}^{(k)}, \boldsymbol{\theta}^{(k)} | \mathbf{y})$  for  $k = 1, \dots, N$  and visually assess convergence and mixing properties of the chain to evaluate ergodicity. The sampling methods used in this thesis possess proven ergodic properties, and we therefore refer the reader to the corresponding literature for further details.

### 2.5.1 Metropolis- within Gibbs sampling

As introduced in Section 2.3.1, when using the MTC method we sample separately from  $\pi(\boldsymbol{\theta} | \mathbf{y})$  and  $\pi(\mathbf{x} | \boldsymbol{\theta}, \mathbf{y})$ . To sample from  $\pi(\boldsymbol{\theta} | \mathbf{y})$ , we use a Metropolis-within-Gibbs sampler as described in [6]. In this thesis, the sampler is applied to the two-dimensional case only, with  $\boldsymbol{\theta} = (\theta_1, \theta_2)$ , where we perform a Metropolis step in the  $\theta_1$  direction and a Gibbs step in the  $\theta_2$  direction. Ergodicity for this approach is proven in [15].

The Metropolis-within-Gibbs algorithm begins with an initial guess  $\boldsymbol{\theta}^{(t)}$  at  $t = 0$ . We then propose a new sample  $\theta_1 \sim q(\theta_1 | \theta_1^{(t-1)})$ , conditioned on the previous state, using a symmetric proposal distribution  $q(\theta_1 | \theta_1^{(t-1)}) = q(\theta_1^{(t-1)} | \theta_1)$ , which is a special

case of the Metropolis-Hastings algorithm [15]. We accept and set  $\theta_1^{(t)} = \theta_1$  with the acceptance probability

$$\alpha(\theta_1|\theta_1^{(t-1)}) = \min \left\{ 1, \frac{\pi(\theta_1|\theta_2^{(t-1)}, \mathbf{y}) q(\theta_1^{(t-1)}|\theta_1)}{\pi(\theta_1^{(t-1)}|\theta_2^{(t-1)}, \mathbf{y}) q(\theta_1|\theta_1^{(t-1)})} \right\} \quad (2.24)$$

or reject and keep  $\theta_1^{(t)} = \theta_1^{(t-1)}$ , which we do by comparing  $\alpha$  to a uniform random number  $u \sim \mathcal{U}(0, 1)$ .

Next, we perform a Gibbs step in the  $\theta_2$  direction, where Gibbs sampling is again a special case of the Metropolis-Hastings algorithm with acceptance probability equal to one, and draw the next sample  $\theta_2^{(t)} \sim \pi(\cdot|\theta_1^{(t)}, \mathbf{y})$ , conditioned on the current value  $\theta_1^{(t)}$ .

We repeat this procedure  $N'$  times and ensure convergence independently of the initial sample (irreducibility) by discarding the initial  $N_{\text{burn-in}}$  samples after a so-called burn-in period, resulting in a Markov chain of length  $N = N' - N_{\text{burn-in}}$ .

**Algorithm 1:** Metropolis within Gibbs

```

1: Initialize and suppose two dimensional vector  $\boldsymbol{\theta}^{(0)} = (\theta_1^{(0)}, \theta_2^{(0)})$ 
2: for  $k = 1, \dots, N'$  do
3:   Propose  $\theta_1 \sim q(\cdot|\theta_1^{(t-1)}) = q(\theta_1^{(t-1)}|\cdot)$ 
4:   Compute

$$\alpha(\theta_1|\theta_1^{(t-1)}) = \min \left\{ 1, \frac{\pi(\theta_1|\theta_2^{(t-1)}, \mathbf{y}) q(\theta_1^{(t-1)}|\theta_1)}{\pi(\theta_1^{(t-1)}|\theta_2^{(t-1)}, \mathbf{y}) q(\theta_1|\theta_1^{(t-1)})} \right\}$$

5:   Draw  $u \sim \mathcal{U}(0, 1)$ 
6:   if  $\alpha \geq u$  then
7:     Accept and set  $\theta_1^{(t)} = \theta_1$ 
8:   else
9:     Reject and keep  $\theta_1^{(t)} = \theta_1^{(t-1)}$ 
10:  end if
11:  Draw  $\theta_2^{(t)} \sim \pi(\cdot|\theta_1^{(t)}, \mathbf{y})$ 
12: end for
13: Output:  $\boldsymbol{\theta}^{(0)}, \dots, \boldsymbol{\theta}^{(k)}, \dots, \boldsymbol{\theta}^{(N)} \sim \pi(\boldsymbol{\theta}|\mathbf{y})$ 
```

### 2.5.2 Draw a sample from a multivariate normal distribution

As part of the MTC scheme, we only draw samples from the conditional distribution  $\pi(\mathbf{x}|\boldsymbol{\theta}, \mathbf{y})$  after sampling from the marginal posterior  $\pi(\boldsymbol{\theta}|\mathbf{y})$ . For linear-Gaussian Bayesian hierarchical models, samples from the multivariate normal distribution  $\pi(\mathbf{x}|\boldsymbol{\theta}, \mathbf{y})$  can be efficiently generated using the Randomise-then-Optimise (RTO) method [16].

The full conditional distribution can be rewritten as

$$\pi(\mathbf{x}|\mathbf{y}, \boldsymbol{\theta}) \propto \pi(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}) \pi(\mathbf{x}|\boldsymbol{\theta}) \quad (2.25)$$

$$= \exp \left( - \left\| \hat{\mathbf{A}}\mathbf{x} - \hat{\mathbf{y}} \right\|^2 \right), \quad (2.26)$$

where

$$\hat{\mathbf{A}} = \begin{bmatrix} \Sigma^{-1/2}(\boldsymbol{\theta}) \mathbf{A} \\ \mathbf{Q}^{1/2}(\boldsymbol{\theta}) \end{bmatrix}, \quad \hat{\mathbf{y}} = \begin{bmatrix} \Sigma^{-1/2}(\boldsymbol{\theta}) \mathbf{y} \\ \mathbf{Q}^{1/2}(\boldsymbol{\theta}) \boldsymbol{\mu} \end{bmatrix} \quad [17]. \quad (2.27)$$

A sample  $\mathbf{x}_i$  can be computed by minimising the following equation with respect to  $\hat{\mathbf{x}}$ :

$$\mathbf{x}_i = \arg \min_{\hat{\mathbf{x}}} \|\hat{\mathbf{A}}\hat{\mathbf{x}} - (\hat{\mathbf{y}} + \mathbf{b})\|^2, \quad \mathbf{b} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad (2.28)$$

where we add a randomised perturbation  $\mathbf{b}$ . Similar to Section 2.4, this expression can be rewritten as

$$(\mathbf{A}^T \Sigma^{-1}(\boldsymbol{\theta}) \mathbf{A} + \mathbf{Q}(\boldsymbol{\theta})) \mathbf{x}_i = \mathbf{A}^T \Sigma^{-1}(\boldsymbol{\theta}) \mathbf{y} + \mathbf{Q}(\boldsymbol{\theta}) \boldsymbol{\mu} + \mathbf{v}_1 + \mathbf{v}_2, \quad (2.29)$$

where the term  $-\hat{\mathbf{A}}^T \mathbf{b}$  is decomposed as  $\mathbf{v}_1 + \mathbf{v}_2$ , with  $\mathbf{v}_1 \sim \mathcal{N}(\mathbf{0}, \mathbf{A}^T \Sigma^{-1}(\boldsymbol{\theta}) \mathbf{A})$  and  $\mathbf{v}_2 \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}(\boldsymbol{\theta}))$ , representing independent Gaussian random variables [6, 16].

If the Markov chain over the marginal posterior  $\pi(\boldsymbol{\theta}|\mathbf{y})$  is ergodic, and the conditional samples  $\mathbf{x}^{(k)} \sim \pi(\mathbf{x}|\boldsymbol{\theta}^{(k)}, \mathbf{y})$  are drawn independently, then the resulting joint chain  $\{(\mathbf{x}, \boldsymbol{\theta})^{(1)}, \dots, (\mathbf{x}, \boldsymbol{\theta})^{(N)}\} \sim \pi(\mathbf{x}, \boldsymbol{\theta}|\mathbf{y})$  is also ergodic [18].

### 2.5.3 t-walk sampler as black box

If the parameters  $\mathbf{x}$  are functionally dependent on the hyper-parameters  $\boldsymbol{\theta}$ , i.e.,  $\mathbf{x} = \mathbf{x}(\boldsymbol{\theta})$ , we can sample directly from the marginal posterior  $\pi(\boldsymbol{\theta}|\mathbf{y})$  using the t-walk algorithm by Christen and Fox [19]. The t-walk is employed as a black-box sampler, requiring only the specification of the number of samples, burn-in period, support region, and the sampling distribution. Convergence to the target distribution is guaranteed by construction of the algorithm.

## 2.6 Numerical Approximation Methods - Tensor Train

First, we provide a short overview of probability spaces and their associated measures, as a foundation for deriving marginal probability distribution, and then we give a brief introduction to the tensor train format. The motivation to use the tensor train format is that we can approximate a d-dimensional grid with far fewer data points compared to the total number of grid points.

Assume that the triple  $(\Omega, \mathcal{F}, \mathbb{P})$  defines a probability space, where  $\Omega$  denotes the complete sample space,  $\mathcal{F}$  is a  $\sigma$ -algebra consisting of a collection of countable subsets  $\{A_n\}_{n \in \mathbb{N}}$  with  $A_n \subseteq \Omega$ , and  $\mathbb{P}$  is a probability measure defined on  $\mathcal{F}$ . The formal conditions for  $\mathbb{P}$  to be a probability measure, and for  $\mathcal{F}$  to be a  $\sigma$ -algebra over  $\Omega$ , are given in Appendix C. We denote

$$\mathbb{P}(A) = \int_A d\mathbb{P} \quad (2.30)$$

as the probability of an event  $A \in \mathcal{F}$ . By applying the Radon-Nikodym theorem [20], we can change variables

$$\mathbb{P}(A) = \int_A \frac{d\mathbb{P}}{dx} dx = \int_A \pi(x) dx, \quad (2.31)$$

where  $dx$  is a reference measure on the same probability space, commonly referred to as the Lebesgue measure. The Radon-Nikodym derivative  $\frac{d\mathbb{P}}{dx}$  of  $\mathbb{P}$  with respect to  $x$ , and is often interpreted as the probability density function (PDF)  $\pi(x)$ . Thus, we say that  $\mathbb{P}$  has a density  $\pi(x)$  with respect to  $x$  [21, Chapter 10].

Now, let  $X : \Omega \rightarrow \mathbb{R}^d$  be a  $d$ -dimensional random variable mapping from the probability space  $(\Omega, \mathcal{F}, \mathbb{P})$  to the measurable space  $(\mathbb{R}^d, \mathcal{X})$ , where  $\mathcal{X}$  is a collection of subsets in  $\mathbb{R}^d$ . Then the associated PDF  $\pi(x)$ , is a joint density of  $X$ , induced by the probability measure on  $\Omega$  [20, 22]. As by Cui et al. [23], we can define the parameter space as the Cartesian product  $\mathcal{X} = \mathcal{X}_1 \times \mathcal{X}_2 \times \cdots \times \mathcal{X}_d$  with  $x_k \in \mathcal{X}_k \subseteq \mathbb{R}$  and  $x = (x_1, \dots, x_k, \dots, x_d)$ . The marginal density function for the  $k$ -th component is then given by

$$f_{X_k}(x_k) = \int_{\mathcal{X}_1} \cdots \int_{\mathcal{X}_d} \lambda(x) \pi(x) dx_1 \cdots dx_{k-1} dx_{k+1} \cdots dx_d, \quad (2.32)$$

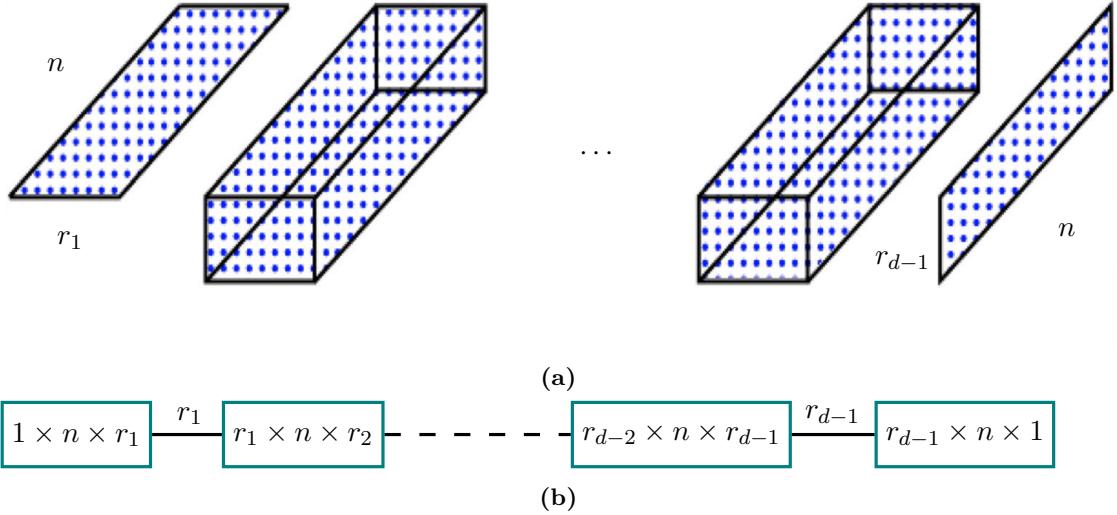
where we integrate over all dimensions except the  $k$ -th. Here, we introduce a weight function  $\lambda(x)$  [24], which can be useful for quadrature rules???. Cui et al. [23] refer to  $\lambda(x)$  as a "product-form Lebesgue-measurable weighting function" and define it as

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

Using the tensor train (TT) format, we can efficiently approximate a  $d$ -dimensional function  $\pi(x)$  and compute marginal probability distributions at low computational cost. To do so, we first define a  $d$ -dimensional discrete univariate grid over the parameter space  $\mathcal{X}$ , with  $n$  grid points in each dimension. In the tensor train format we can represent the function over this  $d$ -dimensional grid as a product train of 2D matrices (rank-2 tensor) and 3D matrices (rank-3 tensors), which we call TT-cores, see Fig. 2.4. More specifically each core  $\pi_k \in \mathbb{R}^{r_{k-1} \times n \times r_k}$  has ranks  $r_{k-1}$  and  $r_k$ , for  $k = 1, \dots, d$ , connecting it with its neighbouring cores, as illustrated in Figure 2.4. For the first and last cores, the outer ranks are set to  $r_0 = r_d = 1$ . This enables us to write the value  $\pi(x)$ , for a fixed point  $x = (x_1, \dots, x_d)$  on the grid, as a sequence of matrix multiplications

$$\pi_1(x_1) \pi_2(x_2) \cdots \pi_d(x_d) = \pi(x) \in \mathbb{R},$$

where each core  $\pi_k(x_k)$ , becomes a matrix of size  $r_{k-1} \times r_k$ . Clearly this shows that we only need  $dn^2$  evaluation points instead of  $n^d$  grid points to approximate the whole parameter space. Consequently, with a tensor train approximation, the marginal target function



**Figure 2.4:** Here, we visualise the tensor train cores as two- and three-dimensional matrices. Each core has a length  $n$ , corresponding to the number of grid points in one dimension, and the cores are connected through ranks  $r_k$ . More specifically, a core  $\pi_k$  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  $dn^2$  evaluation points instead of  $n^d$  grid points. Figure (a) is adapted from [25].

$$f_{X_k}(x_k) = \frac{1}{z} \left| \left( \int_{\mathbb{R}} \lambda_1(x_1) \pi_1(x_1) dx_1 \right) \cdots \left( \int_{\mathbb{R}} \lambda_{k-1}(x_{k-1}) \pi_{k-1}(x_{k-1}) dx_{k-1} \right) \lambda_k(x_k) \pi_k(x_k) \right. \\ \left. \left( \int_{\mathbb{R}} \lambda_{k+1}(x_{k+1}) \pi_{k+1}(x_{k+1}) dx_{k+1} \right) \cdots \left( \int_{\mathbb{R}} \lambda_d(x_d) \pi_d(x_d) dx_d \right) \right| \quad (2.33)$$

is computed by integrating over all TT cores except  $\pi_k$ , as in [26], including a normalisation constant  $z$  [23].

In practice, tensor train approximations may suffer from numerical instability, particularly because it is not advantageous to approximate the target function  $\pi(x)$  in for example, the logarithmic space. To address this, we follow the notation and procedure of Cui et al. [23] and instead approximate the square root of the probability density

$$\sqrt{\pi(x)} \approx g(x) = \mathbf{G}_1(x_1), \dots, \mathbf{G}_k(x_k), \dots, \mathbf{G}_d(x_d). \quad (2.34)$$

Here, each TT-core is given by

$$G_k^{(\alpha_{k-1}, \alpha_k)}(x_k) = \sum_{i=1}^{n_k} \phi_k^{(i)}(x_k) \mathbf{A}_k[\alpha_{k-1}, i, \alpha_k], \quad k = 1, \dots, d, \quad (2.35)$$

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 approximated density is written as:

$$\pi(x) \approx \gamma' + g^2(x), \quad (2.36)$$

where  $\gamma'$  is a small positive constant added to ensure positivity and is chosen such that

$$\gamma' \leq \frac{1}{\lambda(\mathcal{X})} \|g - \sqrt{\pi}\|_2^2. \quad (2.37)$$

This leads to the normalised target function

$$f_X(x) = \frac{1}{z} \lambda(x) \pi(x) = \frac{1}{z} \left( \lambda(x) \gamma' + \lambda(x) g^2(x) \right), \quad (2.38)$$

where  $z$  is the normalisation constant. Given the tensor train approximation of  $\sqrt{\pi}$ , the marginal function  $f_{X_k}(x_k)$  can be expressed as

$$\begin{aligned} f_{X_k}(x_k) &= \frac{1}{z} \left( \gamma' \prod_{i=1}^{k-1} \lambda_i(\mathcal{X}_i) \prod_{i=k+1}^d \lambda_i(\mathcal{X}_i) \right. \\ &\quad + \left( \int_{\mathbb{R}} \lambda_1(x_1) \mathbf{G}_1^2(x_1) dx_1 \right) \cdots \left( \int_{\mathbb{R}} \lambda_{k-1}(x_{k-1}) \mathbf{G}_{k-1}^2(x_{k-1}) dx_{k-1} \right) \\ &\quad \left. \lambda_k(x_k) \mathbf{G}_k^2(x_k) \right. \\ &\quad \left. \left( \int_{\mathbb{R}} \lambda_{k+1}(x_{k+1}) \mathbf{G}_{k+1}^2(x_{k+1}) dx_{k+1} \right) \cdots \left( \int_{\mathbb{R}} \lambda_d(x_d) \mathbf{G}_d^2(x_d) dx_d \right) \right). \end{aligned} \quad (2.39)$$

To compute these marginals efficiently, one can use a procedure similar to left and right orthogonalisation of TT-cores [27]. For this, we define the mass matrix  $\mathbf{M}_k \in \mathbb{R}^{n_k \times n_k}$  as

$$\mathbf{M}_k[i, j] = \int_{\mathcal{X}_k} \phi_k^{(i)}(x_k) \phi_k^{(j)}(x_k) \lambda(x_k) dx_k, \quad i, j = 1, \dots, n_k, \quad (2.40)$$

where  $\{\phi_k^{(i)}(x_k)\}_{i=1}^{n_k}$  denotes the set of basis functions for the  $k$ -th coordinate.

### 2.6.1 Marginal Functions

We compute the marginal functions using two procedures, referred to as backward marginalisation [23] and forward marginalisation. The backward marginalisation provides us with the coefficient matrices  $\mathbf{B}_k$ , while the forward marginalisation gives the coefficient matrices  $\mathbf{B}_{\text{pre},n}$ . These matrices enable the efficient evaluation of marginal functions, similar to [23]. The proposition used to compute  $\mathbf{B}_k$ , stated in Proposition 1, is adapted directly from [23].

**Proposition 1** (Backward Marginalisation): 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  $\mathbf{B}_{k-1} \in \mathbb{R}^{r_{k-2} \times n_{k-1} \times r_{k-1}}$ , which we need 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  $\mathbf{C}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ :

$$\mathbf{C}_k[\alpha_{k-1}, \tau, l_k] = \sum_{i=1}^{n_k} \mathbf{B}_k[\alpha_{k-1}, i, l_k] \mathbf{L}_k[i, \tau]. \quad (2.41)$$

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

$$\mathbf{Q}_k \mathbf{R}_k = (\mathbf{C}_k^{(R)})^\top. \quad (2.42)$$

3. Compute the new coefficient tensor:

$$\mathbf{B}_{k-1}[\alpha_{k-2}, i, l_{k-1}] = \sum_{\alpha_{k-1}=1}^{r_{k-1}} \mathbf{A}_{k-1}[\alpha_{k-2}, i, \alpha_{k-1}] \mathbf{R}_k[l_{k-1}, \alpha_{k-1}]. \quad (2.43)$$

**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 the coefficient tensor  $\mathbf{B}_{\text{pre},k+1} \in \mathbb{R}^{r_k \times n_{k+1} \times r_{k+1}}$  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  $\mathbf{C}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ :

$$\mathbf{C}_{\text{pre},k}[\alpha_{k-1}, \tau, l_k] = \sum_{i=1}^{n_k} \mathbf{L}_k[i, \tau] \mathbf{B}_{\text{pre},k}[\alpha_{k-1}, i, l_k]. \quad (2.44)$$

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

$$\mathbf{Q}_{\text{pre},k} \mathbf{R}_{\text{pre},k} = (\mathbf{C}_{\text{pre},k}^{(R)}). \quad (2.45)$$

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

$$\mathbf{B}_{\text{pre},k+1}[l_{k+1}, i, \alpha_{k+1}] = \sum_{\alpha_k=1}^{r_k} \mathbf{R}_{\text{pre},k}[l_{k+1}, \alpha_k] \mathbf{A}_{k+1}[\alpha_k, i, \alpha_{k+1}]. \quad (2.46)$$

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

$$f_{X_k}(x_k) = \frac{1}{z} \left( \gamma' \prod_{i=1}^{k-1} \lambda_i(X_i) \prod_{i=k+1}^d \lambda_i(X_i) + \sum_{l_{k-1}=1}^{r_{k-1}} \sum_{l_k=1}^{r_k} \left( \sum_{i=1}^n \phi_k^{(i)}(x_k) \mathbf{D}_k[l_{k-1}, i, l_k] \right)^2 \right) \lambda_k(x_k), \quad (2.47)$$

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

$$\mathbf{D}_k[l_{k-1}, i, l_k] = \sum_{\alpha_{k-1}=1}^{r_{k-1}} \mathbf{R}_{\text{pre},k-1}[l_{k-1}, \alpha_{k-1}] \mathbf{B}_k[\alpha_{k-1}, i, l_k]. \quad (2.48)$$

For the first dimension,  $f_{X_1}(x_1)$  can be expressed as

$$f_{X_1}(x_1) = \frac{1}{z} \left( \gamma' \prod_{i=2}^d \lambda_i(\mathcal{X}_i) + \sum_{l_1=1}^{r_1} \left( \sum_{i=1}^n \phi_1^{(i)}(x_1) \mathbf{D}_1[i, l_1] \right)^2 \right) \lambda_1(x_1), \quad (2.49)$$

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

$$f_{X_d}(x_d) = \frac{1}{z} \left( \gamma' \prod_{i=1}^{d-1} \lambda_i(\mathcal{X}_i) + \sum_{l_{n-1}=1}^{r_{d-1}} \left( \sum_{i=1}^n \phi_d^{(i)}(x_d) \mathbf{D}_d[l_{n-1}, i] \right)^2 \right) \lambda_d(x_d), \quad (2.50)$$

where  $\mathbf{D}_d[l_{n-1}, i] = \mathbf{B}_{\text{pre},d}[l_{n-1}, i, \alpha_{n+1}]$  and  $\alpha_{d+1} = 1$ .

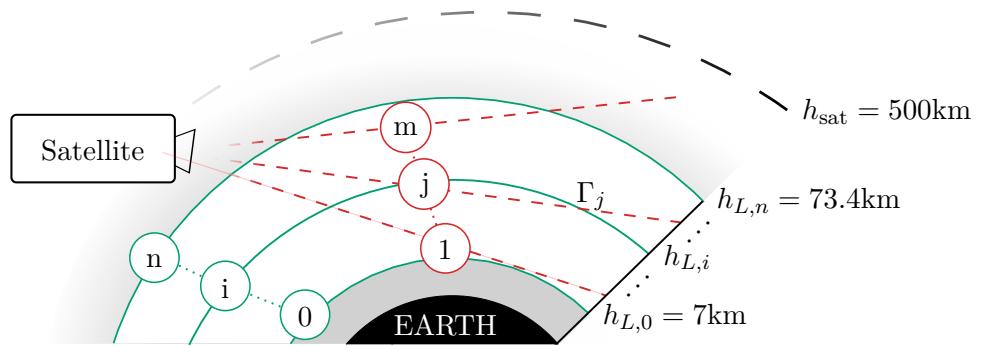


# 3

## Results

In this chapter we explain how we use the forward model to generate data and how we set up a Bayesian framework to then give distribution of solutions. Here we make it explicit and provide all information to be able to replicate our results. In this work we simulate data with an ozone profile from [1]. We follow the U.S. standard atmosphere, 1976 [2] to relate pressure and temperature and height and the HITRANonline [3] database to calculate the measured signal. We follow the mipas instrument description from the forward model [4].

### 3.1 Simulate Data



**Figure 3.1:** Schematic of measurement and analysis geometry, not to scale. The stationary satellite, at a constant height  $h_{\text{sat}}$  above Earth, takes  $m = 36$  measurements along its line-of-sight defining by the line  $\Gamma_j$ . Each measurement has a limb height  $\ell_j$ ,  $j = 1, 2, \dots, m$  defined as the closest distance of  $\Gamma_j$  to the Earth surface, see Fig. 2.1. Between  $h_{L,0} = 7\text{km}$  and  $h_{L,n} = 73.4\text{km}$ , the stratosphere is discretised into  $n = 41$  layers as illustrated by the solid green lines.

We simulate some data by taking an ozone profile from the retrieval from the MLS

limb sounder form [1]. When taking this ozone profile we get given ozone volume mixing ratios and pressure values. [28] [29] [30] [31] [32] [1] [2] [33]

### Pressure to Height to Temperature

we relate pressure and height following the book [33] where we use the equation

$$d \ln p = \frac{dp}{p} = \frac{-gM}{R^*T} dh, \quad (3.1)$$

with the universal gas constant  $R^* \approx 8.314 \text{ N m/mol/K}$ . The moledus numebr ... is  $M = M_0 \approx 28.97 \text{ kg/mol}$  for altiudes below 79km [1]. At altitude  $h$  the gravitational constant Up until 86km we can relate pressure  $p$  and geometric height  $h$  through the hydrostatic equation

$$g = g_0 \left( \frac{r_0}{r_0 + h} \right), \quad (3.2)$$

with  $r_0 \approx 6356 \text{ km}$  (also known as the polar radius of the earth) and  $g_0 \approx 9.81 \text{ m/s}^2$  and [1].

We can formulate a temperature function from [33]

$$T(h) = \begin{cases} T_0, & h = 0 \\ T_0 + a_0 h, & 0 \leq h < h_1 \\ T_0 + a_0 h_1, & h_1 \leq h < h_2 \\ T_0 + a_0 h_1 + a_1(h - h_2), & h_2 \leq h < h_3 \\ T_0 + a_0 h_1 + a_1(h_3 - h_2) + a_2(h - h_3), & h_3 \leq h < h_4 \\ T_0 + a_0 h_1 + a_1(h_3 - h_2) + a_2(h_4 - h_3), & h_4 \leq h < h_5 \\ T_0 + a_0 h_1 + a_1(h_3 - h_2) + a_2(h_4 - h_3) + a_3(h - h_5), & h_5 \leq h < h_6 \\ T_0 + a_0 h_1 + a_1(h_3 - h_2) + a_2(h_4 - h_3) + a_3(h_6 - h_{T5}) + a_4(h - h_6), & h_6 \leq h \lesssim 85 \end{cases} \quad (3.3)$$

depending on 12 parameters with values provided by [1], also see table ???. We set this as our true temperature profile and refer to [1] for temperature values above 79 km.

### Source

- RTE again?
- assumptions

We calculate the source function  $B(\nu, T)$  and the absorption constant  $k(\nu, T)$  as follows. assumption local thermaodynamic equilibrium For one species at one specific wave-number the weighted absorption constant becomes

$$\overline{k(\nu, T, r)} = \sum_{m=1}^{molec} k_m(\nu, T) x_m(r) = k(\nu, T) x(r), \quad (3.4)$$

with the volume mixing ratio of ozone  $x(r)$  at location  $r$ . The absorption constant

$$k(\nu, T) = L(\nu, T_{ref}) \frac{Q(T_{ref})}{Q(T)} \frac{\exp\{-c_2 E''/T\}}{\exp\{-c_2 E''/T_{ref}\}} \frac{1 - \exp\{-c_2 \nu/T\}}{1 - \exp\{-c_2 \nu/T_{ref}\}} \quad (3.5)$$

is depend on the line intensity  $L(\nu, T_{ref})$  at reference temperature  $T_{ref} = 296K$ , the lower-state energy of the transition  $E''$ , the second radiation constant  $c2 = 1.4387769\text{cmK}$  all provided by [1]. Since we only consider one transition namely the lower-state one the partition function becomes

$$Q(T) = g'' \exp\left\{-\frac{c_2 E''}{T}\right\}, \quad (3.6)$$

with the the statistical weight  $g''$  (also called the degeneracy factor), see [2]. M. Šimečková, D. Jacquemart, L. S. Rothman, R. R. Gamache, and A. Goldman, "Einstein A-coefficients and statistical weights for molecular absorption transitions in the HITRAN database", J. Quant. Spectrosc. Radiat. Transfer 98, 130-155 (2006)

Under the assumption of local thermodynamic (LTE) equilibrium t source function is given by the black body radiation

$$B(\nu, T) = \frac{2hc^2\nu^3}{\exp\left\{\frac{hc\nu}{k_B T}\right\} - 1}, \quad (3.7)$$

with Planck's constant  $h$ , velocity of light  $c$  and Boltzmann's constant  $k_B$  [1].

Then we can calculate measurement with the RTE in Eq. 3.8 using the trapezoidal rule

$$y_j = \int_{\Gamma_j} B(\nu, T) k(\nu, T) \frac{p(T)}{k_B T(r)} x(r) \tau(r) dr + \eta_j \quad (3.8)$$

$$\tau(r) = \exp\left\{-\int_{r_{obs}}^r k(\nu, T) \frac{p(T)}{k_B T(r')} x(r') dr'\right\}, \quad (3.9)$$

Note we assume infinte spectral resulution and no poisnting errors. atmopsheric model and now intrumetcn model

## 3.2 Bayesian Model and prior analysis

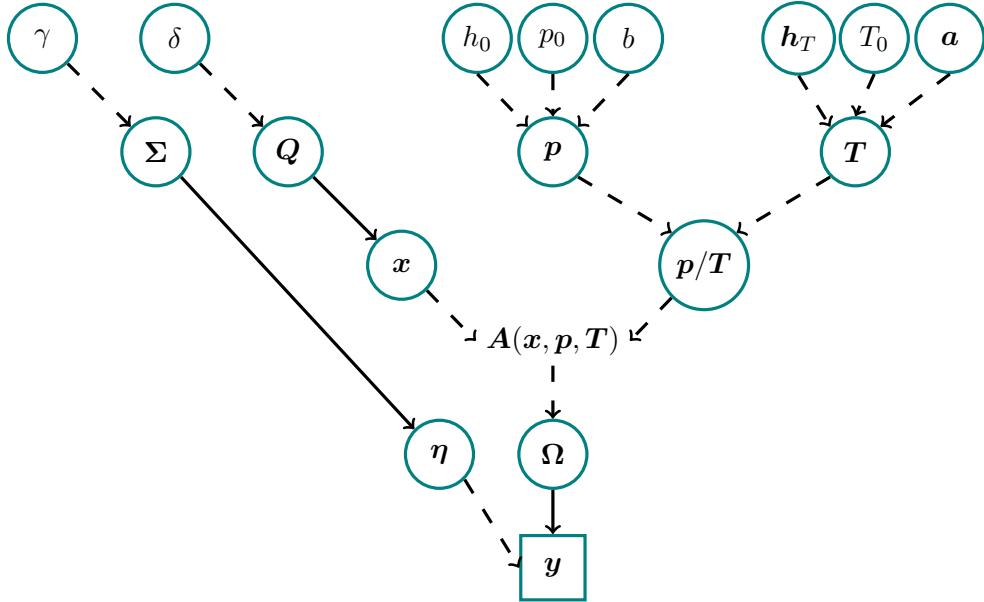
- fill in what we describe beofre
- describe parametres and hyper paraemrets set up model to make dag
- then prior modelling

In this section we present the explicit Bayesian we will use to recover pressure temperature and ozone values.

### 3.2.1 DAG

Again we draw a DAG and specify prior distribution over those

- correlation structure between ozone and temperature and pressure



**Figure 3.2:** Complete directed acyclic graph of the forward model. The hyper-parameters at the top deterministically (dotted line) describe the parameters  $(\mathbf{p}/\mathbf{T})$  or the noise covariance  $\Sigma = \gamma^{-1} \mathbf{I}$  of the random (solid line) noise  $\boldsymbol{\eta} \sim \mathcal{N}(0, \gamma^{-1} \mathbf{I})$  and precision matrix  $\mathbf{Q} = \delta \mathbf{L}$  of the distribution of  $\mathbf{x} \sim \mathcal{N}(0, \delta \mathbf{L})$ , where  $\mathbf{L}$  is a graph Laplacian as in Eq. 3.10. We can group the noise precision  $\gamma$  and the smoothness parameter  $\delta$  to define the marginal posterior over those hyper-parameters and then condition on them for the conditional posterior distribution, for further details see Fig. 3.7. In this whole process where we condition on the pressure  $\mathbf{p}$  and temperature  $\mathbf{T}$ , which we retrieve separately, see Fig. 3.15. The hyper-parameters  $h_0, p_0, b$  deterministically describe the pressure function in Eq. 3.11, note that we only need three parameters here since  $h_0 < h_{L,0}$  and  $\mathbf{h} = \{h_1, h_2, h_3, h_4, h_5, h_6\}$ ,  $\mathbf{a} = \{a_0, a_1, a_2, a_3, a_4\}$  and  $T_0$  determine the temperature function. The parameters  $\mathbf{x}$  and  $\mathbf{p}/\mathbf{T}$  determine the space of all measurable noise free data  $\Omega$  through the forward model  $A(\mathbf{x}, \mathbf{p}, \mathbf{T})$  from which we randomly observe data set plus some random noise.

### 3.2.2 Prior Modelling

- physical meaning by choosing priors
- eventuel dependencies
- draw samples from priors should be as loose as possible

In practise we operate OPzone and condition on temperature and pressure or vice versa.

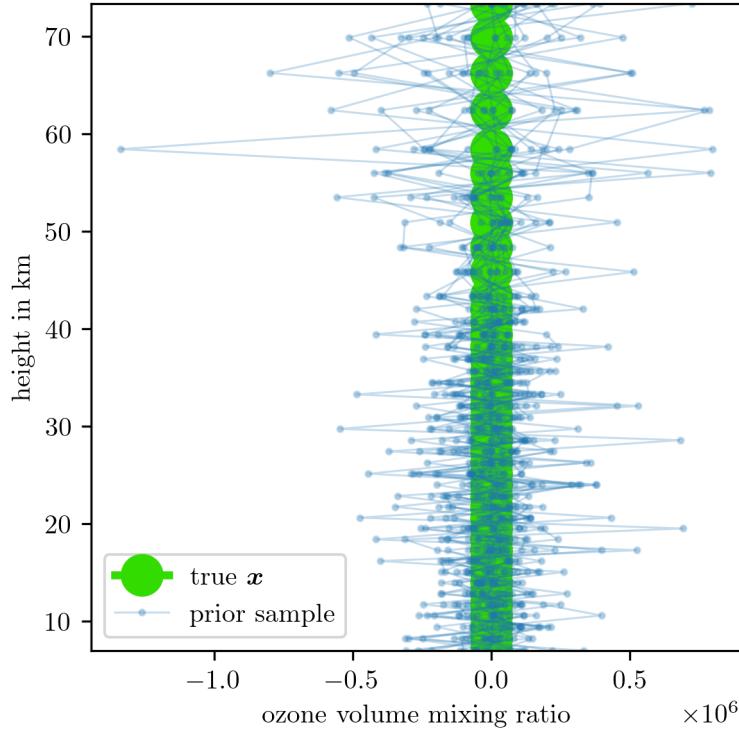
model parameters	priors	TT bounds		Context
		lower	upper	
$\gamma$	$\mathcal{T}(1, 10^{-10})$	$10^{-8}$	$4 \cdot 10^{-7}$	$\mathbf{y}$
$\delta$	$\mathcal{T}(1, 10^{-10})$	-	-	$\mathbf{x}$
$\lambda$	-	150	5000	$\mathbf{x}$
$\mathbf{x}$	$\mathcal{N}(0, \delta \mathbf{L})$	-	-	$\mathbf{x}$
$h_0$	$\mathcal{N}(6, 0.6)$	5.3	6.1	$\mathbf{p}/\mathbf{T}$
$p_0$	$\mathcal{N}(460, 4)$	443	471	$\mathbf{p}/\mathbf{T}$
$b$	$\mathcal{N}(0.167, 5 \cdot 10^{-4})$	0.166	0.169	$\mathbf{p}/\mathbf{T}$
$h_1$	$\mathcal{N}(11, 0.5)$	10.6	11.3	$\mathbf{p}/\mathbf{T}$
$h_2$	$\mathcal{N}(20, 3)$	16.6	22.7	$\mathbf{p}/\mathbf{T}$
$h_3$	$\mathcal{N}(32, 1)$	23.6	43.3	$\mathbf{p}/\mathbf{T}$
$h_4$	$\mathcal{N}(47, 2)$	45.2	48.9	$\mathbf{p}/\mathbf{T}$
$h_5$	$\mathcal{N}(51, 2)$	49.2	52.9	$\mathbf{p}/\mathbf{T}$
$h_6$	$\mathcal{N}(71, 2)$	57.8	84.1	$\mathbf{p}/\mathbf{T}$
$a_0$	$\mathcal{N}(-6.5, 0.01)$	-6.54	-6.46	$\mathbf{p}/\mathbf{T}$
$a_1$	$\mathcal{N}(1, 0.01)$	0.96	1.04	$\mathbf{p}/\mathbf{T}$
$a_2$	$\mathcal{N}(2.8, 0.1)$	2.43	3.18	$\mathbf{p}/\mathbf{T}$
$a_3$	$\mathcal{N}(-2.8, 0.01)$	-3.18	-2.43	$\mathbf{p}/\mathbf{T}$
$a_4$	$\mathcal{N}(-2, 0.01)$	-2.04	-1.96	$\mathbf{p}/\mathbf{T}$
$T_0$	$\mathcal{N}(288.15, 2)$	282	295	$\mathbf{p}/\mathbf{T}$

**Table 3.1:** Gaussian  $\mathcal{N}(\mu, \sigma)$  and gamma distribution  $\mathcal{T}(\alpha = \text{scale}, \beta = \text{rate})$  Bounds for t and p 2.8 times the variance around the mean round pressure approx and test if would work with previous gamma prior or fix gamma prior with set values

## Ozone

graph lacoiacn wigthing in between similiar to a ciuop;led osscialtors what heught is change of weights

$$\mathbf{Q} = \delta \mathbf{L} = \delta \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 6 & -5 \\ & & & \ddots & \ddots & \ddots \\ & & & & -5 & 10 & -5 \\ & & & & & -5 & 10 \end{bmatrix} \quad (3.10)$$



**Figure 3.3:** 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 spread/variance of prior samples is very large compared to the ozone volume mixing ratios, the ozone profile appears to be constant, which it is not, as seen e.g. in Fig. 3.10.

### pressure over temperature

We parametrize the pressure by fitting one exponential to the pressure values  $p$  related to the height  $h$  by Eq. ??.

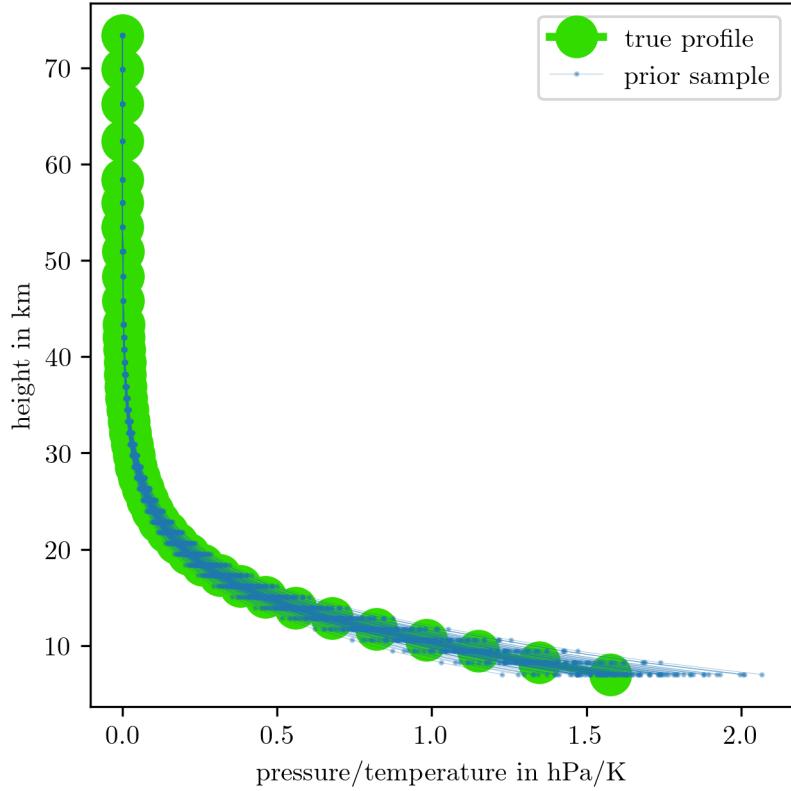
The pressure function,

$$p(h) = \exp \{-b(h - h_0)\} p_0, \quad (3.11)$$

is depending on three different parameters, the gradient  $a_{p,1}$  and the tuple  $(p_0, h_{p,0})$ .

- show that pressure is dominant
- correlation structure
- appendix

PriorTempOverPostMeanSigm



**Figure 3.4:** We draw samples from the hyper-prior distribution of  $h_0, b, p_0, h_1, h_2, h_3, h_4, h_5, h_6, a_0, a_1, a_2, a_3, a_4$  and  $T_0$  as defined in table 3.1 and then calculate  $p/T$  according to the functions in Eq. 3.11 and 3.3.

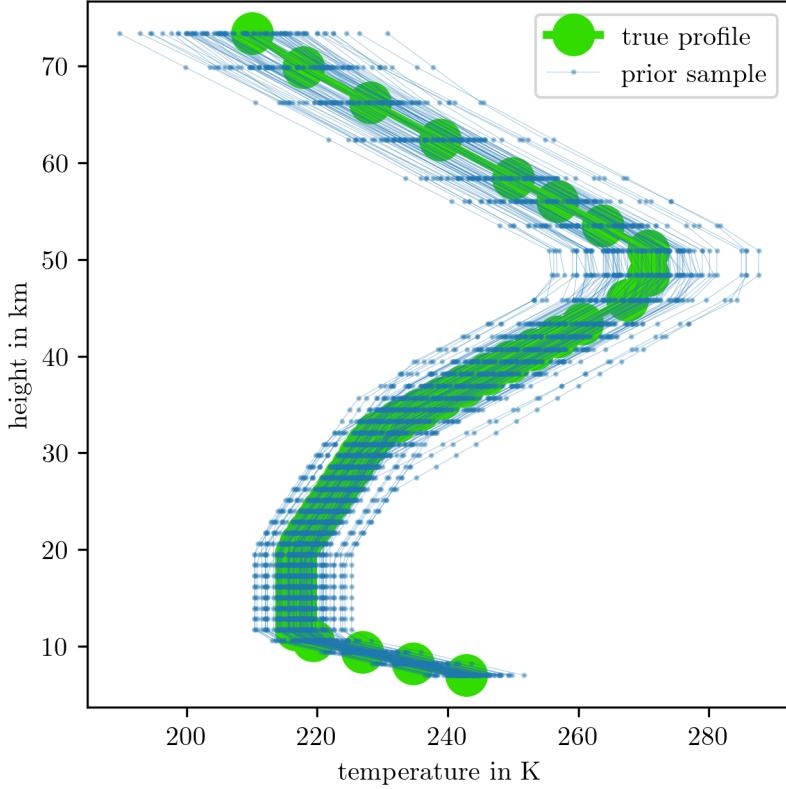
### 3.2.3 Posterior distributions

- explain where we use MTC and that  $T/p$  is spereate
- marginal posterior, noise and covarince and perciosn matrix
- picture of  $f$  and  $g$
- taylor expansion
- maybe make metroplis explixit

conditioned on a ozone profile

**pressure over temperature**

conditioned on a temperauter opver pressure profile



**Figure 3.5:** We draw samples from the hyper-prior distribution of  $h_1, h_2, h_3, h_4, h_5, h_6, a_0, a_1, a_2, a_3, a_4$  and  $T_0$  as defined in table 3.1 and then calculate  $\mathbf{T}$  according to the function in Eq. 3.3.

### Ozone – marginal posterior

## 3.3 MTC posterior sampling

In this Section we discuss sampling from the posterior distribution. But you don't need to.

### 3.3.1 Sampling from the marginal posterior distribution over hyper-parameters

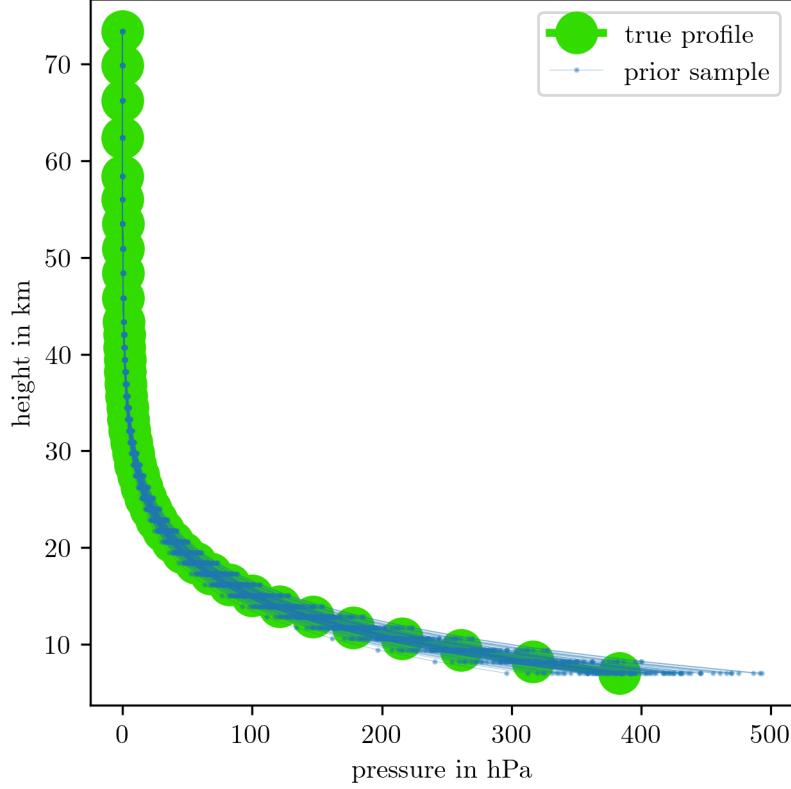
Now, to sample from the marginal posterior of the hyper-parameters

$$\pi(\lambda, \gamma | \mathbf{y}) \propto \lambda^{n/2} \gamma^{m/2} \exp\left\{-\frac{1}{2}g(\lambda) - \frac{\gamma}{2}f(\lambda)\right\} \pi(\lambda, \gamma), \quad (3.12)$$

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

$$f(\lambda) = \mathbf{y}^T \mathbf{y} - (\mathbf{A}^T \mathbf{y})^T (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L})^{-1} (\mathbf{A}^T \mathbf{y}), \quad (3.13a)$$

$$\text{and } g(\lambda) = \log \det(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{L}). \quad (3.13b)$$



**Figure 3.6:** We draw samples from the hyper-prior distribution of  $h_0, b$  and  $p_0$  as defined in table 3.1 and then calculate  $\mathbf{p}$  according to the function in Eq. 3.11.

we employ a so-called MWG (Metropolis within Gibbs) algorithm, summarised in the algorithmic Box 1. One may implement a Metropolis random walk on the full conditional

$$\pi(\lambda|\mathbf{y}, \gamma) \propto \lambda^{n/2+\alpha_\delta-1} \exp\left\{-\frac{1}{2}g(\lambda) - \frac{\gamma}{2}f(\lambda) - \beta_\delta\gamma\lambda\right\} \quad (3.14)$$

and do a Gibbs steps on

$$\gamma|\mathbf{y}, \lambda \sim \Gamma\left(\frac{m}{2} + \alpha_\delta + \alpha_\gamma, \frac{1}{2}f(\lambda) + \beta_\gamma + \beta_\delta\lambda\right) \quad (3.15)$$

to generate marginal posterior samples  $(\lambda, \gamma)^{(1)}, \dots, (\lambda, \gamma)^{(N)} \sim \pi(\lambda, \gamma|\mathbf{y})$ . Note that, when changing variables from  $\delta = \lambda\gamma$  to  $\lambda$  the hyper-prior distribution changes to  $\pi(\lambda) \propto \lambda^{\alpha_\delta-1}\gamma^{\alpha_\delta} \exp(-\beta_\delta\lambda\gamma)$ , due to  $d\delta/d\lambda = \gamma$ . We find the full conditionals by factorisation.

As part of the Metropolis random walk, a new  $\lambda'$  given the previous  $\lambda^{(k)}$ , with  $k = 1, \dots, N$ , is proposed according to the distribution  $q(\lambda'|\lambda^{(k)}) \sim \mathcal{N}(\lambda^{(k)}, w_\lambda)$ . The proposed sample is rejected or accepted with the acceptance probability  $\alpha(\lambda'|\lambda^{(k)})$ , see Equation (??). Here, calculating the difference  $\Delta f = f(\lambda') - f(\lambda^{(k)})$  and  $\Delta g = g(\lambda') - g(\lambda^{(k)})$  is crucial. Since the functions  $f(\lambda)$  and  $g(\lambda)$  are well-behaved over a large range of  $\lambda$  and almost linear around the mode of the marginal posterior  $\lambda_0$ , a Taylor expansion

around the mode is sufficient, see Figure ???. Then, computing the acceptance ratio does not involve evaluating  $f(\lambda)$  and  $g(\lambda)$ , but the difference  $\Delta f = \sum f^{(r)}(\lambda_0)(\lambda' - \lambda^{(k)})^r$  and  $\Delta g = \sum g^{(r)}(\lambda_0)(\lambda' - \lambda^{(k)})^r$ . The derivatives are

$$f^{(r)}(\lambda_0) = (-1)^{r+1} r! (\mathbf{A}^T \mathbf{y})^T (\mathbf{B}_0^{-1} \mathbf{L})^r \mathbf{B}_0^{-1} \mathbf{A}^T \mathbf{y} \quad (3.16)$$

$$\text{and } g^{(r)}(\lambda_0) = (-1)^{r+1} \text{tr}((\mathbf{B}_0^{-1} \mathbf{L})^r) \quad (3.17)$$

with  $\mathbf{B}_0 = \mathbf{A}^T \mathbf{A} + \lambda_0 \mathbf{L}$ .

Finally, a Gibbs step provides a new  $\gamma^{(k+1)} \sim \gamma | \mathbf{y}, \lambda^{(k+1)}$ , see Equation (??).

### Ozone – conditional posterior

Conditioned on the hyper-parameters  $\boldsymbol{\theta} = (\delta, \gamma)$  we utilise the so-called RTO (randomize then optimize) method [6, 16, 34] to draw an independent sample of the conditional posterior distribution. By perturbation of the exponent of

$$\mathbf{x} | \mathbf{y}, \delta, \gamma \sim \mathcal{N}((\mathbf{A}^T \mathbf{A} + \delta/\gamma \mathbf{L})^{-1} \mathbf{A}^T \mathbf{y}, (\gamma \mathbf{A}^T \mathbf{A} + \delta \mathbf{L})^{-1}), \quad (3.18)$$

we obtain one independent sample  $\mathbf{x} \sim \pi(\mathbf{x} | \mathbf{y}, \boldsymbol{\theta})$  for each solve of Equation (2.29), see algorithmic Box 2.

We use the same discretization of the atmosphere as given by the ozone profile taken from [29] [https://disc.gsfc.nasa.gov/datasets/ML203\\_005/summary?keywords=mls%20o3](https://disc.gsfc.nasa.gov/datasets/ML203_005/summary?keywords=mls%20o3). We use ozone values between a height of 10km up to 38km, which results in  $n = 37$  layers. We set the number of measurements to  $m = 105$ . (I can't think of any good reason why I chose that, it is a good number not too big not too small and gives consistent results for various datasets)

When finding the mode we use the `scipy.optimize.fmin` function and limit the number of function evaluations to 25. We use Cholesky factorisation to evaluate  $g(\lambda)$  and  $f(\lambda)$  and to construct the coefficients of the Taylor series, where we have to calculate  $\mathbf{B}^{-1} \mathbf{L}$  and  $\mathbf{B}^{-1} \mathbf{A}^T \mathbf{y}$  once at  $\lambda_0$ .

We bin the samples into a normalised histogram and use the height of the bars as quadrature weights  $\pi(\lambda_i | \mathbf{y})$ , where the quadrature point  $\lambda_i$  denotes the centre of each bin. To calculate the conditional posterior mean we use approximate quadrature

$$\mu_{\mathbf{x} | \mathbf{y}} = \int x_\lambda \pi(\lambda | \mathbf{y}) d\lambda \approx \sum x_{\lambda_i} \pi(\lambda_i | \mathbf{y}), \quad (3.19)$$

with  $\sum \pi(\lambda_i | \mathbf{y}) = 1$ , so that the integral can be interpreted as the weighted average. See Sec. 2.1 [35] <https://www.cambridge.org/core/journals/acta-numerica/article/>

highdimensional-integration-the-quasimonte-carlo-way/03F126DDF465F915B22D5D709CD28946.

We bin the samples into 3 bins and stop increasing the number of bins by one if the relative error between the previous and the current conditional posterior mean is less than 0.1%. This gives a total number of  $3 + 4 + 5 = 12$  solves for  $x_\lambda$ . In addition, we calculate the covariance matrix  $(\gamma \mathbf{B}_\lambda)^{-1}$ , where we use Cholesky factorisation to invert  $\mathbf{B}$ , solving the integral

$$\Sigma_{\mathbf{x}|\mathbf{y}} = \int \gamma^{-1} \pi(\gamma|\mathbf{y}) d\gamma \int \mathbf{B}_\lambda^{-1} \pi(\lambda|\mathbf{y}) d\lambda \approx \sum \gamma_i^{-1} \pi(\gamma_i|\mathbf{y}) \sum \mathbf{B}_{\lambda_i}^{-1} \pi(\lambda_i|\mathbf{y}). \quad (3.20)$$

It takes us less than 0.1s to draw 10000 samples from the marginal posterior and to calculate the conditional posterior mean or to solve for 200 different  $x_\lambda$  and to find the regularised solution at the point of maximum curvature using the kneedle algorithm.

### 3.4 Affine Map

- introduce affine sapce and how we get affine map, to motivate samples from posterir space
- explicit, why we need ozone profiles, because it is faster and temperature and pressure are more well defined within the atmosphere
- generate affine space every samples is a feasable sample
- generate data without noise to find affine map

We do MTC with linear forward map no updadeted In this specific case we find the affine map

$$\mathbf{M} = \begin{bmatrix} - & \mathbf{M}_0 & - \\ & \vdots & \\ - & \mathbf{M}_j & - \\ & \vdots & \\ - & \mathbf{M}_m & - \end{bmatrix} \in \mathbb{R}^{m \times m}, \quad (3.21)$$

with rows  $\mathbf{M}_j$  using a linear solver for

$$W \mathbf{M}_j^\top = V_j. \quad (3.22)$$

Here  $V_j$  denotes the  $j$ th row of

$$V = \begin{bmatrix} | & | & | \\ \mathbf{A}_{NL}(\mathbf{x}^{(1)}) & \cdots & \mathbf{A}_{NL}(\mathbf{x}^{(j)}) & \cdots & \mathbf{A}_{NL}(\mathbf{x}^{(m)}) \\ | & | & | & & | \end{bmatrix} \quad (3.23)$$

and

$$W = \begin{bmatrix} | & | & | \\ \mathbf{A}_L \mathbf{x}^{(1)} & \cdots & \mathbf{A}_L \mathbf{x}^{(j)} & \cdots & \mathbf{A}_L \mathbf{x}^{(m)} \\ | & | & | & & | \end{bmatrix} \quad (3.24)$$

is a  $\mathbb{R}^{m \times m}$  matrix as well as  $\mathbf{A}_{NL}$ . Then the non-linear forward model can be approximated so that

$$\mathbf{A}_{NL}(\mathbf{x}) \approx \mathbf{M} \mathbf{A}_L \mathbf{x}. \quad (3.25)$$

### 3.4.1 First MTC

- make table with set up for TT and sampling , number of samples
- normalize in evrey step
- we use RTO to generate samples

#### Marginal Posterior

- samples vs calc values
- taylor expansion

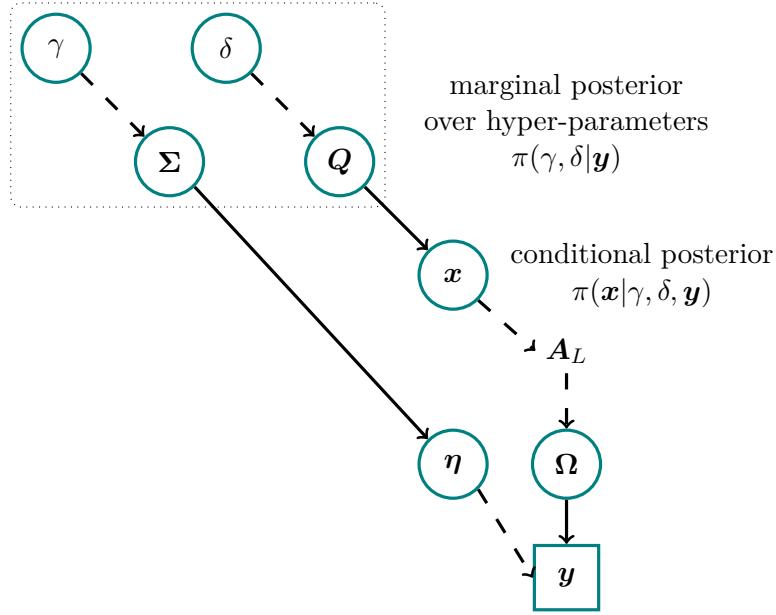
#### sampling from conditional posterior Posterior

- draw samples using RTO no need to calc variance yet, when variance is hard to calculate, we use Cholesky defactorization (maybe put in appendix)
- or calc mean and variance using see other section

### 3.4.2 Generate and Asses Affine Map

## 3.5 Updated Forward map

- updated forward map
- do mtc again but this time with weighted integration and then condition on pressure and temperature, samples
- for sake of completeness regularised solution and say disadvantage, maybe include in table



**Figure 3.7:** Directed acyclic graph for ozone retrieval and MTC scheme as described in Fig. 3.2. The hyper-parameters  $\delta$  and  $\gamma$  determine the noise covariance  $\Sigma$  for the random noise vector  $\eta \sim \mathcal{N}(0, \gamma^{-1} \mathbf{I})$  and the prior precision matrix  $\mathbf{Q} = \delta \mathbf{L}$  for the distribution over  $\mathbf{x} \sim \mathcal{N}(0, \delta \mathbf{L})$ , where  $\mathbf{L}$  is the graph Laplacian, see Eq. 3.10. In the MTC scheme we evaluate the marginal posterior over the hyper-parameters  $\pi(\gamma, \delta | \mathbf{y})$  as in Eq. ?? first and then conditional posterior  $\pi(\mathbf{x} | \gamma, \delta, \mathbf{y})$  as in Eq. ???. The parameter  $\mathbf{x}$  determine the space of all measurable noise free data  $\Omega$  through the forward model  $\mathbf{A}(\mathbf{x}, \mathbf{p}, \mathbf{T})$  from which we randomly observe a data set plus some random noise. Note that once we found an affine map we update the forward model to  $\mathbf{MA}_L$ .

### 3.5.1 Ozone Retrieval

MTC – sampling vs TT

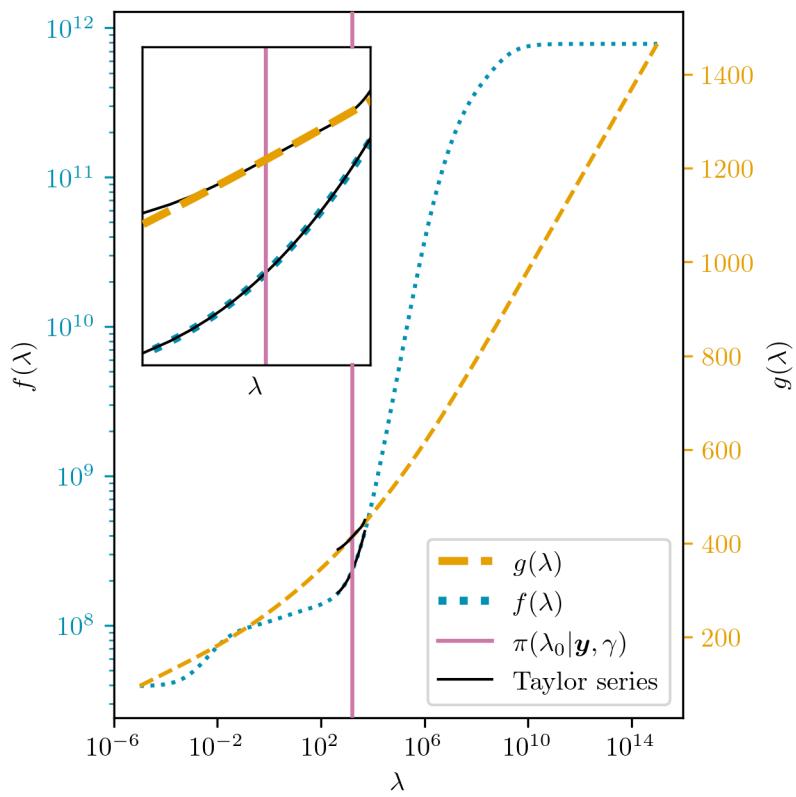
Regularized Solution

- similar to MTC model
- picture of L-Curve and samples
- include in reg paraemter in histograms

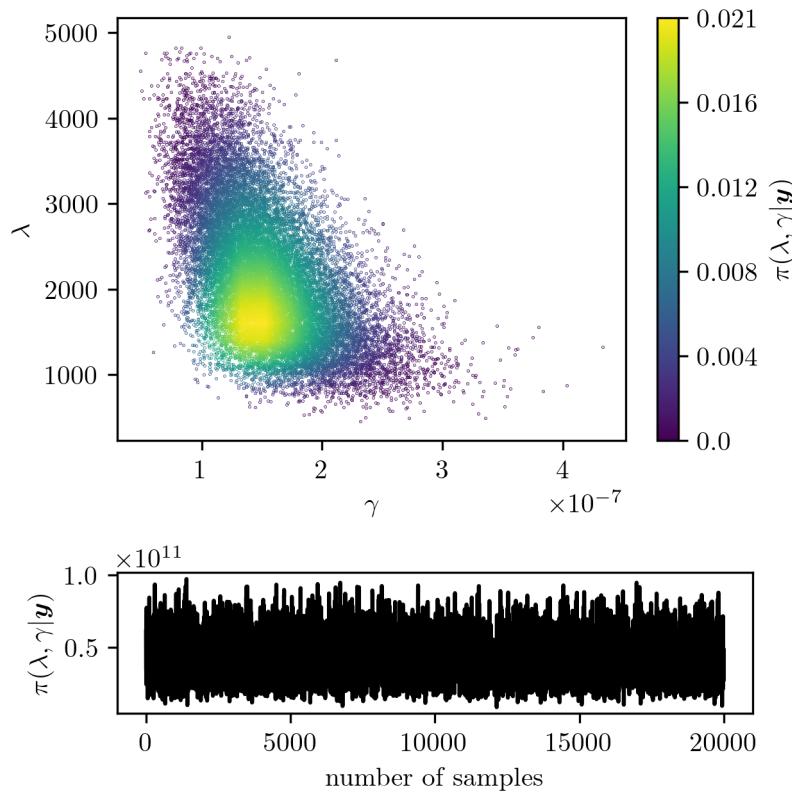
### 3.5.2 Posterior Pressure and Temperature

- make table with set up for TT and sampling t-walk

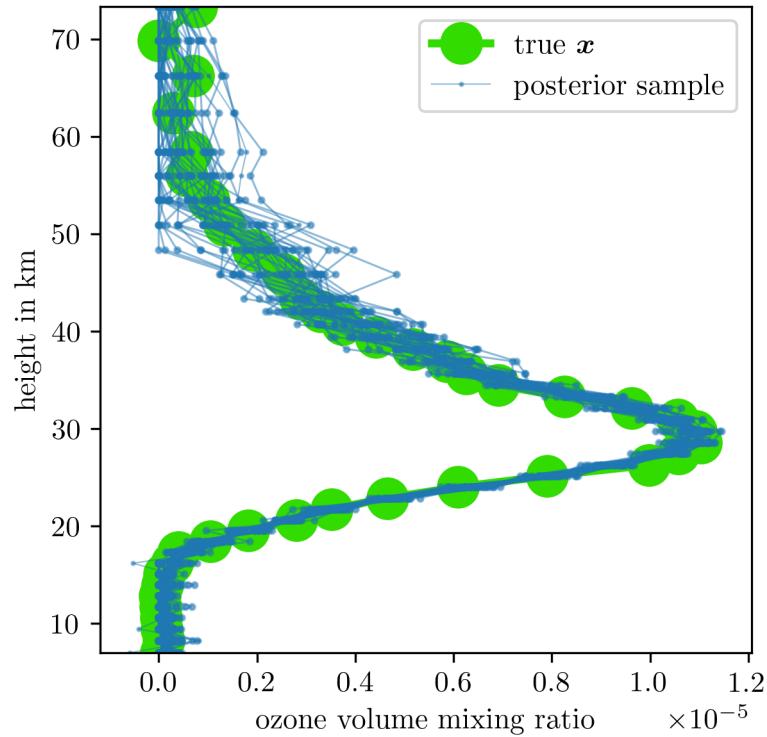
```
@misc{MLSdata, title= MLS/Aura Level 2 Ozone (O3) Mixing Ratio V005, author = Schwartz, M., Froidevaux, L., Livesey, N. and Read, W., year = 2020, howpublished = \url{https://disc.gsfc.nasa.gov/datasets/ML203_005/summary?keywords=mls%20o3}, publisher = Goddard Earth Sciences Data and Information Services Center (GES DISC), address = Greenbelt, MD, USA, note = "[Online; accessed 25/04/24, 10.5067/Aura/MLS/DATA2516]"}
```



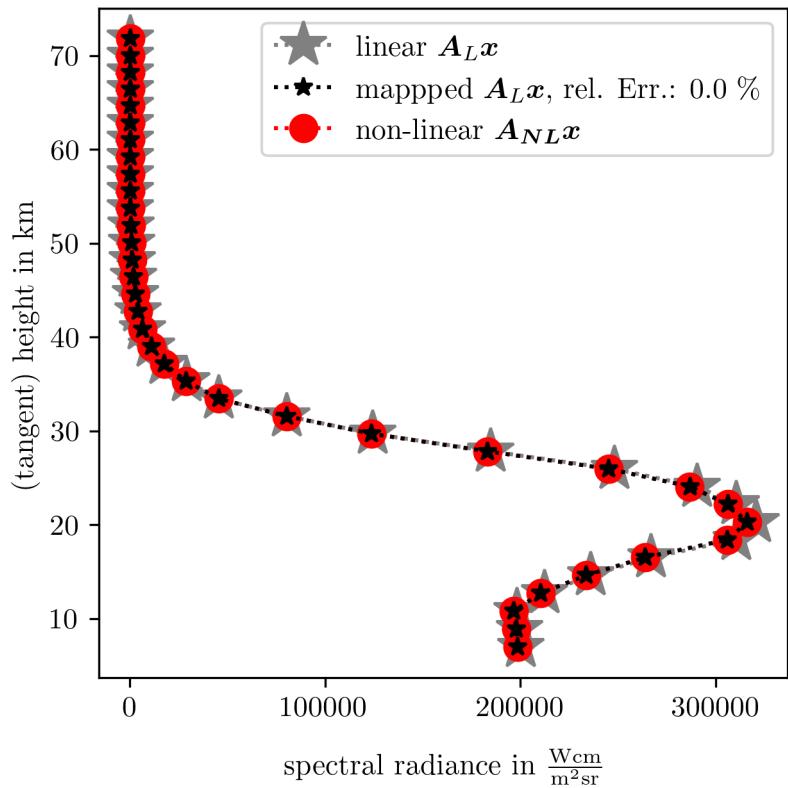
**Figure 3.8:** Plot of the functions  $f(\lambda)$  and  $g(\lambda)$  for marginal posterior for a wide range of  $\lambda = \delta/\gamma$ . We plot the third Taylor series expansion in black around the mode of the marginal posterior (vertical line) for the sampling range of  $\lambda$  within the MTC scheme.



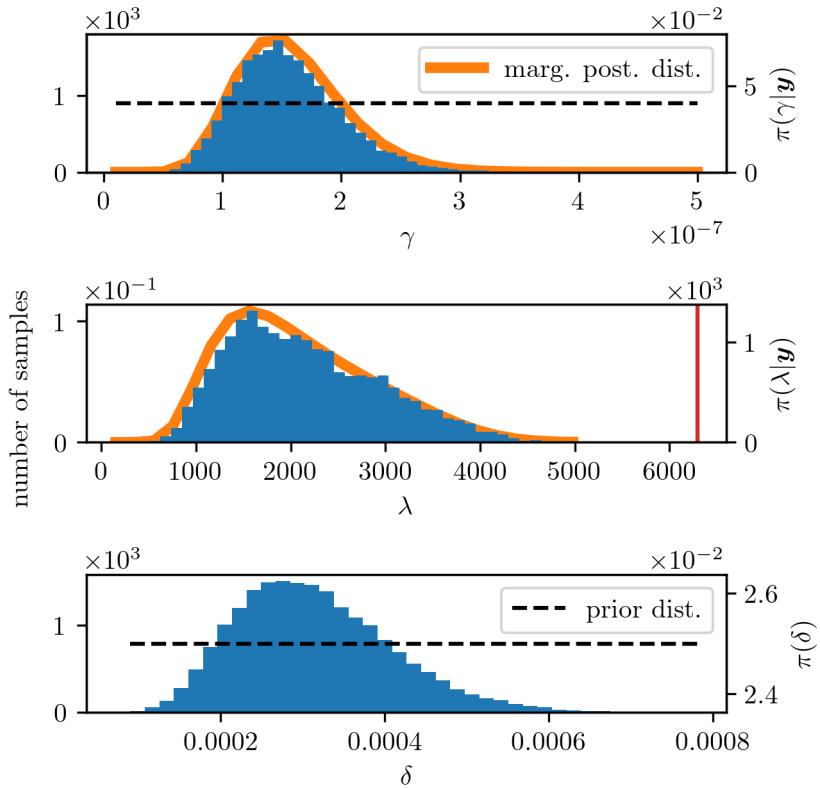
**Figure 3.9:** We scatter plot the samples of  $\lambda = \delta/\gamma$  and  $\gamma$  from the marginal posterior  $\pi(\lambda, \gamma | \mathbf{y})$  and colour code the samples using the TT approximation of  $\pi(\lambda, \gamma | \mathbf{y})$ . To show ergodicity we plot the trace of the samples of the Metropolis-within-Gibbs sampler below.



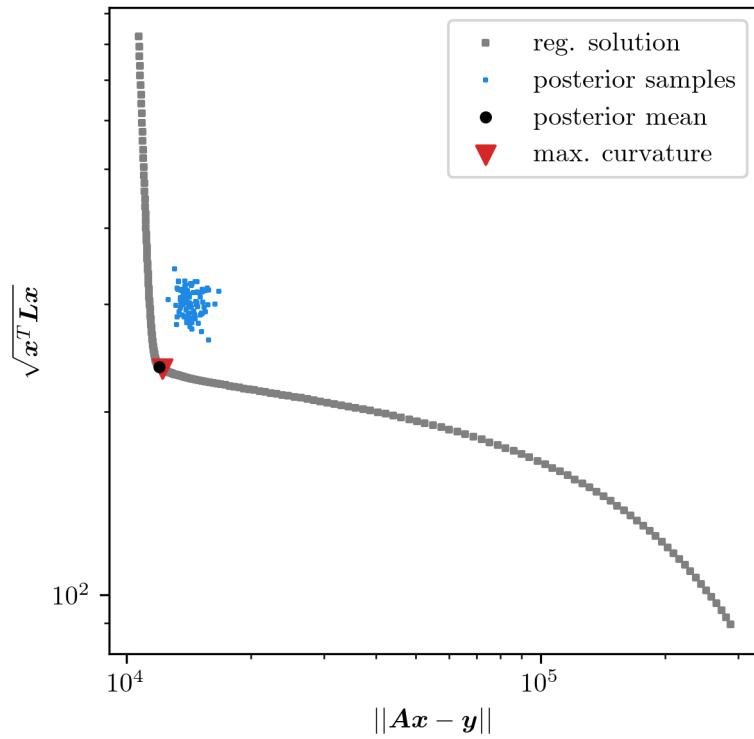
**Figure 3.10:** We draw samples from the conditional posterior distribution  $\pi(\mathbf{x}|\lambda, \gamma, \mathbf{y})$  after characterising the marginal posterior  $\pi(\lambda, \gamma|\mathbf{y})$  through sampling or TT approximation using the linear forward map  $\mathbf{A}_L$ . We will use those samples to find the affine map  $\mathbf{M}$ , see section 3.4



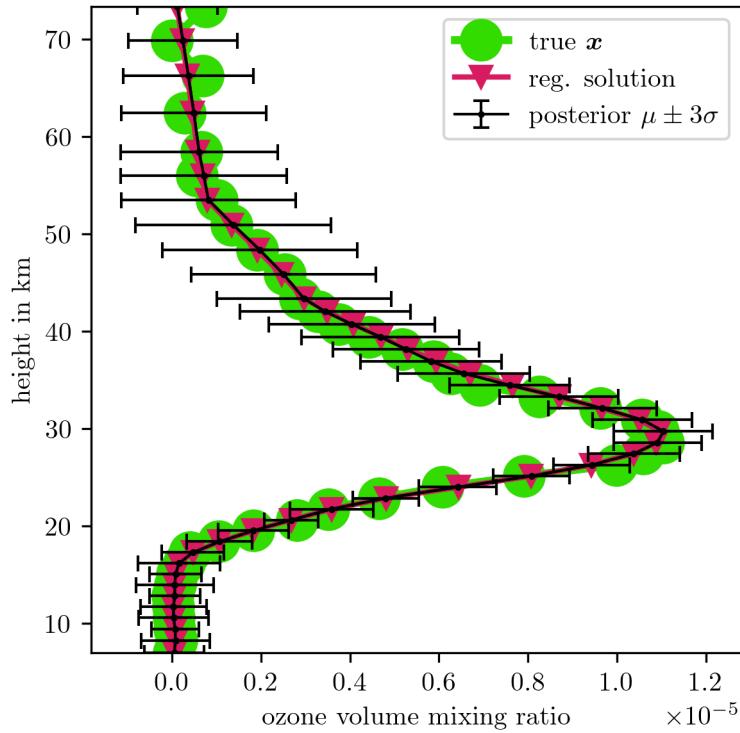
**Figure 3.11:** We asses how good we can map the linear forward model onto the non-linear forward model using the previous calculated affine map. The gray stars represent noise free linear data, where as the red circles present noise free non-linear data. Then we map the linear noise free data onto the non-linear noise free data and give the relative error in between the mapped noise free data and the non-linear data. the needs M



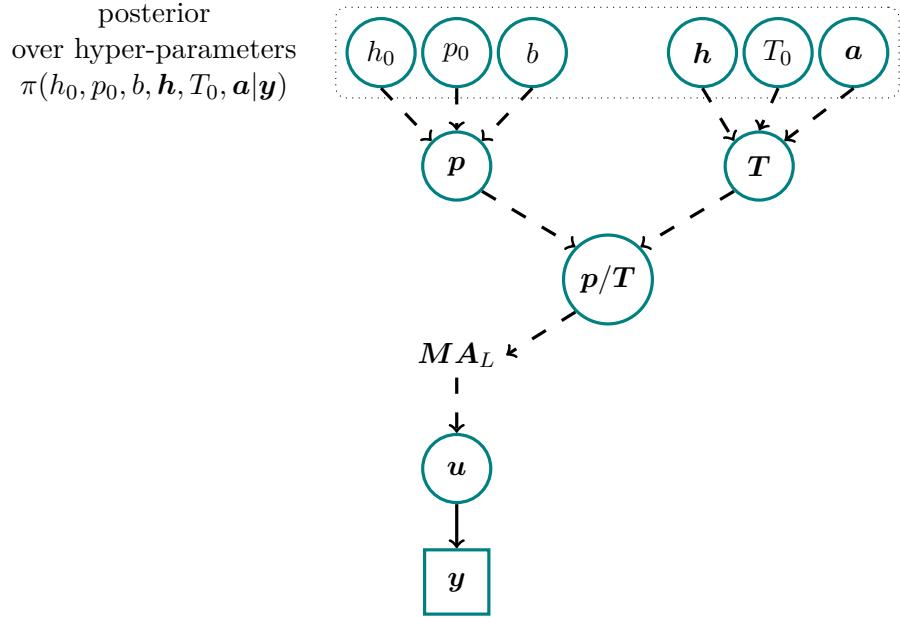
**Figure 3.12:** We plot the TT approximation of marginal posterior in orange and the samples as a histogram as well as the prior distribution with a dotted line. Note that we sample  $\lambda$  and  $\gamma$  using the Metropolis-within-Gibbs sampler and can calculate  $\delta$  for every sample of the marginal posterior, we can not do this for the TT approximation. The regularised parameter corresponding to the regularised solution is marked thought the red vertical line at  $\lambda_{\text{reg}} =$ .



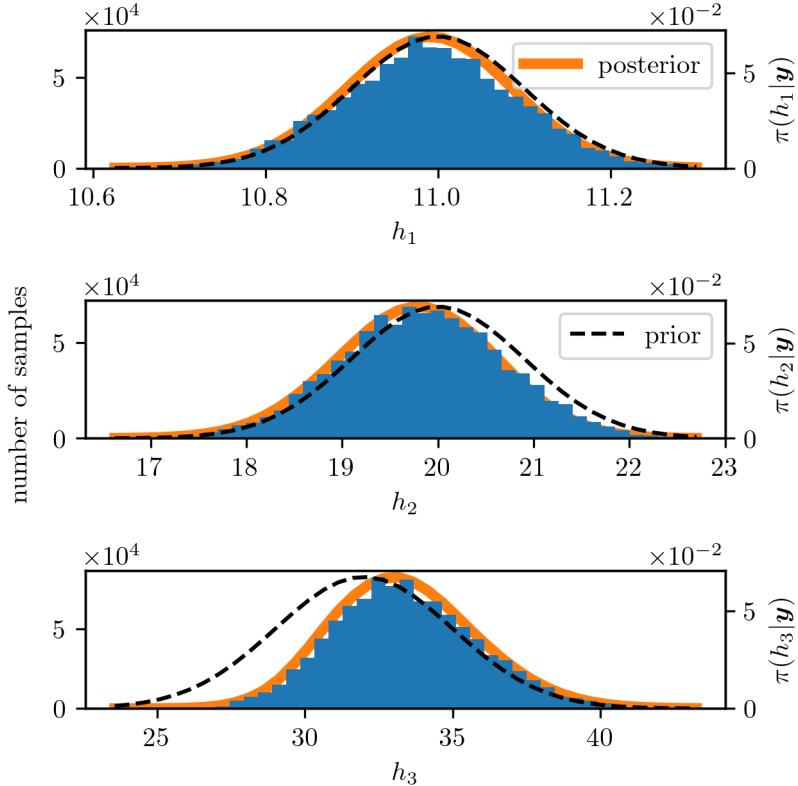
**Figure 3.13:** We calculate regularised solution as in Eq. ?? and plot the regularised semi norm  $\sqrt{\mathbf{x}^T \mathbf{L} \mathbf{x}}$  against the data misfit norm  $\|\mathbf{A}\mathbf{x} - \mathbf{y}\|$  to find the regularised solution at the point of maximum curvature of the so-called L-Curve. Additionally we calculate the data misfit norm and the regularised norm for the ozone posterior and for samples of the conditional posterior distribution.



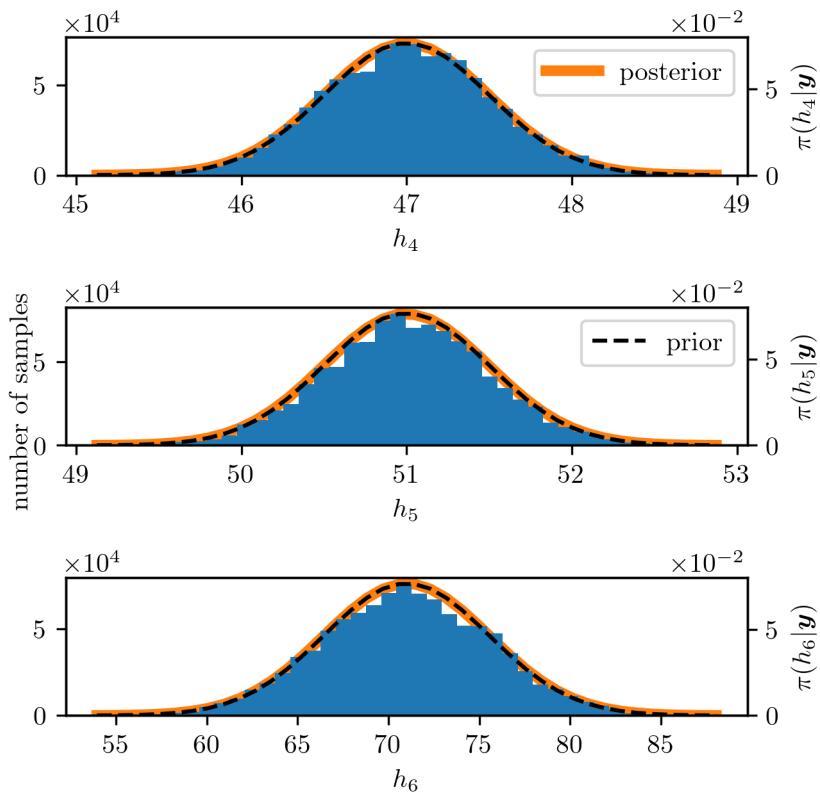
**Figure 3.14:** We plot the conditional posterior mean and variance in black and the regularised solution on top of the ground truth ozone profile in green. We use the updated forward map  $MA_L$



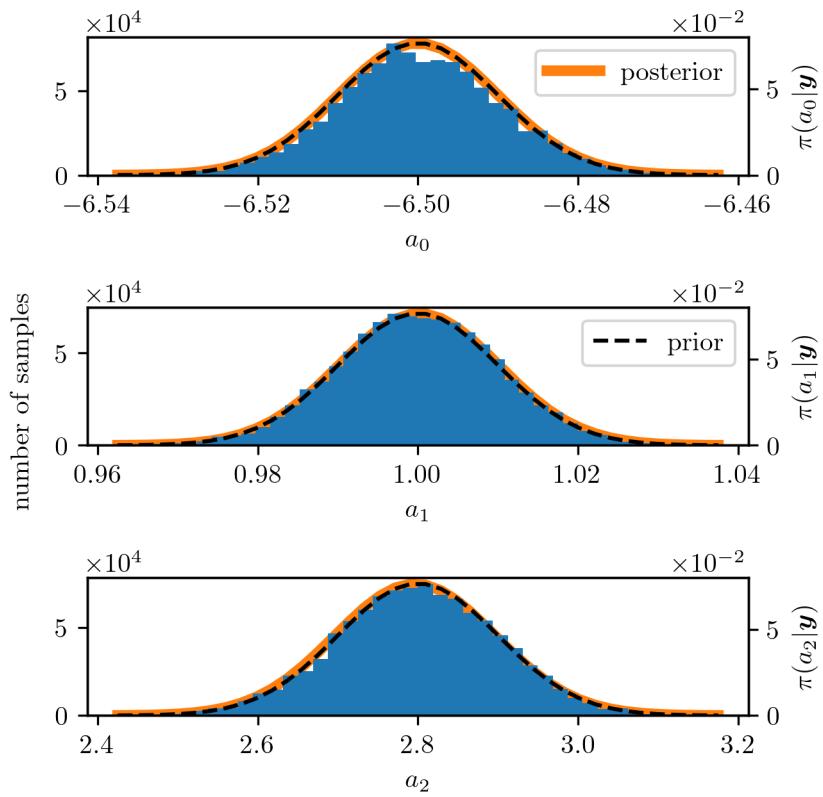
**Figure 3.15:** Conditioned on an ozone profile the posterior of the hyper-parameters describing pressure and temperature is given as in Eq. ???. Since pressure and temperature go into the forward model as  $p/T$  they are highly correlated but the pressure is the dominant parameter, see Fig. 3.4 and D.5. Note that here we use the updated forward model  $MA_L$  and conditioned on a  $\gamma$  sample from the previously evaluated marginal posterior see Fig. 3.12.



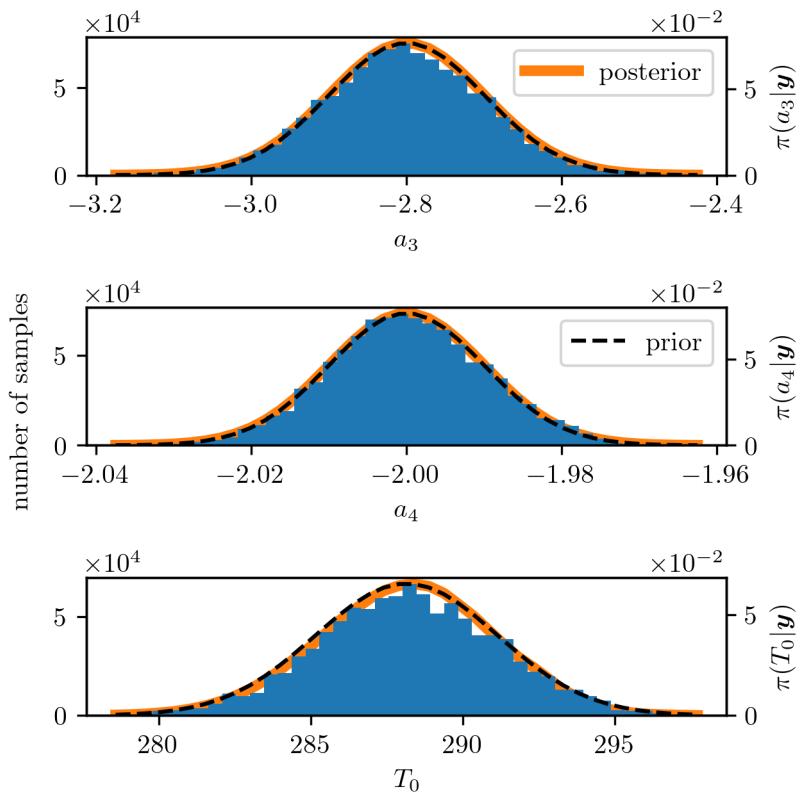
**Figure 3.16:** We plot the TT approximation of marginal posterior in orange and the samples as a histogram as well as the prior distribution with a dotted line.



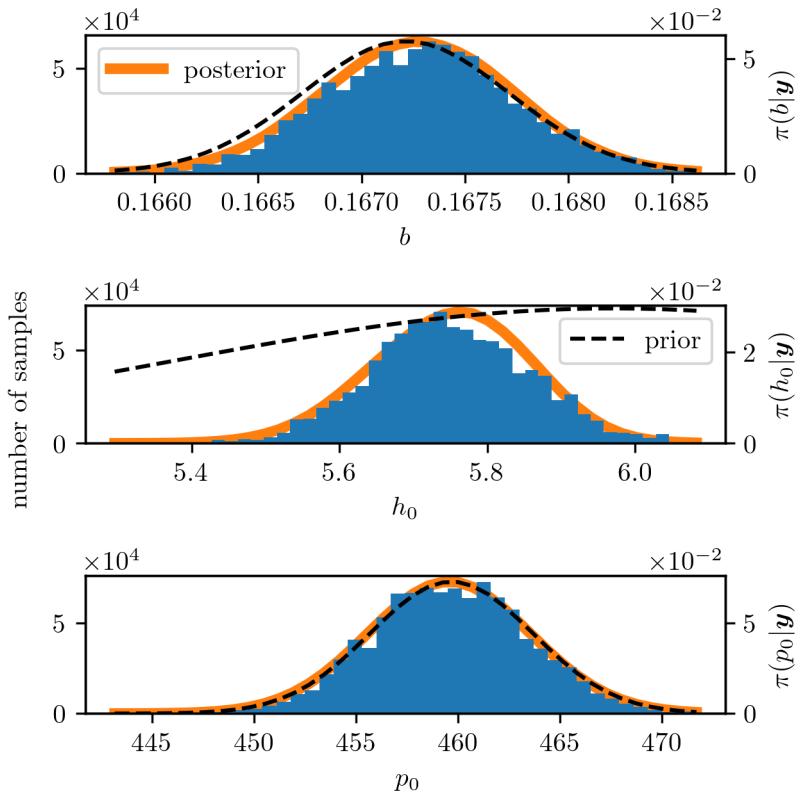
**Figure 3.17:** We plot the TT approximation of marginal posterior in orange and the samples as a histogram as well as the prior distribution with a dotted line.



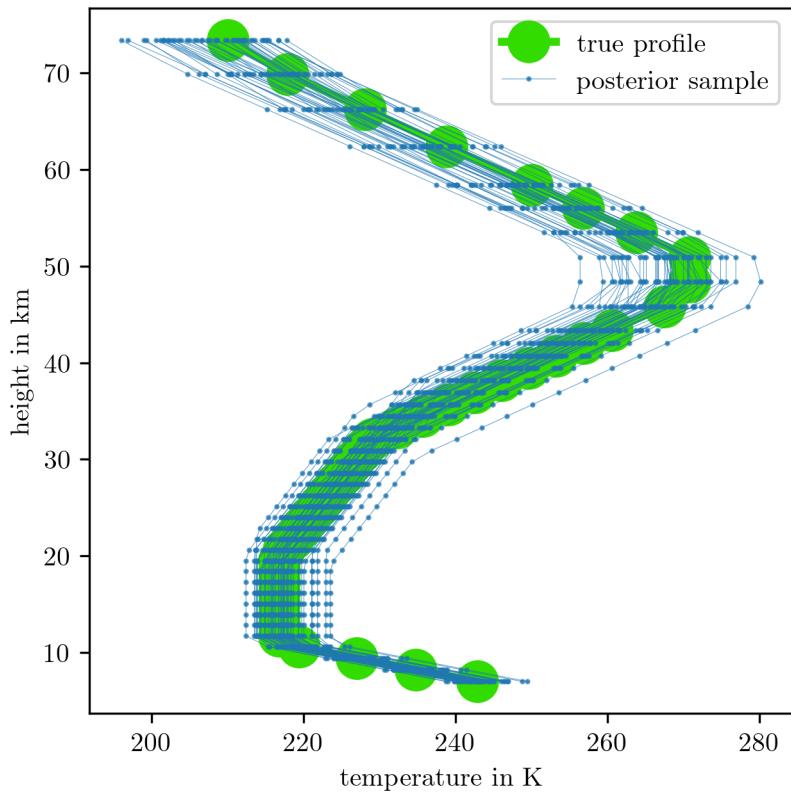
**Figure 3.18:** We plot the TT approximation of marginal posterior in orange and the samples as a histogram as well as the prior distribution with a dotted line.



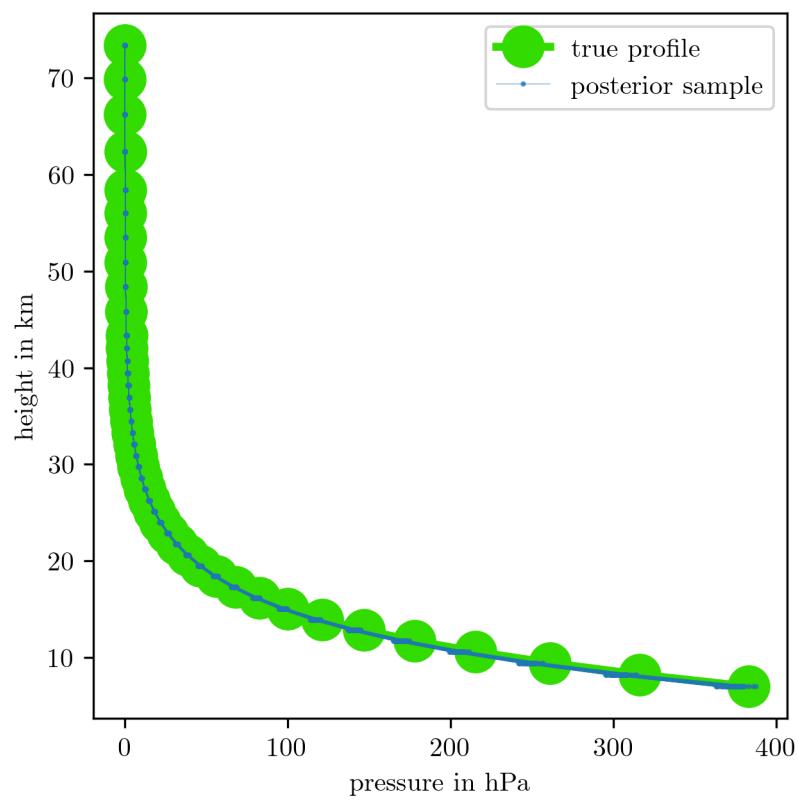
**Figure 3.19:** We plot the TT approximation of marginal posterior in orange and the samples as a histogram as well as the prior distribution with a dotted line.



**Figure 3.20:** We plot the TT approximation of marginal posterior in orange and the samples as a histogram as well as the prior distribution with a dotted line.



**Figure 3.21:** We take samples from the posterior distribution, as plotted in Figures 3.16 to 3.19 and plot the corresponding temperature function, see Eq: 3.3.



**Figure 3.22:** We take samples from the posterior distribution, as plotted in Fig. 3.20 and plot the corresponding pressure function, see Eq: 3.11.



# Appendices



# A

## Additional MCMC analysis

- integrated autocorrelation time, cite Ulli Wolf [36] python and matlab
- acceptance rate for one D and multi D, cite roberts



# B

## Correlation Structure

In the book Gaussian Markov Random Fields [10], Rue and Held demonstrate that a strong correlation between the hyper-parameter  $\mu$  and the latent field  $\mathbf{x}$  can significantly slow down convergence when using samplers, in particular Gibbs samplers. They consider the hierarchical model

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

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

and apply a Gibbs sampler based on the full conditional distributions

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

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

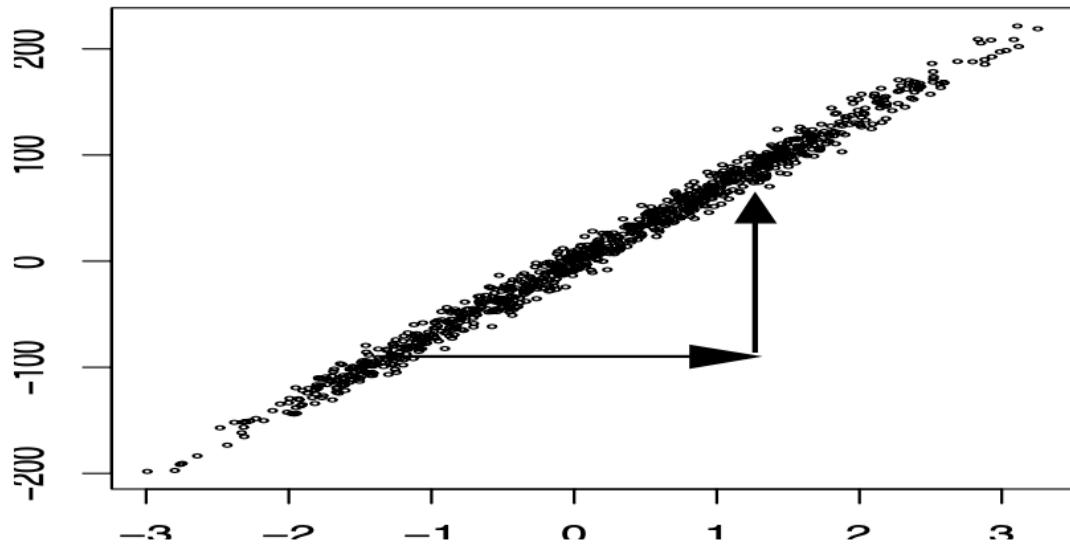
As illustrated in Figure B.1, when the sampler is restricted to steps only in the  $\mu$ -direction (horizontal axis) or the  $\mathbf{x}$ -direction (vertical axis), it requires many iterations to adequately explore the parameter space. This inefficiency arises from the high correlation between  $\mu$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

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

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

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

With a simple MCMC algorithm targeting  $\mu$  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  $\mu^*$  has been accepted.



**Figure B.1:** The figure taken from [10, Figure 4.1 (b)], shows samples from a marginal chain for  $\mu$  and  $\mathbf{1}^T \mathbf{Q} \mathbf{x}^{(k)}$  over 1000 iterations, based on the hierarchical model in Eq. B.1, with an autoregressive process encoded in  $\mathbf{Q}$ . The algorithm updates  $\mu$  and  $\mathbf{x}$  successively from their full conditional distributions. 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  $\mu$  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.

# C

## Mesure theroy

Recall the probability space  $(\Omega, \mathcal{F}, \mathbb{P})$ , where  $\Omega$  denotes the sample space, and  $\mathcal{F}$  is a collection of countable subsets  $\{A_n\}_{n \in \mathbb{N}}$  of  $\Omega$ . Each  $A_n \subseteq \Omega$  is called an event, and a map  $\mathbb{P} : \mathcal{F} \rightarrow \mathbb{R}$  is referred to as a measure. In the following, we describe the conditions required for  $\mathcal{F}$  to be a  $\sigma$ -algebra, and for  $\mathbb{P}$  to qualify as a probability measure. We refer to [37] [20] for further reading.

### C.1 probailty measure

For a probability measure, we require:

- $\mathbb{P}(\Omega) = 1$  and  $\mathbb{P}(\emptyset) = 0$
- $\mathbb{P}(A) \in [0, 1]$
- $\mathbb{P}(\bigcup_{j \in \mathbb{N}} A_j) = \sum_{j \in \mathbb{N}} \mathbb{P}(A_j)$  if we have pairwise disjoint sets or  $A_i \cap A_j = \emptyset$  for  $i \neq j$

In other words, the probability assigned to the entire sample space must be equal to one,  $\mathbb{P}(\Omega) = 1$ , and the probability of the empty set must be zero,  $\mathbb{P}(\emptyset) = 0$ . For any subset  $A \subseteq \Omega$ , the probability  $\mathbb{P}(A)$  must lie between zero and one, i.e.,  $\mathbb{P}(A) \in [0, 1]$ . If e.g. two subsets  $A$  and  $B$  are disjoint (i.e.,  $A \cap B = \emptyset$ ), then the probability of their union satisfies  $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B)$ . This property must also hold for a countable sequence of disjoint sets  $\{A_j\}_{j \in \mathbb{N}}$ , such that  $\mathbb{P}\left(\bigcup_{j \in \mathbb{N}} A_j\right) = \sum_{j \in \mathbb{N}} \mathbb{P}(A_j)$ .

## C.2 $\sigma$ -algebra

A collections of subsets  $\mathcal{F}$  is called  $\sigma$ -algebra if:

- $\emptyset, \Omega \in \mathcal{F}$ ,
- if  $A \in \mathcal{F}$  then  $A^C := A/\Omega \in \mathcal{F}$
- if  $A_1, A_2, \dots \in \mathcal{F}$  then  $\bigcup_{j \in \mathbb{N}} A_j \in \mathcal{F}$

In other words, the empty set  $\emptyset$  and the entire sample space  $\Omega$  must always be elements of  $\mathcal{F}$ . If a set  $A \in \mathcal{F}$ , then its complement  $A^C = \Omega \setminus A$  must also be in  $\mathcal{F}$ . If, in terms of a probability measure, we are able to assign a probability  $\mathbb{P}(A)$  to an event  $A$ , we must also be able to assign a probability to the event “not  $A$ ”, i.e.,  $\mathbb{P}(A^C)$ . Finally, if a countable collection of sets  $A_1, A_2, \dots \in \mathcal{F}$ , then their union  $\bigcup_{j \in \mathbb{N}} A_j$  must also be in  $\mathcal{F}$ . These three properties define the requirements for  $\mathcal{F}$  to be a  $\sigma$ -algebra.

# D

prior modelling

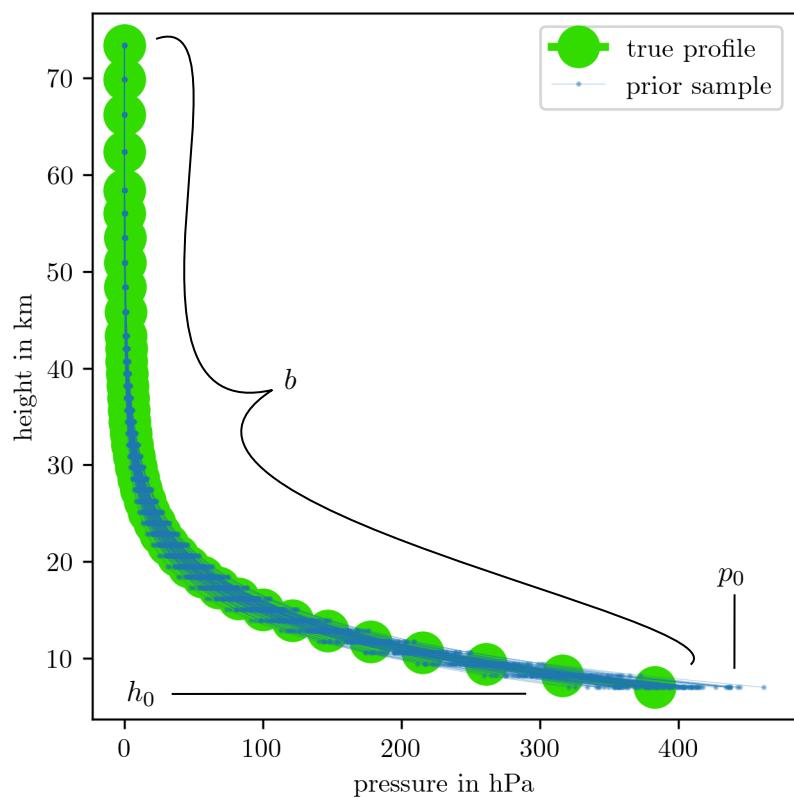


Figure D.1

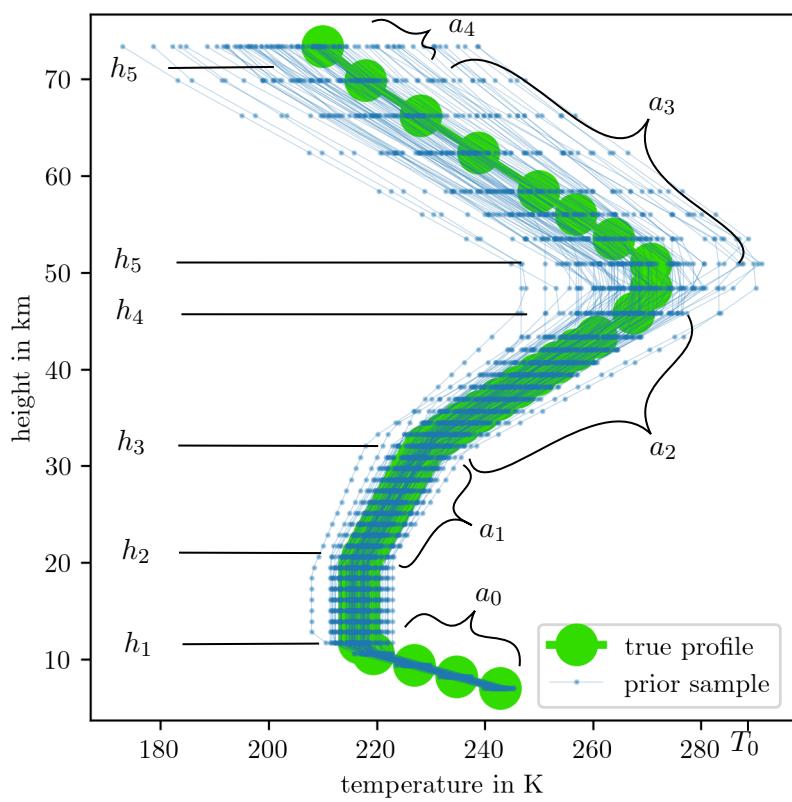


Figure D.2

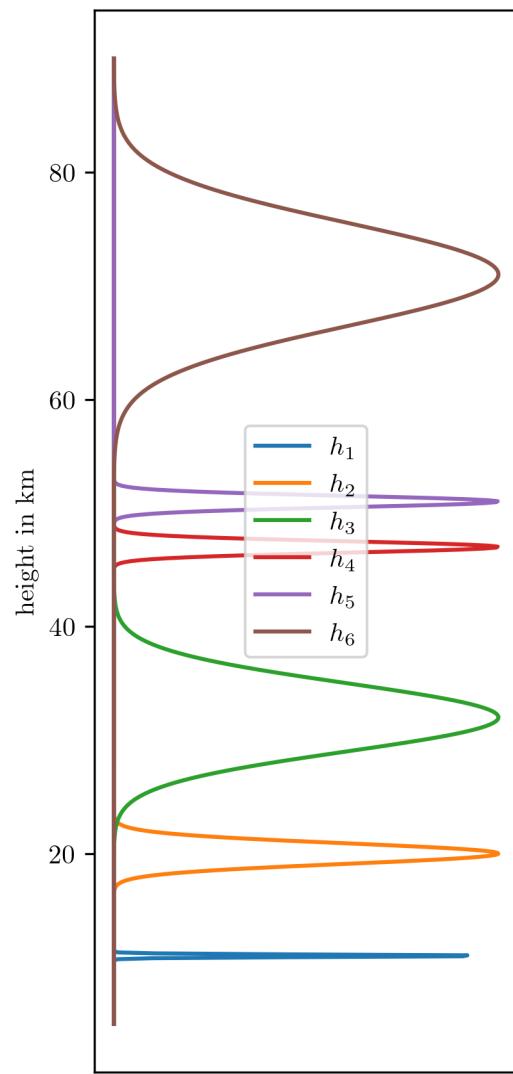
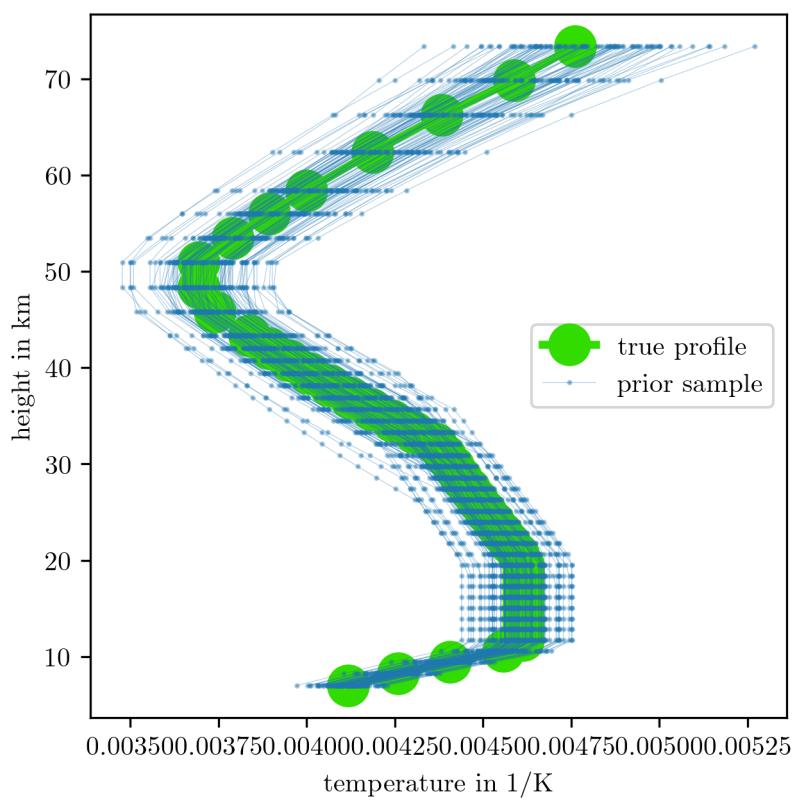


Figure D.3

**Figure D.4**

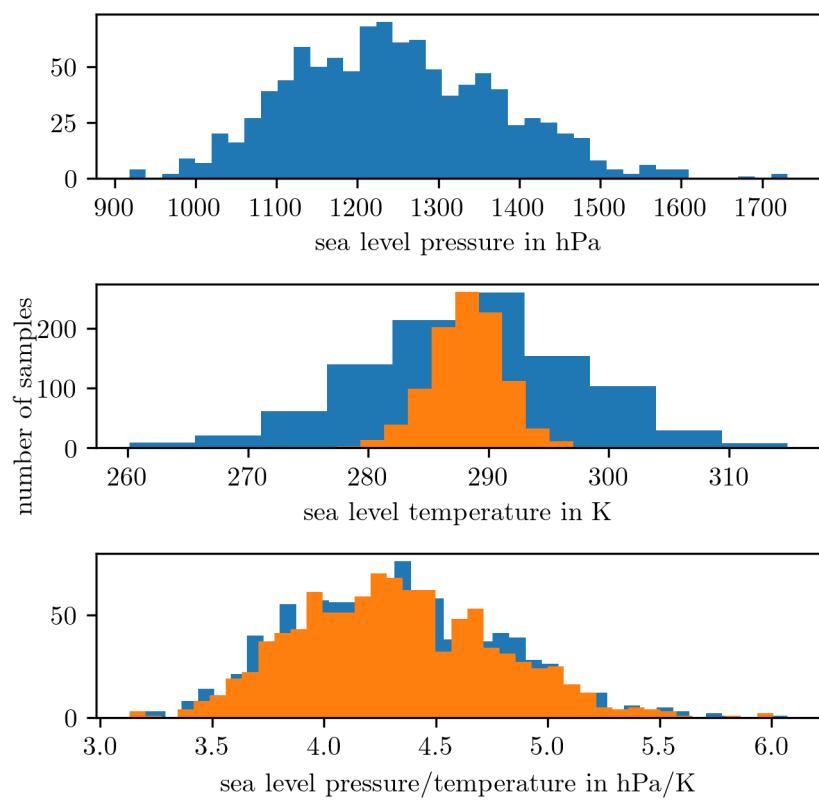


Figure D.5



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