Weierstraß-Institut
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Bayesian inversion with a hierarchical tensor representation

Martin Eigel[1], Manuel Marschall[1], Reinhold Schneider[2]

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[1] Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: martin.eigel@wias-berlin.de
manuel.marschall@wias-berlin.de

[2] TU Berlin
Straße des 17. Juni 136
10623 Berlin
Germany
E-Mail: schneidr@math.tu-berlin.de

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Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract. The statistical Bayesian approach is a natural setting to resolve the ill-posedness of inverse problems by assigning probability densities to the considered calibration parameters. Based on a parametric deterministic representation of the forward model, a sampling-free approach to Bayesian inversion with an explicit representation of the parameter densities is developed. The approximation of the involved randomness inevitably leads to several high dimensional expressions, which are often tackled with classical sampling methods such as MCMC. To speed up these methods, the use of a surrogate model is beneficial since it allows for faster evaluation with respect to calibration parameters. However, the inherently slow convergence can not be remedied by this. As an alternative, a complete functional treatment of the inverse problem is feasible as demonstrated in this work, with functional representations of the parametric forward solution as well as the probability densities of the calibration parameters, determined by Bayesian inversion.

The proposed sampling-free approach is discussed in the context of hierarchical tensor representations, which are employed for the adaptive evaluation of a random PDE (the forward problem) in generalized chaos polynomials and the subsequent high-dimensional quadrature of the log-likelihood. This modern compression technique alleviates the curse of dimensionality by hierarchical subspace approximations of the involved low rank (solution) manifolds. All required computations can be carried out efficiently in the low-rank format. A priori convergence is examined, considering all approximations that occur in the method. Numerical experiments demonstrate the performance and verify the theoretical results.

1. Introduction

Mathematical models in engineering and science applications are typically characterized by calibration parameters, which are uncertain due to incomplete knowledge. It hence is a common task to identify these parameters based on noisy and incomplete measurement data related to the system response. For this, the response of the model is evaluated with different parameter realizations ("exitations"), a functional of which is used to adjust the guess for the parameters. This so-called inverse problem of identification has been tackled with a variety of methods. In a deterministic setting, the problem is ill-posed in the sense of Hadamard and has to be regularized in some way in order to become solvable. As an alternative approach, we are concerned with the Bayesian setting in which the parameters are considered as random variables. The aim then is to determine the posterior density subject to measurements corrupted by some predetermined noise assumption. With this Bayesian notion of the task, the problem is regularized in the sense that a posterior probability distribution can be obtained.

Computational methods for the efficient evaluation of (the expectation of) the parameter densities have received considerable interest in recent years, in particular as part of the research efforts in the field of Uncertainty Quantification (UQ). The most widely used methods are based on statistical sampling from the posterior measure, namely Monte Carlo (MC) type algorithms such as the popular Markov-Chain Monte Carlo method (MCMC). While these methods are well-understood analytically and are relatively simple to implement, a major drawback is the inherently slow convergence, which is limited by the convergence order $1/2$ of MC methods. Since for each sampling of the Markov chain a realization of the governing equation has to be computed, these methods can quickly become very costly computationally.

For the solution of random forward problems, significant progress could be witnessed over the last decade. In particular methods which aim at the construction of an adequate surrogate model were shown to potentially converge at much higher rates than classical MC methods. These findings are also supported by recent analytical results regarding the sparsity of the solution manifold. In addition to a priori results, adaptive algorithms can be derived which steer the problem-dependent adjustment of the discretization parameters based on some a posteriori error indicator or even a reliable error estimator. To improve the efficiency of the Bayesian

inversion, such surrogate models, e.g. given as a functional representation in generalized chaos polynomials, can be used in combination with sampling methods.

However, also a complete functional representation of the posterior density is feasible, leading to a sampling-free method of the statistical inverse problem. For this, we employ a hierarchical tensor representation of the stochastic forward solution. Hierarchical tensor formats have only recently been investigated more thoroughly in the community of numerical mathematics, although these techniques have been used for a long time in physics and chemistry. With hierarchical tensor representations, the low-rank structure of the solution operator and the solution manifold can be fully exploited, which leads to very efficient methods for the evaluation of the system response. We make use of our previous results on adaptive stochastic Galerkin methods in tensor representations.

With a functional representation in the tensor train (TT) format at hand, we derive the representation of the Bayesian potential. Subsequently, the entire Bayesian inversion can be carried out in the low-rank approximation. To describe the posterior density, we introduce a collocation ansatz in parameter space. For the computation of the high-dimensional likelihood in tensor format, we suggest an adaptive Euler scheme.

All employed approximations, i.e. for the forward problem, the tensor exponential and the polynomial interpolation of the probability densities, can be estimated a priori. With this, we provide a convergence analysis of the posterior measure in the Hellinger distance.

The structure of this work is as follows: Section 2 reviews the Bayesian setting and introduces the used notation. Moreover, the parametric model problem is defined. Section 3 is concerned with hierarchical tensor formats, which form the basis for the derived method. As a special case, the popular TT format is introduced and functional representations with this format are discussed. Key to this work is the low-rank approximation of the Bayesian potential using an adaptively computed stochastic Galerkin solution of the parametric problem. In order to carry out the Bayesian inversion, the evaluation of the likelihood makes use of an adaptive Euler method for which numerical observations are presented. These preparations are culminated in Section 4 where the Bayesian inversion in the hierarchical tensor representation is described. Section 5 is devoted to the derivation of an a posteriori convergence result for the Bayesian posterior, taking into account all occurring approximations. The concluding Section 6 demonstrates the performance of the proposed novel approach.

2. Bayesian Inversion of Operator Equations

2.1. **Bayes setup.** We consider a class of operator equations depending on some uncertain datum u taking values in a separable Banach space $\tilde{X}$. The datum u, which for instance is a random coefficient field in a PDE, is determined by a countable infinite set of parameters $y = (y_j)_{j\in\mathbb{N}}$. By the observation of the system response δ in the separable Banach space Y, the goal is to gain knowledge about the unknown u by means of Bayesian estimation with respect to some prior measure π_0 on a full measure subset of $X \subset \tilde{X}$. The measurement data is corrupted by Gaussian noise $\eta \sim N(0, \Gamma)$ on Y. We assume that Y is finite-dimensional and the covariance operator Γ is non-degenerate, i.e. $Y \subseteq \mathbb{R}^K$ for $K < \infty$ noisy measurements. $\mathcal{O} = (o_1, \dots, o_K)^T \in (\mathcal{X}')^K$ models the observation at K sensors including estimated noise from model and measurement errors such that

$$\delta = (\mathcal{O} \circ G)(u) + \eta. \tag{2.1}$$

Assume a "forward" response operator $G : X \to \mathcal{X}$ mapping from a separable Banach space X of uncertain distributed parameters u into the reflexive Banach space of responses $\mathcal{X}$. The spaces are equipped with the norms $\|\cdot\|_X$ and $\|\cdot\|_{\mathcal{X}}$, respectively.

As model response, we consider solutions of the linear operator equation

$$\text{Given } u \in X,\ f \in \mathcal{Y}' \quad \text{find} \quad q \in \mathcal{X} \quad \text{s.t.} \quad A(u)q = f \tag{2.2}$$

with a uniformly boundedly invertible random linear operator $A(u) \in \mathcal{L}(\mathcal{X}, \mathcal{X}')$ with respect to the random data $u \in X$ sufficiently close to the expectation $\langle u \rangle$. With known forcing $f \in \mathcal{X}'$, the response of (2.2) is given by

$$X \ni u \mapsto q(u) := G(u, f) =: G(u) = (A(u))^{-1} f \in \mathcal{X}. \tag{2.3}$$

(2.2) is referred as the *forward* problem throughout this article. The main goal of this work is to solve the *backward* problem

$$\text{Given } \delta = (\mathcal{O} \circ G)(u) + \eta \colon X \to L^2_\Gamma(\mathbb{R}^K) \quad \text{find} \quad u \in X. \tag{2.4}$$

$L^2_\Gamma(\mathbb{R}^K)$ denotes the *weighted* space of square integrable functions over $\mathbb{R}^K$ equipped with the norm

$$\|v\|^2_\Gamma := \langle v, v \rangle_\Gamma = \langle v, \Gamma^{-1} v \rangle \tag{2.5}$$

where $\langle \cdot, \cdot \rangle$ is the Euclidean inner product in $\mathbb{R}^K$ and Γ is the symmetric positive definite covariance matrix of the noise η.

As a deterministic problem, (2.4) is usually ill-posed, e.g. due to the possible dimension gap between the solution space and the measurement space. Interpreting the involved objects as random variable over some probability space, solvability can be deduced by the theorem of Bayes.

As a measure to quantify the probability of u given δ, we introduce a likelihood model by

$$L \colon \mathcal{B}(\mathbb{R}^K) \times X \to [0, 1]. \tag{2.6}$$

The likelihood explains how well the uncertain data u fits the measurements δ. For any set $E \in \mathcal{B}(\mathbb{R}^K)$ and with the Lebesgue density of η denoted by ϱ, a convenient choice is

$$L(E|u) = \mathbb{P}(\delta \in E|u) = \int_E (\delta - (\mathcal{O} \circ G)(u)) \varrho \, \mathrm{d}\delta. \tag{2.7}$$

The joint random variable (u, δ) is distributed according to the joint (possibly non product) measure μ. For $\tilde{E} \in \mathcal{B}(X \times \mathbb{R}^K)$ it is given by

$$\mu(\tilde{E}) := \int_X \int_{\mathbb{R}^K} \mathbb{1}_{\tilde{E}}(u, \delta) L(\, \mathrm{d}\delta|u) \pi_0(\, \mathrm{d}u), \tag{2.8}$$

where π_0 is a *prior* measure on the uncertain data u, containing à priori information about the unknown with $\pi_0(X) = 1$. The suitable choice of the prior is a challenging task and depends on the effective problem.

The sought posterior measure π_δ describes the distribution of u given δ. It follows from conditioning the joint measure to the $\mathbb{R}^K$-fibre represented by the measurement vector. Usually, one defines the *Bayesian potential*[1] by

$$\Phi(u; \delta) := -\log \varrho(\delta - (\mathcal{O} \circ G)(u)) \tag{2.9}$$

[1] also called *misfit* or *negative log likelihood*

Theorem 2.1 (Bayes theorem)**.** *Assume that the norming factor Z satisfies*

$$Z := \int_X \varrho(\delta - (\mathcal{O} \circ G)(u))\pi_0(\,\mathrm{d}u) > 0. \tag{2.10}$$

Then, the measure of u given δ is absolutely continuous and has the Radon-Nikodym derivative with respect to π_0

$$\frac{\mathrm{d}\pi_\delta}{\mathrm{d}\pi_0}(u) = \frac{1}{Z}\varrho\left(\delta - (\mathcal{O} \circ G)(u)\right) = \frac{1}{Z}\exp(-\Phi(u;\delta)). \tag{2.11}$$

Since we have chosen η to be a centered Gaussian noise, there exists an explicit expression of the Bayesian posterior in (2.11). Using that the translation of a $\mathcal{N}(0,\Gamma)$ random variable by $(\mathcal{O} \circ G)(u)$ is distributed according to $\mathcal{N}((\mathcal{O} \circ G)(u),\Gamma)$, we obtain

$$\Phi(u;\delta) = \|\delta - (\mathcal{O} \circ G)(u)\|_\Gamma^2 = \frac{1}{2}\langle \delta - (\mathcal{O} \circ G)(u), \Gamma^{-1}(\delta - (\mathcal{O} \circ G)(u))\rangle. \tag{2.12}$$

Remark 2.2. In general, Bayes theorem requires the measurability of the potential Φ. In our setting, this fact follows immediately by using the local Lipschitz property of the forward operator and the continuity of the observation operator.

Remark 2.3. To show the positivity of the normalization constant Z in (2.11), we need boundedness of $\Phi(u;y)$, which can directly be deduced from the boundedness of $(\mathcal{O} \circ G)(u)$ in $\mathbb{R}^K$ and the η-almost sure finiteness of δ. Hence, the potential is bounded in X by some constant $C(\delta) = C < \infty$ and it follows that

$$Z = Z(y) = \int_X \exp(-\Phi(u;\delta))\pi_0(\,\mathrm{d}u) \geq \int_X \exp(-C)\pi_0(\,\mathrm{d}u) = \exp(-C) > 0. \tag{2.13}$$

2.2. **Connection to Deterministic Regularized Optimization.** The Bayesian approach is a tool to ensure solvability of usually non well-posed problems. From the optimization perspective, the problem (2.4) is intuitively solved by minimizing a least squares functional. This deterministic approach suffers from the possible non-uniqueness of the solution and probably high sensitivity of the data δ. A widely used technique to overcome this issue is by introducing a penalty or constraint term to regularize the optimization.

In this outlook we will show that minimizing a regularized minimizing problem is equivalent to calculating the Bayesian potential.

Assume there is a complete orthonormal system $(b_j)_{j\geq 1}$ on $\mathcal{X}$ which yields the expression

$$(\mathcal{O} \circ G)(u) = \mathcal{O}(\sum_{k\geq 1} \alpha_k b_k) = B^T\alpha, \quad B = [o_j(b_k)]_{k,j} \in \mathbb{R}^{\infty,K}. \tag{2.14}$$

The coefficient $\alpha = (\alpha_k)_{k\in\mathbb{N}}$ is now the unknown parameter which has to be identified. Moreover, we assume a Gaussian prior $\pi_0 = \mathcal{N}(0,\Sigma)$ for some positive definite and symmetric covariance operator Σ on X. Then, to calculate the Bayesian posterior density (2.11) with respect to π_0 we have to estimate

$$\varrho(\alpha) = e^{-\frac{1}{2}\|\delta - B^T\alpha\|_\Gamma} e^{-\frac{1}{2}\|\alpha\|_\Sigma} = e^{-(\frac{1}{2}\|\delta\|_\Gamma - \langle B\Gamma^{-1}\delta,\alpha\rangle + \frac{1}{2}\langle B\Gamma^{-1}B^T - \Sigma^{-1})\alpha,\alpha\rangle)}. \tag{2.15}$$

Then, the exponent can be expressed in a quadratic form

$$\langle Q(\alpha - \alpha_0), \alpha - \alpha_0\rangle = \langle Q\alpha,\alpha\rangle - 2\langle Q\alpha_0,\alpha\rangle + \langle \alpha_0,\alpha_0\rangle \tag{2.16}$$

for some $\alpha_0 \in \mathbb{R}$. By equating coefficients we obtain

$$Q := \frac{1}{2}(B\Gamma^{-1}B^T - \Sigma^{-1}) \tag{2.17}$$

and

$$Q\alpha_0 = B\Gamma^{-1}\delta \quad \Longleftrightarrow \quad \alpha_0 = Q^{-1}B\Gamma^{-1}\delta. \tag{2.18}$$

Completing the square yields finally

$$\varrho(\alpha) = e^{-(\langle Q(\alpha-\alpha_0),\alpha-\alpha_0\rangle + \|\delta\|_\Gamma - \langle\alpha_0,\alpha_0\rangle)} \tag{2.19}$$

The estimation of α_0 is now equivalent to minimizing the empirical loss functional

$$J(\alpha) = \frac{1}{2}\|\delta - (\mathcal{O}\circ G)(u)\|_\Gamma^2 + \frac{1}{2}\|u\|_\Sigma^2 \tag{2.20}$$

$$= \frac{1}{2}\langle \delta - B^T\alpha, \Gamma^{-1}(\delta - B^T\alpha)\rangle + \frac{1}{2}\langle\alpha, \Sigma^{-1}\alpha\rangle, \tag{2.21}$$

since by the sufficient Gaussian normal equation we obtain

$$0 = \langle \nabla J, v\rangle = -\langle B\Gamma^{-1}\delta, v\rangle + \frac{1}{2}\langle B\Gamma^{-1}B^T - \Sigma^{-1})\alpha, v\rangle. \tag{2.22}$$

This computation highlights the connection between a deterministic optimization problem using a regularization in terms of a hyperparameter Σ and the statistical Bayesian approach by considering a Gaussian prior distribution.

The main reason to express ϱ as a quadratic function in the exponent is the usability in further estimations. By introducing the substitution $\widetilde{\alpha} = \alpha - \alpha_0$ we can simplify the process of moment estimation of the forward solution $G(u)$ with respect to the posterior measure

$$\mathbb{E}_{\pi_\delta}[G(u)] = \int_X G(u)\pi_\delta = \frac{1}{Z}\int_{\ell^2(\mathbb{N})}\left(\sum_{k\geq 1}\alpha_k b_j\right)\varrho(\alpha)\,\mathrm{d}\alpha. \tag{2.23}$$

With (2.19) and the substitution we have

$$\mathbb{E}_{\pi_\delta}[G(u)] = \frac{1}{Z}\sum_{k\geq 1} b_k \int_{\ell^2(\mathbb{N})}(\alpha_{0,k} + \widetilde{\alpha}_k)e^{-\langle Q\widetilde{\alpha},\widetilde{\alpha}\rangle + \|\delta\|_\Gamma - \|\alpha_0\|}\,\mathrm{d}\alpha = B^T\alpha_0. \tag{2.24}$$

The first equation follows by splitting the integral and observing that the second term vanishes for it being the mean of a centered Gaussian distribution. And the second equation uses that probability densities have unit L^1 norm.

2.3. **Parametric uncertainty model.** Since the data of the model G depends on a countable infinite number of parameters $y = (y_1, \ldots)$, the same holds for the solution $G(u(y))$ and consequently also the Bayesian formulation in (2.11). For numerical computations to become feasible, several approximations have to be applied.

We make the representation of u more specific and assume that some set $\{\psi_j\}_{j=1}^\infty$ forms a basis of X. Moreover, $y = \{y_j\}_{j=1}^\infty$ is an independent identically distributed set of random variables with $y \sim \pi_0 = \bigotimes_{j\geq 1}\pi_0^j$. With this, we assume an unconditionally L^2-convergent expansion of the form

$$u = u(x,y) := \langle u\rangle(x) + \sum_{j\geq 1}\psi_j(x)y_j, \tag{2.25}$$

where $\langle u\rangle$ is a deterministic nominal value of u. Examples for such decompositions are the Karhunen-Loève expansion [4, Prop. 2.1.6] and [9, 15, 14], or the principal component analysis. Throughout this article we assume $y \in \Xi = [-1,1]^\infty$ which results in π_0^j being the uniform distribution on $[-1,1]$.

In the common stationary diffusion problem

$$\operatorname{div}(u(x,y))\nabla q(x,y)) = f(x) \quad \text{in } D\times\Xi \tag{2.26}$$

$$q(x,y) = 0 \quad \text{on } \partial D\times\Xi \tag{2.27}$$

the expansion (2.25) gives rise to the operator representation

$$A(y) = A_0 + \sum_{j\geq 1} A_j y_j. \tag{2.28}$$

with

$$A_j : H_0^1(D) \to H^{-1}(D), \quad v \mapsto -\operatorname{div}(\psi_j \nabla v), \quad j\in\mathbb{N}_0, \tag{2.29}$$

for $\psi_0 := \langle u\rangle$. We assume bounded invertability for every component of $(A_j)_{j\geq 1}$ such that the parametric operator equation

$$A(y)q = f \tag{2.30}$$

admits a unique solution $G(y) := G(u(y)) = A^{-1}(y)f$, see e.g. [19, Sec. 2] for details.

With these assumptions, we obtain a parametric formulation of the Bayesian posterior (2.11).

Theorem 2.4. *The Bayesian posterior π_δ of $u\in X$ given data $\delta\in\mathbb{R}^K$ is absolutely continuous with respect to the prior π_0 and it holds*

$$\frac{\mathrm{d}\pi_\delta}{\mathrm{d}\pi_0}(y) = \frac{1}{Z}\exp(-\Phi(u(y);\delta))|_{u=\langle u\rangle+\sum_{j\geq 1}\psi_j y_j}. \tag{2.31}$$

One is often interested in functionals depending on the uncertain data, so-called quantities of interest, denoted by $\varphi\colon X\to\mathbb{R}$. Common such functions are moments of u, i.e. $\varphi_m(u) = \int_X u^m \,\mathrm{d}\pi_\delta$.

Proposition 2.5. *Given a quantity of interest $\varphi\colon X\to\mathbb{R}$ and noisy data $\delta\in\mathbb{R}^K$, the Bayesian estimate takes the form*

$$\mathbb{E}_{\pi_\delta}[\varphi] = \frac{1}{Z}\mathbb{E}_{\pi_0}\Big[\exp(-\Phi(u;\delta))\varphi(u)\big|_{u=\langle u\rangle+\sum_{j\geq 1}\psi_j y_j}\Big]. \tag{2.32}$$

2.4. **Dimension Truncation and Forward Operator Approximation.** For practical computations, the infinite expansion (2.25) has to be truncated to a finite number $M<\infty$ of terms, which results in the *truncated, parametrized forward solution*

$$G^M\colon \Xi\to\mathcal{X}, \quad (y_1,\dots,y_M,0,\dots)\mapsto G\Big(\langle u\rangle + \sum_{j=1}^M \psi_j y_j\Big). \tag{2.33}$$

The error introduced by the approximation of the data can be estimated as follows, see [17, Prop. 2.2.].

Proposition 2.6. *For a sufficiently small, closed neighborhood $\widehat{X}\subset X$ of the nominal value $\langle u\rangle\in X$, we assume that the forward solution $G(u)$ is well-posed for every $u\in\widehat{X}$, i.e. $G\colon\widehat{X}\to\mathcal{X}$ is injective and continuous and the sequence $\{\|\psi_j\|_X\}_{j\geq 1}\in\ell^p(\mathbb{N})$ for some $0<p\leq 1$. Then, there exists a constant $C_{Trun}>0$ such that*

$$\sup_{y\in\Xi}\|G(y)-G^M(y)\|_{\mathcal{X}} \leq C_{Trun} M^{-\frac{1}{p}-1}. \tag{2.34}$$

If not stated otherwise, we assume that the forward operator is approximated by a Galerkin finite element solution, which admits a well-known quasi-optimality result.

Proposition 2.7 ([17] Prop 2.3)**.** *Let $\{\mathcal{X}_h\}_{h>0} \subset \mathcal{X}$, be a sequence of finite dimensional subspaces. Then, given solvability of the forward problem corresponding to G, for every $y \in \Xi$ there exists the Galerkin approximation $G^h(y)$ to $G(y)$. Furthermore, it converges quasi optimally, i.e., there exists a constant $C_{Gal} > 0$ independent of h and y such that*

$$\|G(y) - G^h(y)\|_{\mathcal{X}} \leq C_{Gal} \inf_{0 \neq v \in \mathcal{X}_h} \|G(y) - v\|_{\mathcal{X}}. \tag{2.35}$$

Moreover, assume a sequence of subspaces $\{\mathcal{X}_t\}_{t>0} \subset \mathcal{X}$ with $\mathcal{X}_{t_2} \subset \mathcal{X}_{t_1}$ for $t_1 < t_2$, scaling regularity, and $G(y) \in \mathcal{X}_t$. Then,

$$\|G(y) - G^h(y)\|_{\mathcal{X}} \leq C_{Gal} h^t \sup_{y \in \Xi} \|G(y)\|_{\mathcal{X}_t}. \tag{2.36}$$

Remark 2.8. The regularity denoted by the subspace $\mathcal{X}_t$ usually corresponds to a faster decay rate of the basis $\{\psi_j\}_{j\geq 1}$ and can be seen as a Sobolev scale, for example $\mathcal{X}_t = H^{1+t}(D)$.

Remark 2.9. From Propositions 2.6 and 2.7 we can deduce a combined error bound for the forward operator,

$$\|G(y) - G^{h,M}(y)\|_{\mathcal{X}} \leq C_{\mathrm{Trun,Gal}}(h^t + M^{-\frac{1}{p}-1}), \quad y \in \Xi. \tag{2.37}$$

3. Hierarchical Tensor Formats

Representation of multivariate functions in a geometric tensor setting was introduced in [12] and we relate mainly on the article [21]. By introducing the notion of hierarchical tensor networks we build up the setting for the Bayesian inversion using tensor trains, a subclass of hierarchical tensors. To systematically present the idea of hierarchical tensor product spaces one usually relay on the definition of dimension partition trees. For a given topological tensor space $\bigotimes_{m=1}^{M} \mathcal{V}_m$ and an element $\mathbf{V}$ of it define $\mathbb{T} \subset \mathcal{F}(\{1, \dots, M\})$, a subset of the powerset of the index set, as *dimension partition tree* with the following properties

1 The root $\alpha^* := \{1, \dots, M\}$ corresponds to the full index set.
2 Every *node* $\alpha \in \mathbb{T}$ is either a *leaf*, i.e. $|\alpha| = 1$ or there exists $\alpha_1, \alpha_2 \in \mathbb{T}$ such that $\alpha = \alpha_1 \cup \alpha_2$ and $\alpha_1 \cap \alpha_2 = \emptyset$.

This construction is used for binary trees and gives direct access to the length of the tree and suitable traversal techniques. Connecting to every node $\alpha \in \mathbb{T}\backslash\{\alpha^*\}$ with sons α_1, α_2 a subspace $\mathcal{U}_\alpha \subset \bigotimes_{j\in\alpha} \mathcal{V}_j$ of dimension r_α using the nestedness property

$$\mathcal{U}_\alpha \subset \mathcal{U}_{\alpha_1} \otimes \mathcal{U}_{\alpha_2}, \quad \alpha \in \mathbb{T}\backslash\{\widehat{\alpha} \colon \widehat{\alpha} \text{ is a leaf or the root}\} =: \widehat{\mathbb{T}}, \tag{3.1}$$

we recursively construct the corresponding basis $\{U^\alpha[\cdot, k_\alpha] \colon k_\alpha = 1, \dots, r_\alpha\}$ of $\mathcal{U}_\alpha$ by

$$U^\alpha[x_\alpha, k_\alpha] = \sum_{k_1=1}^{r_{\alpha_1}} \sum_{k_2=1}^{r_{\alpha_2}} B^\alpha[k_1, k_2, k_\alpha] U^{\alpha_1}[x_{\alpha_1}, k_1] U^{\alpha_2}[x_{\alpha_2}, k_2], \quad \alpha \in \widehat{\mathbb{T}}. \tag{3.2}$$

Here, B^α is an order three coefficient tensor. With $\mathcal{U}_{\alpha^*} = \mathcal{U}_{\alpha_1^*} \otimes \mathcal{U}_{\alpha_2^*}$, we can find a basis representation with respect to the according subspaces

$$\mathbf{V}[\mathbf{x}_{\alpha^*}] = \sum_{k_1=1}^{r_{\alpha_1^*}} \sum_{k_2=1}^{r_{\alpha_2^*}} B^{\alpha^*}[k_{\alpha_1^*}, k_{\alpha_2^*}, k_\alpha] U^{\alpha_1^*}[x_{\alpha_1^*}, k_{\alpha_1^*}] U^{\alpha_2^*}[x_{\alpha_2^*}, k_{\alpha_2^*}]. \tag{3.3}$$

Expanding this structure recursively using (3.2) one obtains a tree network structure which depicts a multi-linear low-rank subspace approximation. See [2] for more details. To make the essential point, we need only the component tensors (here of order 3) $B^{\alpha^*}[k_{\alpha_1^*}, k_{\alpha_2^*}, k_\alpha]$, $\alpha \in \mathbb{T}$. Depending on the ranks r_α this format gives rise to efficient algorithms. The overall

storage reduces to the order three component tensor tuple $(B^\alpha)_{\alpha\in\mathbb{T}}$ which, in contrast to e.q. the Tucker format, does not scale exponentially in the dimension. Moreover, linear algebra operation can be carried out with a similar but slightly larger complexity.

3.1. **Tensor Train Format.** A popular subclass of the hierarchical tensors introduced above is the tensor train (TT) format. It corresponds to a degenerated, unsymmetric tree, where for every $\alpha \in \widehat{\mathbb{T}}$ we have $\alpha := \{1,\dots,j\} = \{1,\dots,,j-1\}\cup\{j\} = \alpha_1 \cup \alpha_2$ with $\alpha_1 \in \widehat{\mathbb{T}}$ and α_2 is a leaf. Its parametrized form renders it simpler to handle while maintaining the main features of more general hierarchies, see [2] and [10, Sec. 11]. Historically, this format has been known for a long time in quantum chemistry and physics under the name of *matrix product states* (MPS). The TT format became known to a broader community in applied mathematics by recent publications such as [18, 11] and [22]. We provide a brief overview in what follows. In the sequel, we will write for the nodes of the tree $\{1,\dots,j\}$ simply j.

Let $\mathcal{V}_1,\dots,\mathcal{V}_M$ be real Hilbert spaces and consider $\mathbf{V} \in \bigotimes_{m=1}^M \mathcal{V}_m$ an element in the topological tensor product of function spaces $\mathcal{V}_i$ depending on the variable x_i. We say $\mathbf{V}$ is in TT-format if there exists a rank vector $\mathbf{r} = (r_1,\dots,r_M) \in \mathbb{N}^M$ such that $\mathbf{V}$ admits the representation

$$\mathbf{V}[x_1,\dots,x_M] = \sum_{k_1=1}^{r_1} \cdots \sum_{k_{M-1}=1}^{r_{M-1}} V_1[k_1,x_1]V_2[k_1,x_2,k_2]\cdots V_M[k_{M-1},x_M] \tag{3.4}$$

with *core* matrices $V_j[x_j] := (V_j[k_{j-1},x_j,k_j])_{k_{j-1},k_j} \in \mathbb{R}^{r_{j-1},r_j}$ and $r_0 = r_M = 1$ by construction. Hence, every entry of $\mathbf{V}$ can be determined by the matrix product

$$\mathbf{V}[x_1,\dots,x_M] = V_1[x_1]\cdots V_M[x_M]. \tag{3.5}$$

The key element to construct the TT format is the *higher order singular value decomposition* [18, Thm 2.1]. We will shortly discuss the algorithm of obtaining a TT representation and afterwards we point out the possibility to reduce the obtained complexity by truncation.

We describe this procedure for the finite-dimensional case. Given a tensor $\mathbf{U} \in \bigotimes_{m=1}^M \mathbb{R}^{n_m}$ and multi-rank $\mathbf{r} = (r_1,\dots,r_M)$ consider the unfolding matrix

$$A_k := \mathbf{U}(\mu_1,\dots,\mu_k;\mu_{k+1},\dots,\mu_M) \tag{3.6}$$

corresponding to a numerical reshape of the tensor. By assumption of $\mathbf{U}$ admitting a TT-representation, the unfolding A_1 of $\mathbf{U}$ has rank r_1. Hence, there exists the QR decomposition $A_1 = QR^T$

$$A_1[\mu_1;\mu_2,\dots,\mu_M] = Q[\mu_1]R[\mu_2,\dots,\mu_M] = \sum_{\alpha_1=1}^{r_1} Q[\mu_1,\alpha_1]R[\alpha_1,\mu_2,\dots,\mu_M]. \tag{3.7}$$

Expressing $R = A_1^T Q(Q^TQ)^{-1} =: A_1^T G_1$ we obtain

$$R[\mu_1,\mu_2,\dots,\mu_M] = \sum_{\alpha_1=1}^{r_1} \mathbf{U}[\alpha_1,\mu_2,\dots,\mu_M]G_1[\mu_1,\alpha_1]. \tag{3.8}$$

By construction of the unfolding matrices of $\mathbf{U}$ one can deduce that rank $R_k \le r_k$. Thus, the process can be repeated inductively for the next index (α_1,μ_2) to obtain the remaining cores $G_k(\alpha_{k-1},\mu_k,\alpha_k)$ for $k = 2,\dots,M$, giving the TT representation

$$\mathbf{U}[\mu_1,\dots,\mu_M] = \sum_{\alpha_1,\dots,\alpha_{M-1}}^{r_1,\dots,r_{M-1}} G_1[\mu_1,\alpha_1]G_2[\alpha_1,\mu_2,\alpha_2]\dots G_M[\alpha_{M-1},\mu_M]. \tag{3.9}$$

Replacing the QR decomposition in the construction with a singular value decomposition $A_1 = U\Sigma V^T$ with $\Sigma = \operatorname{diag}(\sigma_1,\dots,\sigma_{r_1})$ containing the singular values of A_1, we can replace

Σ by some $\Sigma_s = \operatorname{diag}(\sigma_1, \dots, \sigma_s)$ for $s \leq r_1$. This truncation (hard thresholding) yields an approximation to A_1 which is optimal in the Frobenius norm of matrices. This thresholding algorithm can be used to *round* a tensor to some prescribed rank and granting numerical feasibility. Nevertheless, this process is an approximation and the error must be controlled. For a more rigorous treatment we refer to [2, sec. 3.7]

An error bound for the approximation with a rank-$\mathbf{r}$ tensor is given by the next lemma.

Lemma 3.1 ([18] Cor. 2.4)**.** *Given a tensor $\mathbf{U} \in \bigotimes_{m=1}^{M} \mathbb{R}^{n_m}$ and a rank vector $\mathbf{r}$, there exists an approximation $\mathbf{V}$ of $\mathbf{U}$ with maximal rank $\mathbf{r}$. The approximation can be obtained by the* Higher Order Singular Value Decomposition *(HOSVD) and it holds*

$$\|\mathbf{U} - \mathbf{V}\|_F \leq \sqrt{M-1}\|\mathbf{U} - \mathbf{V}^*\|_F, \tag{3.10}$$

where $\mathbf{V}^*$ is the best approximation of $\mathbf{V}$ with bound ranks $\mathbf{r}$ and $\|\cdot\|_F$ denotes the Frobenius norm, which is the square root of the sum of square magnitudes of the tensor elements.

Proof. The existence follows immediately by the sequential closedness of the fixed rank manifolded spanned by all TT tensors of some prescribed multi-rank and the quasi-optimally bound is the result of the reiterated singular value decomposition and its optimality for matrices. □

Remark 3.2. The storage complexity for a tensor in the tensor train format can be estimated by

$$\mathcal{O}(nr^2d). \tag{3.11}$$

where $n = \max\{n_i : i \in \{1, \dots, d\}\}$, $r = \max\{r_i : i \in \{1, \dots, d-1\}\}$. Hence, the exponential growth with the number of dimensions (curse of dimensionality) can be reduced to a polynomial complexity.

Remark 3.3. The *Hadamard* product of two TT-tensors $\mathbf{U}$ and $\mathbf{V}$ is the element-wise multiplication in the full tensor representation, and can be extended easily to the infinite-dimensional setting of multivariate continuous functions where it is the point-wise multiplication. It is defined by

$$\mathbf{C}[x_1, \dots, x_M] = \mathbf{U}[x_1, \dots, x_M] \circ \mathbf{V}[x_1, \dots x_M]. \tag{3.12}$$

The Hadamard product is a binary operation between two tensors, e.g. two TT tensors. When applying this operation in the TT-format, the resulting TT-tensor has a rank which is at most the product of the individual representation ranks,

$$\begin{aligned}\mathbf{C}[x_1, \dots, x_M] &= U_1[x_1] \cdots U_M[x_M] V_1[x_1] \cdots V_M[x_M] \\ &= (U_1[x_1] \otimes V_1[x_1]) \cdots (U_M[x_M] \otimes V_M[x_M]) \\ &=: C_1[x_1] \cdots C_M[x_M].\end{aligned}$$

3.2. **Functional Representation in TT-Format.** As in [8], we employ the tensor train formalism for functional approximations of stochastic operators and functions with appropriate polynomials in the parameters. Concerning our model problem (2.26), we have to consider a basis approximation in both physical and stochastic space. We refer to the approximation of [7] in $H_0^1(D) \times \left(\bigotimes_{m=1}^{M} L^2_{\pi_m}([-1,1])\right)$ given by a polynomial basis in $L^2_{\pi_m}([-1,1])$ for the stochastic dimensions. This fact concludes the *extended* TT format, possessing a polynomial basis on the leafs of the dimension tree, instead of a general Tucker basis, i.e. $U^j[x_j, k_j] = P_{k_j}(x_j)$, where $(P_k)_{k\in\mathbb{N}}$ are the orthonormal Legendre polynomials with respect to the weighted inner product in $\langle\cdot,\cdot\rangle_{\pi_j}$ on $L^2[-1,1]$ for $j = 1, \dots, M$. For an element $\mathbf{V} \in \bigotimes_{m=1}^{M} L^2_{\pi_m}([-1,1]) =: \mathcal{Y}$, the corresponding core tensor is denote by $\tilde{\mathbf{V}}$, i.e.

$$\mathbf{V}[\mathbf{x}] = \sum_{\mu_1=1}^{\infty} \cdots \sum_{\mu_M}^{\infty} \tilde{\mathbf{V}}[\mu_1, \dots, \mu_M] \prod_{i=1}^{M} P_{\mu_i}(x_i), \quad \mathbf{x} \in \Xi^M := [-1,1]^M \tag{3.13}$$

To appropriately use the extended TT format we have to consider a finite dimensional approximation $\mathcal{P}_M(N) \subset \mathcal{Y}$ by polynomials of degree at most $N \in \mathbb{N}$ in every dimension $m = 1, \dots, M$, i.e. $\Lambda = \{(\mu_1, \dots, \mu_m) : \mu_i = 1, \dots, N\}$. Choosing an appropriate set of interpolation points $\Xi^M = \{y_{\mu_1}, \dots, y_{\mu_1} : \mu \in \Lambda\}$, the interpolation in Ξ^M follows from tensorization of the univariate Lagrange polynomials $L_\mu(y) := \prod_{m=1}^M L_{\mu_m}(y_m)$ such that $L_\mu(\hat{y}_\nu) = \delta_{\mu\nu}$ for $\mu, \nu \in \Lambda_L$ and $y \in \Xi^M$. Given some function $f : \Xi^M \to \mathbb{R}$, we define the N-th order *tensor product interpolation operator* $\mathcal{I}_N$ by a univariate interpolation basis $\mathbf{L} = (L_m)_{m=1}^N$ and collocation nodes $\hat{y}_j \in \Xi^M$, $j = 1, \dots, N$, such that for all $(x_1, \dots, x_M) \in \Xi^M$,

$$\mathcal{I}_N f(x_1, \dots, x_M) := \sum_{\mu \in \Lambda} f(\hat{y}_{\mu_1}, \dots, \hat{y}_{\mu_M}) L_{\mu_1}(x_1) \cdots L_{\mu_M}(x_M) \in \mathcal{P}_M(N). \tag{3.14}$$

Here, the multi-index set $\Lambda \subset \{0, \dots, N\}^M$ specifies the polynomial degrees used in the representation (3.14). We define the tensor

$$\mathbf{F}[\mu_1, \dots, \mu_d] := f(\hat{y}_{\mu_1}, \dots, \hat{y}_{\mu_M}) \ .$$

The interpolation operator $\mathcal{I}_N$ yields the usual error bounds [20], namely for $f \in H^s(\Xi^M)$ there exists a constant $C > 0$ such that

$$\|f - \mathcal{I}_N f\|_{\mathcal{Y}} \leq C N^{-s} \|f\|_{H^s(\Xi^M)}. \tag{3.15}$$

The error of (3.15) using the quasi best rank-$\mathbf{r}$ TT compression of $\mathbf{F}$, denoted by $\mathbf{F}^* := HOSVD(\mathbf{F})$ and the best rank-$\mathbf{r}$ TT approximation $\mathbf{F}^+$, can be bounded with the previous results (3.10) and (3.14)

$$\|f - \sum_{\mu \in \Lambda} \mathbf{F}^*[\mu] \mathbf{L}_\mu\|_{\mathcal{Y}} \leq \|f - \mathcal{I}_N f\|_{\mathcal{Y}} + \|\sum_{\mu \in \Lambda} (\mathbf{F}[\mu] - \mathbf{F}^+[\mu]) \mathbf{L}_\mu\|_{\mathcal{Y}}$$

which yields the bound

$$\|f - \sum_{\mu \in \Lambda} \mathbf{F}^*[\mu] \mathbf{L}_\mu\|_{\mathcal{Y}} \leq C(N^{-s} \|f\|_{H^s(\Xi^M)} + c_2 \sqrt{M-1} \|\mathbf{F} - \mathbf{F}^+\|_F). \tag{3.16}$$

The bound $c_2 \|\mathbf{F} - \mathbf{F}^+\|_F$ can be significantly improved by expanding $\mathcal{I}_N f$ into an ortho-normal Legendre basis instead of the interpolation basis with an ill-conditioned Gram matrix. Ths can be achieved by a rank-one transformation $\otimes_{i=1}^M T_i : \mathbf{F} \to \hat{\mathbf{F}}$. For details see section 3.4.

Remark 3.4. If we apply the Hadamard product to two tensors $\mathbf{U}, \mathbf{V}$ in the extended TT format, the resulting polynomial degree has doubled, and it is not given by the Hadamard poduct of $\tilde{\mathbf{U}}, \tilde{\mathbf{V}}$. Therefore, we approximate the Hadamar poduct of $\mathbf{U}, \mathbf{V}$, by collocation at the interpolation points, i.e. we compute

$$\mathbf{T}[\mu_1, \dots, \mu_d] := \mathbf{U}[\hat{y}_{\mu_1}, \dots, \hat{y}_{\mu_d}] \mathbf{V}[\hat{y}_{\mu_1}, \dots, \hat{y}_{\mu_d}].$$

Usage of (3.16) with $\mathbf{F} = \mathbf{U} \circ \mathbf{V}$ and $\mathbf{F}^+ = \mathbf{T}^+$ yields an error bound for the coefficient tensor Hadamard product.

3.3. **(Adaptive) Stochastic Galerkin Method.** By the introduced tensor train format and the approximation in stochastic and physical space, we present the solution of the forward problem in $\mathcal{Y} = H_0^1(D) \otimes \left(\bigotimes_{m=1}^M L^2_{\pi_m}([-1,1]) \right)$ for the model problem (2.2) using approximation in finite elements and a tensorized Legendre basis, respectively. Therefore, consider the set of finitely supported multi-indices

$$\widehat{\mathcal{F}} := \{\mu \in \mathbb{N}_0^M \ : \ |\operatorname{supp} \mu| < \infty\} \tag{3.17}$$

and for any $\Lambda \subset \widehat{\mathcal{F}}$ the family of orthogonal Legendre polynomials $(P_\mu)_{\mu\in\Lambda}$. For a given dimension vector $(d_m)_{m=1,\dots,M} \in \mathbb{N}_0^M$ we define the multi-index set

$$\Lambda := \left\{(\mu_1,\dots,\mu_M) \in \widehat{\mathcal{F}} : \ \mu_m = 0,\dots,d_m-1;\ m=1,\dots,M\right\}. \tag{3.18}$$

By that we obtain the semi-discrete space

$$\mathcal{Y}(\Lambda) := \left\{ v_\Lambda(x,y) = \sum_{\mu\in\Lambda} v_{\Lambda,\mu}(x) P_\mu(y) \ :\ v_{\Lambda,\mu} \in H_0^1(D) \right\} \subset \mathcal{Y}. \tag{3.19}$$

Discretizing $H_0^1(D)$ in conforming finite element spaces $(\mathcal{X}(\Lambda)_p)_{p\geq 1}$ by piecewise polynomials of degree p on some triangulation $\mathcal{T}$ of D yields a nodal basis $(\varphi_i)_{i=0}^{h-1}$ with $h = \dim(\mathcal{X}_p)$. The fully discrete space is given by

$$\mathcal{Y}_p(\Lambda,\mathcal{T}) := \left\{ v_h(x,y) = \sum_{\mu\in\Lambda} v_{h,\mu}(x) P_\mu(y) \ :\ v_{h,\mu} \in \mathcal{X}_p \right\} \subset \mathcal{Y}(\Lambda) \tag{3.20}$$

and the Galerkin projection of the solution of the variational problem obtained from (2.2) is the unique $G^{h,M} \in \mathcal{Y}_p(\Lambda,\mathcal{T})$ satisfying

$$\int_{\Xi^M}\int_D u(x,y)\nabla G^{h,M}(x,y)\nabla v(x,y) = \int_{\Xi^M}\int_D f(x)\nabla v(x,y) \quad \text{for all } v \in \mathcal{Y}_p(\Lambda,\mathcal{T}). \tag{3.21}$$

Hence, we get the representation

$$G^{h,M}(x,y) = \sum_{k=1}^{N}\sum_{\mu\in\Lambda} U[k,\mu]\varphi_k(x)P_\mu(y) \quad x\in D, y\in\Xi^M. \tag{3.22}$$

Using a tensor train recompression of the coefficient tensor $U \in \mathbb{R}^{N\times d_1\times\dots,d_M}$ by e.q. a HOSVD we can write in abuse of the same notation

$$\begin{aligned} G^{h,M}(x,y) &= \sum_{k=1}^{N}\sum_{\mu\in\Lambda} U[k,\mu]\varphi_k(x)P_\mu(y) \\ &= \sum_{k_1,\dots,k_{M-1}=1}^{r_1,\dots,r_{M-1}} \left(\sum_{\mu_0=0}^{d_0} U_0[\mu_0,k_1]\varphi_{\mu_0}(x)\right)\dots\left(\sum_{\mu_M=0}^{d_M} U_M[k_{M-1},\mu_M]P_{\mu_M}(y_M)\right). \\ &= U[x,y_1,\dots,y_M] = U_0[x]U_1[y_1]U_2[y_2]\dots U_M[y_M] \quad x\in D, y\in\Xi^M. \end{aligned} \tag{3.23}$$

In fact, the defining parameters M, Λ and $\mathcal{T}$ can be obtained adaptive using error estimators for the stochastic and physical space, introduced in [7] and for the TT tensor setting adapted in [8]. An example of the resulting procedure is mentioned in section 6

3.4. **Low rank approximation of the Bayesian potential.** A key point for the proposed sampling-free Bayesian approach is the explicit representation of the posterior measure (and consequently the marginals) in terms of the functional representation in the TT format as described in the preceding sections. For efficient calculations, it is paramount to carry out all evaluations in the TT format. We recall the Radon-Nikodym derivative which has to be computed subsequently,

$$\frac{\mathrm{d}\pi_\delta}{\mathrm{d}\pi_0}(u) = \frac{1}{Z}\exp(-\frac{1}{2}\langle\delta-(\mathcal{O}\circ G)(u), \Gamma^{-1}(\delta-(\mathcal{O}\circ G)(u))\rangle). \tag{3.24}$$

In actual computations, we use the approximate solution $G^{h,M}$ of the forward problem given as a multivariate polynomial representation in TT format (3.23) where the discretization parameters h and M determine the FE mesh width and the length of the parameter vector used in the

expansion of the data, respectively. Furthermore, $\hat{x} = (x_1, \dots, x_K)$ are the nodes in the physical domain D employed with the measure operator $\mathcal{O}$. The observed approximated system response $\mathcal{O} \circ G^{h,M}$ again is a TT tensor whose first core is of rank 1 and which is indexed by $k \in \{1, \dots, K\}$ denoting the physical measurement x_k,

$$(\mathcal{O} \circ G^{h,M})(\hat{x}, y) = \sum_{k_1=1}^{r_1} \cdots \sum_{k_{M-1}=1}^{r_{M-1}} \left(\sum_{k=1}^{K} U_0[k, k_1] \right) \cdots \left(\sum_{\mu_M=0}^{d_M} U_M[k_{M-1}, \mu_M] P_{\mu_M}(y_M) \right). \tag{3.25}$$

Note that this tensor object represents the stochastic solution at certain measure points $\hat{x}$ parametrized with a polynomial basis in y. This has to be considered when evaluating the inner product (3.24) in $\mathbb{R}^K$. In order to make the computation feasible and avoid handling the large product polynomial basis which would normally arise, we introduce a collocation ansatz in the parametric dimensions and then interpolate the solution. For this, we employ univariate *Chebyshev* nodes of the same order L in every dimension to obtain a full tensor grid in $\Xi^M = [-1, 1]^M$. To make the construction precise, choose $\hat{y}_{\hat{\nu}} = \cos\left(\frac{2\nu - 1}{2L}\pi\right)$ with $1 \leq \hat{\nu} \leq L$. We then evaluate the sum over every tensor core at any combination of nodes and store the results in the corresponding tensor cores,

$$(\mathcal{O} \circ G^{h,M})(\hat{x}_\ell, \hat{y}_\nu) = \sum_{k_1=1}^{r_1} \cdots \sum_{k_{M-1}=1}^{r_{M-1}} \left(\sum_{k=1}^{K} U_0[\ell, k_1] \right) \left(\sum_{\mu_1=0}^{d_1} U_1[k_1, \mu_1, k_2] P_{\mu_1}(\hat{y}_{\nu_1}) \right) \times \tag{3.26}$$

$$\times \cdots \left(\sum_{\mu_M=0}^{d_M} U_M[k_{M-1}, \mu_M] P_{\mu_M}(\hat{y}_{\nu_M}) \right) \tag{3.27}$$

$$= \sum_{k_1=1}^{r_1} \cdots \sum_{k_{M-1}=1}^{r_{M-1}} \tilde{U}_0[\ell, k_1] \tilde{U}_1[k_1, \nu_1, k_2] \cdots \tilde{U}_M[k_{M-1}, \nu_M] \tag{3.28}$$

$$= \tilde{U}_0[\ell] \tilde{U}_1[\nu_1] \cdots \tilde{U}_M[\nu_M] =: \tilde{U}[\ell, \nu_1, \dots, \nu_M], \tag{3.29}$$

for $\ell = 1, \dots, K$ and $\nu = (\nu_1, \dots, \nu_M) \in \{1, \dots, L\}^M =: \Lambda_L$. The resulting tensor of the Bayesian potential can then be evaluated pointwise at the L^M collocation nodes $\nu \in \Lambda_L$,

$$\hat{U}_L^{h,M}[\nu] := \frac{1}{2}(\delta - \tilde{U}[\cdot, \nu])^T \Gamma^{-1} (\delta - \tilde{U}[\cdot, \nu]), \tag{3.30}$$

where the Euclidean inner product (expanded in (3.23)) is calculated by the sum of the terms

$$A := \delta^T \Gamma^{-1} \delta, \tag{3.31}$$

$$B := -2\delta^T \Gamma^{-1} \tilde{U}[\cdot, \nu], \tag{3.32}$$

$$C := \tilde{U}[\cdot, \nu]^T \Gamma^{-1} \tilde{U}[\cdot, \nu]. \tag{3.33}$$

The first term A is a order and rank 1 tensor product which has to be raised to a M dimensional tensor, which is constant in the remaining dimensions. This can be carried out by taking $\tilde{A} = A \otimes e \otimes \cdots \otimes e$, where e is the vector $(1, \dots, 1)$. The matrix tensor product in the mixed term B acts only on the first core of the collocated solution. In order to avoid rank increasing operations, we do not implement the summation of the remaining vector product but instead treat the physical and stochastic dimensions separately. For this, we create a copy of the TT tensor $\tilde{U}[\cdot, \nu]$, set all entries in the first core to zero, multiply it by $K - 1$ and add the result to the already calculated $\Gamma^{-1}\tilde{U}[\cdot, \nu]$. Computationally more involved is the quadratic term C. Usually the TT-ranks add up with every summation and are multiplied with every multiplication. Hence, while increasing the number of measurements K clearly adds information to the problem,

this may also lead to a substantial growth in the tensor ranks which has to be compensated by recompression of the low-rank representation. Nevertheless, the proposed splitting of the inner product allows for a parallel computation and reduces the rank increase when compared to a straightforward approach.

The interpolation in Ξ^M follows from tensorization of the univariate Lagrange polynomials $L_\mu(y) := \prod_{m=1}^M L_{\mu_m}(y_m)$ such that $L_\mu(\hat{y}_\nu) = \delta_{\mu\nu}$ for $\mu, \nu \in \Lambda_L$ and $y \in \Xi^M$. An approximation of the Bayesian misfit function (2.12) is then given by

$$\Phi_L^{h,M}(y;\delta)\colon \Xi \to \mathbb{R}, \quad (y_1, \dots, y_M, 0, \dots) \mapsto \sum_{\mu\in\Lambda_L} \hat{U}_L^{h,M}[\mu] L_\mu(y). \tag{3.34}$$

This representation does not depend on the physical space anymore and satisfies the following property.

Lemma 3.5. *Let $\Phi^{h,M}(\cdot;\delta) \in H^s(\Xi)$, $s > 0$, be an approximation of the Bayesian potential which is Lipschitz in the first component. Given a prescribed maximal tensor rank $\mathbf{r} \in \mathbb{N}^M$, there holds*

$$\Phi_L^{h,M}(\cdot;\delta)\colon \Xi \to \mathbb{R}, \quad (y_1, \dots, y_M, 0, \dots) \mapsto \sum_{\mu\in\Lambda_L} U_L^{h,M}[\mu] \mathbf{P}_\mu(y), \tag{3.35}$$

where $(\mathbf{P}_\mu)_{\mu\in\Lambda_L} = \left(\prod_{m=1}^L P_{\mu_m}\right)_{\mu\in\Lambda_L}$ denotes the orthonormal Legendre basis of

$$\mathcal{P}(\Lambda_L) := \left\{ p(y) = \prod_{m=1}^M p_m(y_m) \,:\, y \in \Xi^M,\ p_m \text{ polynomial of degree } L \right\} \tag{3.36}$$

$$\subset L^\infty(\Xi^M), \tag{3.37}$$

and $U_L^{h,M}$ is the coefficient tensor of $\Phi_L^{h,M}$, resulting from (3.30) *with additional one dimensional basis change in every tensor core by $T = (t_{i,j})_{i,j=1,\dots,L}$ given by*

$$t_{i,i} := \langle L_i, P_j \rangle = \int_{-1}^1 L_\mu(x) P_\nu(x) \,\mathrm{d}x. \tag{3.38}$$

Furthermore, there exists a constant $C > 0$ such that

$$\|\Phi^{h,M} - \Phi_L^{h,M}\|_{L^2_{\pi_0}(\Xi)} \le C\bigg(\sqrt{M-1} \|U_L^{h,M} - U_L^{h,M*}\|_F \tag{3.39}$$

$$+ L^{-s} \|\Phi^{h,M}\|_{H^s(\Xi)} \bigg), \tag{3.40}$$

where $U_L^{h,M*}$ is the best rank-$\mathbf{r}$ approximation of the coefficient tensor $U_L^{h,M}$.

Proof. The proof is an immediate consequence of (3.16) applied to the construction of the Bayesian potential approximation. □

Remark 3.6. Note that the proposed collocation and interpolation approach is exact for $L \in \mathbb{N}$ sufficiently large, i.e. twice the maximal degree of the solution of the operator in (3.23). The Bayesian potential calculated from the tensor representation,

$$\Phi^{h,M}(y,\delta) = \|\delta - (\mathcal{O} \circ G^{h,M})(y)\|_\Gamma, \tag{3.41}$$

is a polynomial depending on the active index set $\Lambda \subset \mathcal{F}$. With this adaptively constructed set at hand, we can easily choose the collocation degree L for an exact interpolation. To make this more efficient and consider the anisotropy in the active set Λ, we can choose the collocation degree seperately in each dimension which results in a sparser non-product structure in Ξ^M.

Remark 3.7. The basis change in (3.35) can be implemented computationally robust since it contains only one dimensional basis functions.

3.5. **Exponential of a TT-Tensor.** As presented in section 3.4 we have an almost optimal functional representation of the Bayesian potential in terms of an orthonormal basis, which exhibits important properties to become a useful surrogate model. Nevertheless, we want to present a sampling free Bayesian inversion method, therefore we have to consider the remaining terms in (3.24). From a practical point of view, the exponential of the functional representation of the potential is a critical part. Obtaining a closed form representation is subject to collocation and interpolation, i.e. we take collocation nodes $\hat{y} \in \Xi^M$ and create a tensor from (3.34) analog to (3.26), which is used for multivariate interpolation using Lagrange polynomials and a rank one basis change to obtain orthonormal Legendre polynomials. This procedure needs to be consistent in the tensor train format, which additionally gives the possibility to work with tensor meshes of magnitudes unsustainable even in modern devices.

In [5] several possibilities to calculate the matrix exponential are described, which in principle could be applied in the tensor framework. We make use of the well-known fact that the exponential is the solution of a simple ordinary differential equation (ODE)

$$\frac{\mathrm{d}}{\mathrm{d}t} W(t, \hat{y}, \delta) = -W(t, \hat{y}; \delta) \circ \Phi(\hat{y}, \delta) \tag{3.42}$$

$$W(0, \hat{y}, \delta) = 1. \tag{3.43}$$

The solution to this initial value problem is given by

$$W(t, \hat{y}, \delta) = \exp(-t\Phi(\hat{y}, \delta)), \tag{3.44}$$

and $W(1, \hat{y}, \delta)$ is equivalent to the exponential of the negative Bayesian potential. It is to mention that, in abuse of notation, $\Phi(\hat{y}, \delta)$ denotes the discrete collocation tensor of the approximated potential in (3.34). Hence, the initial value problem (3.42) is a low-rank approximation of the original system interpreting the point-wise multiplication as Hadamard product. It remains to solve this ODE in tensor format. [16] explains the problem of quasi-optimal approximation on larger time-scales and gives rise to dynamical algorithms maintaining in the desired rank manifold, without the use of hard-thresholding.

3.5.1. *Runge-Kutta methods.* Numerical methods for the solution of ODEs are a classical topic [13, 3]. For our purposes, we adapt a well-known class of explicit s-stage Runge-Kutta methods to the TT-tensor framework. Runge-Kutta schemes are usually described by Butcher-Tableaus of the form

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b^T} \end{array} \tag{3.45}$$

where, in explicit approaches, $A = [a_{i,j}]$ is a strict lower-triangular $s \times s$ matrix. We cite a result for the general scheme.

Proposition 3.8. *Let $Y(t)$ be the unique solution to the initial value problem*

$$\frac{\mathrm{d}}{\mathrm{d}t} Y(t) = f(t, Y(t)), \tag{3.46}$$

$$Y(0) = Y_0. \tag{3.47}$$

Then, the approximation method given by a temporal grid $t_i = ih$*, a Butcher-Tableau* (3.45) *and the iterative procedure*

$$Y_{n+1} = Y_n + h \sum_{i=1}^{s} b_i k_i, \tag{3.48}$$

$$k_i = f\left(t_n + c_i h, Y_n + h \sum_{j=1}^{i-1} a_{i,j} k_j\right), \tag{3.49}$$

is consistent if and only if $\sum_{i=1}^{s} b_i = 1$.

Assuming an admissible rhs f, i.e. continuous in the first and Lipschitz in the second argument, we obtain convergence rates equal to the resulting consistency rate, which depends on the choice of A, b and c. Examples are the explicit Euler scheme with convergence order 1,

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}, \tag{3.50}$$

the Heun method with convergence order 2,

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}, \tag{3.51}$$

and the classical Runge-Kutta method which is convergent of order 4,

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}. \tag{3.52}$$

Remark 3.9. For our context, we only need to consider a stationary rhs f. Hence, the calculations are independent of the nodes vector c. However, the stability and convergence of the considered method still also depends on c.

For the evaluation of the Bayes potential in TT format, we have to consider (3.42) as tensor ODE and extend the iteration scheme (3.48) to TT tensors. This is formally described in Algorithm 1. Figure 1 pictures the convergence of V_{exp} for different numerical schemes. The computation was executed for a randomly created order five TT-tensor with dimensions up to 10 and ranks up to 20. The error for this plot is determined approximately by Monte-Carlo sampling of the tensor and comparison with the exact pointwise exponential. One can observe the mentioned convergence rates for the different numerical schemes. The implicit and explicit Euler display the same convergence but the implicit method yields an approximation already for less than 10 iteration steps.

Remark 3.10. Note that the tensor multiplication in line 11 has to be carried out element-wise, i.e. in the Hadamard sense. It is apparent that with regard to complexity, the iteration process is dominated by these tensor multiplications. As mentioned above, this leads to a strong increase of tensor ranks due to the multiplication of the respective ranks of the involved tensors.

Since explicit schemes are not unconditionally stable and hence may require a very small step size and many iterations, the inevitable increase of tensor ranks in each step becomes a pressing issue. To keep the scheme computationally feasible, the tensor has to be recompressed to a prescribed tolerance in each iteration.

Algorithm 1: explicit Runge-Kutta method for TT-tensors

Require: TT-tensor V, number of iterations N, maximal rank r, rounding precision ϵ, Butcher-Tableau (A, b)

$V_{exp} = (1, \dots, 1) \otimes \cdots \otimes (1, \dots, 1)$ according to dimensions and ranks of V.
for $l = 1 : N$ **do**
  if $\max$(TT-ranks of V_{exp}) $> r$ **then**
    $V_{exp} \leftarrow$ hard-thresholding to maximal rank r and precision ϵ.
  end if
  $\mathrm{summ} = 0$
  for $j = 1 : s$ **do**
    for $i = 1 : j - 1$ **do**
      $\mathrm{summ} = \mathrm{summ} + a_{i,j} k_i$
    end for
    $k_j = hf(V_{exp} + \mathrm{summ}) = hV \circ V_{exp}$
  end for
  $\mathrm{summ} = 0$
  for $j = 1 : s$ **do**
    $\mathrm{summ} = \mathrm{summ} + b_j k_j$
  end for
  $V_{exp} = V_{exp} + \mathrm{summ}$
end for
return V_{exp}

While this may become impossible with general tensors, the convenient structure of the Bayesian misfit (element-wise negative and hopefully small), this procedure turns out to be relatively stable.

3.5.2. *Adaptive step size Runge-Kutta algorithm.* Adaptivity can often greatly reduce the computational complexity while maintaining a high accuracy of the solution. We hence discuss embedded step size control of Runge-Kutta methods as described in Section 3.5.1. The main idea is to take a second Runge-Kutta approximation of higher order $q > p$ which reuses the already calculated increments k_i of the order p scheme, i.e.,

$$Y^*_{n+1} = Y^*_n + h_n \sum_{i=1}^{s} b^*_i k_i.$$

The resulting error

$$e_{n+1} = \|Y_{n+1} - Y^*_{n+1}\|_F = h_n \|\sum_{i=1}^{s} (b_i - b^*_i) k_i\|_F \tag{3.53}$$

is of order p and it can be used as an error estimator to adaptively adjust the step size. Given a desired approximation tolerance $\tau > 0$ and a delay parameter $0 < \beta < 1$, we obtain an optimal step size for the next step in the iteration process by

$$h_{n+1} = \begin{cases} \beta h_n \left(\frac{\tau}{e_{n+1}}\right)^{\frac{1}{p}} & e_{n+1} >= \tau \\ \beta h_n \left(\frac{\tau}{e_{n+1}}\right)^{\frac{1}{p}+1} & else. \end{cases}$$

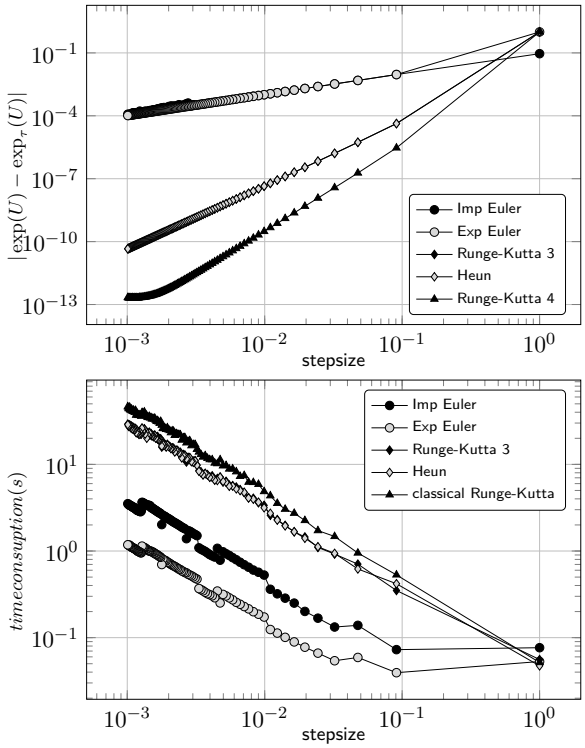

FIGURE 1. Convergence rates (top) and measured time (bottom) of different Runge-Kutta schemes for the evaluation of the tensor exponential for decreasing step sizes. The error is determined by Monte-Carlo sampling with respect to the point-wise exact exponential.

Proposition 3.11. *Assume $0 < p < q < \infty$ and two Runge-Kutta methods with convergence of order p and q. Then, the embedded Runge-Kutta method for* (3.46) *converges with order p.*

3.5.3. *Implicit Method.* Usually, the above defined methods are stable only in specific restricted regions. In order to alleviate such limitations, we can take advantage of implicit methods which are unconditionally stable. The simplest implicit method is the first order convergent backward Euler scheme which can be written as

$$W_{k+1}(\hat{y}, \delta) = W_k(\hat{y}, \delta) + h\Phi(\hat{y}, \delta) \circ W_{k+1}(\hat{y}, \delta)$$

In every iteration step of the implicit Euler scheme a system of linear equations has to be solved, which in our setting consists of TT tensors. Solving linear equation system involving TT-tensors is e.g. examined in [22]. For our computations, we use the *Alternating Minimal Energy* (AMEN) [6] algorithm with a random starting tensor. In experiments, as a result of its unconditional stability, the implicit Euler scheme already converges for a small number of steps, i.e., a large step size. We now express the main result of this section.

Lemma 3.12. *Let $\Phi_L^{h,M}(\cdot;\delta) \in \mathcal{P}(\Lambda_L)$ be an approximation of the Bayesian potential which is Lipschitz in the first component. Assume there is a stable one-step Runge-Kutta method of convergence order $p \geq 1$ with step size $\tau > 0$. Then, for a prescribed maximal tensor rank $\mathbf{r} \in \mathbb{N}^M$, the following mapping is well-defined*

$$\exp_\tau\left(-\frac{1}{2}\Phi_L^{h,M}(\cdot;\delta)\right) : \Xi \to \mathbb{R}, \quad (y_1, \ldots, y_M, 0, \ldots) \mapsto \sum_{\mu \in \Lambda_L} U_{L,\tau}^{h,M}[\mu] P_\mu(y), \tag{3.54}$$

Algorithm 2: Implicit Euler method for TT-tensors

Require: TT-tensor V, number of iterations N, maximal rank r, rounding precision ϵ
1: $O = (1,\dots,1)\otimes\cdots\otimes(1,\dots,1)$ according to dimensions and ranks of V
2: $V_{\exp} = O$
3: **for** $j = 1 : N$ **do**
4: **if** $\max($TT-ranks of $V_{\exp})> r$ **then**
5: $V_{\exp} \leftarrow$ hard-thresholding to maximal rank r and precision ϵ
6: **end if**
7: $\operatorname{diag}(O - \frac{1}{N}V,\dots,O-\frac{1}{N}V)V_{\exp} = V_{exp}$
8: **end for**
9: **return** $V_{\exp}$

where $U_{L,\tau}^{h,M}$ is the resulting coefficient tensor of $\Phi_L^{h,M}$ from (3.35) *applied to* (3.42)*. Furthermore, if $(e^{-\frac{1}{2}\Phi_L^{h,M}}) \in H^{\tilde{s}}(\Xi)$ for some $\tilde{s} > 0$, then there exists a constant $\widetilde{C} > 0$ such that*

$$\|\exp_\tau\left(-\frac{1}{2}\Phi_L^{h,M}\right) - \exp\left(-\frac{1}{2}\Phi_L^{h,M}\right)\|_{L^2_{\pi_0}(\Xi)} \le \widehat{C}\Big(\sqrt{M-1}\|U_{L,\tau}^{h,M} - U_{L,\tau}^{h,M*}\|_F \tag{3.55}$$

$$+ L^{-\tilde{s}}\|e^{-\frac{1}{2}\Phi_L^{h,M}}\|_{H^{\tilde{s}}(\Xi)} + \tau^{-p}\Big), \tag{3.56}$$

where $U_{L,\tau}^{h,M*}$ is the best rank-$\mathbf{r}$ approximation of the coefficient tensor $U_{L,\tau}^{h,M}$.

Proof. The result follows directly from the stability of the Runge-Kutta method and (3.16). □

4. Bayesian Inversion Using Low-Rank Tensor Approximation

This section is concerned with the derivation of of an explicit representation of the Bayesian posterior density based on the results of the preceding sections.

We pointed out the usability of the tensor train format to express the Bayesian potential in terms of multivariate polynomials (3.34). Moreover, we have shown that we can calculate the point-wise exponential of a TT-tensor with higher order Runge-Kutta methods efficiently, or at least stable using the implicit Euler approach from section 3.5. Combining both ideas with a suitable interpolation basis leads to a functional representation of the Bayesian posterior density

$$\exp_\tau\left(-\frac{1}{2}\Phi_L^{h,M}(y;\delta)\right) = \sum_{\mu\in\Lambda_L} U_{L,\tau}^{h,M}[\mu]P_\mu(y), \quad \text{for } y\in\Xi. \tag{4.1}$$

Employing the TT tensor structure and the shorthand $V_k := (U_{L,\tau}^{h,M})_k$ for the tensor cores $k = 0,\dots,M$ we have

$$\exp_\tau\left(-\frac{1}{2}\Phi_L^{h,M}(y;\delta)\right) = \sum_{k_1=1}^{r_1}\cdots\sum_{k_{M-1}=1}^{r_{M-1}} V_0[k_1]\left(\sum_{\mu_1=0}^{L} U_1[k_1,\mu_1,k_2]P_{\mu_1}(y_1)\right)\times \tag{4.2}$$

$$\times\cdots\left(\sum_{\mu_M=0}^{L} V_M[k_{M-1},\mu_M]P_{\mu_M}(y_M)\right).$$

The usability of (4.2) becomes apparent when estimating usually expensive quantities as e.q. the norming factor Z from (2.31)

$$Z = \mathbb{E}_{\pi_\delta}[1] = \mathbb{E}_{\pi_0}\left[\exp\left(-\frac{1}{2}\Phi(\cdot,\delta)\right)\right]. \tag{4.3}$$

This high dimensional integral equation is a challenging task for direct integration methods. Method classes like MCMC are favored partly due to the benefit of not having to calculate this constant. Contrasting, in the TT tensor setting using a functional representation in orthogonal polynomials, the approximation to the normalization constant is worked out by

$$Z^{h,M}_{L,\tau} = \mathbb{E}_{\pi_0}[\exp_\tau(-\Phi^{h,M}_L(y,\delta))] = \int_{\Xi^M} \exp_\tau(-\Phi^{h,M}_L(y,\delta))\,\mathrm{d}\frac{1}{2}\lambda(y) \tag{4.4}$$

$$= 2^{-M}\sum_{\mu\in\Lambda_L} V[\mu]\int_{-1}^{1} P_{\mu_1}(y_1)\,\mathrm{d}\lambda(y_1)\cdots\int_{-1}^{1} P_{\mu_M}(y_M)\,\mathrm{d}\lambda(y_M) \tag{4.5}$$

$$= 2^{-M}V[0,0,\ldots,0]. \tag{4.6}$$

This one tensor evaluation, consisting of $M+1$ Matrix vector multiplications, yields the expression for our approximated Bayesian density in (2.11)

$$\frac{d\pi^{h,M}_{\delta,L,\tau}}{d\pi_0}(y) = \frac{1}{Z^{h,M}_{L,\tau}}\exp_\tau\left(-\frac{1}{2}\Phi^{h,M}_L(y,\delta)\right). \tag{4.7}$$

This joint density contains all information about the unknown parameter in our model parametrized by the expansion (2.25). Concerning parameter estimation, the tensor train decomposed Bayesian potential can be used to estimate the marginals as well. Setting $y_{-k} = (y_1,\ldots,y_{k-1},y_{k+1},\ldots,y_M)$ the k-th marginal density for the parameter y_k is given by

$$\left(\frac{d\pi^{h,M}_{\delta,L,\tau}}{d\pi_0}\right)_k(y_k) = \frac{1}{Z^{h,M}_{L,\tau}}\int_{-1}^{1}\exp_\tau\left(-\frac{1}{2}\Phi^{h,M}_L(y,\delta)\right)\mathrm{d}\pi_0(y_{-k}) \tag{4.8}$$

$$= 2^{-M+1}\sum_{j=1}^{L} V[0,0,\ldots,0,j,0,\ldots,0]P_j(y_k), \tag{4.9}$$

using again the orthogonality of the Legendre polynomials.

Another advantage can be employed by estimating a quantity of interest (2.32), e.q. moments of the forward solution with respect to the posterior measure.

Example 4.1. *Given the representation* (3.23) *of the forward map in* [8, sec 3.3] *it is shown that the estimation of the mean of the solution with respect to the prior measure is a simple tensor evaluation as in* (4.4)*. Employing the same argument for the posterior measure gives the calculation*

$$\mathbb{E}_{\pi^{h,M}_{L,\tau,\delta}}\left[G^{h,M}(y)\right] = \left(\frac{1}{2}\right)^M\int_{\Xi}\left(\sum_{i=1}^{N}\sum_{\mu\in\Lambda}U[i,\mu]P_\mu(y)\right)\left(\sum_{\nu\in\Lambda_L}V[\nu]P_\nu(y)\right)\mathrm{d}y. \tag{4.10}$$

Here we use again the orthogonality of the Legendre polynomials and moreover the fact that the index sets Λ and consequently Λ_L are monotone. Thus,

$$\mathbb{E}_{\pi^{h,M}_{L,\tau,\delta}}\left[G^{h,M}(y)\right] = \left(\frac{1}{2}\right)^M\sum_{i=1}^{N}\sum_{\mu\in\Lambda\cap\Lambda_L}U[i,\mu]V[\mu]. \tag{4.11}$$

Obviously, the extended TT format grants easy access to important quantities which, by sampling or integration in general, are hard to obtain.

5. Error Analysis

5.1. **Convergence of the posterior.** In considering the Hellinger distance,

$$d_{Hell}(\pi_\delta, \pi_{\delta,L,\tau}^{h,M}) = \left(\frac{1}{2} \int_{\xi \in [-1,1]^{|\mathbb{J}|}} \left(\sqrt{\frac{d\pi_\delta}{d\pi_0}} - \sqrt{\frac{d\pi_{\delta,L,\tau}^{h,M}}{d\pi_0}} \right)^2 d\pi_0 \right)^{\frac{1}{2}} , \tag{5.1}$$

there is a tool to measure the distance of the analytical posterior measure π_y and an approximation $\pi_{\delta,L,\tau}^{h,M}$, containing possible approximations of the forward operator by an M-term series truncation and a finite element method with meshsize h as described in (3.23), a collocation with polynomial interpolation of degree L (3.30) and a stepsize parameter τ for the ODE solver of (3.42) In [1], it is shown that an alternative approximation by Gaussian processes yields sole dependence on the $L^2_{\pi_0}(X)$-norm of the solution operator.

The approach designed in this article is an analogous method using a different basis representation and due to parametrization and tensor compression we are able to use more design points.

With the same arguments as in [1] Lemma 4.1. we can show

$$Z_L^{h,M} > 0 \tag{5.2}$$

and therefore the following theorem holds.

Theorem 5.1. *Assume that* $sup_{y\in\Xi}|\mathcal{O}(G(y))| < \infty$ *and* $\sup_{y\in\Xi} \|G(y) - G^{h,M}(y)\|_{\mathcal{X}} \to 0$ *as* $N \to \infty$. *Then, there exists a constant* $C > 0$ *independent of* M, h, L *and* τ, *such that*

$$d_{Hell}(\pi_\delta, \pi_{\delta,L,\tau}^{h,M}) \leq C\|G - G^{h,M}\|_{L^2_{\pi_0}(X)} + \widetilde{C}(h, M, L, \tau), \tag{5.3}$$

where $\widetilde{C}(L,\tau) \to 0$ *as* $h, \tau \to 0$ *and* $M, L \to \infty$.

Proof. We consider the *Bayesian posterior* density (2.31) and the calculated approximation

$$\frac{d\pi_{\delta,L,\tau}^{h,M}}{d\pi_0}(\xi) = \frac{1}{Z_L^{h,M}} \exp_\tau(-\Phi_L^{h,M}(\xi;\delta)) , \tag{5.4}$$

with $\Phi_L^{h,M}(\xi;\delta)$ from (3.34) and $\exp_\tau$ is the approximated exponential as solution of the ODE (3.42).

Given that setup, by Hölders inequality we have

$$
\begin{aligned}
2d_{Hell}(\pi_\delta, \pi^{h,M}_{\delta,L,\tau})^2 &= \mathbb{E}_{\pi_0}\left[\left(\frac{e^{-\frac{1}{2}\Phi(\cdot,\delta)}}{\sqrt{Z}} - \frac{e_\tau^{-\frac{1}{2}\Phi_L^{h,M}(\cdot,\delta)}}{\sqrt{Z_L^{h,M}}}\right)^2\right] \\
&= \underbrace{\frac{2}{Z}\mathbb{E}_{\pi_0}\left[\left(e^{-\frac{1}{2}\Phi(\cdot;\delta)} - e_\tau^{-\frac{1}{2}\Phi_L^{h,M}(\cdot,\delta)}\right)^2\right]}_{:=I} - \frac{2}{Z}\mathbb{E}_{\pi_0}\left[e^{-\Phi_L^{h,M}(\cdot,\delta)}\right] \\
&\quad + \left(\frac{4}{Z} - \frac{2}{\sqrt{ZZ_L^{h,M}}}\right)\mathbb{E}_{\pi_0}\left[e^{-\frac{1}{2}\Phi(\cdot,\delta)}e_\tau^{\frac{1}{2}\Phi_L^{h,M}(\cdot,\delta)}\right] \\
&\leq I - \frac{2Z_L^{h,M}}{Z} + \frac{4\sqrt{ZZ_L^{h,M}}}{Z} - 2 \\
&= I - \underbrace{2Z_L^{h,M}\left(\frac{1}{\sqrt{Z}} - \frac{1}{\sqrt{Z_L^{h,M}}}\right)^2}_{:=II} \leq I + II\ . \qquad (5.5)
\end{aligned}
$$

Using the triangle inequality we can split the difference in I into two distinct error terms

$$
\left|e^{-\frac{1}{2}\Phi(\xi;\delta)} - e_\tau^{-\frac{1}{2}\Phi_L^{h,M}(\xi;\delta)}\right| \leq \left|e^{-\frac{1}{2}\Phi(\xi;\delta)} - e^{-\frac{1}{2}\Phi_L^{h,M}(\xi;\delta)}\right| + \left|e^{-\frac{1}{2}\Phi_L^{h,M}(\xi;\delta)} - e_\tau^{-\frac{1}{2}\Phi_L^{h,M}(\xi;\delta)}\right|. \quad (5.6)
$$

Due to the continuity of the observation operator $\mathcal{O}$ and the convergence of the forward operator, we have that the exponential expression in the first term is locally Lipschitz, which means there exists a $Q > 0$, such that

$$
|e^{-\frac{1}{2}\Phi(\xi;\delta)} - e^{-\frac{1}{2}\Phi_L^{h,M}(\xi;\delta)}| \leq \frac{1}{4}Q|\Phi(\xi;\delta) - \Phi_L^{h,M}(\xi;\delta)|\ . \qquad (5.7)
$$

Here, the second term of (5.6) models the error of the exponential approximation with a chosen ODE solver. Another triangle inequality yields the splitting of the potential interpolation error

$$
|\Phi(\xi;\delta) - \Phi_L^{h,M}(\xi;\delta)| \leq |\Phi(\xi;\delta) - \Phi^{h,M}(\xi;\delta)| + |\Phi^{h,M}(\xi;\delta) - \Phi_L^{h,M}(\xi;\delta)|, \qquad (5.8)
$$

where the second term is the interpolation error of the potential itself.

To reduce notation we omit the functional dependence of $\Phi := \Phi(\cdot,\delta)$ and their approximations. Thus,

$$\begin{aligned}\frac{Z}{2}I &\leq \frac{1}{16}Q^2\mathbb{E}_{\pi_0}\left[\left(\left|\Phi-\Phi^{h,M}\right|+\left|\Phi^{h,M}-\Phi_L^{h,M}\right|\right)^2\right] \\ &\quad+\frac{1}{2}Q\mathbb{E}_{\pi_0}\left[\left(\left|\Phi-\Phi^{h,M}\right|+\left|\Phi^{h,M}-\Phi_L^{h,M}\right|\right)\left|e^{-\frac{1}{2}\Phi_L^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\right|\right] \\ &\quad+\mathbb{E}_{\pi_0}\left[\left|e^{-\frac{1}{2}\Phi_L^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\right|^2\right] \\ &= \frac{1}{16}Q^2\mathbb{E}_{\pi_0}\left[\left(\left|\Phi-\Phi^{h,M}\right|\right)^2\right]+\frac{1}{8}Q^2\mathbb{E}_{\pi_0}\left[\left|\Phi-\Phi^{h,M}\right|\left|\Phi^{h,M}-\Phi_L^{h,M}\right|\right] \\ &\quad+\frac{1}{16}Q^2\mathbb{E}_{\pi_0}\left[\left(\left|\Phi^{h,M}-\Phi_L^{h,M}\right|\right)^2\right]+\frac{1}{2}Q\mathbb{E}_{\pi_0}\left[\left|\Phi-\Phi^{h,M}\right|\left|e^{-\frac{1}{2}\Phi_L^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\right|\right] \\ &\quad+\frac{1}{2}Q\mathbb{E}_{\pi_0}\left[\left|\Phi^{h,M}-\Phi_L^{h,M}\right|\left|e^{-\frac{1}{2}\Phi_L^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\right|\right]+\frac{1}{2}Q\mathbb{E}_{\pi_0}\left[\left|e^{-\frac{1}{2}\Phi_L^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\right|^2\right]\end{aligned} \tag{5.9}$$

and using the reverse triangle as well as Hölder's inequality

$$\begin{aligned}\frac{Z}{2}I &\leq \frac{1}{16}Q^2\mathbb{E}_{\pi_0}\left[\left|\Phi^{\frac{1}{2}}+(\Phi^{h,M})^{\frac{1}{2}}\right|^2\|\mathcal{O}\|^2_{\mathcal{L}(\mathcal{X},Y)}\|G-G^{h,M}\|^2_{L^2(X;\mathcal{X})}\right] \\ &\quad+\frac{1}{8}Q^2\mathbb{E}_{\pi_0}\left[\left|\Phi^{\frac{1}{2}}+(\Phi^{h,M})^{\frac{1}{2}}\right|\|\mathcal{O}\|_{\mathcal{L}(\mathcal{X},Y)}\|G-G^{h,M}\|_{L^2(X;\mathcal{X})}|\Phi^{h,M}-\Phi_L^{h,M}|\right] \\ &\quad+\frac{1}{16}Q^2\|\Phi^{h,M}-\Phi_L^{h,M}\|^2_{L^2_{\pi_0}(\Xi)} \\ &\quad+\frac{1}{2}Q\mathbb{E}_{\pi_0}\left[\left|\Phi^{\frac{1}{2}}+(\Phi^{h,M})^{\frac{1}{2}}\right|\|\mathcal{O}\|_{\mathcal{L}(\mathcal{X},Y)}\|G-G^{h,M}\|_{L^2(X;\mathcal{X})}\left|e^{-\frac{1}{2}\Phi_L^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\right|\right] \\ &\quad+\frac{1}{2}Q\|\Phi^{h,M}-\Phi_L^{h,M}\|_{L^2_{\pi_0}(\Xi)}\|e^{-\frac{1}{2}\Phi^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\|_{L^2_{\pi_0}(\Xi)} \\ &\quad+\frac{1}{2}Q\|e^{-\frac{1}{2}\Phi^{h,M}}-e^{-\frac{1}{2}\Phi_L^{h,M}}\|^2_{L^2_{\pi_0}(\Xi)} \\ &\leq \frac{1}{16}Q^2\sup_{y\in\Xi}\left|\Phi(y)^{\frac{1}{2}}+\Phi^{h,M}(y)^{\frac{1}{2}}\right|^2\|\mathcal{O}\|^2_{\mathcal{L}(\mathcal{X},Y)}\|G-G^{h,M}\|^2_{L^2_{\pi_0}(\Xi)} \\ &\quad+\frac{1}{8}Q^2\sup_{y\in\Xi}\left|\Phi(y)^{\frac{1}{2}}+\Phi^{h,M}(y)^{\frac{1}{2}}\right|\|\mathcal{O}\|_{\mathcal{L}(\mathcal{X},Y)}\|G-G^{h,M}\|_{L^2_{\pi_0}(\Xi)}\|\Phi^{h,M}-\Phi_L^{h,M}\|_{L^2_{\pi_0}(\Xi)} \\ &\quad+\frac{1}{2}Q\sup_{y\in\Xi}\left|\Phi(y)^{\frac{1}{2}}+\Phi^{h,M}(y)^{\frac{1}{2}}\right|\|\mathcal{O}\|_{\mathcal{L}(\mathcal{X},Y)}\|G-G^{h,M}\|_{L^2_{\pi_0}(\Xi)}\|e^{-\frac{1}{2}\Phi^{h,M}}-e^{-\frac{1}{2}\Phi_L^{h,M}}\|_{L^2_{\pi_0}(\Xi)} \\ &\quad+\frac{1}{2}Q\|\Phi^{h,M}-\Phi_L^{h,M}\|_{L^2_{\pi_0}(\Xi)}\|e^{-\frac{1}{2}\Phi^{h,M}}-e_\tau^{-\frac{1}{2}\Phi_L^{h,M}}\|_{L^2_{\pi_0}(\Xi)} \\ &\quad+\frac{1}{16}Q^2\|\Phi^{h,M}-\Phi_L^{h,M}\|^2_{L^2_{\pi_0}(\Xi)} \\ &\quad+\frac{1}{2}Q\|e^{-\frac{1}{2}\Phi^{h,M}}-e^{-\frac{1}{2}\Phi_L^{h,M}}\|^2_{L^2_{\pi_0}(\Xi)}\end{aligned}$$

By assumption, we can bound the supremum uniformly and independent of M and h. Therefore, we can rewrite I as

$$I \leq C_1\|G-G^{h,M}\|^2_{L_{\pi_0}(\mathcal{X})}+\widetilde{C}_1(h,M,L,\tau), \tag{5.10}$$

where $\widetilde{C}_1(h,M,L,\tau)$ goes to zero as L increases toward twice the maximal gpc degree of Λ, $\tau\to 0$, $h\to 0$ and $M\to\infty$. Using the L^2 bounds from Lemma 3.5 and 3.12, we can estimate a convergence rate of $\widetilde{C}_1$.

The second therm, II can be bounded by multiplication with $\left(\frac{Z-Z_L^{h,M}}{Z-Z_L^{h,M}}\right)^2$ and factoring out an appropriate term

$$\begin{aligned} II &= 2Z_L^{h,M}\left(\frac{1}{\sqrt{Z}}-\frac{1}{\sqrt{Z_L^{h,M}}}\right)^2 \\ &\leq 2Z_L^{h,M}\max\left\{Z^{-3},\left(Z_L^{h,M}\right)^{-3}\right\}\left(Z-Z_L^{h,M}\right)^2 \\ &= 2Z_L^{h,M}\max\left\{Z^{-3},\left(Z_L^{h,M}\right)^{-3}\right\}\left(\mathbb{E}_{\pi_0}\left[e^{-\Phi(\cdot;\delta)}-e^{-\Phi_L^{h,M}(\cdot;\delta)}\right]\right)^2 . \end{aligned} \tag{5.11}$$

Finally, by Jensens inequality and a similar argument as in (5.9), we obtain the upper bound on II

$$II \leq C_2\|G-G^{h,M}\|^2_{L_{\pi_0}(\mathcal{X})}+\widetilde{C}_2(h,M,L,\tau). \tag{5.12}$$

The remainder $\widetilde{C}_2(h,M,L,\tau)$ is a rescaling of $\widetilde{C}_1(h,M,L,\tau)$. □

6. Numerical Experiments

To verify the introduced setting, we consider the model parametric stationary diffusion problem on the unit square

$$-\mathrm{div}(u\nabla p) = f \qquad \text{in } D := [0,1]^2 \tag{6.1}$$

$$p = 0 \qquad \text{on } \partial D, \tag{6.2}$$

with force term $f \equiv 1$. The unknown coefficient admits an affine-parametric presentation analog to [8, sec. 7.2]

$$u(x,y) = 2+\sum_{m=1}^{M}\psi_m(x)y_m \tag{6.3}$$

with

$$\psi_m(x) = \alpha_m\cos(2\pi\varrho_1(m)x_1)\cos(2\pi\varrho_2(m)x_2), \tag{6.4}$$

where α_m is of the form $\bar{\alpha}m^{-\sigma}$ for some $0<\bar{\alpha}<\frac{1}{\zeta(\sigma)}$ with $\sigma>0$ and ζ the Riemann zeta function. Moreover, we say

$$\varrho_1(m) := \frac{m-k(m)(k(m)+1)}{2} \quad \varrho_2(m) := k(m)-\varrho_1(m) \tag{6.5}$$

with $k(m) = \lfloor -\frac{1}{2}+\sqrt{\frac{1}{4}+2m}\rfloor$. More precisely, the coefficient functions enumerate all planar Fourier sine modes in increasing total order. The random variables are assumed to be uniformly distributed $y_m \sim \mathcal{U}[-1,1]$.

The goal is to estimate the distribution of u, resp. of the parameter y, from knowledge of noisy measurement data

$$\delta = (\mathcal{O}\circ G)(y)+\eta. \tag{6.6}$$

η is assumed to be Gaussian $\eta\sim\mathcal{N}(0,\Gamma)$ with covariance $\Gamma=\gamma I$ and $\gamma<1$. To approximate the forward solution $G(y)$ we use the presented adaptive stochastic Galerkin approach and, for reference, usual finite elements approximation with adaptive mesh refinements and order $p=1,2,3$. The adaptive solution algorithm is driven by the calibration of the physical mesh acuteness h, the amount of stochastic modes M and the tensor rank $\mathbf{r}=(r_0,\dots,r_M)$. Due to the design of the error estimators, those parameters are chosen to balance the overall approximation error. A suitable stopping criteria is given by the amount of information stored in the tensor object, represented by the compressed amount of degrees of freedom. Therefore,

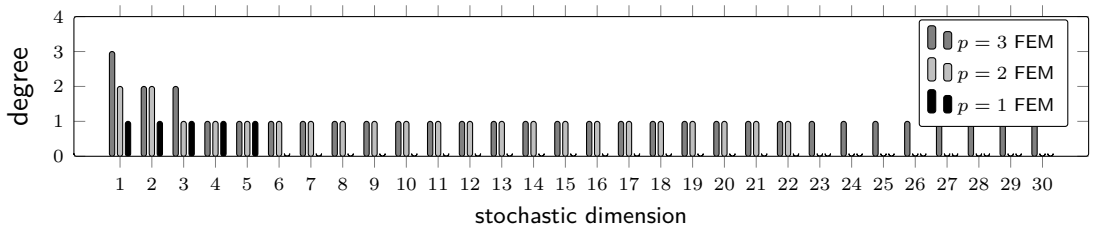

FIGURE 2. Three resulting degrees of polynomials in the solution representation (3.23) after reaching the threshold $ndofs = 5 \cdot 10^4$ for finite elements of order $p = 1, 2, 3$. We show the dimension with their respective polynomial degree.

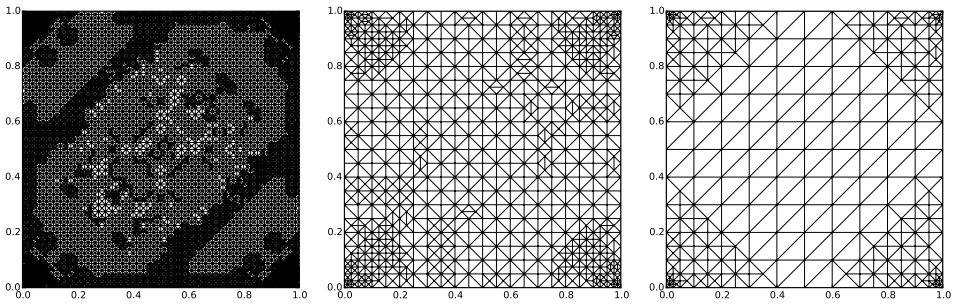

FIGURE 3. Physical mesh results of the adaptive stochastic Galerkin approach for finite elements $p = 1$ (left), $p = 2$ (middle), $p = 3$ (right) after reaching the threshold of $ndofs = 5 \cdot 10^4$.

let $G^{h,M}(x, y) = U[x, y]$ the system response (3.23) with coefficient tensor $\tilde{U} \in \mathbb{R}^{N \times d_0 \times \ldots \times d_M}$. Then we define the *TT-dofs* as

$$ndofs := Nr_0 + \sum_{m=1}^{M} r_{m-1} d_m r_m. \tag{6.7}$$

Remember, the first tensor rank r_0 for the ASGFEM solution (3.23) is in fact nonzero and to be precise, we consider $r_{-1} = 0$ to be part of the rank vector.

Nevertheless, we stop the refinement process when a given amount of TT-dofs is reached. For a threshold of $ndofs = 5 \cdot 10^4$ the resulting polynomial degrees can be seen in figure 2 and the mesh refinement is exemplarily shown in figure 3 for $P1$ elements. As one would expect, a finite elements discretization with higher order elements is already accurate in the physical space and hence the algorithm refines the stochastic space, which results in higher polynomial degrees and a larger consideration of coefficients in the uncertainty expansion. For $p = 3$ we in fact obtained $M = 67$, whereas all spaces $m \geq 4$ contain linear polynomials only.

The accuracy of the solution approximation can be seen in figure 4. We sampled the mean error of the ASGFEM solution and a reference FEM solution with the same concinnity, using Monte Carlo integration and $N = 200$ samples. It can be seen that we reach quasi-optimal convergence orders in $L^1(\Xi; L^2(D))$ and $L^1(\Xi; H_0^1(D))$ for the respective finite elements order.

Having a set of approximations of the forward solution $G^{h,M}$, we can focus on the inverse problem. The designed algorithm contains measurements $\delta \in \mathbb{R}^K$, which are observed at $K = 20$ uniformly chosen nodes in D and obtained from the finest reference solution, disturbed by a Gaussian noise with covariance factor $\gamma = 10^{-3}$.

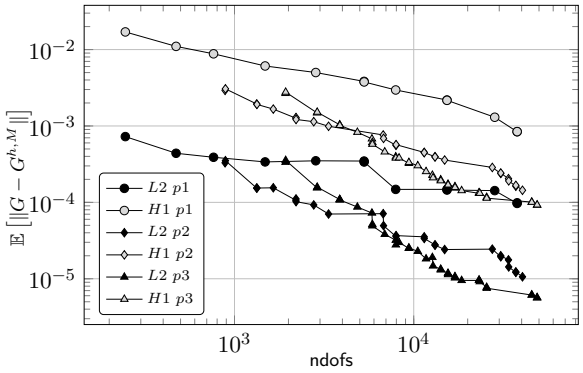

FIGURE 4. Sampled mean of the forward solution error in $L^2(D)$ and $H_0^1(D)$ norm of the stationary diffusion problem on the square with homogeneous Dirichlet boundary conditions and $p = 1, 2, 3$ FEM approximation w.r.t. number of TT degrees of freedom ($ndofs$).

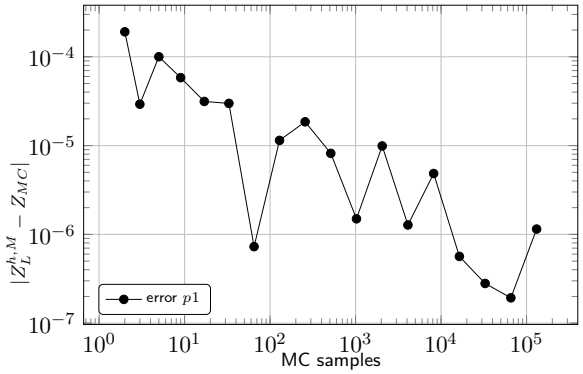

FIGURE 5. Sampled error of the approximated normalization constant and Monte Carlo sampling results for varying number of samples. The used $Z_L^{h,M}$ is the finest solution of the $p = 1$ approximation.

The first experiment involves the normalization constant

$$Z = \int_{[-1,1]^M} e^{-\frac{1}{2}\|\delta - (\mathcal{O} \circ G)(y)\|^2} d\pi_0(y) \tag{6.8}$$

and its corresponding approximation $Z_{L,\tau}^{h,M}$ in (4.4).

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