## A BENCHMARK FOR THE BAYESIAN INVERSION OF COEFFICIENTS IN PARTIAL DIFFERENTIAL EQUATIONS

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Abstract. Bayesian methods have been widely used in the last two decades to infer statistical properties of spatially variable coefficients in partial differential equations from measurements of the solutions of these equations. Yet, in many cases the number of variables used to parameterize these coefficients is large, and obtaining meaningful statistics of their values is difficult using simple sampling methods such as the basic Metropolis-Hastings (MH) algorithm – in particular if the inverse problem is ill-conditioned or ill-posed. As a consequence, many advanced sampling methods have been described in the literature that converge faster than MH, for example by exploiting hierarchies of statistical models or hierarchies of discretizations of the underlying differential equation.

At the same time, it remains difficult for the reader of the literature to quantify the advantages of these algorithms because there is no commonly used benchmark. This paper presents a benchmark Bayesian inverse problem – namely, the determination of a spatially-variable coefficient, discretized by 64 values, in a Poisson equation, based on point measurements of the solution – that fills the gap between widely used simple test cases (such as superpositions of Gaussians) and real applications that are difficult to replicate for developers of sampling algorithms. We provide a complete description of the test case, and provide an open source implementation that can serve as the basis for further experiments. We have also computed  $2 \times 10^{11}$  samples, at a cost of some 30 CPU years, of the posterior probability distribution from which we have generated detailed and accurate statistics against which other sampling algorithms can be tested.

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1. Introduction. Inverse problems are parameter estimation problems in which one wants to determine unknown, spatially variable material parameters in a partial differential equation (PDE) based on measurements of the solution. In the deterministic approach, one in essence seeks that set of parameters for which the solution of the PDE would best match the measured values; this approach is widely used in many applications. On the other hand, the Bayesian approach to inverse problems recognizes that all measurements are subject to measurement errors and that models are also inexact; as a consequence, we ought to pose the inverse problem as one that seeks a probability distribution describing how likely it is that parameter values lie in a given interval or set. This generalization of the perspective on inverse problems has long roots, but first came to the attention of the wider scientific community through a 1987 book by Tarantola [49]. It was later followed by a significantly revised and more accessible version by the same author [50] as well as numerous other books on the subject; we mention [35] as one example, along with [2,3,17] for tutorial-style introductions to the topic. The Bayesian approach to inverse problems has been used in a wide variety of inverse applications: Too many to mention in detail, but including acoustics [12], flow in the Earth's mantle [59], laminar and turbulent flow [13], ice sheet modeling [42], astronomy [15], chemistry [26, 39], and groundwater modeling [33].

From a computational perspective, the primary challenge in Bayesian inverse problems is that after discretizing the spatially variable parameters one seeks to infer, one generally ends up with trying to characterize a finite- but high-dimensional probability distribution  $\pi(\theta)$  that describes the relative likelihood of parameters  $\theta$ . In particular, we are typically interested in computing the mean and standard deviation

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of this probability distribution (i.e., which set of parameters  $\langle \theta \rangle$  on average fits the measured data best, and what we know about its variability given the uncertainty in the measured data). Computing these integral quantities in high dimensional spaces can only be done through sampling methods such as Monte Carlo Markov Chain (MCMC) algorithms. On the other hand, sampling in high-dimensional spaces often suffers from a number of problems: (i) Long burn-in times until a chain finally finds the region where the probability distribution  $\pi(\theta)$  has values substantially different from zero; (ii) long autocorrelation length scales if  $\pi(\theta)$  represents elongated, curved, or "ridged" distributions; (iii) for some inverse problems, multi-modality of  $\pi(\theta)$  is also a problem that complicates the interpretation of the posterior probability distribution; (iv) in many ill-posed inverse problems, parameters have large variances that result in rather slow convergence to reliable and accurate means.

In most high-dimensional applications, the result of these issues is then that one needs very large numbers of samples to accurately characterize the desired probability distribution. In the context of inverse problems, this problem is compounded by the fact that the generation of every sample requires the solution of the forward problem – i.e., generally, the expensive numerical solution of a PDE. As a consequence, the solution of Bayesian inverse problems is computationally exceptionally expensive.

The community has stepped up to this challenge over the past two decades: Numerous algorithms have been developed to make the sampling process more efficient. Starting from the simplest sampler, the Metropolis-Hastings algorithms with a symmetric proposal distribution [32], ideas to alleviate some of the problems include nonsymmetric proposal distributions [44], delayed rejection [53], non-reversible samplers [21], piecewise deterministic Markov processes [11,54] including Hamiltonian Monte Carlo [38], adaptive methods [6,31,43], randomize-then-optimize methods [7–9], affine invariant samplers [24,29], and combinations thereof [16,30].

Other approaches introduce parallelism (e.g., the differential evolution method and variations [51,52,56]), or hierarchies of models (see, for example, the survey by Peherstorfer et al. [41] and references therein, as well as [14,23,25,45,57]). Yet other methods exploit the fact that discretizing the underlying PDE gives rise to a natural multilevel hierarchy (see [20] among many others) or that one can use the structure of the discretized PDE for efficient sampling algorithms [36,55].

Many of these methods are likely vastly faster than the simplest sampling methods that are often used. Yet, the availability of a whole zoo of possible methods and their various possible combinations has also made it difficult to assess which method really should be used if one wanted to solve a particular inverse problem, and there is no consensus in the community on this topic. Underlying this lack of consensus is that there is no widely used benchmark for Bayesian inverse problems: Most of the papers above demonstrate the qualities of their particular innovation using some small but artificial test cases such as a superposition of Gaussians, and often a more elaborate application that is insufficiently well-described and often too complex for others to reproduce. As a consequence, the literature contains few examples of comparisons of algorithms using test cases that reflect the properties of actual inverse problems.

Our contribution here seeks to address this lack of widely used benchmarks. In particular:

• We provide a complete description of a benchmark that involves characterizing a posterior probability distribution  $\pi(\theta)$  on a 64-dimensional parameter space that results from inverting data for a discretized coefficient in a Poisson equation.

- We explain in detail why this benchmark is at once simple enough to make reproduction by others possible, yet difficult enough to reflect the real challenges one faces when solving Bayesian inverse problems.
- We provide highly accurate statistics for  $\pi(\theta)$  that allow others to assess the correctness of their own algorithms and implementations. We also provide a performance profile for a simple Metropolis-Hastings sampler as a baseline against which other methods can be compared.

To make adoption of this benchmark simpler, we also provide an open-source implementation of the benchmark that can be adapted to experimentation on other sampling methods with relative ease.

The remainder of this paper is structured as follows: In Section 2, we provide a complete description of the benchmark. In Section 3, we then evaluate highly accurate statistics of the probability distribution that solves the benchmark, based on  $2 \times 10^{11}$  samples we have computed. Section 4 provides a short discussion of what we hope the benchmark will achieve, along with our conclusions. An appendix presents details of our implementation of the benchmark (Appendix A), discusses a simple 1d benchmark for which one can find solutions in a much cheaper way (Appendix B), and provides some statistical background relevant to Section 3 (in Appendix C).

## 2. The benchmark for sampling algorithms for inverse problems.

**2.1. Design criteria.** In the design of the benchmark described in this paper, we were guided by the following principle:

A good benchmark is neither too simple nor too complicated. It also needs to reflect properties of real-world applications.

Specifically, we design a benchmark for inferring posterior probability distributions using sampling algorithms that correspond to the Bayesian inversion of coefficients in partial differential equations. In other words, cases where the relative posterior likelihood is computed by comparing (functionals of) the forward solution of partial differential equations with (simulations of) measured data.

The literature has many examples of papers that consider sampling algorithms for such problems (see the references in the introduction). However, they are typically tested only on cases that fall into the following two categories:

• Simple posterior probability density functions (PDFs) that are given by explicitly known expressions such as Gaussians or superpositions of Gaussians. There are advantages to such test cases: (i) the probability distributions are cheap to evaluate, and it is consequently possible to create essentially unlimited numbers of samples; (ii) because the PDF is exactly known, exact values for statistics such as the mean, covariances, or maximum likelihood (MAP) points are often computable exactly, facilitating the quantitative assessment of convergence of sampling schemes. On the other hand, these test cases are often so simple that any reasonable sampling algorithm converges relatively quickly, making true comparisons between different algorithms difficult. More importantly, however, such simple test cases do not reflect real-world properties of inverse problems: Most inverse problems are ill-posed, nonlinear, and high-dimensional. They are often unimodal, but with PDFs that are typically quite insensitive along certain directions in parameter space, reflecting the ill-posedness of the underlying problem. Because real-world problems are so different from simple artificial test cases, it is difficult to draw conclusions from the performance of a new sampling algorithm when applied to a simple test case.

• Complex applications, such as the determination of the spatially variable oil reservoir permeability from the production history of an oil field, or the determination of seismic wave speeds from travel times of earthquake waves from their source to receivers. Such applications are of course the target for applying advanced sampling methods, but they make for poor benchmarks because they are very difficult to replicate by other authors. As a consequence, they are almost exclusively used in only the single paper in which a new sampling algorithm is first described, and it is difficult for others to compare this new sampling algorithm against previous ones, since they have not been tested against the same, realistic benchmark.

We position the benchmark in this paper between these extremes. Specifically, we have set out to achieve the following goals:

- Reflect real properties of inverse problems: Our benchmark should reflect properties one would expect from real applications such as the permeability or seismic wave speed determinations mentioned above. We do not really know what these properties are, but intuition and knowledge of the literature suggest that they include very elongated and nonlinear probability distributions, quite unlike Gaussians or their superpositions. In order for our benchmark to reflect these properties, we base it on a partial differential equation.
- High dimensional: Inverse problems are originally infinite dimensional, i.e., we seek parameters that are functions of space and/or time. In practice, these need to be discretized, leading to finite- but often high-dimensional problems. It is well understood that the resulting curse of dimensionality leads to practical problems that often make the Bayesian inverse problem extremely expensive to solve. At the same time, we want to reflect these difficulties in our benchmark.
- Computable with acceptable effort: A benchmark needs to have a solution that is known to an accuracy sufficiently good to compare against. This implies that it can't be so expensive that we can only compute a few thousand or tens of thousands of samples of the posterior probability distribution. This rules out most real applications for which each forward solution, even on parallel computers may take minutes, hours, or even longer. Rather, we need a problem that can be solved in at most a second on a single processor to allow the generation of a substantial number of samples.
- Reproducible: To be usable by anyone, a benchmark needs to be completely specified in all of its details. It also needs to be simple enough so that others can implement it with reasonable effort.
- Available: An important component of this paper is that we make the software that implements the benchmark available as open source, see Appendix A. In particular, the code is written in a modular way that allows evaluating the posterior probability density for a given set of parameter values i.e., the key operation of all sampling methods. The code is also written in such a way that it is easy to use in a multilevel sampling scheme where the forward problem is solved with a hierarchy of successively more accurate approximations.
- **2.2. Description of the benchmark.** Given the design criteria discussed in the previous subsection, let us now present the details of the benchmark. Specifically, we seek (statistics of) a non-normalized posterior probability distribution  $\pi(\theta|\hat{z})$  on a parameter space  $\theta \in \Theta = \mathbb{R}^{64}$  of modestly high dimension 64 large enough to be interesting, while small enough to remain feasible for a benchmark. Here, we think of  $\hat{z}$

| 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 |
|----|----|----|----|----|----|----|----|
| 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 |
| 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 |
| 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 |
| 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 |
| 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 |
| 8  | 9  | 10 | 11 | 12 | 13 | 14 | 15 |
| 0  | 1  | 2  | 3  | 4  | 5  | 6  | 7  |

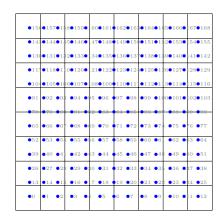


Fig. 2.1. Left: Numbering of the 64 cells on which the parameters are defined. Right: Numbering and locations of the  $13^2=169$  evaluation points at which the solution is evaluated.

as a set of measurements made on a physical system that is used to infer information about the internal parameters  $\theta$  of the system. As is common in Bayesian inverse problems,  $\pi(\theta|\hat{z})$  is defined as the product of a likelihood times a prior probability:

$$\pi(\theta|\hat{z}) \propto L(\hat{z}|\theta) \,\pi_{\rm pr}(\theta).$$
 (2.1)

Here,  $L(z|\theta)$  describes how likely it would be to measure values z if  $\theta$  were the "true" values of the internal parameters.  $\pi_{\rm pr}$  is a (not necessarily normalized) probability distribution encoding our prior beliefs about the parameters. A complete description of the benchmark then requires us to describe the values of z and ways to evaluate the functions L and  $\pi_{\rm pr}$ . We will split the definition of L into a discussion of the forward model and a statistical model of measurements in the following.

**2.2.1.** The forward model. The setting we want to pursue is as follows: Let us imagine a membrane stretched over a frame that bounds a domain  $\Omega$  which, for simplicity we assume to be the unit square  $\Omega = (0,1)^2$ . The membrane is subject to an external vertical force  $f(\mathbf{x})$  which for the purpose of this benchmark we choose constant as  $f(\mathbf{x}) = 10$ . Furthermore, the membrane has a spatially variable resistance  $a(\mathbf{x})$  to deflection (for example, it may have a variable thickness or may be made from different materials). In this benchmark, we assume that  $a(\mathbf{x})$  is piecewise constant on a uniform  $8 \times 8$  grid as shown in Fig. 2.1, with the 64 values that parameterize  $a(\mathbf{x})$  given by the elements of the vector  $\theta_0, \ldots, \theta_{63}$  as also indicated in the figure. In other words, there is a 1:1 relationship between the vector  $\theta$  and the piecewise constant coefficient function  $a(\mathbf{x}) = a^{\theta}(\mathbf{x})$ .

Then, an appropriate model to describe the vertical deflection  $u(\mathbf{x})$  of the membrane would express u as the solution of the following partial differential equation that generalizes the Poisson equation:

$$-\nabla \cdot [a(\mathbf{x})\nabla u(\mathbf{x})] = f(\mathbf{x}) \qquad \text{in } \Omega, \tag{2.2}$$

$$u(\mathbf{x}) = 0$$
 on  $\partial\Omega$ . (2.3)

This model is of course not exactly solvable. But its solution can be approximated using discretization. The way we define the likelihood L then requires us to specify exactly how we discretize this model. Concretely, we define  $u_h(\mathbf{x})$  as the solution

of a finite element discretization of (2.2)–(2.3) using a uniform  $32 \times 32$  mesh and a  $Q_1$  (bilinear) element. Because  $f(\mathbf{x})$  is given, and because there is a 1:1 relationship between  $\theta$  and  $a(\mathbf{x})$ , this discretized model then implies that for each  $\theta$  we can find a  $u_h(\mathbf{x}) = u_h^{\theta}(\mathbf{x})$  that can be thought of as being parameterized using the 1089 degrees of freedom of the  $Q_1$  discretization on the  $32 \times 32$  mesh. (However, of these 1089 degrees of freedom, 128 are on the boundary and are constrained to zero.) In other words, using the  $Q_1$  shape functions  $\varphi_k(\mathbf{x})$ , we can express  $u_h(\mathbf{x}) = \sum_{k=0}^{1088} U_k \varphi_k(\mathbf{x})$ . It is important to stress that the mapping  $\theta \mapsto u_h^{\theta}(\mathbf{x})$  (or equivalently,  $\theta \mapsto U^{\theta}$ ) is nonlinear.

The function  $u_h^{\theta}(\mathbf{x})$  can be thought of as the predicted displacement at every point  $\mathbf{x} \in \Omega$  if  $\theta$  represented the spatially variable stiffness coefficient of the membrane. In practice, however, we can only measure finitely many things, and consequently define a measurement operator  $\mathcal{M}: u_h \mapsto z \in \mathbb{R}^{169}$  that evaluates  $u_h$  on a uniform  $13 \times 13$  grid of points  $\mathbf{x}_k \in \Omega$  so that  $\mathbf{x}_k = \left(\frac{i}{13+1}, \frac{j}{13+1}\right), 1 \leq i, j \leq 13$  with k = 13(i-1) + (j-1). The locations of these points are also indicated in Fig. 2.1. This last step then defines a linear mapping. Because of the equivalence between the function  $u_h$  and its nodal vector U, the linearity of the measurement operator implies that we can write z = MU with a matrix  $M \in \mathbb{R}^{169 \times 1089}$  that is given by  $M_{kl} = \varphi_l(\mathbf{x}_k)$ .

In summary, a parameter vector  $\theta \in \mathbb{R}^{64}$  then predicts measurements  $z^{\theta} \in \mathbb{R}^{169}$  using the following chain of maps:

$$\theta \mapsto a^{\theta}(\mathbf{x}) \mapsto U^{\theta} \mapsto z^{\theta}.$$
 (2.4)

The mapping  $\theta \mapsto z^{\theta}$  is commonly called the "forward model" as it *predicts* measurements  $z^{\theta}$  if we knew the parameter values  $\theta$ . The "inverse problem" is then of course the inverse operation: to *infer* the parameters  $\theta$  that describe a system based on measurements z of its state u.

All of the steps of the forward model have been precisely defined above and are easily computable with some basic knowledge of finite element methods (or using the code discussed in Appendix A). The expensive step is to solve for the nodal vector  $U^{\theta}$ , as this requires the assembly and solution of a linear system of size 1089.

Remark 2.1. The  $32 \times 32$  mesh to define the forward model is chosen sufficiently fine to resolve the exact solution u reasonably well. At the same time, it is coarse enough to allow for the rapid evaluation of the solution – even a rather simple implementation should yield a solution in less than a second, and a highly optimized implementation such as the one discussed in Appendix A.1 will be able to do so in less than 5 milliseconds on modern hardware. As a consequence, this choice of mesh allows for computing a large number of samples, and consequently accurate quantitative comparisons of sampling algorithms.

We also mention that the  $32 \times 32$  mesh for  $u_h(\mathbf{x})$  is twice more globally refined than the  $8 \times 8$  mesh used to define  $a(\mathbf{x})$  in terms of  $\theta$ . It is clear to practitioners of finite element discretizations of partial differential equations that the mesh for  $u_h$  must be at the very least as fine as the one for the coefficient  $a^{\theta}$  to obtain any kind of accuracy. On the other hand, these choices then leave room for a hierarchy of models in which the forward model uses  $8 \times 8$ ,  $16 \times 16$ , and  $32 \times 32$  meshes; we expect that multilevel sampling methods will use this hierarchy to good effect.

REMARK 2.2. In our experiments, we will choose the values of  $\theta$  (and consequently of  $a(\mathbf{x})$ ) clustered around one. With the choice f = 10 mentioned above, this leads to a solution  $u(\mathbf{x})$  with values in the range 0...0.95. This then also implies that we should think of the numerical magnitude of our measurements  $z_k^{\theta}$  as  $\mathcal{O}(1)$ .

**2.2.2.** The likelihood  $L(z|\theta)$ . Given the predicted measurements  $z^{\theta}$  that correspond to a given set of parameters  $\theta$ , the likelihood  $L(z|\theta)$  can be thought of as expressing the (non-normalized) probability of actually obtaining z in a measurement if  $\theta$  were the "correct" set of parameters. This is a statement that encodes the measurement error of our measurement device.

For the purposes of this benchmark, we assume that these measurement errors are identical and independently distributed for all 169 measurement points. More specifically, we define the likelihood as the following (non-normalized) probability function:

$$L(z|\theta) = \exp\left(-\frac{\|z - z^{\theta}\|^2}{2\sigma^2}\right) = \prod_{k=0}^{168} \exp\left(-\frac{(z_k - z_k^{\theta})^2}{2\sigma^2}\right),\tag{2.5}$$

where we set  $\sigma = 0.05$  and where  $z^{\theta}$  is related to  $\theta$  using the chain (2.4).

Remark 2.3. We can think of (2.5) as encoding our belief that our measurement system produces a Gaussian-distributed measurement  $z_k \sim N(z_k^{\theta}, \sigma)$ . Given that  $z_k^{\theta} = \mathcal{O}(1)$ ,  $\sigma = 0.05$  implies a measurement error of 5%. This is clearly much larger than the accuracy with which one would be able to determine the deflection of a membrane in practice. On the other hand, we have chosen  $\sigma$  this large to ensure that the Bayesian inverse problem does not lead to a probability distribution  $\pi(\theta|\hat{z})$  that is so narrowly centered around a value  $\bar{\theta}$  that the mapping  $\theta \mapsto z^{\theta}$  can be linearized around  $\bar{\theta}$  – in which case the likelihood  $L(\hat{z}|\theta)$  would become Gaussian, as also discussed in Appendix B. We will demonstrate in Section 3.4 that indeed  $\pi(\theta|\hat{z})$  is not Gaussian and, moreover, is large along a curved ridge that can not easily be approximated by a Gaussian either.

**2.2.3.** The prior probability  $\pi_{\mathbf{pr}}(\theta)$ . Our next task is to describe our prior beliefs for the values of the parameters. Given that the 64 values of  $\theta$  describe the stiffness coefficient of a membrane, it is clear that they must be positive. Furthermore, as with many mechanical properties that can have values over vast ranges, <sup>1</sup> reasonable priors are typically posed on the "order of magnitude" (that is, the *logarithm*), not the size of the coefficient itself. We express this through the following (non-normalized) probability distribution:

$$\pi_{\rm pr}(\theta) = \prod_{i=0}^{63} \exp\left(-\frac{(\ln(\theta_i) - \ln(1))^2}{2\sigma_{\rm pr}^2}\right),$$
(2.6)

where we choose  $\sigma_{\rm pr} = 2$ . We recognize the prior density of  $\ln(\theta_k)$  as a Gaussian with mean  $\sigma_{\rm pr}^2$  and standard deviation  $\sigma_{\rm pr}$ .

Because this prior distribution is posed on the logarithm of the parameters, the prior on the parameters themselves is very heavy-tailed, with mean values  $\langle \theta_k \rangle_{\pi_{\rm pr}}$  for each component much larger than the value at which  $\pi_{\rm pr}$  takes on its maximum (which is at  $\theta_k = 1$ ): Indeed, the mean of each  $\theta_k$  with respect to  $\pi_{\rm pr}$  is about 403.43.

We note that this prior probability is quite weak and, in particular, does not assume any (spatial) correlation between parameters as is often done in inverse problems [35, 48, 55]. The correlations we will observe in our posterior probability (see Section 3.3) are therefore a consequence of the likelihood function only.

<sup>&</sup>lt;sup>1</sup>For example, the Young's modulus that is related to the stiffness of a membrane, can range from 0.01 GPa for rubber to 200 GPa for typical steels. Similarly, the permeability of typical oil reservoir rocks can range from 1 to 1000 millidarcies.

Table 2.1

The "true" measurement values  $\hat{z}_k$ ,  $k=0,\ldots,168$  used in the benchmark. The values are also available in the electronic supplemental material and are shown in full double precision accuracy to allow for exact reproduction of the benchmark.

| $\hat{z}_0$    | 0.060 765 117 622 593 69                 | $\hat{z}_{60}$  | 0.6235300574156917                       | $\hat{z}_{120}$ | 0.5140091754526943                                 |
|----------------|--|-----------------|--|-----------------|--|
|                | 0.096 019 101 208 484 81                 | 00              | 0.5559332704045935                       | 120             | 0.555 933 270 404 596 9                            |
|                | 0.1238852517838584                       |                 | 0.4670304994474178                       |                 | 0.5677443693743304                                 |
|                | 0.1495184117375201                       |                 | 0.349 980 914 381 1                      |                 | 0.547 825 166 529 545 3                            |
|                | 0.1841596127549784                       |                 | 0.19688263746294                         |                 | 0.4895759664908982                                 |
|                | 0.2174525028261122                       |                 | 0.2174525028261253                       |                 | 0.4109641743019171                                 |
|                | 0.225 099 616 089 869 8                  |                 | 0.4122329537843404                       |                 | 0.395727260284338                                  |
|                | 0.219 795 476 900 299 3                  |                 | 0.5779452419831566                       |                 | 0.3778949322004734                                 |
|                | 0.2074695698370926                       |                 | 0.6859683749254372                       |                 | 0.3596268271857124                                 |
|                | 0.188 999 647 766 301 6                  |                 | 0.737 310 833 139 606 3                  |                 | 0.2191250268948948                                 |
| $\hat{z}_{10}$ | 0.1632722532153726                       | $\hat{z}_{70}$  | 0.7458811983178246                       | $\hat{z}_{130}$ | 0.1632722532153683                                 |
| 10             | 0.1276782480038186                       | 10              | 0.7278968022406559                       | 130             | 0.2850397806663325                                 |
|                | 0.077 118 459 157 893 12                 |                 | 0.690 479 353 535 775 1                  |                 | 0.373 006 008 206 081                              |
|                | 0.096 019 101 208 485 52                 |                 | 0.636 917 645 271 028 8                  |                 | 0.432 532 550 635 420 7                            |
|                | 0.200 058 953 336 798 3                  |                 | 0.567 744 369 374 321 5                  |                 | 0.467 030 499 447 431 5                            |
|                | 0.3385592591951766                       |                 | 0.4784738764865867                       |                 | 0.4784738764866023                                 |
|                | 0.393 430 002 464 780 6                  |                 | 0.360 219 063 282 326 2                  |                 | 0.467 712 268 759 904 1                            |
|                | 0.404 022 389 246 154 1                  |                 | 0.203 179 205 473 732 5                  |                 | 0.434 171 688 106 105 5                            |
|                | 0.412 232 953 784 309 2                  |                 | 0.225 099 616 089 881 8                  |                 | 0.388 186 479 011 099                              |
|                | 0.410 048 009 154 555 4                  |                 | 0.4100480091545787                       |                 | 0.3778949322004602                                 |
| $\hat{z}_{20}$ | 0.394 915 163 718 996 8                  | $\hat{z}_{80}$  | 0.555 561 595 613 713 7                  | $\hat{z}_{140}$ | 0.363 336 256 718 736 4                            |
| 20             | 0.3697873264791232                       | 80              | 0.656 123 536 696 093 8                  | 140             | 0.3464457261905399                                 |
|                | 0.33401826235924                         |                 | 0.7116558878070715                       |                 | 0.2096362321365655                                 |
|                | 0.2850397806663382                       |                 | 0.727896802240657                        |                 | 0.1276782480038148                                 |
|                | 0.2184260032478671                       |                 | 0.7121928678670187                       |                 | 0.2184260032478634                                 |
|                | 0.1271121156350957                       |                 | 0.6712187391428729                       |                 | 0.2821694983395252                                 |
|                | 0.1238852517838611                       |                 | 0.6139157775591492                       |                 | 0.3248315148915535                                 |
|                | 0.3385592591951819                       |                 | 0.5478251665295381                       |                 | 0.3499809143811097                                 |
|                | 0.7119285162766475                       |                 | 0.4677122687599031                       |                 | 0.3602190632823333                                 |
|                | 0.8175712861756428                       |                 | 0.3587654911000848                       |                 | 0.3587654911000799                                 |
| $\hat{z}_{30}$ | 0.6836254116578105                       | $\hat{z}_{90}$  | 0.2050734291675918                       | $\hat{z}_{150}$ | 0.3534389974779268                                 |
|                | 0.5779452419831157                       |                 | 0.2197954769003094                       |                 | 0.3642640090182283                                 |
|                | 0.5555615956136897                       |                 | 0.3949151637190157                       |                 | 0.35962682718569                                   |
|                | 0.5285181561736719                       |                 | 0.5285181561736911                       |                 | 0.3464457261905295                                 |
|                | 0.491439702849224                        |                 | 0.6213197201867471                       |                 | 0.3260728953424643                                 |
|                | 0.4409367494853282                       |                 | 0.6745179049094407                       |                 | 0.180670595355394                                  |
|                | 0.3730060082060772                       |                 | 0.690479353535786                        |                 | 0.07711845915789244                                |
|                | 0.2821694983395214                       |                 | 0.6712187391428787                       |                 | 0.1271121156350963                                 |
|                | 0.1610176733857739                       |                 | 0.6178408289359514                       |                 | 0.1610176733857757                                 |
|                | 0.149 518 411 737 525 7                  |                 | 0.545 360 502 723 788 3                  |                 | 0.1834600412730144                                 |
| $\hat{z}_{40}$ | 0.393 430 002 464 792 9                  | $\hat{z}_{100}$ | 0.489 575 966 490 909                    | $\hat{z}_{160}$ | 0.196 882 637 462 944 3                            |
|                | 0.817 571 286 175 656 2                  |                 | 0.434 171 688 106 127 8                  |                 | 0.203 179 205 473 735 4                            |
|                | 0.943 915 462 552 765 3                  |                 | 0.353 438 997 477 945 6                  |                 | 0.205 073 429 167 588 5                            |
|                | 0.801 590 411 509 512 8                  |                 | 0.208 322 749 696 134 7                  |                 | 0.208 322 749 696 124 5                            |
|                | 0.685 968 374 925 402 4                  |                 | 0.207 469 569 837 099                    |                 | 0.217 959 990 927 999 8                            |
|                | 0.656 123 536 696 059 9                  |                 | 0.369 787 326 479 136 6                  |                 | 0.219 125 026 894 882 2                            |
|                | 0.6213197201867315<br>0.5753611315000049 |                 | 0.4914397028492412<br>0.5753611315000203 |                 | 0.209 636 232 136 555 1<br>0.180 670 595 355 388 7 |
|                | 0.514 009 175 452 682 3                  |                 | 0.623 530 057 415 701 7                  |                 | 0.180 670 595 355 388 7                            |
|                | 0.432 532 550 635 416 5                  |                 | 0.636 917 645 271 049 7                  | $\hat{z}_{168}$ | 0.106 796 555 001 001 5                            |
|                | 0.324 831 514 891 548 2                  |                 | 0.613 915 777 559 157 9                  |                 |  |
| $\hat{z}_{50}$ | 0.183 460 041 273 008 6                  | $\hat{z}_{110}$ | 0.545 360 502 723 793 5                  |                 |  |
|                | 0.184 159 612 754 991 7                  |                 | 0.433 660 492 961 285 1                  |                 |  |
|                | 0.404 022 389 246 183 2                  |                 | 0.410 964 174 301 931 2                  |                 |  |
|                | 0.683 625 411 657 843 9                  |                 | 0.388 186 479 011 124 5                  |                 |  |
|                | 0.801 590 411 509 539 6                  |                 | 0.364 264 009 018 259 2                  |                 |  |
|                | 0.787 011 956 114 497 7                  |                 | 0.217 959 990 928 014 5                  |                 |  |
|                | 0.737 310 833 139 580 8                  |                 | 0.188 999 647 766 301 1                  |                 |  |
|                | 0.711 655 887 807 046 3                  |                 | 0.334 018 262 359 246 1                  |                 |  |
|                | 0.674 517 904 909 428 3                  |                 | 0.440 936 749 485 338 1                  |                 |  |
|                |  |                 |  | 1               |  |

**2.2.4.** The "true" measurements  $\hat{z}$ . The last piece necessary to describe the complete benchmark is the choice of the "true" measurements  $\hat{z}$  that we want to use to infer the statistical properties of the parameters  $\theta$ . For the purposes of this benchmark, we will use the 169 values for  $\hat{z}$  given in Table 2.1.

In some sense, it does not matter where these values come from – we could have measured them in an actual experiment, and used these values to infer the coefficients of the system we measured on. On the other hand, for the purposes of a benchmark, it might be interesting to know whether these "true measurements"  $\hat{z}$  correspond to a "true set of parameters"  $\hat{\theta}$  against which we can compare statistics such as the mean  $\langle \theta \rangle$  of the posterior probability  $\pi(\theta|\hat{z})$ .

Indeed, this is how we have generated  $\hat{z}$ : We chose a set of parameters  $\hat{\theta}$  that corresponds to a membrane of uniform stiffness  $a(\mathbf{x}) = 1$  except for two inclusions in

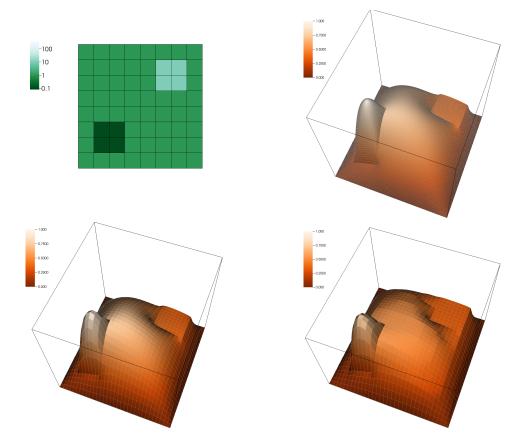


Fig. 2.2. Top left: The  $8\times 8$  grid of values  $\hat{\theta}$  used in generating the "true measurements"  $\hat{z}$  via the forward model discussed in Section 2.2.4. The color scale matches that in Fig. 3.3. Top right: The solution of the Poisson equation corresponding to  $\hat{\theta}$  on the  $256\times 256$  mesh and using  $Q_3$  finite elements. "True" measurements  $\hat{z}$  are obtained from this solution by evaluation at the points shown in the right panel of Fig. 2.1. Bottom left: For comparison, the solution obtained for the same set of parameters  $\hat{\theta}$ , but using the  $32\times 32$  mesh and  $Q_1$  element that defines the forward model. Bottom right: The solution of this discrete forward model applied to the posterior mean  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  that we will compute later; the values of  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  are tabulated in Table 3.1, and visualized in Fig. 3.3.

which a=0.1 and a=10, respectively. This set up is shown in Fig. 2.2.<sup>2</sup> Using  $\hat{\theta}$ , we then used the series of mappings as shown in (2.4) to compute  $\hat{z}$ . However, to avoid an inverse crime, we have used a 256 × 256 mesh and a bicubic ( $Q_3$ ) finite element to compute  $\hat{\theta} \mapsto \hat{u}_h \mapsto \hat{z} = \mathcal{M}\hat{u}_h$ , rather than the 32 × 32 mesh and a bilinear ( $Q_1$ ) element used to define the mapping  $\theta \mapsto u_h \mapsto z^\theta = \mathcal{M}u_h$ .

<sup>&</sup>lt;sup>2</sup>This set up has the accidental downside that both the set of parameters  $\hat{\theta}$  and the set of measurement points  $\mathbf{x}_k$  at which we evaluate the solution are symmetric about the diagonal of the domain. Since the same is true for our finite element meshes, the exact solution of the benchmark results in a probability distribution that is invariant to permutations of parameters about the diagonal as well, and this is apparent in Fig. 3.3, for example. A better designed benchmark would have avoided this situation, but we only realized the issue after expending several years of CPU time. At the same time, the expected symmetry of values allows for a basic check of the correctness of inversion algorithms: If the inferred mean value  $\langle \theta_7 \rangle_{\pi(\theta|\hat{z})}$  is not approximately equal to  $\langle \theta_{63} \rangle_{\pi(\theta|\hat{z})}$  – see the numbering shown in the left panel of Fig. 2.1 – then something is wrong.

As a consequence of this choice of higher accuracy (and higher computational cost), we can in general not expect that there is a set of parameters  $\theta$  for which the forward model of Section 2.2.1 would predict measurements  $z^{\theta}$  that are equal to  $\hat{z}$ . Furthermore, the presence of the prior probability  $\pi_{\rm pr}$  in the definition of  $\pi(\theta|\hat{z})$  implies that we should not expect that either the mean  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  nor the MAP point  $\theta_{\rm MAP} = \arg \max_{\theta} \pi(\theta|\hat{z})$  are equal or even just close to the "true" parameters  $\hat{\theta}$ .

3. Statistical assessment of  $\pi(\theta|\hat{z})$ . The previous section provides a concise definition of the non-normalized posterior probability density  $\pi(\theta|\hat{z})$ . Given that the mapping  $\theta \mapsto z^{\theta}$  is nonlinear and involves solving a partial differential equation, there is no hope that  $\pi(\theta|\hat{z})$  can be expressed as an explicit formula. On the other hand, all statistical properties of  $\pi(\theta|\hat{z})$  can of course be obtained by sampling, for example using algorithms such as the Metropolis-Hastings sampler [32].

In order to provide a useful benchmark, it is necessary that at least some properties of  $\pi(\theta|\hat{z})$  are known with sufficient accuracy to allow others to compare the convergence of their sampling algorithms. To this end, we have used a simple Metropolis-Hastings sampler to compute  $2\times 10^{11}$  samples that characterize  $\pi(\theta|\hat{z})$ , in the form of N=2000 Markov chains of length  $N_L=10^8$  each. (Details of the sampling algorithm used to obtain these samples are given in Appendix A.2.) Using the program discussed in Appendix A.1, the effort to produce this many samples amounts to approximately 30 CPU years on current hardware. On the other hand, we will show below that this many samples are really necessary in order to provide statistics of  $\pi(\theta|\hat{z})$  accurately enough to serve as reference values – at least, if one insists on using an algorithm as simple as the Metropolis-Hastings method. In practice, we hope that this benchmark is useful in the development of algorithms that are substantially better than the Metropolis-Hastings method. In addition, when assessing the convergence properties of a sampling algorithm, it is of course not necessary to achieve the same level of accuracy as we obtain here.

In the following let us therefore provide a variety of statistics computed from our samples, along with an assessment of the accuracy with which we believe that we can state these results. In the following, we will denote by  $0 \le L < N = 2000$  the number of the chain, and  $0 \le \ell < N_L = 10^8$  the number of a sample  $\theta_{L,\ell}$  on chain L. If we need to indicate one of the 64 components of a sample, we will use a subscript index k for this purpose as already used in Section 2.2.1.

3.1. How informative is our data set?. While we have N=2000 chains, each with a large number  $N_L=10^8$  of samples per chain, a careful assessment needs to include an evaluation how informative all of these samples really are. For example, if the samples on each chain had a correlation length of  $10^7$  because our Metropolis-Hastings sampler converges only very slowly, then each chain really only contains approximately ten statistically independent samples of  $\pi(\theta|\hat{z})$ . Consequently, we could not expect great accuracy in estimates of the mean value, covariance matrices, and other quantities obtained from each of the chains. Similarly, if the "burn-in" time of the sampler is a substantial fraction of the chain lengths  $N_L$ , then we would have to throw away many of the early samples.

To assess these questions, we have computed the autocovariance matrices

$$AC_{L}(s) = \left\langle [\theta_{L,\ell} - \langle \theta \rangle_{L}] [\theta_{L,\ell-s} - \langle \theta \rangle_{L}]^{T} \right\rangle_{L}$$

$$= \frac{1}{N_{L} - s - 1} \sum_{\ell=s}^{N_{L} - 1} [\theta_{L,\ell} - \langle \theta \rangle_{L}] [\theta_{L,\ell-s} - \langle \theta \rangle_{L}]^{T}$$
(3.1)

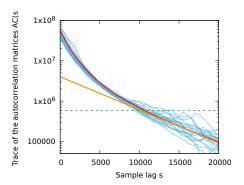


Fig. 3.1. Decay of the trace of the autocovariance matrices  $AC_L(s)$  with the sample lag s. The light blue curves show the traces of  $AC_L(s)$  for twenty of our chains. The red curve shows the trace of the averaged autocovariance matrices,  $AC(s) = \frac{1}{N} \sum_{L=0}^{N-1} AC_L(s)$ . The thick yellow line corresponds to the function  $4 \cdot 10^6 \cdot e^{-s/5300}$  and shows the expected, asymptotically exponential decay of the autocovariance. The dashed green line indicates a reduction of the autocovariance by roughly a factor of 100 compared to its starting values.

between samples s apart on chain L. We expect samples with a small lag s to be highly correlated (i.e.,  $AC_L(s)$  to be a matrix that is large in some sense), whereas for large lags s, samples should be uncorrelated and  $AC_L(s)$  should consequently be small. A rule of thumb is that samples at lags s can be considered decorrelated from each other if  $AC_L(s) \leq 10^{-2}AC_L(0)$  entrywise; see Appendix C.

Fig. 3.1 shows the trace of these autocovariance matrices for several of our chains. (We only computed the autocovariance at lags  $s=0,100,200,300,\ldots$  up to s=20,000 because of the cost of computing  $AC_L(s)$ .) The curves show that the autocovariances computed from different chains all largely agree, and at least asymptotically decay roughly exponentially with s as expected. The data also suggest that the autocorrelation length of our chains is around  $N_{AC}=10^4$  — in other words, each of our chains should result in approximately  $N_L/N_{AC}=10^4$  meaningful and statistically independent samples.

To verify this claim, we estimated the integrated autocovariance [47] using

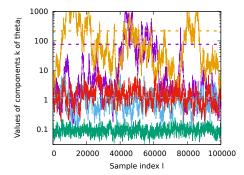
$$IAC \approx \frac{1}{N} \sum_{L=0}^{N-1} 100 \sum_{s=-200}^{200} AC_L(|100s|).$$
 (3.2)

The integrated autocovariance is obtained by summing up the autocovariance. (The factor of 100 appears because we only computed  $AC_L(s)$  at lags that are multiples of 100.) We show in Appendix C that the integrated autocovariance leads to the following estimate of the effective sample size:

Effective sample size per chain 
$$\approx \frac{N_L}{\lambda_{\rm max}(C^{-1} \cdot IAC)} \approx 1.3 \times 10^4$$
, (3.3)

where  $\lambda_{\text{max}}$  indicates the maximum eigenvalue and  $C = \frac{1}{N} \sum_{L=0}^{N-1} AC_L(0)$  is the covariance matrix; see also (3.4) below. This is in good agreement with Fig. 3.1 and the effective sample size derived from it.

This leaves the question of how long the burn-in period of our sampling scheme is. Fig. 3.2 shows two perspectives on this question. The left panel of the figure shows



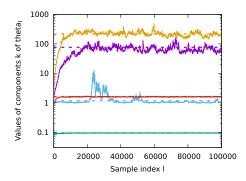


Fig. 3.2. Two perspectives on the length of the burn-in phase of our sampling scheme. Left: Values of components k=0,9,36,54, and 63 of samples  $\theta_\ell$  for  $\ell=0,\ldots,100,000$ , for one, randomly chosen chain. (For the geometric locations of the parameters that correspond to these components, see Fig. 2.1.) Right: Across-chain averages  $\frac{1}{N}\sum_{L=0}^{N-1}\theta_{L,\ell}$  for the same components k as above. Both images also shows the mean values  $\langle\theta\rangle_{\pi(\theta|\hat{z})}$  for these five components as dashed lines.

several components  $\theta_{\ell,k}$  of the samples of one of our chains for the first few autocorrelation lengths. The data shows that there is at least no obvious "burn-in" period on this scale that would require us to throw away a substantial part of the chain. At the same time, it also illustrates that the large components of  $\theta$  are poorly constrained and vary on rather long time scales that make it difficult to assess convergence to the mean. The right panel shows across-chain averages of the  $\ell$ th samples, more clearly illustrating that the burn-in period may only last around 20,000 samples – that is, that only around 2 of the approximately 10,000 statistically independent samples of each chain are unreliable.

Having thus convinced ourselves that it is safe to use all  $10^8$  samples from all chains, and that there is indeed meaningful information contained in them, we will next turn our attention towards computing statistical information that characterizes  $\pi(\theta|\hat{z})$  and against which other implementations of sampling methods can compare their results.

**3.2.** The mean value of  $\pi(\theta|\hat{z})$ . The simplest statistic one can compute from samples of a distribution is the mean value. Table 3.1 shows the 64 values that characterize the mean

$$\langle \theta_k \rangle_{\pi(\theta|\hat{z})} = \frac{1}{N} \sum_{L=0}^{N-1} \left( \frac{1}{N_L} \sum_{\ell=0}^{N_L-1} \theta_{L,\ell,k} \right).$$

A graphical representation of  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  is shown Fig. 3.3 and can be compared to the "true" values  $\hat{\theta}$  shown in Fig. 2.2.<sup>3</sup>

<sup>&</sup>lt;sup>3</sup>By comparing Fig. 2.2 and the data of Table 3.1 and Fig. 3.3, it is clear that for some parameters, the mean  $\langle \theta_k \rangle_{\pi(\theta|\hat{z})}$  is far away from the value  $\hat{\theta}_k$  used to generate the original data  $\hat{z}$  – principally for those parameters that correspond to large values  $\hat{\theta}_k$ , but also the "white cross" below and left of center. For the first of these two places, we can first note that the prior probability  $\pi_{\rm pr}$  defined in (2.6) is quite heavy-tailed, with a mean far larger than where its maximum is located. And second, by realizing that a membrane that is locally very stiff is not going to deform in a substantially different way in response to a force from one that is even stiffer in that region – in other words, in areas where the coefficient  $a^{\theta}(\mathbf{x})$  is large, the likelihood function (2.5) is quite insensitive to the exact values of  $\theta$ , and the posterior probability will be dominated by the prior  $\pi_{\rm pr}$  with its large mean.

Table 3.1

Sample means  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  for the 64 parameters, along with their estimated 2-sigma uncertainties.

```
\begin{array}{c} \langle\theta\rangle_{24} = & 0.881\,977\,\pm\,0.000\,039 \\ & 0.5828\,\pm\,0.0020 \\ & 267.72\,\pm\,0.62 \\ & 369.35\,\pm\,0.64 \\ & 234.59\,\pm\,0.53 \\ & 13.29\,\pm\,0.14 \\ & 23.69\,\pm\,0.16 \end{array}
                                  \begin{array}{c} 76.32\,\pm\,0.30 \\ 1.2104\,\pm\,0.0094 \\ 0.977\,380\,\pm\,0.000\,051 \end{array}
                                                                                                                                                                                                                                                                                           \begin{array}{c} \langle\theta\rangle_{48} = \ 1.085\,21\,\pm\,0.000\,11 \\ 9.386\,\pm\,0.089 \\ 12.44\,\pm\,0.12 \end{array}
\langle \theta \rangle_0 =
                                  0.882\ 007\ \pm\ 0.000\ 039
0.971\ 859\ \pm\ 0.000\ 048
0.947\ 832\ \pm\ 0.000\ 064
1.085\ 29\ \pm\ 0.000\ 11
                                                                                                                                                                                                                                                                                                                                \begin{array}{c} 12.44 \pm 0.12 \\ 22.50 \pm 0.17 \\ 88.57 \pm 0.33 \\ 283.41 \pm 0.57 \\ 218.65 \pm 0.49 \end{array}
                                                                                                                                                                                        22.36 \pm 0.16
                             \begin{array}{c} 11.39 \pm 0.10 \\ 11.19 \pm 0.011 \\ 0.093 \ 721 \ 5 \pm 0.000 \ 002 \ 7 \\ 0.115 \ 799 \ 2 \pm 0.000 \ 003 \ 9 \end{array}
                                                                                                                                                                      \begin{array}{c} 22.00 \pm 0.10 \\ 0.988806 \pm 0.000074 \\ = 0.971900 \pm 0.000049 \\ 0.9509 \pm 0.0079 \end{array}
                                                                                                                                                                                                                                                                                                                      0.933451 \pm 0.000087
                                                                                                                                                                                                                                                                                                                        0.949\,869\,\pm\,0.000\,074
                                                                                                                                                                                  233.93 \pm 0.52
1.169 \pm 0.012
0.8327 \pm 0.0057
                                                                                                                                                                                                                                                                                                                       0.988770 \pm 0.000074

0.987866 \pm 0.000083

0.914247 \pm 0.000077
                                            0.5815 \pm 0.0022
                                            0.9472 \pm 0.0079
6.258 \pm 0.079
                                               9.334 \pm 0.090
                                                                                                                                                                                        88.52 \pm 0.33
                                                                                                                                                                                                                                                                                                                        0.933426 \pm 0.000087
                             9.534 \pm 0.090
1.08151 \pm 0.00011
0.977449 \pm 0.000052
0.1157962 \pm 0.000038
                                                                                                                                                                          0.987\,809 \pm 0.000\,079
=0.947 816 ± 0.000 065
                                                                                                                                                                                                                                                                                                                            1.59984 \pm 0.00030
                                                                                                                                                                                       6.260 \pm 0.076
7.119 \pm 0.087
                                               0.461 \pm 0.020
                                                                                                                                                                          \begin{array}{c} 7.119 \pm 0.087 \\ 13.20 \pm 0.13 \\ 0.8327 \pm 0.0035 \\ 176.73 \pm 0.44 \\ 283.38 \pm 0.58 \\ 0.914 \, 212 \, \pm \, 0.000 \, 077 \end{array}
                                           0.461 \pm 0.020

267.01 \pm 0.55

30.87 \pm 0.19

7.189 \pm 0.089

12.39 \pm 0.11
```

To assess how accurately we know this average, we consider that we have N=2000 chains of length  $N_L=10^8$  each, and that each of these has its own chain averages

$$\langle \theta_k \rangle_L = \frac{1}{N_L} \sum_{\ell=0}^{N_L-1} \theta_{L,\ell,k}.$$

The ensemble average  $\langle \theta_k \rangle_{\pi(\theta|\hat{z})}$  is of course the average of the chain averages  $\langle \theta_k \rangle_L$  across chains, but the chain averages vary between themselves and we can compute the standard deviation of these chain averages as

stddev 
$$(\langle \theta_k \rangle_L) = \left[ \frac{1}{N} \sum_{L=0}^{N-1} \left( \langle \theta_k \rangle_L - \langle \theta_k \rangle_{\pi(\theta|\hat{z})} \right)^2 \right]^{1/2}.$$

Under standard assumptions, and assuming that the posterior is Gaussian, we can then estimate that we know the ensemble averages  $\langle \theta_k \rangle_{\pi(\theta|\hat{z})}$  to within an accuracy of  $\pm \frac{1}{\sqrt{N}} \text{stddev} (\langle \theta_k \rangle_L)$  with 68% (1-sigma) certainty, and with an accuracy of  $\pm \frac{2}{\sqrt{N}} \text{stddev} (\langle \theta_k \rangle_L)$  with 95% (2-sigma) certainty. In reality, the posterior is not Gaussian (see Section 3.4), and the argument is not true as stated; however, computing 2-sigma values for all parameters is still a useful metric for how accurately we know each of the parameters.

This 2-sigma accuracy is also provided in Table 3.1. For all but parameter  $\theta_{18}$  (for which the relative 2-sigma uncertainty is 4.5%), the relative uncertainty in  $\langle \theta \rangle$  is between 0.003% and 1.3%. In other words, the table provides nearly two certain digits for all but one parameter, and four digits for at least half of all parameters.

For the "white cross", one can make plausible that the likelihood is uninformative and that, consequently, mean value and variances are again determined by the prior. To understand why this is so, one could imagine by analogy what would happen if one could measure the solution  $u(\mathbf{x})$  of (2.2)–(2.3) exactly and everywhere, instead of only at a discrete set of points. In that case, we would have  $u(\mathbf{x}) = z(\mathbf{x})$ , and we could infer the coefficient  $a(\mathbf{x})$  by solving (2.2)–(2.3) for the coefficient instead of for u. This leads to the advection-reaction equation  $-\nabla z(\mathbf{x}) \cdot \nabla a(\mathbf{x}) - (\Delta z(\mathbf{x}))a(\mathbf{x}) = f(\mathbf{x})$ , which is ill-posed and does not provide for a stable solution  $a(\mathbf{x})$  at those places where  $\nabla z(\mathbf{x}) = \nabla u(\mathbf{x}) \approx 0$ . By comparison with Fig. 2.2, we can see that at the location of the white cross, we could not identify the coefficient at one point even if we had measurements available everywhere, and not stably so in the vicinity of that point. We can expect that this is also so in the discrete setting of this benchmark – and that consequently, at this location, only the prior provides information.

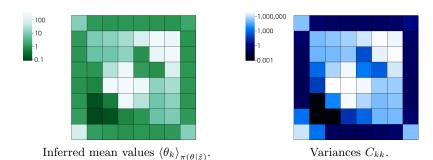


Fig. 3.3. Left: Visualization on an  $8 \times 8$  grid of mean values  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  obtained from our samples. This figure should be compared with the values  $\hat{\theta}$  used as input to generate the "true measurements"  $\hat{z}$  and shown in Fig. 2.2. Right: Variances  $C_{kk}$  of the parameters. Dark colors indicate that a parameter is accurately known; light colors that the variance is large. Standard deviations (the square roots of the variances) are larger than the mean values in some cases because of the heavy tails in the distributions of parameters.

**3.3.** The covariance matrix of  $\pi(\theta|\hat{z})$  and its properties. The second statistic we demonstrate is the covariance matrix,

$$C_{L} = \frac{1}{N_{L} - 1} \sum_{\ell=0}^{N_{L} - 1} \left( \theta_{L,\ell} - \langle \theta \rangle_{\pi(\theta|\hat{z})} \right) \left( \theta_{L,\ell} - \langle \theta \rangle_{\pi(\theta|\hat{z})} \right)^{T},$$

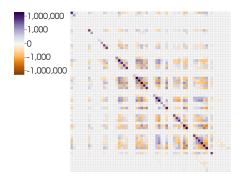
$$C = \frac{1}{N} \sum_{L=0}^{N-1} C_{L}.$$
(3.4)

While conceptually easy to compute, in practice it is substantially harder to obtain accuracy in C than it is to compute accurate means  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$ : While we know the latter to two or more digits of accuracy, see Table 3.1, there is substantial variation between the matrices  $C_L$ .<sup>4</sup> The remainder of this section therefore only provides qualitative conclusions we can draw from our estimate of the covariance matrix, rather than providing quantitive numbers.

First, the diagonal entries of C,  $C_{kk}$ , provide the variances of the statistical distribution of  $\theta_k$ , and are shown on the right of Fig. 3.3; the off-diagonal entries  $C_{k\ell}$  suggest how *correlated* parameters  $\theta_k$  and  $\theta_\ell$  are and are depicted in Fig. 3.4.

In the context of inverse problems related to partial differential equations, it is well understood that we expect the parameters to be highly correlated. This can be understood intuitively given that we are thinking of a membrane model: If we increased the stiffness value on one of the  $8\times 8$  pixels somewhat, but decreased the stiffness value on a neighboring correspondingly, then we would expect to obtain more or less the same global deformation pattern – maybe there are small changes at measurement points close to the perturbation, but for measurement points far away the local perturbation will make little difference. As a consequence, we should expect that  $L(\hat{z}|\theta)\approx L(\hat{z}|\tilde{\theta})$  where  $\theta$  and  $\tilde{\theta}$  differ only in two nearby components, one component of  $\tilde{\theta}$  being slightly larger and the other being slightly smaller than the

<sup>&</sup>lt;sup>4</sup>For diagonal entries  $C_{L,kk}$ , the standard deviation of the variation between chains is between 0.0024 and 37.7 times the corresponding entry  $C_{kk}$  of the average covariance matrix. The variation can be even larger for the many small off-diagonal entries. On the other hand, the average (across chains) difference  $||C_L - C||_F$  is  $0.9||C||_F$ . This would suggest that we don't know very much about these matrices, but as shown in the rest of the section, qualitative measures can be extracted robustly.



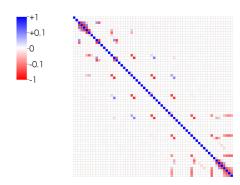
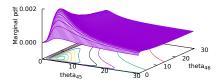


FIG. 3.4. Left: A visualization of the covariance matrix C computed from the posterior probability distribution  $\pi(\theta|\hat{z})$ . The sub-structure of the matrix in the form of  $8\times 8$  tiles represents that geographically neighboring – and consequently correlated – parameters are either a distance of  $\pm 1$  or  $\pm 8$  apart. Right: Correlation matrix  $D_{ij} = \frac{C_{ij}}{\sqrt{C_{ii}}\sqrt{C_{jj}}}$ .



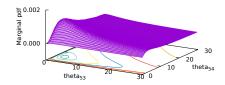


Fig. 3.5. Pairwise marginal probabilities for  $\theta_{45}$  and  $\theta_{46}$  (left) and for  $\theta_{53}$  and  $\theta_{54}$  (right), respectively. See Fig. 2.1 for the relative locations of these parameters. These marginal distributions illustrate the anti-correlation of parameters: If one is large, the other is most likely small, and vice versa.

corresponding component of  $\theta$ . If the changes are small, then we will also have that  $\pi(\theta|\hat{z}) \approx \pi(\tilde{\theta}|\hat{z})$  – in other words, we would expect that  $\pi$  is approximately constant in the secondary diagonal directions  $(0,\ldots,0,+\varepsilon,0,\ldots,0,-\varepsilon,0,\ldots)$  in  $\theta$  space.

On the other hand, increasing (or decreasing) the stiffness value in both of two adjacent pixels just makes the membrane overall more (or less) stiff, and will yield different displacements at all measurement locations. Consequently, we expect that the posterior probability distribution  $\pi(\theta|\hat{z})$  will strongly vary in the principal diagonal directions  $(0,\ldots,0,+\varepsilon,0,\ldots,0,+\varepsilon,0,\ldots 0)$  in  $\theta$  space.

We can illustrate this by computing two-dimensional histograms of the samples for parameters  $\theta_k$  and  $\theta_l$  corresponding to neighboring pixels – equivalent to a two-dimensional marginal distribution. We show such histograms in Fig. 3.5. These also indicate that the posterior probability distribution  $\pi(\theta|\hat{z})$  is definitely not Gaussian – see also Remark 2.3.

A better way to illustrate correlation is to compute a singular value decomposition of the covariance matrix C. Many inverse problems have only a relatively small number of large singular values of C [12,13,22,42,55,59], suggesting that only a finite number of modes is resolvable with the data available – in other words, the problem is ill-posed. Fig. 3.6 shows the singular values of the covariance matrix C for the current case. The data suggests that from the 169 measured pieces of (noisy) data, a deterministic inverse problem could only recover some 25-30 modes of the parameter

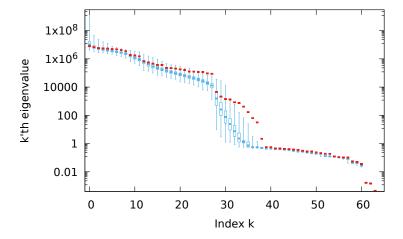


Fig. 3.6. Singular values of the covariance matrix C as defined in (3.4). Red bars indicate eigenvalues of the across-chain averaged covariance matrix. Blue boxes correspond to the 25th and 75th percentiles of the corresponding eigenvalues of the covariance matrices  $C_L$  of individual chains; vertical bars extend to the minimum and maximum across chains for the kth eigenvalue of the matrices  $C_L$ ; blue bars in the middle of boxes indicate the median of these eigenvalues.

vector  $\theta \in \mathbb{R}^{64}$  with reasonable accuracy.<sup>5</sup>

**3.4.** Higher moments of  $\pi(\theta|\hat{z})$ . In some sense, solving Bayesian inverse problems is not very interesting if the posterior distribution  $p(\theta|\hat{z})$  for the parameters is Gaussian, or at least approximately so, because it can be done much more efficiently by computing the maximum likelihood estimator through a deterministic inverse problem, and then computing the covariance matrix via the Hessian of the deterministic (constrained) optimization problem. For example, [55] provides an excellent overview of the techniques that can be used in this case. Because of these simplifications, it is of interest to know how close the posterior density of this benchmark is to a multi-dimensional Gaussian.

To evaluate this question, Fig. 3.7 shows histograms of all of the parameters, using 1000 bins that are equally spaced in logarithmic space; i.e., for each component k, we create 1000 bins between -3 and +3 and sort samples into these bins based on  $\log_{10}(\theta_k)$ . It is clear that many of the parameters have heavy tails and can,

<sup>&</sup>lt;sup>5</sup>The figure shows the spread of each of the eigenvalues of the within-chain matrices  $C_L$  in blue, and the eigenvalues of the across-chain matrix C in red. One would expect the latter to be well approximated by the former, and that is true for the largest and smallest eigenvalues, but not for the ones in the middle. There are two reasons for this: First, each of the  $C_L$  is nearly singular, but because each chain is finite, the poorly explored directions are different from one chain to the next. At the same time, it is clear that the sum of (different) singular matrices may actually be "less singular", with fewer small eigenvalues, and this is reflected in the graph. A second reason is that we computed the eigenvalues of each of the  $C_L$  and ordered them by size when creating the plot, but without taking into account the associated eigenspaces. As a consequence, if one considers the, say, 32nd largest eigenvalue of C, the figure compares it with the 32nd largest eigenvalues of all of the  $C_L$ , when the correct comparison would have been with those eigenvalues of the matrices  $C_L$  whose eigenspace is most closely aligned; this may be an eigenvalue elsewhere in the order, and the effect will likely be the most pronounced for those eigenvalues whose sizes are the least well constrained.

The conclusions to be drawn from Fig. 3.6 are therefore not the actual sizes of eigenvalues, but the number of "large" eigenvalues. This observation is robust, despite the inaccuracies in our determination of C.

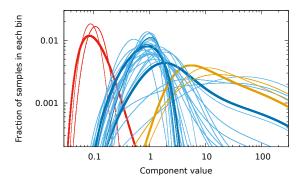


Fig. 3.7. Histograms (marginal distributions) for all 64 components of  $\theta$ , accumulated over all  $2 \times 10^{11}$  samples. The histograms for those parameters whose values were 0.1 for the purposes of generating the vector  $\hat{z}$  are shown in red, those whose values were 10 in orange, and all others in blue. The figure highlights histograms for some of those components  $\theta_k$  whose marginal distributions are clearly neither Gaussian nor log-Gaussian. Note that the histograms were generated with bins whose size increases exponentially from left to right, so that they are depicted with equal size in the figure given the logarithmic  $\theta_k$  axis. Histograms with equal bin size on a linear scale would be more heavily biased towards the left, but with very long tails to the right. See Fig. 3.5 for (pair) histograms using a linear scale.

consequently, not be approximated well by Gaussians. On the other hand, given the prior distribution (2.6) we attached to each of the parameters, it would make sense to conjecture that the logarithms  $log(\theta_k)$  might be Gaussian distributed.

If that were so, the double-logarithmic plot shown in the figure would consist of histograms in the form of parabolas open to the bottom, and again a simpler – and presumably cheaper to compute – representation of  $\pi(\theta|\hat{z})$  would be possible. However, as the figure shows, this too is clearly not the case: While some parameters seem to be well described by such a parabola, many others have decidedly non-symmetric histograms, or shapes that are simply not parabolic. As a consequence, we conclude that the benchmark is at least not boring in the sense that its posterior distribution could be computed in some comparably much cheaper way.

3.5. Rate of convergence to the mean. The data provided in the previous subsections allows checking whether a separate implementation of this benchmark converges to the same probability distribution  $\pi(\theta|\hat{z})$ . However, it does not help in assessing whether it does so faster or slower than the simplistic Metropolis-Hastings method used herein. Indeed, as we will outline in the next section, we hope that this work spurs the development and evaluation of methods that can achieve the same results without needing more than  $10^{11}$  samples.

To this end, let us here provide metrics for how fast our method converges to the mean  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  discussed in Section 3.2. More specifically, if we denote by  $\langle \theta \rangle_{L,n} = \frac{1}{n} \sum_{\ell=0}^{n-1} \theta_{L,\ell}$  the running mean of samples zero to n-1 on chain L, then we are interested in how fast it converges to the mean. We measure this using the following error norm

$$e_{L}(n) = \left\| \operatorname{diag} \left( \langle \theta \rangle_{\pi(\theta|\hat{z})} \right)^{-1} \left( \langle \theta \rangle_{L,n} - \langle \theta \rangle_{\pi(\theta|\hat{z})} \right) \right\|$$

$$= \left[ \left( \langle \theta \rangle_{L,n} - \langle \theta \rangle_{\pi(\theta|\hat{z})} \right)^{T} \operatorname{diag} \left( \langle \theta \rangle_{\pi(\theta|\hat{z})} \right)^{-2} \left( \langle \theta \rangle_{L,n} - \langle \theta \rangle_{\pi(\theta|\hat{z})} \right) \right]^{1/2}. \tag{3.5}$$

The weighting by a diagonal matrix containing the inverses of the estimated parameters  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  (given in Table 3.1 and known to sufficient accuracy) ensures that the large parameters with their large variances do not dominate the value of  $e_L(n)$ . In other words,  $e_L(n)$  corresponds to the "root mean squared relative error".<sup>6</sup>

Fig. 3.8 shows the convergence of a few chains to the ensemble average. While there is substantial variability between chains, it is clear that for each chain  $e_L(n)^2 \to 0$  and, furthermore, that this convergence follows the classic one-over-n convergence of statistical sampling algorithms. Indeed, averaging  $e_L(n)^2$  over all chains,

$$e(n)^2 = \frac{1}{N} \sum_{L=0}^{N-1} e_L(n)^2,$$

the behavior of this decay of the "average" square error  $e(n)^2$  can be approximated by the following formula that corresponds to the orange line in the figure:

$$e(n)^2 \approx \frac{1.9 \times 10^8}{n}.$$
 (3.6)

While we have arrived at the factor  $1.9 \times 10^8$  by fitting a curve "by eye", it turns out – maybe remarkably – that we can also theoretically support this behavior: using the Markov chain central limit theorem [34] (see Appendix C for details), we can estimate the mean of  $ne(n)^2$  by

$$\mathrm{tr}\left(\mathrm{diag}(\langle\theta\rangle_{\pi(\theta|\hat{z})})^{-1}\cdot IAC\cdot\mathrm{diag}(\langle\theta\rangle_{\pi(\theta|\hat{z})})^{-1}\right)\approx 1.9\times 10^8,$$

where the matrix IAC is defined in (3.2).

If one measures computational effort by how many times an algorithm evaluates the probability distribution  $\pi(\theta|\hat{z})$ , then n in (3.5) can be interpreted as work units and (3.6) provides an approximate relationship between work and error. Similar relationships can be obtained experimentally for other sampling algorithms that we hope this benchmark will be used for, and (3.6) therefore allows comparison among other algorithms as well as against the one used here.

4. Conclusions and what we hope this benchmark achieves. As the data presented in the previous section illustrates, it is possible to obtain reasonably accurate statistics about the Bayesian solution of the benchmark introduced in Section 2, even using a rather simple method: The standard Metropolis-Hastings sampler. At the same time, using this method, it is not at all trivial to compute posterior statistics accurately: We had to compute  $2 \times 10^{11}$  samples, and expended 30 CPU years on this task (plus another two CPU years on postprocessing the samples).

But all of this also makes this a good benchmark: Simple algorithms, with known performance, can solve it to a reasonable accuracy, and more advanced algorithms should be able to do so in a fraction of time without making the test case trivial. For example, it is not unreasonable to hope that advanced sampling software [1,19,37,40], using multi-level and multi-fidelity expansions [20,23,41,45], and maybe in conjunction with methods that exploit the structure of the problem to approximate covariance matrices [55], might be able to reduce the compute time by a factor of 100 to 1000,

 $<sup>^6\</sup>mathrm{A}$  possibly better choice for the weighting would be to use the inverses of the diagonal entries of the covariance matrix – i.e., the variances of the recovered marginal probability distributions of each parameter. However, these are only approximately known – see the discussion in Section 3.3 – and consequently do not lend themselves for a concise definition of a reproducible benchmark.

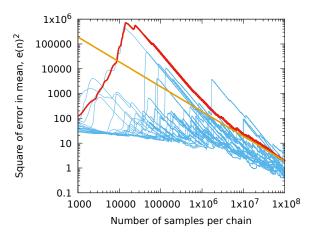


FIG. 3.8. Convergence of the square of the relative error  $e_L(n)^2$  between the running mean up to sample n and the true mean  $\langle \theta \rangle_{\pi(\theta|z)}$ , measured in the weighted norm (3.5), for a subset of chains. The thick red curve corresponds to the average of these squared errors over all chains. This average squared error is dominated by some chains with large errors and so lies above the curves  $e_L(n)^2$  of most chains. The thick orange line corresponds to the decay  $\frac{1.9 \times 10^8}{n}$  and represents an approximately average convergence behavior of the chains.

possibly also running computations in parallel. This would move characterizing the performance of such algorithms for the case at hand to the range of a few hours or days on moderately parallel computers; practical computations might not actually need the same level of accuracy and could be solved even more rapidly.

As a consequence of these considerations, we hope that providing a benchmark that is neither too simple nor too hard, and for which the solution is known to good accuracy, spurs research in the development of better sampling algorithms for Bayesian inverse problems. Many such algorithms of course already exist, but in many cases, their performance is not characterized on standardized test cases that would allow a fair comparison. In particular, their performance is often characterized using probability distributions whose characteristics have nothing to do with those that result from inverse problems – say, sums of Gaussians. By providing a standardized benchmark that matches what we expect to see in actual inverse problems – along with an open source implementation of a code that computes the posterior probability function  $\pi(\theta|\hat{z})$  (see Appendix A) – we hope that we can contribute to more informed comparisons between newly proposed algorithms: Specifically, that their performance can be compared with the relationship shown in (3.6) and Fig. 3.8 to provide a concrete factor of speed-up over the method used here.

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with Mantautas Rimkus and Dawson Eliasen on the SampleFlow library that was used for the statistical evaluation of samples. Finally, the feedback given by Noemi Petra, Umberto Villa, and Danny Long are acknowledged with gratitude.

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Appendix A. An open source code to sample  $\pi(\theta|\hat{z})$ . We make a code that implements this benchmark available as part of the "code gallery" for DEAL.II at https://dealii.org/developer/doxygen/deal.II/code\_gallery\_MCMC\_Laplace.html, using the name MCMC-Laplace, and using the Lesser GNU Public License (LGPL) version 2.1 or later as the license. DEAL.II is a software library that provides the basic tools and building blocks for writing finite element codes that solve partial differential equations numerically. More information about DEAL.II is available at [4, 5]. The DEAL.II code gallery is a collection of programs based on DEAL.II that were contributed by users as starting points for others' experiments.

The code in question has essentially three parts: (i) The forward solver that, given a set of parameters  $\theta$ , produces the output  $z^{\theta}$  using the map discussed in Section 2.2.1; (ii) the statistical model that implements the likelihood  $L(z|\theta)$  and the prior probability  $\pi_{\rm pr}(\theta)$ , and combines these to the posterior probability  $\pi(\theta|\hat{z})$ ; and (iii) a simple Metropolis-Hastings sampler that draws samples from  $\pi(\theta|\hat{z})$ . The second of these pieces is quite trivial, encompassing only a couple of functions; we will therefore only comment on the first and the third piece below.

**A.1. Details of the forward solver.** The forward solver is a C++ class whose main function performs the following steps:

- 1. It takes a 64-dimensional vector  $\theta$  of parameter values, and interprets it as the coefficients that describe a piecewise constant field  $a(\mathbf{x})$ ;
- 2. It assembles a linear system that corresponds to the finite element discretization of equations (2.2)–(2.3) using a  $Q_1$  (bilinear) element on a uniformly refined mesh;
- 3. It solves this linear system to obtain the solution vector  $U^{\theta}$  that corresponds to the function  $u_h^{\theta}(\mathbf{x})$ ; and
- 4. It evaluates the solution  $u_h^{\theta}$  at the measurement points  $\mathbf{x}_k$  to obtain  $z^{\theta}$ . It then returns  $z^{\theta}$  to the caller for evaluation with the statistical model.

Such a code could be written in DEAL.II with barely more than 100 lines of C++ code, and this would have been sufficient for the purpose of evaluating new ideas of sampling methods. However, we wanted to draw as large a number of samples as possible, and consequently decided to see how fast we can make this code.

To this end, we focused on accelerating three of the operations listed above, resulting in a code that can evaluate  $\pi(\hat{z}|\theta)$  in 4.5 ms on an Intel Xeon E5-2698 processor with 2.20GHz (on which about half of the samples used in this publication were computed), 3.1 ms on an AMD EPYC 7552 processor with 2.2 GHz (the other half), and 2.7 ms on an Intel Core i7-8850H processor with 2.6 GHz in one of the authors' laptops.

The first part of the code that can be optimized for the current application uses the fact that the linear system that needs to be assembled is the sum of contributions from each of the cells of the mesh. Specifically, the contribution from cell K is

$$A^K = P_K^T A_{\text{local}}^K P_K$$

where  $P_K$  is the restriction from the global set of degrees of freedom to only those degrees of freedom that live on cell K, and  $A_{\text{local}}^K$  is – for the  $Q_1$  element used here –

a  $4 \times 4$  matrix of the form

$$(A_{\text{local}}^K)_{ij} = \int_K a^{\theta}(\mathbf{x}) \nabla \varphi_i(\mathbf{x}) \cdot \nabla \varphi_j(\mathbf{x}) \, \mathrm{d}x.$$

This suggests that the assembly, including the integration above that is performed via quadrature, has to be repeated every time we consider a new set of parameters  $\theta$ . However, since we discretize  $u_h$  on a mesh that is a strict refinement of the one used for the coefficient  $a^{\theta}(\mathbf{x})$ , and because  $a^{\theta}(\mathbf{x})$  is piecewise constant, we can note that

$$(A_{\text{local}}^K)_{ij} = \theta_{k(K)} \underbrace{\int_K \nabla \varphi_i(\mathbf{x}) \cdot \nabla \varphi_j(\mathbf{x}) \, \mathrm{d}x}_{(A_{\text{local}})_{ij}},$$

where k(K) is the index of the element of  $\theta$  that corresponds to cell K. Here, the matrix  $A_{\text{local}}$  no longer depends on  $\theta$  and can, consequently, be computed once and for all at the beginning of the program. Moreover,  $A_{\text{local}}$  does not actually depend on the cell K as long as all cells have the same shape, as is the case here. We therefore have to store only one such matrix. This approach makes the assembly substantially faster since we only have to perform the local-to-global operations corresponding to  $P_K$  on every cell for every new  $\theta$ , but no longer any expensive integration/quadrature.

Secondly, we have experimented with solving the linear systems so assembled as fast as possible. For the forward solver used for each sample, the size of these linear systems is  $1089 \times 1089$ , with at most 9 entries per row. Following a substantial amount of experimentation, we found that a sparse direct solver is faster than any of the other approaches we have tried, and we use the UMFPACK [18] interfaces in DEAL.II for this purpose. In particular, this approach is faster than attempting to use an algebraic multigrid method as a solver or preconditioner for the Conjugate Gradient method. We have also tried to use a sparse decomposition via UMFPACK as a preconditioner for the CG method, updating the decomposition only every few samples – based on the assumption that the samples change only relatively slowly and so a decomposition of the matrix for one sample is a good preconditioner for the matrix corresponding to a subsequent sample. However, this turned out to be slower than using a new decomposition for each sample.

The linear solver described above consumes about 90% of the time necessary to evaluate each sample. As a consequence, there is certainly further room for improvements. After all numerical results had been generated for this publication, we have followed up on a suggestion by Martin Kronbichler to replace the linear solver by a conjugate gradient method preconditioned by an incomplete LU decomposition. This accelerates the computations by about a factor of three, from 2.7 ms to less than 0.9 ms per sample on the Intel Core i7-8850H processor mentioned above. It is this accelerated version that is available at the website mentioned above; we have verified that the new version results in the same results up to at least 11 digits in computing the posterior probability using the techniques mentioned in Appendix A.4.

Finally, evaluating the solution of a finite element field  $u_h(\mathbf{x})$  at arbitrary points  $\mathbf{x}_k$  is an expensive operation since one has to find which cell K the point belongs to and then transform this point into the reference coordinate system of the cell K. On the other hand, the point evaluation is a linear and bounded operation, and so there must exist a vector  $m_k$  so that  $u_h(\mathbf{x}_k) = m_k \cdot U$  where U is the vector of coefficients that describe  $u_h$ . This vector  $m_k = (\varphi_i(\mathbf{x}_k))_{i=0}^{1089-1}$  can be computed once and for all. The computation of  $z = (u_h(\mathbf{x}_k))_{k=0}^{169-1}$  can then be facilitated by building a matrix

M whose rows are the vectors  $m_k$ , and then the evaluation at all measurement points reduces to the operation z = MU. M is a sparse matrix with at most 4 entries per row, making this a very economical approach.

The code with all of these optimizations is not very large – it contains  $197 \text{ semi-colons.}^7$ 

**A.2.** Details of the Metropolis-Hastings sampler. The steps described at the start of this appendix yield an algorithm that, given a sample  $\theta$ , can evaluate  $\pi(\theta|\hat{z})$ . We use this functionality to drive a Metropolis-Hastings sampler to obtain a large number of samples characterizing the posterior probability distribution.

While the basic algorithm of the Metropolis-Hastings sampler is well known [32, 35], its practical implementation depends crucially on a number of details that we will describe in the following.

First, we start the sampling process with a fixed sample  $\theta_0 = (1, ..., 1)^T$ , corresponding to a coefficient  $a^{\theta}(\mathbf{x}) = 1$ .

Secondly, an important step in the Metropolis-Hastings algorithm is the generation of a "trial" sample  $\tilde{\theta}_{\ell}$  based on the current sample  $\theta_{\ell}$ . To this end, we use the following strategy: We define the components of  $\tilde{\theta}_{\ell,k}$  of  $\tilde{\theta}_{\ell}$  as

$$\tilde{\theta}_{\ell,k} = e^{\ln(\theta_{\ell,k}) + \xi_k} = \theta_{\ell,k} e^{\xi_k},$$

where  $\xi_k$ ,  $k = 0, \dots, 63$ , are iid Gaussians with mean 0 and standard deviation  $\sigma_{\text{prop}}$ . In other words, the "proposal distribution" for the trial samples is an isotropic Gaussian ball centered at  $\theta_{\ell}$  in log space. This has the effect that all elements of samples always stay positive, as one would expect given that they correspond to material stiffness coefficients. The use of a ball in log space is also consistent with the description of our prior probability distribution in Section 2.2.3, which is also defined in log space.

To compute the Metropolis-Hastings acceptance probability, we first need to compute the proposal probability density. By definition

$$\begin{split} \mathbb{P}(\tilde{\theta}_{\ell,k} \leq \tilde{t}_k | \theta_{\ell,k} = t_k) &= \mathbb{P}(t_k e^{\xi_k} \leq \tilde{t}_k) \\ &= \mathbb{P}(\xi_k \leq \log \tilde{t}_k - \log t_k) \\ &= \frac{1}{\sqrt{2\pi\sigma_{\text{prop}}^2}} \int_{-\infty}^{\log \tilde{t}_k - \log t_k} \exp\left(\frac{-x^2}{2\sigma_{\text{prop}}^2}\right) \, dx. \end{split}$$

The probability density  $p_{\text{prop}}(\tilde{\theta}_{\ell,k}|\theta_{\ell,k})$  of proposing  $\tilde{\theta}_{\ell,k}$  given  $\theta_{\ell,k}$  is then the derivative of this expression with respect to  $\tilde{t}_k$ , with  $\tilde{\theta}_{\ell,k}$  and  $\theta_{\ell,k}$  in place of  $\tilde{t}_k$  and  $t_k$ :

$$p_{\text{prop}}(\tilde{\theta}_{\ell,k}|\theta_{\ell,k}) = \frac{1}{\tilde{\theta}_{\ell,k}} \frac{1}{\sqrt{2\pi\sigma_{\text{prop}}^2}} \exp\left(\frac{-(\log \tilde{\theta}_{\ell,k} - \log \theta_{\ell,k})^2}{2\sigma_{\text{prop}}^2}\right).$$

By definition, the components  $\tilde{\theta}_{\ell,k}$  of the proposal vector  $\tilde{\theta}_{\ell}$  are independent conditional on the current state  $\theta_{\ell}$ . Thus the joint probability density,  $p_{\text{prop}}(\tilde{\theta}_{\ell}|\theta_{\ell})$ , of

<sup>&</sup>lt;sup>7</sup>Counting semicolons is a commonly used metric in C and C++ programs. It roughly coincides with the number of declarations and statements in a program, and is a better metric for *code size* than the number of lines of code, as the latter also includes comments and empty lines used to help the readability of a code.

proposing vector  $\tilde{\theta}_{\ell}$  given vector  $\theta_{\ell}$  is the product of the probabilities above:

$$p_{\text{prop}}(\tilde{\theta}_{\ell}|\theta_{\ell}) = \frac{1}{\prod_{k=0}^{63} \tilde{\theta}_{\ell,k}} \times \frac{1}{(2\pi\sigma_{\text{prop}}^2)^{32}} \exp\left(-\frac{\sum_{k=0}^{63} (\log \tilde{\theta}_{\ell,k} - \log \theta_{\ell,k})^2}{2\sigma_{\text{prop}}^2}\right).$$

The Metropolis-Hastings acceptance probability,  $A(\tilde{\theta}_{\ell}|\theta_{\ell})$ , to accept proposal  $\tilde{\theta}_{\ell}$  given the current state  $\theta_{\ell}$ , is then

$$\begin{split} A(\tilde{\theta}_{\ell}|\theta_{\ell}) &= \min \left\{ 1, \frac{\pi(\tilde{\theta}_{\ell}|\hat{z})}{\pi(\theta_{\ell}|\hat{z})} \times \frac{p_{\text{prop}}(\theta_{\ell}|\tilde{\theta}_{\ell})}{p_{\text{prop}}(\tilde{\theta}_{\ell}|\theta_{\ell})} \right\} \\ &= \min \left\{ 1, \frac{\pi(\tilde{\theta}_{\ell}|\hat{z})}{\pi(\theta_{\ell}|\hat{z})} \times \prod_{k=0}^{63} \frac{\tilde{\theta}_{\ell,k}}{\theta_{\ell,k}} \right\}. \end{split}$$

As usual, with probability  $A(\tilde{\theta}_{\ell}|\theta_{\ell})$  the proposal  $\tilde{\theta}_{\ell}$  is accepted, in which case it becomes the next sample  $\theta_{\ell+1} = \tilde{\theta}_{\ell}$ ; otherwise the proposal is rejected and we keep the current sample,  $\theta_{\ell+1} = \theta_{\ell}$ .

In our experiments, we use  $\sigma_{\text{prop}} = 0.0725$ , corresponding to changing  $\theta$  by a factor  $e^{\xi}$  that with 65% probability lies within the range  $[e^{-\sigma_{\text{prop}}}, e^{+\sigma_{\text{prop}}}] = [0.93, 1.075]$ . This results in an acceptance rate for the Metropolis-Hastings algorithm of just under 24%. This is close to the recommended value of 0.234 for Metropolis-Hastings sampling algorithms that can be derived for specific probability distributions that are generally simpler than the one we are interested in here [27,46]; the theory guiding the derivation of the 0.234 value may not be applicable here (see [10]), but absent better guidance, we stuck with it.

Finally, all steps in the Metropolis-Hastings algorithms that require the use of a random number use the MT19937 random number generator, as implemented by C++11 compilers in the std::mt19937 class.

A.3. Implementations of the benchmark in alternative languages. We consider the C++ implementation discussed above as the "reference implementation" of the benchmark. However, we recognize that it is rather heavy-weight in the sense that it requires the installation of the DEAL.II library. While this readily facilitates otherwise non-trivial modifications (e.g., for multilevel sampling schemes that require the solution of the forward problem on coarser meshes), it is clear that for simple experiments, it would be nice to have stand-alone implementations of the benchmark.

As a consequence, we have also developed Matlab and Python versions of the benchmark. These are available from the same website from which the C++ implementation is available – see the link at the top of the appendix. These alternative implementations provide everything one needs to build a sampler: Namely, the functionality to provide an input vector  $\theta$  and to compute the prior  $\pi_{\rm pr}(\theta)$  and the likelihood  $L(\hat{z}|\theta)$  from such an input. Using (2.1), these can then be used to compute the posterior probability  $\pi(\theta|\hat{z})$  that forms the basis of most sampling algorithms. The Matlab version includes a basic Metropolis-Hastings sampler with parallel functionality.

On a recent laptop, the Matlab version is able to compute the posterior probability for a sample in about 4 ms, not substantially slower than the C++ version we have used for our results. The Python version – although an almost literal transcription of the Matlab version – requires approximately 25 ms. One imagines that it could be optimized further (for example, a substantial part of the run time is spent in the

insertion of the cell-local  $4 \times 4$  matrices into the global matrix), but we have not attempted to do so.

**A.4. Testing of alternative implementations.** In order to facilitate testing of alternative implementations such as the ones discussed in the previous section (or testing modifications made to the C++ implementation itself), the website from which the benchmark can be obtained (see the top of this appendix) also contains a set of known input/output pairs. Specifically, it contains files for ten different input vectors  $\theta$ , along with the corresponding outputs  $z^{\theta}$ , likelihood  $L(\hat{z}|\theta)$ , and prior  $\pi_{\rm pr}(\theta)$  for each input vector. The latter two can be combined via (2.1) to the posterior probability  $\pi(\theta|\hat{z})$  associated with the input vector  $\theta$ .

We have used these known input/output pairs obtained from our reference implementation to verify that the alternative implementations of the benchmark discussed in the previous sub-section are correct. For example, the Matlab implementation provides the vectors  $z^{\theta}$  to relative errors on the order of  $10^{-13}$ ; log priors and likelihoods are computed to relative errors less than  $10^{-11}$ . The Python version achieves the same level of accuracy.

Appendix B. One dimensional version of the benchmark. Many of the features of the posterior probability on the 64-dimensional parameter space that we have experimentally observed in Section 3 match those that one would expect for inverse problems of the kind discussed herein. In particular, the fact that we have a large spread between the large and small eigenvalues of the covariance matrix, the non-Gaussianity of the probability distribution, and the anticorrelation of parameters defined on neighboring cells did not come as a surprise. Yet, strict proofs for these properties are hard to come by.

At the same time, we can investigate an analogous situation in a one-dimensional model with parameters  $\theta_k$ , for which one can derive the posterior probability distribution analytically. In this Appendix, we work out some details of a one-dimensional version of the benchmark. Consider the generalized Poisson equation

$$-\frac{d}{dx}\left(a(x)\frac{du}{dx}(x)\right) = f(x), \qquad 0 < x < 1, \qquad (B.1)$$

$$u(x) = 0,$$
  $x \in \{0, 1\}.$  (B.2)

Again we assume  $a(x) = a^{\theta}(x)$  is parametrized by  $\theta = (\theta_0, \dots, \theta_{N-1})$  where

$$a(x) = \theta_k, \quad \text{if} \quad \frac{k}{N} < x < \frac{k+1}{N},$$
 (B.3)

and we take  $f(x) \equiv 1$ . The solution to (B.1) is then of the form

$$u(x) = -\int_0^x \frac{y+c}{a(y)} \, dy,\tag{B.4}$$

where c is constant determined by requiring u(1) = 0. Due to the piecewise constant form of a = a(x), this rewrites as

$$u(x) = u_k(x) := -\frac{1}{\theta_k} \left( \frac{x^2}{2} + cx \right) + d_k, \quad \text{if} \quad \frac{k}{N} < x < \frac{k+1}{N}.$$
 (B.5)

There are N-1 continuity constraints and two boundary conditions, namely,

$$u_{k-1}\left(\frac{k}{N}\right) = u_k\left(\frac{k}{N}\right), \qquad k = 1, \dots, N-1,$$
 (B.6)

$$u_0(0) = 0, \quad u_{N-1}(1) = 0.$$
 (B.7)

This translates, via (B.5), into N+1 linear equations for the N+1 coefficients  $c,d_0,\ldots,d_{N-1}$ . The boundary conditions show that

$$d_0 = 0, c = -\frac{\int_0^1 \frac{y}{a(y)} dy}{\int_0^1 \frac{1}{a(y)} dy} = -\frac{1}{2N} \frac{\sum_{k=0}^{N-1} \theta_k^{-1} (2k+1)}{\sum_{k=0}^{N-1} \theta_k^{-1}}. (B.8)$$

The remaining N-1 equations for  $d_1, \ldots, d_{N-1}$  can be solved using the continuity constraints, which give the equations

$$d_{k-1} - d_k = \left(\frac{1}{2} \left(\frac{k}{N}\right)^2 + c\frac{k}{N}\right) \left(\theta_{k-1}^{-1} - \theta_k^{-1}\right), \qquad k = 1, \dots, N - 1,$$
 (B.9)

which have solution

$$d_k = -\sum_{j=1}^k \left(\frac{1}{2} \left(\frac{j}{N}\right)^2 + c\frac{j}{N}\right) \left(\theta_{j-1}^{-1} - \theta_j^{-1}\right), \qquad k = 1, \dots, N-1.$$

Let us specifically consider the case with N=2 parameters to understand some qualitative features of the benchmark. In this case,  $c=-\frac{1}{4}(3\theta_0+\theta_1)/(\theta_0+\theta_1)$  and

$$u_0(x) = -\frac{x^2}{2\theta_0} + \frac{3\theta_0 + \theta_1}{4\theta_0(\theta_0 + \theta_1)}x, \qquad u_1(x) = -\frac{x^2}{2\theta_1} + \frac{3\theta_0 + \theta_1}{4\theta_1(\theta_0 + \theta_1)}x + \frac{\theta_1 - \theta_0}{4\theta_1(\theta_0 + \theta_1)}.$$

This solution is shown in Fig. B.1.

Let us assume that we have measurements at  $x_0 = 0.25$  and  $x_1 = 0.75$ . Then the "exact" measurements we would get are<sup>8</sup>

$$\hat{z}_0 = -\frac{x_0^2}{2\theta_0} + \frac{3\theta_0 + \theta_1}{4\theta_0(\theta_0 + \theta_1)} x_0, \qquad \hat{z}_1 = -\frac{x_1^2}{2\theta_1} + \frac{3\theta_0 + \theta_1}{4\theta_1(\theta_0 + \theta_1)} x_1 + \frac{\theta_1 - \theta_0}{4\theta_1(\theta_0 + \theta_1)}.$$

We can use these values to exactly and cheaply evaluate the posterior probability (without sampling), and Fig. B.2 shows  $\pi(\theta|\hat{z})$  in this simple case, using "true" parameters  $\hat{\theta}_0 = 0.1$  and  $\hat{\theta}_1 = 1$  to define  $\hat{z}$ . We use the prior and likelihoods defined before, with the prior standard deviation  $\sigma_{\rm pr} = 2$  and two different values for the likelihood standard deviations used in (2.5):  $\sigma = 0.01$  and  $\sigma = 0.1$ .

The figure illustrates more concisely the strong correlation between parameters that we have experimentally observed in Fig. 3.5. It also illustrates that if  $\sigma$  in the likelihood (2.5) is chosen small (i.e., if the measurement error is small), then the posterior is approximately Gaussian. The observation here therefore validates our choice of a relatively large  $\sigma$ , see also Remark 2.3.

Appendix C. Estimating the essential sample size. Section 3.1 assessed how much information is actually present in the many samples we have computed,

<sup>&</sup>lt;sup>8</sup>Unlike in Section 2, these values are computed using the exact solution, instead of a finite element approximation.

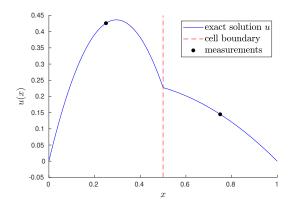


FIG. B.1. Exact solution to (B.1)–(B.2) when a(x)=0.1 for 0< x<1/2 and a(x)=1 for 1/2< x<1, corresponding to "true" parameters  $\hat{\theta}_0=0.1$  and  $\hat{\theta}_1=1$ , with measurements at  $x_0=0.25$  and  $x_1=0.75$ .

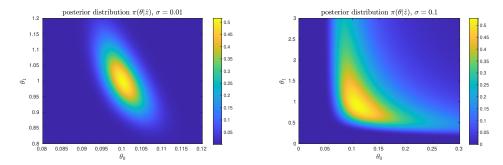


Fig. B.2. Left: Non-normalized posterior distribution  $\pi(\theta|\hat{z})$  when  $\sigma=0.01$  in the 1D model. Notice the distribution is approximately Gaussian for this very small  $\sigma$ . Right: When using  $\sigma=0.1$  in the 1D model. For this larger value of  $\sigma$ , the posterior distribution extends to larger values of  $\theta_0$  and  $\theta_1$ , and has a non-Gaussian, "banana" shape, reminiscent of the pair histograms in Fig. 3.5.

and we have also used the results shown there in providing theoretical support for the key cost-accuracy estimate (3.6). Many of the statistical errors described there can be estimated from the autocovariance  $AC_L(s)$  defined in (3.1). The basis for this is the Markov chain central limit theorem. Informally, the Markov chain central limit theorem says that, for large n and  $N_L$ , the running means  $\langle \theta \rangle_{L,n}$  are approximately normally distributed with mean  $\langle \theta \rangle_{\pi(\theta|\hat{z})}$  and covariance

$$\operatorname{Cov}\left(\langle\theta\rangle_{L,n}\right) \approx \frac{IAC}{n},$$
 (C.1)

where IAC is the integrated autocovariance, obtained by summing up the autocovariance  $AC_L(s)$ ; we estimate IAC from the data in (3.2). Equation (C.1) then justifies the formula for the scaling of  $e(n)^2$  below (3.6).

To establish the effective sample size formula (3.3), we cite the "Delta method" in statistics [58]. Informally, the Delta method states that, for large n and  $N_L$ , a continuously differentiable function f of the running means is nearly normally distributed with variance

$$\operatorname{Var}(f(\langle \theta \rangle_{L,n})) \approx \frac{1}{n} \nabla f(\langle \theta \rangle_{\pi(\theta|\hat{z})})^T \cdot IAC \cdot \nabla f(\langle \theta \rangle_{\pi(\theta|\hat{z})}), \tag{C.2}$$

provided  $\nabla f(\langle \theta \rangle_{\pi(\theta|\hat{z})})$  is nonzero. The formula (C.2) is obtained by Taylor expanding f and applying the Markov chain central limit theorem. For a Markov chain in which successive samples are all independent, IAC is the covariance matrix, which we estimate from the data in (3.4) and denote by C. Using a standard result on generalized Rayleigh quotients,

$$\frac{\nabla f(\langle \theta \rangle_{\pi(\theta|\hat{z})})^T \cdot IAC \cdot \nabla f(\langle \theta \rangle_{\pi(\theta|\hat{z})})}{\nabla f(\langle \theta \rangle_{\pi(\theta|\hat{z})})^T \cdot C \cdot \nabla f(\langle \theta \rangle_{\pi(\theta|\hat{z})})} \leq \max_{x \neq 0} \frac{x^T \cdot IAC \cdot x}{x^T \cdot C \cdot x} = \lambda_{\max}(C^{-1} \cdot IAC),$$

where  $\lambda_{\text{max}}$  denotes the largest eigenvalue. This means that the variance (C.2) is at most  $\lambda_{\text{max}}(C^{-1} \cdot IAC)$  times the value it would take if all of the samples on chain L were independent. In other words, the minimum number of "effectively independent samples" is approximately  $N_L/\lambda_{\text{max}}(C^{-1} \cdot IAC)$  for each of our chains of length  $N_L$ .

It is quite standard to quantify statistical error in Markov chain Monte Carlo simulations by using the integrated autocovariance [28,47]. In the literature, it is also common to determine an effective sample size by checking to see where autocovariances cross a certain threshold – such as a small percentage of its initial value – as we have done in Figure 3.1 above, where we used a threshold of 1%.

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