BAYESIAN ESTIMATION OF MULTISCALE STRUCTURES IN A BINARY MEDIUM FROM SPARSE OBSERVATIONS

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Summary. We present a multiscale Bayesian method to reconstruct the permeability field of a binary medium. The reconstruction is conditioned on measurements of permeability and tracer test breakthrough times, observed at a limited set of locations. The medium consists of a spatially variable distribution of inclusions, which are too small to be individually resolved at the grid scale. The unknown inclusion proportion is modeled using a multivariate Gaussian, represented using a truncated Karhunen-Loève transformation to reduce dimensionality. An upscaling model is used for the permeability, which is parameterized by the inclusion size. Along with a Darcy flow model, we formulate a Bayesian inverse problem for the Karhunen-Loève modes' weights. The posterior distribution is calculated using an adaptive Markov chain Monte Carlo method and demonstrates that breakthrough times contain information on the small-scale structures. The inclusion sizes can be estimated accurately in certain cases. By selecting a few members of an ensemble of permeability fields consistent with the data, breakthough times at the sensor points are predicted. We combine them using Bayesian Model Averaging and find that the model-averaged ensemble can be predictive over the domain.

1 INTRODUCTION

Many porous media have small, dispersed inclusions in them that impact permeability or other material properties. These materials can be approximated as binary media, if the properties of the two phases are vastly (orders of magnitude) different. The spatial distribution of the inclusions and their size are often central to material property estimation. However, in the context of limited observations, this becomes a challenge – the spatial

distribution may not be smooth and the inclusion size is generally much smaller than the grid resolution. The estimation can be performed if assisted by multiscale modeling, for example, if the inclusion proportion $\mathbf{F}(\mathbf{x})$ can be modeled using a smooth latent variable $\zeta(\mathbf{x})$, which in turn is represented by a multivariate Gaussian. Further, the impact of fine-scale unresolved inclusions can be incorporated into the permeability field, at the grid-block scale, using upscaling. The authors have developed such a procedure [1]. The method is multiscale, in the sense that resolved spatial structures are estimated along with summary statistics of the unresolved ones (the inclusion size δ), and it integrates observations made at separate scales. The method is Bayesian and probabilistically reconstructs the $\mathbf{F}(\mathbf{x})$ field and δ as a joint distribution. The binary medium was discretized with a 30×20 grid and the multiGaussian field, on this grid, was represented using a 30-term Karhunen-Loève expansion, predicated on a prior covariance. This achieved a considerable reduction in problem dimensionality and the inverse problem involved estimating 31 independent parameters (weights of the Karhunen-Loève modes and the δ). This was performed using a Delayed Rejection Adaptive Metropolis (DRAM) [2] sampler. The observations consisted of grid-block scale measurements of permeability ("static") and tracer breakthrough times ("dynamic") from a tracer test at 20 "sensor" points. It was found that the dynamic data was primarily useful for estimating small-scale (partially resolved) spatial structures, and δ was under-estimated. The grid-scale probabilistic reconstruction was used to develop realizations of the binary medium (matrix and inclusions, with a $100\times$ higher permeability) on a fine 3000×2000 mesh, consistent with observations.

In this paper we investigate the conditions under which δ can be estimated and the accuracy of estimation. We also explore whether it is the static or dynamic data that contributes to estimation. Finally, we explore if a small set (of size ≈ 20) of fine-scale binary medium realizations could be combined into a cheap surrogate model to provide probabilistic predictions of the breakthrough time. This would present a contrast to the expense of running multiple (thousands) flow simulations on a 3000×2000 mesh.

Note that the estimation problem mentioned above cannot be solved using multiscale estimation methods based on multiscale finite elements [3] or multi-level models [4, 5] since they resolve (not model) all the estimated structures.

2 PROBLEM STATEMENT

The detailed description of the problem is available in [1] and we provide a summary here. We are given a rectangular binary domain with a spatially variable distribution of the high-prmeability phase $\mathbf{F}(\mathbf{x}), 0 \leq \mathbf{F}(\mathbf{x}) \leq 1$ (and consequently permeability $\mathbf{K}$). The domain is discretized with a 30×20 mesh and has two sets of sensors (SSA, with 20 sensors and SSB, with 34) where permeabilities and tracer breakthrough times are measured (Fig. 1). The inclusions are too small to be resolved and so, the 30×20 grid supports an upscaled permeability field. $\mathbf{F}(\mathbf{x})$ is obtained by an analytical mapping from $\zeta(\mathbf{x})$, a multiGaussian, whose prior covariance is used to obtain its 30-term Karhunen-Loève expansion. The weights of the expansion are the objects of inference.
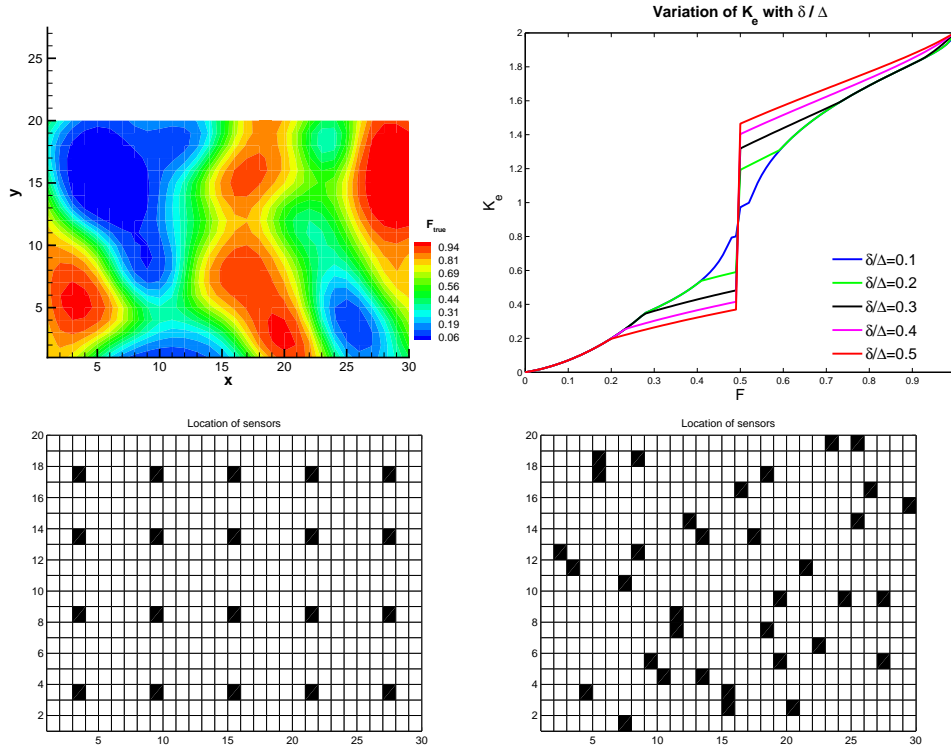
Figure 1: Top left: Distribution of inclusion $\mathbf{F}(\mathbf{x})$ in the domain. Top right: Variation of the effective log-permeability $\mathbf{K}_e$ of a grid-block with $\mathbf{F}(\mathbf{x})$ and δ. Δ is the grid-block size. Bottom left: The SSA set of 20 sensors. Bottom right: The SSB set of 34 sensors.

In a given grid-block, the inclusion proportion is related to the log-permeability field using an upscaling model $\mathbf{K}_e(\mathbf{F}, \delta)$. $\mathbf{K}_e$ is a closed-form expression and its description is in [6]. It represents the sub-grid-block field using a correlated noise field (with δ as correlation length), which is truncated at a given noise level. The excursion sets so formed, of sizes that scale with δ, are designated as the inclusions. The truncation level is determined by $\mathbf{F}$. Thus given a proposed δ and $\mathbf{F}(\mathbf{x})$ (more accurately, $\mathbf{w}$, the weights of the Karhunen-Loève modes, from which $\boldsymbol{\zeta}(\mathbf{x})$ and $\mathbf{F}(\mathbf{x})$ can be constructed), we construct a log-permeability field $\mathbf{K}(x)$. This field is used with a finite-difference Darcy flow model to predict breakthrough times. The observed and predicted breakthrough times and log-transformed permeabilities are compared and their differences are modeled as i.i.d. Gaussian errors ([1]). Base 10 is used for log-transformation and consequently the $100\times$ contrast in permeabilities of the matrix and inclusion leads to $0 \leq \mathbf{K} \leq 2$. The prior distribution for $\ln(\delta)$ is a truncated Gaussian, which restricts the inclusion size to less than a grid-block but larger than a hundredth of it. The 31-dimensional parameter space is explored using DRAM, and a joint degree distribution is constructed. 10,000 samples from the posterior distribution, retained by thinning the samples, are used to generate

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an ensemble of permeability fields on the 30×20 mesh. Applying the upscaling model in reverse, we also generate realizations of the binary field, with discrete inclusions, on a 3000×2000 mesh.

In this work, we concentrate on estimating δ. Fig. 1 (top right) shows the response of $\mathbf{K}_e$ with respect to $\mathbf{F}$ and δ. The permeability shows marked sensitivity to δ/Δ near $\mathbf{F}(\mathbf{x}) \approx 0.5$ and we investigate the degree of accuracy with which δ can be estimated if the variation of $\mathbf{F}$ is confined to a range narrower than $(0, 1.0)$. Δ is the grid-block size.

The dynamic data for the inversion is generated by simulating flow through the true, fine-scale binary medium using MODFLOW/MODPATH [7]. Upscaled permeabilities at the sensor grid-block are obtained by simulating flow under permeameter boundary conditions on the 100×100 set of grid-cells (corresponding to the sensor grid-blocks) on the fine 3000×2000 mesh.

The ensemble of fine-scale binary media realizations, estimated from the observations, can be used for generating probabilistic predictions of breakthrough times in the domain. This can be expensive. We select a small set of 20 fine-scale binary field reconstructions as "models" of the true binary medium, and use the breakthrough times from the 20 models as model predictions. Using the observations at the sensor locations, each of the 20 models can be combined using Bayesian model averaging (BMA) [8], to construct a composite prediction and a Gaussian term for the uncertainty in the models' fit to data. In BMA, the data is first used to determine a bias correction for each of the models. The discrepancy between a bias-corrected model prediction and observation is modeled as a Gaussian with an unknown variance. The likelihood of the observations, given the ensemble of models, is expressed as a mixture of Gaussians and the weights of the mixture components (and the variance) are estimated using Expectation Maximization. This "BMA-ed" composite model can be used for probabilistic breakthrough time predictions in the domain with little expense.

3 TESTS

We explore the ability to estimate δ by creating synthetic inclusion proportionality fields $\mathbf{F}^* = 0.5 + \gamma(\mathbf{F} - 0.5)$ and performing the inversion with them. We consider $\gamma = 0.2$ and 0.5, which limit $\mathbf{F}^*(\mathbf{x})$ to $(0.4, 0.6)$ and $(0.25, 0.75)$. In Fig. 2 we investigate the impact of having more sensors in the domain, using $\gamma = 0.5$. We plot the probability density functions (PDFs) of the weights for 3 Karhunen-Loève modes and δ calculated using the SSA and SSB sensor sets. We see that the weights of the larger modes (w_1, w_{15}) are easily inferred (the posterior PDFs are quite different from the prior), whereas the information on the smallest mode (w_{30}) is limited. Both SSA and SSB sensors allow the estimation of δ, though as the number of sensors increase, the peak in the PDF moves closer to the true figure. This general conclusion is not very different from the results found in [1], where the tests were conducted for $\gamma = 1.0$.

In Fig. 3 (left), we investigate whether δ is estimated from the information in the static or dynamic data. We plot the PDFs constructed using just the static data, as well
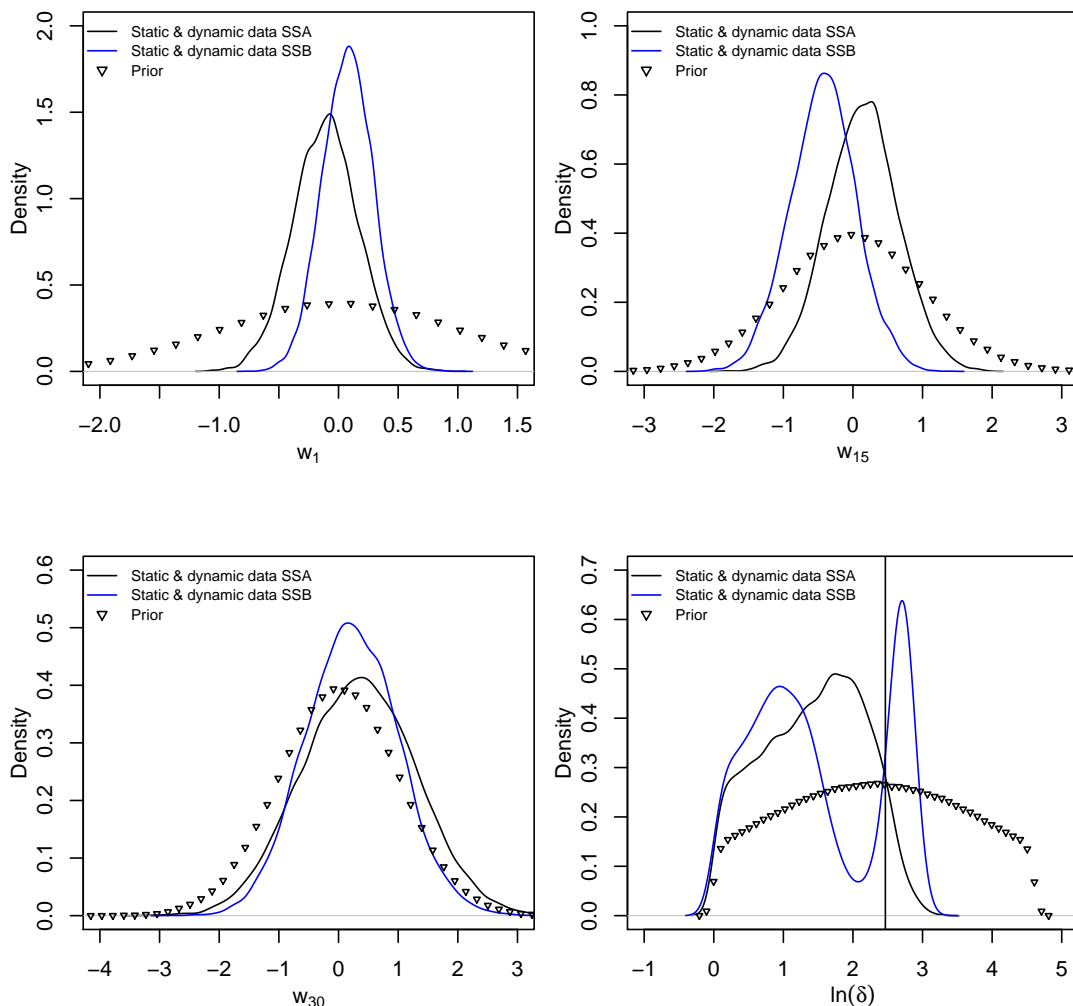
Figure 2: Marginalized PDFs of w_1, w_{15}, w_{30} and $\ln(\delta)$ as inferred jointly from static and dynamic data for SSA (black line) and SSB (blue). The priors are plotted with ∇ for comparison. $\gamma = 0.5$. The true values of w_1, w_{15} and w_{30} are 0.127, 0.814 and 1.607 respectively; that of δ is plotted with a vertical line.

as the static and dynamic data, obtained from the SSA and SSB sets of sensors. The PDFs obtained from the static and dynamic data are little different from those obtained with just the static data, indicating that δ estimates are drawn locally, and its impact on breakthrough times $\mathbf{t}_b$ is small. This can be explained using Fig. 1 (top right). The impact of δ is felt near $\mathbf{F} \approx 0.5$, a feature that is present in only a few grid-blocks (see [1] for the distribution of $\mathbf{F}$ among grid-blocks). In the vast majority of the grid-blocks, permeability is only weakly dependent on δ and flowpaths, which are affected by multiple grid-blocks, are not much affected by δ. A sensitivity analysis [1] confirms this view. In
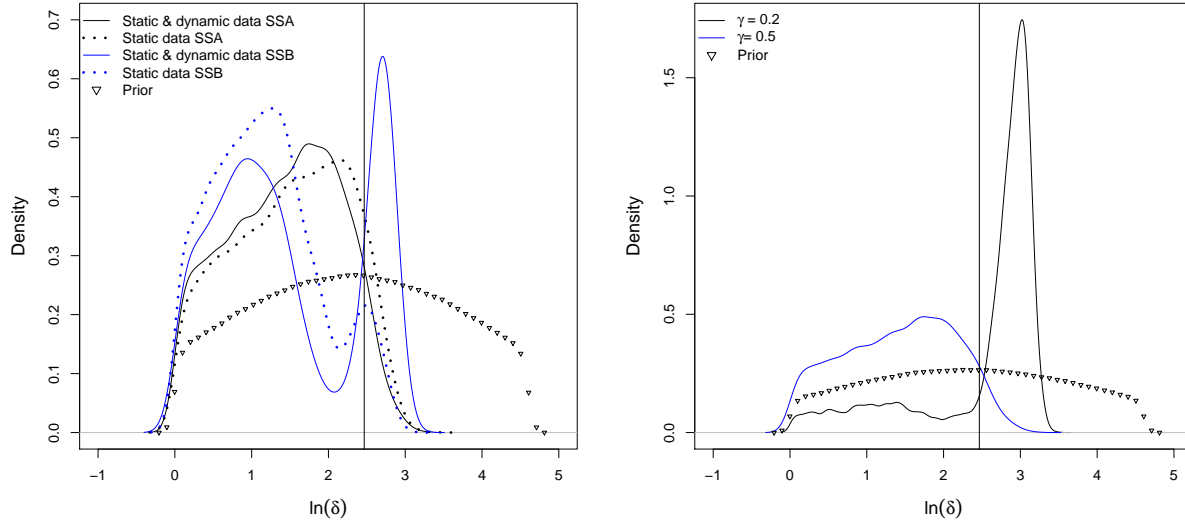
Figure 3: Left: Marginalized PDFs for $\log_{10}(\delta)$ developed using static data and static and dynamic data for the SSA and SSB sensors. Dynamic data contributes little to the estimate of δ. Right: PDFs of $\log_{10}(\delta)$ for different values of γ. The estimate of $\log_{10}(\delta)$ is more specific for low γ (more homogeneous material).

Fig. 3 (right), we plot δ as estimated for $\gamma = 0.2, 0.5$. The $\gamma = 0.2$ constrains $\mathbf{F}^*$ to (0.4, 0.6) where $\mathbf{K}_e$ is very sensitive to δ and we see that δ is estimated both accurately and with specificity. For $\gamma = 0.5$, i.e., $0.25 \leq \mathbf{F}^* \leq 0.75$ the specificity is lost and δ is also under-estimated. SSA sensors were used for both estimations.

We now address combining permeability models to create an inexpensive predictive model for the breakthrough times. We evaluate the posterior density of the samples collected by DRAM, sort them based on their posterior value, and collect 20 evenly spaced samples. These are used to generate binary media realizations (on a 3000×2000 mesh) to serve as models for the true field. The models so constructed may be expected to capture a wide range of spatial patterns that are consistent with observations. The binary media realizations are then used to predict breakthrough times using MODFLOW/MODPATH at the SSA sensors and 12 "testing sites" (see Fig. 4 (left)). The observations, and the 20 model predictions, are combined via BMA and used to predict the breakthrough times at 12 testing sites. In Fig. 4 (right) we see the predictions from the "raw" ensemble, the BMA model and the observations at the 12 testing sites (these were not used in the inversion). There are 20 members in both the "raw" and BMA ensembles. Table 1 shows the CRPS (cumulative rank probability score) and MAE (mean absolute error) [9, 10]. BMA improves the predictive skill of the 20 models at the sensor locations, whereas it worsens them slightly at the testing sites (vis-à-vis the "raw" ensemble). Thus, at points near the sensor sites, the enhanced predictive skill of the BMA model will provide better
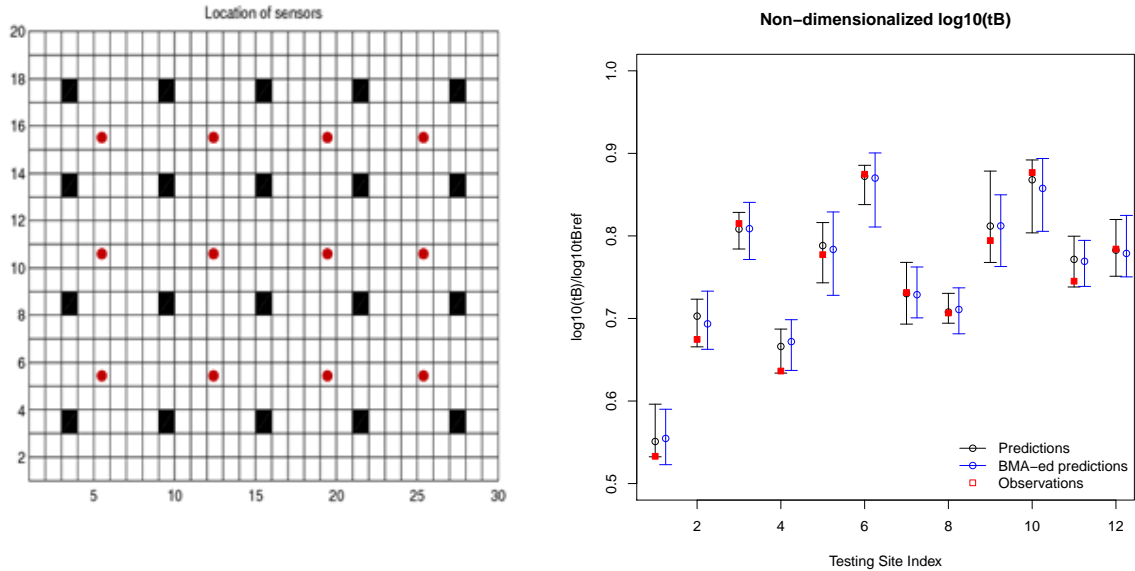
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Figure 4: Left: Sensor set SSA, along with 12 red "testing sites". Right: Predicted $\log_{10}$ tracer break-through times from the "raw" ensemble ("Predictions"), model-averaged ("BMA-ed predictions") and observations.

predictions. At points which are equidistant from sensors (similar to our testing sites), this effect is expected to be the least; further, the statistical re-weighting actually leads to errors compared to predictions by the raw ensemble.

Metric	Sensor points		Testing sites	
	"Raw"	BMA	"Raw"	BMA
CRPS	2.12×10^{-2}	1.92×10^{-2}	6.29×10^{-2}	6.39×10^{-2}
MAE	2.66×10^{-2}	2.38×10^{-2}	9.00×10^{-2}	9.16×10^{-2}

Table 1: CRPS and MAE for the breakthrough times at the sensors and testing sites, using ensemble ("Raw") and model-averaged (BMA) predictions.

4   CONCLUSIONS

We use a Bayesian method, developed in [1], to reconstruct a binary medium from static and dynamic observations. In this paper, we have explored how accurately, and under what conditions, the size δ of the unresolved inclusions may be estimated. We see that δ is estimated almost entirely from static data. Further, permeability is largely insensitive to inclusions, unless its proportionality $\mathbf{F}(\mathbf{x}) \approx 0.5$, at which point significant percolation effects are observed. This makes the estimation of δ difficult, but not impossible.

We also considered using the posterior distribution to create realizations of the fine-

scale binary medium and use them as models of the true binary field. We select a few realizations, use them to predict breakthrough times in the domain, and combine them using BMA. We find that near the sensors, BMA improves the predictive skill of the ensemble of models.

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