

Use of the Bayesian Approximation Error Approach to Account for Model Discrepancy: The Robin Problem Revisited

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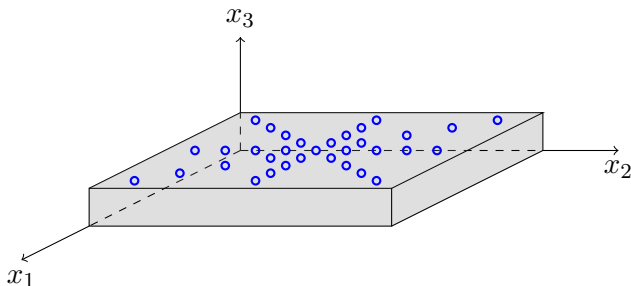
SIAM CSE19

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- 3 Model discrepancy and the Bayesian approximation error (BAE) approach
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The Robin problem

Find $\beta(\mathbf{x})$ on inaccessible part of domain from noisy measurements of u on accessible part of domain

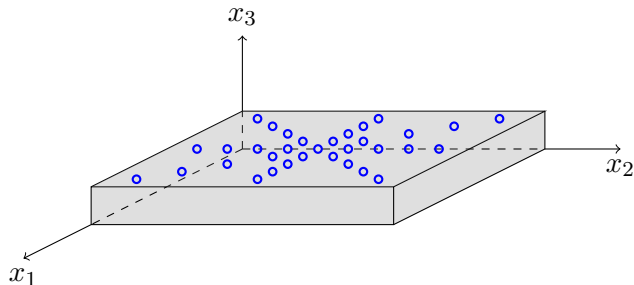
$$\begin{aligned} -\Delta u(\mathbf{x}) &= 0 && \text{in } \Omega, \\ \nabla u(\mathbf{x}) \cdot \mathbf{n}_t &= g(\mathbf{x}) && \text{on } \Gamma_t \\ \nabla u(\mathbf{x}) \cdot \mathbf{n}_b + e^{\beta(\mathbf{x})} u(\mathbf{x}) &= 0 && \text{on } \Gamma_b \\ u(\mathbf{x}) &= 0 && \text{on } \Gamma_s, \end{aligned} \tag{1}$$



The Robin problem revised

Find $\beta(\mathbf{x})$ on inaccessible part of domain from noisy measurements of u on accessible part of domain without knowing $a(\mathbf{x})$

$$\begin{aligned} -\nabla \cdot (e^{a(\mathbf{x})} \nabla u(\mathbf{x})) &= 0 && \text{in } \Omega, \\ e^{a(\mathbf{x})} \nabla u(\mathbf{x}) \cdot \mathbf{n}_t &= g(\mathbf{x}) && \text{on } \Gamma_t \\ e^{a(\mathbf{x})} \nabla u(\mathbf{x}) \cdot \mathbf{n}_b + e^{\beta(\mathbf{x})} u(\mathbf{x}) &= 0 && \text{on } \Gamma_b \\ u(\mathbf{x}) &= 0 && \text{on } \Gamma_s. \end{aligned} \tag{2}$$



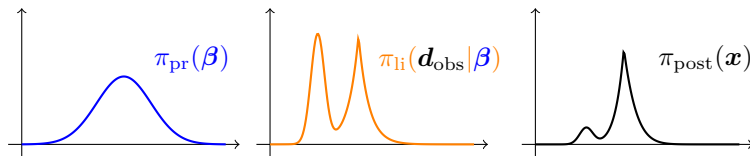
The Bayesian View of Inverse Problems

Inverse problem¹: With observed data, \mathbf{d} , and parameter to observable map \mathbf{f} , find β given

$$\mathbf{d} = \mathbf{f}(\beta, \mathbf{a}) + \mathbf{e}$$

- 1 All unknowns are taken to be random variables.
- 2 Solution to the inverse problem is posterior probability density.

$$\pi_{\text{post}}(\beta) = \pi(\beta|\mathbf{d}) = \frac{\pi_{\text{pr}}(\beta)\pi_{\text{li}}(\mathbf{d}|\beta)}{\pi(\mathbf{d})} \propto \pi_{\text{pr}}(\beta)\pi_{\text{li}}(\mathbf{d}|\beta)$$



¹Details in for example: J. Kaipio, E. Somersalo, *Statistical and Computational Inverse Problems*, Springer, 2005

The MAP Estimate

- **The maximum a posteriori estimate:** The point in parameter space that maximises the posterior probability density function
- Gaussian prior, mean β_* and covariance $\mathbf{\Gamma}_\beta = (\mathbf{A}^T \mathbf{A})^{-1}$
- Additive Gaussian noise in the measurements, $\mathbf{e} \sim \mathcal{N}(\mathbf{0}, \mathbf{\Gamma}_e)$, then the posterior density is²

$$\pi_{\text{post}}(\boldsymbol{\beta}) \propto \exp \left\{ -\frac{1}{2} \left(\|\mathbf{f}(\boldsymbol{\beta}, \mathbf{a}) - \mathbf{d}\|_{\mathbf{\Gamma}_e^{-1}}^2 + \|\mathbf{A}(\boldsymbol{\beta} - \boldsymbol{\beta}_*)\|^2 \right) \right\}$$

and

$$\boldsymbol{\beta}_{\text{MAP}} := \arg \min_{\boldsymbol{\beta} \in \mathbb{R}^n} \left\{ \frac{1}{2} \left(\|\mathbf{f}(\boldsymbol{\beta}, \mathbf{a}) - \mathbf{d}\|_{\mathbf{\Gamma}_e^{-1}}^2 + \|\mathbf{A}(\boldsymbol{\beta} - \boldsymbol{\beta}_*)\|^2 \right) \right\}$$

²Details in for example: J. Kaipio, E. Somersalo, *Statistical and Computational Inverse Problems*, Springer, 2005

We employ a *weighted* squared inverse elliptic operator as our prior covariance operator³:

$\mathbf{A} = \mathbf{K}\mathbf{G}^{-1}$ where

$$K_{ij} = \alpha \int_{\Gamma_b} (\gamma \nabla \phi_i \cdot \nabla \phi_j + \phi_i \phi_j) d\mathbf{x} + \int_{\partial\Gamma_b} \kappa \phi_i \phi_j ds,$$

$$G_{ij} = 4\pi\gamma\alpha^2 \sqrt{K_{ij}^{-1}} \delta_{ij}, \quad i, j \in \{1, 2, \dots, n\},$$

with $\alpha > 0$, $\gamma > 0$ and $\kappa \geq 0$ controlling variance and correlation structure, and δ_{ij} is the Kronecker delta.

- Other approaches include use of *Aristotelian boundary conditions*⁴

³Details in: Y. Daon, G. Stadler, *Mitigating the influence of the boundary on PDE-based covariance operators*, Inverse Problems and Imaging, 2017

⁴Details in: D. Calvetti, J. Kaipio, E. Someralo, *Aristotelian prior boundary conditions*, International Journal of Mathematics and Computer Science, 2006

Model Discrepancy and the BAE Approach

The Bayesian approximation error⁵ (BAE) approach has been used to account for uncertainties and discrepancies in many models.

Ingredients:

- 1 Let $f(\boldsymbol{\beta}, \mathbf{a})$ an *accurate* forward problem
- 2 Let $g_{a_*}(\boldsymbol{\beta})$ a *coarse/approximative* forward problem with auxiliary/nuisance parameter(s) \mathbf{a} set to \mathbf{a}_* .

Notice,

$$\begin{aligned} d &= f(\boldsymbol{\beta}, \mathbf{a}) + e = g_{a_*}(\boldsymbol{\beta}) + e + (f(\boldsymbol{\beta}, \mathbf{a}) - g_{a_*}(\boldsymbol{\beta})) \\ &= g_{a_*}(\boldsymbol{\beta}) + e + \varepsilon(\boldsymbol{\beta}) = g_{a_*}(\boldsymbol{\beta}) + \nu(\boldsymbol{\beta}), \end{aligned}$$

- $\varepsilon(\boldsymbol{\beta})$: *Approximation errors* accounts for model discrepancies
- $\nu(\boldsymbol{\beta})$: *Total errors* accounts for all errors

⁵Introduced in: J. Kaipio, E. Somersalo, *Statistical and Computational Inverse Problems*, Springer, 2005

Calculating the statistics of $\boldsymbol{\varepsilon}(\boldsymbol{\beta})$

$$\boldsymbol{\varepsilon}(\boldsymbol{\beta}) = \mathbf{f}(\boldsymbol{\beta}, \mathbf{a}) - \mathbf{g}_{\mathbf{a}_*}(\boldsymbol{\beta})$$

- In general cannot be computed analytically
- Gaussian approximation of $\pi(\boldsymbol{\varepsilon}, \boldsymbol{\beta})$
- Approximate $\boldsymbol{\varepsilon}$ and $\boldsymbol{\beta}$ as uncorrelated \rightarrow *enhanced error model*⁶
- Total error is then Gaussian with $\boldsymbol{\nu} \sim \mathcal{N}(\boldsymbol{\varepsilon}_*, \boldsymbol{\Gamma}_\varepsilon + \boldsymbol{\Gamma}_\beta)$

To calculate $\boldsymbol{\varepsilon}_*$ and $\boldsymbol{\Gamma}_\varepsilon$ (done *offline*):

- Generate r samples from $\pi(\boldsymbol{\beta}, \mathbf{a})$
- Compute $\boldsymbol{\varepsilon}^{(\ell)} = \mathbf{f}(\boldsymbol{\beta}^{(\ell)}, \mathbf{a}^{(\ell)}) - \mathbf{g}_{\mathbf{a}_*}(\boldsymbol{\beta}^{(\ell)})$, $\ell = 1, 2, \dots, r$
- Calculate

$$\boldsymbol{\varepsilon}_* = \frac{1}{r} \sum_{\ell=1}^r \boldsymbol{\varepsilon}^{(\ell)} \quad \text{and} \quad \boldsymbol{\Gamma}_\varepsilon = \frac{1}{r-1} \sum_{\ell=1}^r (\boldsymbol{\varepsilon}^{(\ell)} - \boldsymbol{\varepsilon}_*)(\boldsymbol{\varepsilon}^{(\ell)} - \boldsymbol{\varepsilon}_*)^T$$

⁶Details in for example: J. Kaipio, V. Kolehmainen, *Approximate marginalization over modelling errors and uncertainties in inverse problems*, Bayesian Theory and Applications, 2013

What Have we Accomplished?

An updated likelihood

⇒ An updated MAP estimate:

$$\beta_{\text{MAP}}^{\text{BAE}} := \arg \min_{\beta \in \mathbb{R}^n} \{ \mathcal{J}(\beta) \}$$

with

$$\begin{aligned} \mathcal{J}(\beta) &= \frac{1}{2} \left(\| \mathbf{g}_{a^*}(\beta) - \mathbf{d} + \boldsymbol{\nu}_* \|_{\Gamma_\nu^{-1}}^2 + \| \mathbf{A}(\beta - \beta_*) \|^2 \right) \\ &= \frac{1}{2} \left(\| \mathcal{B}\mathbf{u} - \mathbf{d} + \boldsymbol{\nu}_* \|_{\Gamma_\nu^{-1}}^2 + \| \mathbf{A}(\beta - \beta_*) \|^2 \right) \end{aligned}$$

\mathcal{B} is the observation operator, and \mathbf{u} is the FEM solution to the forward problem

$$\begin{aligned} -\nabla \cdot (e^{a^*} \nabla u(\mathbf{x})) &= 0 && \text{in } \Omega, \\ e^{a^*} \nabla u(\mathbf{x}) \cdot \mathbf{n}_t &= g(\mathbf{x}) && \text{on } \Gamma_t \\ e^{a^*} \nabla u(\mathbf{x}) \cdot \mathbf{n}_b + e^{\beta(\mathbf{x})} u(\mathbf{x}) &= 0 && \text{on } \Gamma_b \\ u(\mathbf{x}) &= 0 && \text{on } \Gamma_s. \end{aligned}$$

Use an inexact CG adjoint-based Gauss-Newton method

- Set up Lagrangian functional $\mathcal{L} : \mathcal{V} \times \mathcal{V} \times \mathcal{E} \rightarrow \mathbb{R}$ is

$$\mathcal{L}(u, \mathbf{p}, \beta) := \mathcal{J} + \int_{\Omega} e^{a_*} \nabla u \cdot \nabla \mathbf{p} \, d\mathbf{x} - \int_{\Gamma_t} g \mathbf{p} \, ds_t + \int_{\Gamma_b} e^{\beta} u \mathbf{p} \, ds_b,$$

- Gradient of \mathcal{J} found by requiring variations of \mathcal{L} with respect to the forward potential u and the *adjoint potential* \mathbf{p} vanish
- Results in following strong form of gradient \mathcal{G} ,

$$\mathcal{G}(\beta) := \mathcal{A}^2 (\beta - \beta_*) + e^{\beta} u \mathbf{p}$$

where u satisfies the forward problem, and \mathbf{p} satisfies the adjoint Poisson problem for given u and β :

The adjoint Poisson problem:

$$\begin{aligned} -\nabla \cdot (e^{a_*} \nabla p(\mathbf{x})) &= -\mathcal{B}^* \Gamma_{\nu}^{-1} (\mathcal{B}u(\mathbf{x}) - \mathbf{d} + \nu_*) && \text{in } \Omega, \\ e^{a_*} \nabla p(\mathbf{x}) \cdot \mathbf{n}_t &= 0 && \text{on } \Gamma_t, \\ e^{a_*} \nabla p(\mathbf{x}) \cdot \mathbf{n}_b + e^{\beta(\mathbf{x})} p(\mathbf{x}) &= 0 && \text{on } \Gamma_b, \\ p(\mathbf{x}) &= 0 && \text{on } \Gamma_s, \end{aligned}$$

- Action of the Gauss-Newton approximation of the Hessian operator evaluated at β in the direction $\hat{\beta}$ is given by

$$\mathcal{H}(\beta)(\hat{\beta}) := \mathcal{A}^2 \hat{\beta} + e^{\beta} \hat{\beta} u \hat{p}$$

where \hat{p} satisfies the *incremental adjoint Poisson problem* and \hat{u} satisfies the *incremental forward Poisson problem*

The incremental adjoint Poisson problem

$$\begin{aligned} -\nabla \cdot (e^{a^*} \nabla \hat{p}(\mathbf{x})) &= -\mathcal{B}^* \Gamma_{\nu}^{-1} \mathcal{B} \hat{u}(\mathbf{x}) && \text{in } \Omega \\ e^{a^*} \nabla \hat{p}(\mathbf{x}) \cdot \mathbf{n}_t &= 0 && \text{on } \Gamma_t \\ e^{a^*} \nabla \hat{p}(\mathbf{x}) \cdot \mathbf{n}_b + e^{\beta(\mathbf{x})} \hat{p}(\mathbf{x}) &= 0 && \text{on } \Gamma_b, \\ \hat{p}(\mathbf{x}) &= 0 && \text{on } \Gamma_s, \end{aligned}$$

The incremental forward Poisson problem

$$\begin{aligned} -\nabla \cdot (e^{a^*} \nabla \hat{u}(\mathbf{x})) &= 0 && \text{in } \Omega \\ e^{a^*} \nabla \hat{u}(\mathbf{x}) \cdot \mathbf{n}_t &= 0 && \text{on } \Gamma_t \\ e^{a^*} \nabla \hat{u}(\mathbf{x}) \cdot \mathbf{n}_b + e^{\beta(\mathbf{x})} \hat{u}(\mathbf{x}) &= -\hat{\beta} e^{\beta(\mathbf{x})} u(\mathbf{x}) && \text{on } \Gamma_b, \\ \hat{u}(\mathbf{x}) &= 0 && \text{on } \Gamma_s. \end{aligned}$$

Methods for Inversion

The resulting system to be solved (inexactly using CG) for the Gauss-Newton search direction, $\hat{\beta}$, is

$$\mathcal{H}(\beta)(\hat{\beta}) = -\mathcal{G}(\beta).$$

For joint inversion⁷ we would also need to solve

$$\mathcal{H}_a(a)(\hat{a}) = -\mathcal{G}_a(a)$$

for \hat{a} , with

$$\begin{aligned}\mathcal{G}_a(a) &:= \mathcal{A}_a^2(a - a_*) + e^a \nabla u \cdot \nabla p \\ \mathcal{H}_a(a)(\hat{a}) &:= \mathcal{A}_a^2 \hat{a} + e^a \hat{a} \nabla u \cdot \nabla \hat{p}\end{aligned}$$

⁷Such an approach was used in an ice sheet problem, details in N. Petra et al., *An inexact Gauss-Newton method for inversion of basal sliding and rheology parameters in a nonlinear Stokes ice sheet model*, Journal of Glaciology, 2012

Computational Examples Set Up

- Domain $\Omega = [0, 1] \times [0, 1] \times [0, 0.01]$
- 33 point measurements on the top of the domain
- Avoid *inverse crimes* by using finer FEM discretisation to generate data than for inversions

	Mesh use	#Nodes	#Els	#Param
Example 1	Data synthesis	28,611	150,000	2,601
	Inversion	6,727	32,400	961
Example 2	Data synthesis	132,651	750,000	2,601
	Inversion	29,791	162,000	961

- 1% noise added to measurements: $\Gamma_e = \delta_e^2 I$.

Prior for β

- Covariance set by using $\alpha = 7$, $\gamma = 0.01$ and $\kappa = 0$
- Recall, $\Gamma_\beta = (\mathbf{A}^T \mathbf{A})^{-1}$, with $\mathbf{A} = \mathbf{K} \mathbf{G}^{-1}$ where

$$K_{ij} = \alpha \int_{\Gamma_b} (\gamma \nabla \phi_i \cdot \nabla \phi_j + \phi_i \phi_j) d\mathbf{x} + \int_{\partial \Gamma_b} \kappa \phi_i \phi_j ds,$$

and \mathbf{G}^{-1} effectively homogenises the variance of the prior.

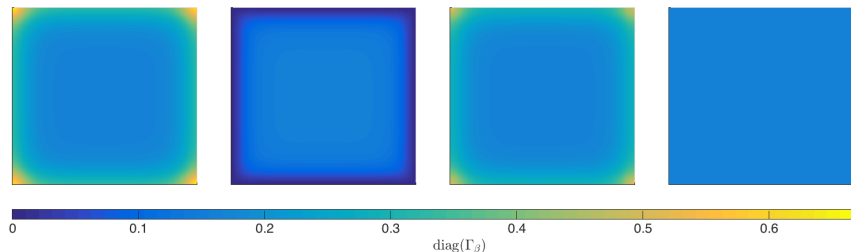


Figure: spatial variance of β for different boundary conditions

Prior for β

- Prior mean set as $\beta_* = 1$
- Same prior for β and true value, β_{true} used for both numerical examples

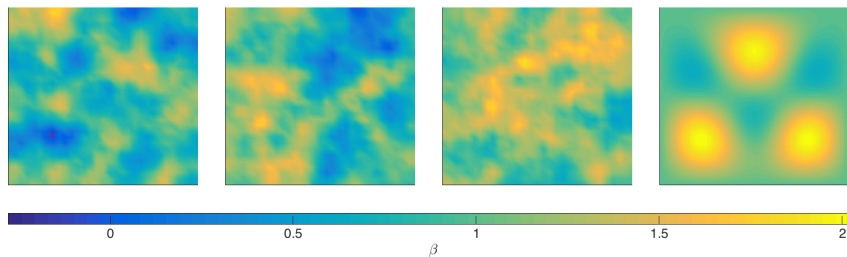


Figure: Three draws from $\pi_{\text{pr}}(\beta)$ and β_{true}

Example One: The Isotropic Case

- Mean and Covariance set using $a_* = 0$, $\alpha_a = 100$, $\gamma_a = 0.001$
- With $\Gamma_a = (\mathbf{A}_a^T \mathbf{A}_a)^{-1}$, with $\mathbf{A}_a = \mathbf{K}$ where

$$K_{ij} = \alpha_a \int_{\Omega} (\gamma_a \nabla \phi_i \cdot \nabla \phi_j + \phi_i \phi_j) dx$$

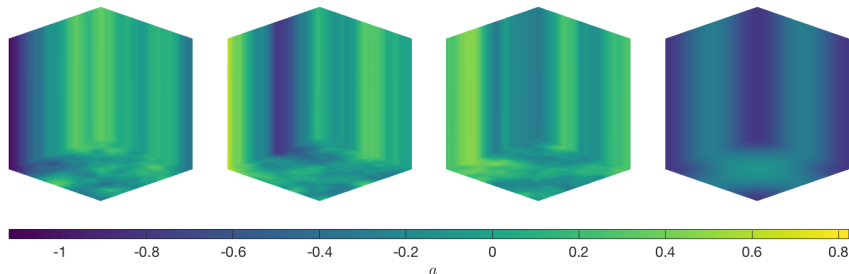


Figure: Three draws from $\pi_{\text{pr}}(a)$ and a_{true}

Approximation Errors for Example One

- $r = 1000$ samples drawn to calculate ϵ_* and Γ_ϵ .
- Some components of Γ_ϵ are $\approx 100\times$ larger than those in Γ_e
- Perhaps more important: **Structured noise**

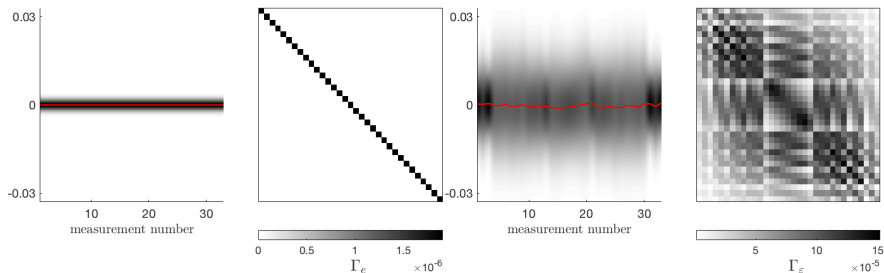


Figure: Statistics of the measurement errors and the approximation errors

Results for Example One

Results are compared for for the following

- **Reference case:** use the correct value of a in the model
- **Conventional error case:** neglect approximation errors
- **BAE case:** take into account approximation errors

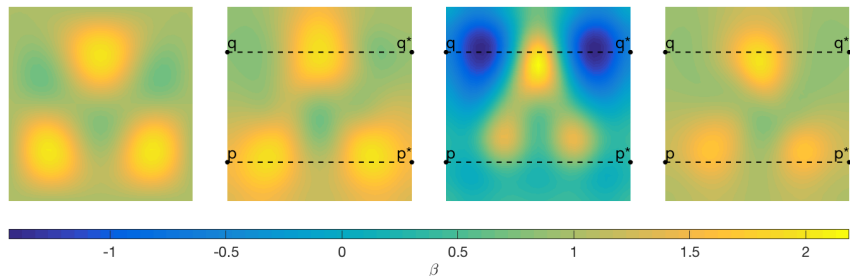


Figure: β_{true} , reference MAP, conventional error MAP, BAE MAP

Results for Example One

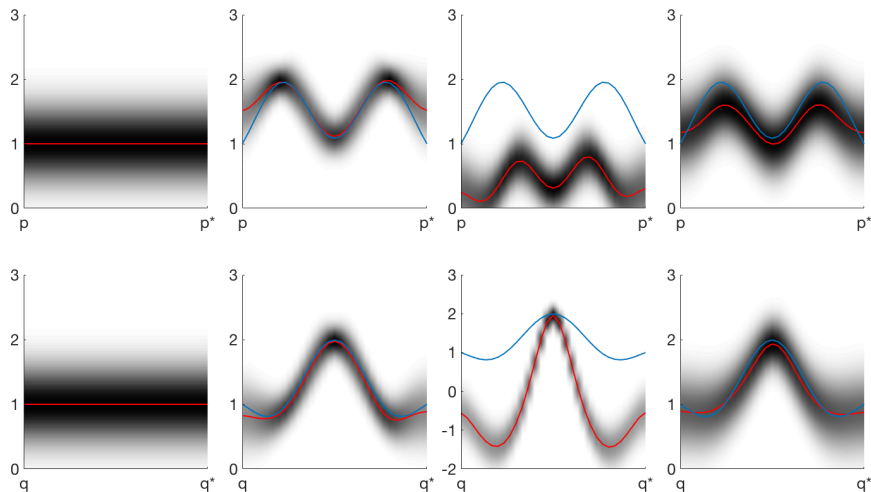


Figure: Prior and posterior variance: reference, conventional error, BAE

Example Two: The Anisotropic Case

- Mean and Covariance set using $a_* = 0$, $\alpha_a = 100$,
 $\gamma_a = \text{diag}(10^{-2}, 10^{-2}, 10^{-8})$
- With $\Gamma_a = (\mathbf{A}_a^T \mathbf{A}_a)^{-1}$, with $\mathbf{A}_a = \mathbf{K}$ where

$$K_{ij} = \alpha_a \int_{\Omega} (\gamma_a \nabla \phi_i \cdot \nabla \phi_j + \phi_i \phi_j) d\mathbf{x}$$

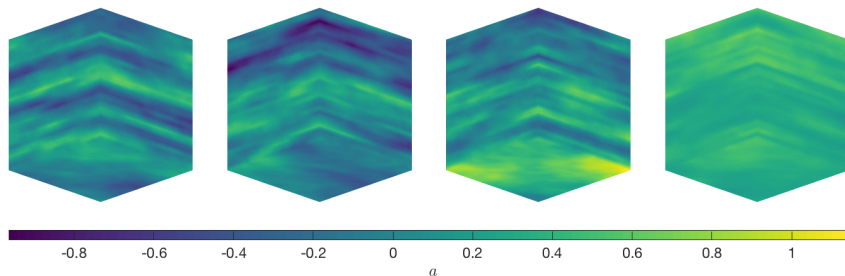


Figure: Three draws from $\pi_{\text{pr}}(a)$ and a_{true}

Approximation Errors for Example Two

- Again, $r = 1000$ samples drawn to calculate ε_* and Γ_ε .
- Some components of Γ_ε are $> 100\times$ larger than those in Γ_e
- We have: **Structured noise**

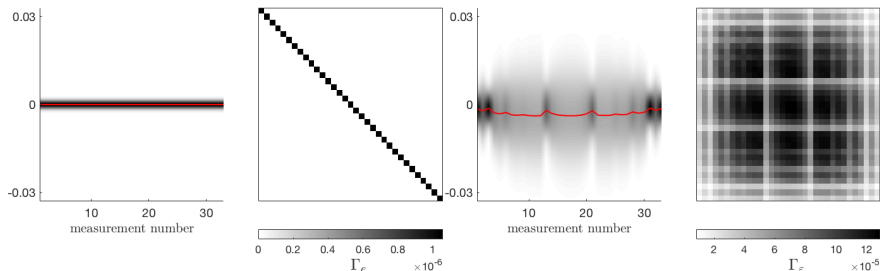


Figure: Statistics of the measurement errors and the approximation errors

Results for Example Two

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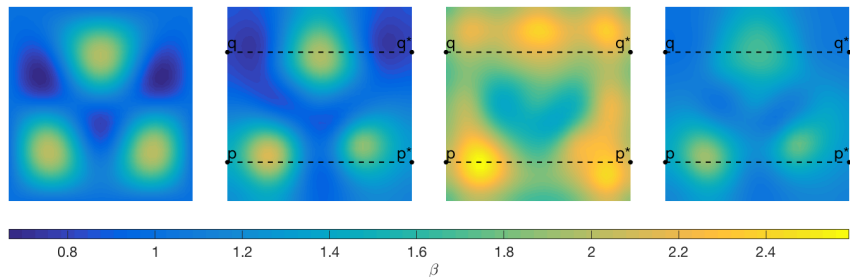


Figure: β_{true} , reference MAP, conventional error MAP, BAE MAP

Results for Example Two

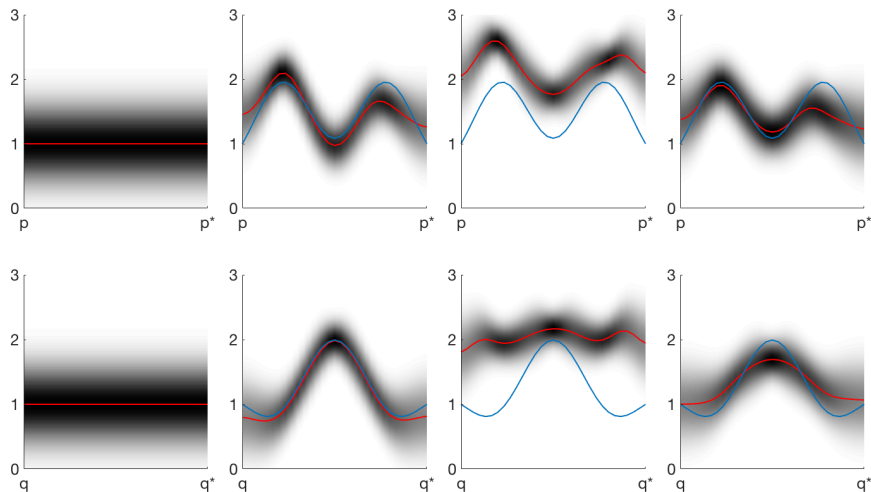


Figure: Prior and posterior variance: reference, conventional error, BAE

Computational Costs

- Gauss-Newton terminated when norm of gradient decreased by factor of 10^7
- CG iterations are terminated using Eisenstat-Walker condition

	MAP	#GN	#CG	avg.CG	#back	#Poisson
<hr/>						
Example 1						
REF	8	117	15	0	250	
CEM	11	101	10	4	228	
BAE	5	57	12	0	124	
<hr/>						
Example 2						
REF	6	54	9	0	120	
CEM	8	95	12	0	206	
BAE	5	97	20	0	204	

Current & Future Work: The Ice Sheet Problem

Consider the incompressible Stokes equations⁸

$$\begin{aligned} -\nabla \cdot \boldsymbol{\sigma}_u &= \rho \mathbf{g} & \mathbf{x} \in \Omega, \\ \nabla \cdot \mathbf{u} &= 0 & \mathbf{x} \in \Omega, \end{aligned} \quad (3)$$

- Basal sliding coefficient β
- Glen's flow-law exponent parameter n : Determines (non-)linearity

$$\boldsymbol{\sigma}_u = -p\mathbf{I} + 2\eta(\mathbf{u}, \mathbf{n})\dot{\boldsymbol{\epsilon}} \quad \text{Cauchy stress tensor}$$

$$\eta(\mathbf{u}, \mathbf{n}) = \frac{1}{2} A^{-\frac{1}{n}} \left(\dot{\boldsymbol{\epsilon}}_{\parallel}(\mathbf{u}) + \epsilon \right)^{\frac{1-n}{2n}} \quad \text{Effective viscosity}$$

$$\dot{\boldsymbol{\epsilon}}(\mathbf{u}) = \frac{1}{2} \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T \right) \quad \text{Strain rate tensor}$$

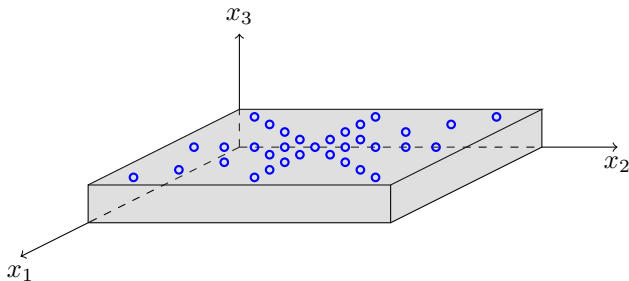
$$\dot{\boldsymbol{\epsilon}}_{\parallel}(\mathbf{u}) = \frac{1}{2} \dot{\boldsymbol{\epsilon}}(\mathbf{u}) : \dot{\boldsymbol{\epsilon}}(\mathbf{u}) \quad \text{Second invariant}$$

⁸See for example N. Petra et al., *An inexact Gauss-Newton method for inversion of basal sliding and rheology parameters in a nonlinear Stokes ice sheet model*, Journal of Glaciology, 2012

The Ice Sheet Problem

$$\begin{aligned} \mathbf{u}|_{\Gamma_l} = \mathbf{u}|_{\Gamma_r} \quad \text{and} \quad \boldsymbol{\sigma}_u \mathbf{n}|_{\Gamma_l} = \boldsymbol{\sigma}_u \mathbf{n}|_{\Gamma_r} & \quad \mathbf{x} \in \Gamma_p \\ \boldsymbol{\sigma}_u \mathbf{n} = \mathbf{0} & \quad \mathbf{x} \in \Gamma_t \\ \mathbf{u} \cdot \mathbf{n} = 0 & \quad \mathbf{x} \in \Gamma_b \\ T \boldsymbol{\sigma}_u \mathbf{n} + e^\beta T \mathbf{u} = \mathbf{0} & \quad \mathbf{x} \in \Gamma_b, \end{aligned} \quad (4)$$

$$\int_{\Omega} 2\eta(\mathbf{u}, \mathbf{n}) \dot{\boldsymbol{\varepsilon}}(\mathbf{u}) : \dot{\boldsymbol{\varepsilon}}(\mathbf{v}) - p \nabla \cdot \mathbf{v} - q \nabla \cdot \mathbf{u} \, dx + \int_{\Gamma_b} e^\beta T \mathbf{u} \cdot T \mathbf{v} \, ds = \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{v} \, dx$$



The Ice Sheet Problem

- Replace nonlinear Stokes model with linear counterpart⁹

$$\mathbf{f}(\boldsymbol{\beta}, \mathbf{n}) = \mathbf{g}_{\mathbf{n}_*}(\boldsymbol{\beta}) + \boldsymbol{\varepsilon}(\boldsymbol{\beta}), \quad \mathbf{n}_* = 1$$



Figure: Nonlinear (left) and Linear (right) velocities for same β_{true} ,

⁹See R. Nicholson, O. Babaniyi, N. Petra, *Incorporating model discrepancy stemming from uncertain rheology in an inverse ice sheet flow problem*, in preparation

Conclusions:

- The Bayesian approximation error (BAE) approach allows use of simpler forward model while *premarginialising* over auxilliary parameters
- Consequential model discrepancy dealt with systematically.
- BAE approach results in an updated likelihood which fits in naturally to the existing framework.
- Neglecting model discrepancy can lead to infeasible results.
- Robin problem details in R. Nicholson, N. Petra, J. Kaipio, *Estimation of the Robin coefficient field in a Poisson problem with uncertain conductivity field*, Inverse Problems 34 (11) 2018
- Ice sheet problem details in R. Nicholson, O. Babaniyi, N. Petra, *Incorporating model discrepancy stemming from uncertain rheology in an inverse ice sheet flow problem*, in preperation
- Thank you