Local point spread function Hessian approximation

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Joint work with:
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CCGO meeting

Outline

- Motivation: **Antartic ice sheet**
- New Hessian approximation: **big idea**
- New Hessian approximation: **technical details**
- Preliminary **numerical results** (heat inverse problem)

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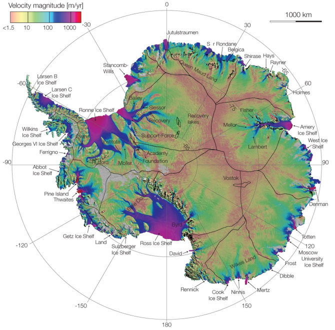
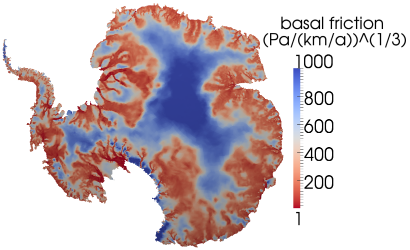
Antartic ice sheet



Observed surface flow velocity from InSAR (Rignot et. al, 2011)



Antarctic ice sheet inversion for the basal friction parameter field from InSAR surface velocities

Details in: T. Isaac, N. Petra, G. Stadler, and O. Ghattas. *Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet*, Journal of Computational Physics, 296, 348-368 (2015).

Ice sheet dynamics: forward and inverse

Balance of linear momentum, mass, and energy

$$-\boldsymbol{\nabla} \cdot [\eta(\theta, \boldsymbol{u})\, \dot{\boldsymbol{\varepsilon}} - \boldsymbol{I}p] = \rho \boldsymbol{g}, \qquad [\dot{\boldsymbol{\varepsilon}} = \tfrac{1}{2}(\boldsymbol{\nabla}\boldsymbol{u} + \boldsymbol{\nabla}\boldsymbol{u}^T)]$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0,$$

$$\rho c \left(\frac{\partial \theta}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}\theta \right) - \boldsymbol{\nabla} \cdot (K \boldsymbol{\nabla}\theta) = 2\,\eta\, \mathrm{tr}(\dot{\boldsymbol{\varepsilon}}^2)$$

We have: Satellite observations of surface velocity

We want: The sliding/friction coefficient β in Robin boundary condition

$$\mathbf{T}(\boldsymbol{\sigma}\mathbf{n}) + \beta(x)\mathbf{T}\mathbf{u} = 0$$

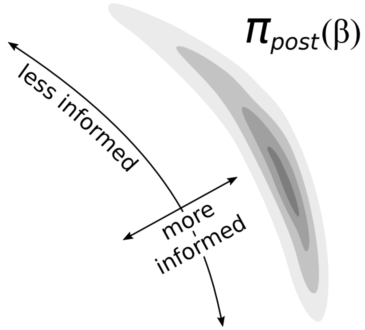
($\mathbf{T}$ is tangential component)

Bayesian approach

Inverse problem: given noisy data $\boldsymbol{d}$ and a model $\boldsymbol{f}$, infer parameters $\boldsymbol{\beta}$ that characterize the model, i.e.,

$$\boldsymbol{f}(\boldsymbol{\beta}) + \boldsymbol{e} = \boldsymbol{d}$$

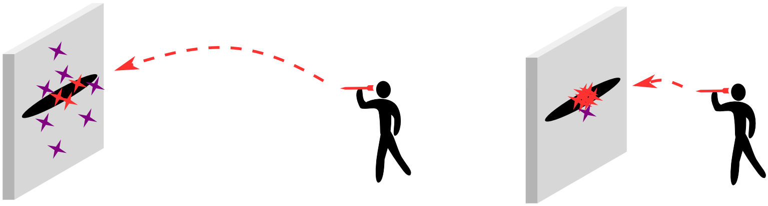
Interpret $\boldsymbol{\beta}$, $\boldsymbol{d}$ as random variables; solution of inverse problem is the "posterior" probability density function $\pi_{\text{post}}(\boldsymbol{\beta})$ found via Bayes' theorem.



Ill-conditioning and sampling

Objective: characterize posterior distribution by drawing samples with Markov chain Monte Carlo.

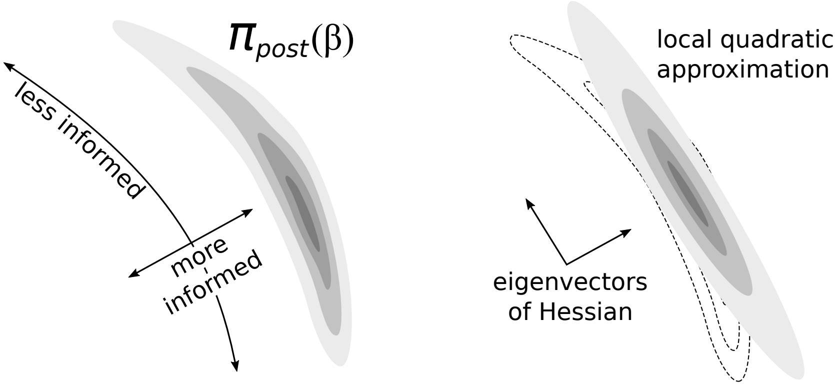
Dilemma: If the directional scalings of the proposal distribution are inconsistent with the directional scalings of the posterior, then sampling will be slow.



Hessian: local Gaussian approximation

Local Gaussian approximation proposal:

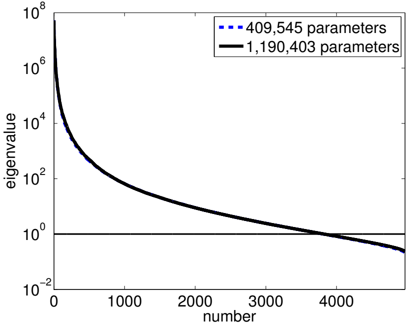
$$\pi_{\mathsf{prop}}(\beta) := \frac{\det \boldsymbol{H}^{1/2}}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}\left(\boldsymbol{y} - \boldsymbol{\beta}_k + \boldsymbol{H}^{-1}\boldsymbol{g}\right)^T \boldsymbol{H}\left(\boldsymbol{y} - \boldsymbol{\beta}_k + \boldsymbol{H}^{-1}\boldsymbol{g}\right)\right)$$



Low-rank approximation/Woodbury formula:

$$\Gamma_{\text{prop}} = H^{-1} = \left(F^T \Gamma_{\text{noise}}^{-1} F + \Gamma_{\text{prior}}^{-1}\right)^{-1} \approx \Gamma_{\text{prior}}^{1/2} (V_r \Lambda_r V_r^T + I)^{-1} \Gamma_{\text{prior}}^{1/2}$$

where V_r and Λ_r are the eigenvectors/values of $F^T \Gamma_{\text{noise}}^{-1} F v_i = \lambda_i \Gamma_{\text{prior}}^{-1} v_i$



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MCMC sampling: stochastic Newton

Performance results / Convergence diagnostics

	MPSRF	IAT	ESS	MSJ	ARR	#Stokes	time (s)
SN	1.348	600	875	64	2	**8400**	420

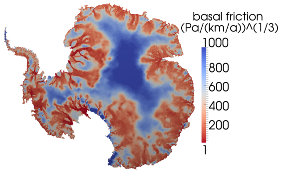
- **MPSRF:** multivariate potential scale reduction factor
- **IAT:** integrated autocorrelation time
- **ESS:** effecitive sample size
- **MSJ:** mean squared jump distance
- **ARR:** average rejection rate
- **#Stokes:** # of Stokes solves per independent sample
- **time:** time per independent sample

- **Statistics:** 21 parallel chains (each 25k); # samples: 525k; dof: 139; rank Hessian: 15

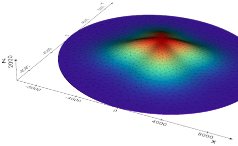
Too many PDE solves!!

Details in: N. Petra, J. Martin, G. Stadler, O. Ghattas. *A computational framework for infinite-dimensional Bayesian inverse problems: Part II. Stochastic Newton MCMC with application to ice sheet inverse problems*, SIAM Journal on Scientific Computing, 2014

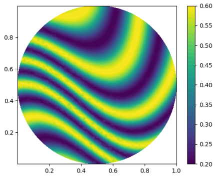
Model problems



(a) Antartica (Stokes)



(b) Ice mountain (Stokes)



(c) Heat swirl (heat)

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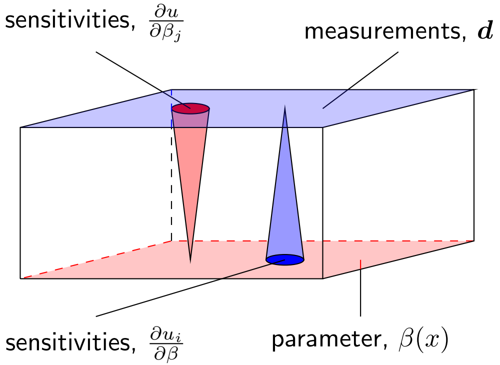
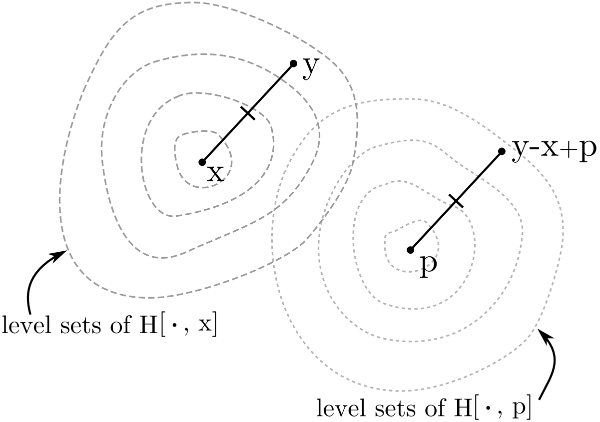
Local sensitivities



Local translation invariance



Hessian impulse responses

Hessian impulse response

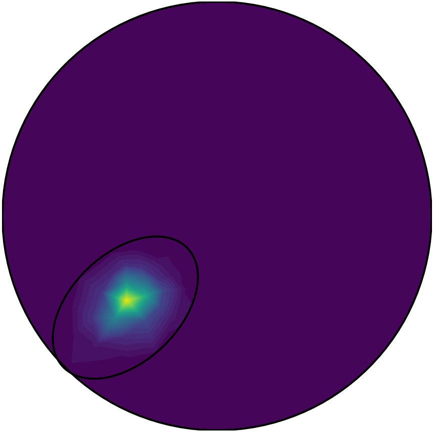


*image shown from ice mountain

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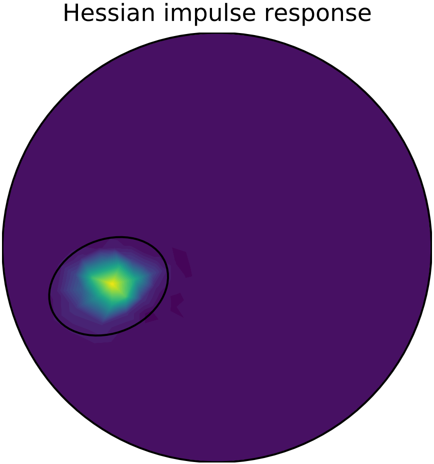

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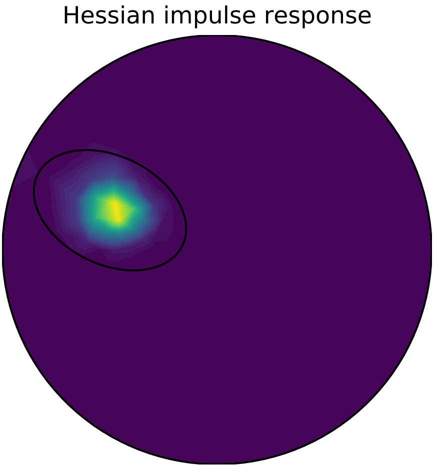

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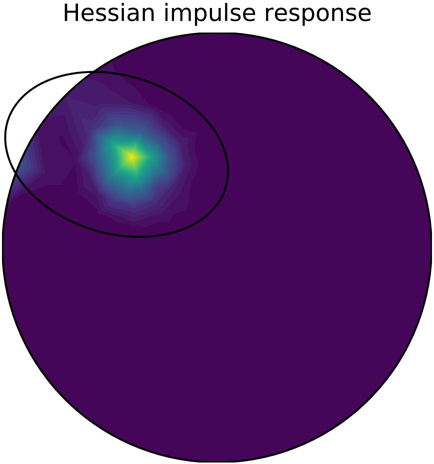

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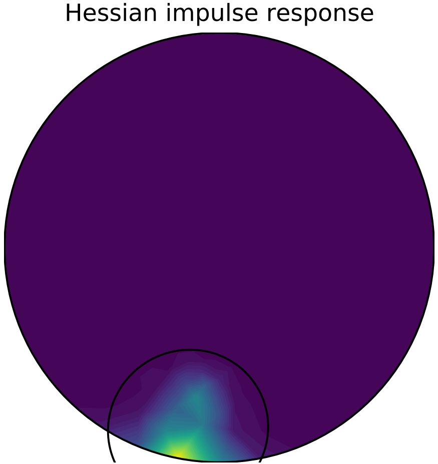

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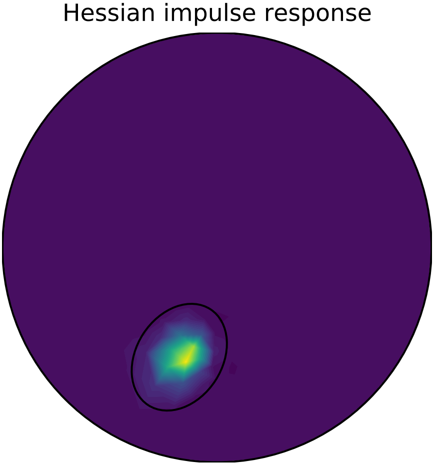

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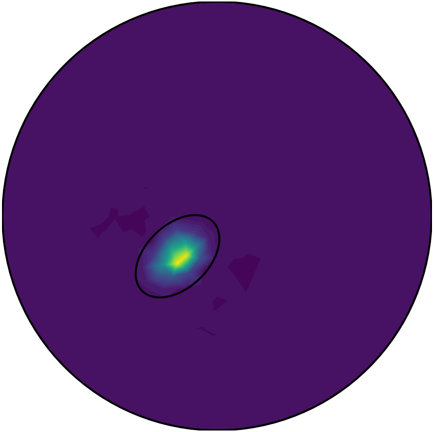

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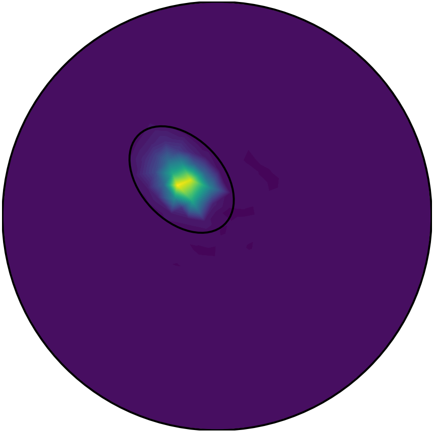

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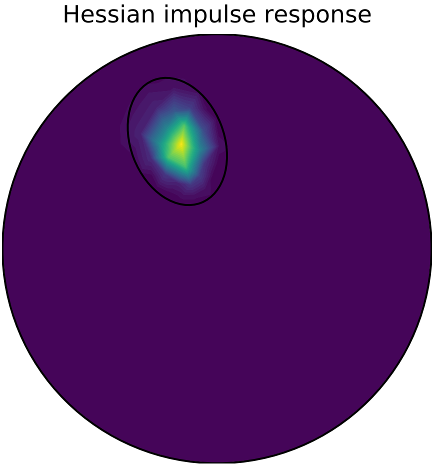

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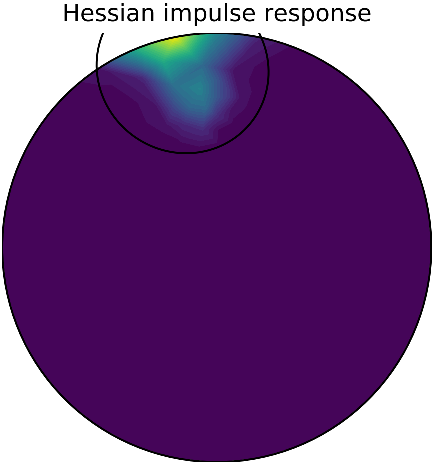

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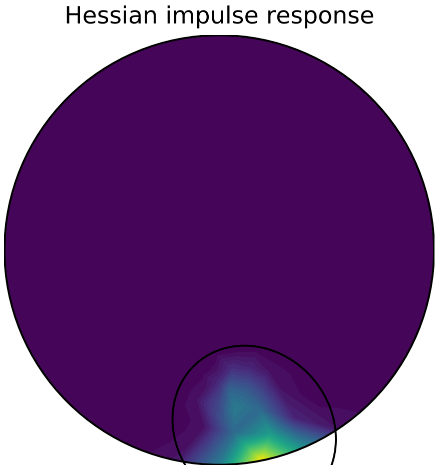

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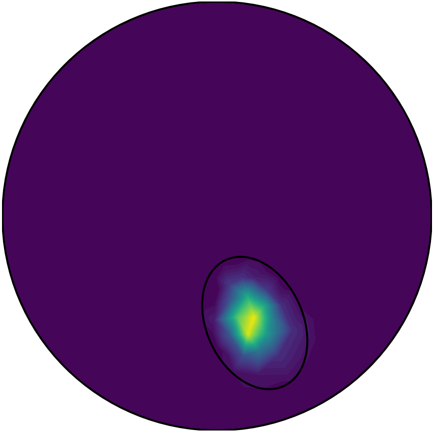

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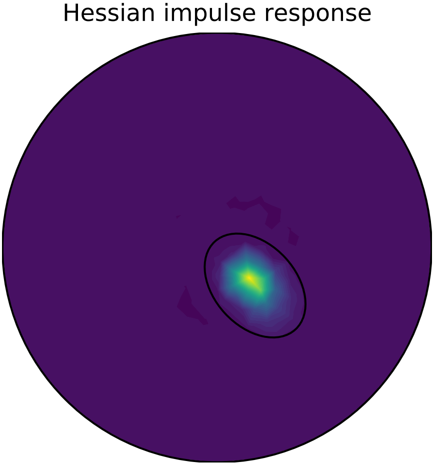

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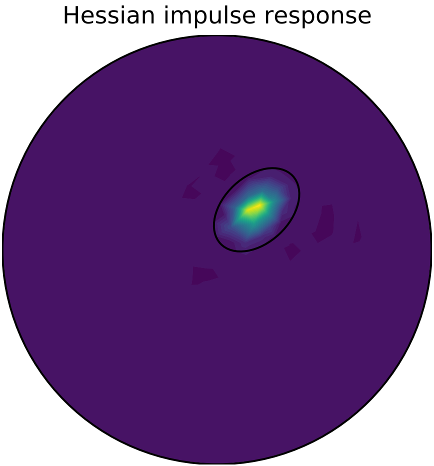

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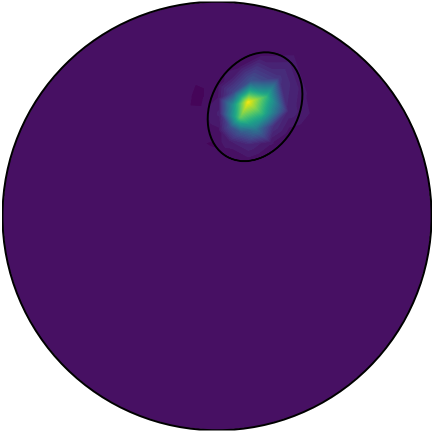

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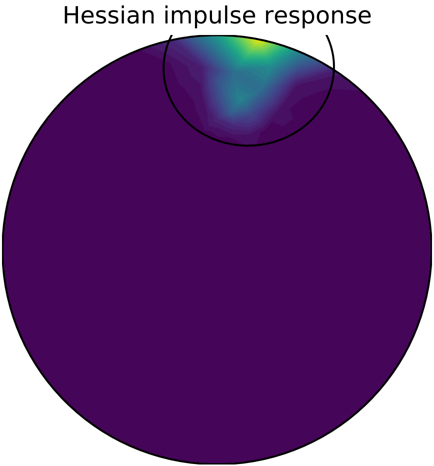

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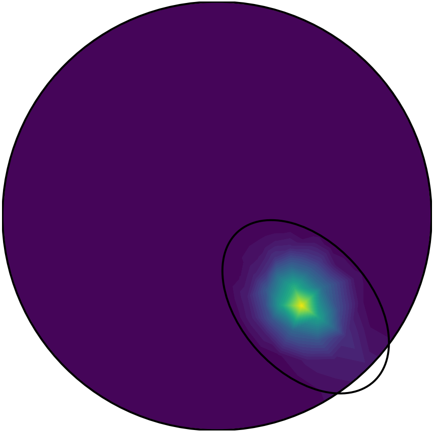

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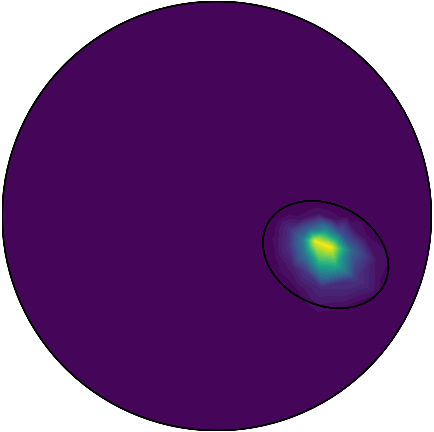

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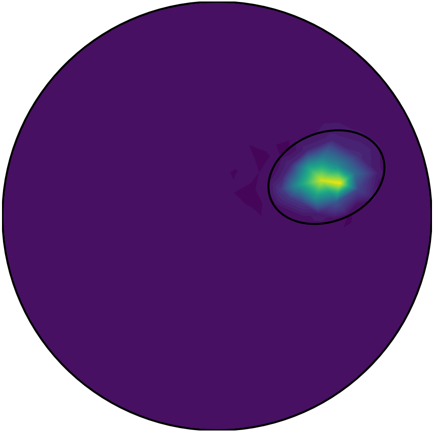

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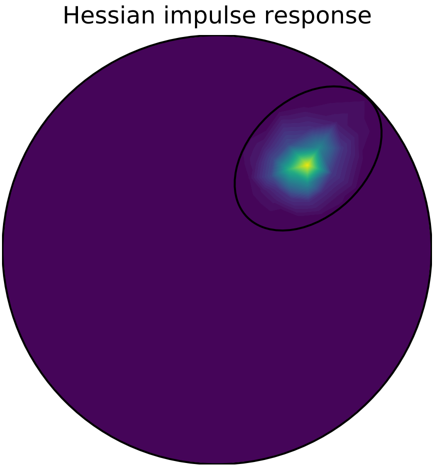

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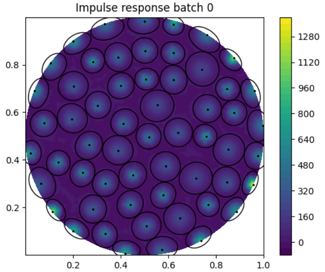
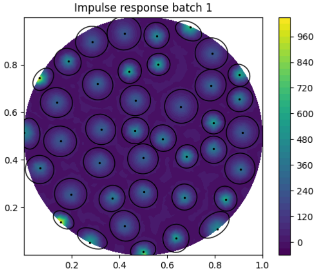
Hessian approximation method: big idea

- **Step 1:** Compute "batches" of impulse responses by applying Hessian to Dirac combs
- **Step 2:** Interpolate known impulse responses to approximate unknown impulse responses
- **Step 3:** Convert to $\mathcal{H}$-matrix to do linear algebra





*images shown from heat swirl

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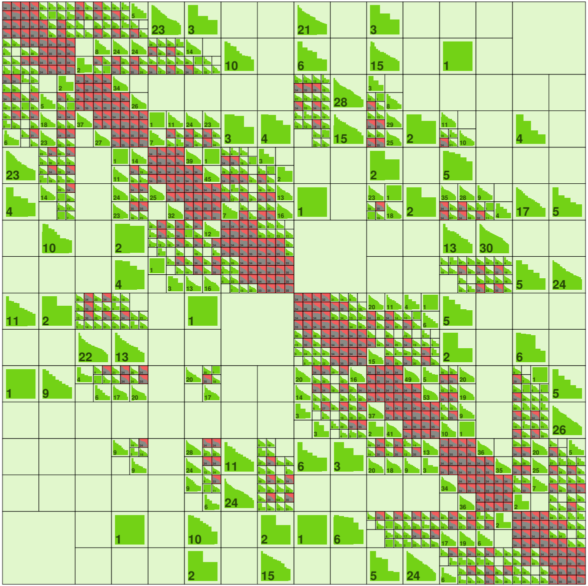
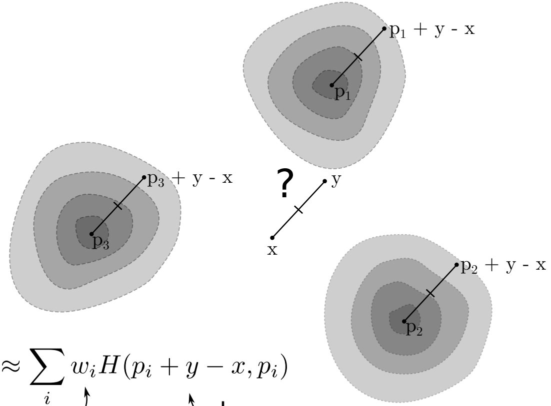
Technical details

- How do we choose the impulse response points?
- How do we interpolate the impulse responses?
  - What about boundary issues?
- What are $\mathcal{H}$-matrices and how do we use them?

Hierarchical matrices ($\mathcal{H}$-matrices)



Radial basis function interpolation



$$H(y,x) \approx \sum_i w_i H(p_i + y - x, p_i)$$

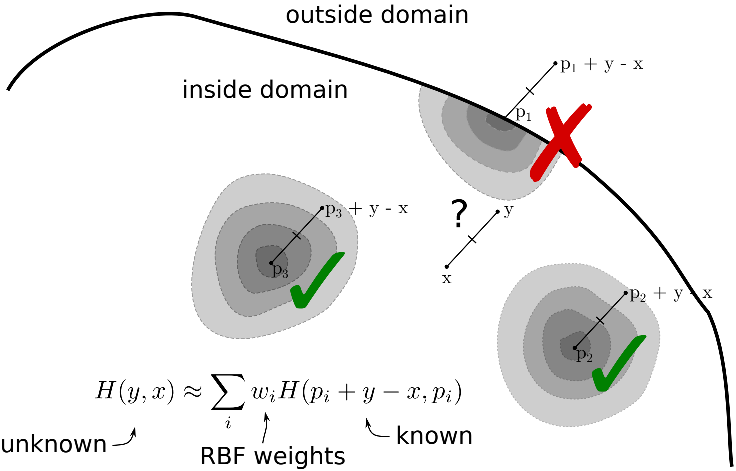
unknown

RBF weights

known

- Interpolate impulse responses using polyharmonic spline radial basis functions.
- Use only k-nearest neighbors (must solve $k \times k$ linear system)

Boundary considerations (1)



$$H(y,x) \approx \sum_i w_i H(p_i + y - x, p_i)$$

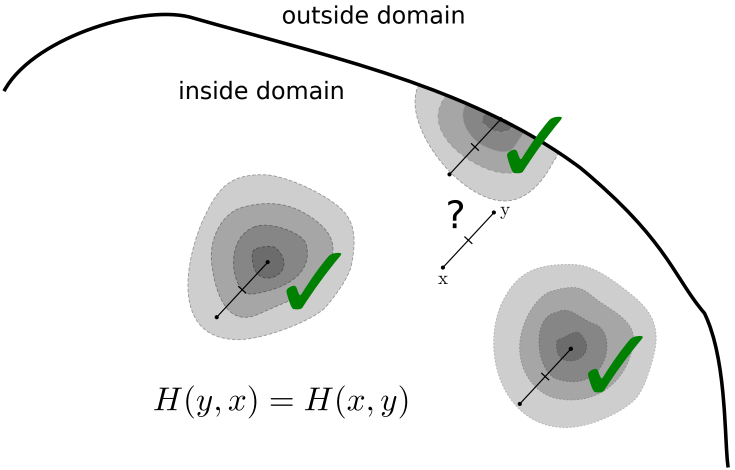
unknown

RBF weights

known

- If $p_i + y - x$ is outside the domain, don't use ith impulse response for $H(y,x)$

Boundary considerations (2)

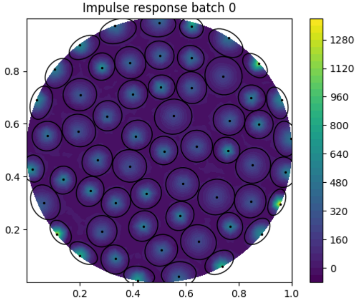


$$H(y, x) = H(x, y)$$

- Take advantage of symmetry

How to choose impulse response points?

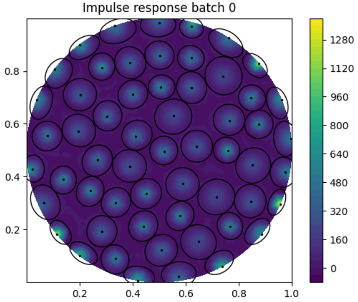
One hessian matrix-vector product $\to$ many impulse responses



- **Goal:** choose as many points as possible, such that the impulse response supports don't overlap
- **Dilemma:** How can we know the impulse response supports before we compute them?

How to choose impulse response points?

One hessian matrix-vector product $\rightarrow$ many impulse responses



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Matrix analogy: getting all row sums

Matrix: let $A \in \mathbb{R}^{N \times N}$. Then

$$A^T \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} \text{sum of } A \text{ col } 1 \\ \text{sum of } A \text{ col } 2 \\ \vdots \\ \text{sum of } A \text{ col } N \end{bmatrix}$$

Apply matrix to vector of ones $\rightarrow$ get row sums for all rows

Operator: let $C(x) = 1$ be the constant function. Then

$$(H^T C)^*(y) = \int_\Omega (H\delta_y)(x) dx$$

Apply Hessian to constant function $\rightarrow$ get volumes of every impulse response

Mean and standard deviations of impulse responses

- Let C, L^i, and Q^{ij} be the following functions:

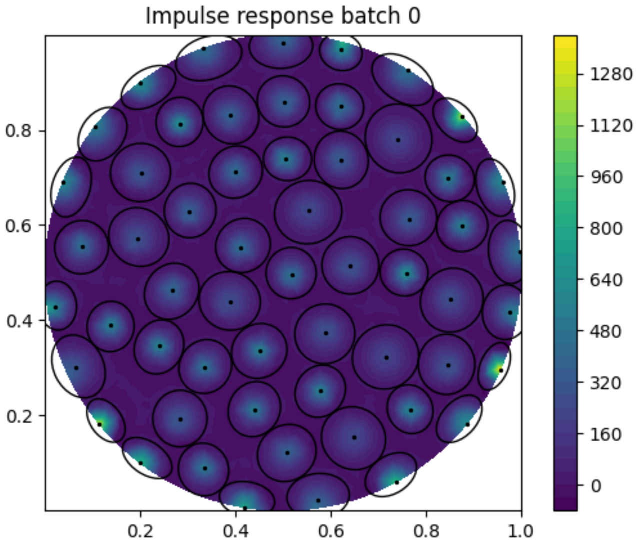
$$C(x) := 1, \qquad L^i(x) := x^i, \qquad Q^{ij}(x) = x^i x^j$$

- Then

$$\begin{aligned} V &= \left(H^T C\right)^* \\ \mu^i &= \left(H^T L^i\right)^* / V \\ \Sigma^{ij} &= \left(H^T Q^{ij}\right)^* / V - \mu^i \cdot \mu^j \end{aligned}$$

- Apply Hessian to constant, linear, and quadratic functions $\rightarrow$ get estimates of support for every impulse response

Impulse response support ellipsoids



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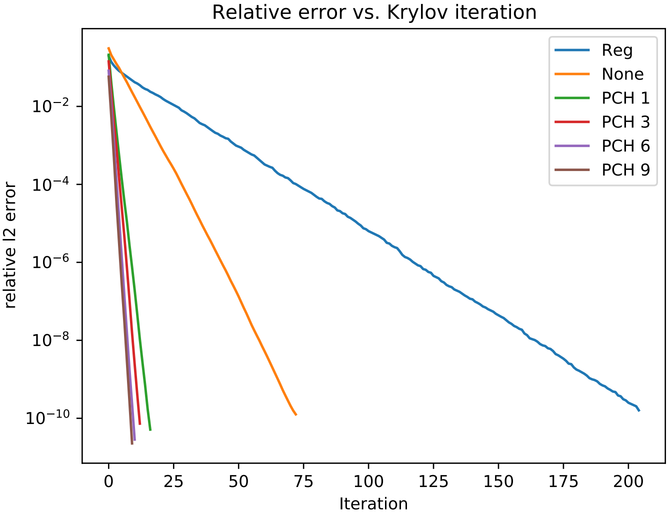
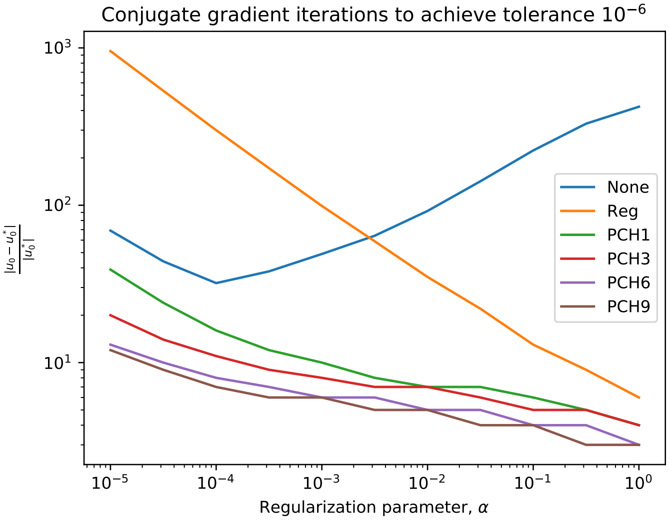
Heat swirl: CG Hessian solve with different preconditioners



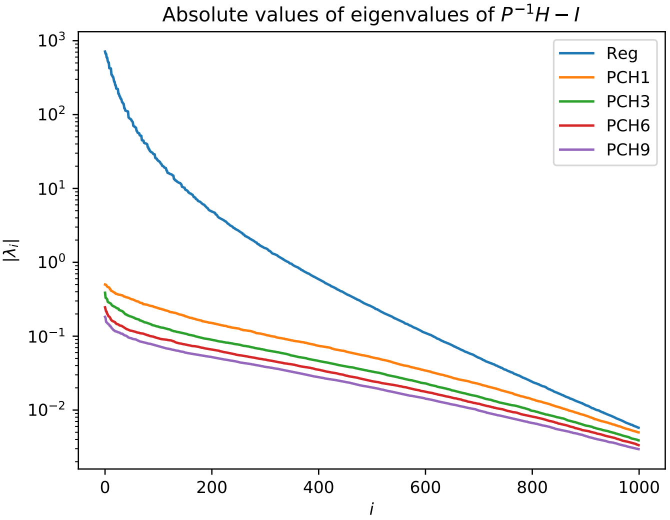
Solving $Hp = -g$ with preconditioned conjutate gradient

Heat swirl: Krylov iter vs. regularization parameter

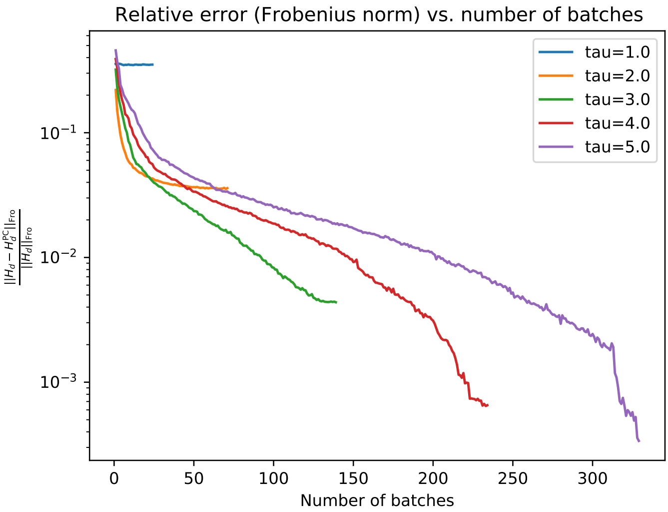


Solving $Hp = -g$ with preconditioned conjutate gradient

Heat swirl: preconditioned spectrum

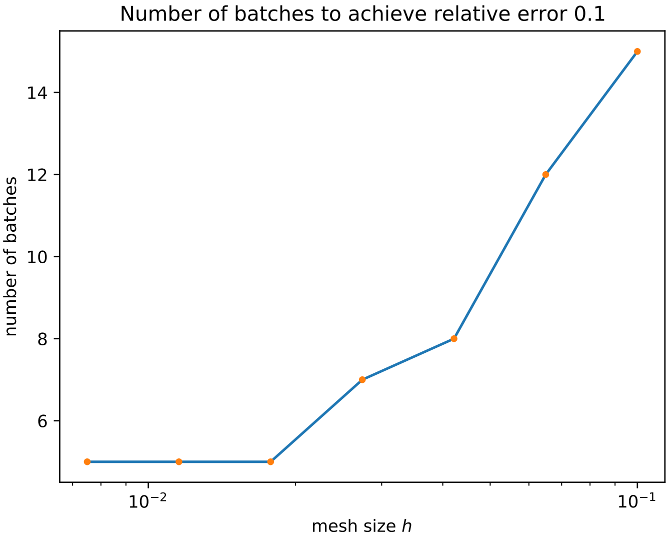


Heat swirl: error vs. num batches



tau: number of standard deviations used for ellipsoids

Heat swirl: error vs. mesh size



Summary

- Hessian approximations or preconditioners are essential for Bayesian sampling in inverse problems governed by partial differential equations.
- Low-rank approximations of the Hessian become prohibitive as the data becomes more informative (as is the case for ice sheet inverse problems).
- Local point spread function interpolation combined with Hierarchical matrix representations promise a more efficient Hessian approximation.