Machine Learning for Sciences

Notes from Recent Experiences

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Variational Bayesian approximation of inverse problems using sparse precision matrices

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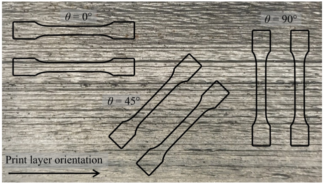
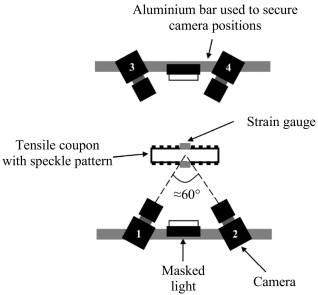
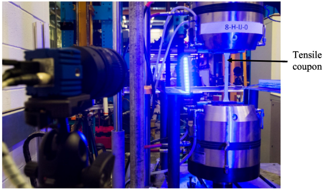
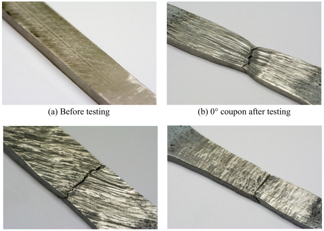








(a) Before testing

(b) 0° coupon after testing

(c) 45° coupon after testing

(d) 90° coupon after testing

Formulating PDE-based Bayesian inverse problem

- We consider an elliptic PDE of the form:

$$-\nabla \cdot (\exp(\kappa(\boldsymbol{x}))\nabla u(\boldsymbol{x})) = f(\boldsymbol{x}),$$

- Using FEM, we obtain a linear system:

$$\mathbf{A}(\boldsymbol{\kappa})\mathbf{u} = \mathbf{f}\,,$$

- The likelihood is given by

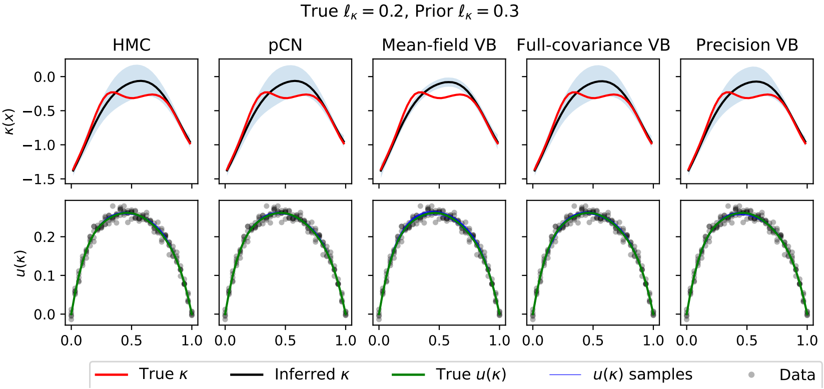
$$p(\boldsymbol{y} \mid \boldsymbol{\kappa}) = p(\boldsymbol{y} \mid \mathbf{u}(\boldsymbol{\kappa})) = \mathcal{N}(\mathbf{A}(\boldsymbol{\kappa})^{-1}\mathbf{f}, \sigma_y^2\mathbf{I})\,.$$

- The prior is:

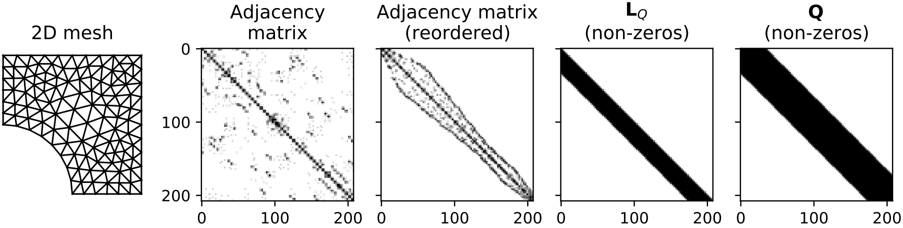
$$\log p(\boldsymbol{\kappa}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_\psi(x, x)).$$

We develop the variational inference scheme for this problem.

Variational Bayesian approximation of inverse problems using sparse precision matrices



Leveraging Sparsity – Outlook



Outlook:

- Leverage sparse linear algebra routines and tailored optimisation schemes.

Physics Informed Generative Models

Scalable Deep probabilistic Models for PDEs

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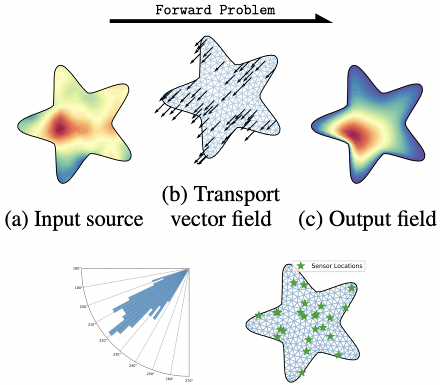
PDE-based generative modelling

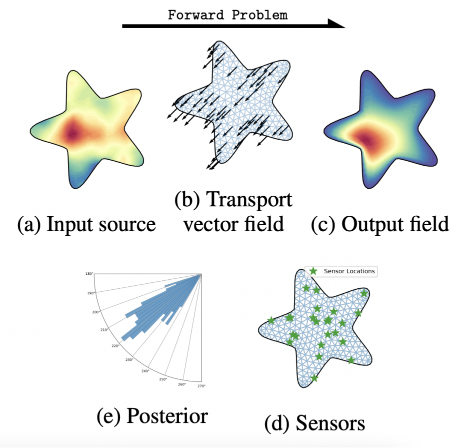


(a) Input source (b) Transport vector field (c) Output field

(e) Posterior (d) Sensors

Variational Autoencoding of PDE Inverse Problems (2020), Tait, Damoulas

PDE-based generative modelling



Broken down:

- Parametric PDE simulation
- Uncertainty Quantification
- Forward and Inverse Solutions
- Data incorporation & Dataless
- Scalable

Methods:

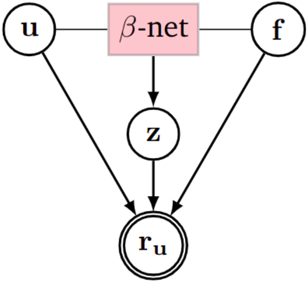
- Weighted residual method
- Neural networks
- Variational inference

Variational Autoencoding of PDE Inverse Problems (2020), Tait, Damoulas

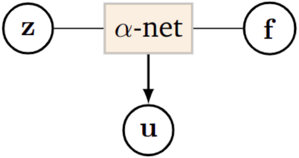
Physics Informed Generative Models

Lower Bound on the Residual Evidence

$$\log p_{\alpha,\beta}(\mathbf{r}) \geq \int \log \frac{p(\mathbf{r_u}|\mathbf{u},\mathbf{z},\mathbf{f},\boldsymbol{\omega})p_\beta(\mathbf{z}|\mathbf{u},\mathbf{f},\boldsymbol{\omega})p(\mathbf{u})}{q_\alpha(\mathbf{u}|\mathbf{z},\mathbf{f},\boldsymbol{\omega})p(\mathbf{z})} \times$$
$$q_\alpha(\mathbf{u}|\mathbf{z},\mathbf{f},\boldsymbol{\omega})p(\mathbf{z})p(\mathbf{f})p(\boldsymbol{\omega})\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{z}\mathrm{d}\mathbf{f}.$$

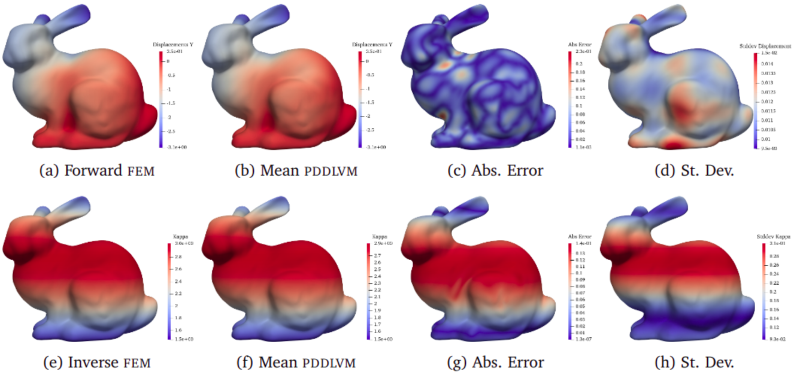


(a) Probabilistic Model with β-Net



(b) Variational Approximation with α-Net

Linear elasticity – Forward and Inverse problem



(a) Forward FEM (b) Mean PDDLVM (c) Abs. Error (d) St. Dev.

(e) Inverse FEM (f) Mean PDDLVM (g) Abs. Error (h) St. Dev.

Outlook:

- Place for generative modelling
- Useful latent variables

Ice Core Dating

via Probabilistic Programming

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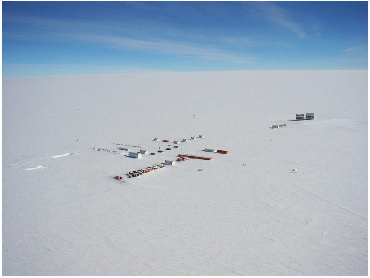
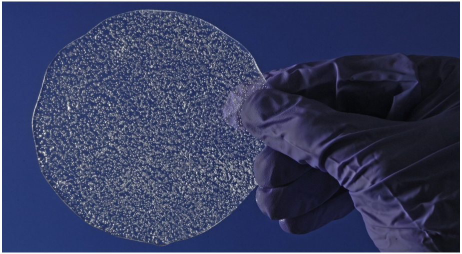
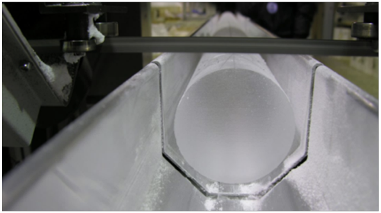
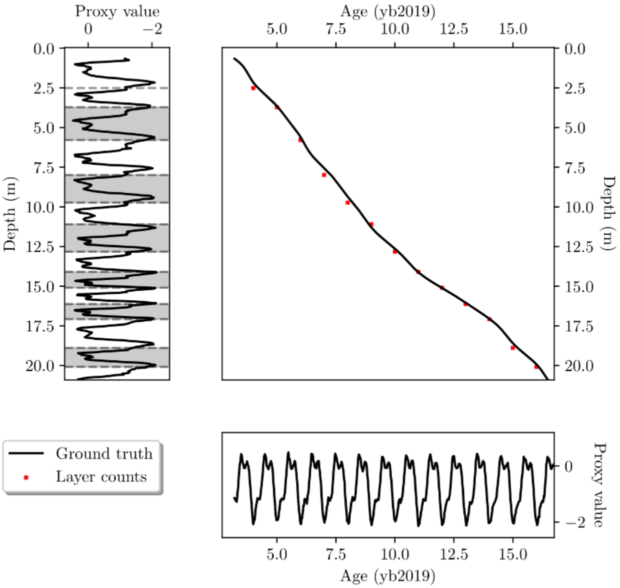
Palaeoclimatology – Ice core dating



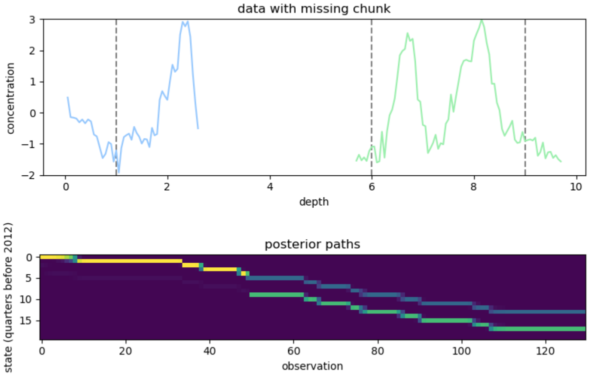




Ice core dating



Hidden Markov model – Probabilistic programming



Outlook:

- Probabilistic Programming Languages (PPLs) enable composability of model blocks while ensuring maintainability
- Interpretation is hard

Multi-fidelity experimental design for simulators

with Application to Ice Sheet Models

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J. Scott Hosking [2, 3] Neil D. Lawrence [1, 2] Ieva Kazlauskaite [1, 3]

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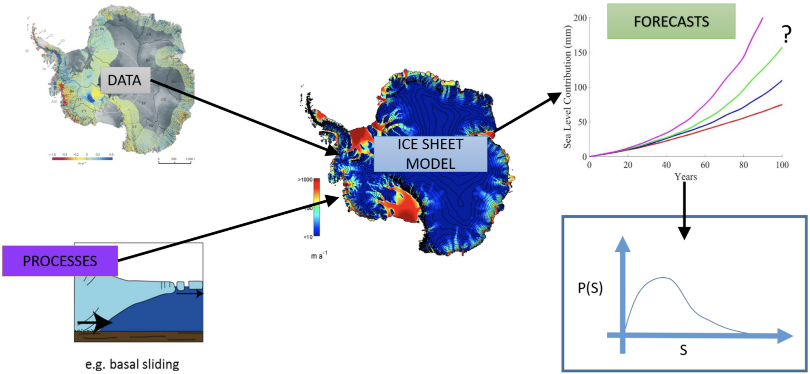
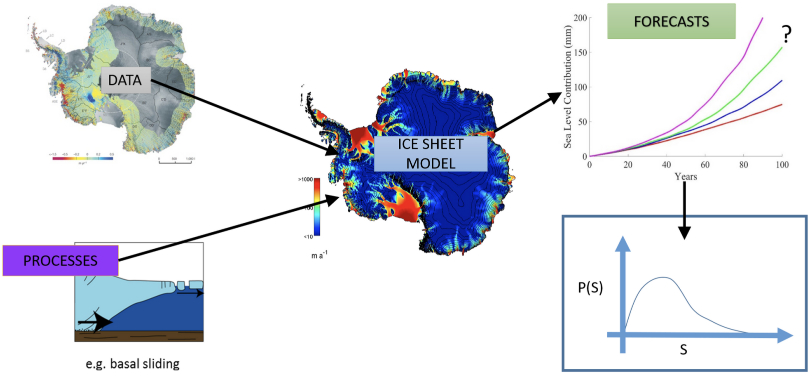
Ice Sheet Models – Hybrid modelling

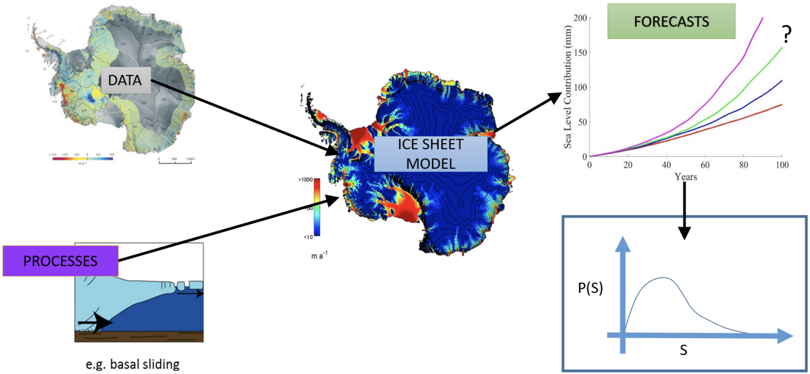


Ice Sheet Models – Hybrid modelling



- Historical data in ensembles
- Empirical priors of parameters (*e.g.*, exponent in Glen's law)

Ice Sheet Models – Hybrid modelling

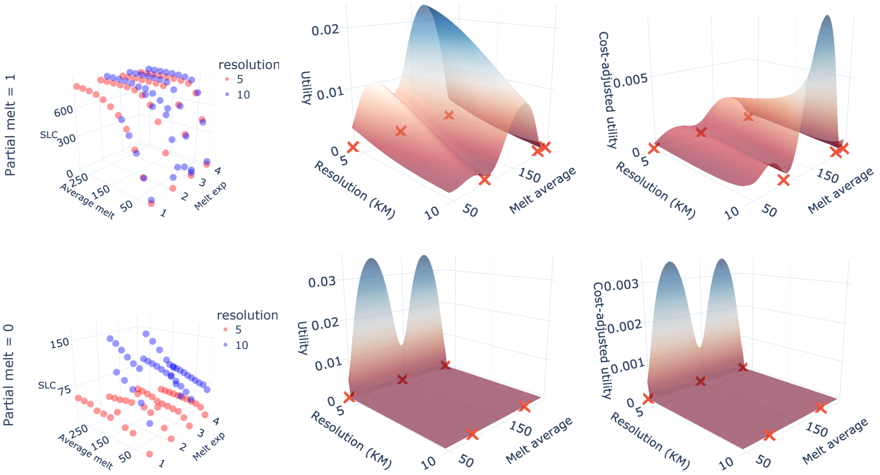


- Historical data in ensembles
- Empirical priors of parameters (*e.g.*, exponent in Glen's law)

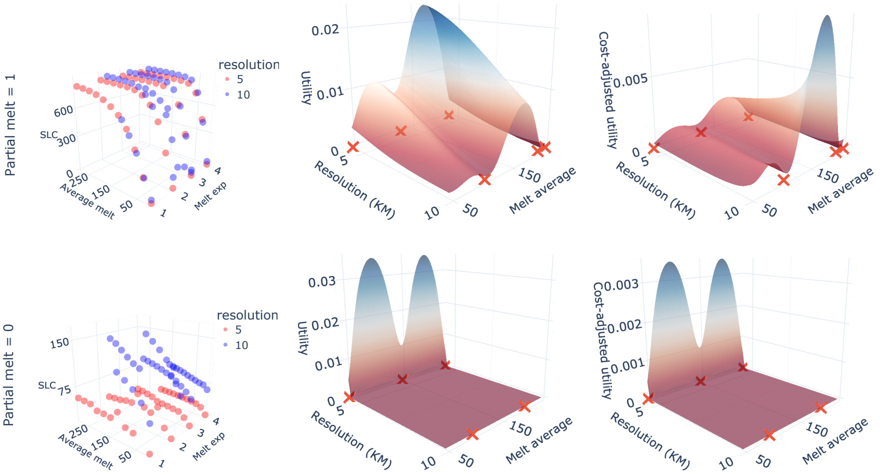
What can ML offer?

Change in prediction based on experimental parameters

Ice sheet experimental design



Ice sheet experimental design



Outlook:

- Place for statistics/machine learning

Discussion

- Sparse algebra in ML
- Application of generative models
- Probabilistic programming languages
- Role of ML