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Optimal Bayesian Design of Borehole Locations for Inferring Past Ice Sheet Surface Temperatures

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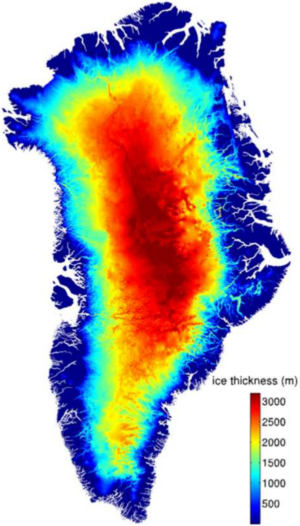
Motivation



Source: (left) National Snow & Ice Data Center, (middle) earth-chronicles.com, (right) Andrew D. Davis

Motivation

Ice sheets impact future global mean sea level

- Greenland: $\approx$ 6 meters   Antarctica: $\approx$ 60 meters

Source: National Geographic

Model calibration from field observations

Generally, we need to. . .

- develop and improve physics-based models
- calibrate models with observation data
- predict with quantified uncertainty

Past surface temperature:

- An indication of past climate and geological events
- Inferred from borehole data
- Drill, insert, equilibrate, measure

$\Rightarrow$ Overall process 2-4 years!

Some measurements are more useful than others

Borehole data acquisition is:

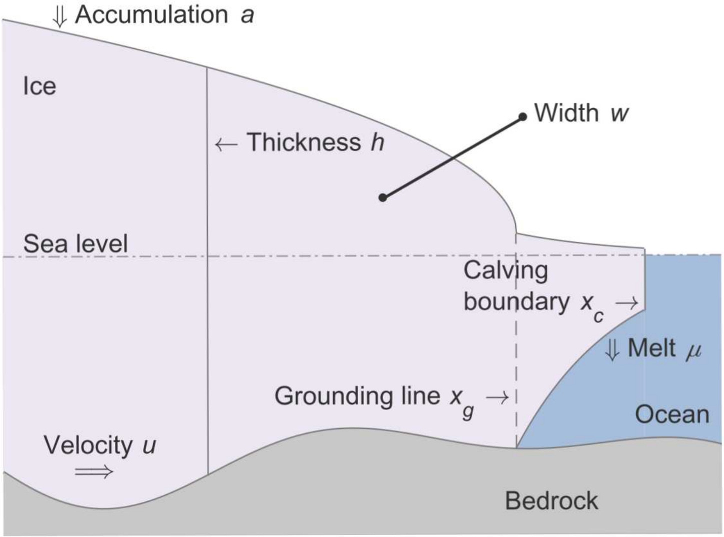
- time-consuming
- expensive
- dangerous

Goal of Optimal Experimental Design:

Select borehole locations that maximize the value of data for inferring past surface temperature

Outline

Anatomy of an ice stream



Three-part physical model

Three-part flowline model:

1. Compute grounded thickness $h(x,t)$ and velocity $\mathbf{u}(x,t)$ from stress and mass balance equations [Dupont 05, Hindmarsh 12, Jamieson 12, Pegler 13, Pegler 16]
2. Select a calving law and solve for the terminus $x_c(t)$ [Nick 10, Schoof 17]
3. Describe temperature $T(x,z,t)$ using advection-diffusion
   - Dirichlet boundary condition at the surface (assumed constant in x)

$$\dot{T} + \kappa\nabla^2 T + \mathbf{u}\cdot\nabla T = 0$$
$$T(x, h(x,t), t) = T_s(t;\theta)$$

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Forward problem: $\theta \to T(x, z, t)$

Inverse problem: noisy $T(\xi, :, t_f) \to \theta$

Optimal experimental design: *best* location ξ^* for noisy $T(\xi^*, :, t_f) \to \theta$

Parameterization of the surface temperature

Surface temperature field...

- assumed independent of x but changes with t
- modeled using a **Gaussian process** [Rasmussen 06]

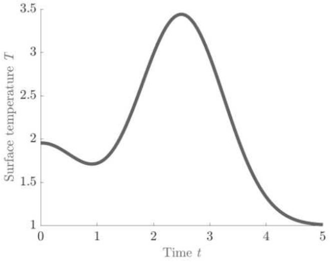
$$T_s(t;\theta) \approx \sum_{k=1}^{k_t} \sqrt{\theta_k} q_k(t) \zeta_k$$

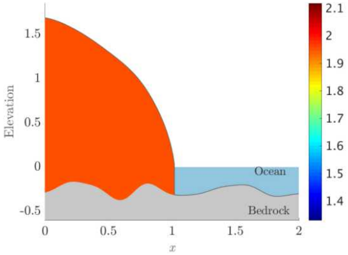
$$\text{with kernel} \quad K(t,t') = \exp\left(-\frac{\| t - t' \|_2^2}{2\ell^2}\right)$$

- k_t: number of terms after truncation (~ 10 in our study)
- K: covariance kernel (square-exponential; hyperparams fixed for now)
- θ_k: k^{th} eigenvalue of K
- $q_k(t)$: k^{th} eigenfunction of K
- ζ_k: $\stackrel{\text{iid}}{\sim} \mathcal{N}(0,1)$

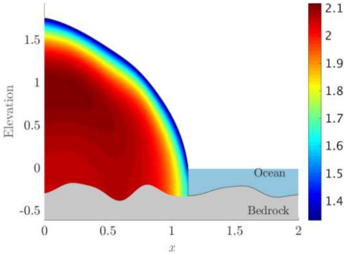
Sample modeling results

Surface temperature:





Initial condition (steady state)



Observable snapshot

Outline

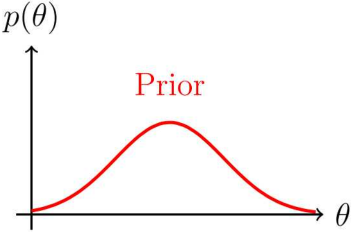
1. Physical model
2. Optimal Bayesian Experimental Design
3. Results

Bayesian inference

Characterize uncertainty using **Bayes' Theorem**:

$$\frac{\overbrace{p(\theta\quad)}^{prior}}{}$$

θ — parameters δ — noisy data



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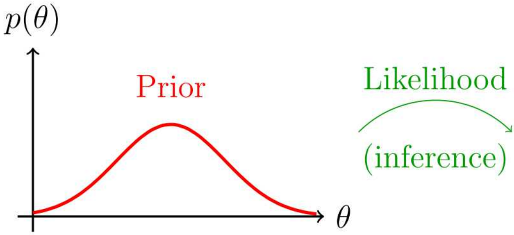

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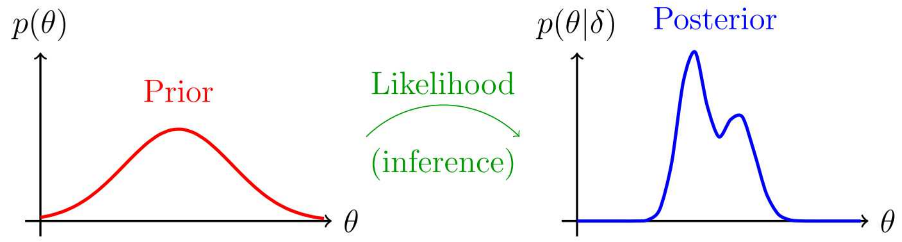
$$\overbrace{p(\theta|\delta)}^{\textit{posterior}} = \frac{\overbrace{p(\delta|\theta)}^{\textit{likelihood}}\overbrace{p(\theta)}^{\textit{prior}}}{\underbrace{p(\delta)}_{\textit{evidence}}}$$

θ — parameters $\qquad \delta$ — noisy data



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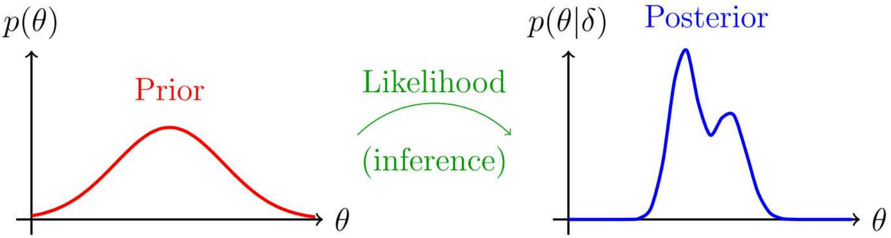
θ — parameters δ — noisy data ξ — design (experimental conditions)



Expected information gain

Expected **Kullback-Leibler (KL)** divergence between posterior and prior ($\iff$ **mutual information** between data and parameters) [Lindley 56]

$$U(\xi) = \mathbb{E}_{\delta|\xi}\left[D_{\mathrm{KL}}(p(\theta|\delta,\xi)||p(\theta|\xi))\right]$$

$$= \int_{\delta}\left[\int_{\theta}\ln\left[\frac{p(\theta|\delta,\xi)}{p(\theta)}\right]p(\theta|\delta,\xi)\,d\theta\right]p(\delta|\xi)\,d\delta$$

$$\approx \frac{1}{N}\sum_{i=1}^{N}\left\{\ln\left[p(\delta^{(i)}|\theta^{(i)},\xi)\right]-\ln\left[p(\delta^{(i)}|\xi)\right]\right\}$$

$$p(\delta^{(i)}|\xi) \approx \frac{1}{M}\sum_{j=1}^{M}p(\delta^{(i)}|\theta^{(i,j)},\xi)$$ (nested Monte Carlo!) [Ryan 03]

U — expected utility

θ — parameters of interest

δ — noisy data

ξ — design variables

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p(\delta^{(i)}|\xi) \approx \frac{1}{M}\sum_{j=1}^{M} p(\delta^{(i)}|\theta^{(i,j)},\xi) \quad \text{(nested Monte Carlo!)}
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Find optimal design: $\xi^* = \underset{\xi}{\operatorname{argmax}}\ U(\xi)$

Computationally prohibitive: $N = M = 10^3$ requires 10^6 forward evaluations

Another perspective on the expected utility

$$U(\xi) = \int_\theta \underbrace{\int_\delta \{\ln[p(\delta|\theta,\xi)] - \ln[p(\delta|\xi)]\}\, p(\delta|\theta,\xi)\, d\delta}_{f(\xi,\theta)}\, p(\theta)\, d\theta$$

$$\approx \frac{1}{N_1}\sum_{i_1=1}^{N_1} \underbrace{\frac{1}{N_2}\sum_{i_2=1}^{N_2}\left\{\ln\left[p(\delta^{(i_2)}|\theta^{(i_1)},\xi)\right] - \ln\left[p(\delta^{(i_2)}|\xi)\right]\right\}}_{\hat{f}(\xi,\theta)}$$

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with $\theta^{(i_1)} \sim p(\cdot)$, $\delta^{(i_2)} \sim p(\cdot|\theta,\xi)$ and an importance sampling estimate

$$p(\delta^{(i_2)}|\xi) \approx \sum_{j=1}^{M} p(\delta^{(i_2)}|\theta^{(i_2,j)},\xi) w^j \quad \text{with} \quad \theta^{(j)} \sim q(\cdot)$$

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- Triple-nested, but no new cost in integration
- Avoids surrogates that involve data δ (high-dimensional)
- Inner loops produce **noisy estimates** $\hat{f}(\theta,\xi) \approx f(\theta,\xi)$

Adaptive surrogate for Bayesian evidence

Given noisy estimates $\{\hat{f}_i(\theta_i, \xi_i)\}_{i=1}^{S}$ with known variance, we compute a **local polynomial surrogate** using regression

$$\eta(\theta, \xi) = \underset{m \in \mathcal{P}}{\operatorname{argmin}} \sum_{i=1}^{S} \left(m(\theta_i, \xi_i) - \hat{f}_i(\theta_i, \xi_i) \right)^2 \mathcal{K}(\theta_i, \xi_i; \theta, \xi)$$

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The error bound can be shown to be

$$\| \eta(\theta, \xi) - f(\theta, \xi) \| \leq C_S \Delta^{p+1}$$

Replacing f with η introduces a bias of $C_S \Delta^{p+1}$; choose S such that

$$\begin{aligned} [\text{Monte Carlo variance}] &\sim [\text{Surrogate bias}]^2 \\ C_{MC} N^{-1} &\sim C_s^2 \Delta^{2(p+1)} \end{aligned}$$

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- Regression averages noise from $\hat{f}$ so we can choose smaller N_2, M
- Choosing $S \approx 50$, $N_2 = M = 10$ requires $SN_2M \approx 5000 \ll 10^6$ model evaluations

Outline

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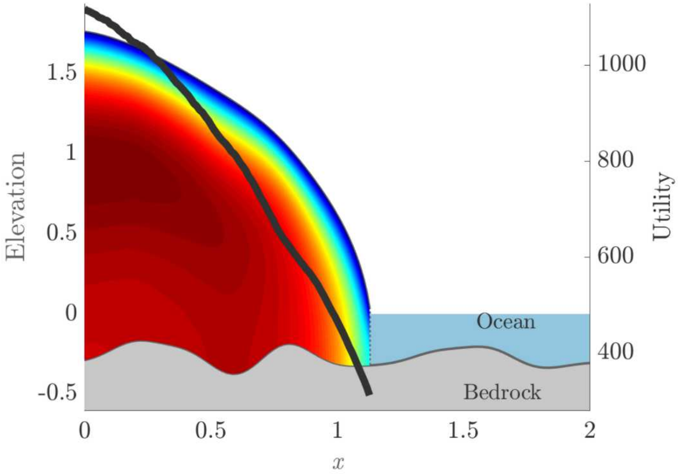
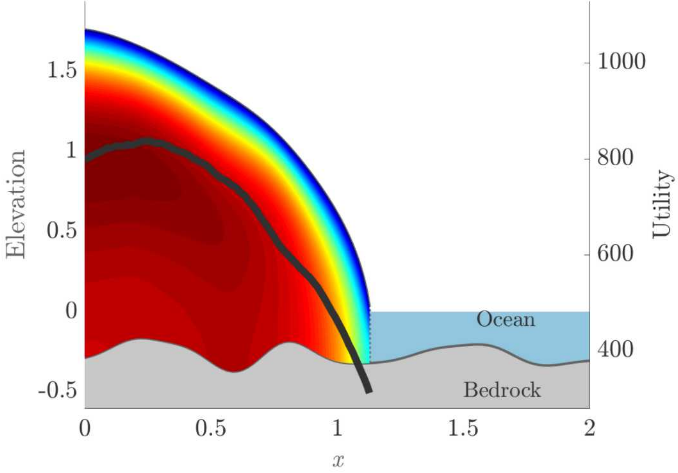


Expected information gain with inland hiking penalty

$$U(\xi) = \mathbb{E}_{\delta|\xi}\left[D_{\mathrm{KL}}(p(\theta|\delta,\xi)||p(\theta|\xi))\right] - 250(x_g - \xi)^2$$



Summary

Conclusions:

- Formulated borehole selection problem in a Bayesian setting and using optimal experimental design
- Constructed surrogate on information gain to significantly reduce computational costs from nested Monte Carlo
- Adapted surrogate based on bias-variance tradeoff
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Future work:

- Incorporate more complex physical model: geothermal heating, frictional heating, internal source/sinks
- Include more sophisticated cost/constraints within a 2D spatial setting
- Design multiple locations on single expedition

Acknowledgment

- Sandia National Laboratories[1]
- Massachusetts Institute of Technology
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- National Science Foundation

[1] Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the presentation do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

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