Uncertainty Quantification and Experimental Design for Large-Scale Linear Inverse Problems under Gaussian Process Priors, with Applications to Geophysics.

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Goal: Find high-density regions in Stromboli

Where should we collect data?



Figure: True density and excursion set (generated from model).



Figure: Proposed data collection plan, wIVR long-range strategy, total budget of 90 observations.



Figure: Estimated excursion set (Vorob'ev Expectation) and coverage function.

- Extend Bayesian experimental design criterion to inverse problems.
- Fine grained reconstruction (50m) \implies big grid (\sim 150k cells) \implies big cov matrix (\sim 150GB).

Implicit Representation of Covariance Matrix

Observation

Posterior covariance information may be extracted via products with *tall and thin* matrices:

 $\tilde{K}A,\ A\in \mathbb{R}^{m\times p},\ p\ll m$

Only need to maintain a multiplication routine.



Implicit Representation: Sequential Setting

$$K^{(n)}A = K^{(0)}A - \sum_{i=1}^{n} \bar{K}_{i}R_{i}^{-1}\bar{K}_{i}^{T}A$$
$$\bar{K}_{i} := K^{(i-1)}G_{i}^{T},$$
$$R_{i}^{-1} := \left(G_{i}K^{(i-1)}G_{i}^{T} + \tau^{2}I\right)^{-1}.$$

• Update representation at evey new data inclusion.

Bayesian Experimental Design for Inverse Problems

Implicit Representation gives access to (and fast updates of) posterior covariance on large grids.



Since implicit representation allows fast inclusion of new datapoints, can study the *limiting distribution*.

Limiting Distribution

- Posterior distribution after data collected at all accessible locations.
- Gives sense of *minimal residual uncertainty* (inherent to this type of data).



Figure: Evolution of true and false positives as a function of the number of observations.

Implicit representation allows sampling through residual kriging.



Figure: Prior (left) and empirical posterior (right) distribution (after 450 observations) of the excursion volume for each ground truth. True volumes are denoted by vertical lines.