The Bayesian framework for calibration and UQ with application to a porous media flow model

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Motivation

Understand physical phenomena

Observations of phenomena

Mathematical model of phenomena (includes some parameters that characterise behaviour)

Numerical model approximating mathematical model

Find parameters in a situation of interest (calibration)

Use the parameters to do something cool

General framework

Model (usually a PDE): $\mathcal{G}(u, \theta)$ where u is the initial condition and θ are model paramaters.

u: perhaps an initial condition

θ: perhaps some interesting model parameters (diffusion, convection speed, permeability field, material properties)

Observations:

$$
\begin{aligned}
& y_{j,k} = u(x_j, t_k) + \eta_{j,k}, \quad \eta_{j,k} \overset{\text{i.i.d}}{\sim} \mathcal{N}(0, \sigma^2) \\
\rightsquigarrow \quad & y = \mathcal{G}(\theta) + \eta, \quad \eta \sim \mathcal{N}(0, \sigma^2 I)
\end{aligned}
$$

Want:

$$p(\theta | y) \propto p(y | \theta) p(\theta)$$

Why?

Do we need Bayes's theorem?

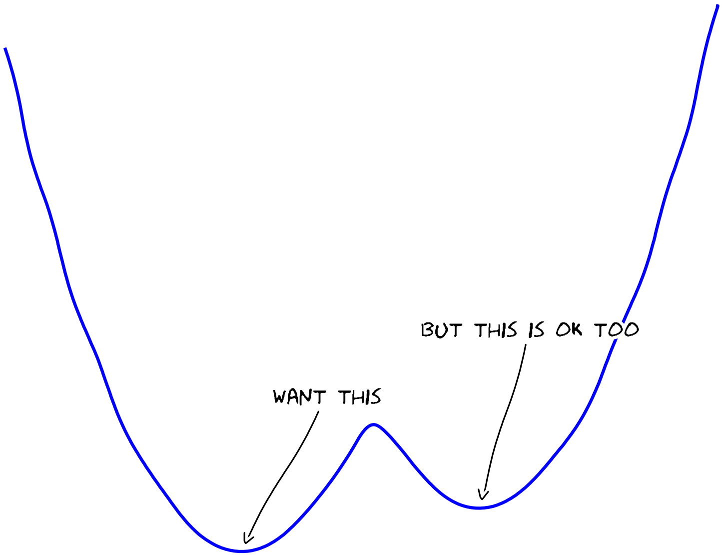
Is Bayes's theorem really necessary? We could minimise

$$J(\theta) = \frac{1}{2\sigma^2}\|\mathcal{G}(\theta) - y\|^2 + \frac{1}{2\lambda^2}\|\theta\|^2$$

to get

$$\theta^* = \text{argmin}_\theta \, J(\theta)$$

Do we need Bayes's theorem?



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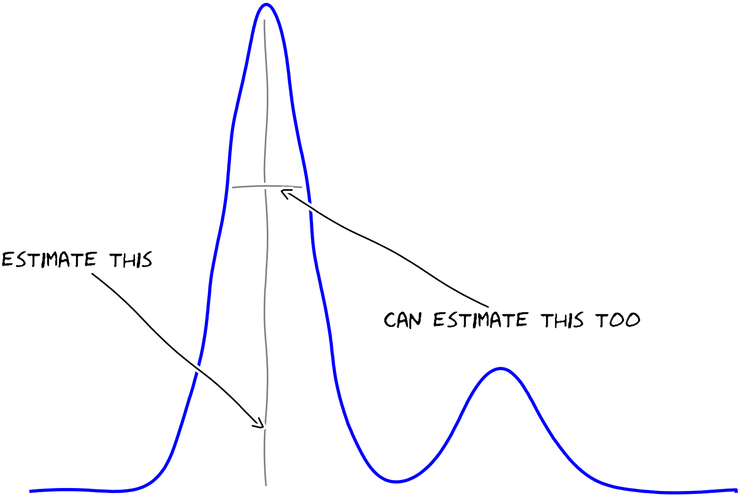


Do we need Bayes's theorem?

Bayesian methods involve estimating *uncertainty* (as well as mean).
They're equivalent.

Deterministic optimisation:

$$J(\theta) = \underbrace{\frac{1}{2\sigma^2}\|\mathcal{G}(\theta) - y\|^2}_{\textit{misfit}} + \underbrace{\frac{1}{2\lambda^2}\|\theta\|^2}_{\textit{regularisation}}$$

Bayesian framework:

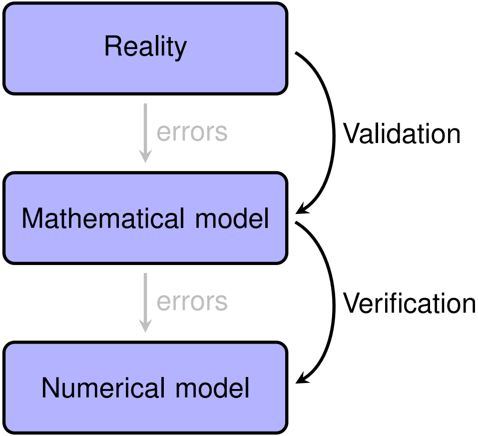
$$\begin{aligned}\exp(-J(\theta)) &= \underbrace{\exp\left(-\frac{1}{2\sigma^2}\|\mathcal{G}(\theta) - y\|^2\right)}_{\textit{likelihood}} \underbrace{\exp\left(-\frac{1}{2\lambda^2}\|\theta\|^2\right)}_{\textit{prior}} \\ &= p(y|\theta)p(\theta) \\ &\propto p(\theta|y)\end{aligned}$$

Method for solving Bayesian inverse problems

- Kalman filtering/smoothing methods
  - Kalman filter (Kalman)
  - Ensemble Kalman filter (Evensen)
- Variational methods
  - 3D VAR (Lorenc)
  - 4D VAR (Courtier, Talagrand, Lawless)
- Particle methods
  - Particle filter (Doucet)
- Sampling methods
  - Markov chain Monte Carlo (Metropolis, Hastings)

This list is not exhaustive. The body of work is prodigious.

Understanding errors



"I reject your reality and substitute my own!"

— Adam Savage (Mythbusters)

Porous media flow application

We will conjur our very own reality. Model is

$$\begin{aligned} \frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} &= \nu \frac{\partial^\alpha c}{\partial x^\alpha}, \quad t > 0, \quad x \in (0,1) \\ c(x,0) &= c_0(x), \\ c(0,t) &= c(1,t), \quad t > 0 \end{aligned}$$

and u is a known fluid velocity independent of x. Observations are

$$\begin{aligned} & y_{jk} = c(x_j, t_k) + \eta_{jk}, \quad \eta_{jk} \overset{\text{i.i.d}}{\sim} \mathcal{N}(0, \sigma^2) \\ \rightsquigarrow \quad & y = (y_{11}, \dots, y_{JK})^\top \in \mathbb{R}^{JK} \end{aligned}$$

We get to play God with our reality.

Porous media flow application

- Write down the mathematical model for what we think is happening.
- Know it's some kind of confusion equation, but there might be errors.
- Perhaps, since medium is porous, the flux is weird?

$$\begin{aligned} \frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} &= \bar{\nu}\frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x} + \mathcal{L}(c)\right), \\ &=: \mathcal{A}c \end{aligned}$$

Same initial and boundary conditions as reality.

What does $\mathcal{L}$ look like given the observations y? Bayes to the rescue,

$$p(r_k, \theta_k | y) \propto p(y | r_k, \theta_k) p(r_k, \theta_k),$$

where,

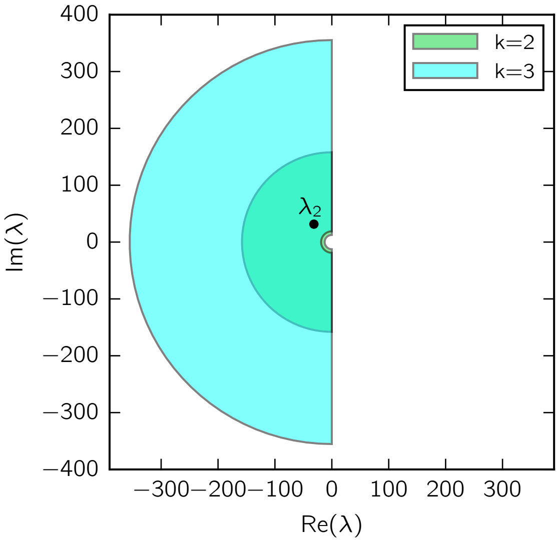
$$\begin{aligned} \lambda_k &= r_k \exp(i\theta_k), \\ \mathcal{A}\phi_k(x) &= \lambda_k \phi_k(x). \end{aligned}$$

The prior: $p(r_k, \theta_k)$

Assumptions:

1. r_j and r_k are independent for $j \neq k$;
2. θ_j and θ_k are independent for $j \neq k$;
3. r_j and θ_k are independent $\forall j, k$;
4. $r_k \sim U[2\pi k, (2\pi k)^2]$;
5. $\theta_k \sim U[-\frac{\pi}{2}, \frac{\pi}{2}]$.

The prior $p(r_k, \theta_k)$

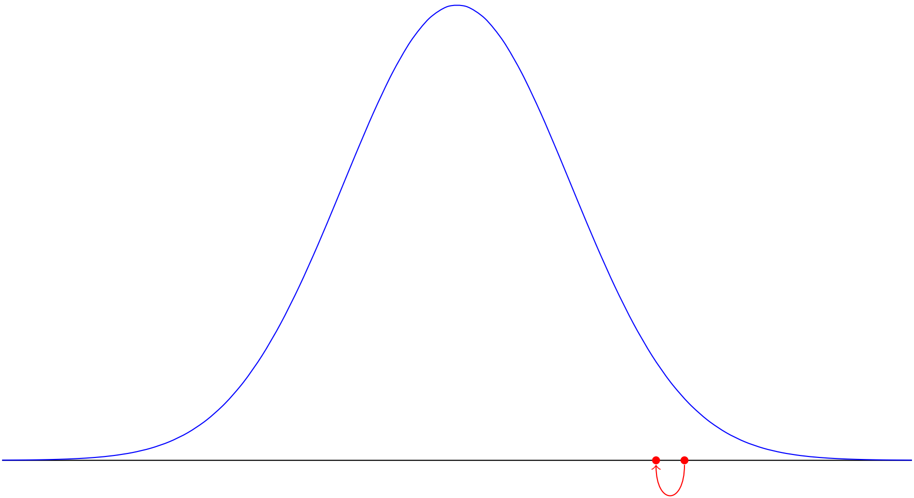


QUESO

Nutshell: QUESO gives samples from $p(\theta|y)$ (called MCMC)

- Library for Quantifying Uncertainty in Estimation, Simulation and Optimisation
- Born in 2008 as part of PECOS PSAAP programme
- Provides robust and scalable sampling algorithms for UQ in computational models
- Open source
- C++
- MPI for communication
- Parallel chains, each chain can house several processes
- Dependencies are MPI, Boost and GSL. Other optional features exist
- http://libqueso.com

What does MCMC look like?



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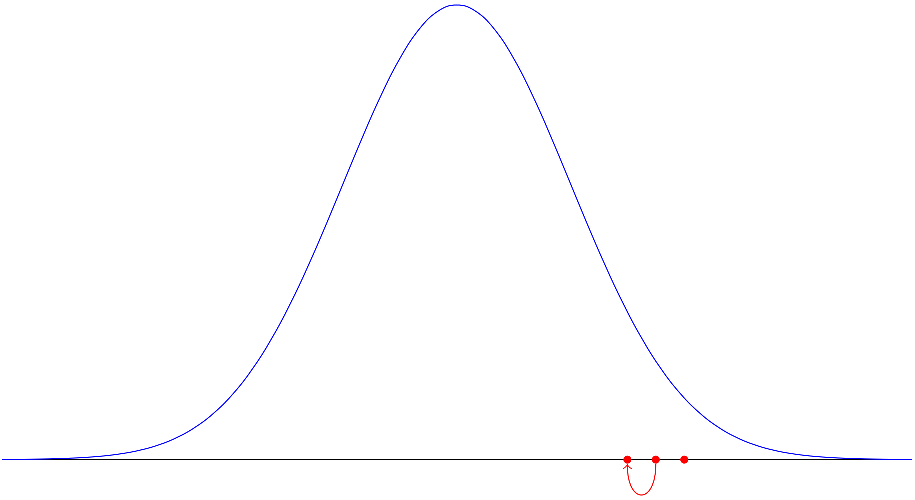

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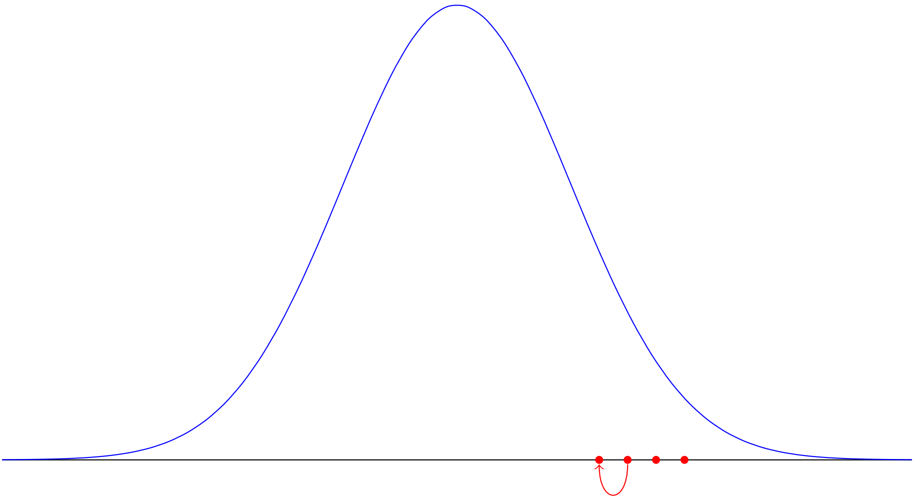

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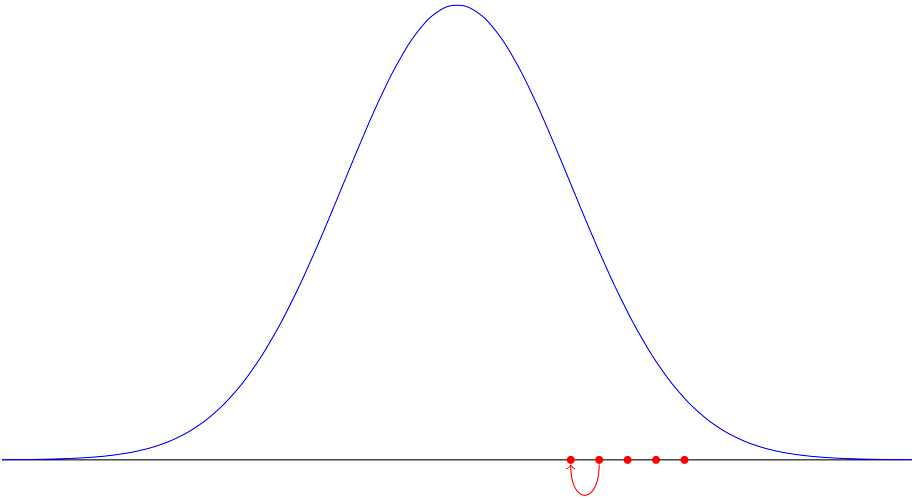

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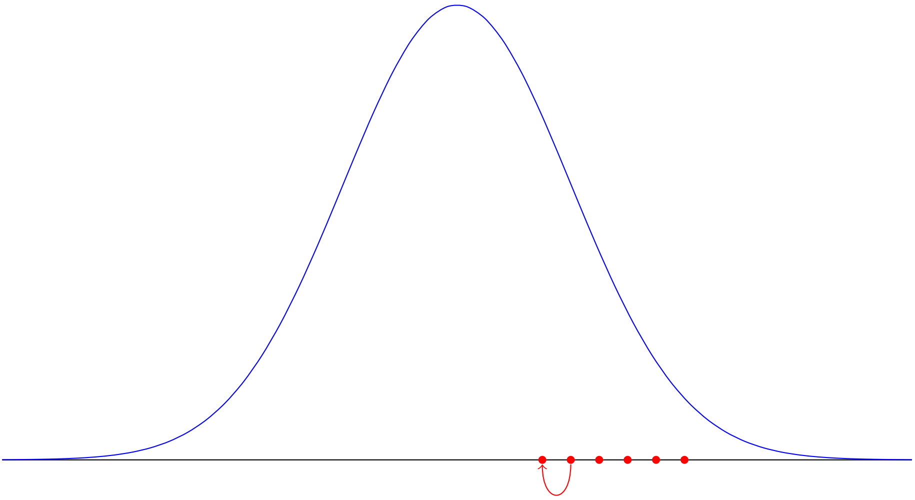

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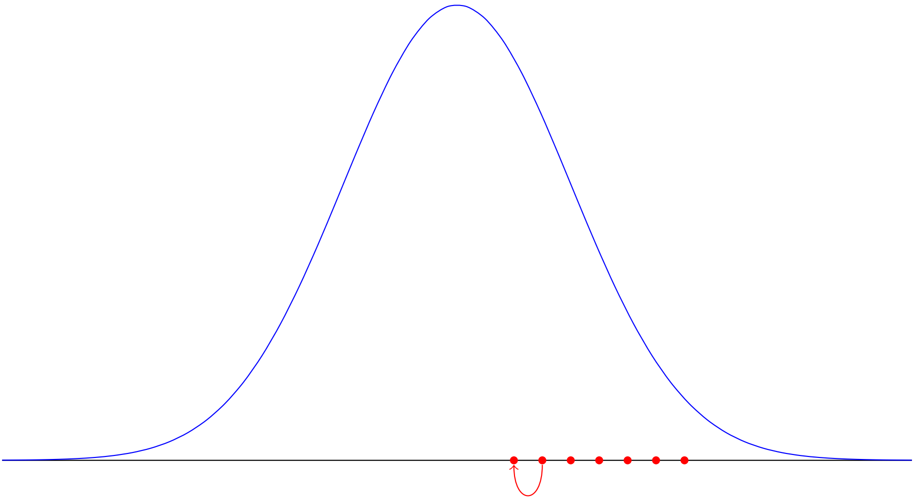

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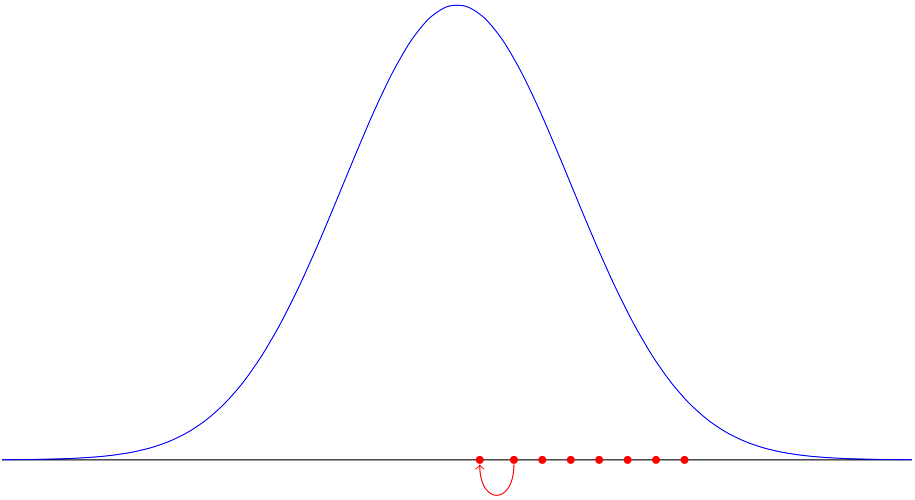

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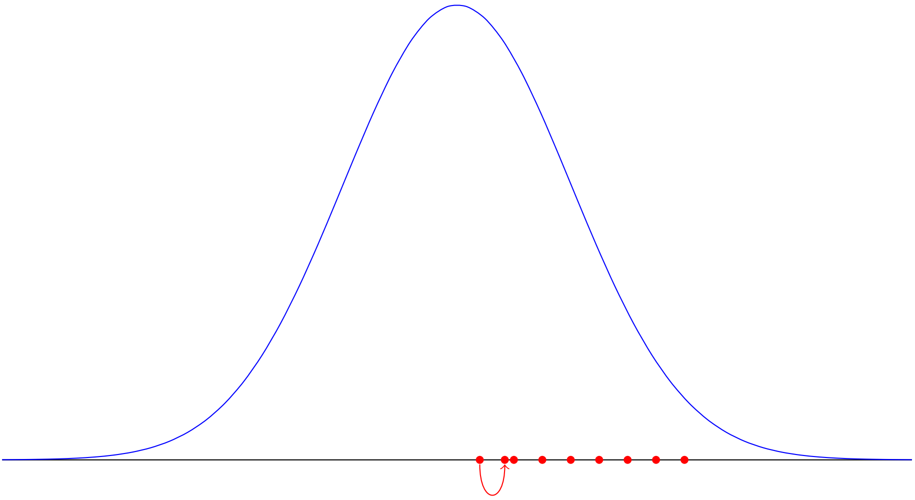

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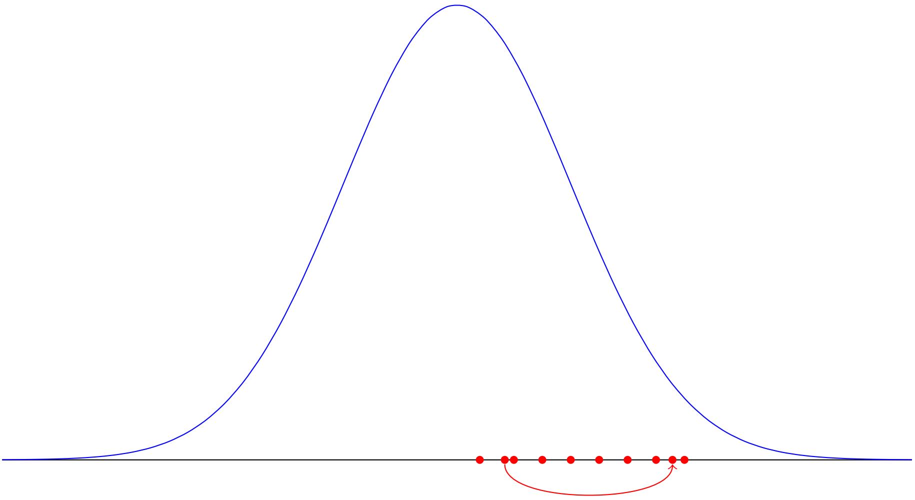

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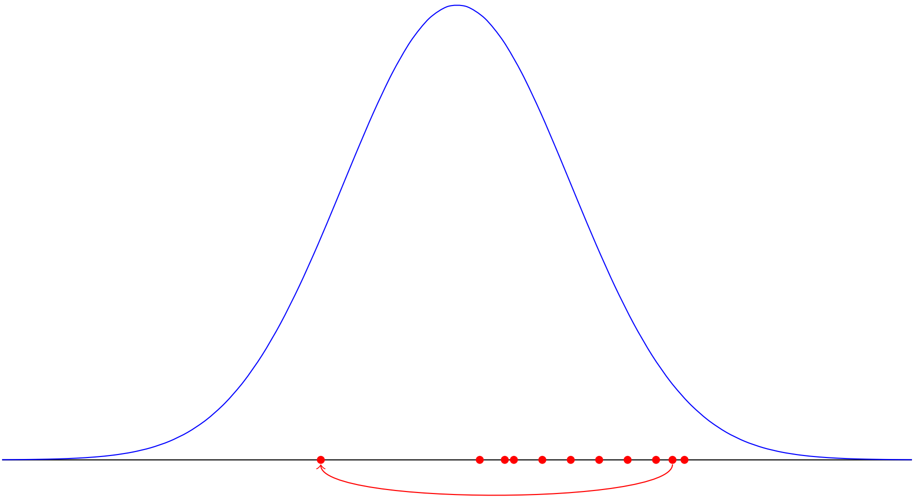

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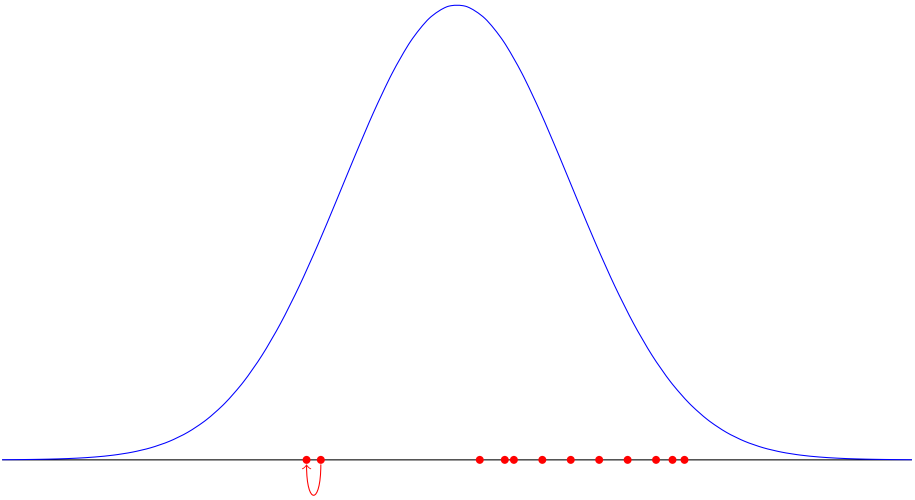

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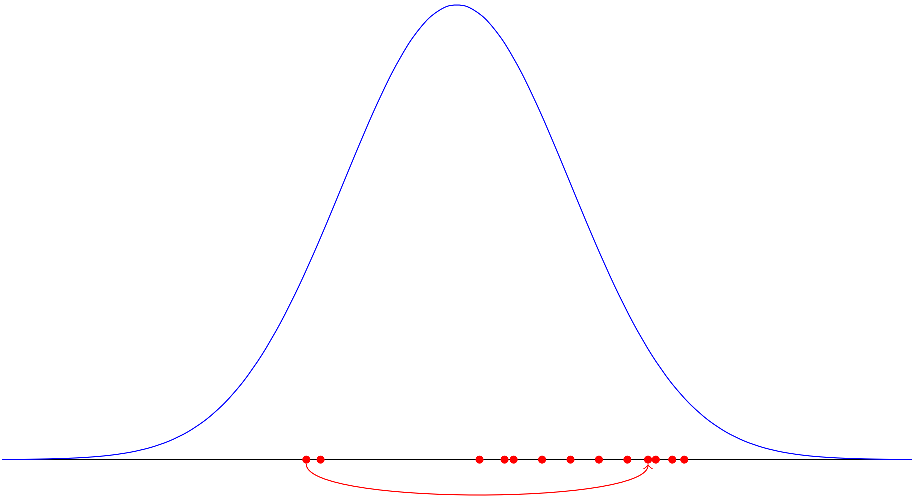

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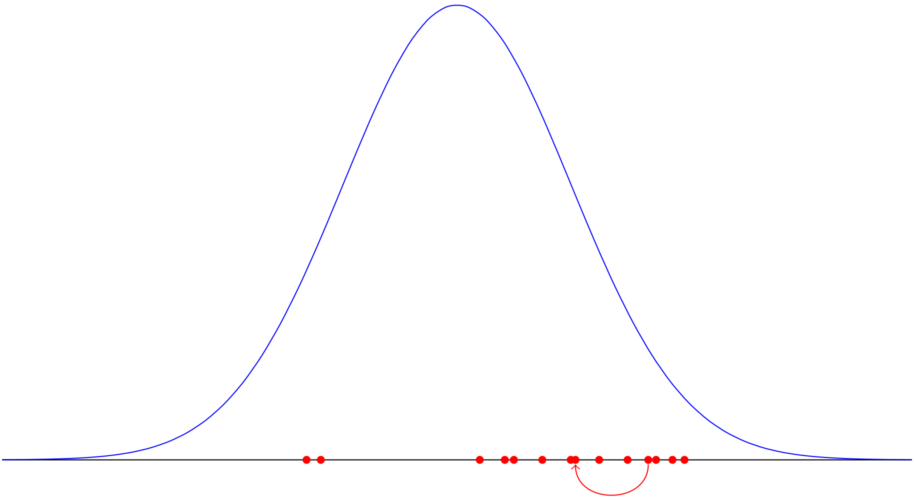

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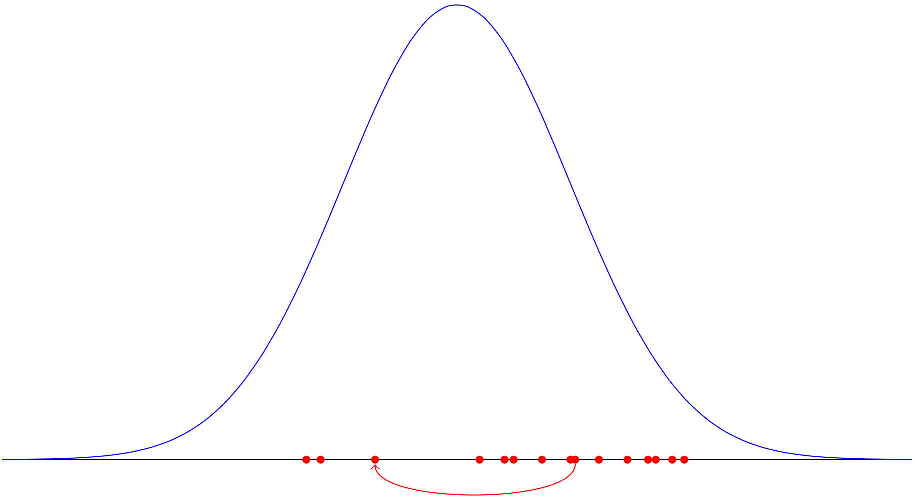

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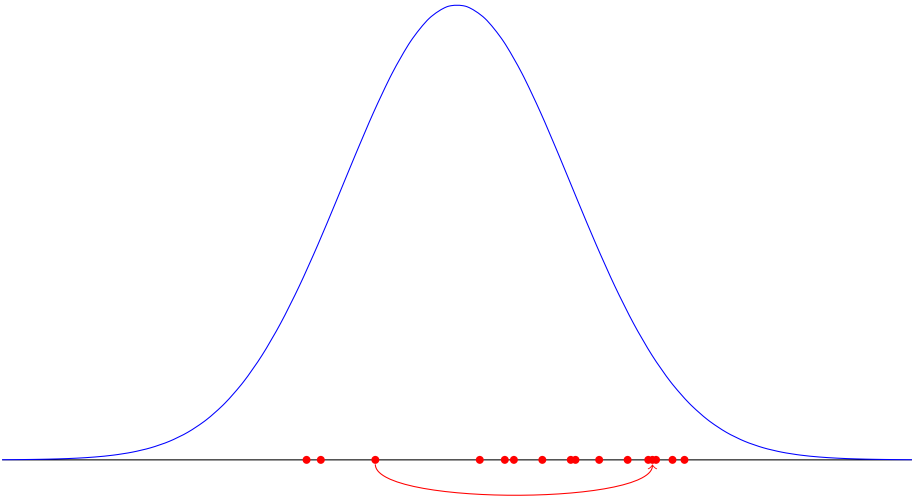

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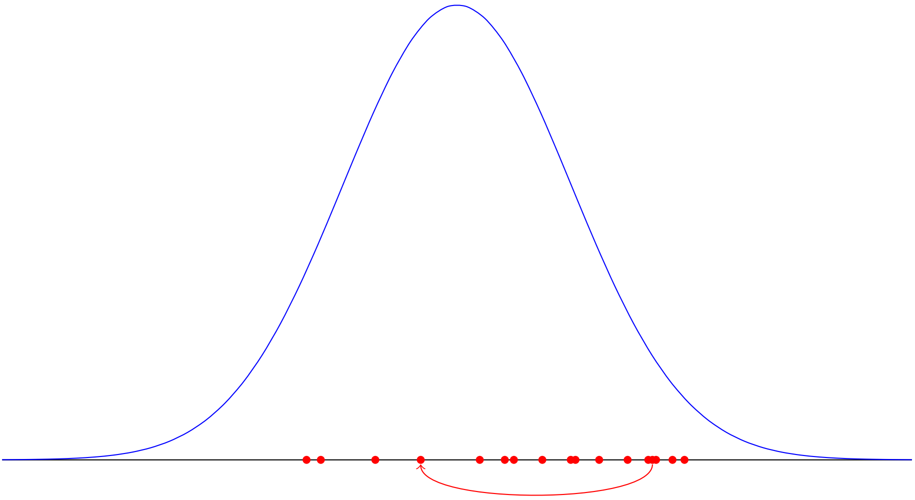

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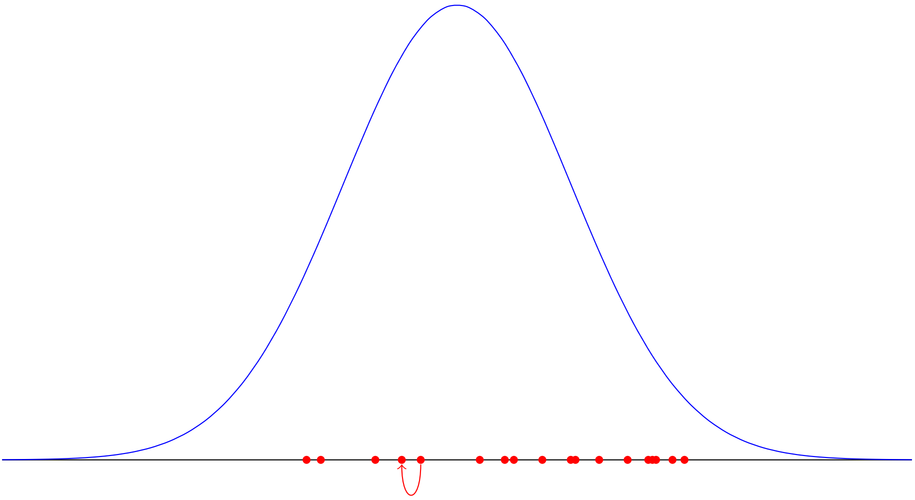

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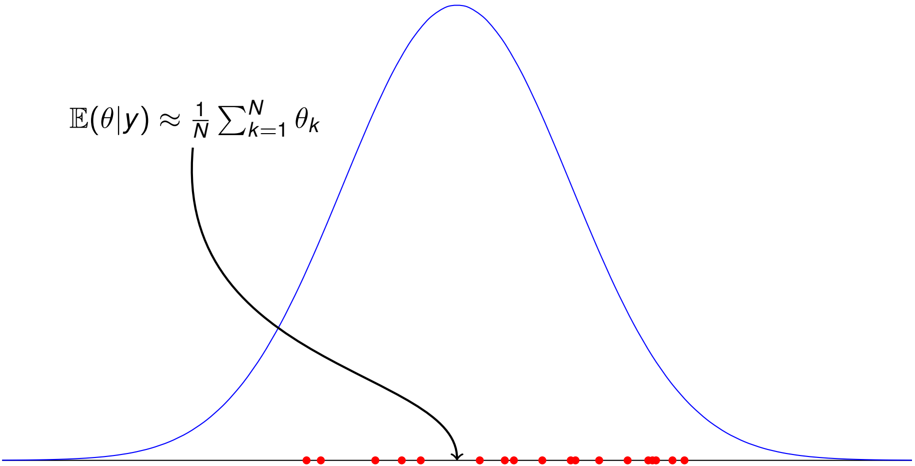

How to do MCMC? Sampling $p(\theta|y)$

- Idea: Construct $\{\theta_k\}_{k=1}^{\infty}$ cleverly such that $\{\theta_k\}_{k=1}^{\infty} \sim p(\theta|y)$
  1. Let θ_j be the 'current' state in the sequence and construct a *proposal*, $z \sim q(\theta_j, \cdot)$

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3. Let

$$\theta_{j+1} = \begin{cases} \theta & \text{with probability } \alpha(\theta_j, z) \\ \theta_j & \text{with probability } 1 - \alpha(\theta_j, z) \end{cases}$$

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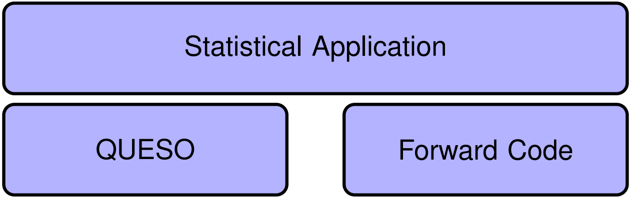
- We can take θ_1 to be a draw from $p(\theta)$

Why use QUESO?

Other solutions are available, e.g. R, PyMC, emcee, MICA, Stan, MUQ.

QUESO solves the same problem, but:

- Has been designed to be used with large forward problems
- Has been used successfully with 5000+ cores
- Leverages parallel MCMC algorithms
- Supports for finite **and** infinite dimensional problems



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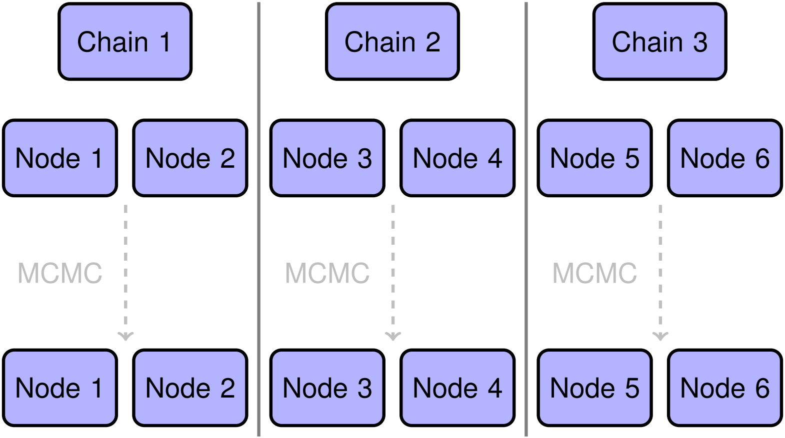
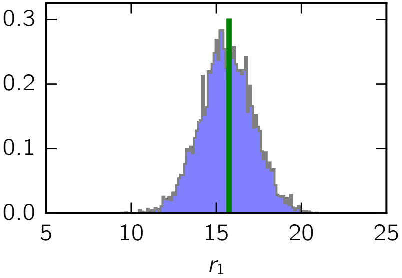
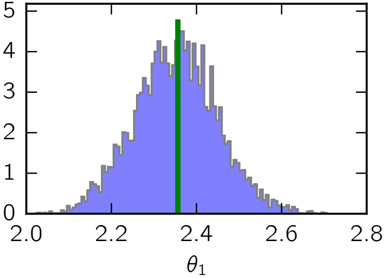


Results

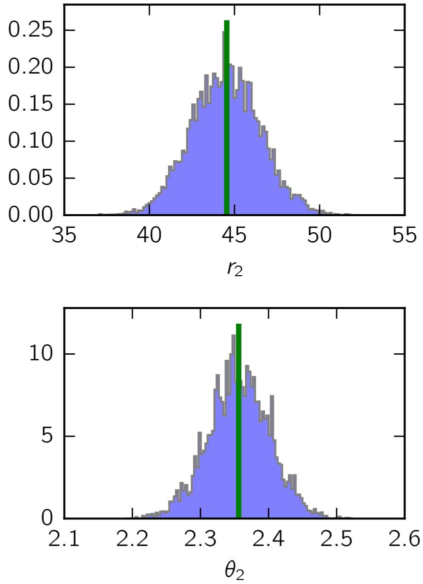
- $c_0(x) = A \exp\left(-\frac{1}{2\tau^2} \|x - 0.5\|\right)$
- $\alpha = 1.5$
- $\sigma = 0.01$
- $J = 8, K = 1 \Rightarrow y \in \mathbb{R}^8$
- `QUESO` DRAM algorithm
  - http://libqueso.com

Results: $p(r_1, \theta_1 | y)$

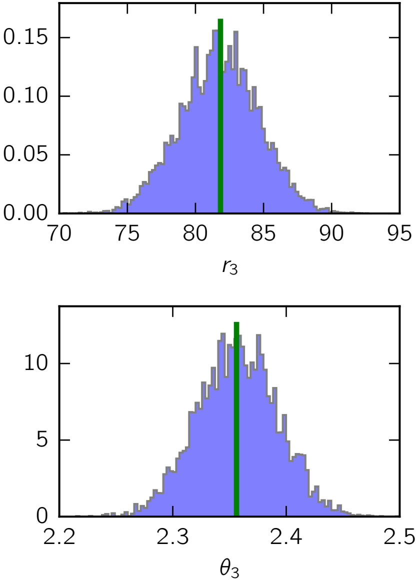




Results: $p(r_2, \theta_2 | y)$



Results: $p(r_3, \theta_3 | y)$



Summary

- Shown how to solve a Bayesian calibration problem.
- Shown what the solution to this calibration problem looks like.
- Described the (open source) software that we use.
- Can infer a differential operator. This is new.
- Framework arises from not knowing the truth.
- Future work:
  - Application to a problem where the inadequacy (operator) does not capture the true inadequacy
  - May still involve operator inference, but the operator is random
  - Are there opportunities to advance the algorithmic component for these types of problems?
  - Will these algorithms be HPC-friendly?

- We're hiring!
  - Post-doctoral research fellows
  - `http://pecos.ices.utexas.edu/job-postings/`