The University of Auckland – Applied Mathematics

Bayesian Methods for Inverse Problems : why and how

Colin Fox

Tiangang Cui, Mike O'Sullivan (Auckland), Geoff Nicholls (Statistics, Oxford)

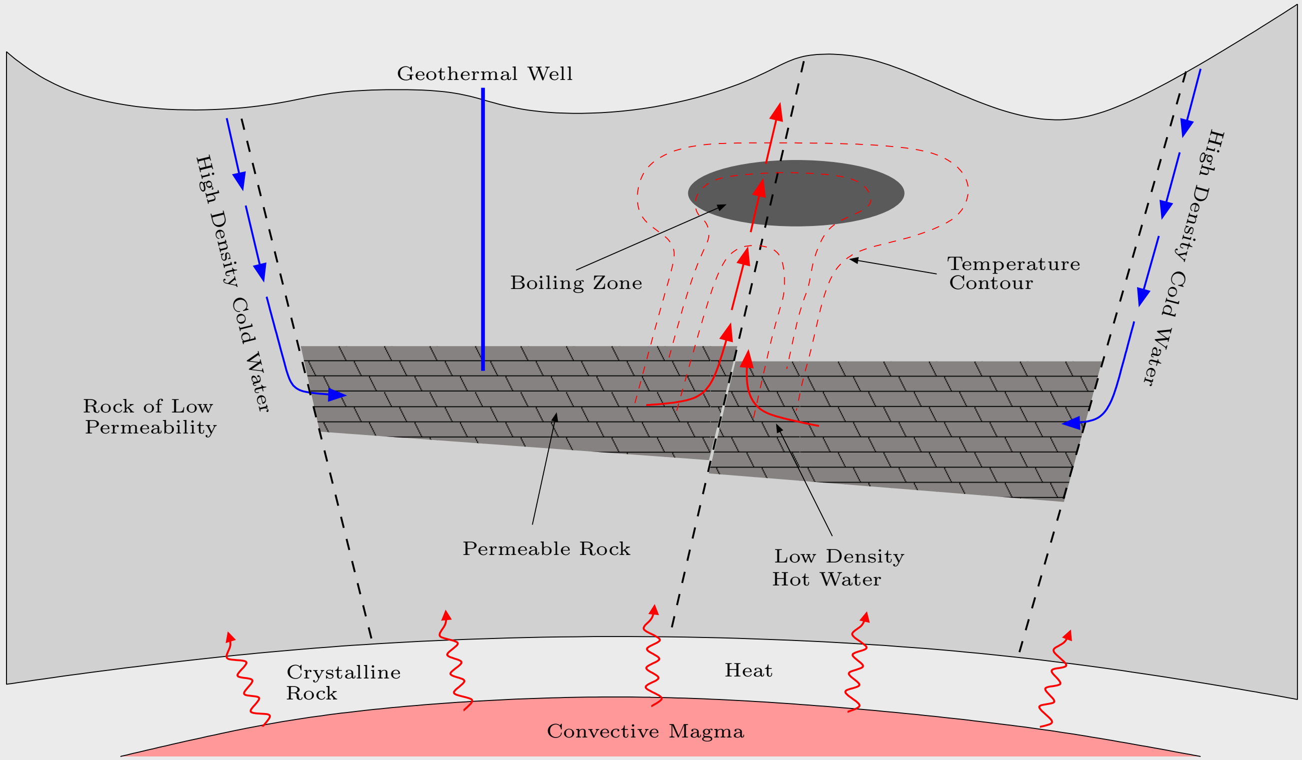
fox@math.auckland.ac.nz

In this talk

- An example in geothermal model calibration
- Inferential solutions to inverse problems, noise and all
- The need to integrate: pixel-wise degraded binary images
- Monte Carlo integration
- Computation (MCMC)
- Output analysis for geothermal problem
- Next talk :: better sampling algorithms

An inverse problem in geothermal fields

Schematic of a geothermal field



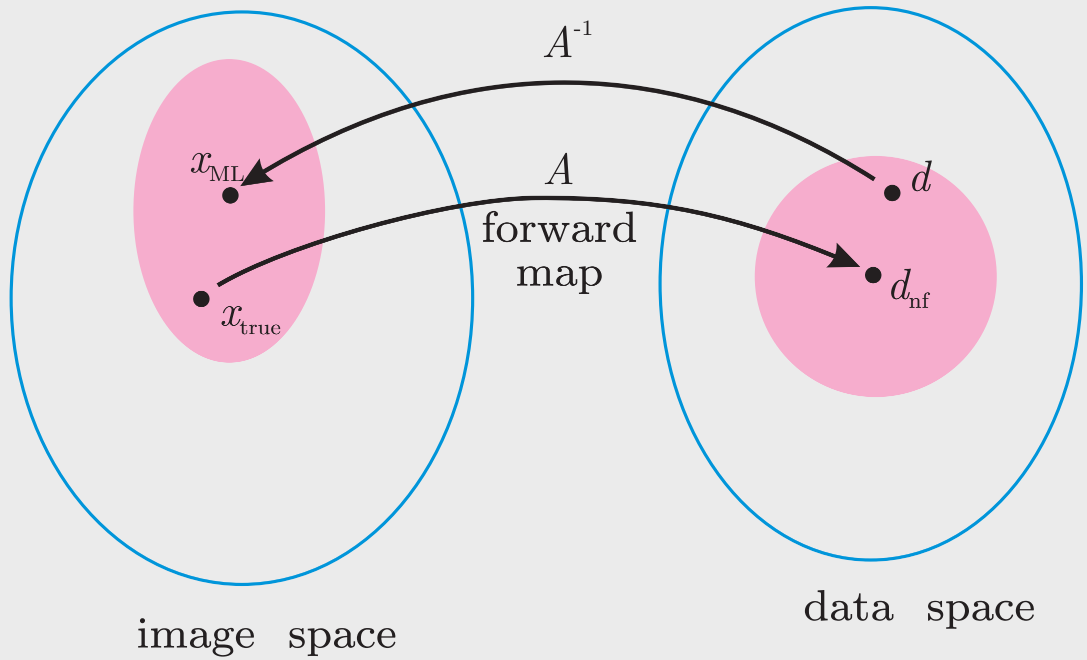
Given near-surface measurements of temperature, pressure, flow, want

- Model calibration :: rock type, porosity, fracture : heat sources
- Predict :: long term (50 year) power generation, land subsidence, etc
- Decide :: robust investment plan

Wairakei geothermal power generator

Bayesian formulation of inverse problems

$d = Ax + n$: data d, image x, measurement noise n, forward map A



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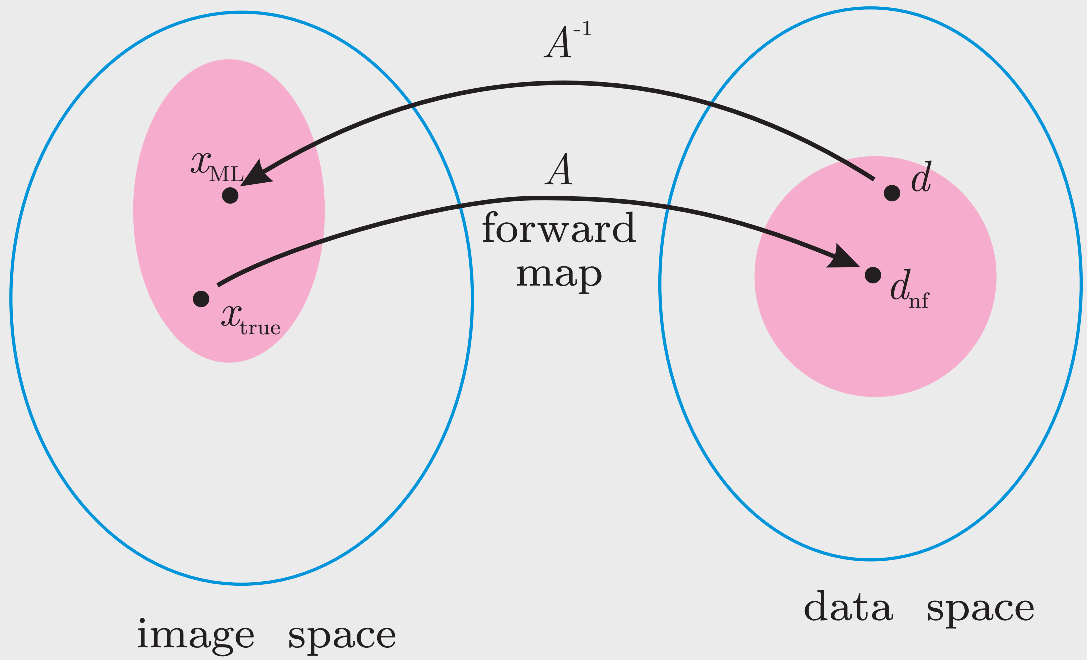

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Likelihood: measurement and noise (Physics, instrumentation, probability)

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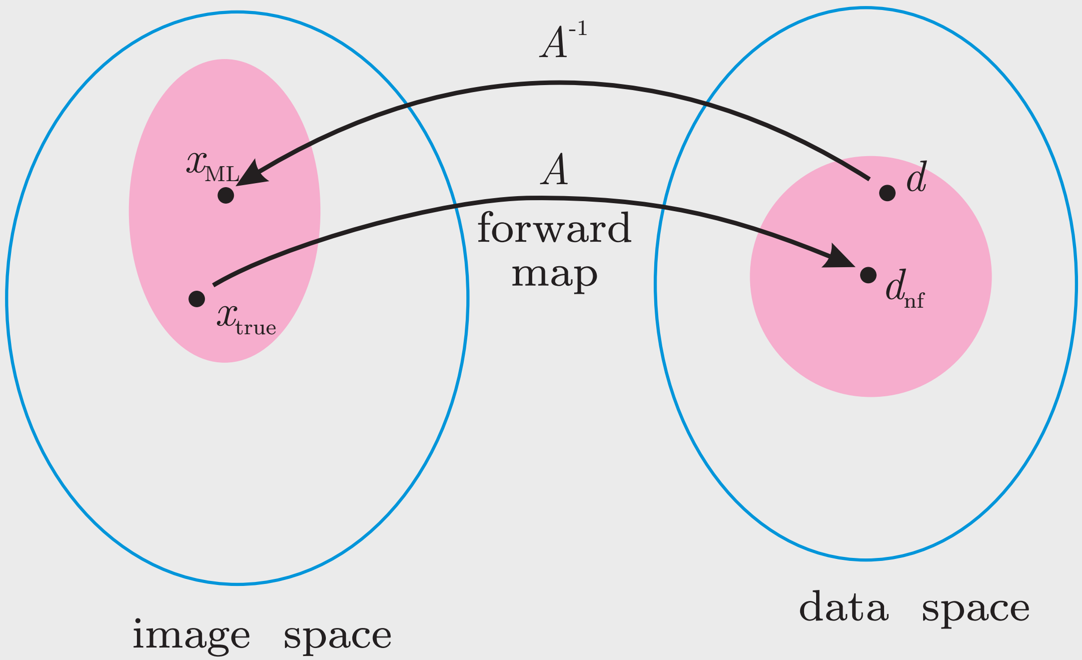

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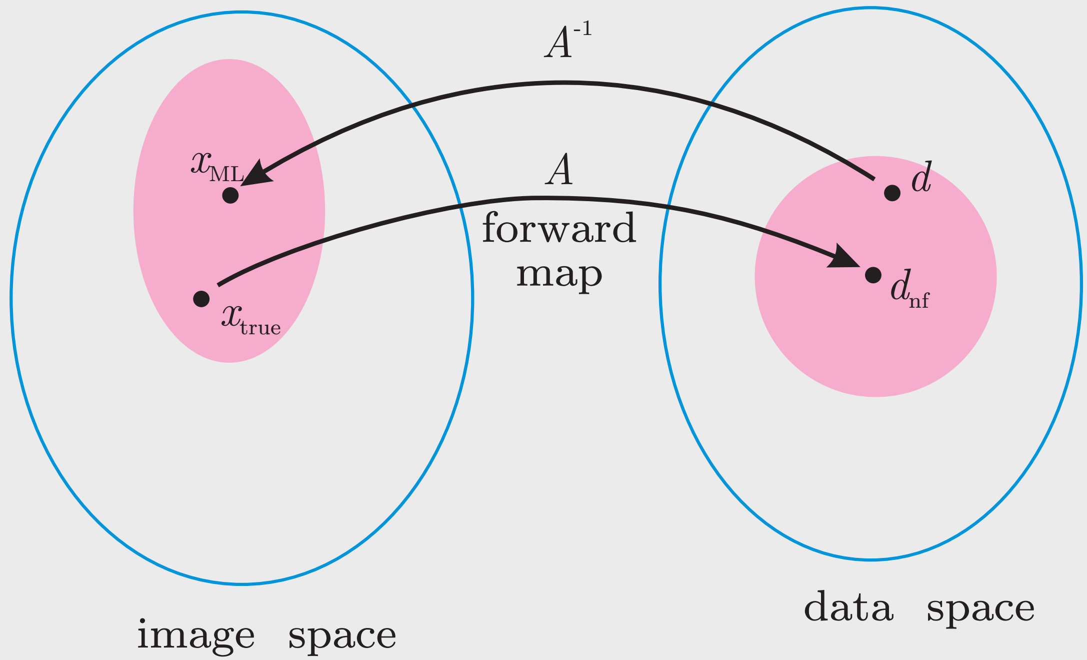

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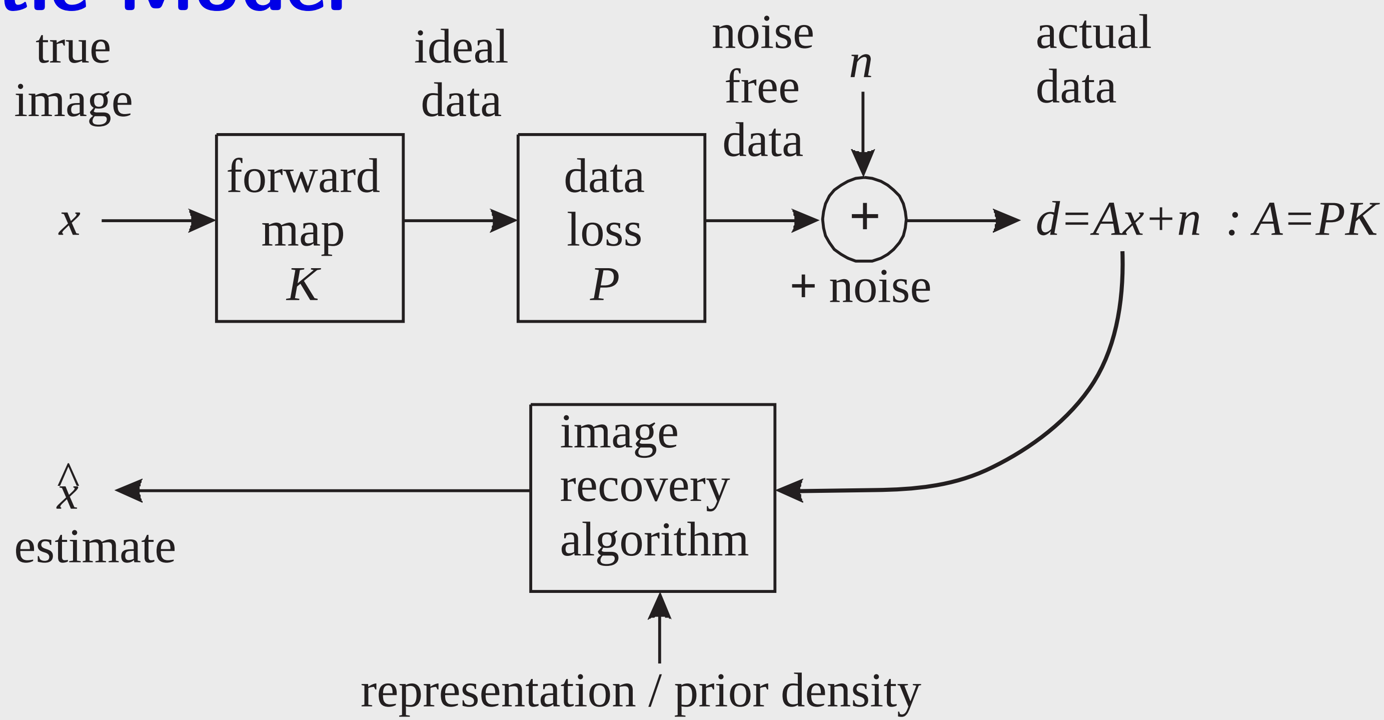
Inference based on posterior distribution conditioned on data (computational statistics)

Stochastic Model



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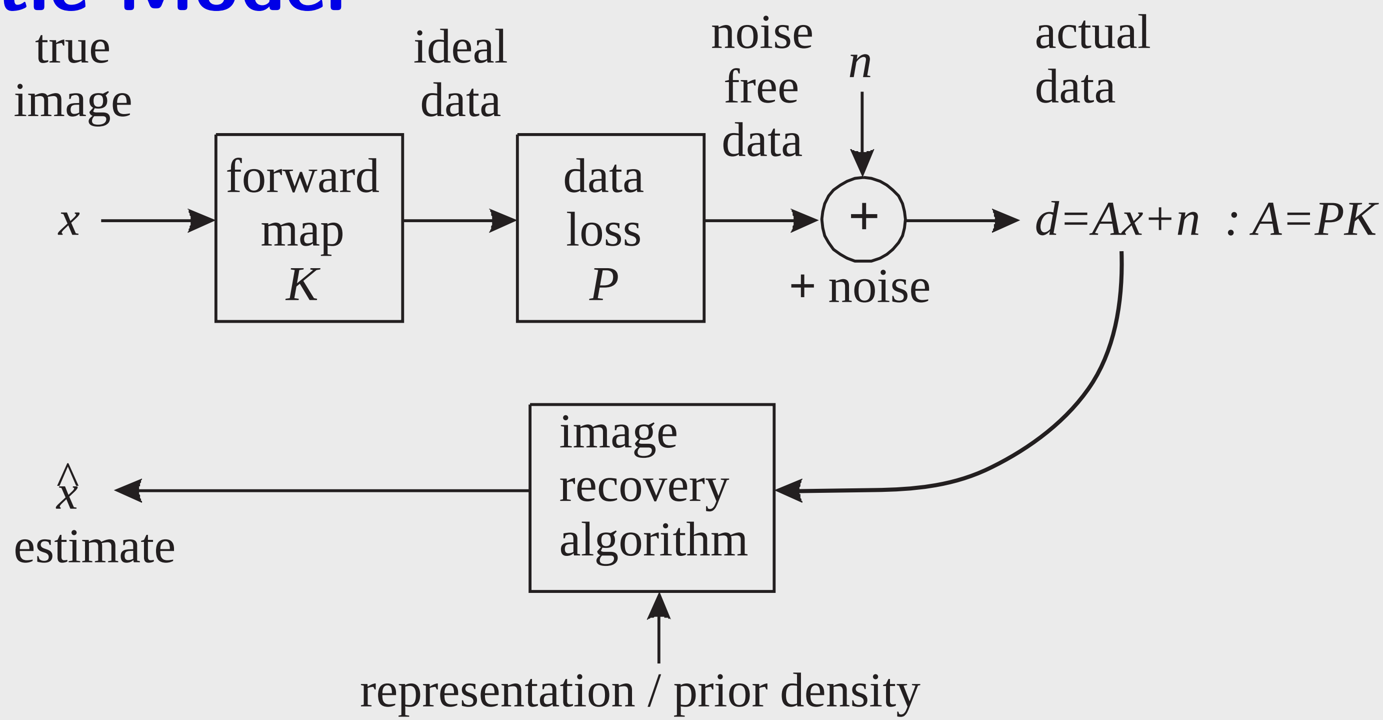

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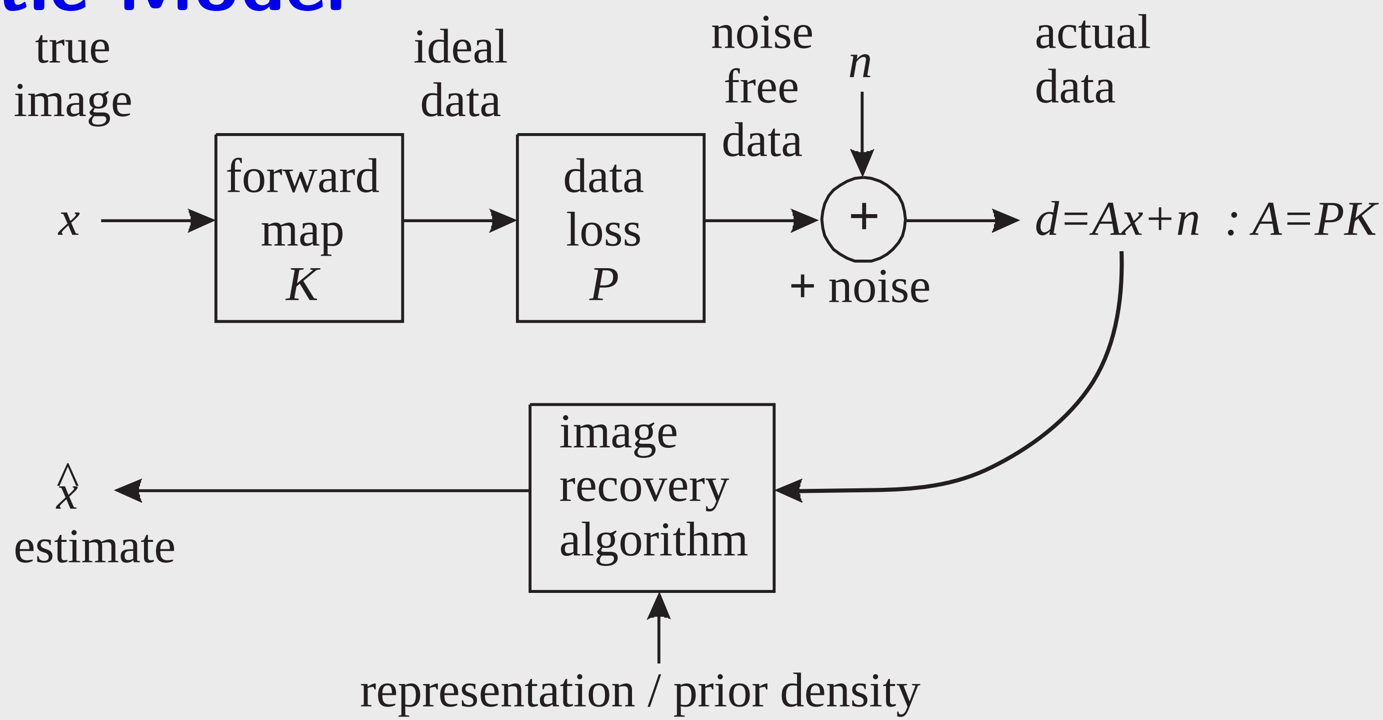

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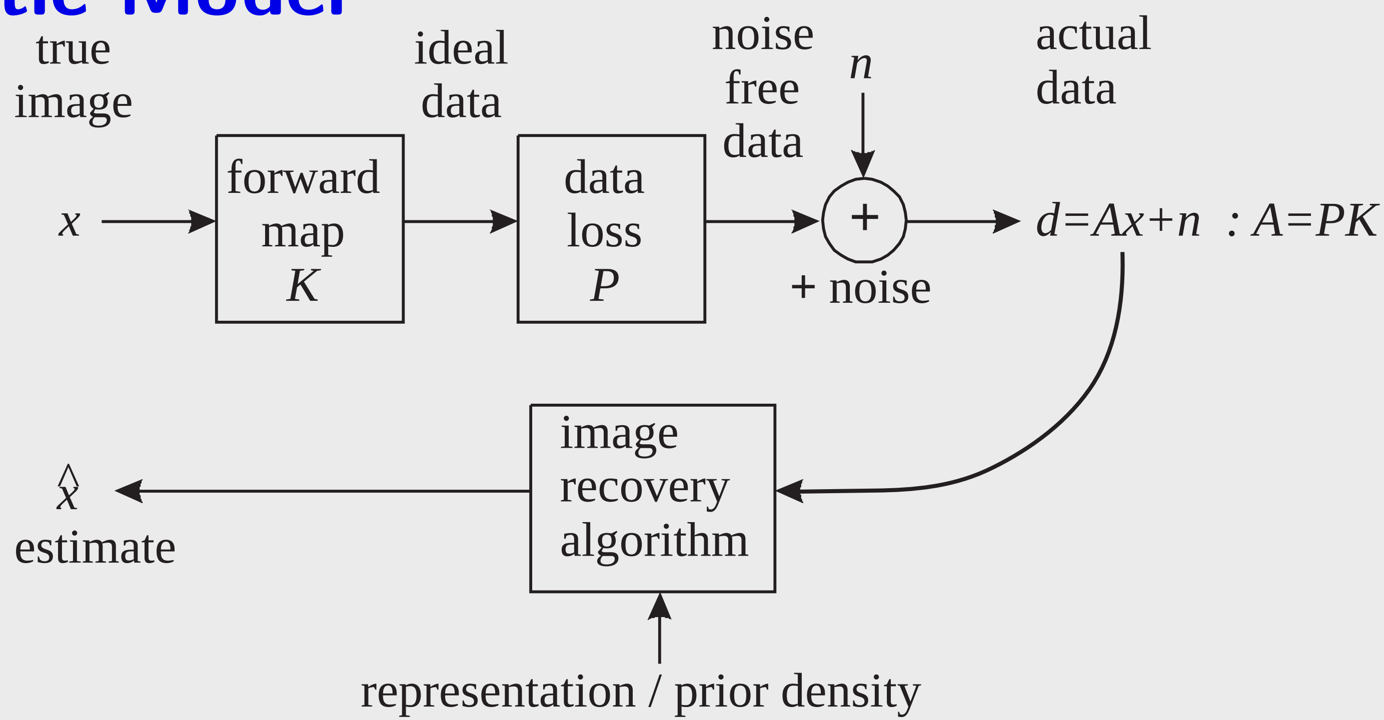

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Focus of inference is posterior distribution for x given d

$$\pi\left(x|d\right) \propto \Pr\left(d|x\right) \pi_{\text{pr}}\left(x\right)$$

Solutions to Inverse Problem = Summary Statistics

Posterior distribution $\pi(x|d)$ encapsulates all information about x

Regularized Inversion - Modes

$$\hat{x}_{\mathsf{MLE}} = \arg\max \Pr(d|x) \qquad \hat{x}_{\mathsf{MAP}} = \arg\max \pi(x|d)$$

(least-squares, Moore-Penrose inverse, Tikhonov regularization, Kalman filtering, Backus-Gilbert, Prussian-hat cleaning)

Inferential Solutions

"Answers" are expectations over the posterior $\pi(x|d)$

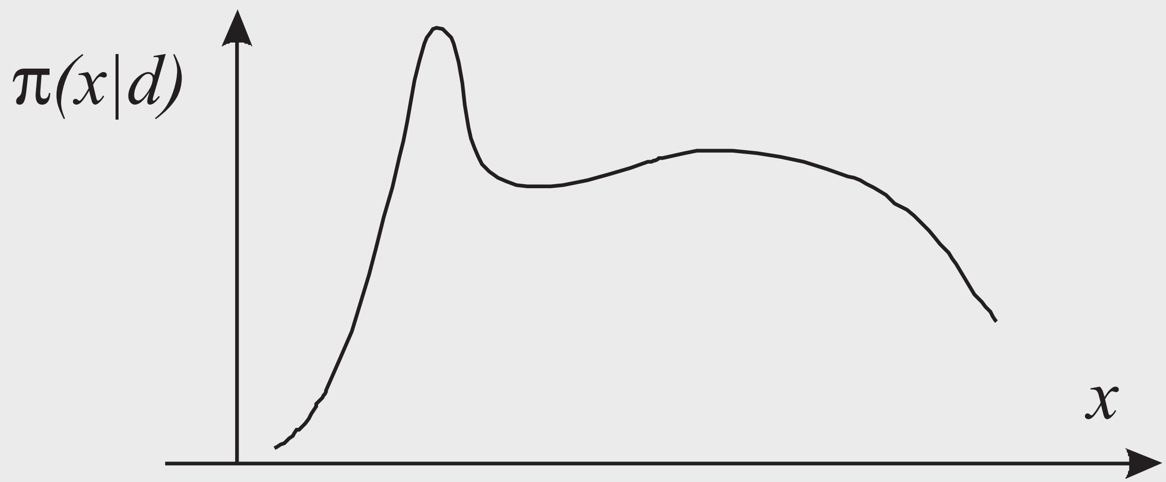
$$\mathsf{E}_\pi[f(x)] = \int_X f(x)\,\pi(x|d)\,dx$$

If

$$f(x) = \text{indicator function that image shows cancer}$$

$\mathsf{E}[f(x)]$ is posterior probability (based on measurements, prior) that patient has cancer.

Two modes over 100×100 pixel image



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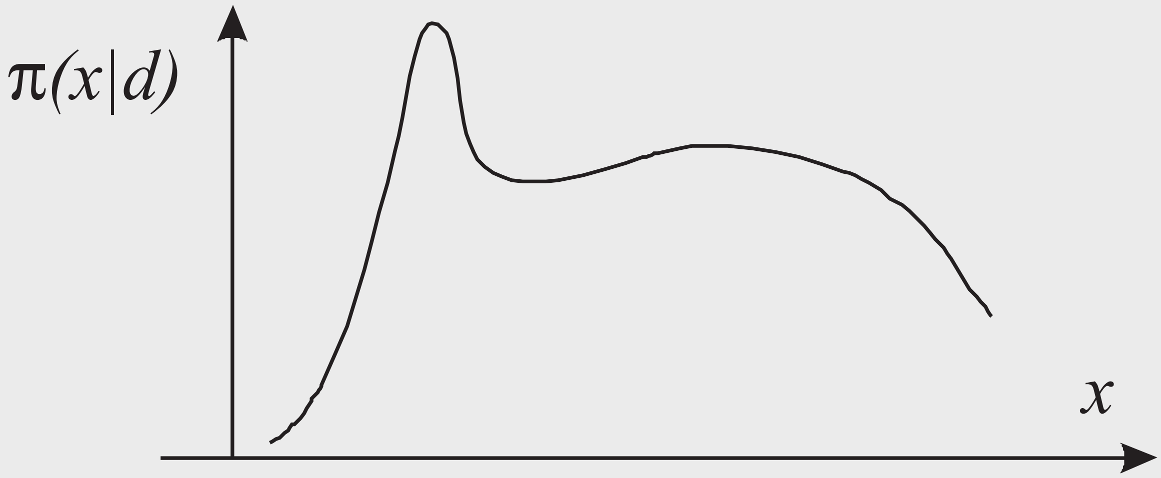

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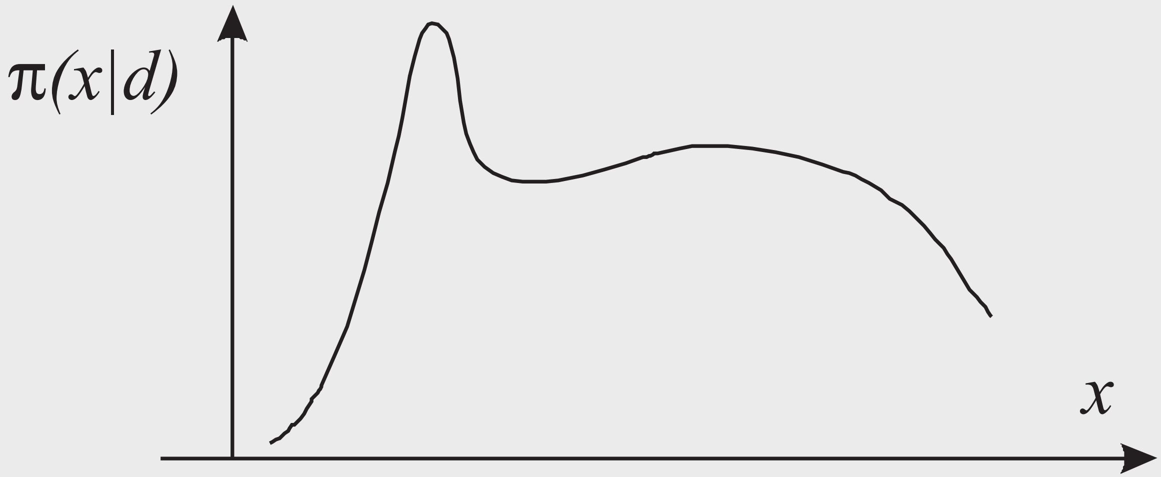

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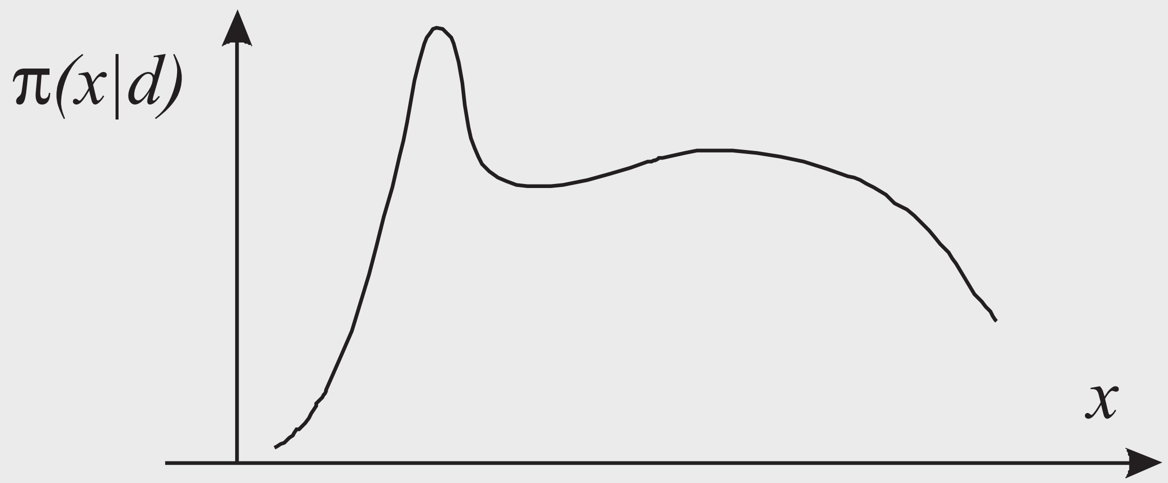

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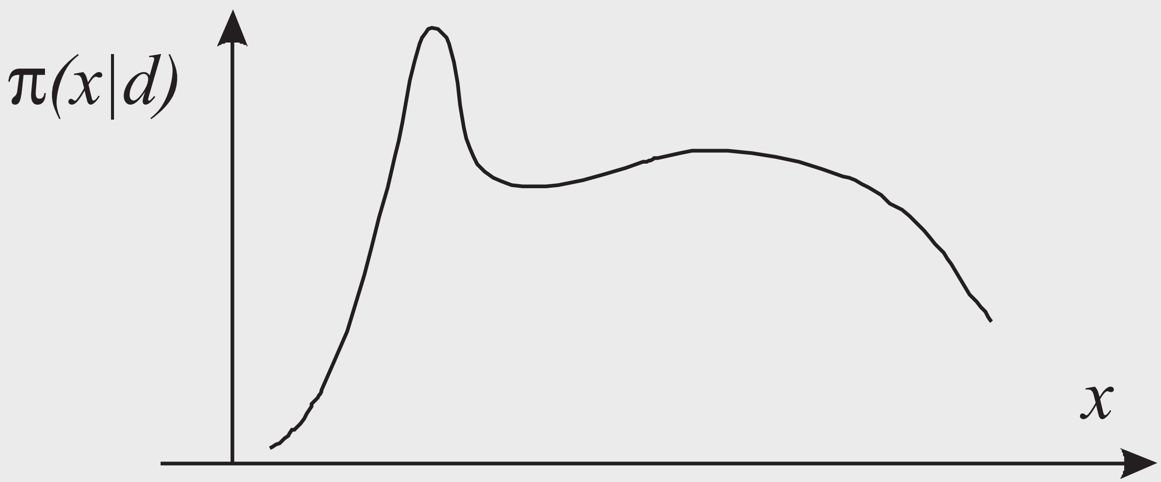

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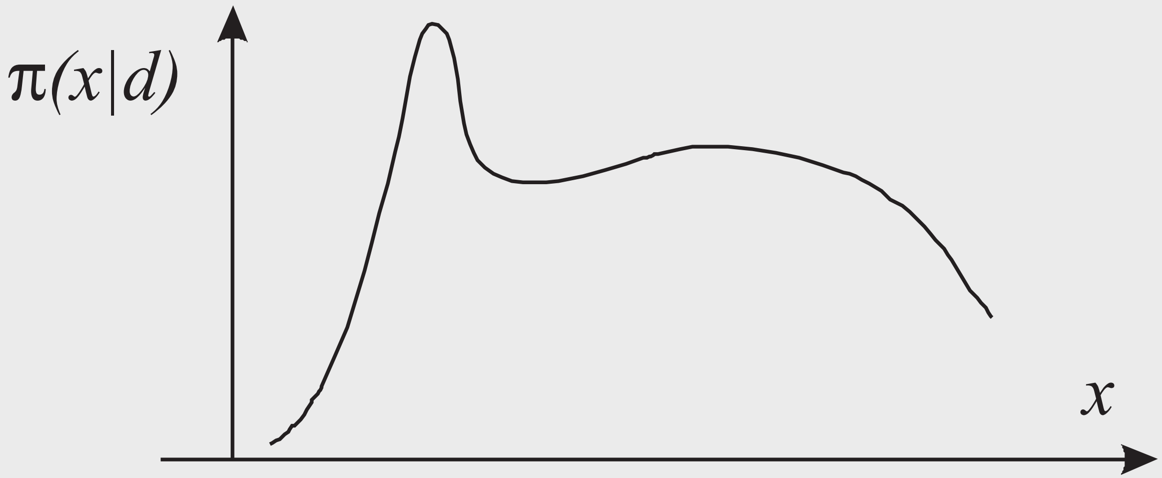

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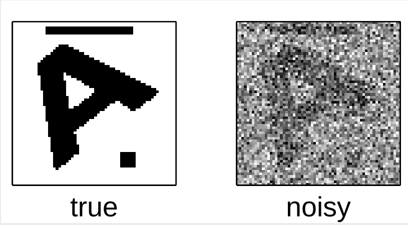
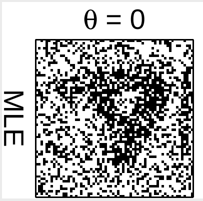
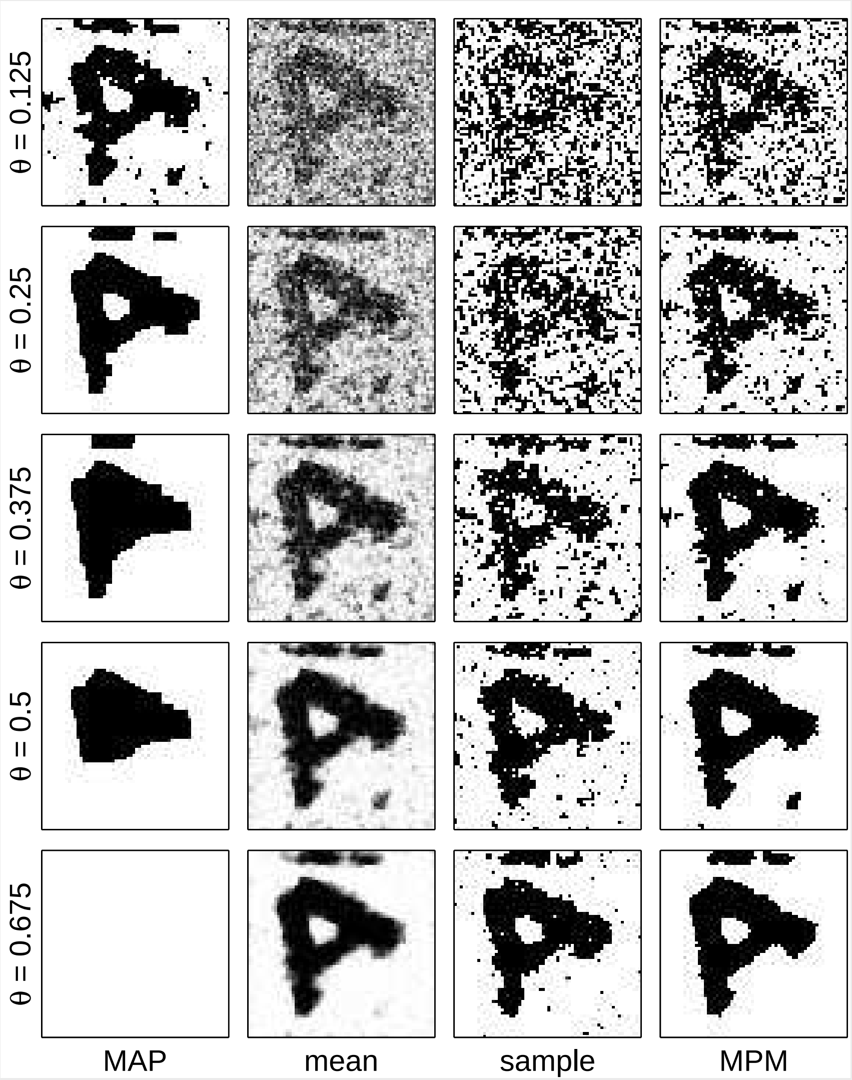
$$\int_X \pi\left(\mathbf{x}|d\right)\, d\mathbf{x} = \int_X \pi\left(\mathbf{x}|d\right)\, dx_1\, dx_2 \cdots dx_{10000}$$

Mode vs Mean







Pixel-wise noise on binary image, Ising prior with "lumping" constant θ

F and Nicholls "Exact MAP states and expectations from perfect sampling: Greig, Porteous and Seheult revisited" 2001

Monte Carlo integration + importance sampling

If $x^{(1)}, \ldots, x^{(n)} \sim \pi\left(\cdot|d\right)$

$$\mathsf{E}_{\pi}\left[f\left(x\right)\right] \approx \frac{1}{n}\sum_{i=1}^{n} f\left(x^{(i)}\right)$$

Construct $x^{(1)}, \ldots, x^{(n)}$ as iterates of an ergodic map

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Deterministic iteration: $x^{(n+1)} = M\left(x^{(n)}\right)$

$$\pi(x) = \sum_{M(y)=x} \frac{\pi(y)}{|M'(y)|} \qquad \text{(Frobenius-Perron)}$$

Stochastic Iteration: Markov chain with transition kernel $p\left(x, y\right)$

$$\int_X \pi\left(x\right) p\left(x, y\right)\, dx = \int_X \pi\left(y\right) p\left(y, x\right)\, dx \qquad \text{(global balance)}$$

$$\pi\left(x\right) p\left(x, y\right) = \pi\left(y\right) p\left(y, x\right) \qquad \text{(detailed balance)}$$

Sampling Algorithms in Physics

Hamiltonian Dynamics

Equate unknowns x to ‘position’ variables q with potential energy

$$E(q) = -T\log\left(\pi(x)\right) - T\log\left(Z\right)$$

Auxiliary 'momentum' variables p with kinetic energy $K(p) = \frac{1}{2}\|p\|^2$.

Hamiltonian $H(q,p) = E(q) + K(p)$ has canonical distribution

$$P(q,p) = \frac{1}{Z_P}\exp\left(-E(q)\right)\frac{1}{Z_K}\exp\left(-K(p)\right)$$

Hamiltonian dynamics leave $P(q,p)$ invariant $+$ stochastic transitions for ergodicity

Langevin diffusion

$$dx = s\,dB + \frac{s^2}{2}\nabla\log\left(\pi(x)\right)\,dt$$

Metropolis-Hastings algorithm

1. given state x_t at time t generate candidate state x' from a proposal distribution $q\left(.|x_t\right)$
2. With probability $\alpha\left(x_t \to x'\right) = \min\left(1, \frac{\pi(x')q\left(x_t|x'\right)}{\pi(x_t)q\left(x'|x_t\right)}\right)$ set $X_{t+1} = x'$
   otherwise $X_{t+1} = x_t$
3. Repeat

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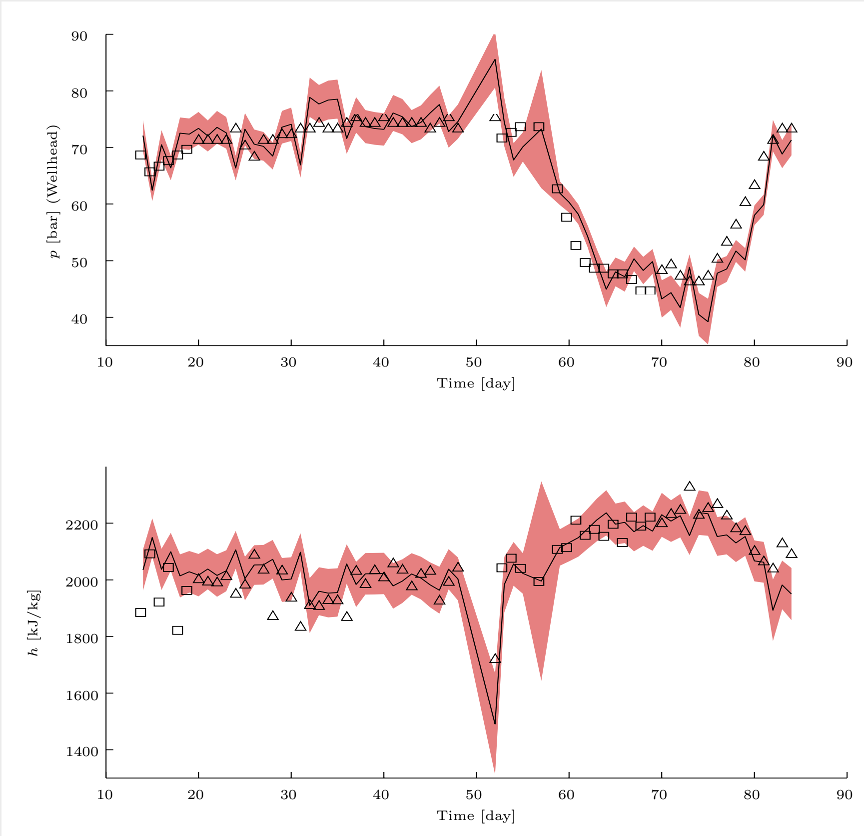
Pros

- Provably convergent under mild requirements
- State space can be continuous, discrete, stochastic, or variable dimension

Cons

- Can be (very) slow

Results for geothermal field

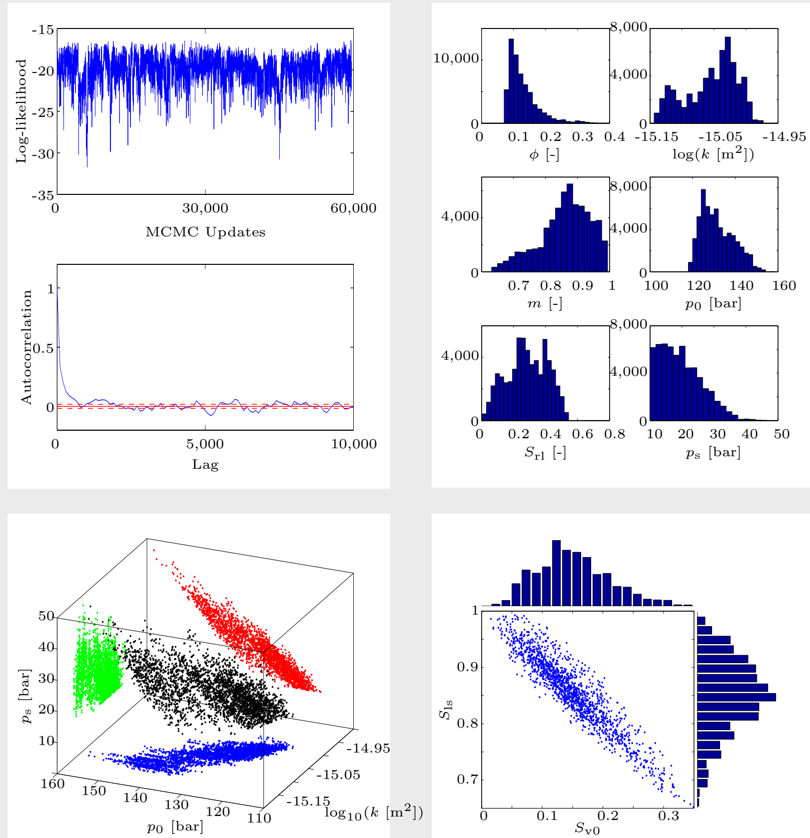


Wellhead pressure (top) and flowing enthalpy (bottom).

Black line is estimated result, triangles and squares are observed data.

Tiangang Cui, *Bayesian Inference for Geothermal Model Calibration* MEng Auckland, 2005

Output analysis for geothermal field



Autocorrelation and MCMC output trace. Histogram for the marginal distribution of parameters. Scatter plot of the joint marginal distribution for $\log(k)$, p_0 and p_s. Histogram for the marginal distribution of S_{v0} and S_{ls} and scatter plot of their joint marginal distribution.

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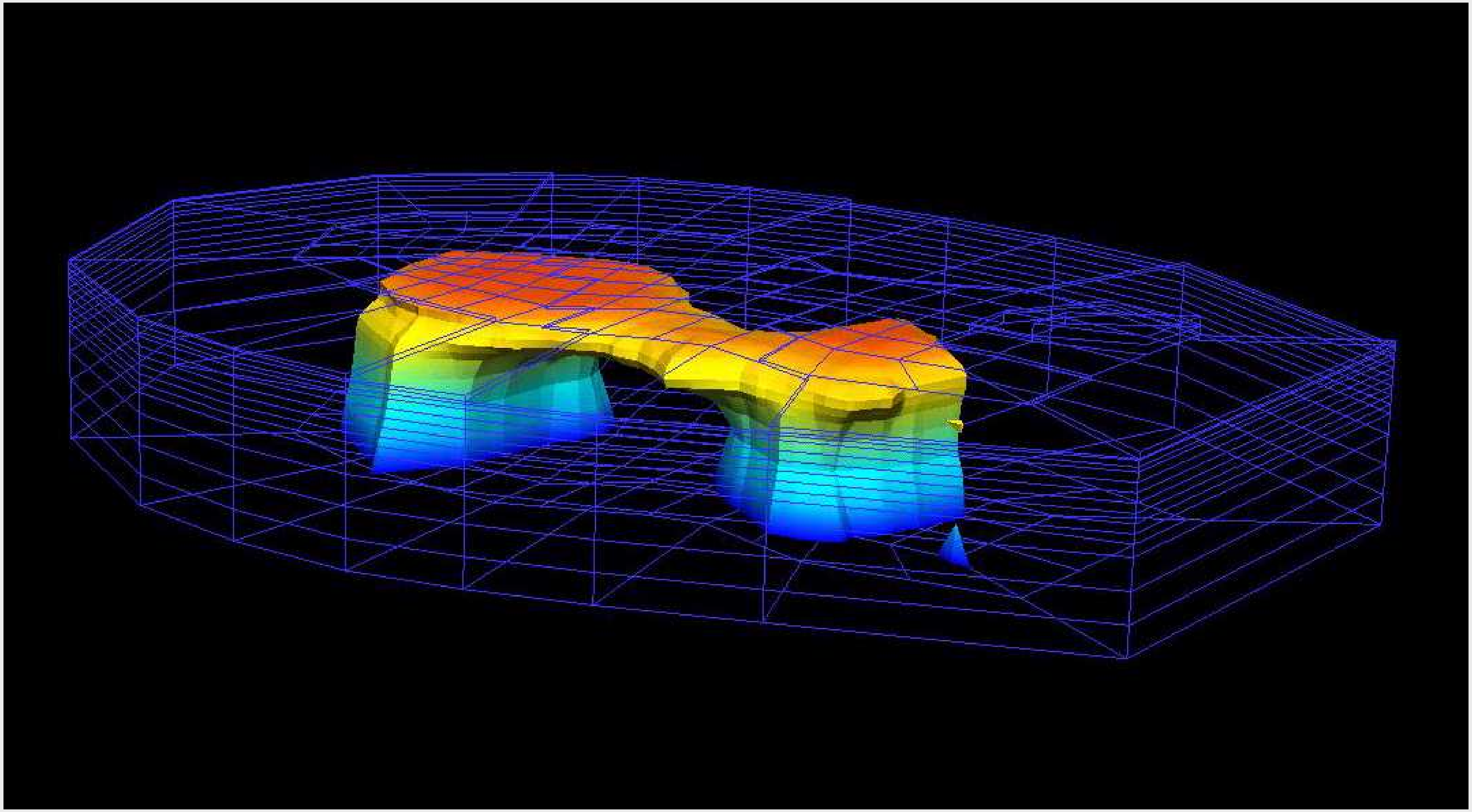
Inferred iso-temperature surface



Conclusions

1. Bayesian methods can solve substantial real-world inverse problems
2. Time to convergence depends on efficient simulation of the forward map, fast MCMC algorithms, good proposal distributions
3. Computation required is feasible