Facing the Curse of Dimensionality

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Ideal Sampling Solutions to the Non-linear Probabilistic Inverse Problem

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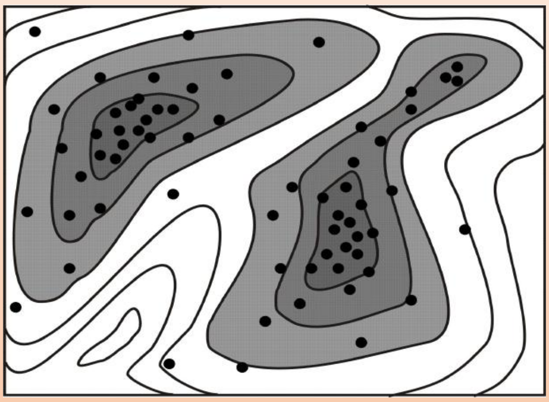
Solution: Sampling the Posterior PDF



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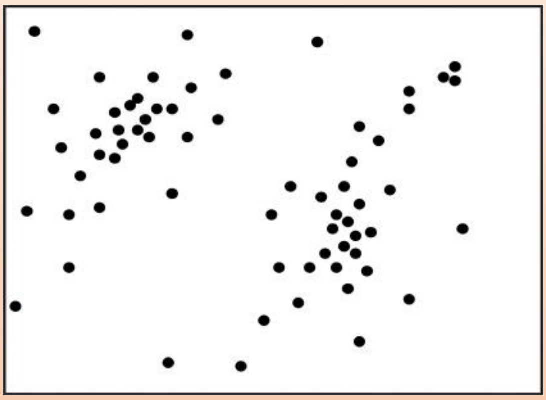

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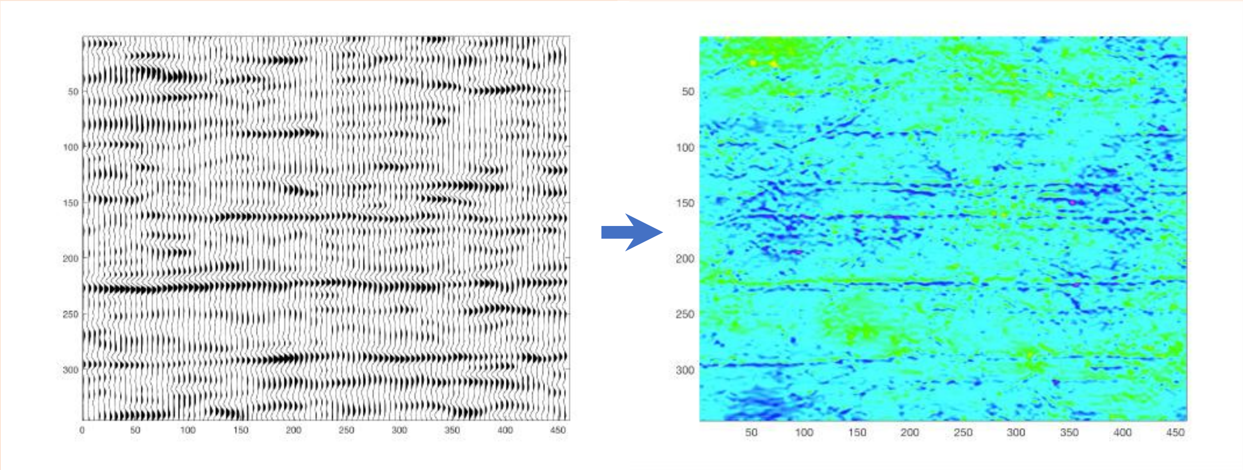
Solution: Sampling the Posterior PDF



(Fernandes and Mosegaard, Geophysical Prospecting 2022)

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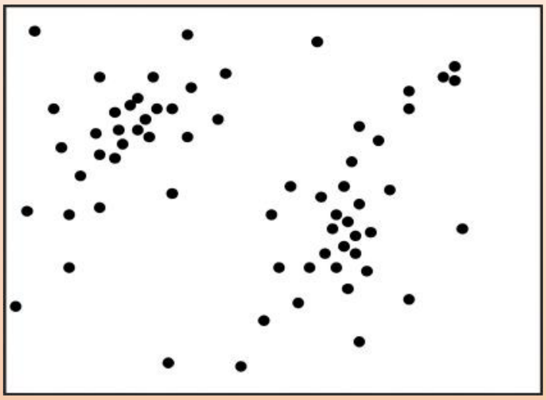
Solution: Sampling the Posterior PDF



...but how difficult is it to obtain such a sample?

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Monte Carlo Algorithms in Spaces of High Dimension

Why pre-knowledge about the distribution is decisive!

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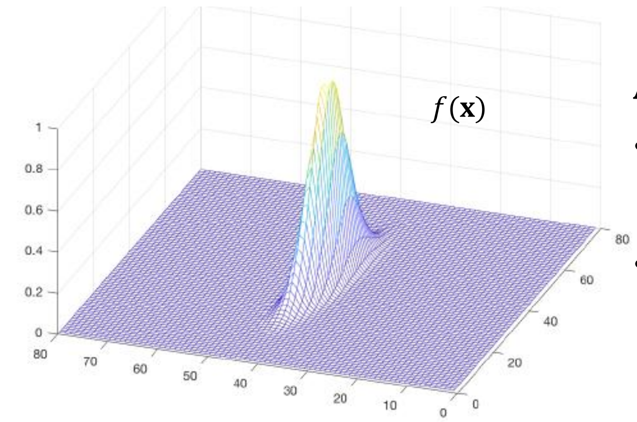
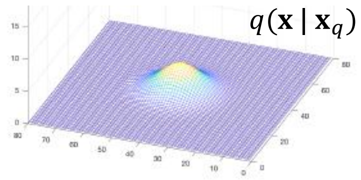
Blind MCMC Sampling of a Gaussian: A Hard Problem!





Assumptions:

- $\mathbf{x}$ is Gaussian:

$$f(\mathbf{x}) = \mathcal{N}_{\mathbf{x}}\,(\mathbf{x}_0, \mathbf{C}).$$

- Proposal distribution is isotropic Gaussian:

$$q(\mathbf{x} \mid \mathbf{x}_q) \;= \mathcal{N}_{\mathbf{x}}\,(\mathbf{x}_q, \mathbf{C}_q).$$

- Start sampling at f's maximum point $\mathbf{x}_0$.

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Sampling a Gaussian **without knowing it is a Gaussian**

Examples: Let us consider the case where $\sigma_q^2 = 1$, and $\sigma_n^2 = \frac{1}{n}$:

1. $N = 2$:
   Expected acceptance probability: 0.4082
   Mean waiting time between accepted moves: $0.4082^{-1} \approx$ 2.5 iterations

2. $N = 10$:
   Expected acceptance probability: $1.5828 \cdot 10^{-4}$
   Mean waiting time between accepted moves: $\approx$ 6318 iterations.

3. $N = 100$:
   Expected acceptance probability: $1.03 \cdot 10^{-80}$
   Mean waiting time between accepted moves: $\approx 10^{80}$ iterations.

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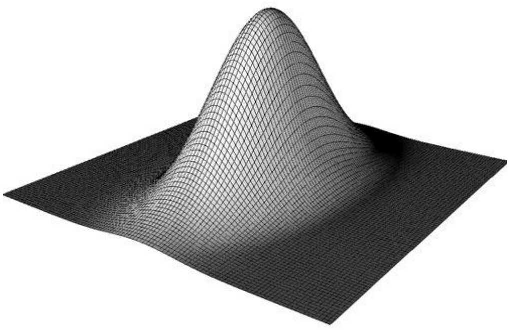
Sampling a Gaussian, **knowing that it is Gaussian**: Easy!



Characterized by:

- N components of its mean vector
- $N\,(N+1)/2$ components of its covariance matrix.

The family of Gaussians over an N-dimensional space is a manifold of dimension

$$N + N\,(N+1)/2$$

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- At least $N + N(N+1)/2$ function evaluations are required to characterize ("reconstruct") an N-dimensional Gaussian.
- Consequently, the best conceivable algorithm needs $\sim N + N(N+1)/2$ function evaluations to produce one exact sample of an N-dimensional Gaussian!

Sampling a Gaussian is **not** a hard problem, if you know it is Gaussian

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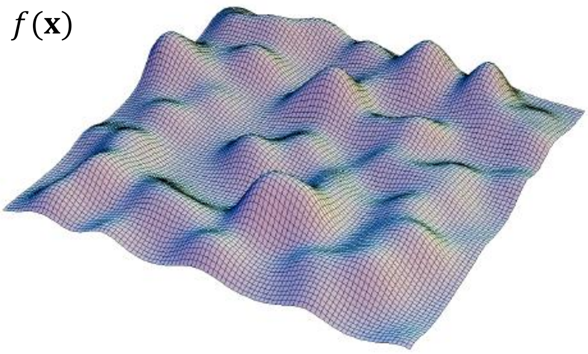
Blind Sampling of a Complex Distribution (Hard)



Assume:

- f can be expanded in terms of basis functions:

$$f(\mathbf{x}) = \sum_{j=1}^{J} u_j \varphi_j(\mathbf{x})$$

- We have K samples $\mathbf{x}_1, \cdots, \mathbf{x}_K$ and sample values:

$$s_k = f(\mathbf{x}_k) = \sum_{j=1}^{J} u_j \varphi_j(\mathbf{x}_k)$$

Hence, $\mathbf{s} = \mathbf{Fu}$ where $\mathbf{s} = (s_1, \cdots, s_K)$, $\mathbf{u} = (u_1, \cdots, u_J)$, and $F_{kj} = \varphi_j(\mathbf{x}_k)$.

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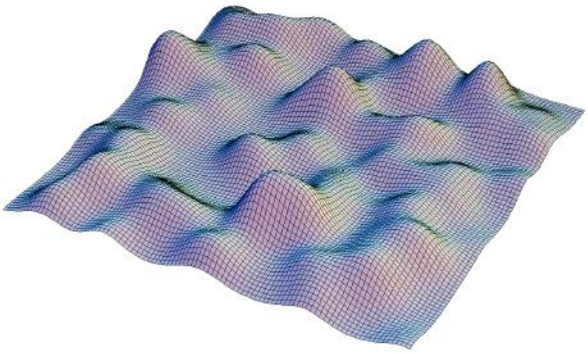
Blind Sampling of a Complex Distribution (Hard)



- We have K samples $\mathbf{x}_1, \cdots, \mathbf{x}_K$ and sample values:

$$s_k = f(\mathbf{x}_k) = \sum_{j=1}^{J} u_j \varphi_j(\mathbf{x}_k)$$

- $\mathbf{s} = \mathbf{F}\mathbf{u}$

$\mathbf{F}^T\mathbf{F}$ singular (e.g., # samples $< J$) $\Longrightarrow$ Incomplete knowledge/sampling
$\Longrightarrow$ Potentially missing "peaks"

If # required base functions grows exponentially with dimension, the problem is **Hard!**

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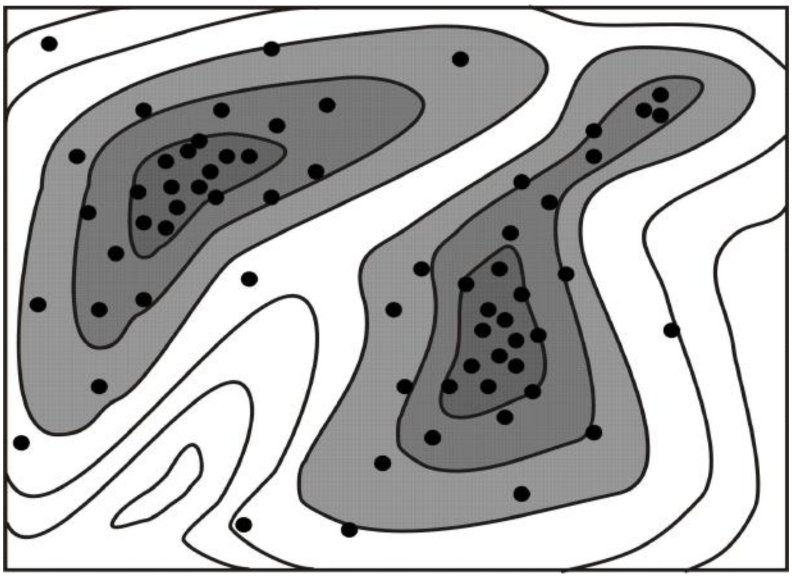
Blind Sampling a Complex Distribution (Hard)



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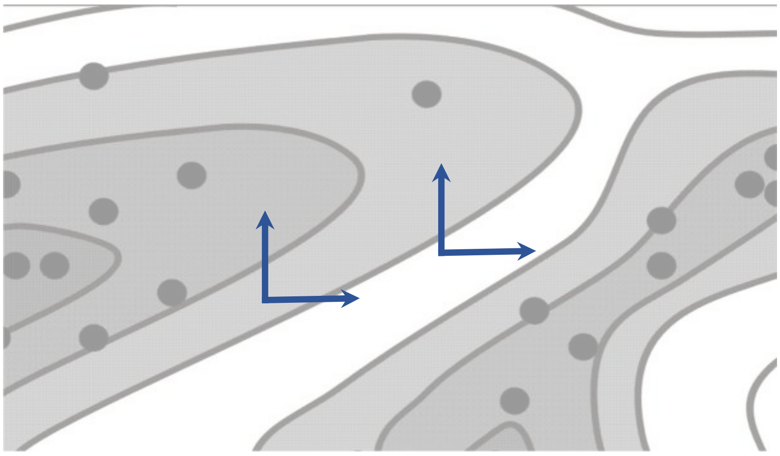
Blind Sampling of a Complex Distribution (Hard)



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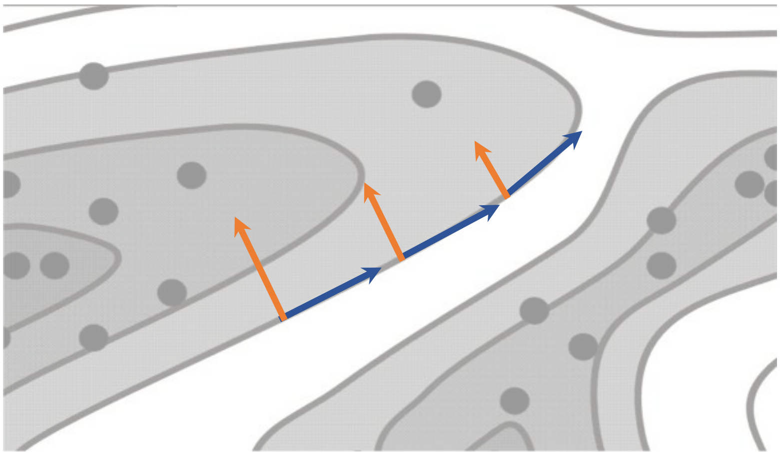
Sampling of a Complex Distribution, **having gradients** (Easier)



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When Solutions are Essentially Located in a Lower-Dimensional Subspace

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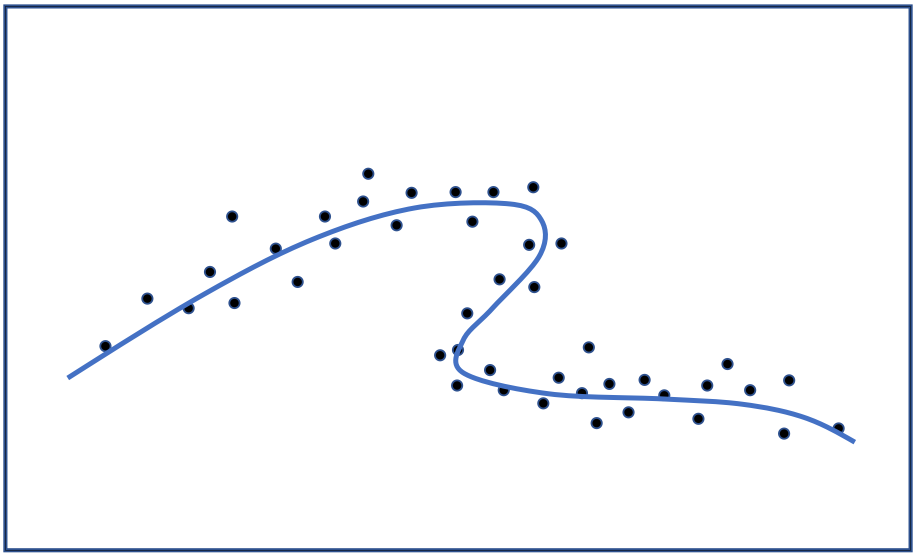
Sometimes solutions are essentially located in a lower-dimensional manifold..



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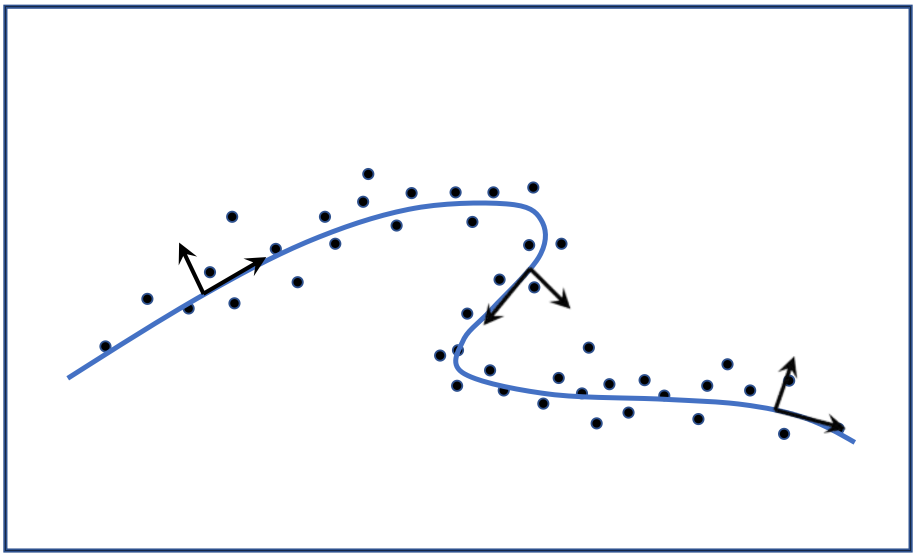

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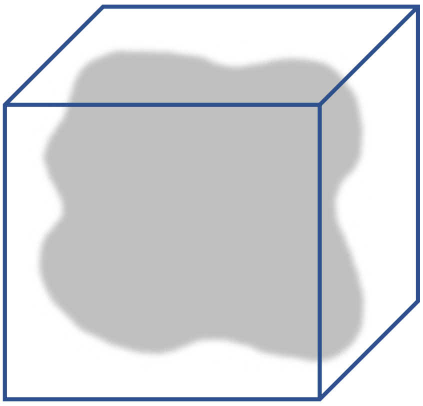
Highly Nonlinear Inverse Problems: Dimensionality and Degrees of Freedom

Easy to find acceptable models, but hard to sample due to the high dimension

- Space-filling Distribution
- N degrees of freedom
- Embedded in ND



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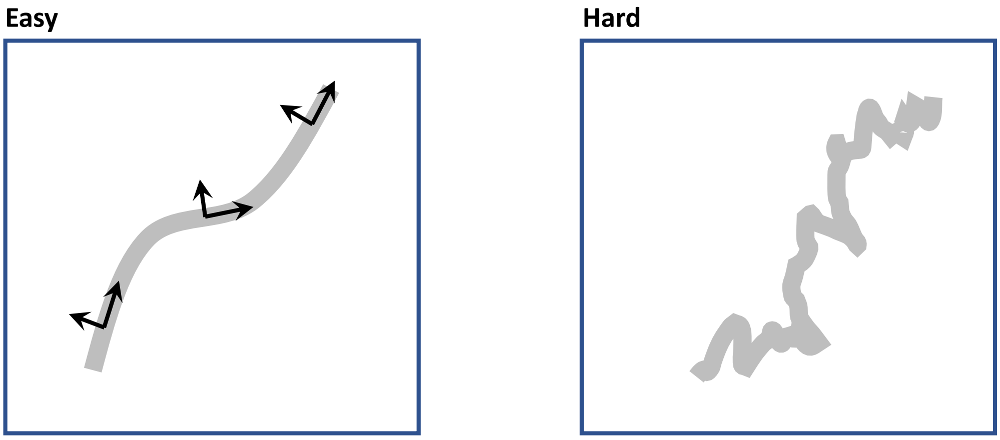
Highly Nonlinear Inverse Problems: Dimensionality and Degrees of Freedom



- Parametric distribution
- 1 degree of freedom
- Embedded in 2D

- Non-parametric distribution
- 1 degree of freedom
- Embedded in 2D

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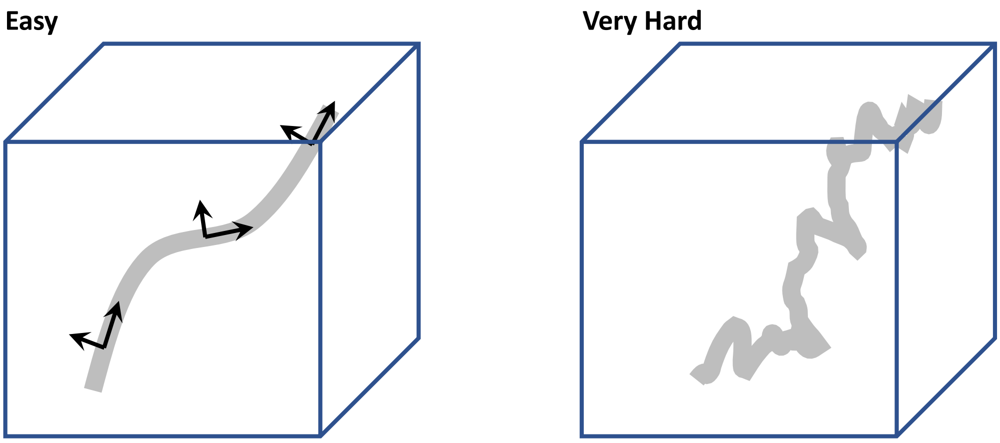
Highly Nonlinear Inverse Problems: Dimensionality and Degrees of Freedom



- Parametric distribution
- 1 degree of freedom
- Embedded in ND

- Non-parametric distribution
- 1 degree of freedom
- Embedded in ND

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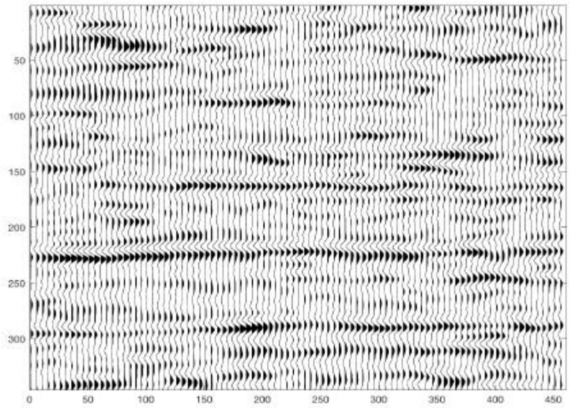
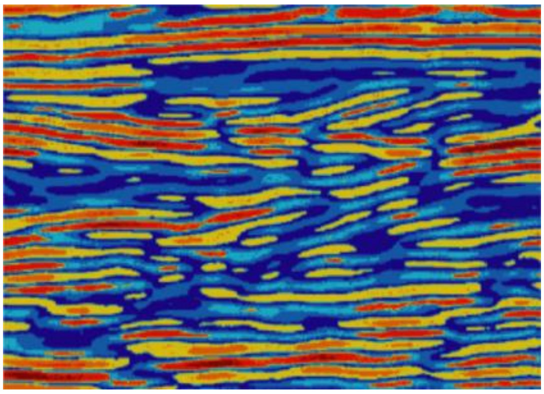
A Non-Parametric Posterior from Inversion of Seismic Data with a Multiple-Point Geostatistical Prior

Seismic Data



Model realization from a Multiple-Point Geostatistical Prior



GAIA LAB: https://wp.unil.ch/gaia/mps/ds/

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Preliminary Conclusion

- A Posterior that is only nonzero close to a **subspace described by (few) local coordinates** is **easy** to sample.
- A Posterior that is only nonzero close to a **subspace without local coordinates** is **difficult** to sample.
- The latter case gets worse when the dimension of the embedding space grows!

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MCMC Algorithms with Informed Proposals

Strategies guided by

the physics of the problem

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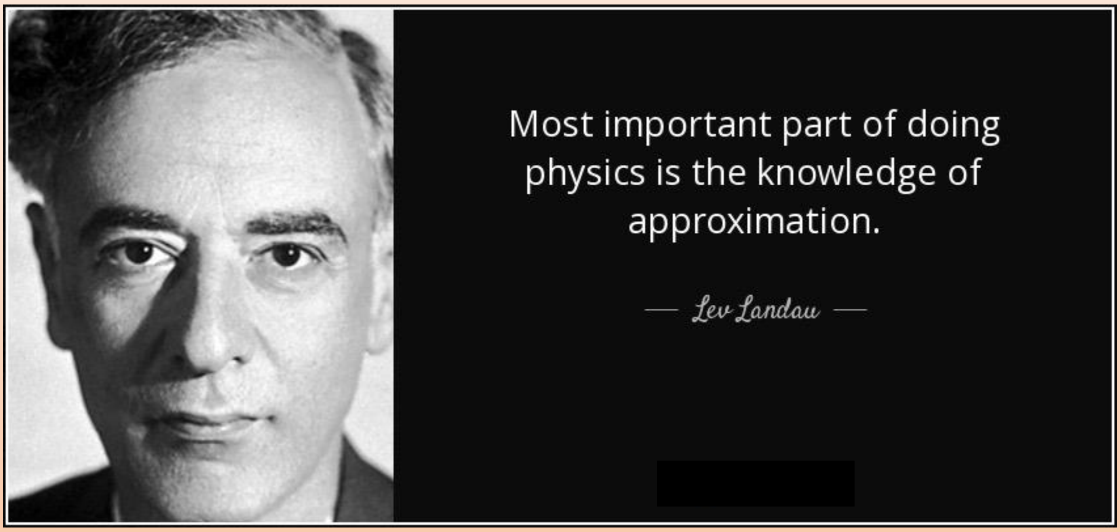

Lev Landau (1908-1968)

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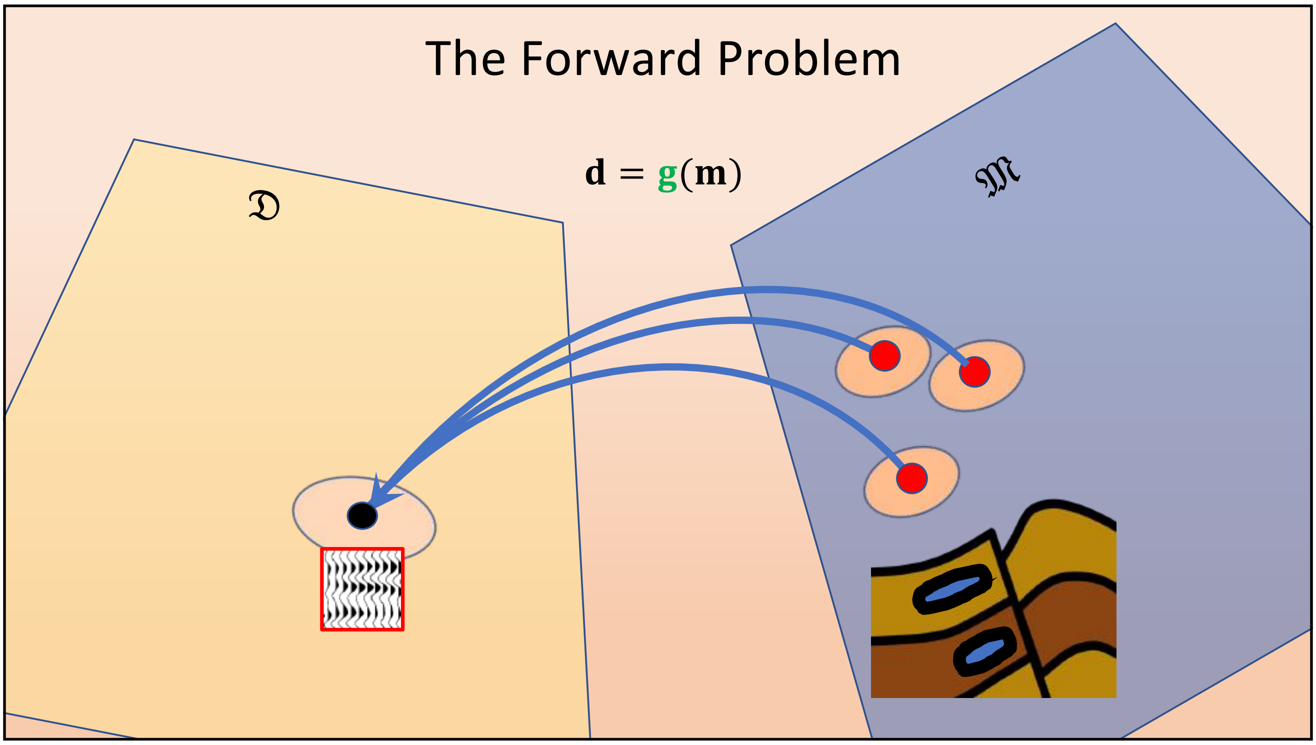

The Forward Problem
$\mathbf{d} = \mathbf{g}(\mathbf{m})$
𝔇
𝔐

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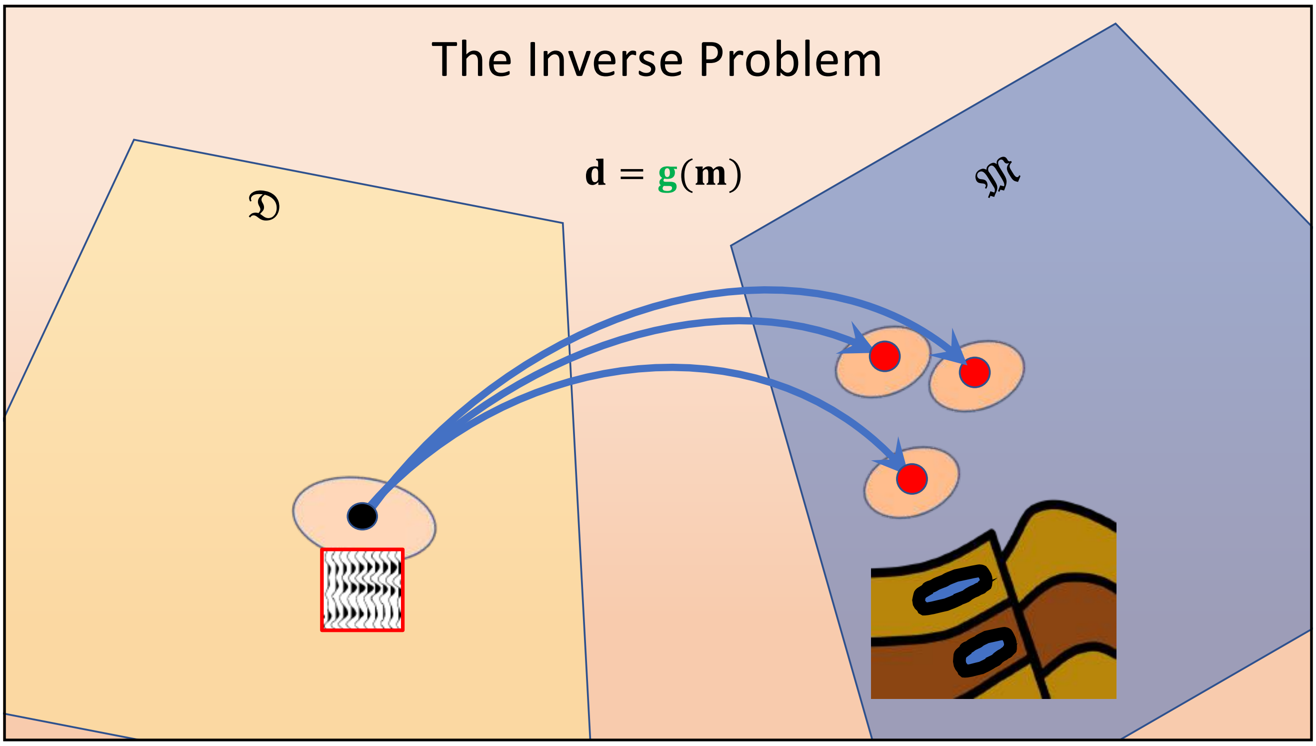

The Inverse Problem
$\mathbf{d} = \mathbf{g}(\mathbf{m})$
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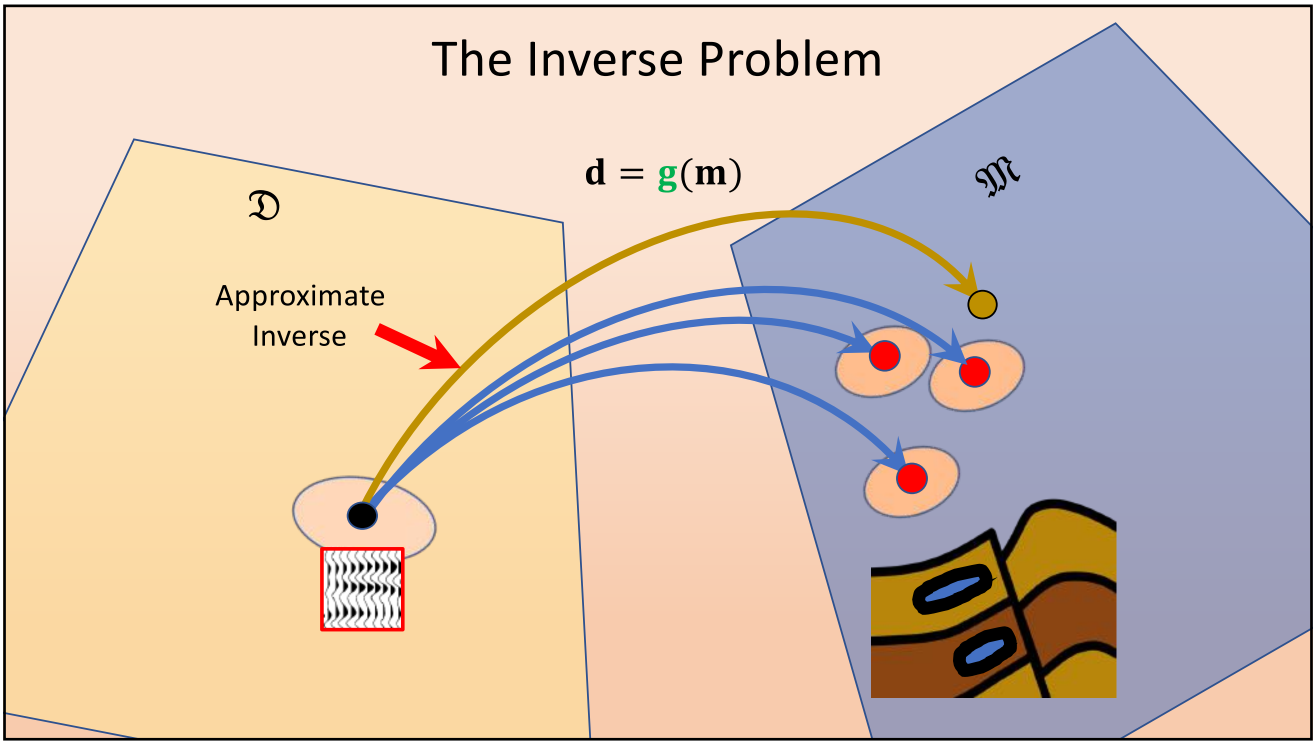
The Inverse Problem
$\mathbf{d} = \mathbf{g}(\mathbf{m})$
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Approximate
Inverse

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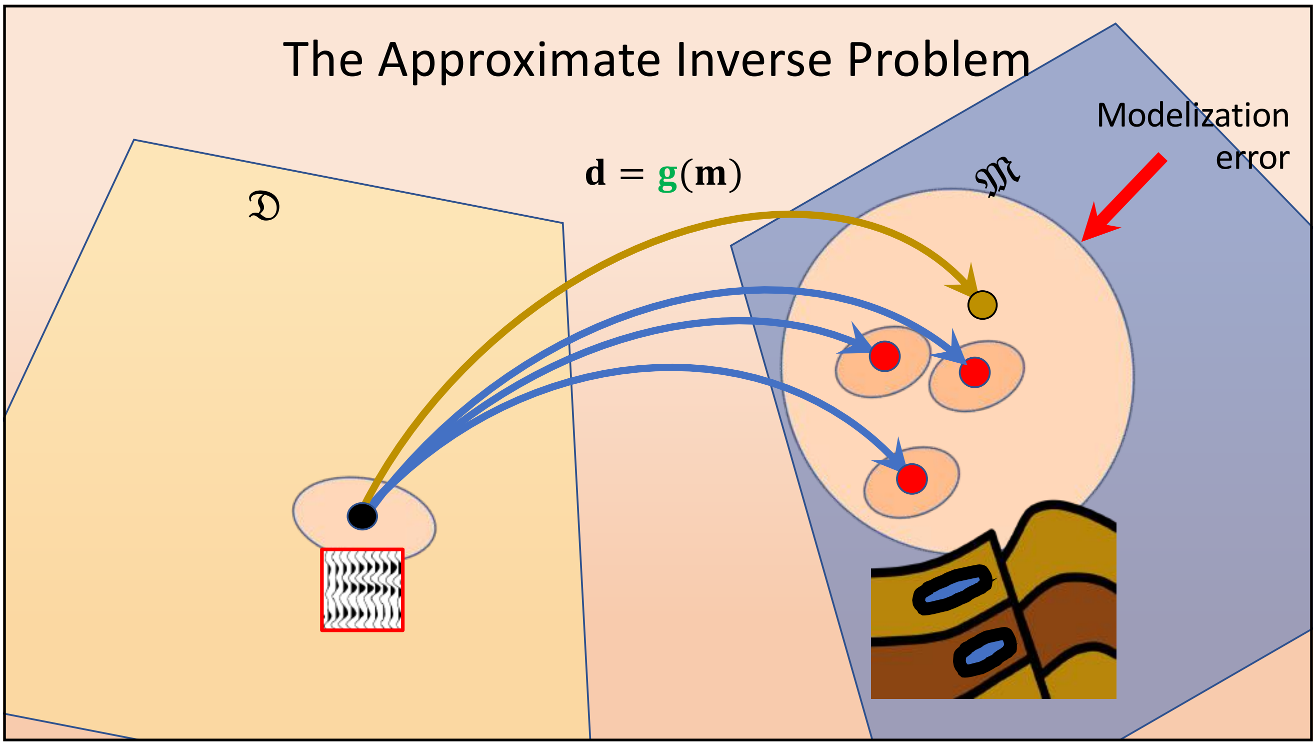
The Approximate Inverse Problem
$\mathbf{d} = \mathbf{g}(\mathbf{m})$
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Modelization
error

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Building Approximate Physics into MCMC Without an (Asympthotic) Bias

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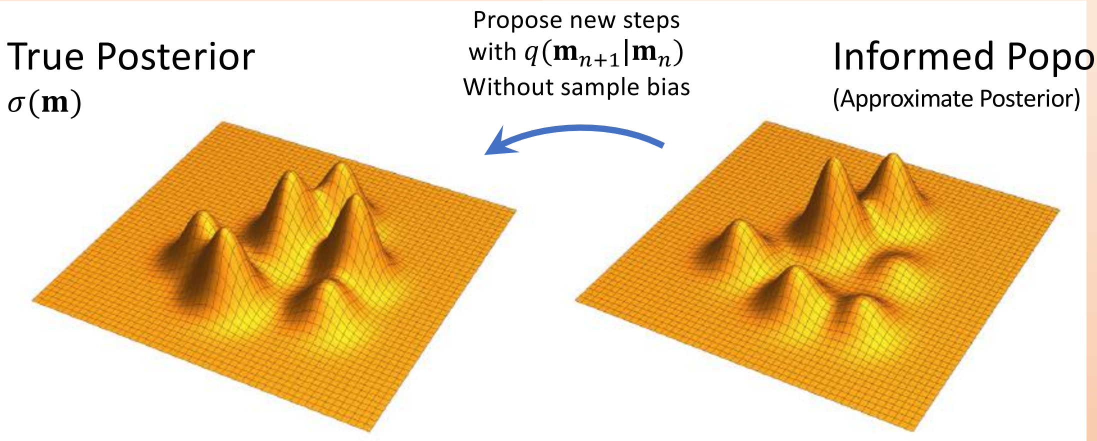
MCMC with Informed Proposals: The Idea



Propose with $q(\mathbf{m}_{n+1}|\mathbf{m}_n)$ Accept with probability:

$$P_{acc} = \frac{\sigma(\mathbf{m}_{n+1})}{\sigma(\mathbf{m}_n)} \frac{q(\mathbf{m}_n|\mathbf{m}_{n+1})}{q(\mathbf{m}_{n+1}|\mathbf{m}_n)}$$

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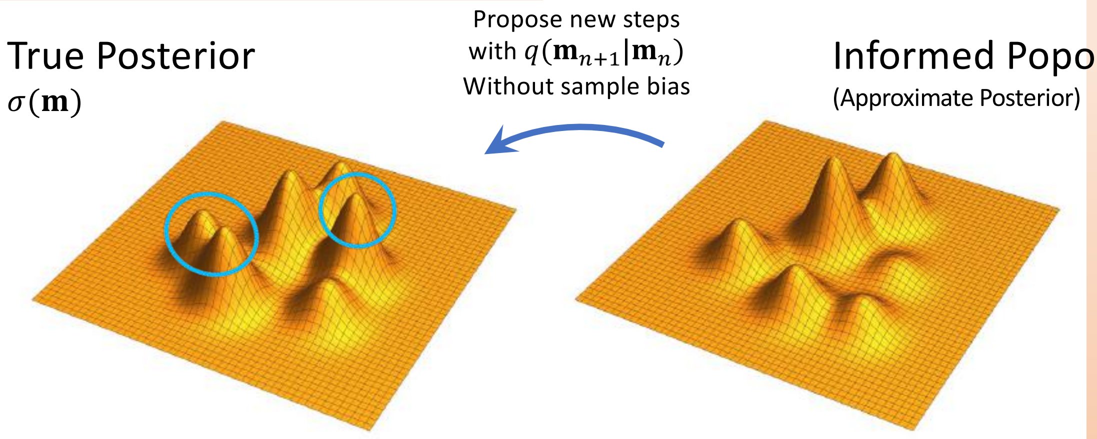
MCMC with Informed Proposals: The Idea



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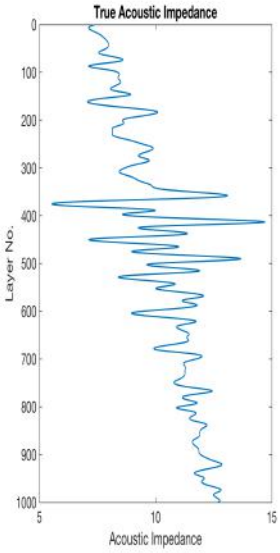
A 1-D Inverse Scattering Problem with 1000-parameters



Khoshkholgh, Zunino and Mosegaard, 2021: Informed Proposal Monte Carlo. Geophys. Journ. Int.

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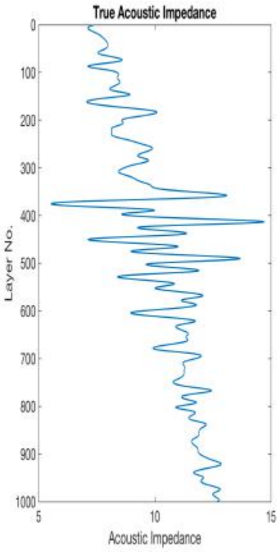
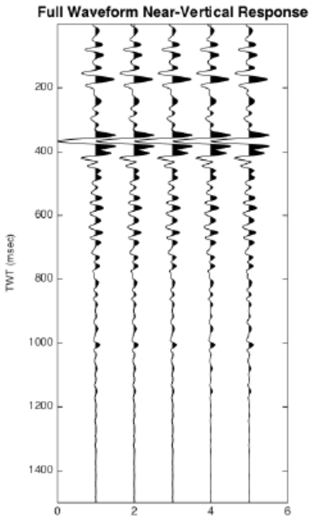
A 1-D Inverse Scattering Problem with 1000-parameters





Khoshkholgh, Zunino and Mosegaard, 2021: Informed Proposal Monte Carlo. Geophys. Journ. Int.

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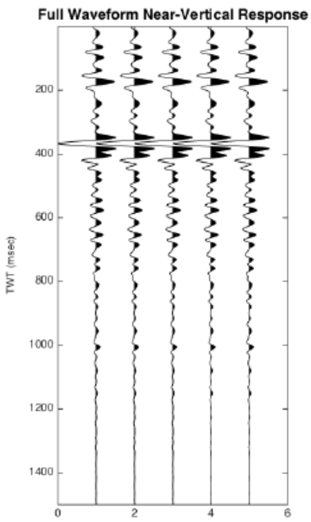
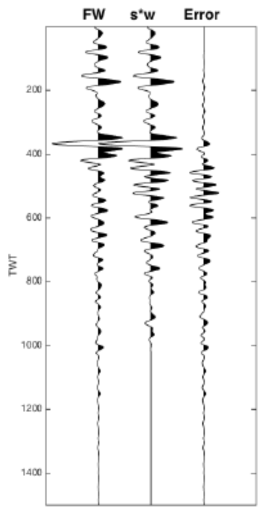
A 1-D Inverse Scattering Problem with 1000-parameters





Khoshkholgh, Zunino and Mosegaard, 2021: Informed Proposal Monte Carlo. Geophys. Journ. Int.

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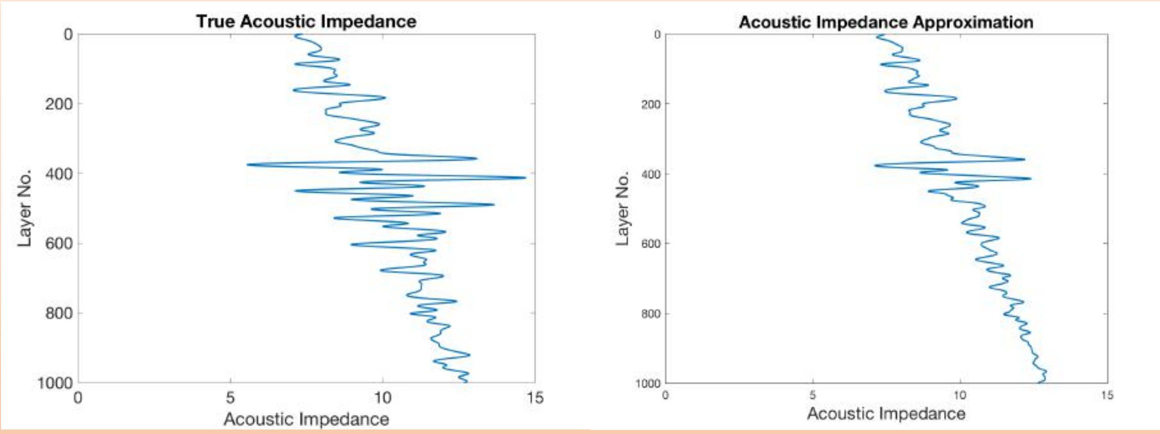
Linear Inversion: An Approximate Solution



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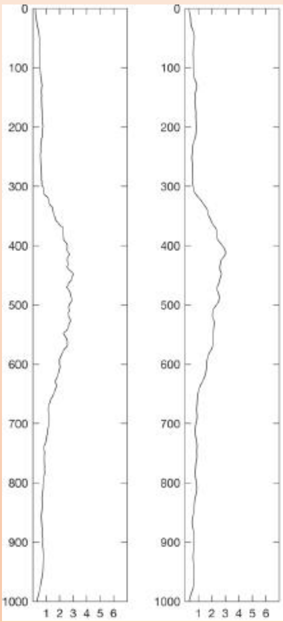
Approximate (Linear) Inversion: Modelization Error

Envelope of true error



Envelope of 2. order error

1. Assume the approximate model is the true model
2. Simulate fully nonlinear data from this model
3. Find (2. order) approximate solution
4. Compute modelization error

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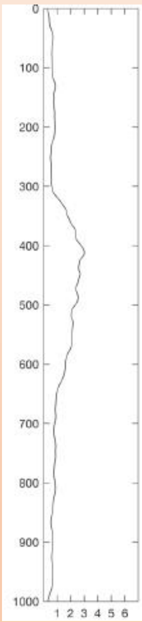
Defining the Informed Proposal Distribution



1. Define proposal distribution as a Gaussian centered at the approx. model
2. Use modelization errors at each depth/TWT as standard dev. in the proposal

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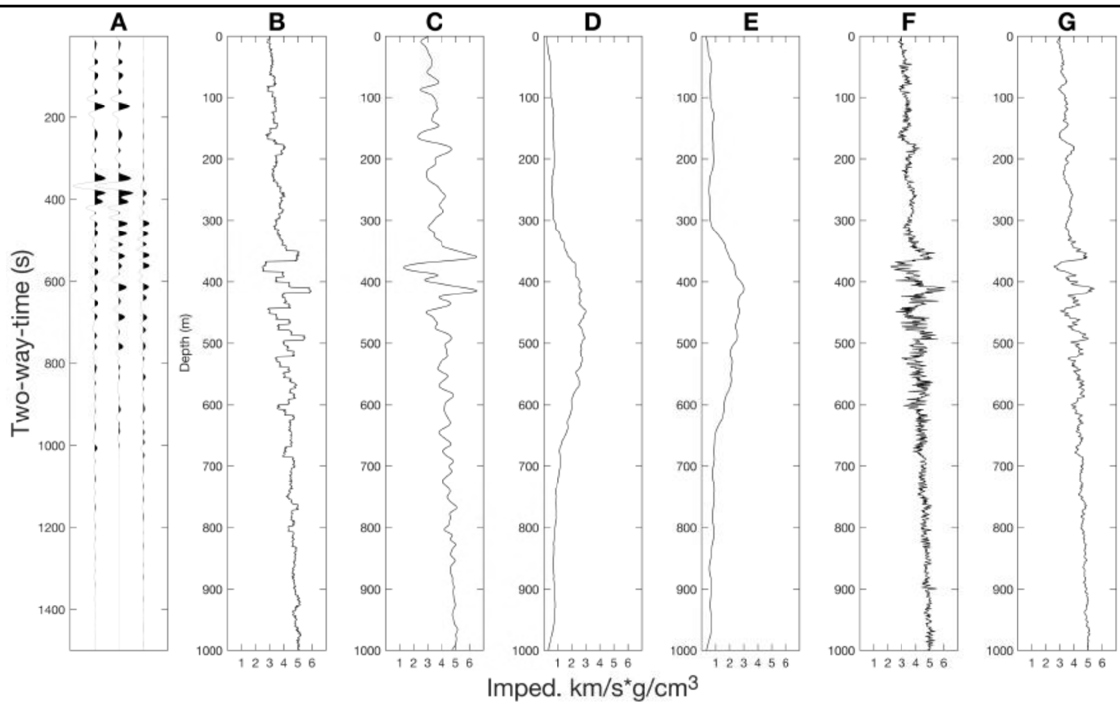

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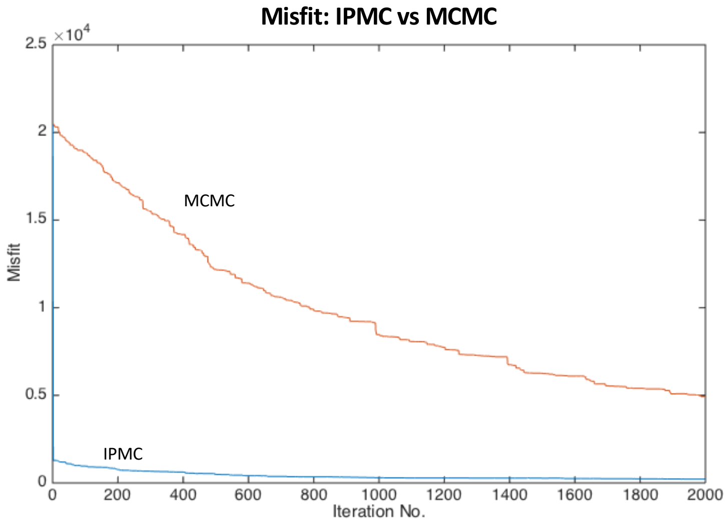
Convergence: Informed-Proposal Monte Carlo



In this example: IPMC equilibrates 10^3 - 10^4 times faster

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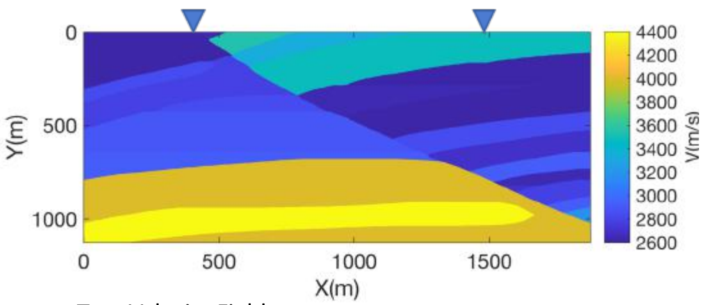
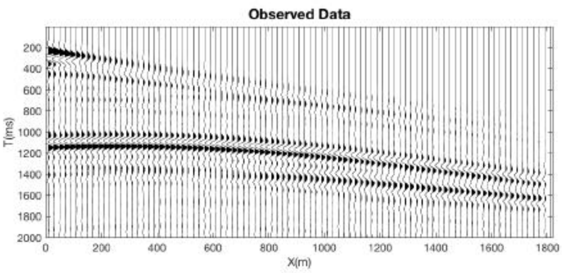
A ~940000-parameter Full-Waveform Acoustic Problem



True Velocity Field



Acoustic wave field recorded at the surface

Khoshkholgh, Mosegaard and Zunino (2022)

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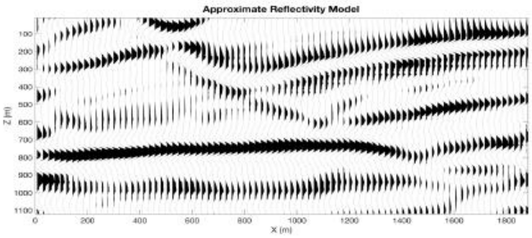
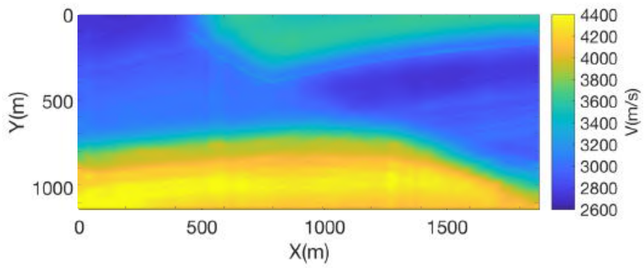
An Approximate Solution



Approximate Reflectivity Model



Estimated Acoustic Velocity Field

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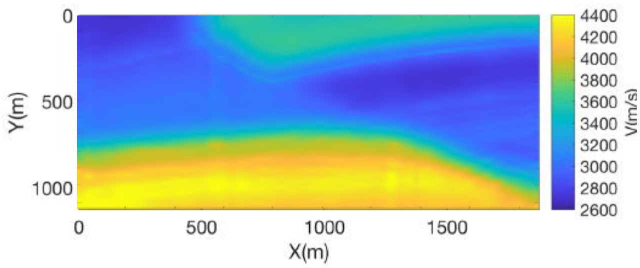
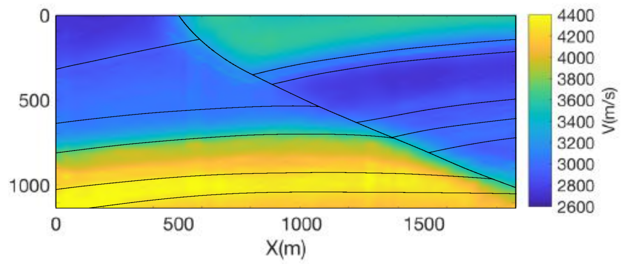
An Approximate Solution from Classical Processing



Estimated Acoustic Velocity Field



Approximate Velocity Model

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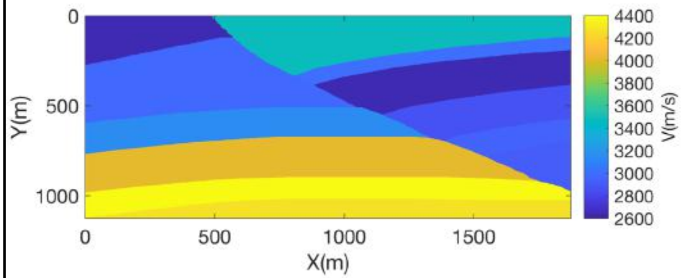
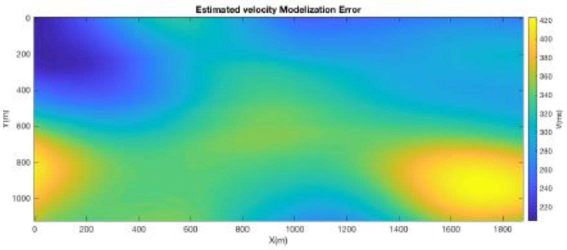
Creating the Modelization Error Distribution



Final Approximate Velocity Model



Envelope $\left(\mathbf{m}_{approx} - \boldsymbol{H}_{approx}\left(\boldsymbol{g}_{precise}(\mathbf{m}_{approx})\right)\right)$

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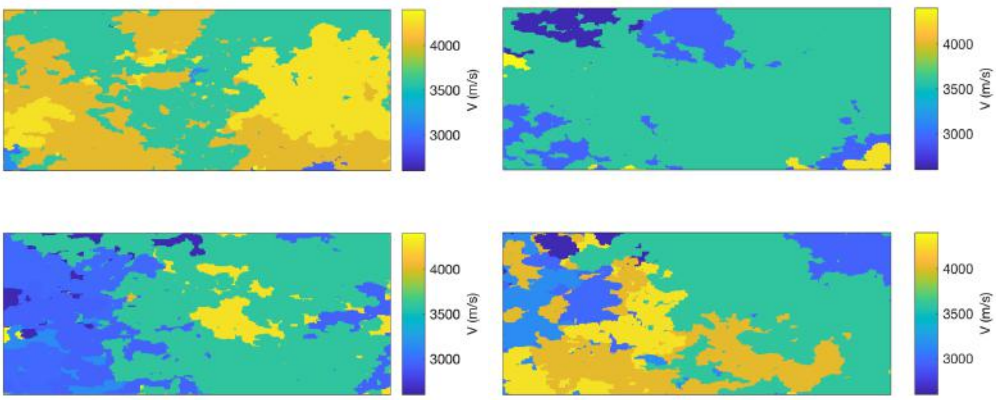
Samples from the combined Prior and Modelization Error Distributions



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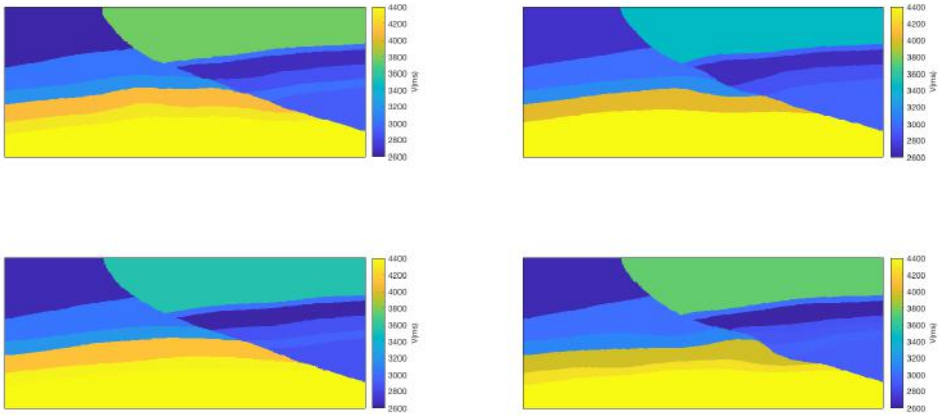
Samples from the Posterior Distribution



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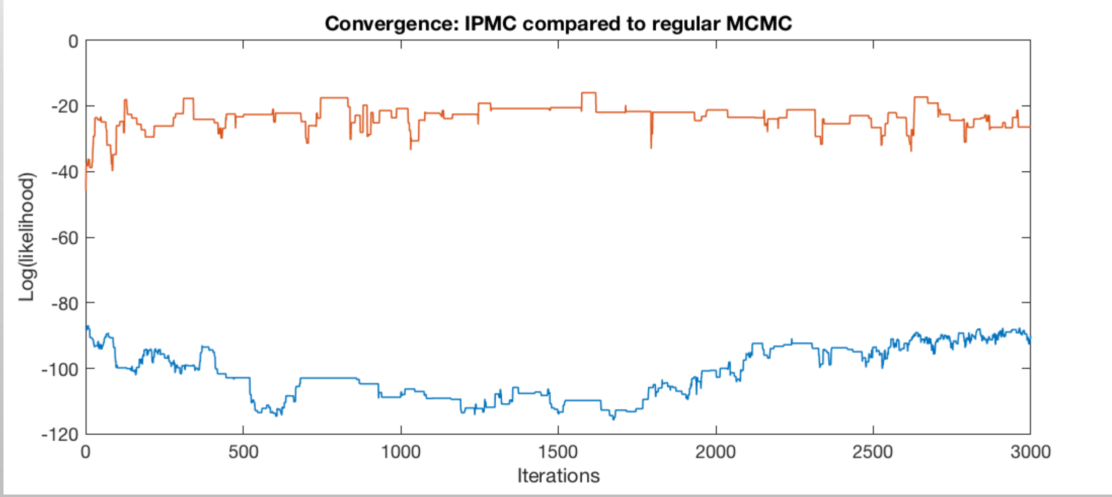
Convergence: Informed Proposal Monte Carlo



In this example: IPMC equilibrates in ~300 iterations

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