PolyChord: Next Generation Nested Sampling

Sampling, Parameter Estimation and Bayesian Model Comparison

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University of Cambridge

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Parameter estimation & model comparison

Metropolis Hastings

Nested Sampling

PolyChord

Applications

Notation

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- Data: D

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- Prior: $\mathrm{P}(\Theta|M) = \pi(\Theta)$
- Evidence: $\mathrm{P}(D|M) = \mathcal{Z}$

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$$\text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Evidence}}$$

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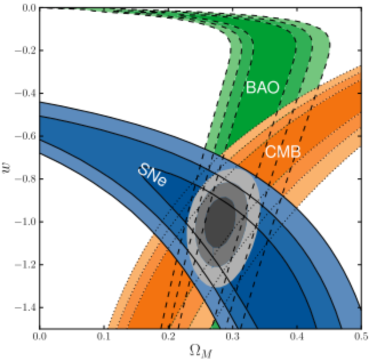
- Nested sampling (NS) promises to solve both simultaneously.

Parameter estimation & model comparison

Why is it difficult?



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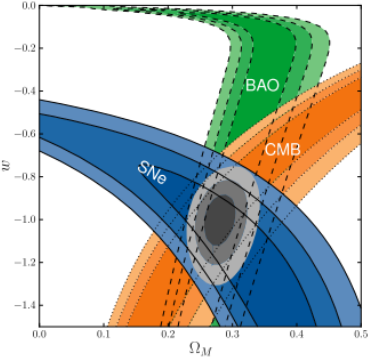

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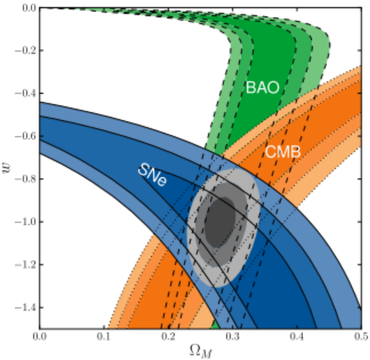

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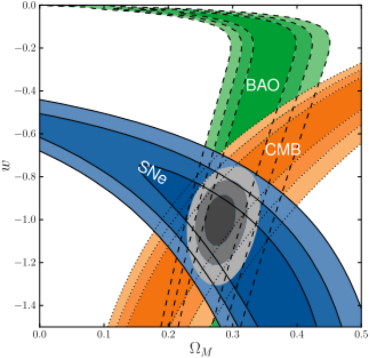

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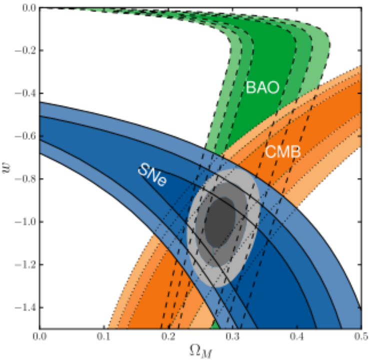

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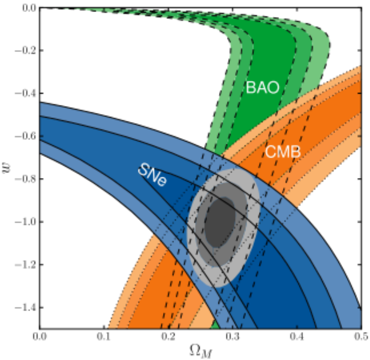

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- *Sampling* the posterior is an excellent compression scheme.

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Metropolis-Hastings, Gibbs, Hamiltonian...

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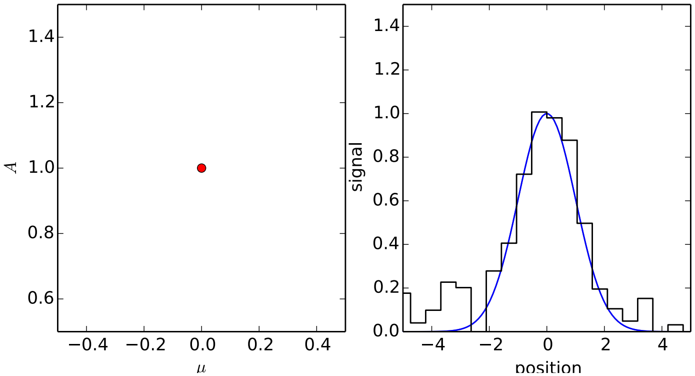
MCMC in action



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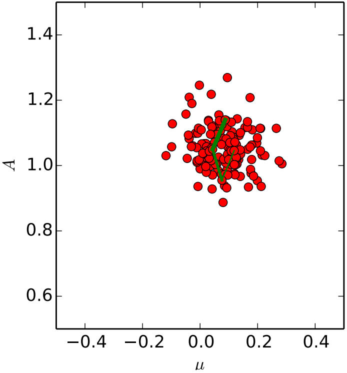
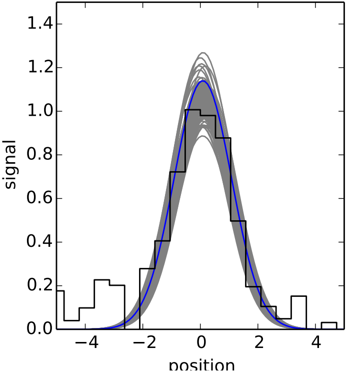
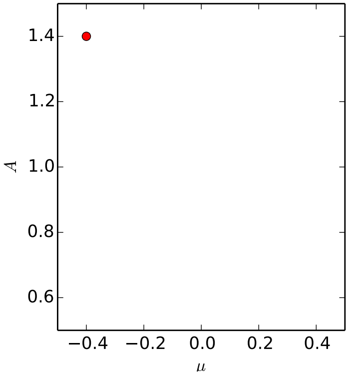
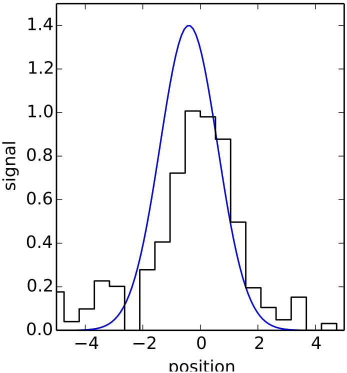




When MCMC fails

Burn in





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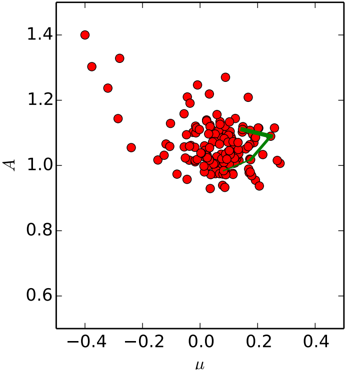

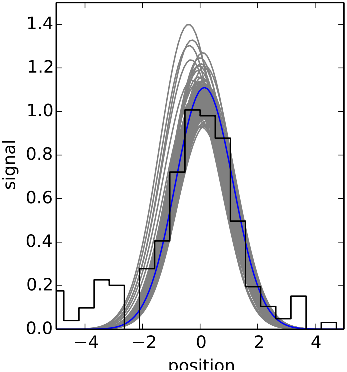

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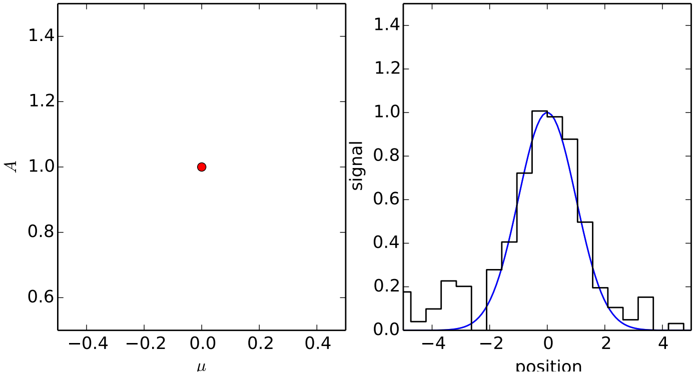

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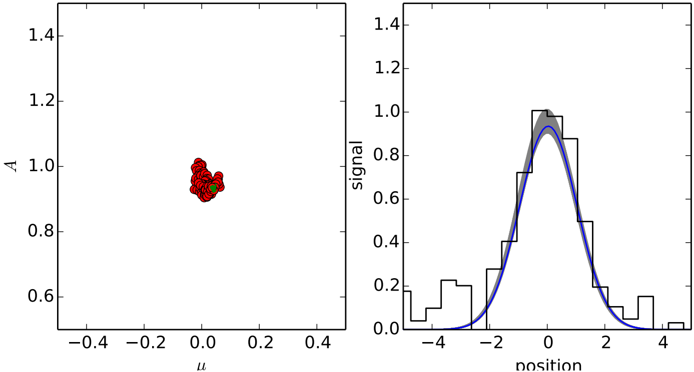

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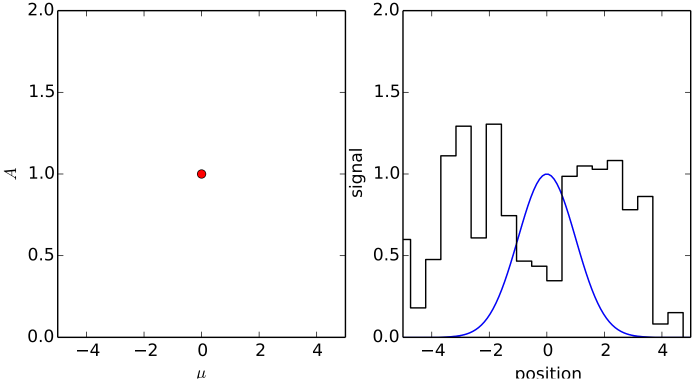
Multimodality



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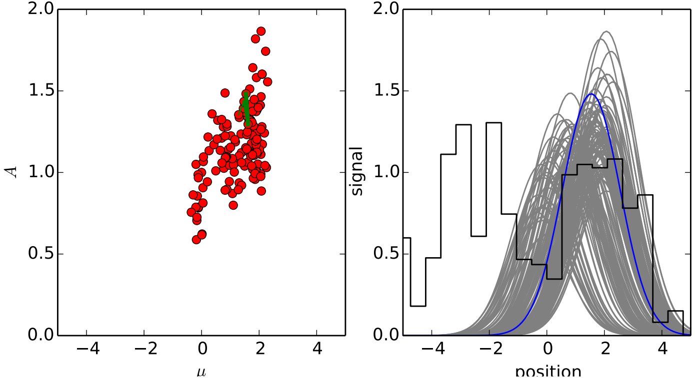

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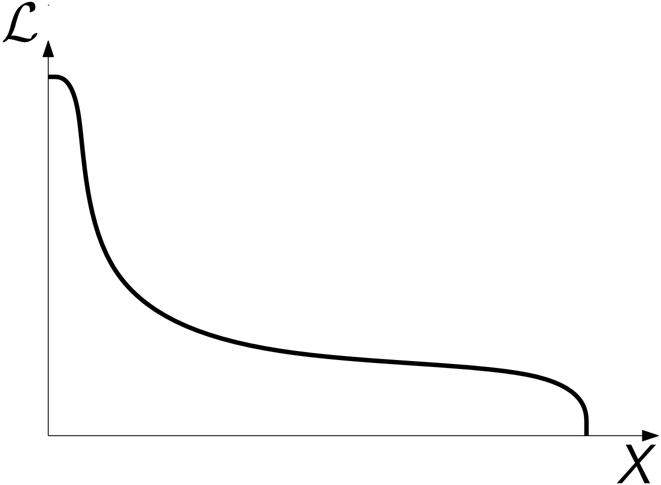
Phase transitions



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- MCMC fundamentally explores the posterior, and cannot average over the prior.

Nested Sampling

John Skilling's alternative to MCMC!

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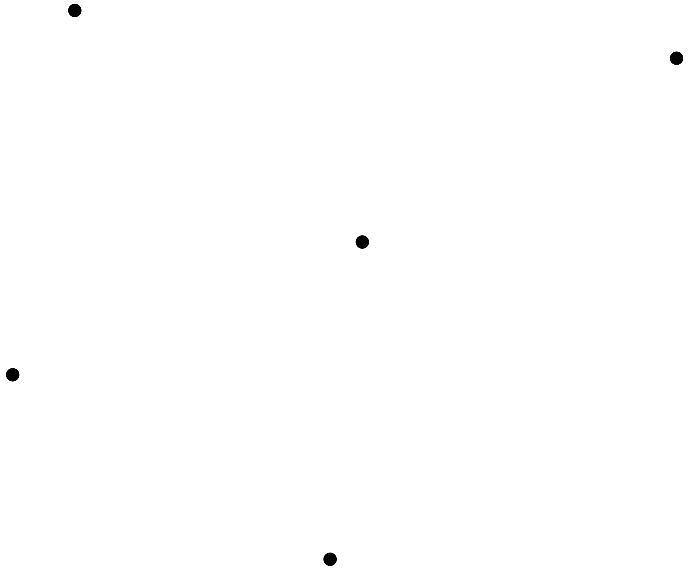
Requires one to be able to sample from the prior, subject to a *hard likelihood constraint*.

Nested Sampling

Graphical aid



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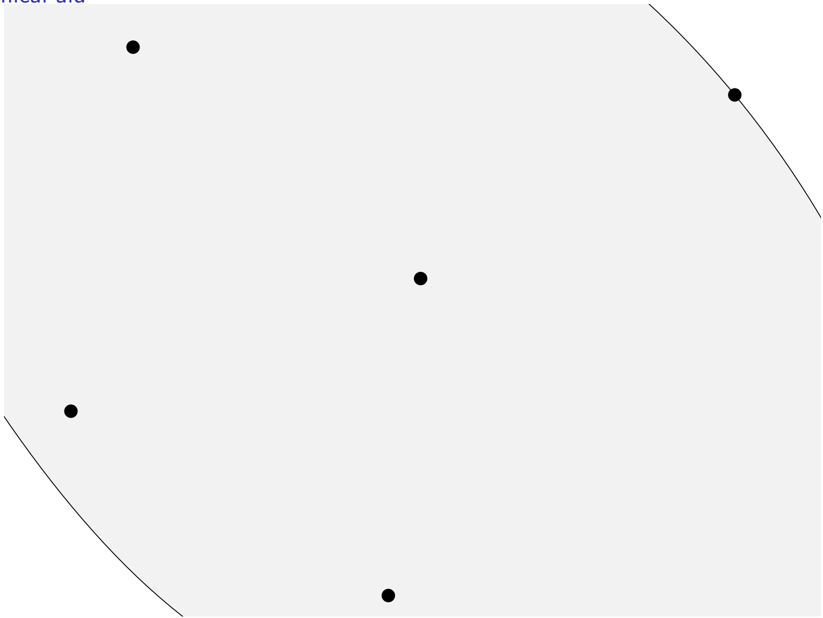

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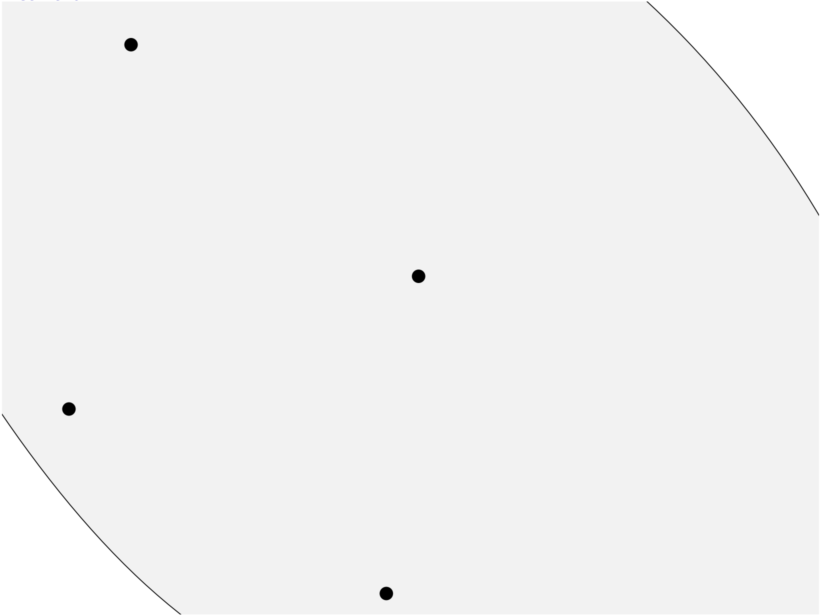

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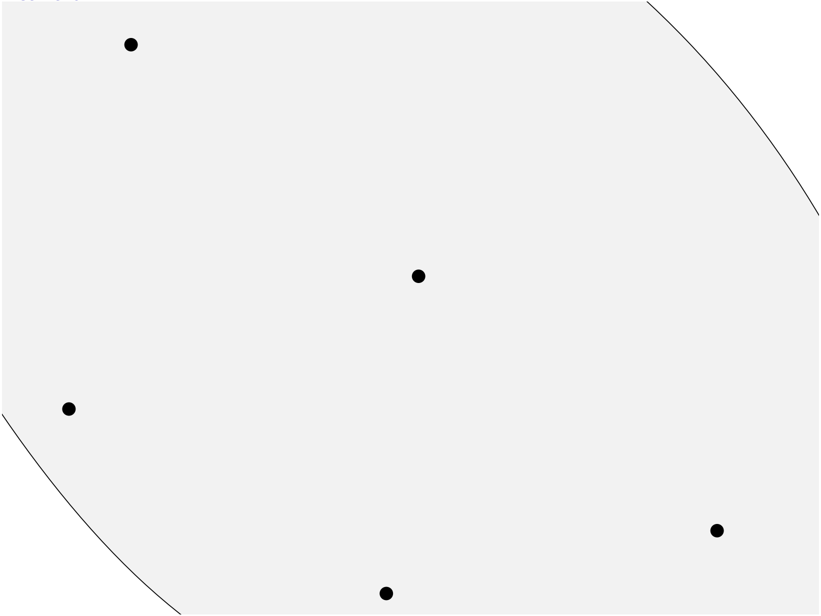

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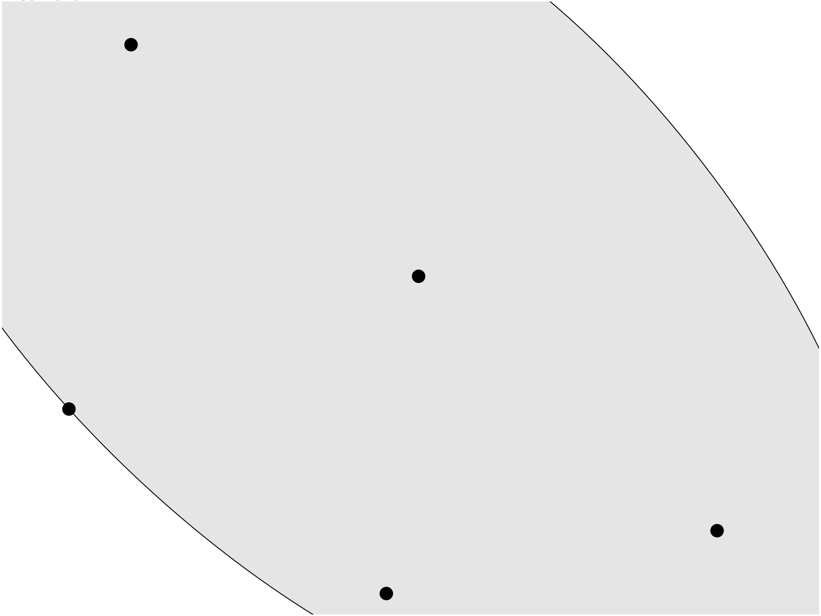

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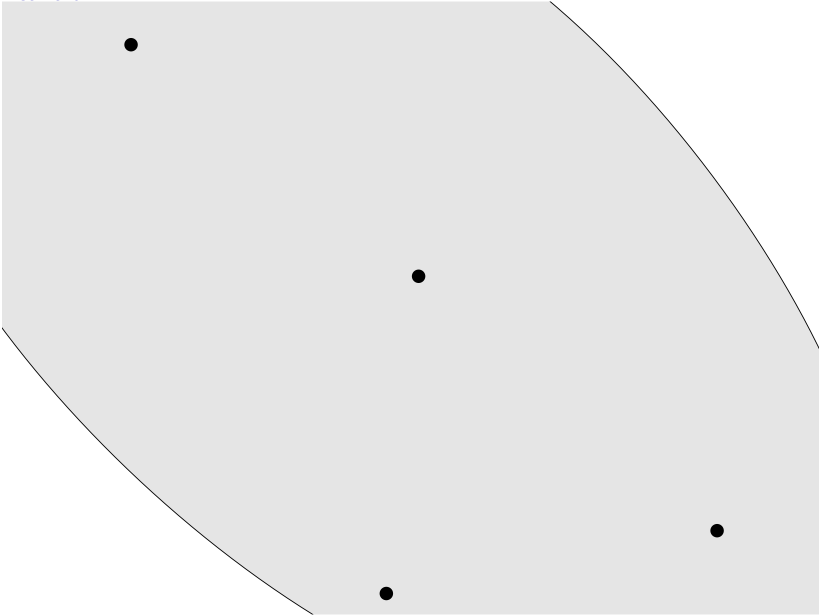

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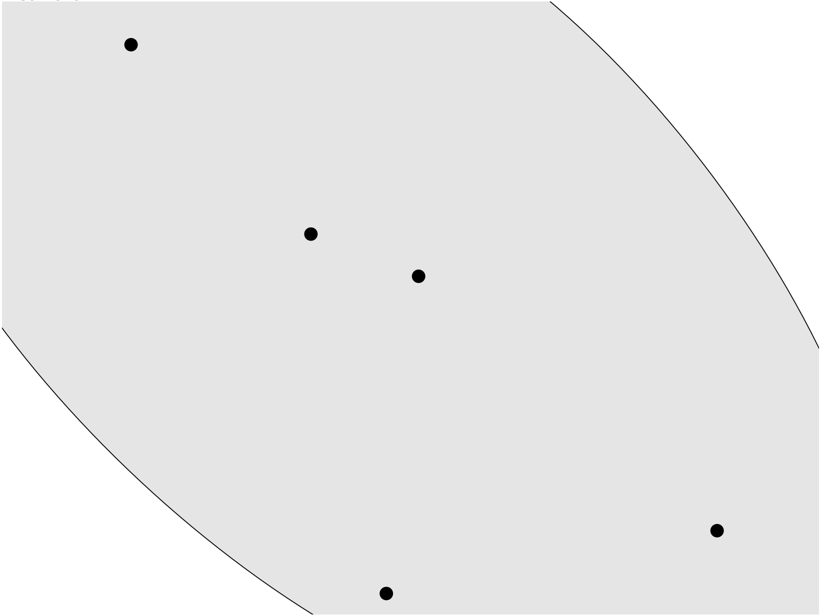

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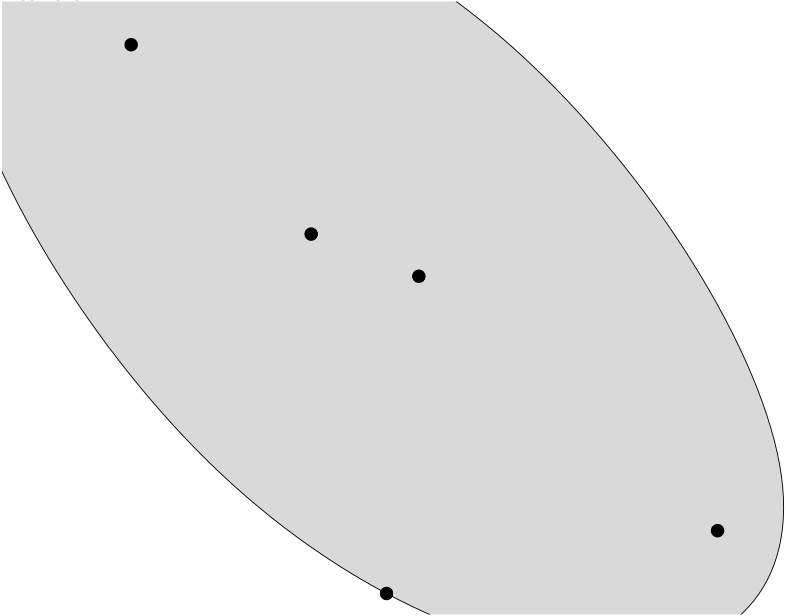

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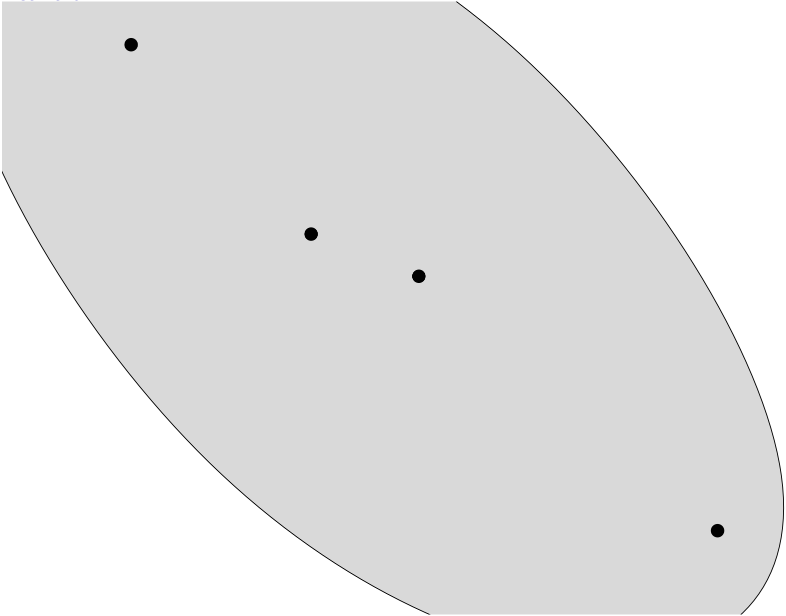

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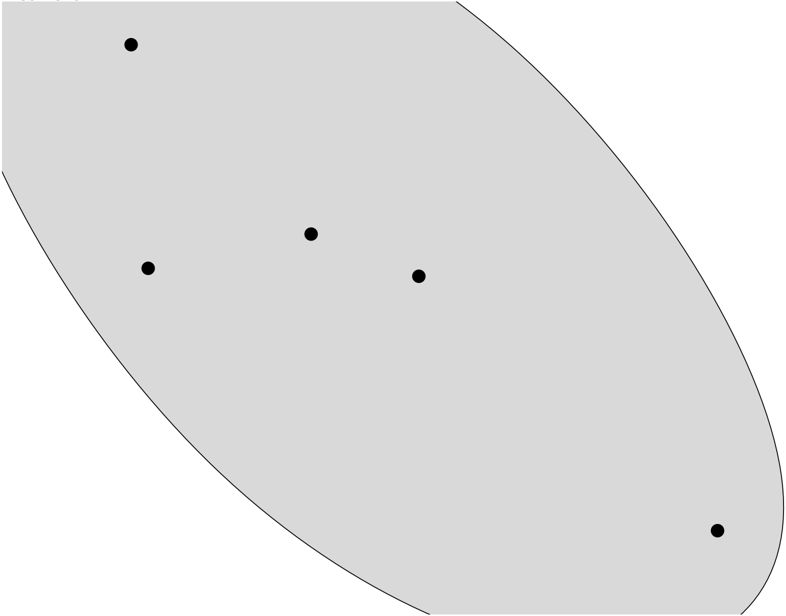

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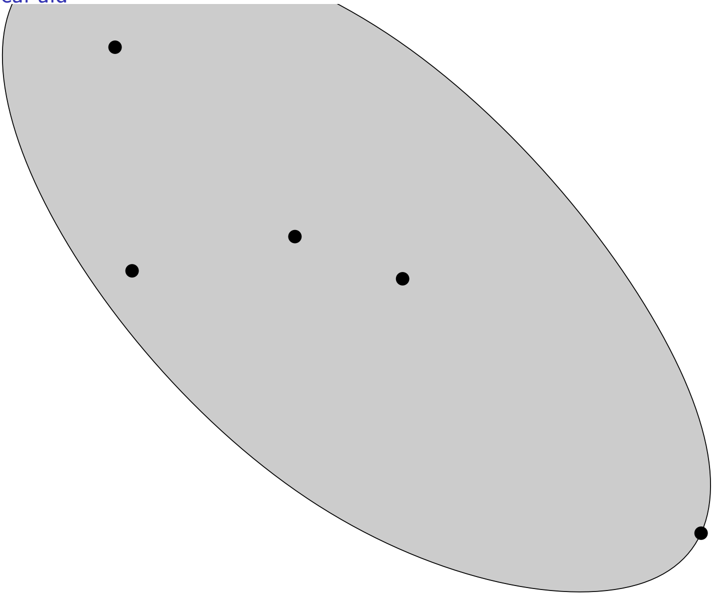

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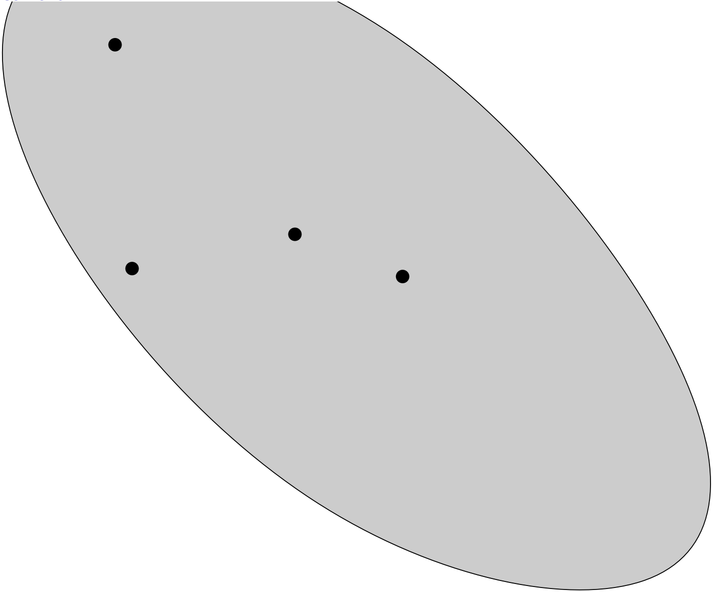

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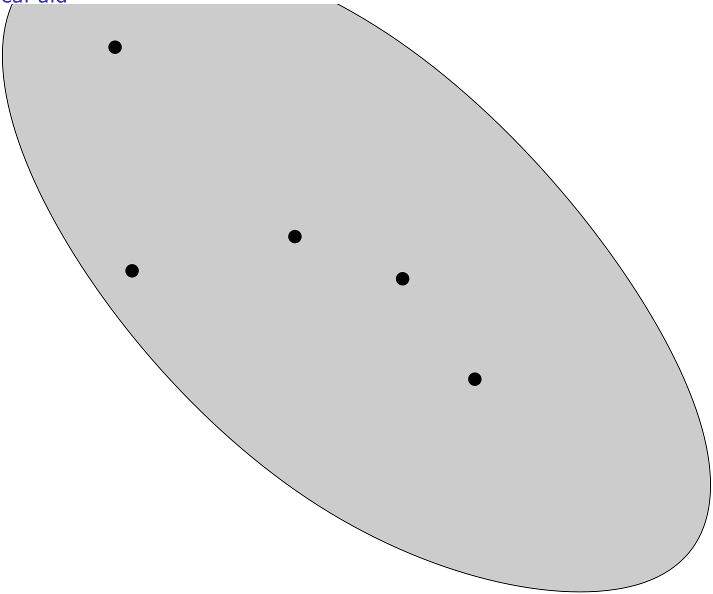

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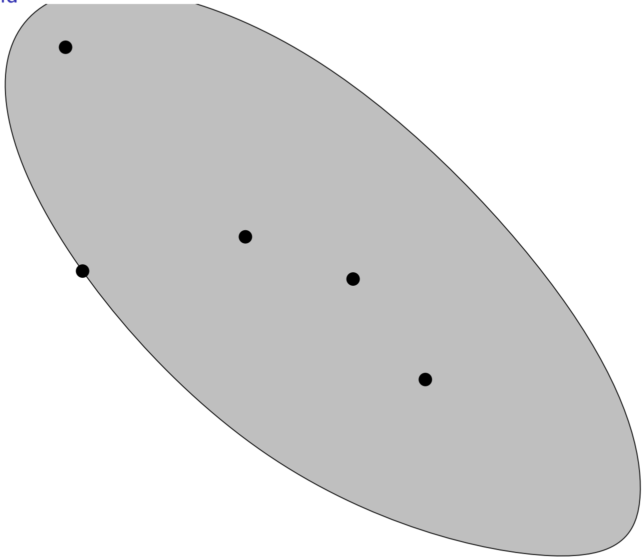

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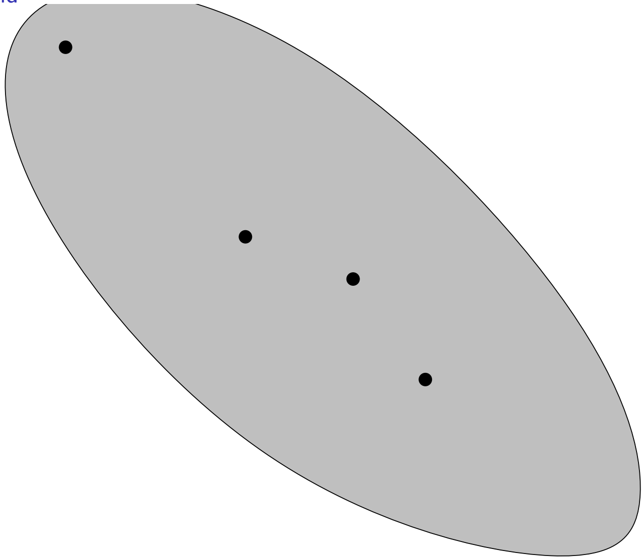

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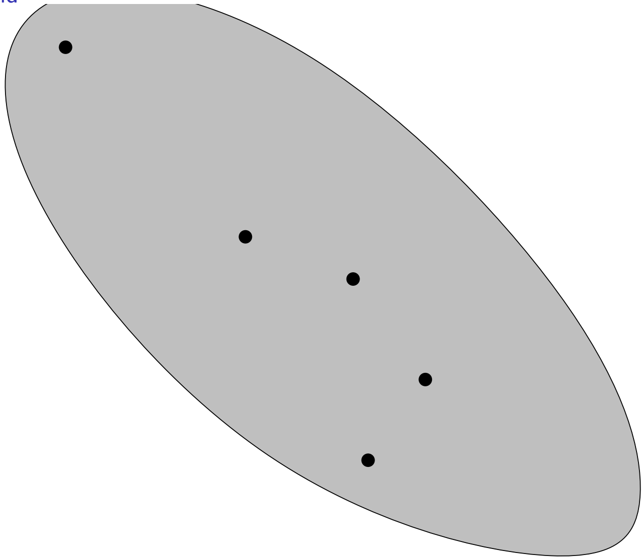

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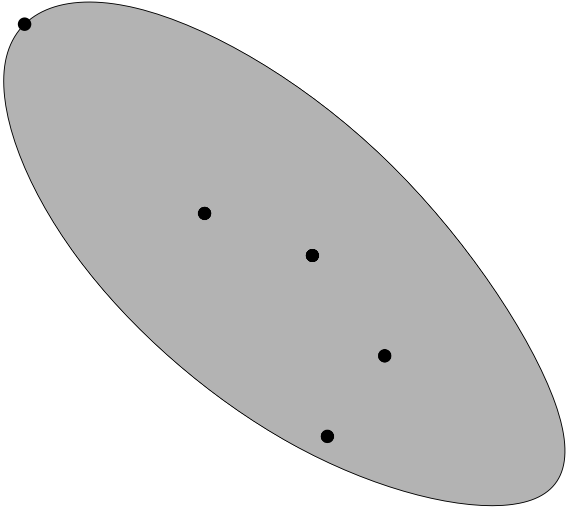

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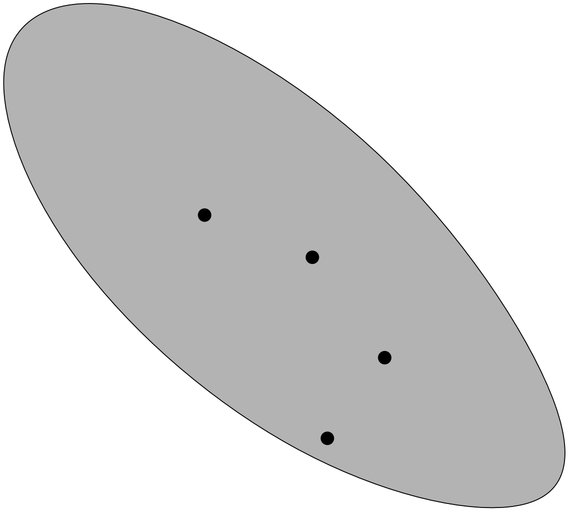

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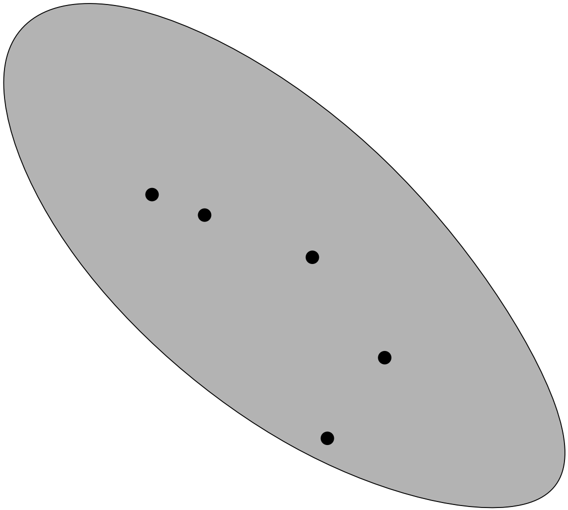

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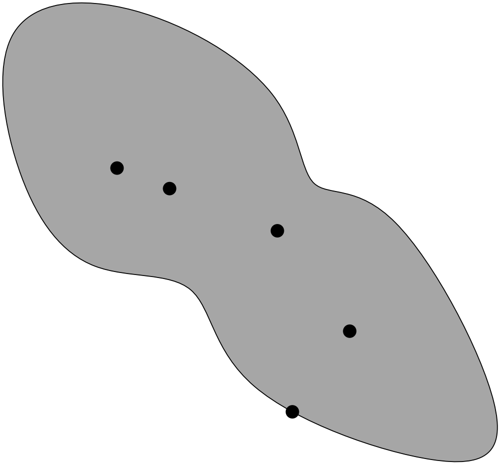

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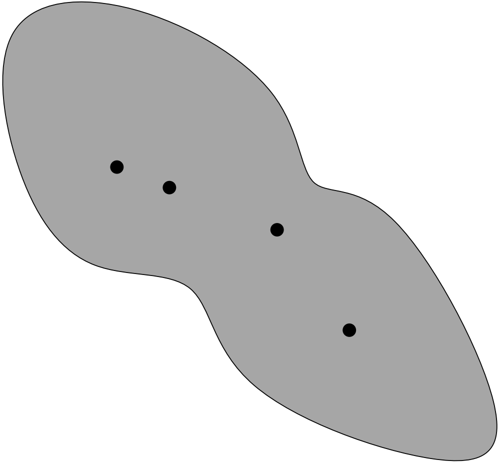

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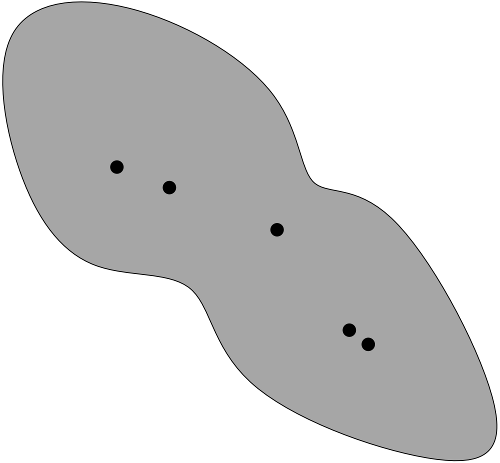

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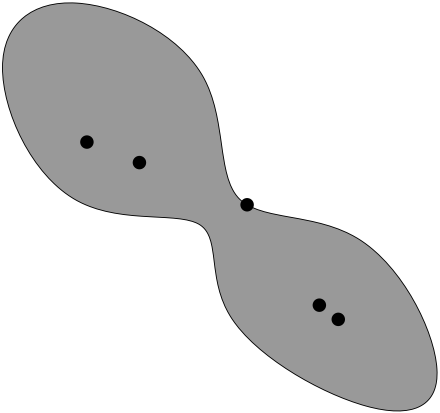

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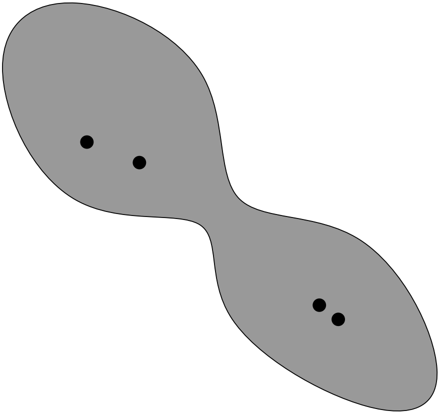

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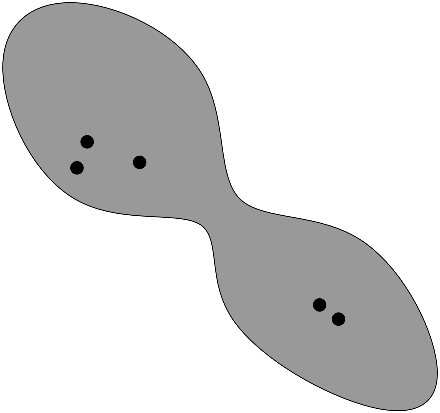

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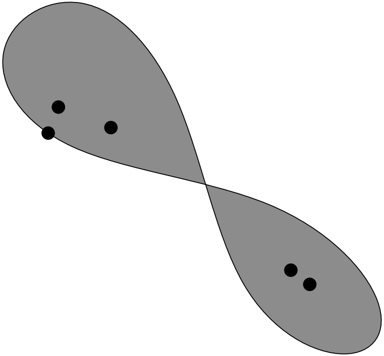

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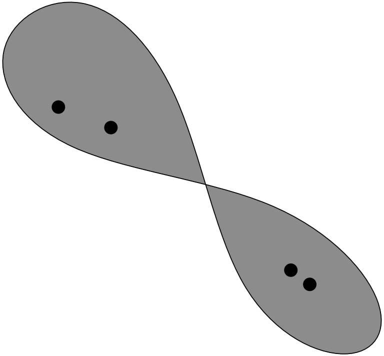

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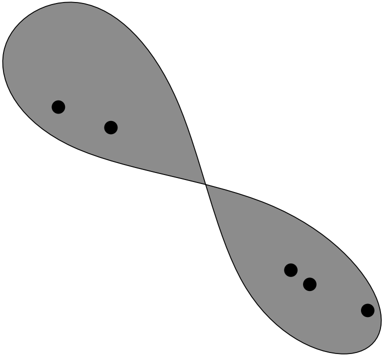

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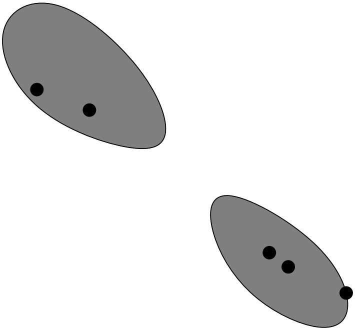

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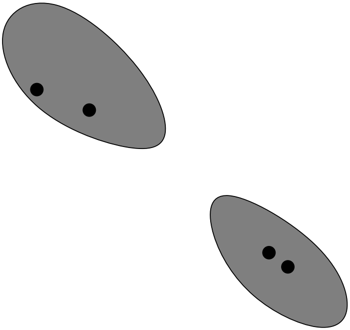

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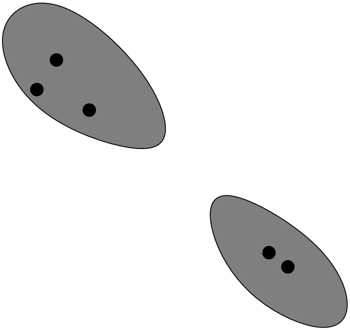

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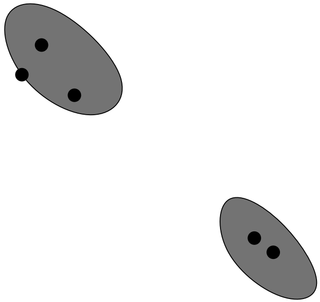

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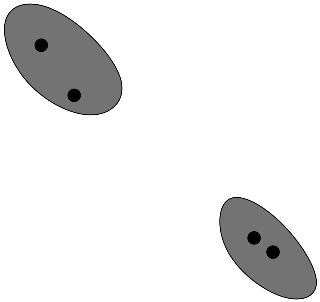

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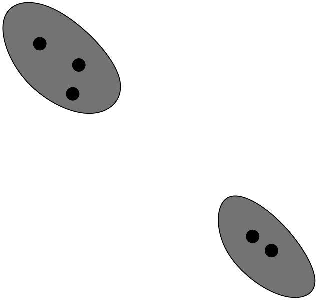

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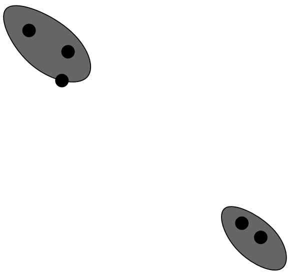

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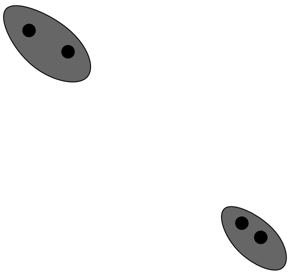

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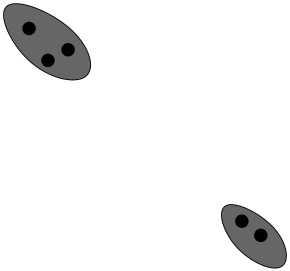

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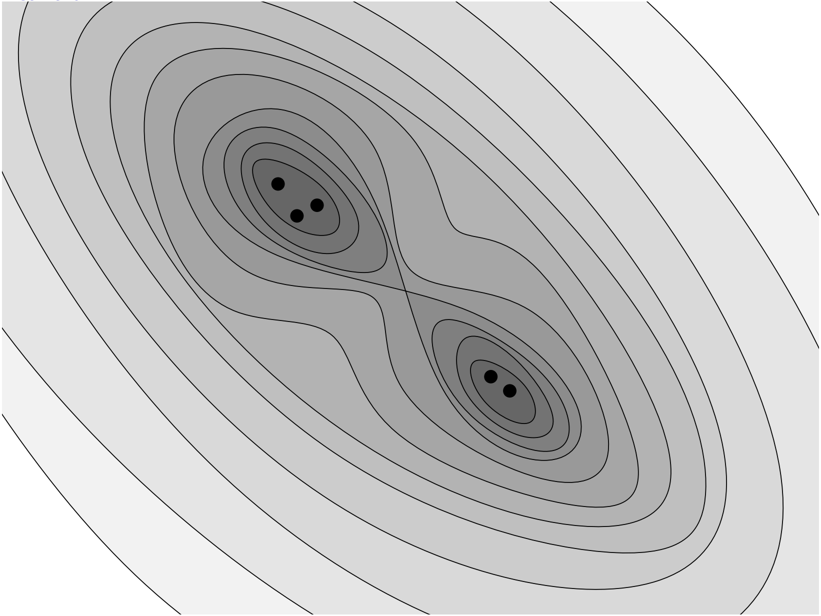

Nested Sampling

Why bother?

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- At each iteration, the likelihood contour will shrink in volume by a factor of $\approx 1/n$.
- Nested sampling zooms in to the peak of the posterior *exponentially*.
- Nested sampling can be used to get evidences!

Calculating evidences

Calculating evidences

$$\mathcal{Z} = \int \mathcal{L}(\theta)\pi(\theta)d\theta$$

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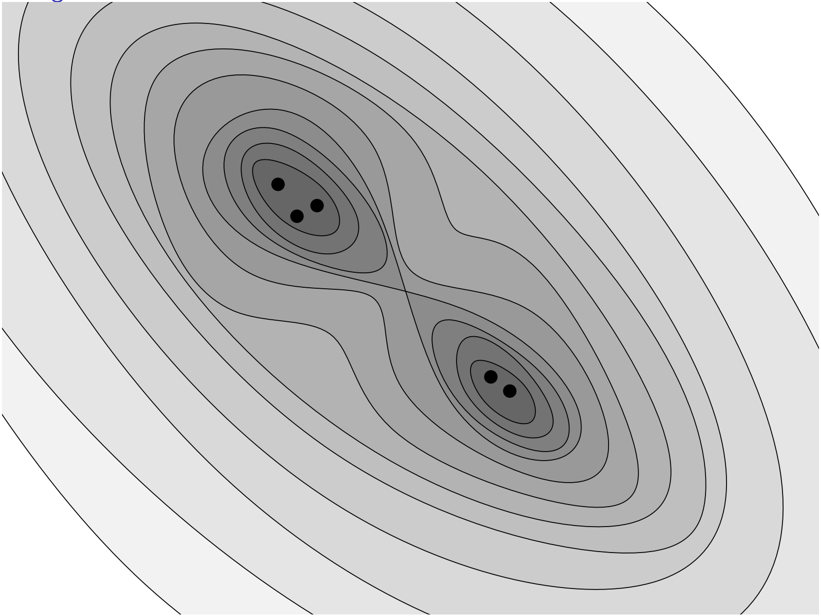
- i.e. the fraction of the prior which the iso-likelihood contour $\mathcal{L}$ encloses.

Nested Sampling

Calculating evidences



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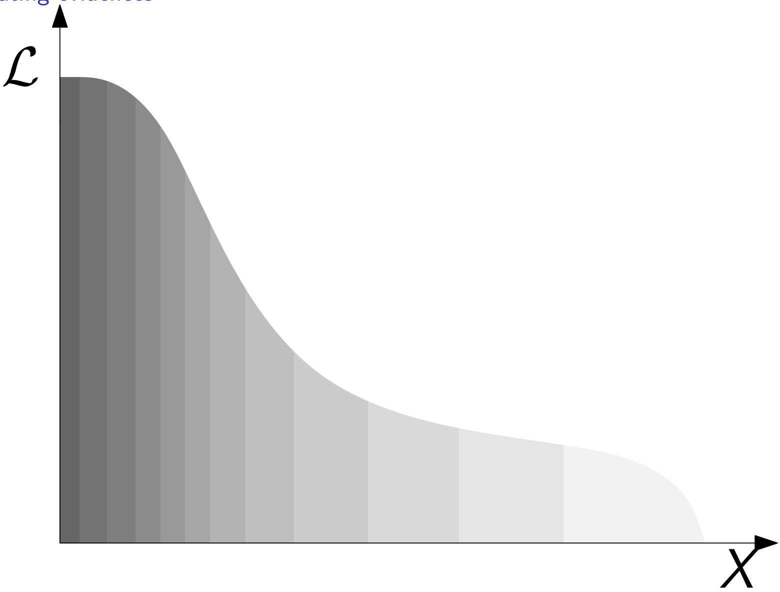

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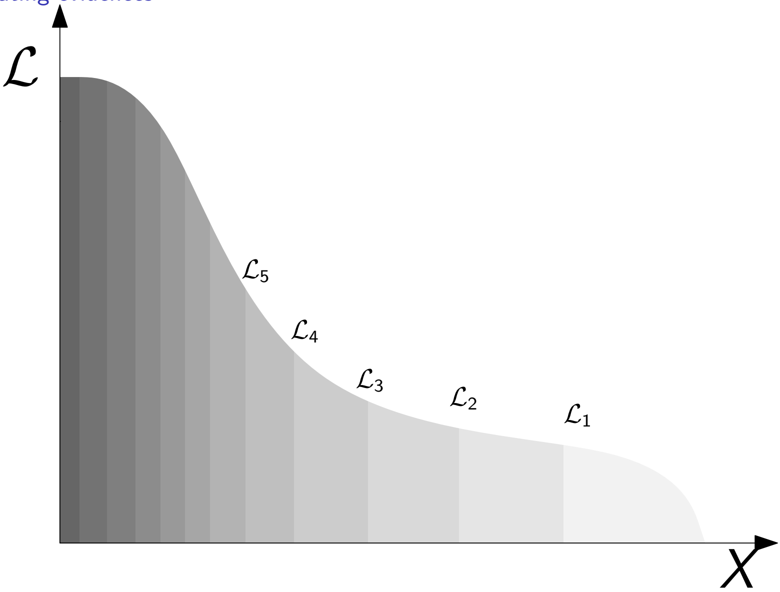

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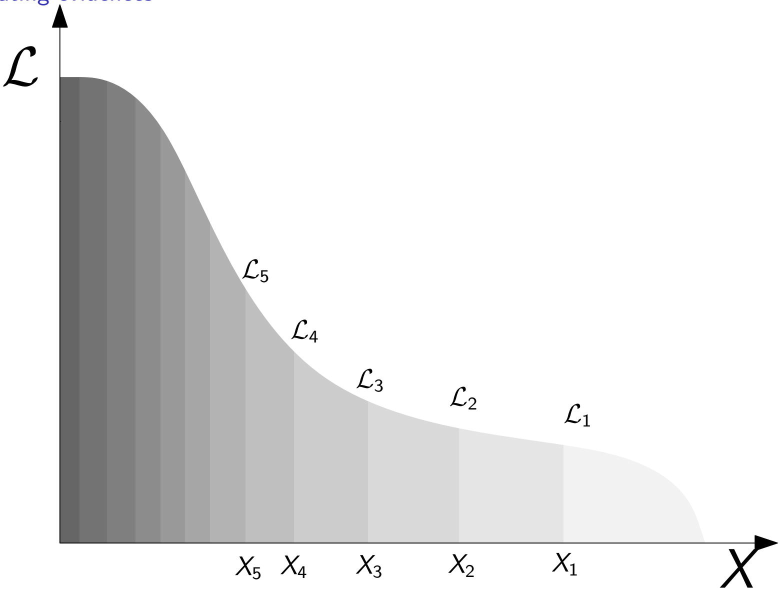

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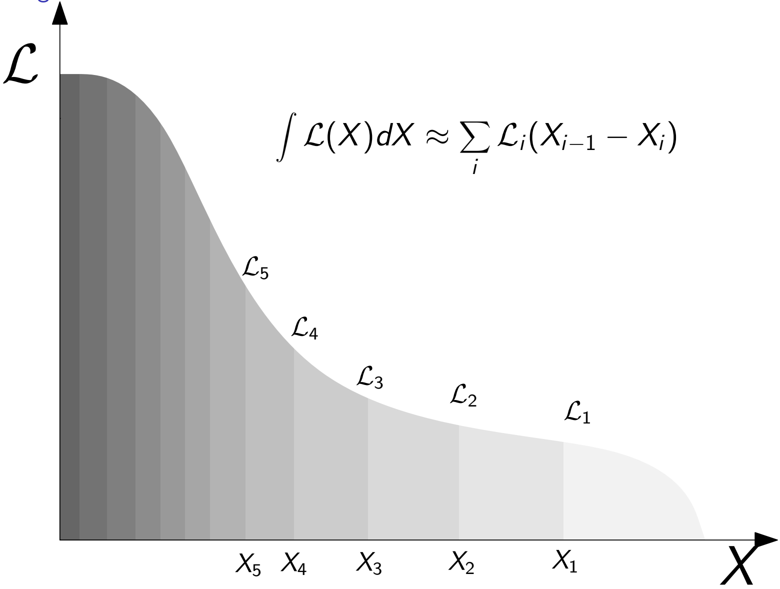

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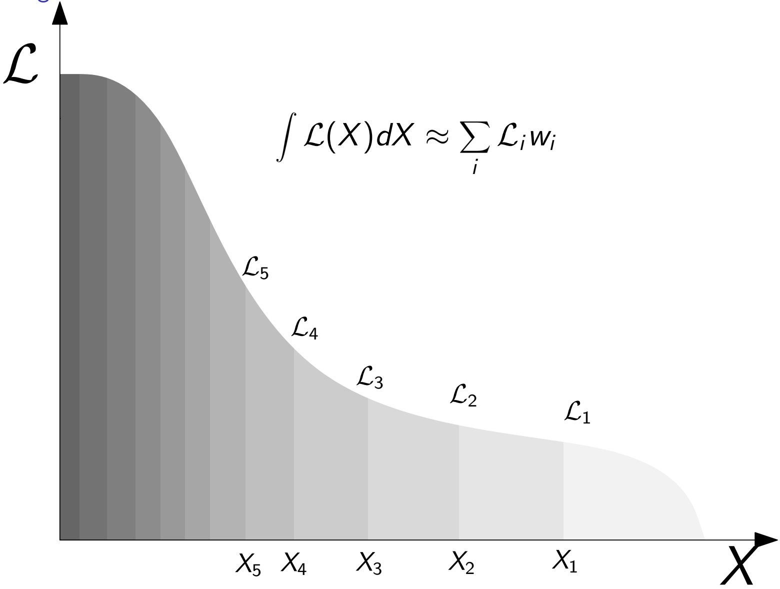
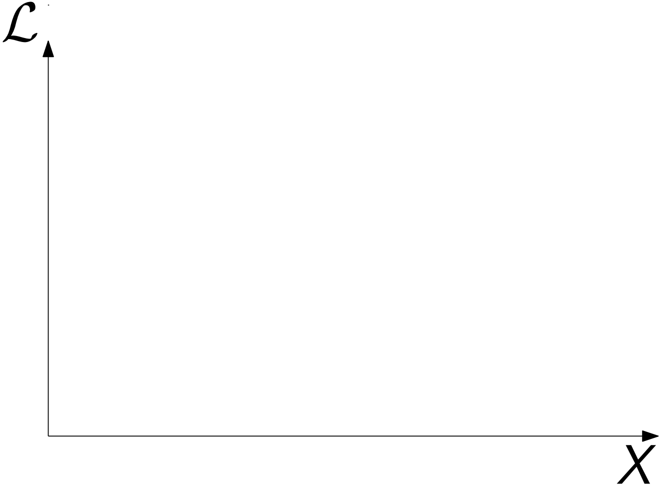


Estimating evidences

Evidence error



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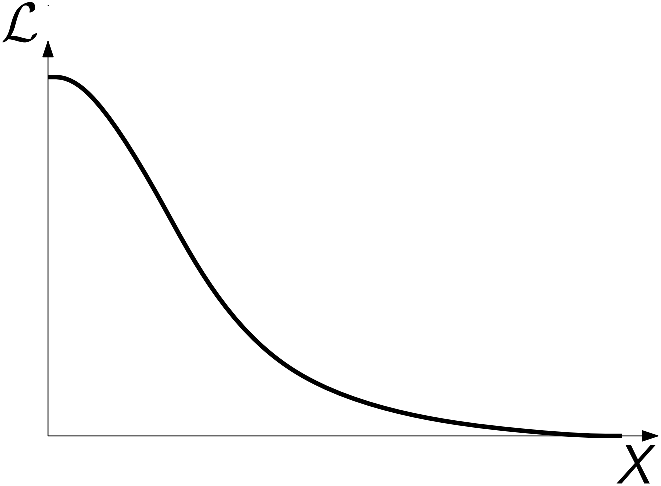

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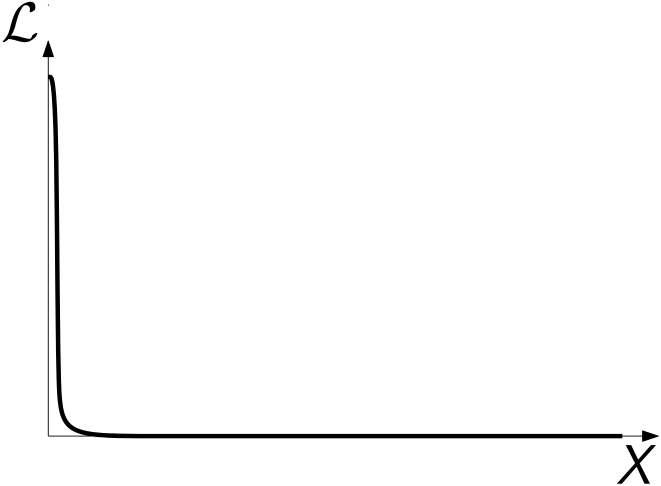

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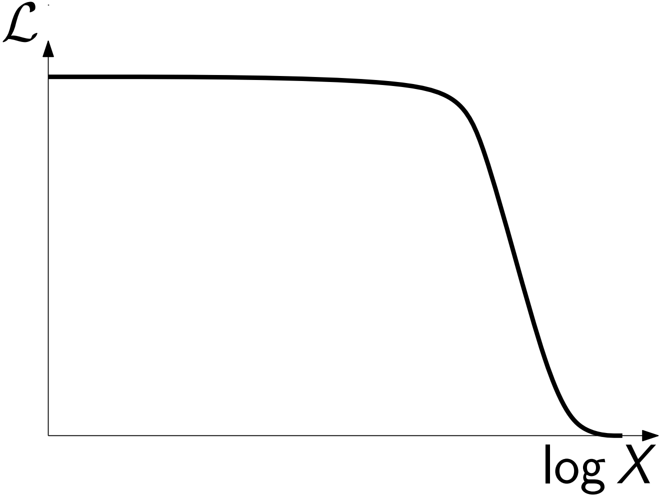

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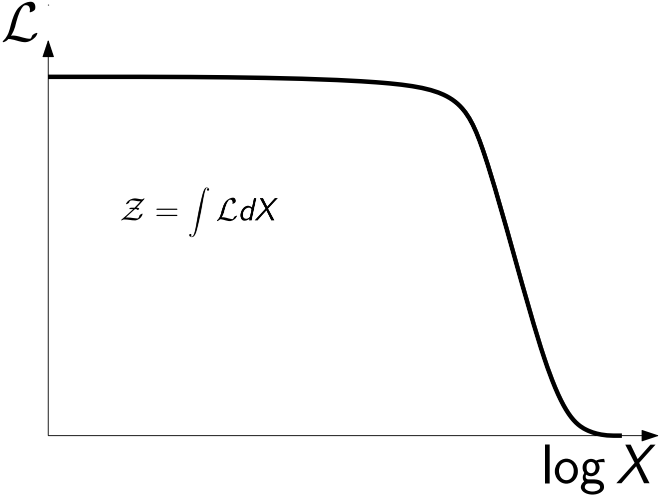

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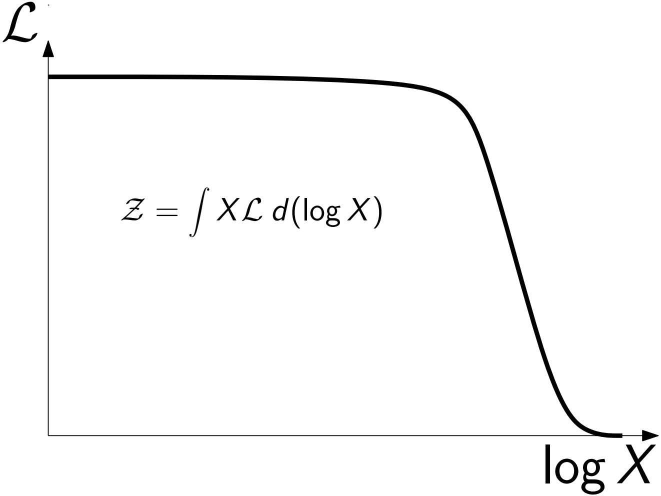

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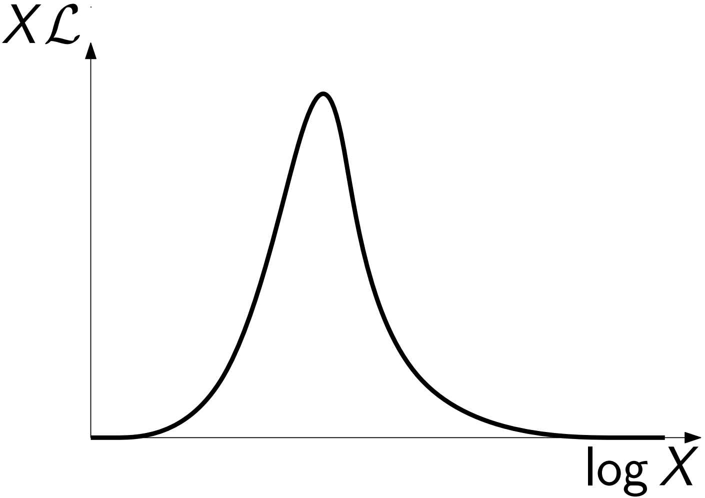

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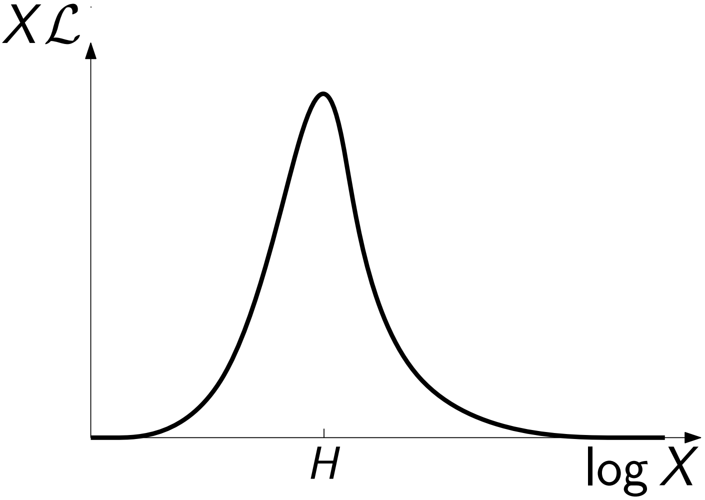

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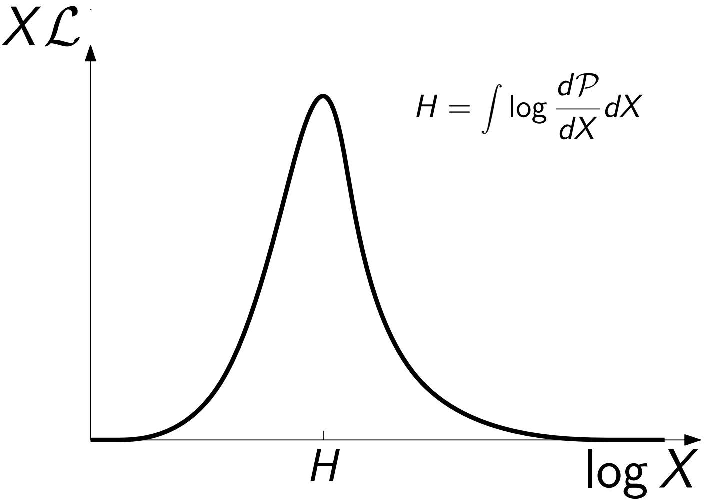

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$$i_H \sim nH$$

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- estimate of evidence error:

$$\log \mathcal{Z} \approx \sum w_i \mathcal{L}_i \pm \sqrt{\frac{H}{n}}$$

Nested sampling

Parameter estimation

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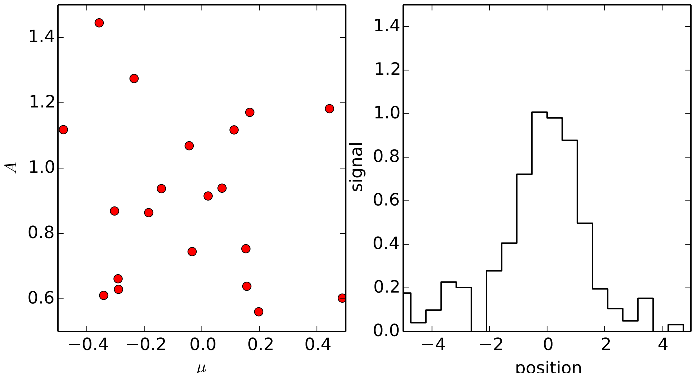
- NS can also be used to sample the posterior

Nested sampling

Parameter estimation

- NS can also be used to sample the posterior
- The set of dead points are posterior samples with an appropriate weighting factor

When NS succeeds



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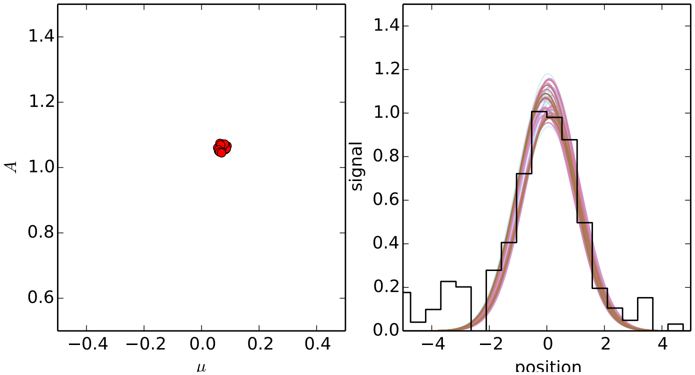

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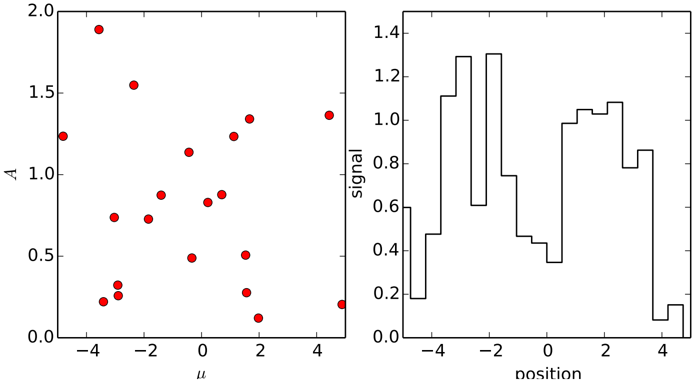

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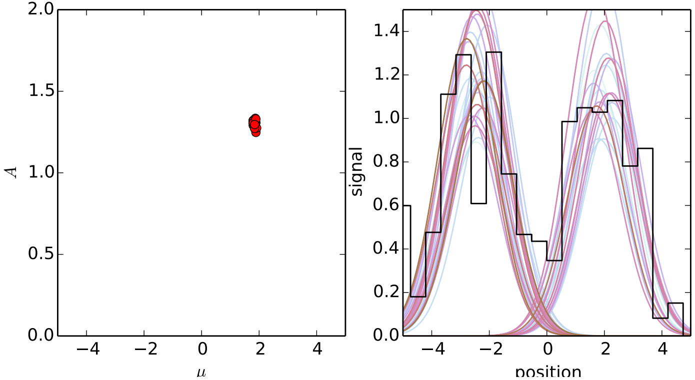

Sampling from a hard likelihood constraint

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> *"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."*
>
> — *John Skilling*

Sampling within an iso-likelihood contour

Previous attempts

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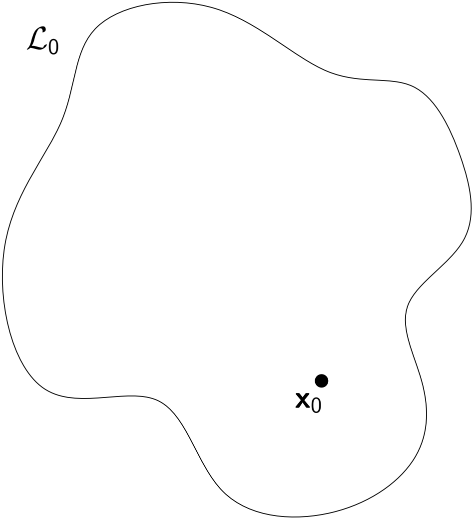
Diffusion Nested Sampling B. Brewer et al. (2009).

- Very promising
- Too many tuning parameters

PolyChord

"Hit and run" slice sampling



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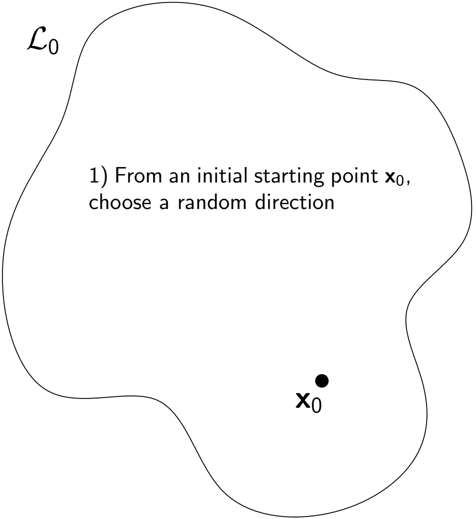

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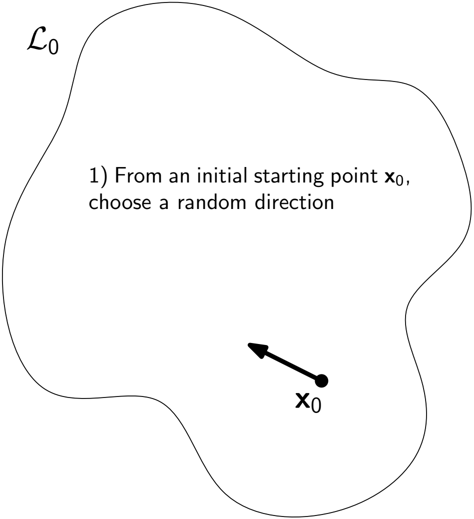

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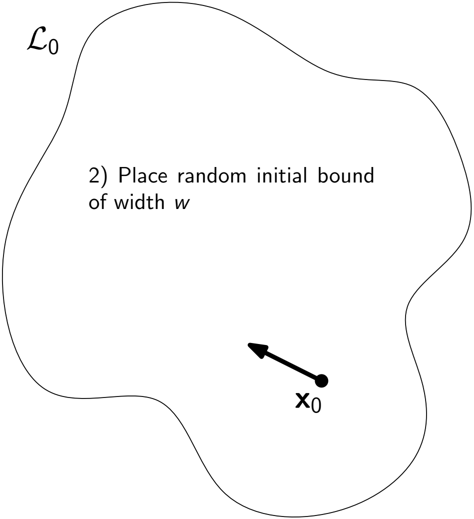

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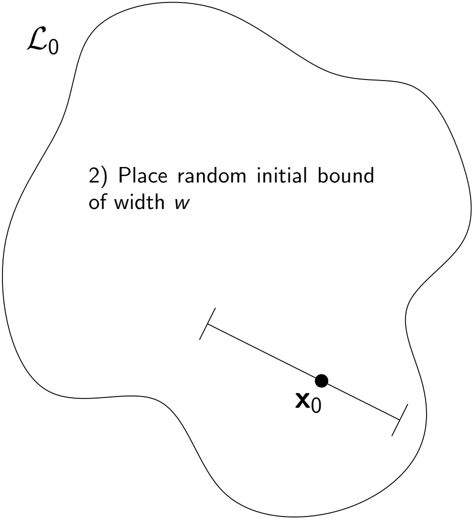

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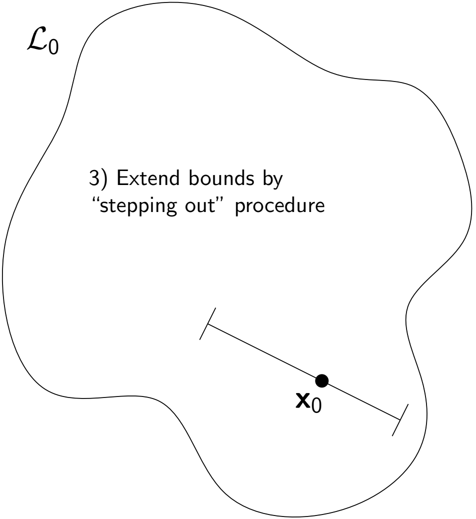

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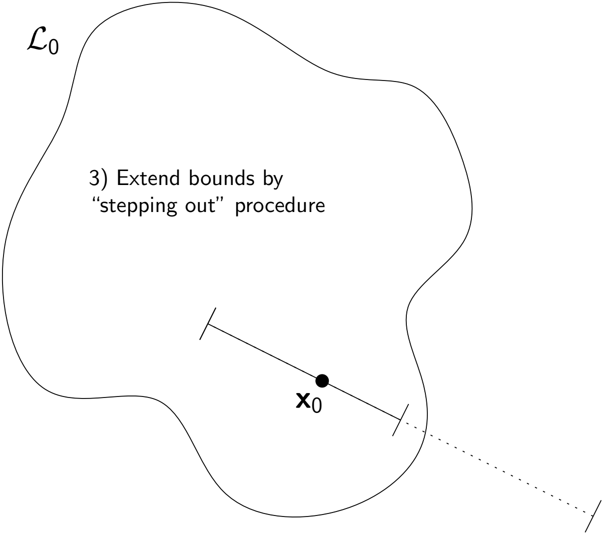

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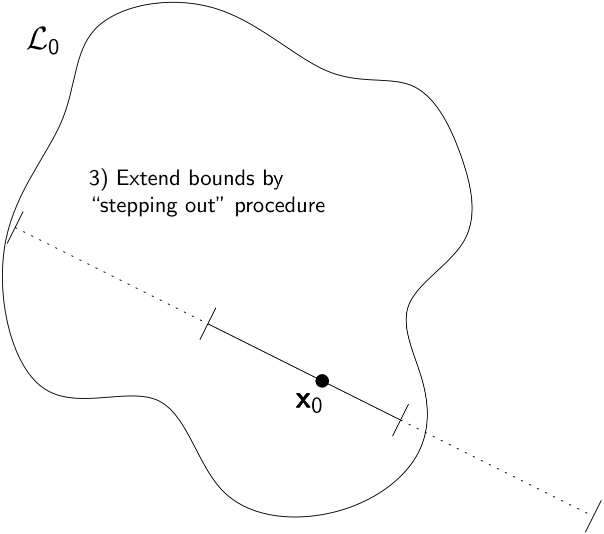

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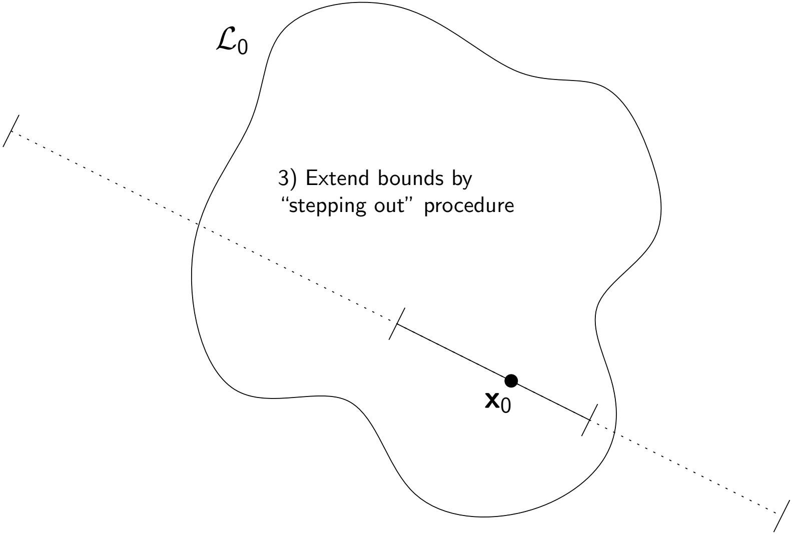

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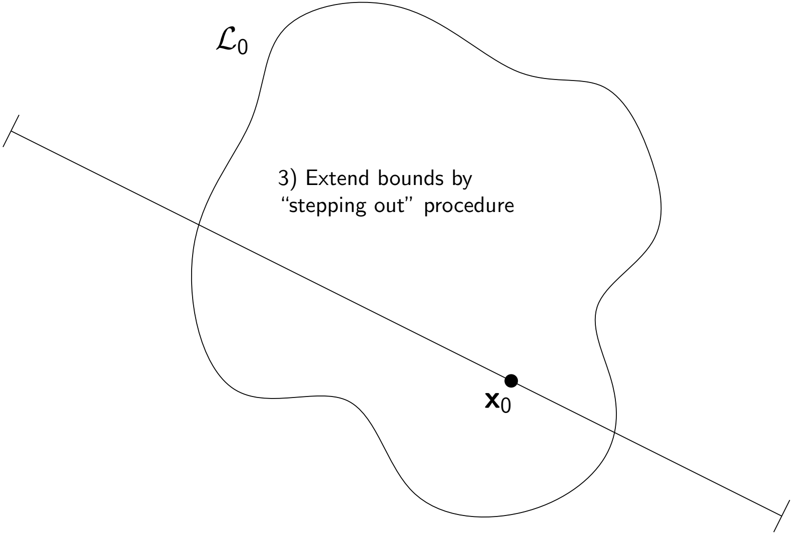

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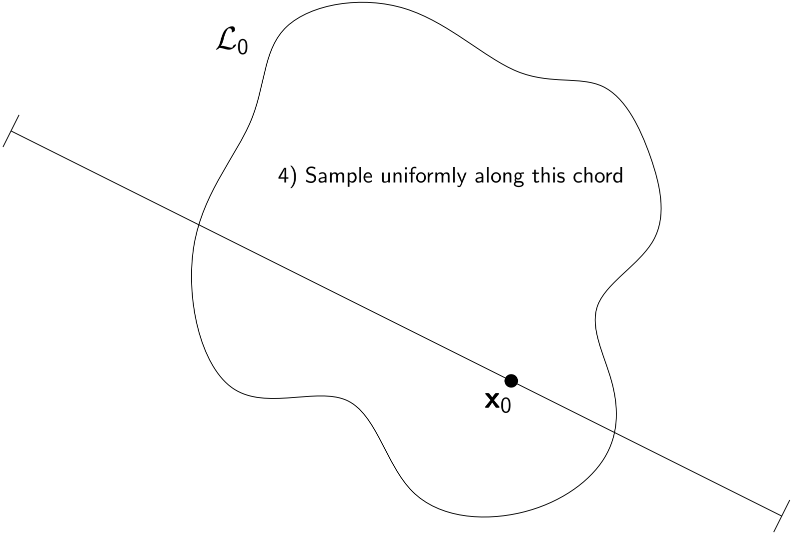

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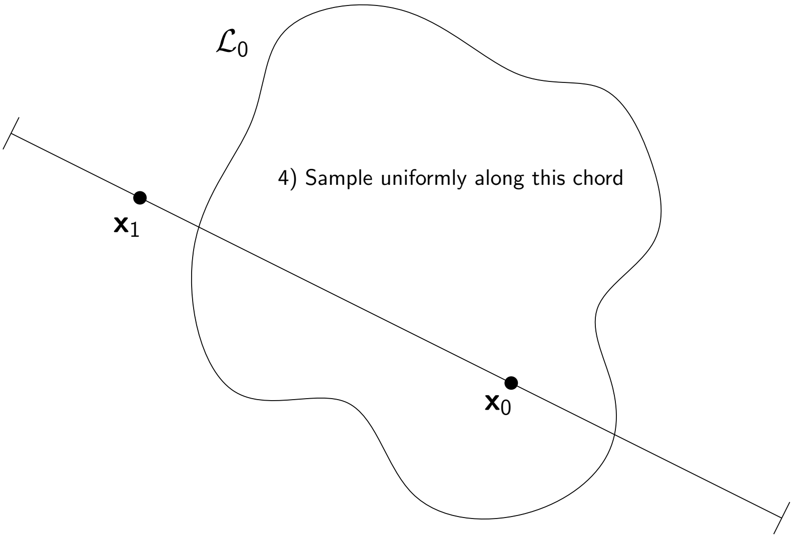

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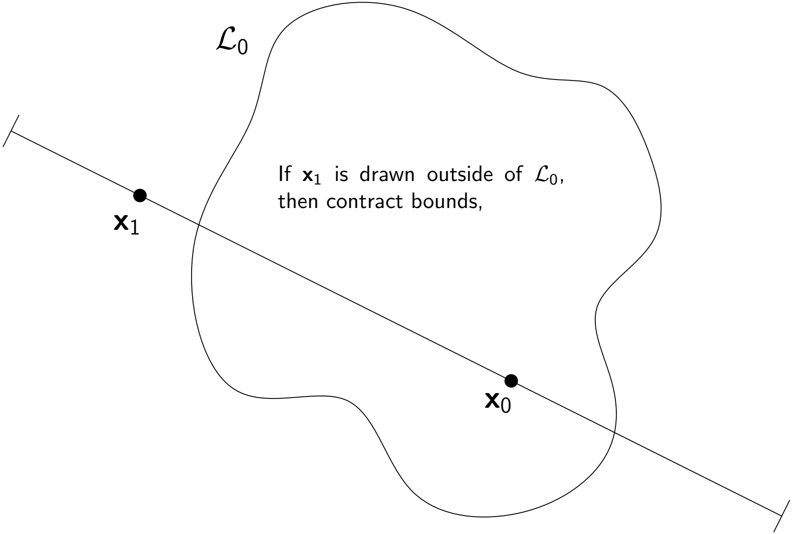

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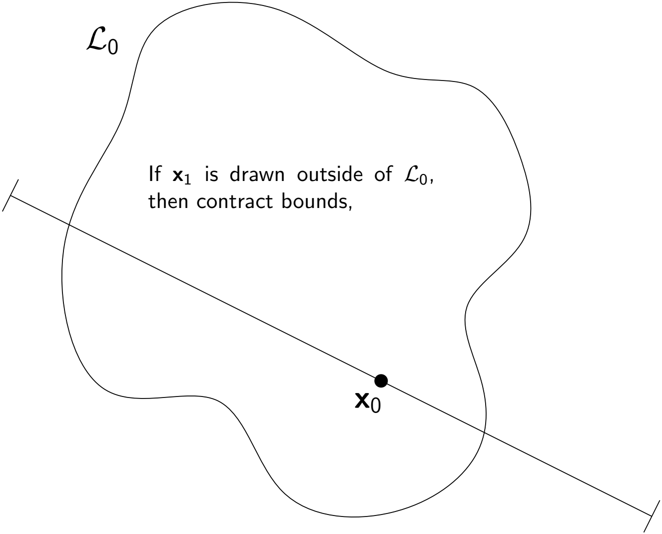

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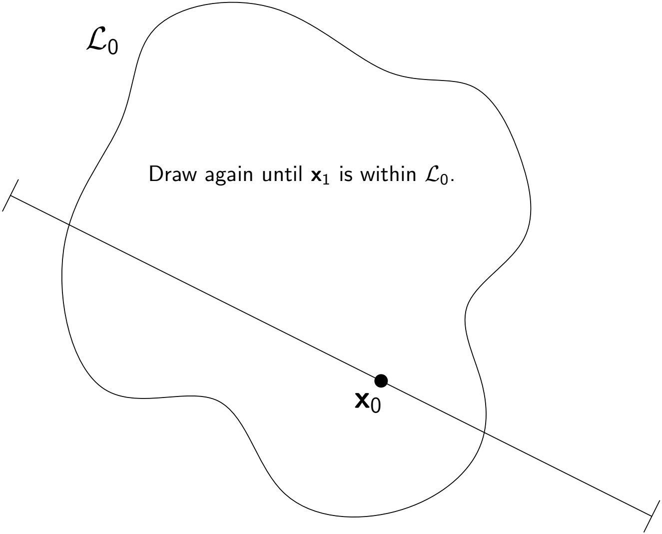

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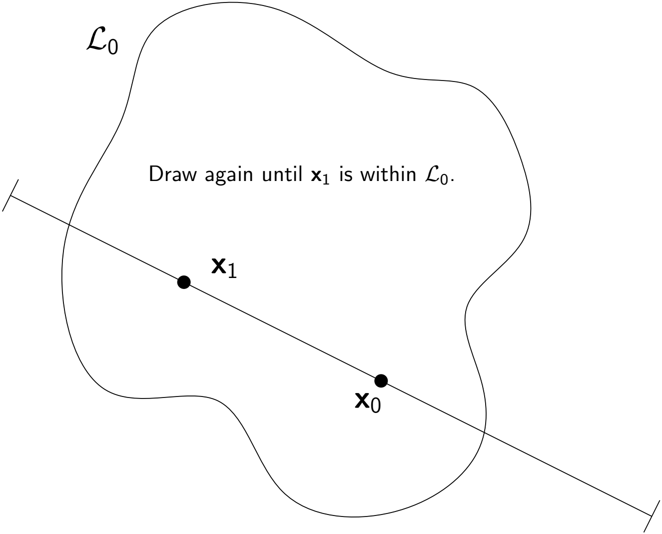

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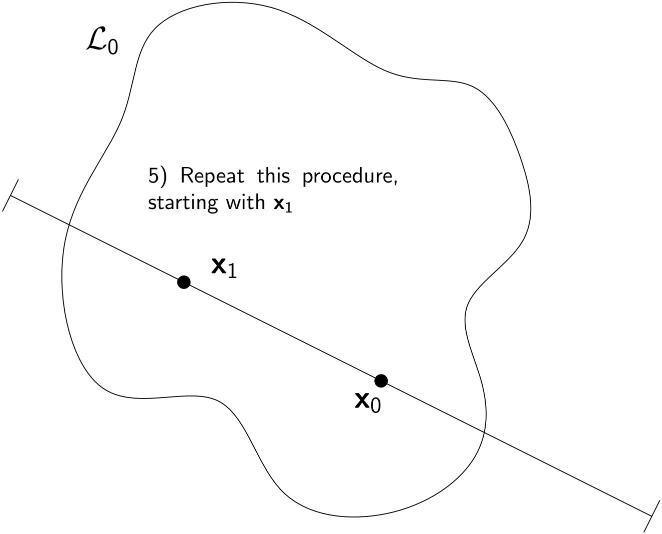

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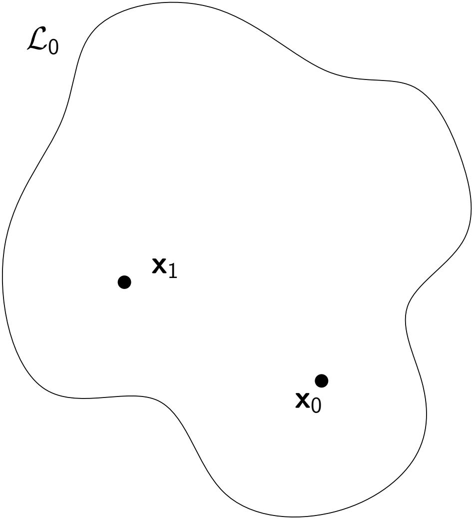

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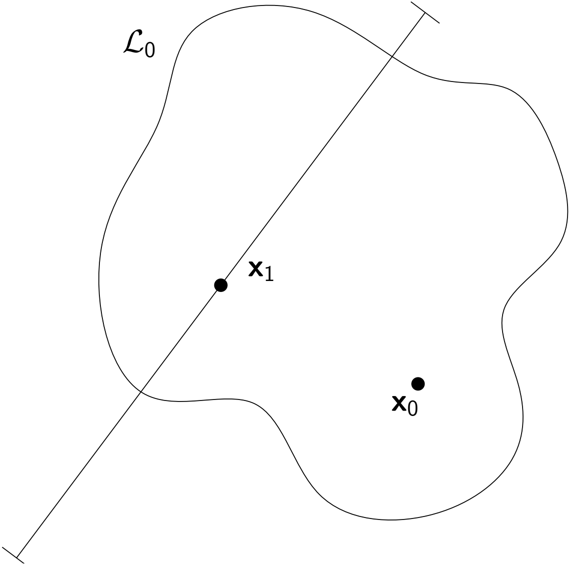

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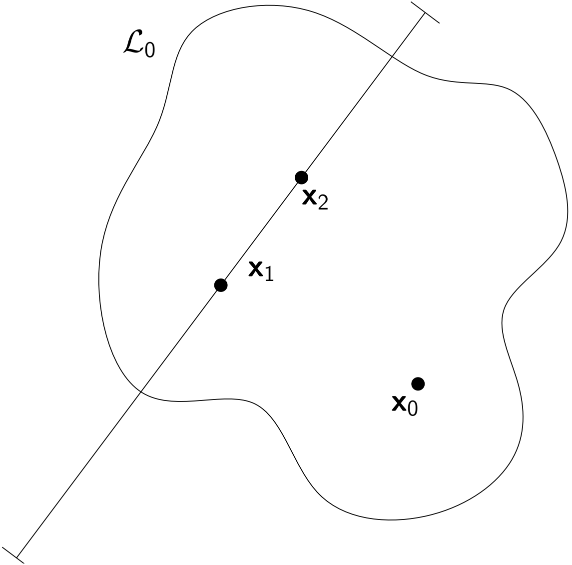

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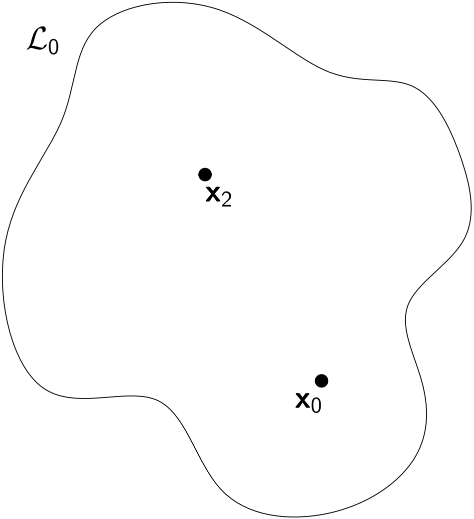

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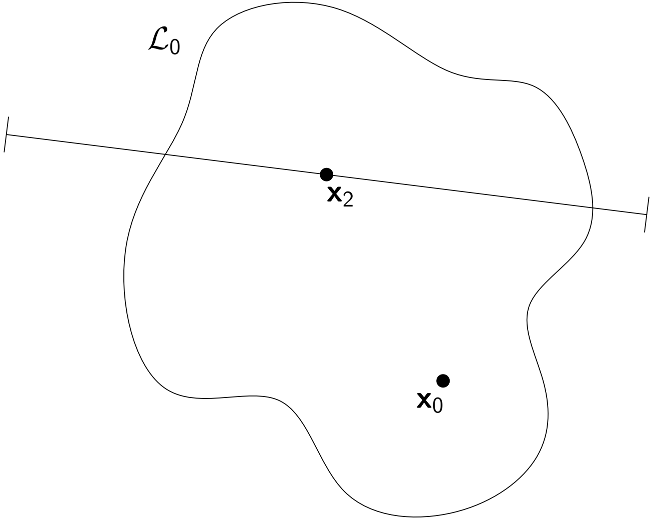

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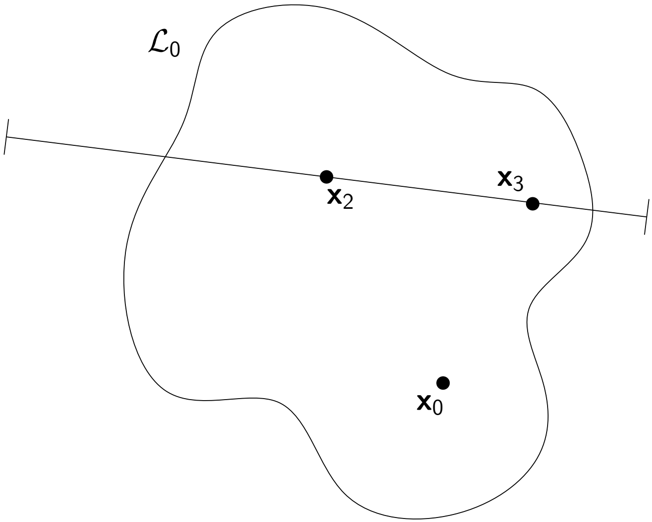

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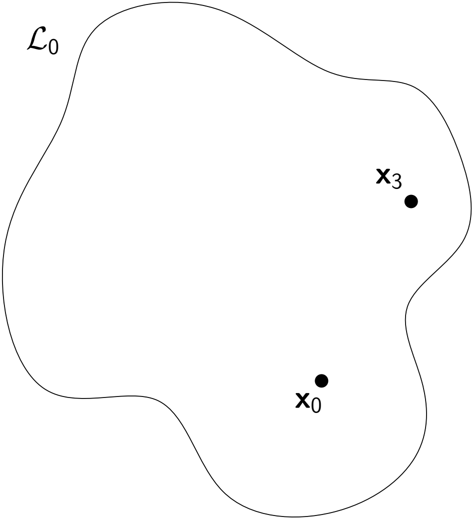

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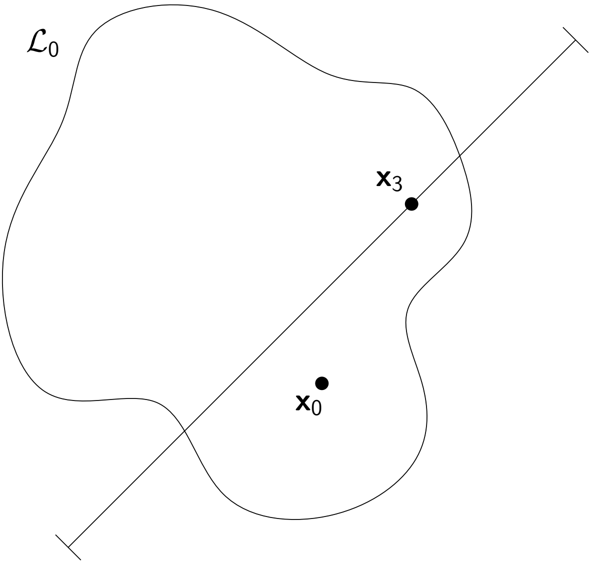

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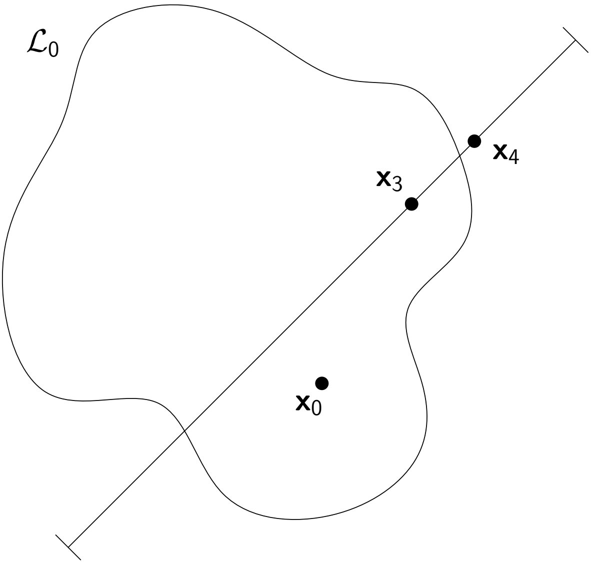

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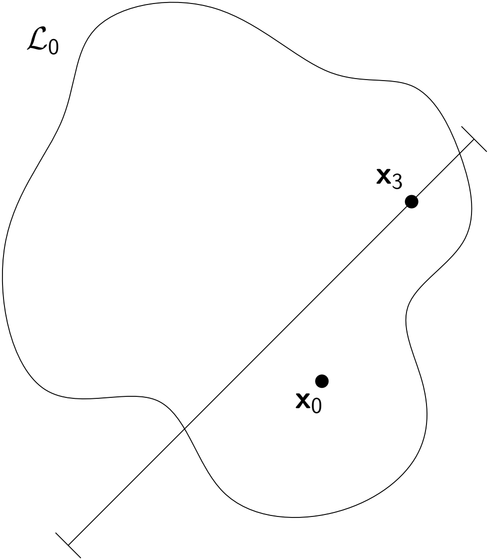

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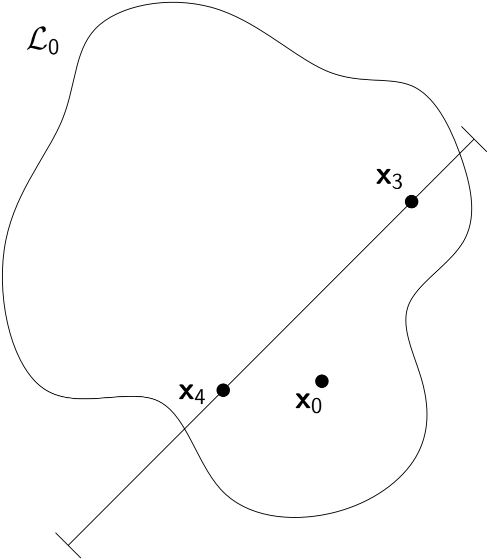

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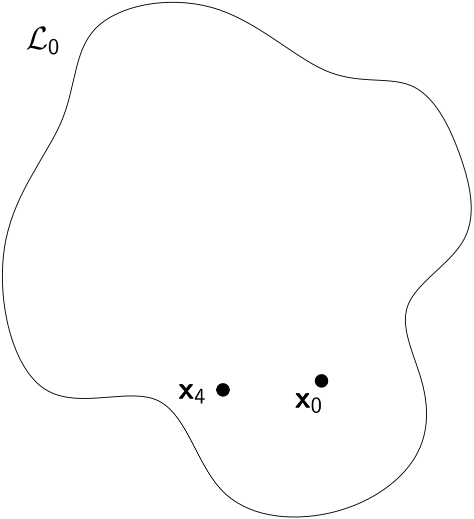

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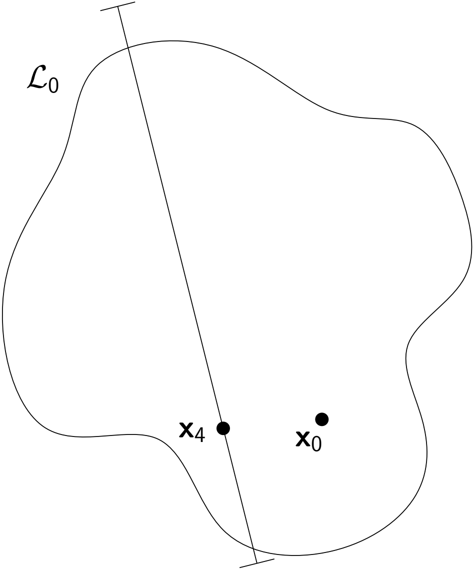

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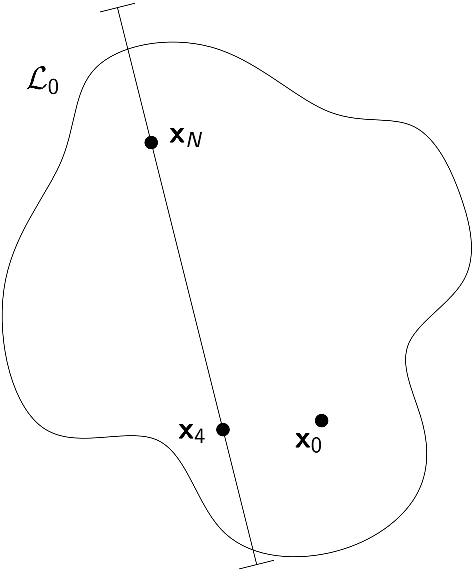

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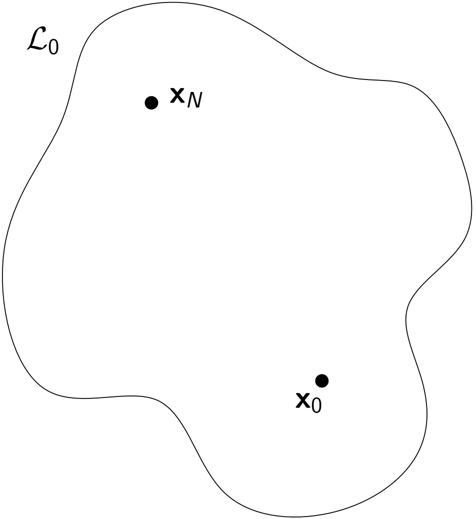

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- Need N reasonably large $\sim \mathcal{O}(n_{\mathrm{dims}})$ so that x_N is de-correlated from x_1.

Issues with Slice Sampling

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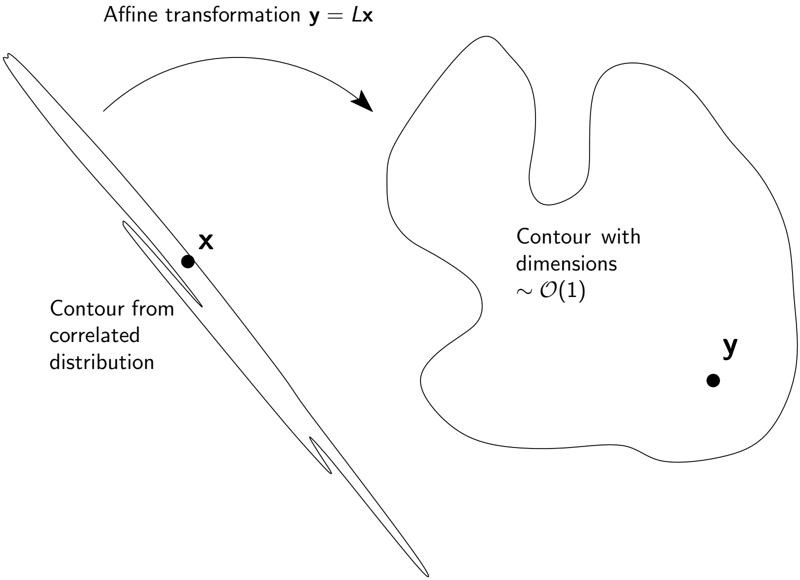
2. Need to “tune” w parameter.

PolyChord's solutions

Correlated distributions



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- $w = 1$ in this transformed space

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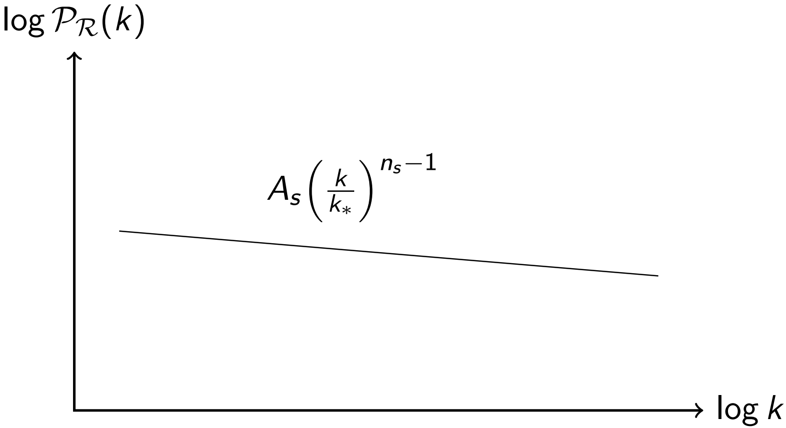
- Novel method for identifying and evolving modes separately.
- Implemented in CosmoMC, as "CosmoChord", with fast-slow parameters.

PolyChord in action

Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction



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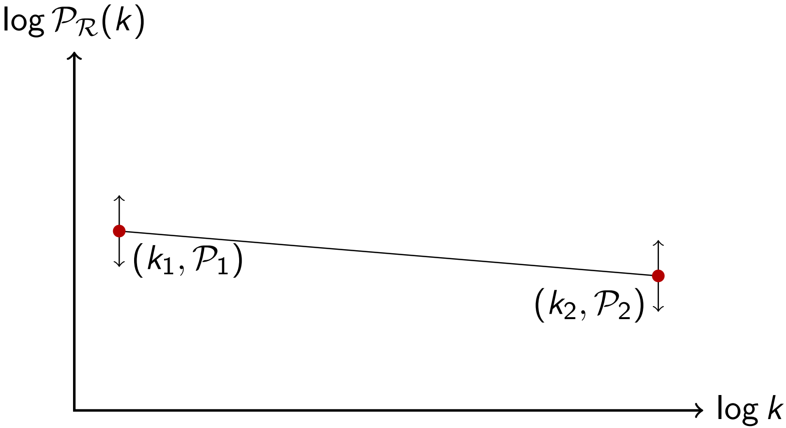

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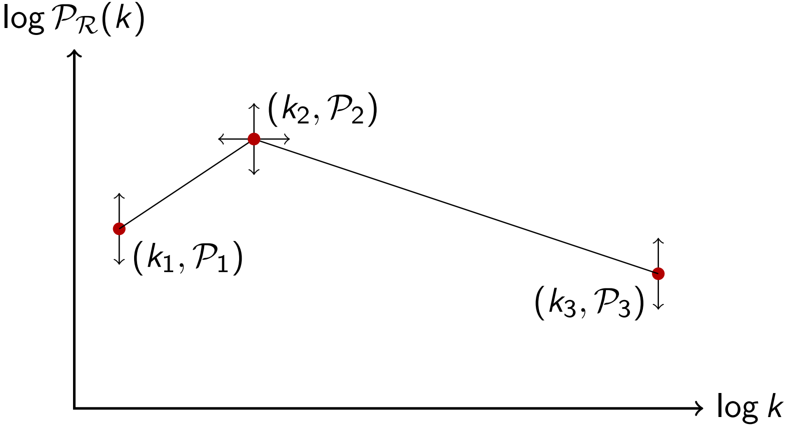

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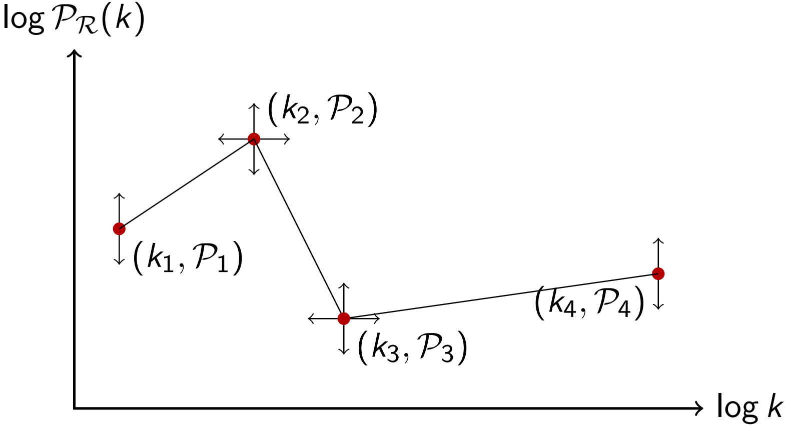

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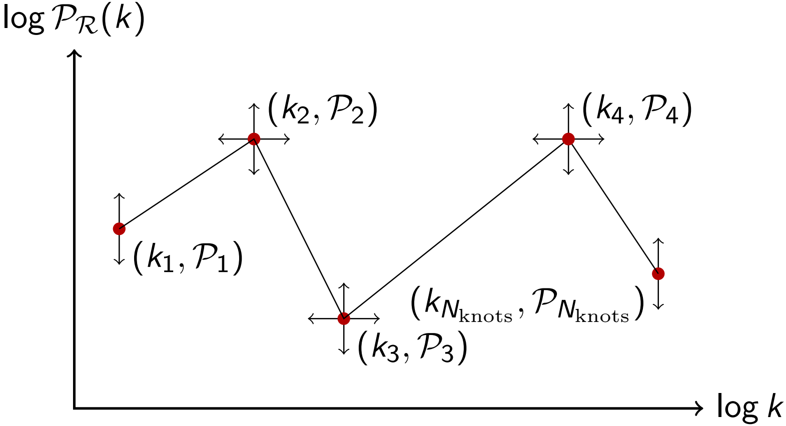

Planck data

Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction

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- Temperature data TT+lowP

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- Marginalised plots of $\mathcal{P}_\mathcal{R}(k)$
- $$\mathrm{P}(\mathcal{P}_\mathcal{R}|k, N_\mathrm{knots}) = \int \delta(\mathcal{P}_\mathcal{R} - f(k;\theta))\mathcal{P}(\theta)d\theta$$

0 internal knots

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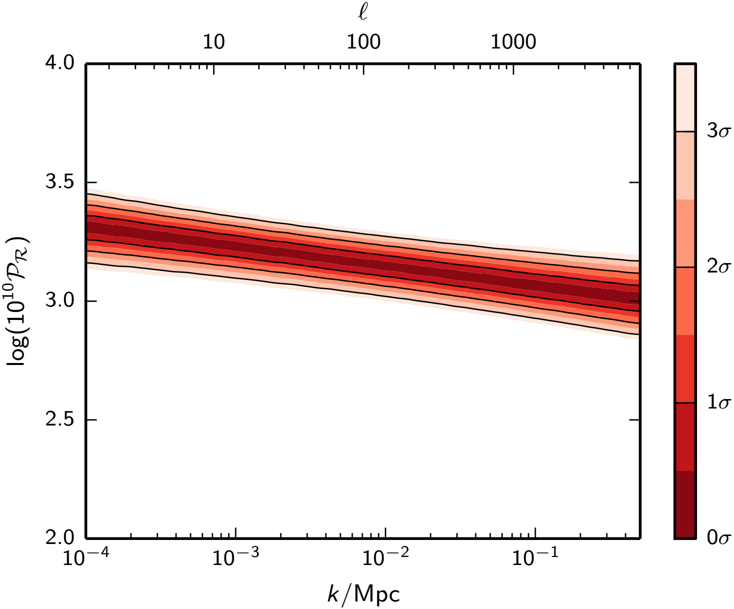

1 internal knots

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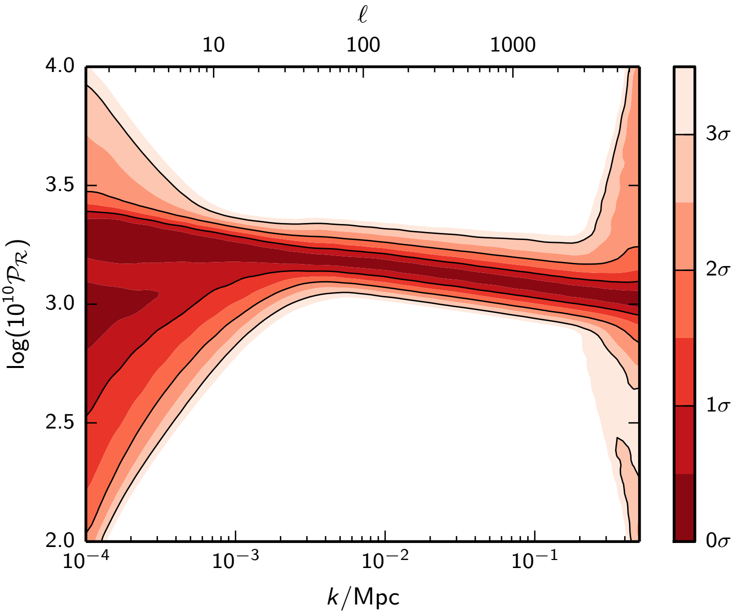

2 internal knots

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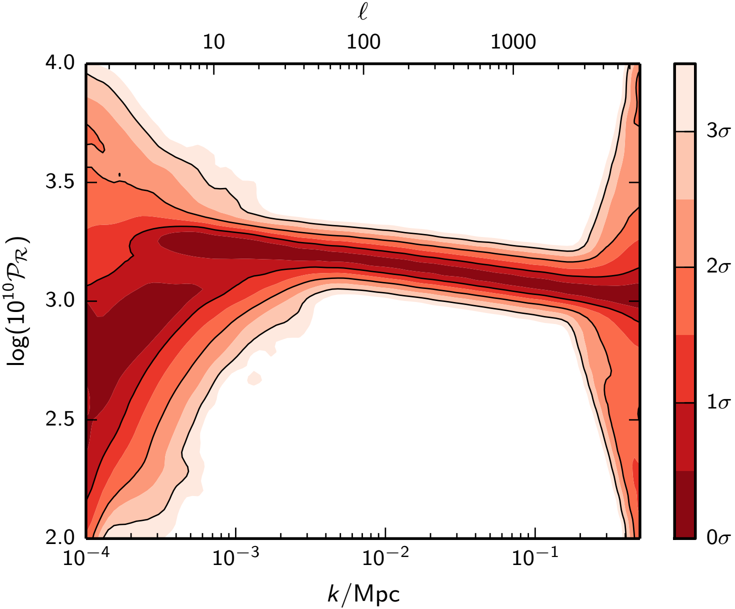

3 internal knots

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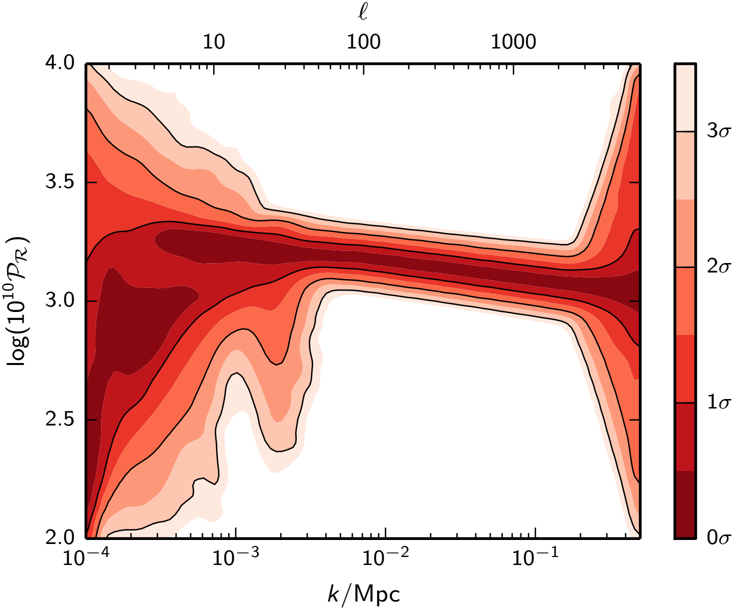

4 internal knots

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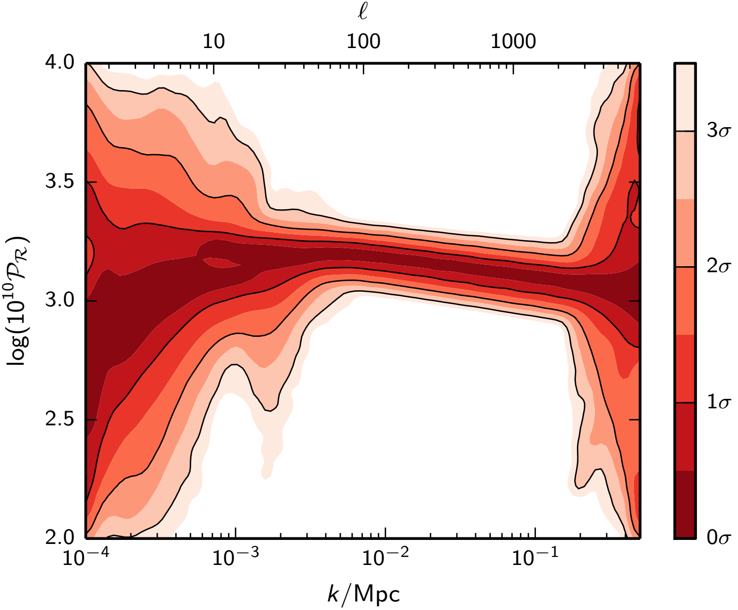
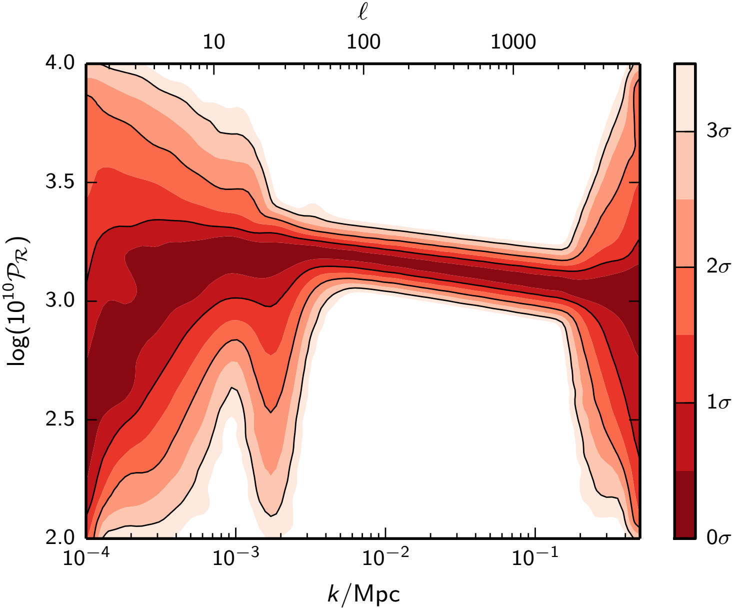


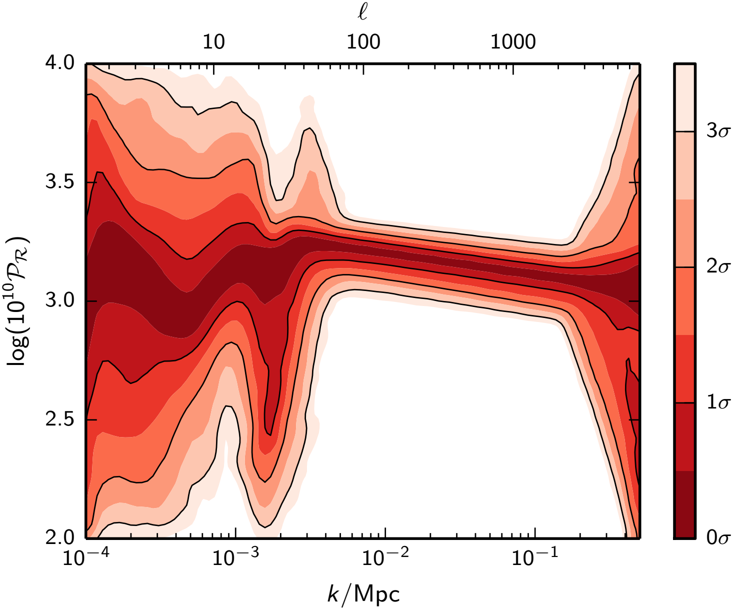
5 internal knots

Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction



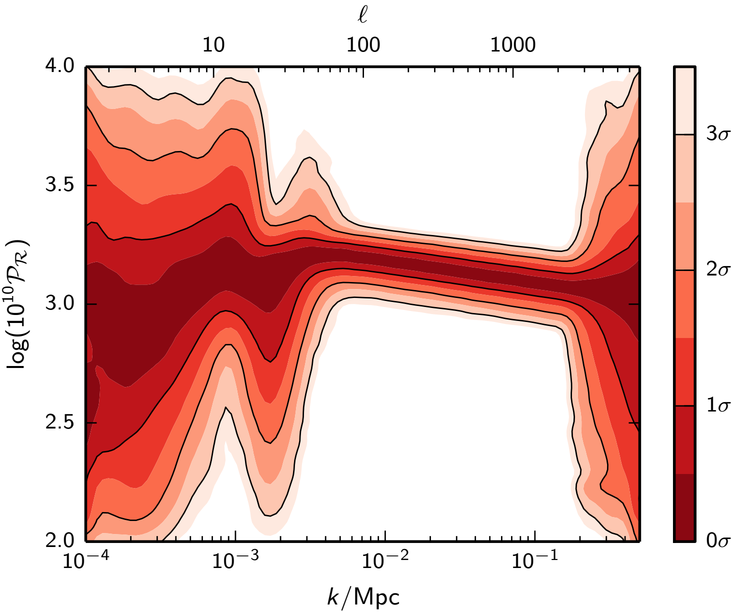
6 internal knots

Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction



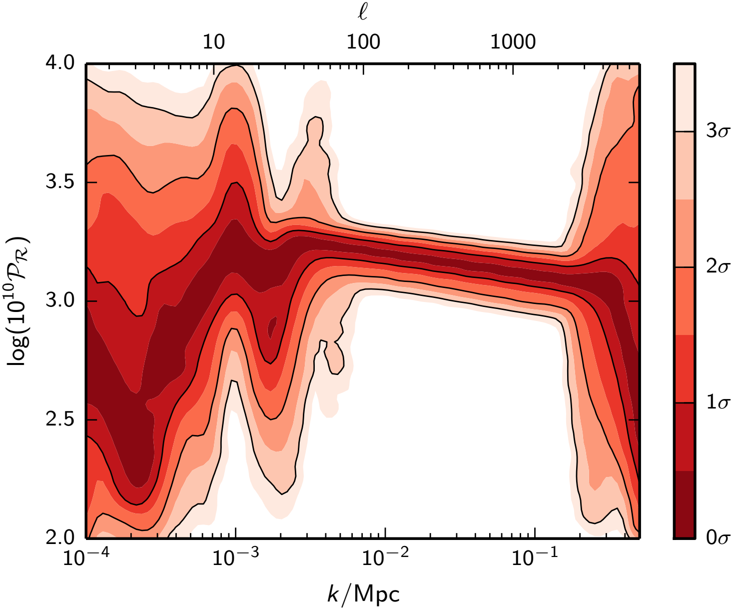
7 internal knots

Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction



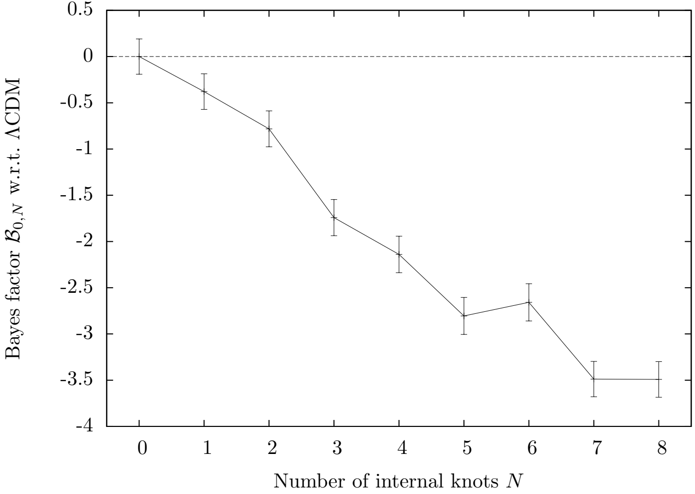
8 internal knots

Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction



Bayes Factors

Primordial power spectrum $\mathcal{P}_\mathcal{R}(k)$ reconstruction



Marginalised plot

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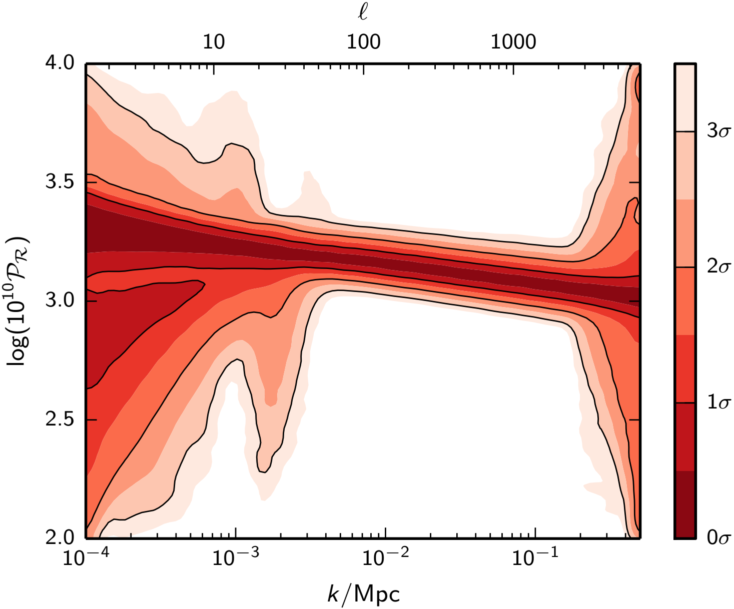
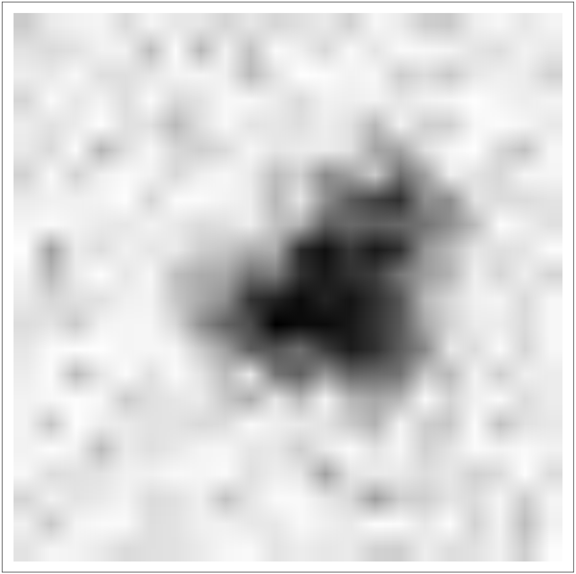


Object detection

Toy problem



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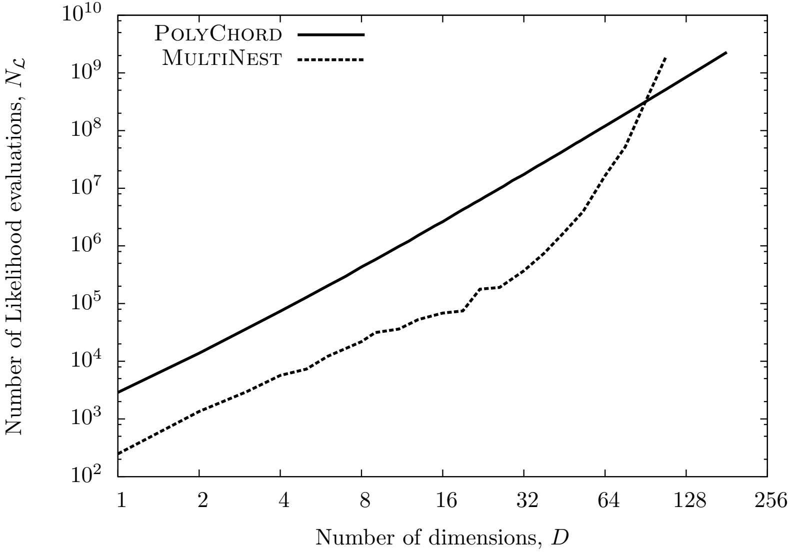
- odds ratio: $10^{-60} : 10^{-19} : 1 : 0.04 : 10^{-10}$

PolyChord vs. MultiNest

Gaussian likelihood



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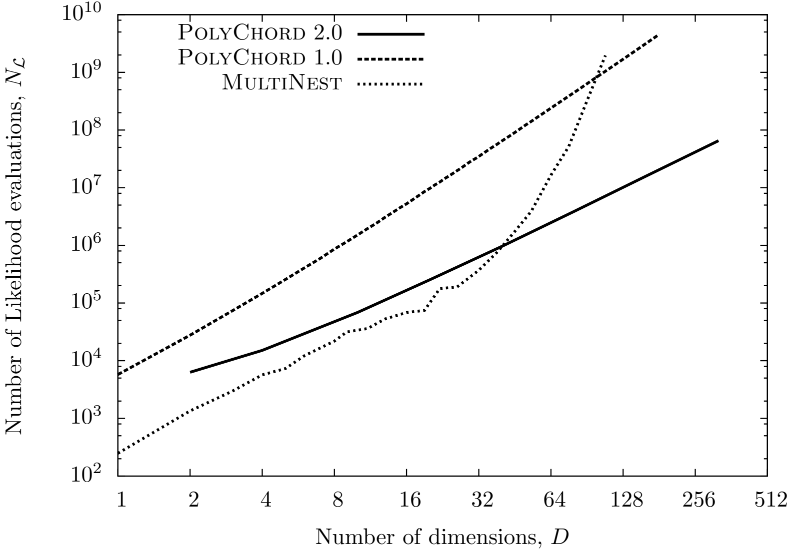

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- http://ccpforge.cse.rl.ac.uk/gf/project/polychord/