

PolyChord: Next Generation Nested Sampling

Sampling, Parameter Estimation and Bayesian Model Comparison

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Cavendish Laboratory
University of Cambridge

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Parameter estimation & model comparison

Metropolis Hastings

Nested Sampling

PolyChord

Applications

Notation

Notation

- ▶ Data: D

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- ▶ Model: M

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

Bayes' theorem

Parameter estimation

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

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Parameter estimation & model comparison

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Parameter estimation: what does the data tell us about a model?
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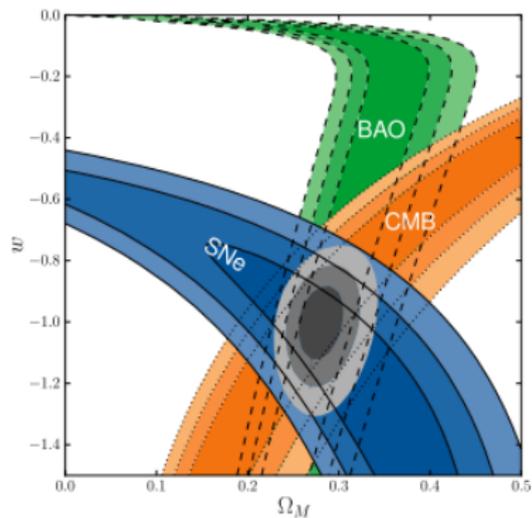
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- ▶ Markov-Chain Monte-Carlo (MCMC) can solve the first of these (kind of)
- ▶ Nested sampling (NS) promises to solve both simultaneously.

Parameter estimation & model comparison

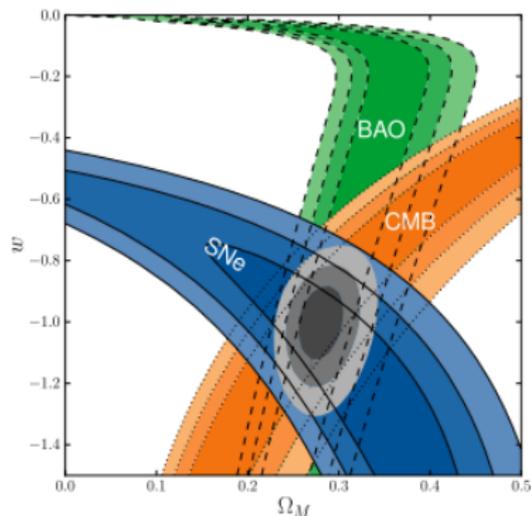
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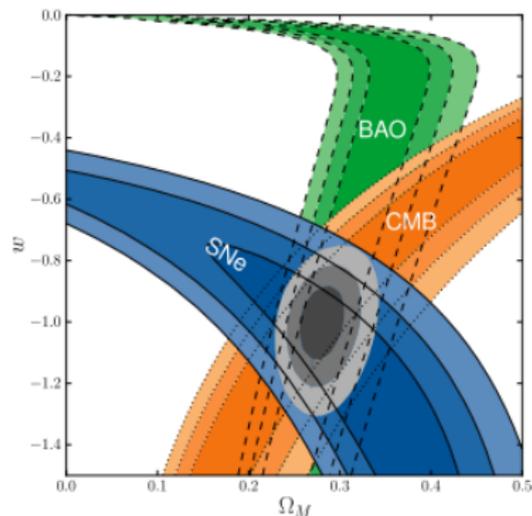
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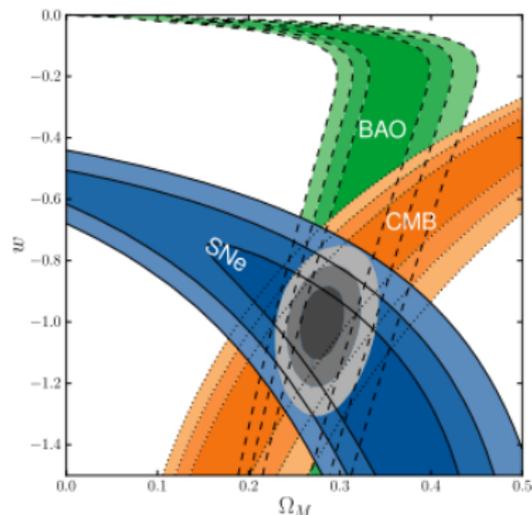
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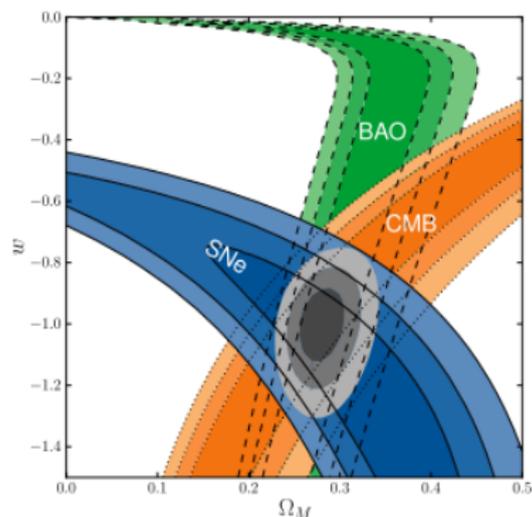


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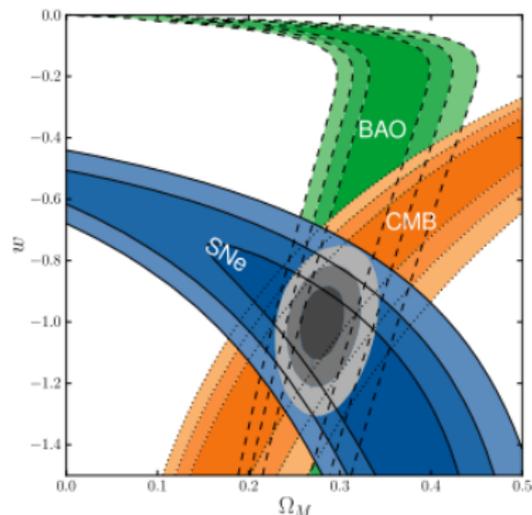


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- ▶ Describing an N -dimensional posterior fully is impossible.
- ▶ Project/marginalise into 2- or 3-dimensions at best
- ▶ *Sampling* the posterior is an excellent compression scheme.

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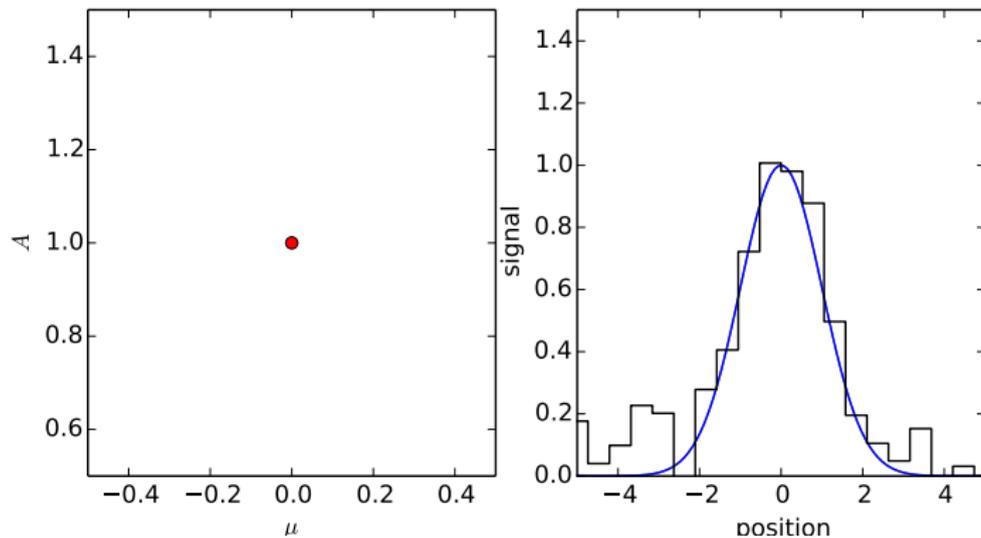
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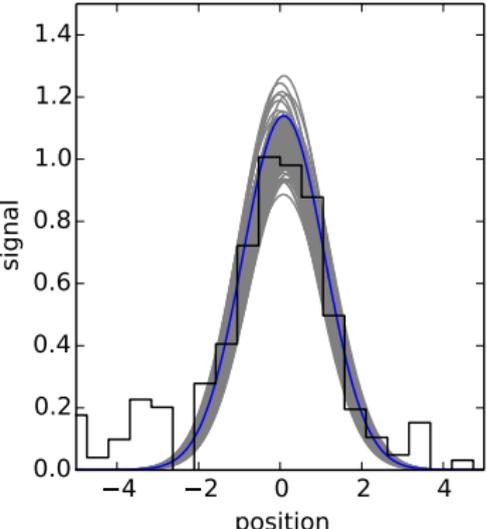
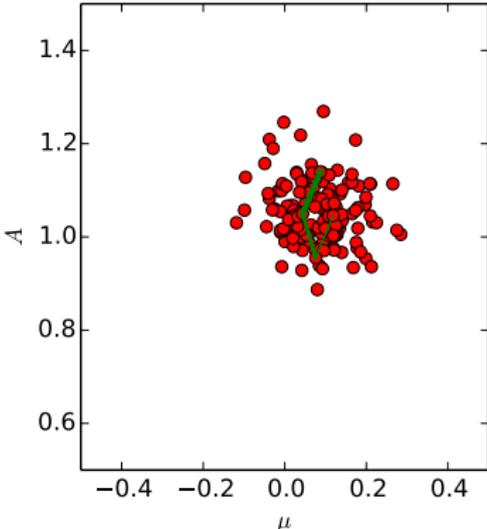
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MCMC in action

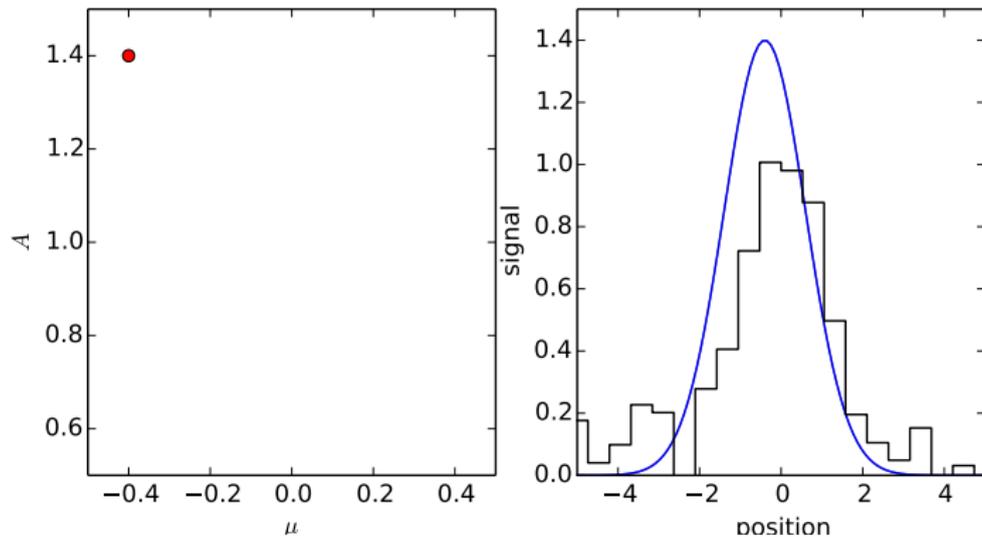


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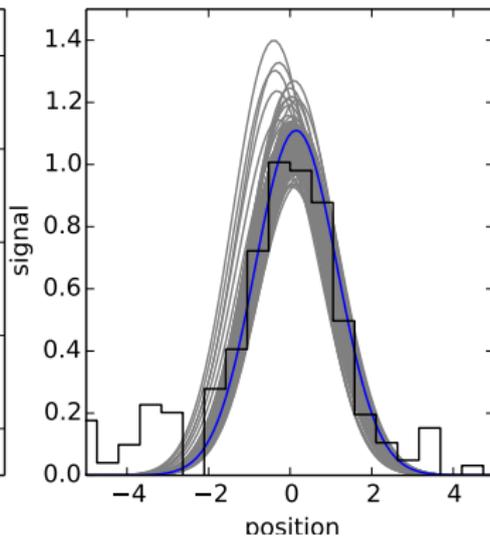
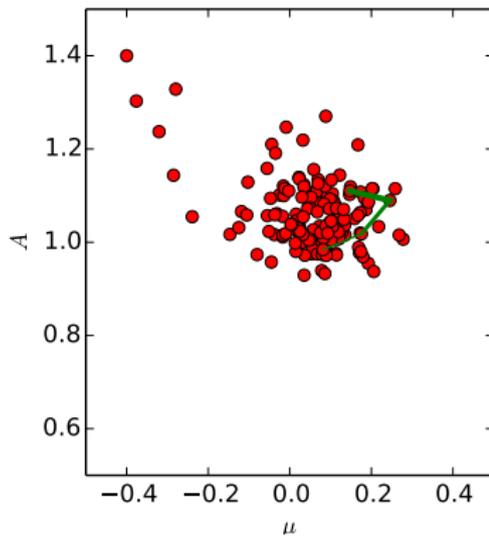
When MCMC fails

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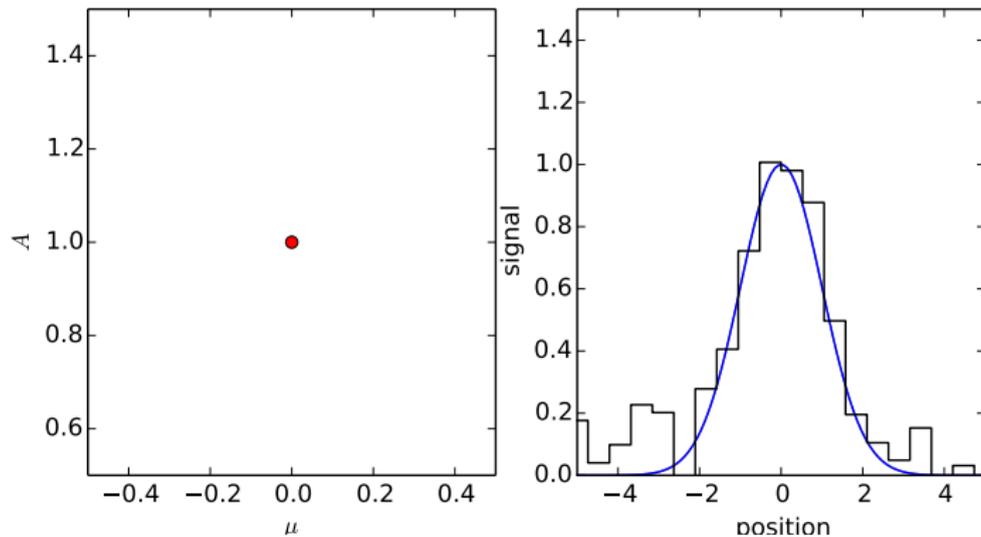
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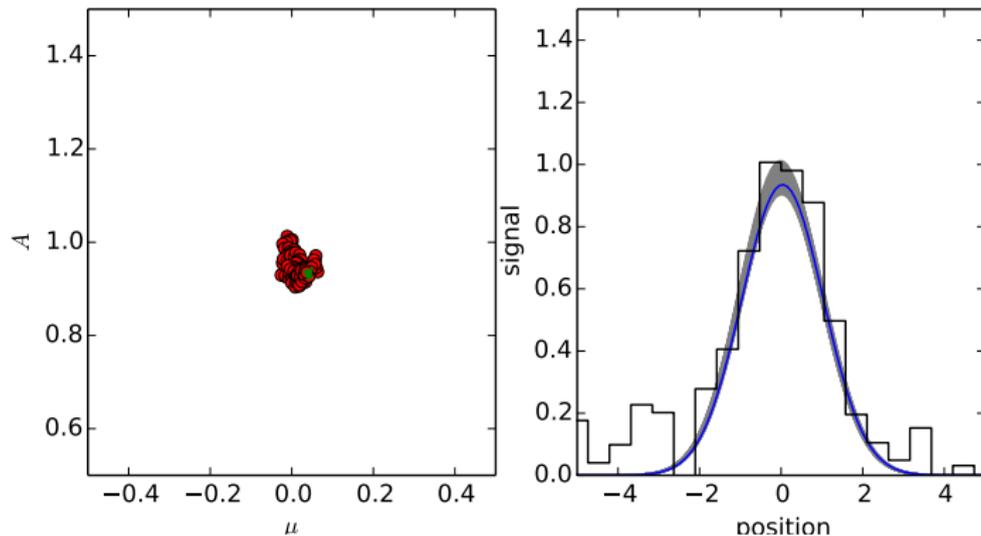
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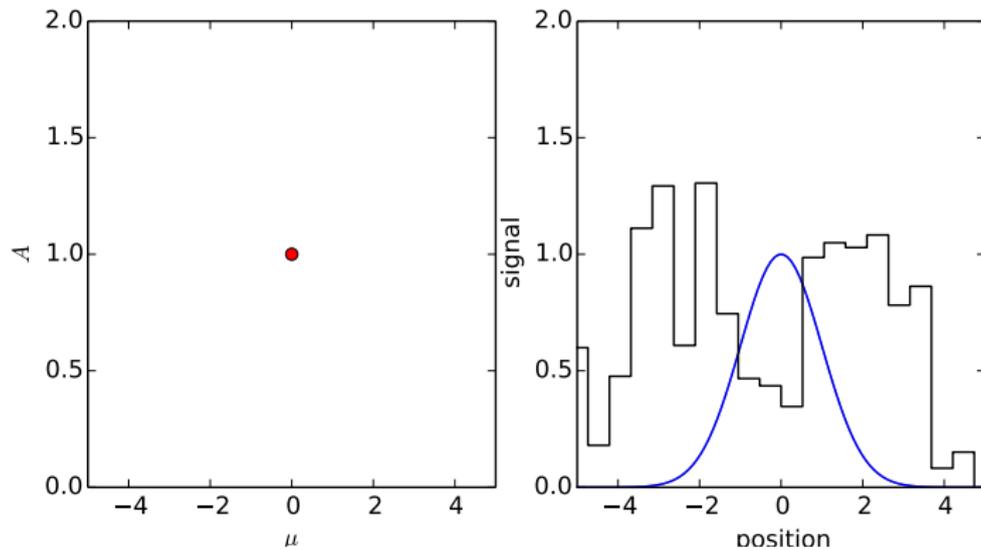
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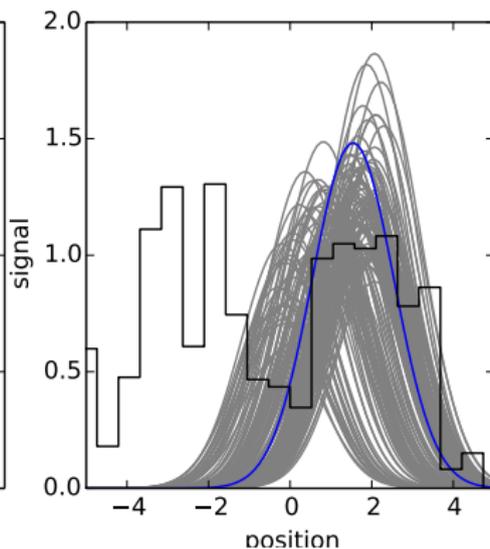
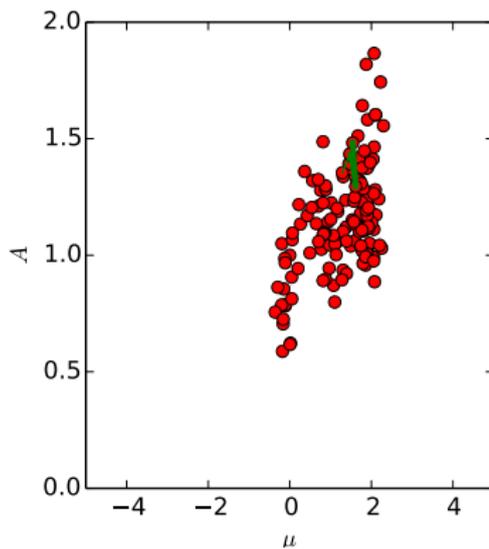
When MCMC fails

Multimodality



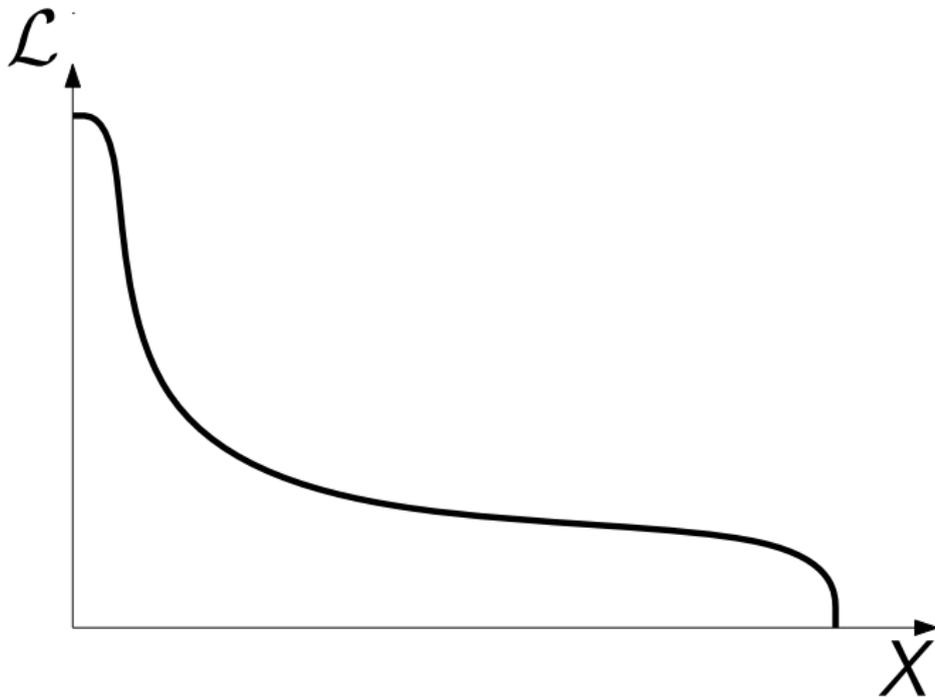
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Phase transitions



When MCMC fails

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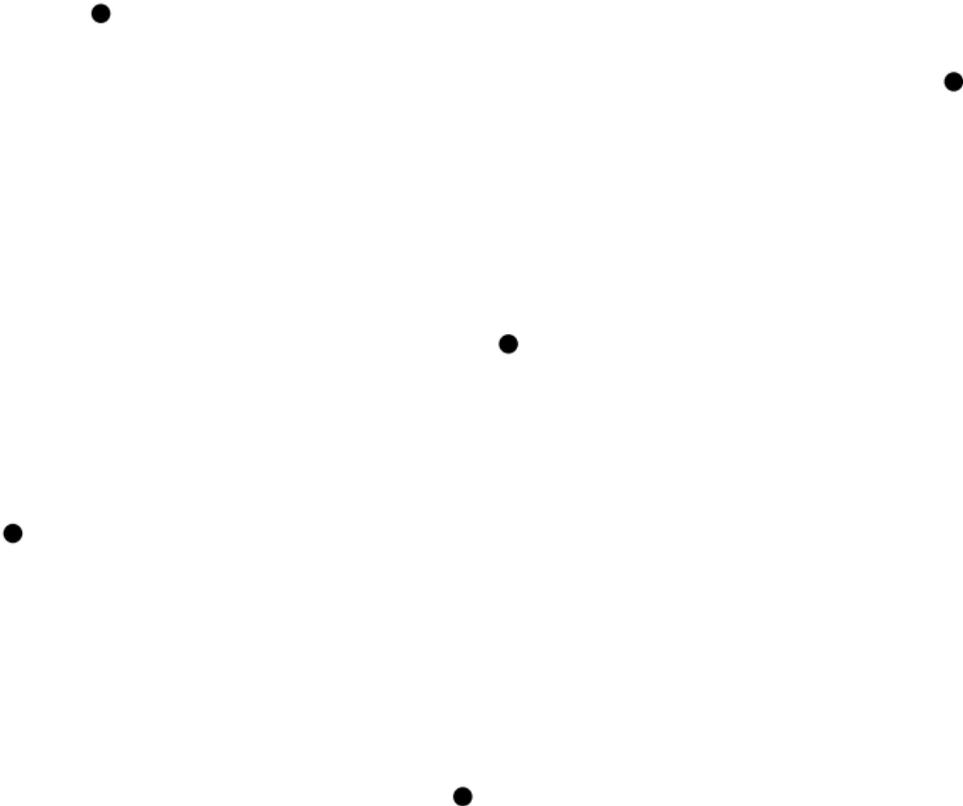
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Requires one to be able to sample from the prior, subject to a *hard likelihood constraint*.

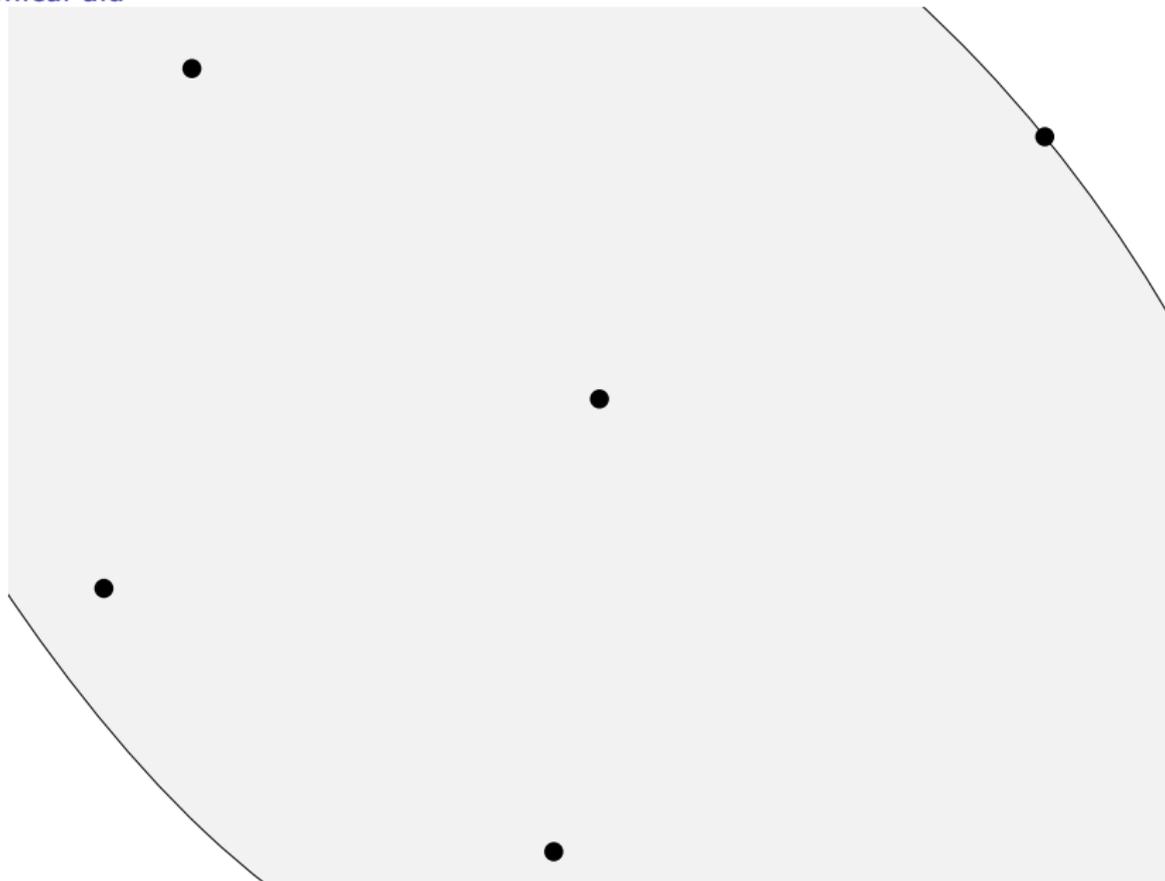
Nested Sampling

Graphical aid



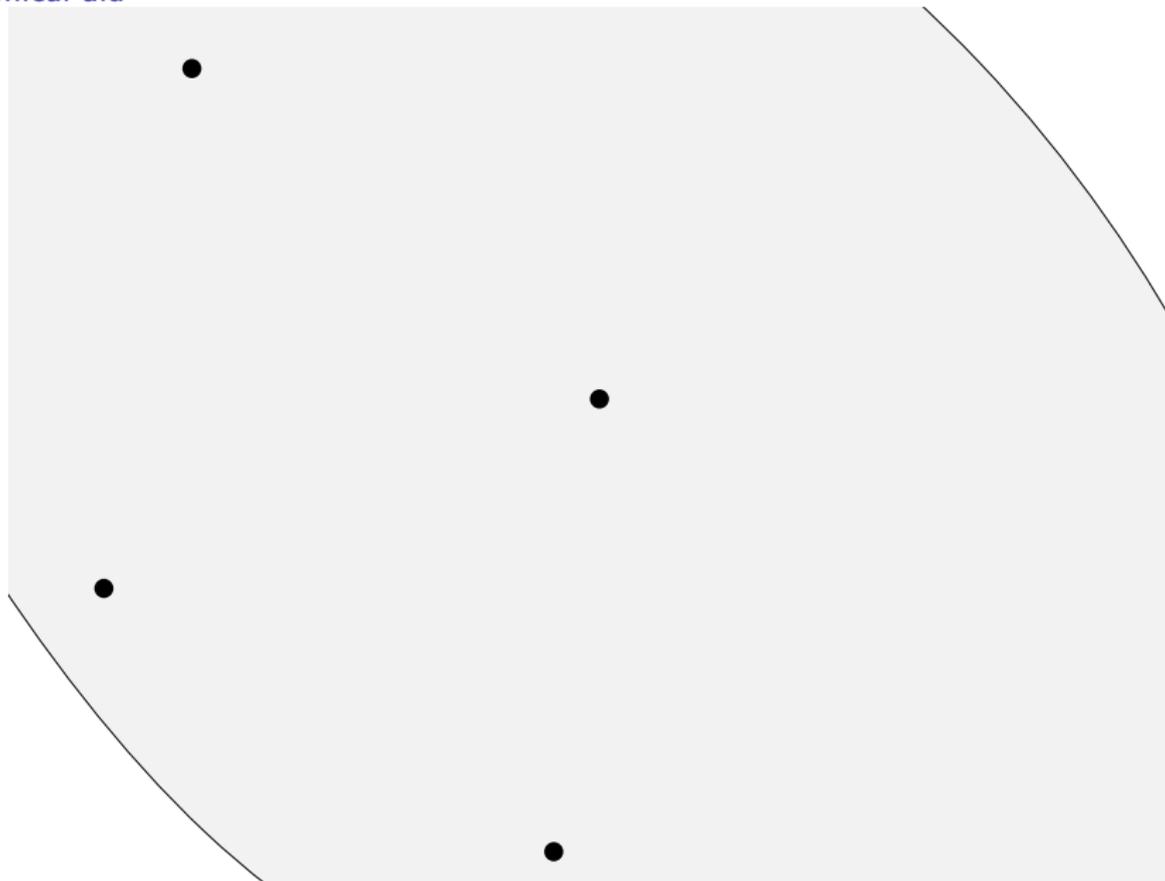
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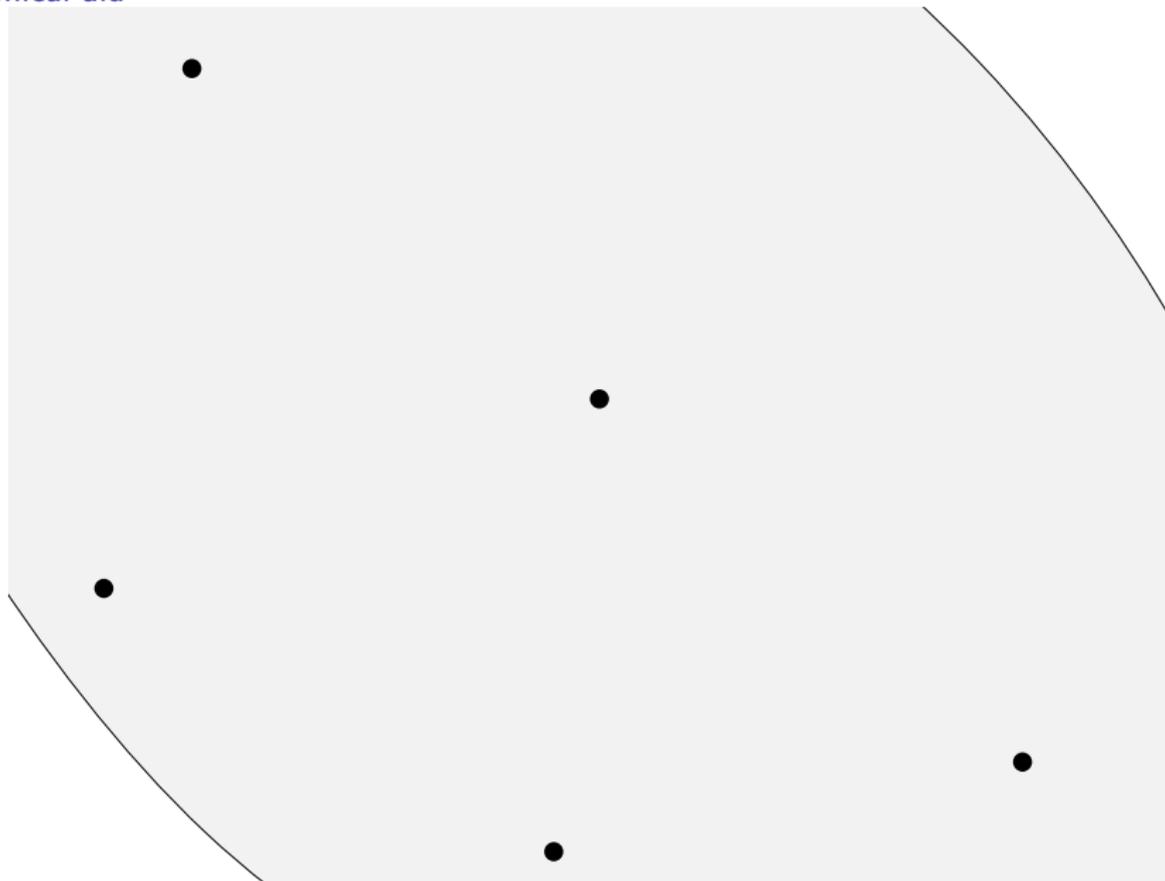
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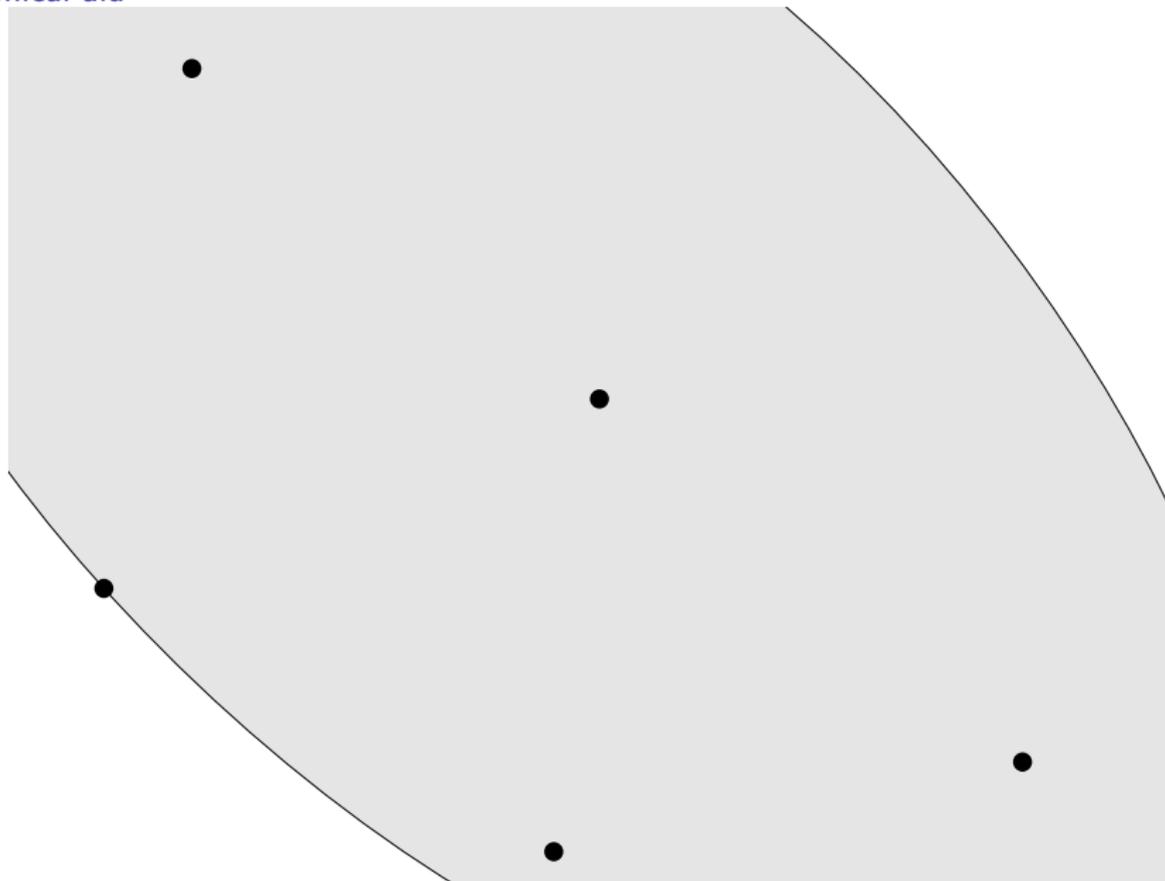
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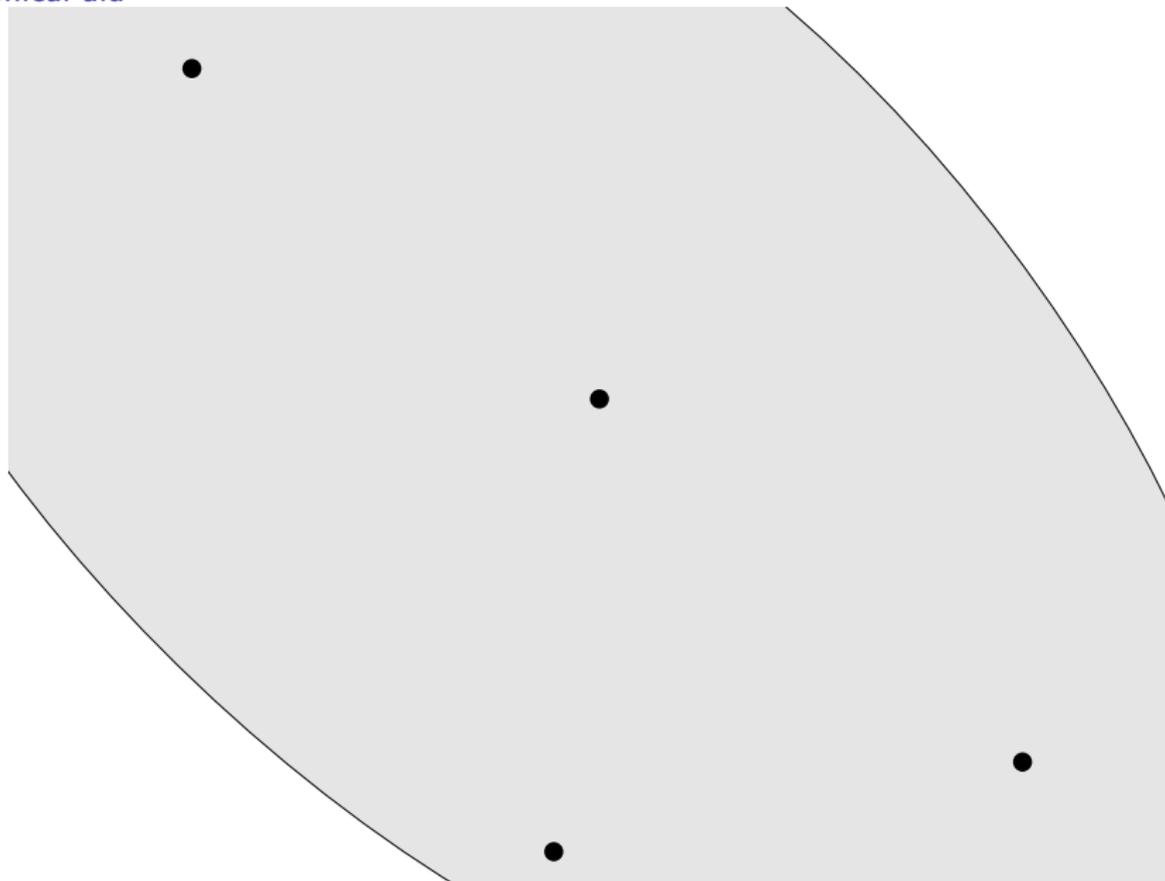
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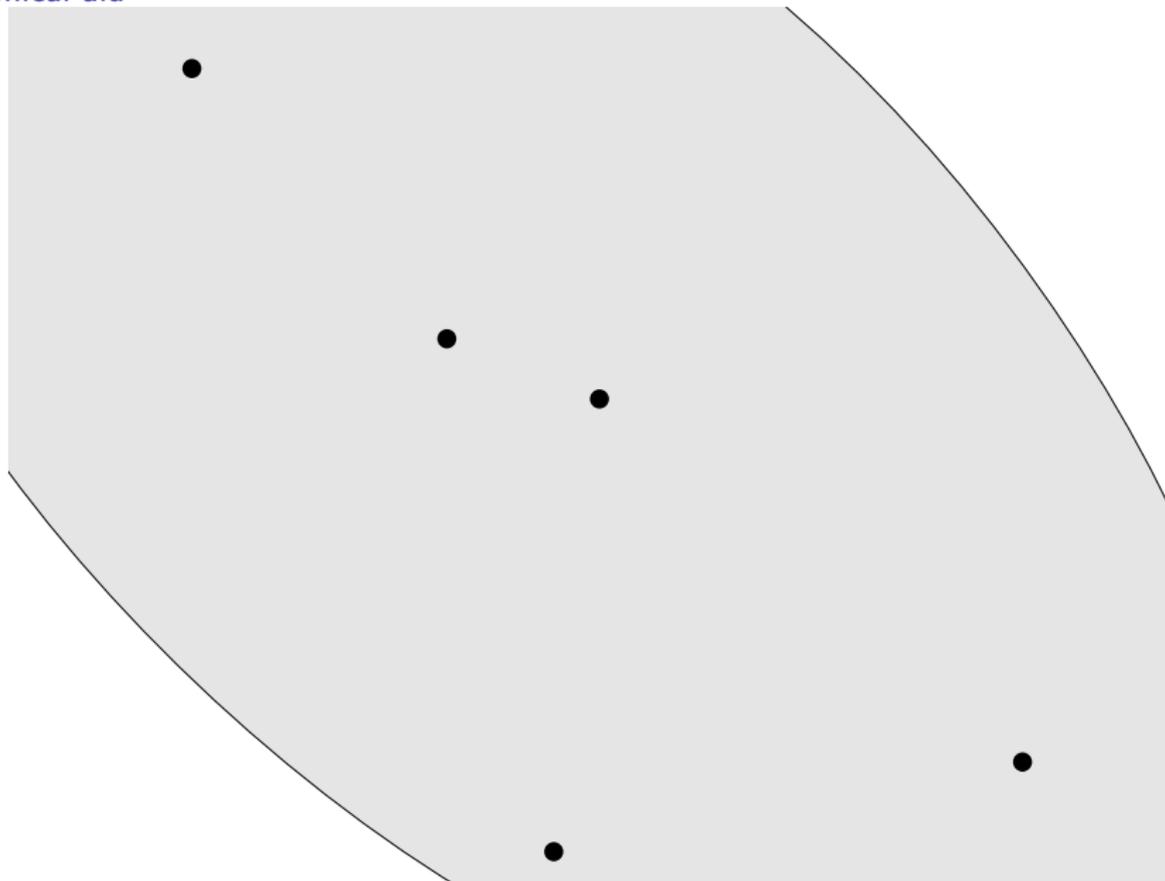
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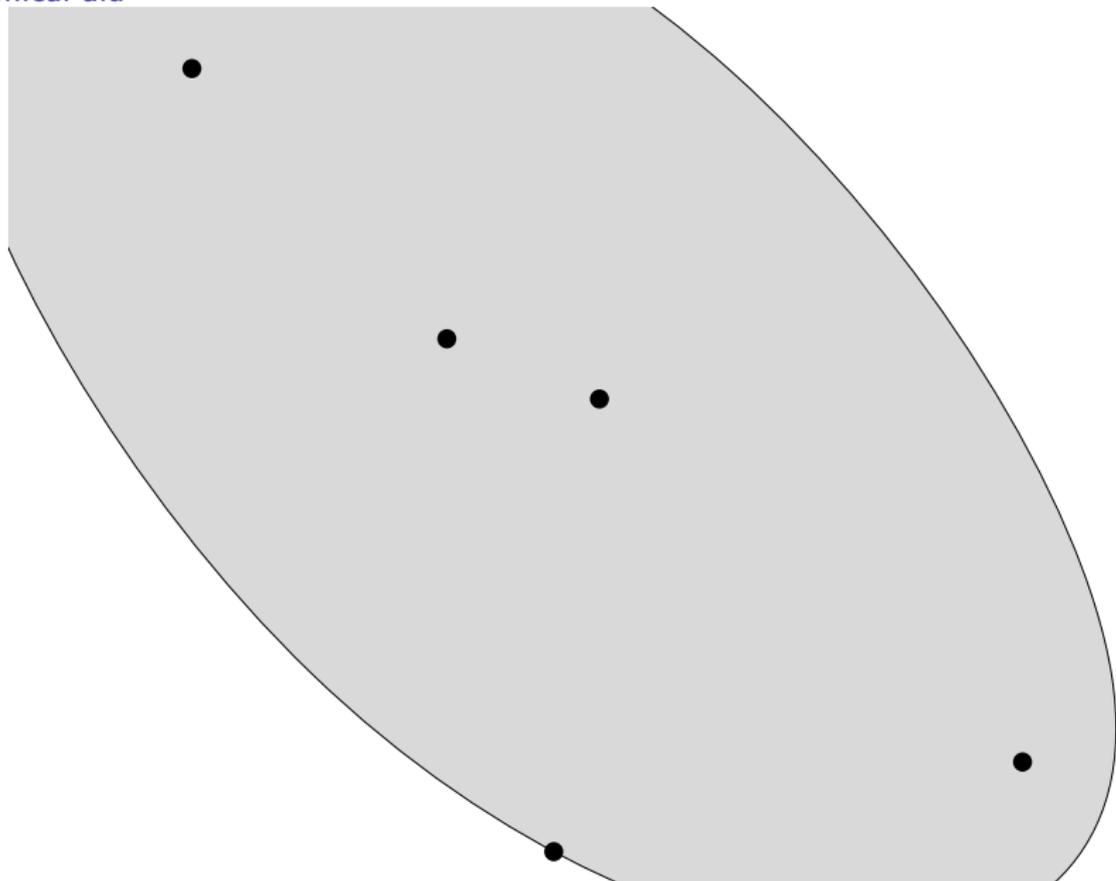
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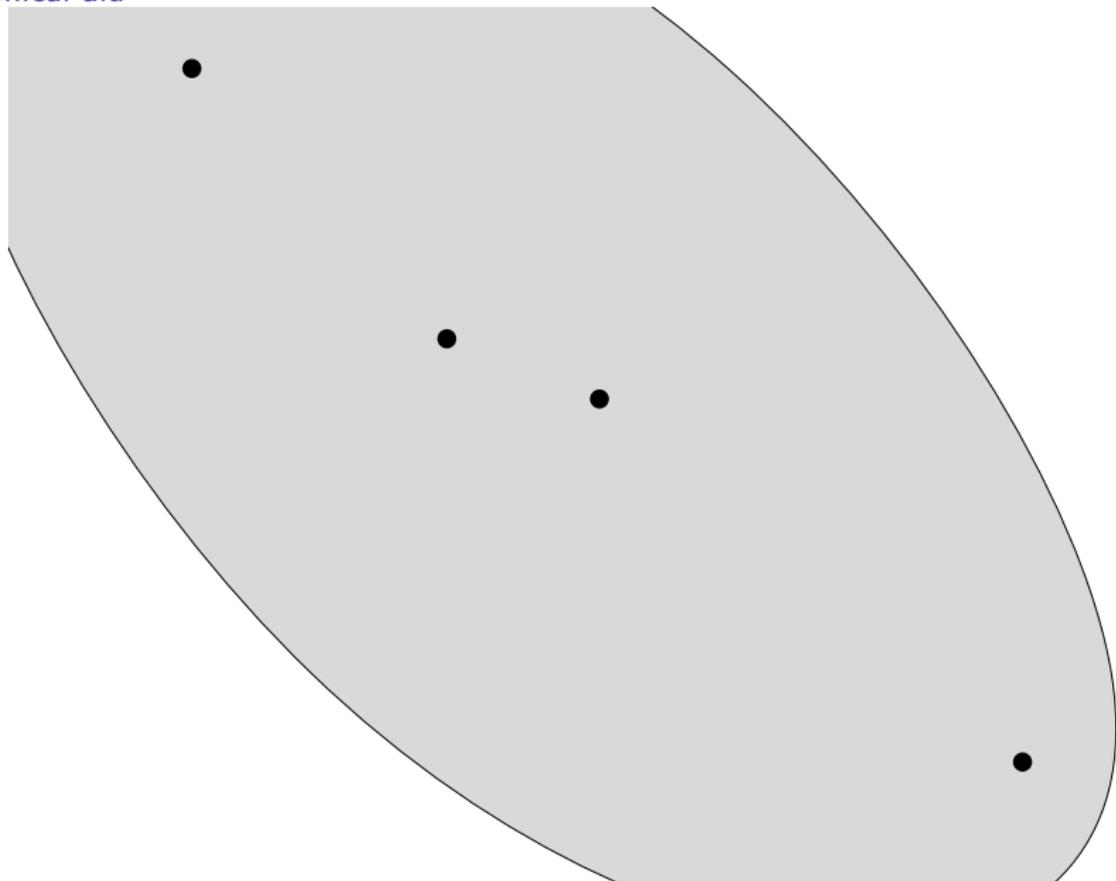
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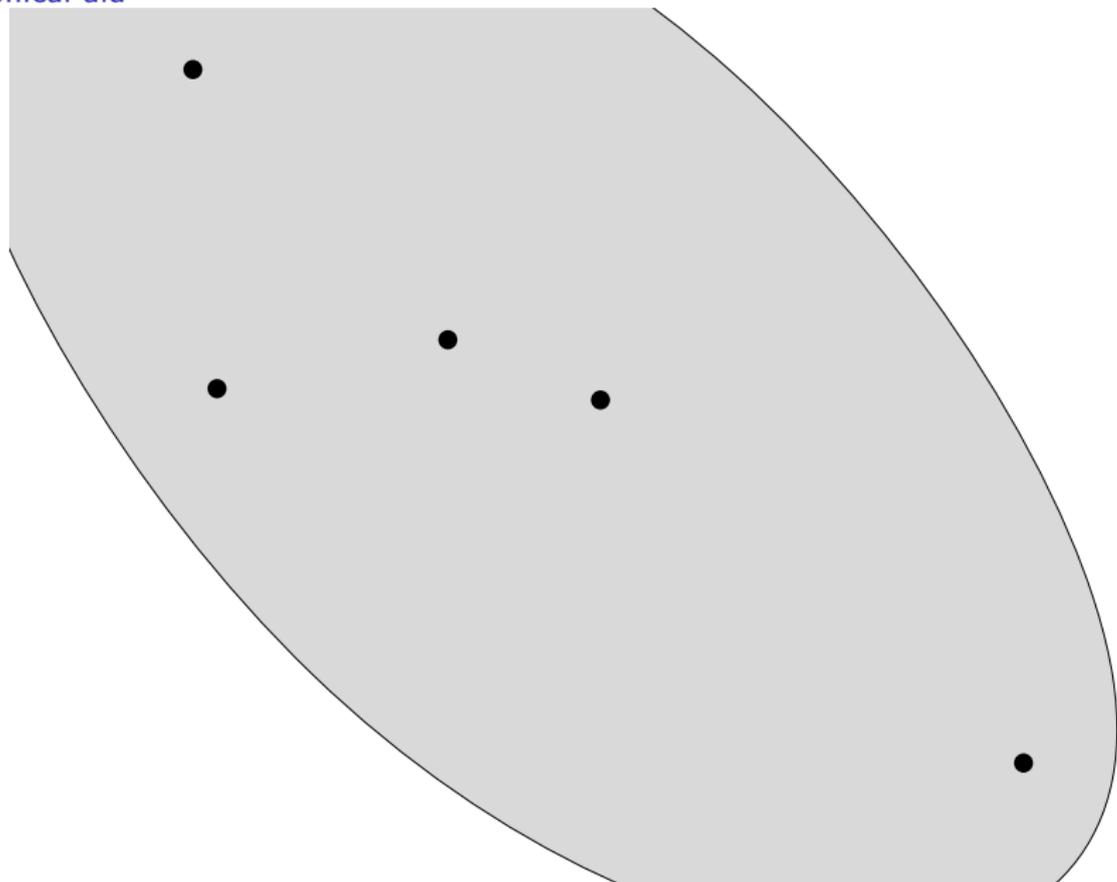
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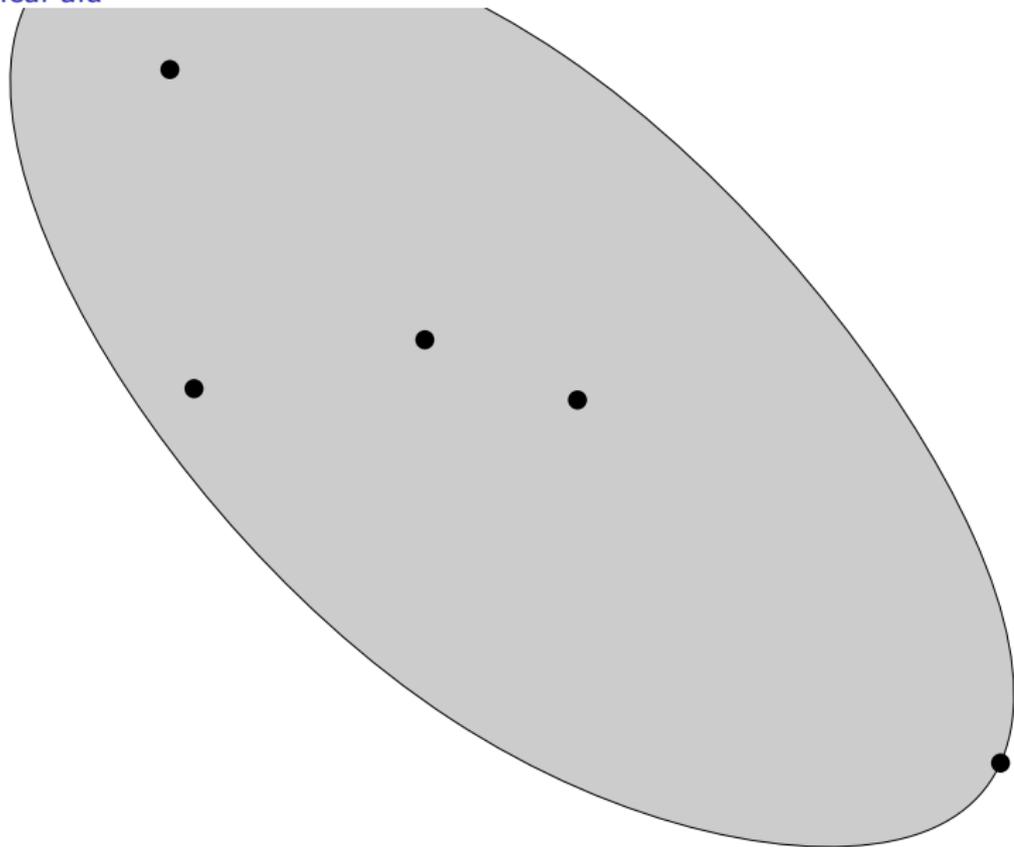
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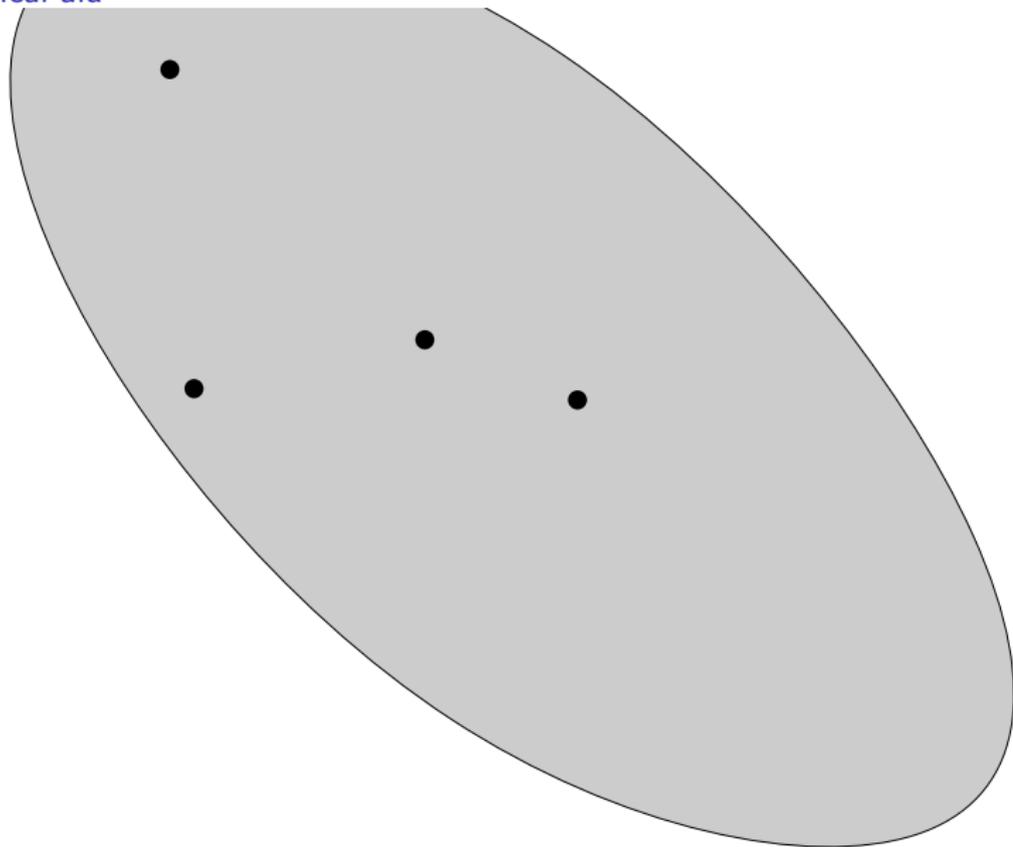
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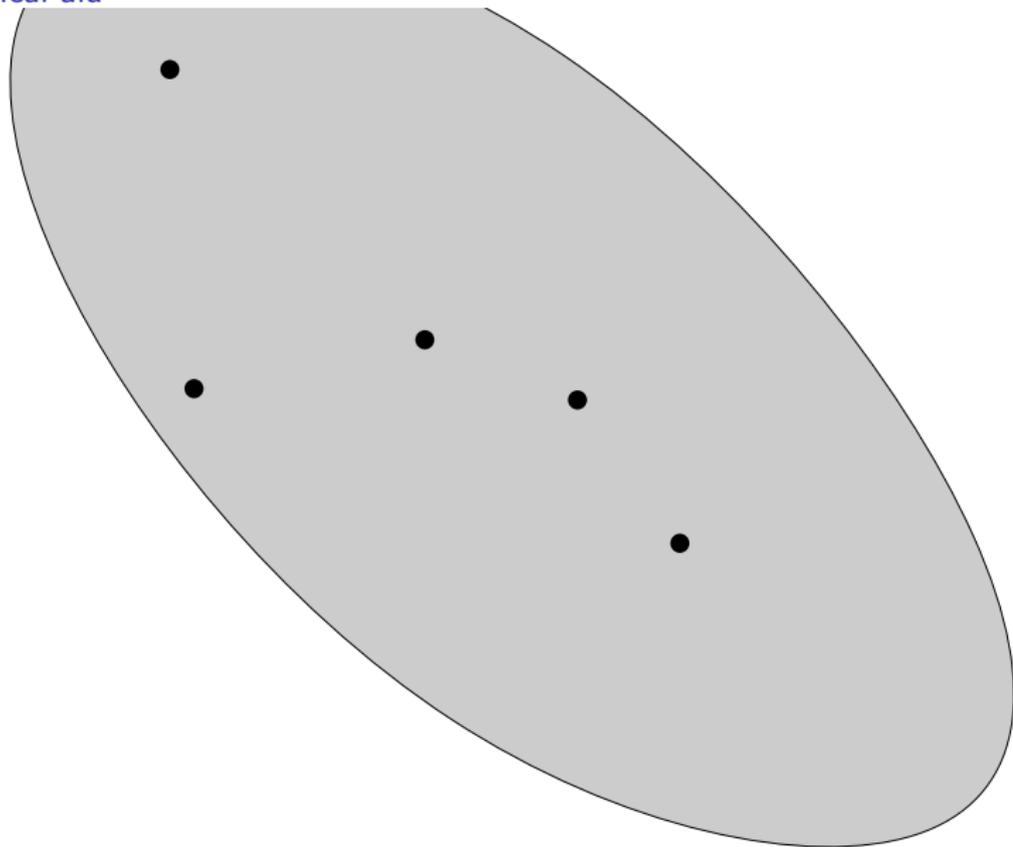
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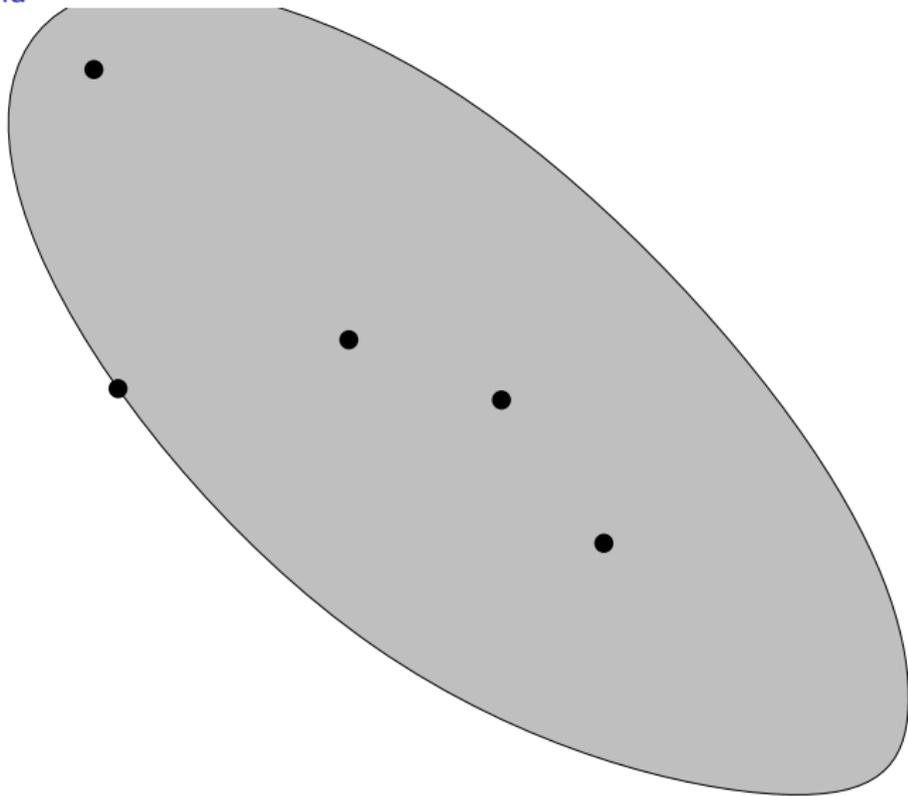
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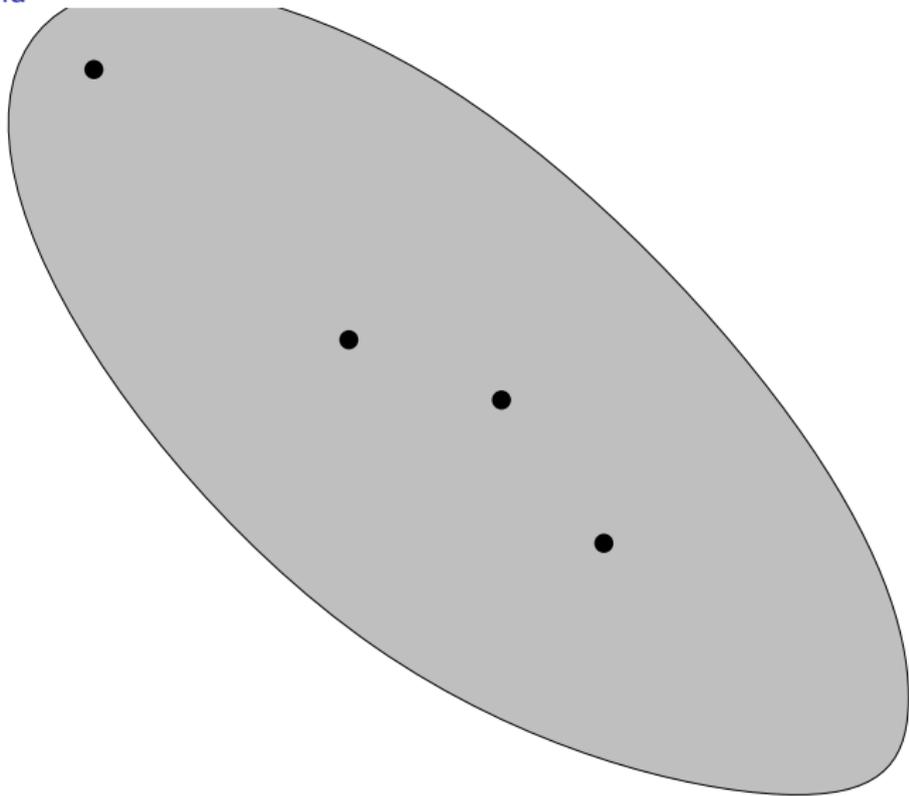
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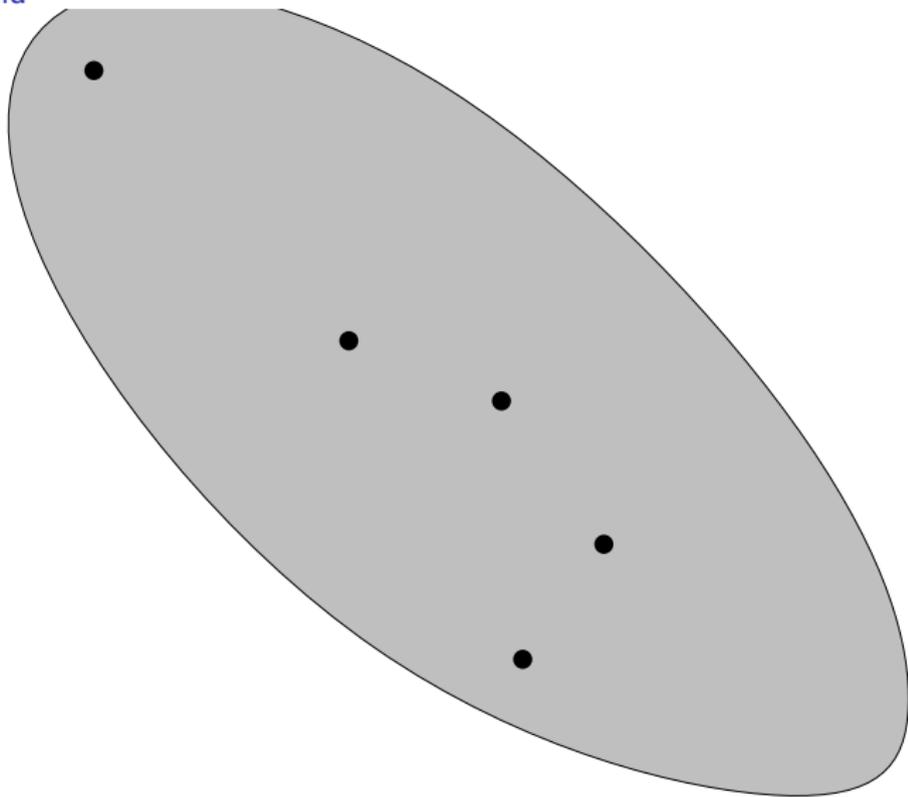
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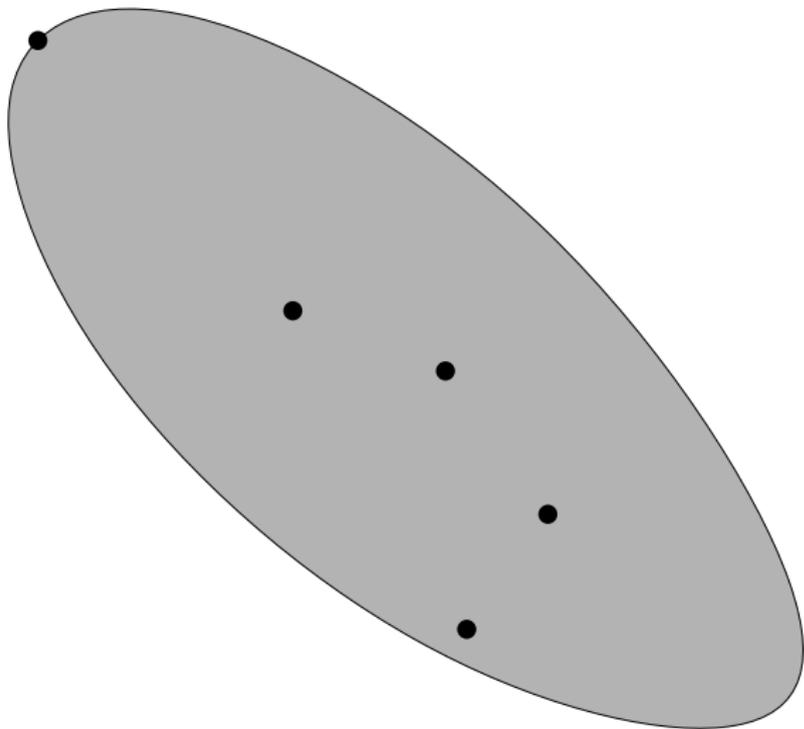
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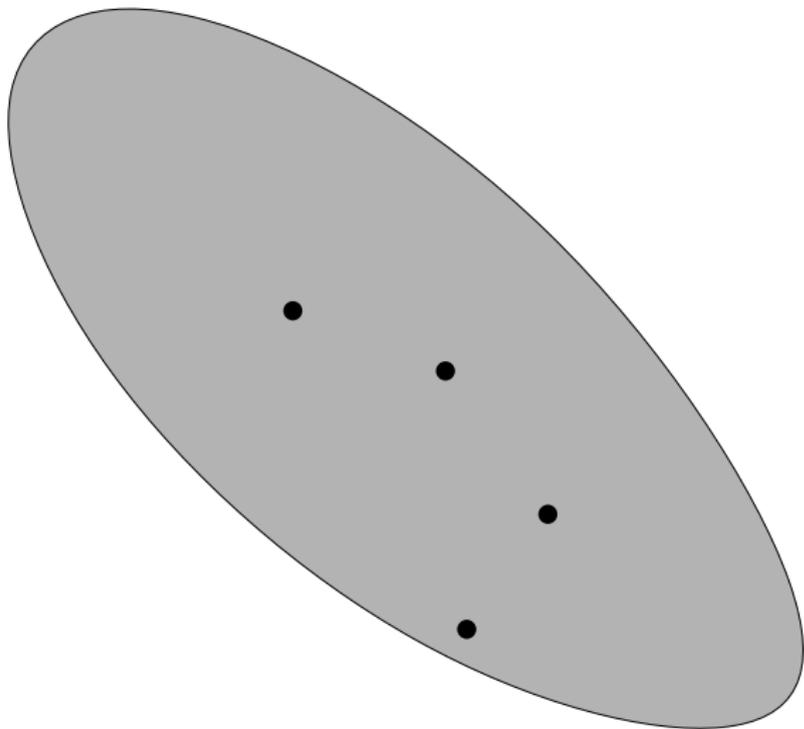
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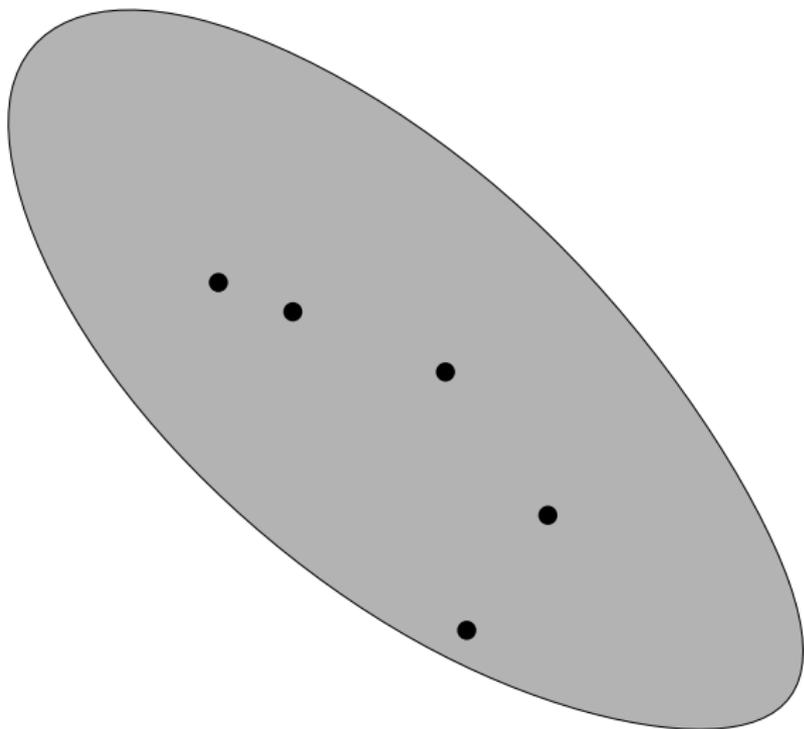
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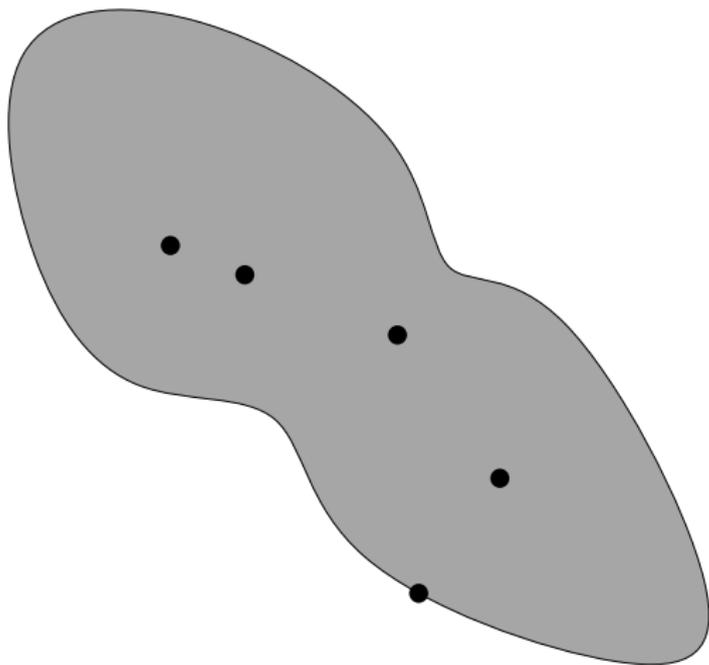
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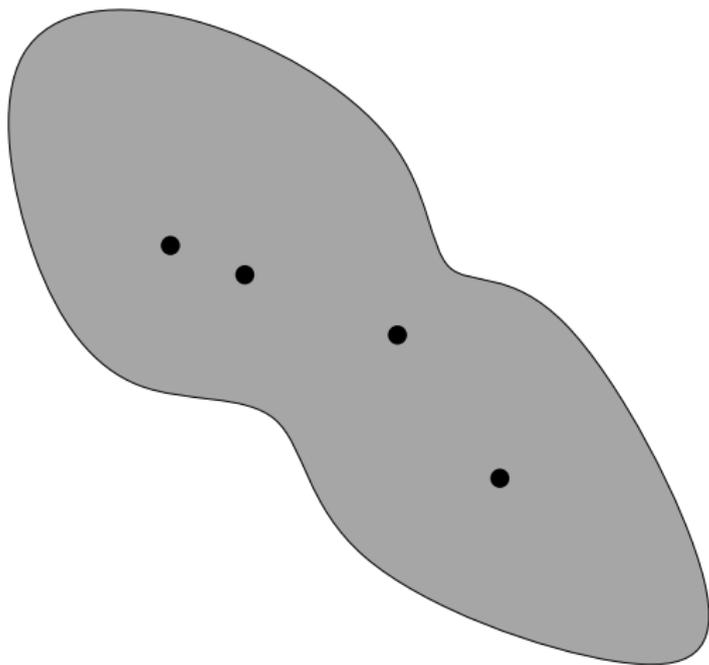
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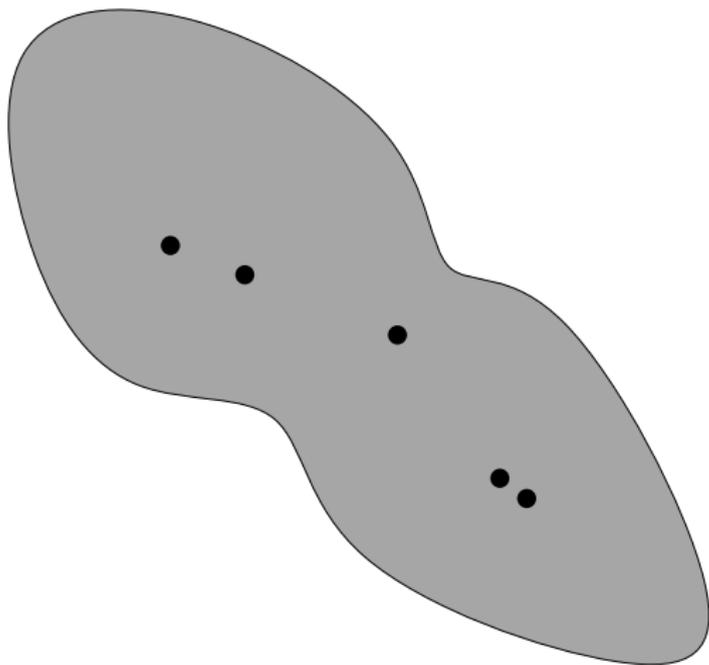
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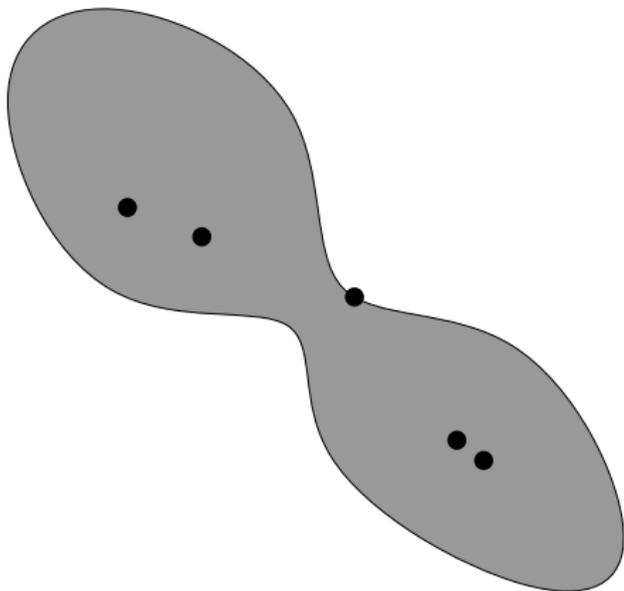
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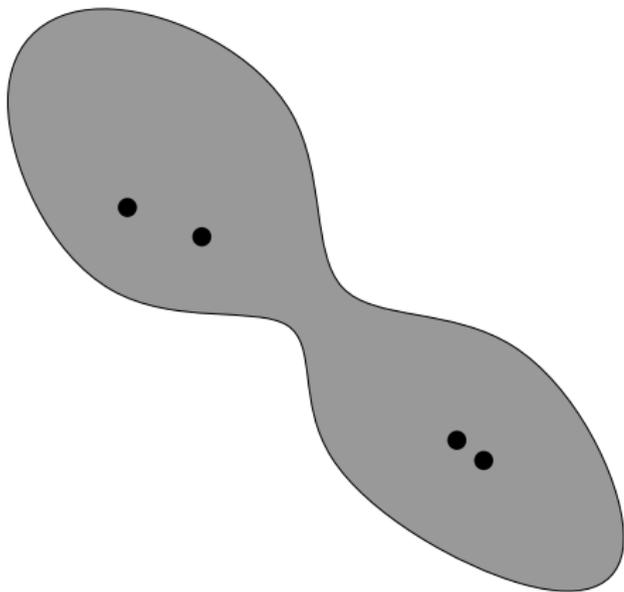
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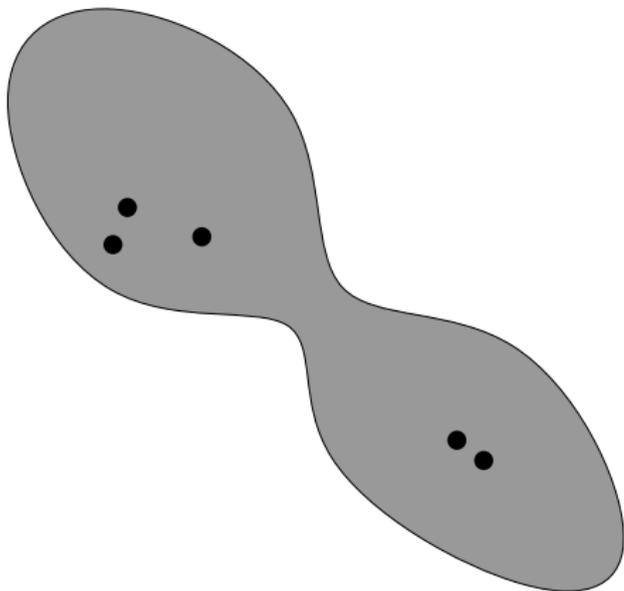
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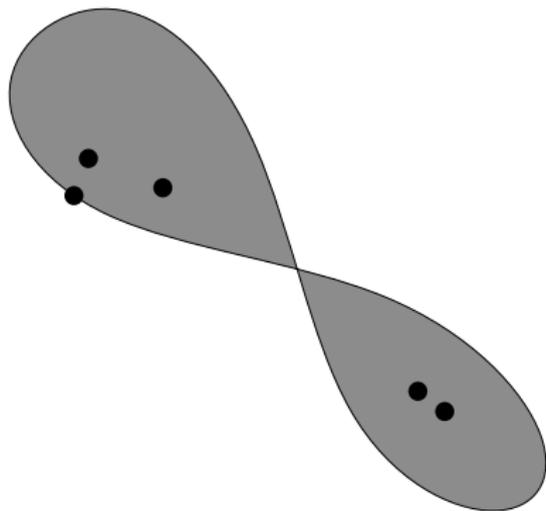
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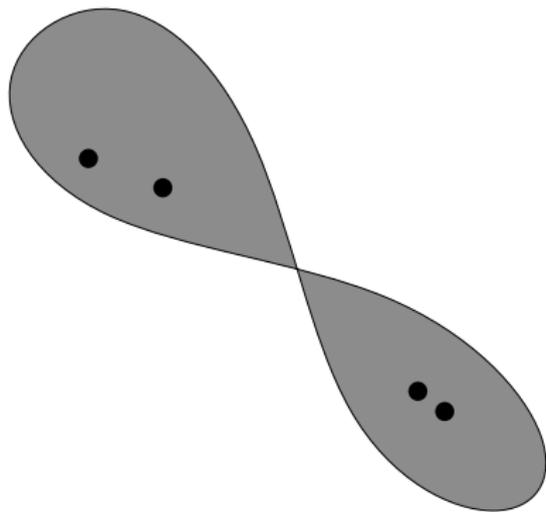
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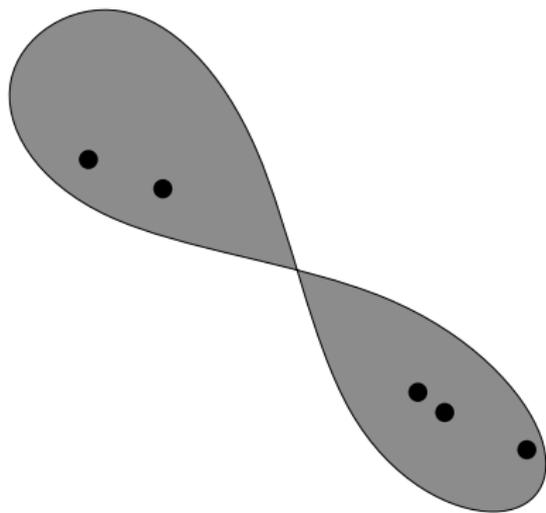
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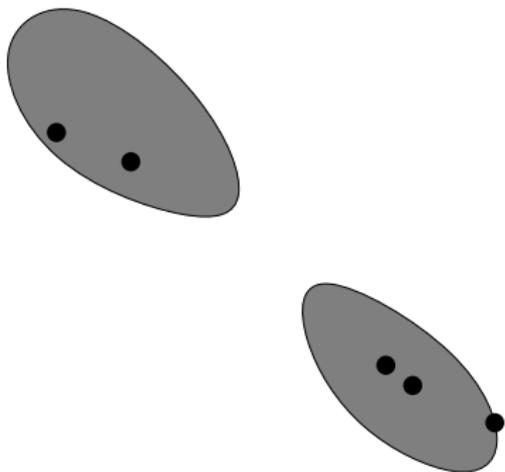
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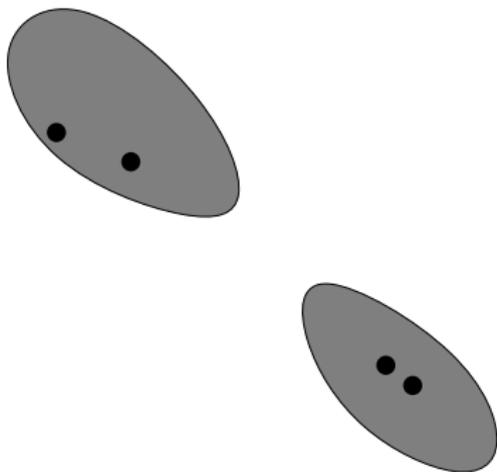
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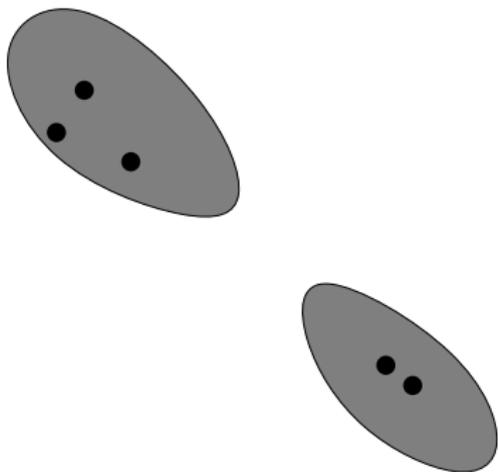
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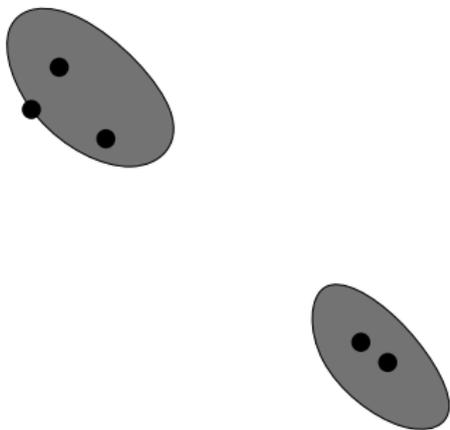
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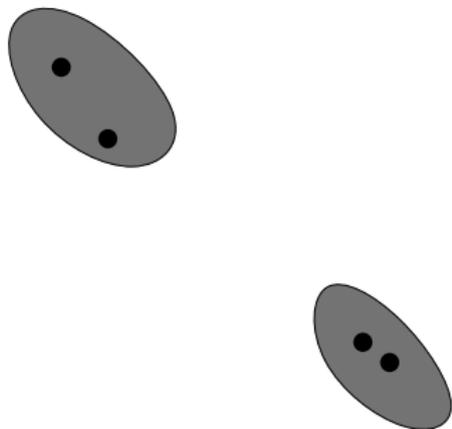
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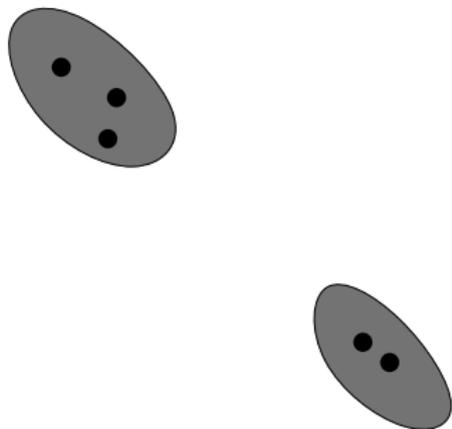
Nested Sampling

Graphical aid



Nested Sampling

Graphical aid



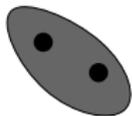
Nested Sampling

Graphical aid



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Graphical aid



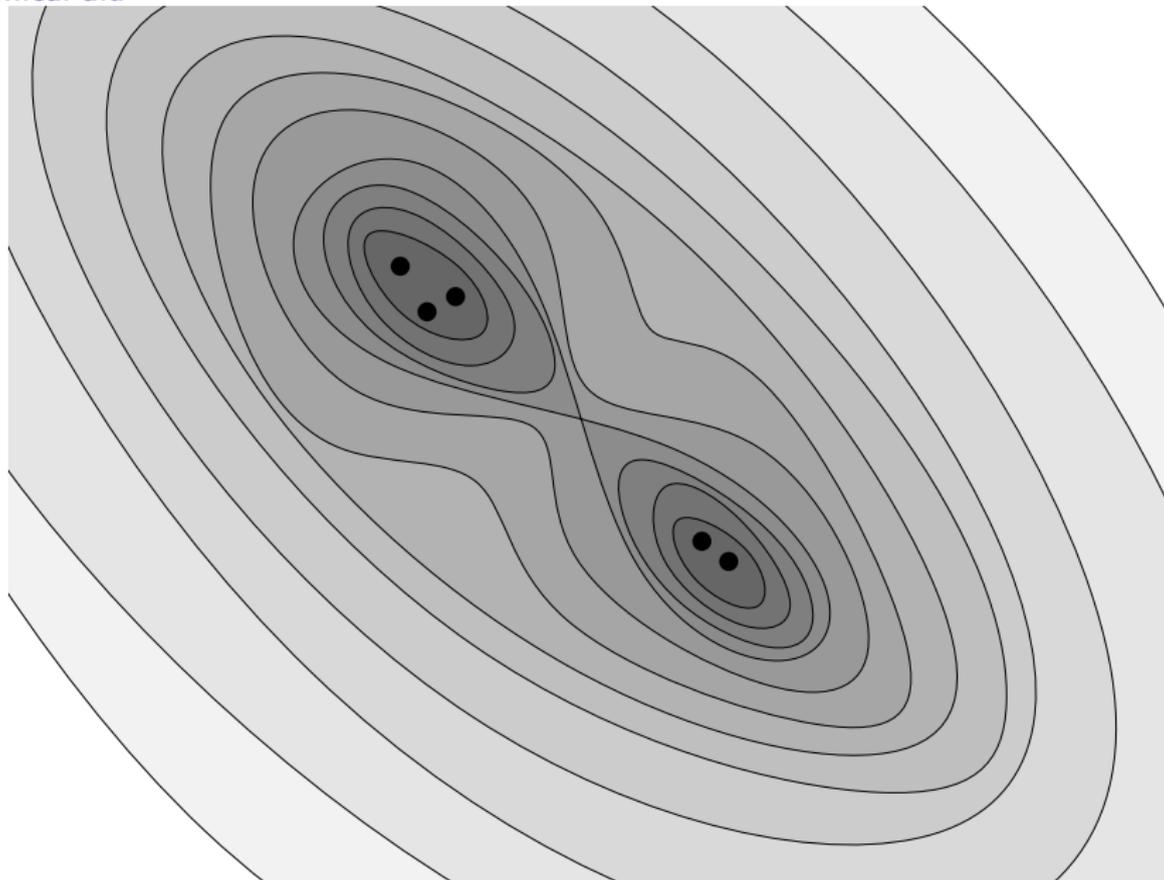
Nested Sampling

Graphical aid



Nested Sampling

Graphical aid



Nested Sampling

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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

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

Calculating evidences

- ▶ Transform to 1 dimensional integral

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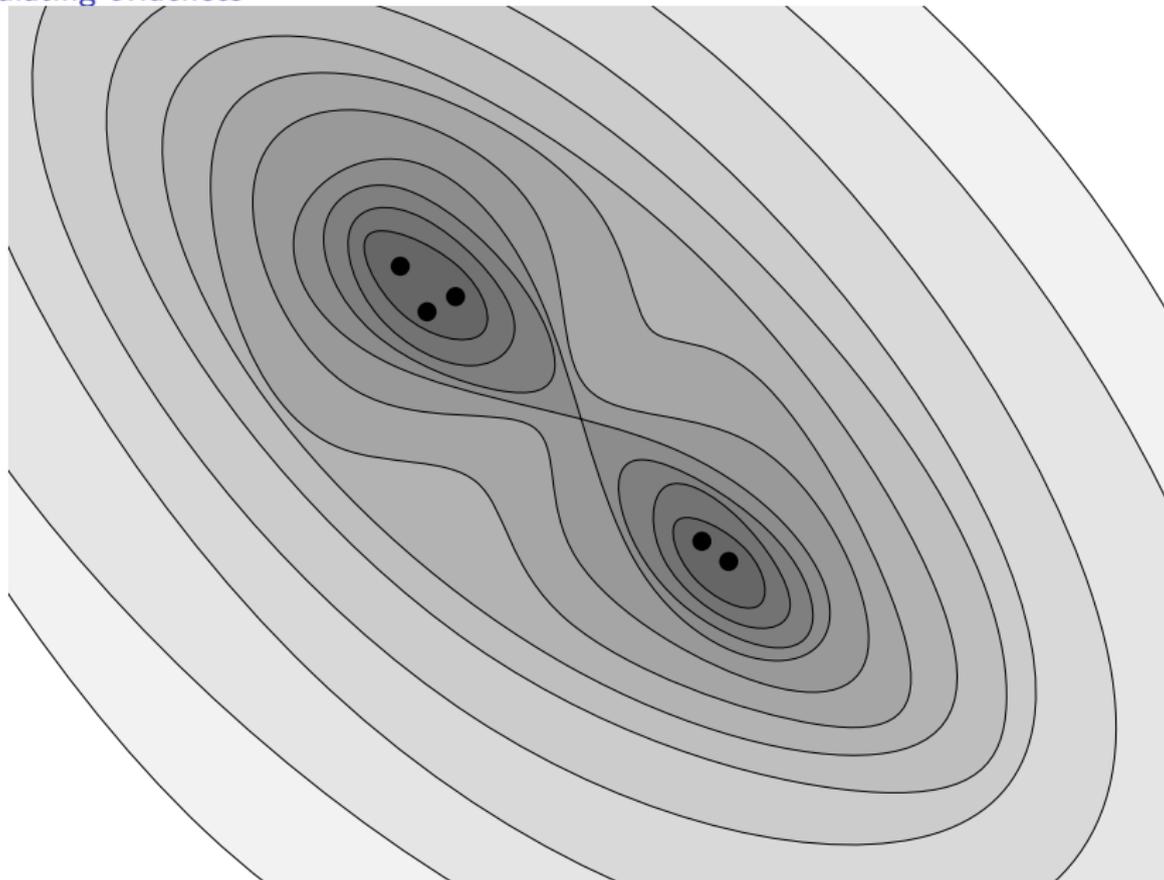
- ▶ X is the *prior volume*

$$X(\mathcal{L}) = \int_{\mathcal{L}(\theta) > \mathcal{L}} \pi(\theta)d\theta$$

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

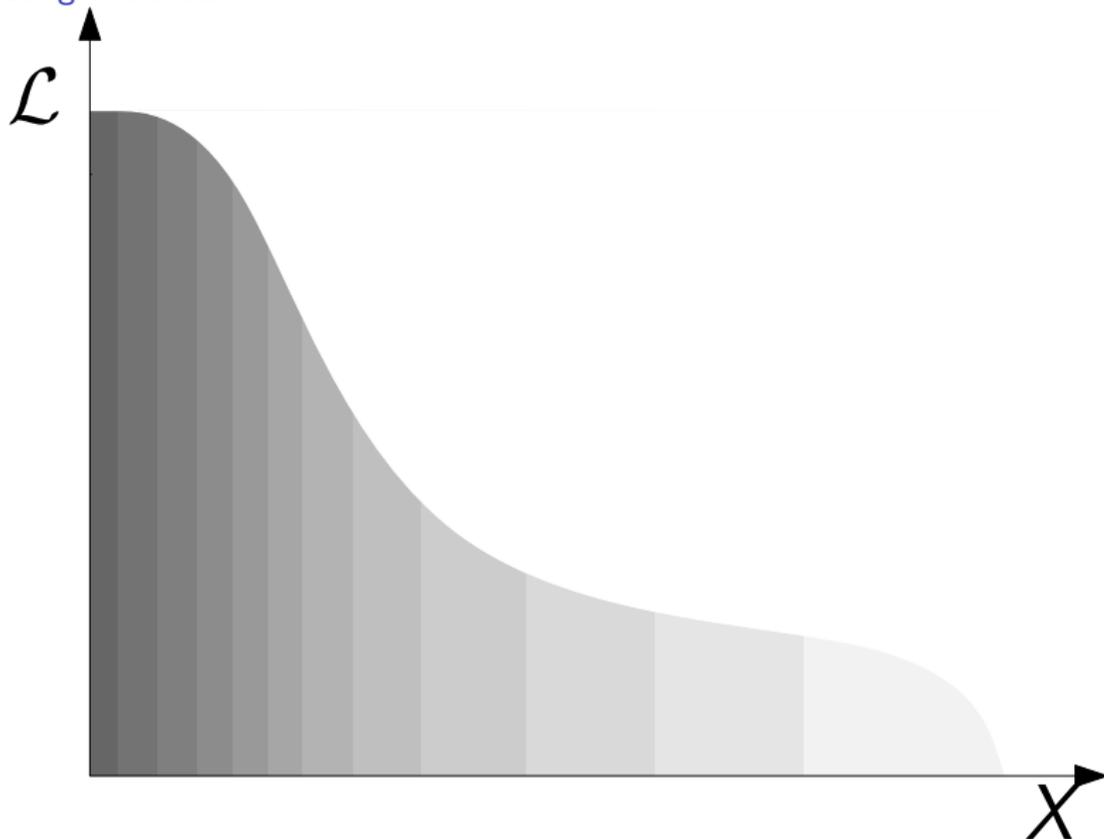
Nested Sampling

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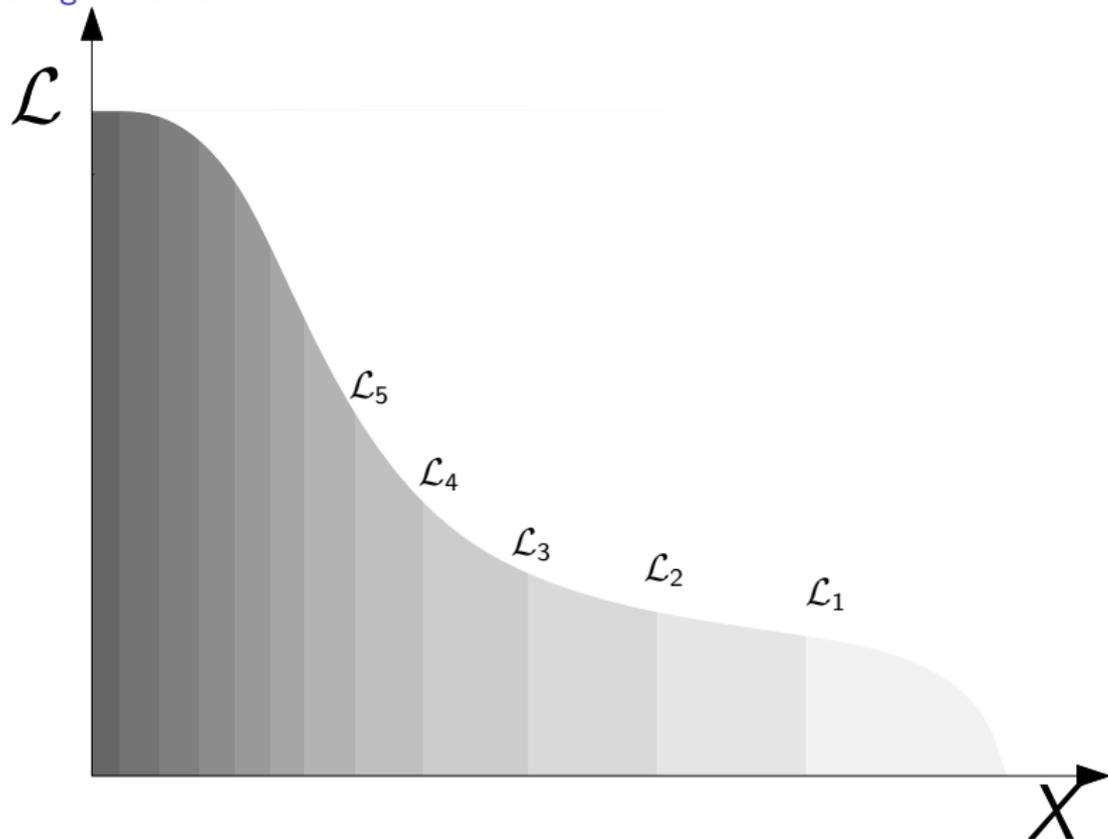
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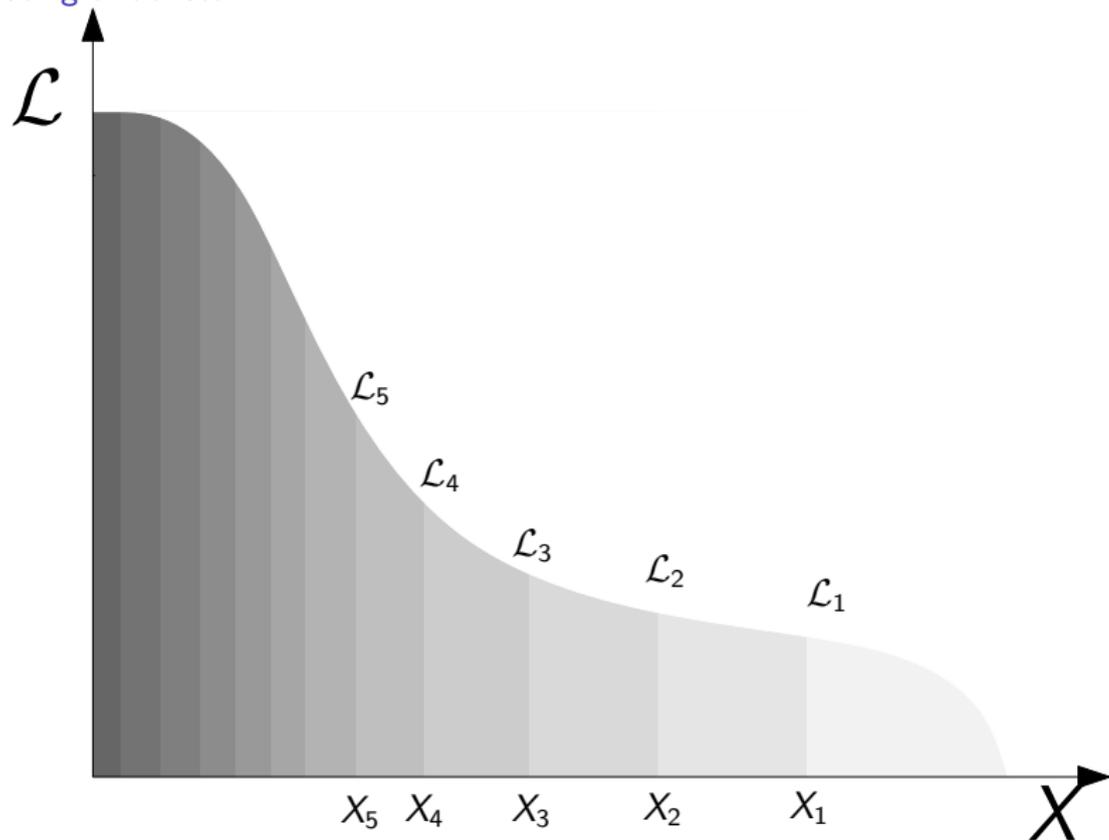
Nested Sampling

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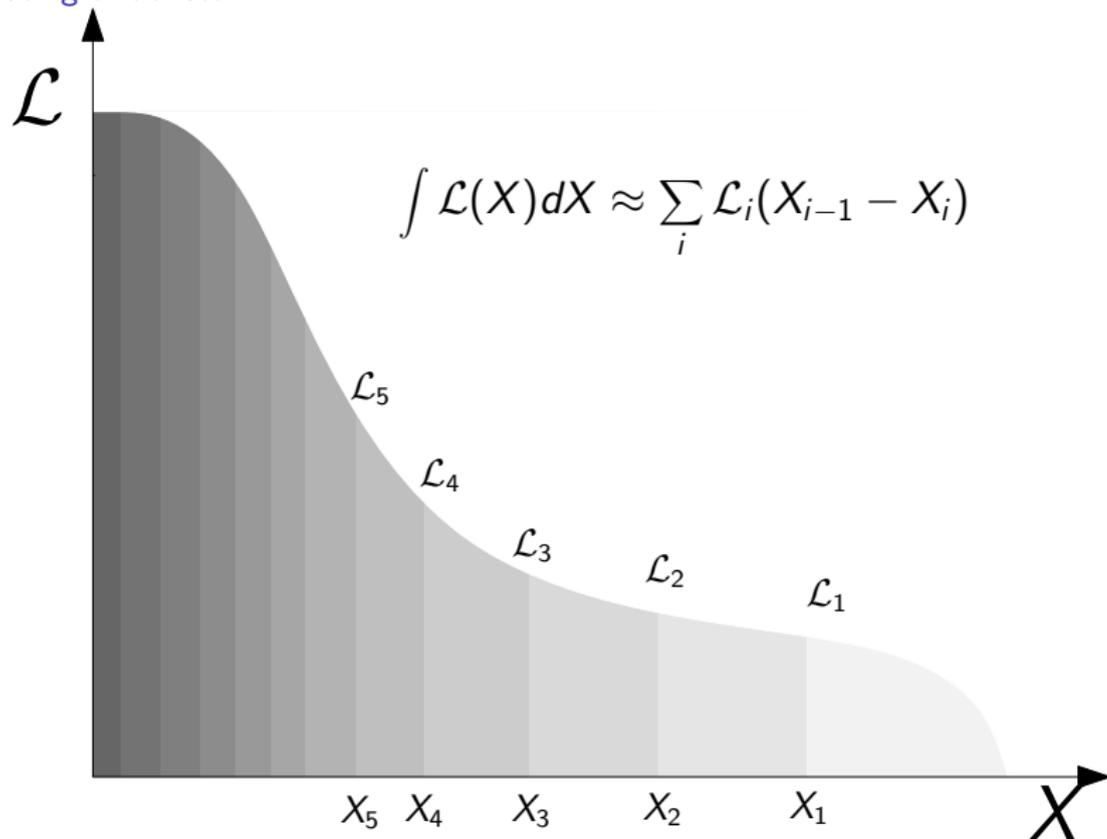
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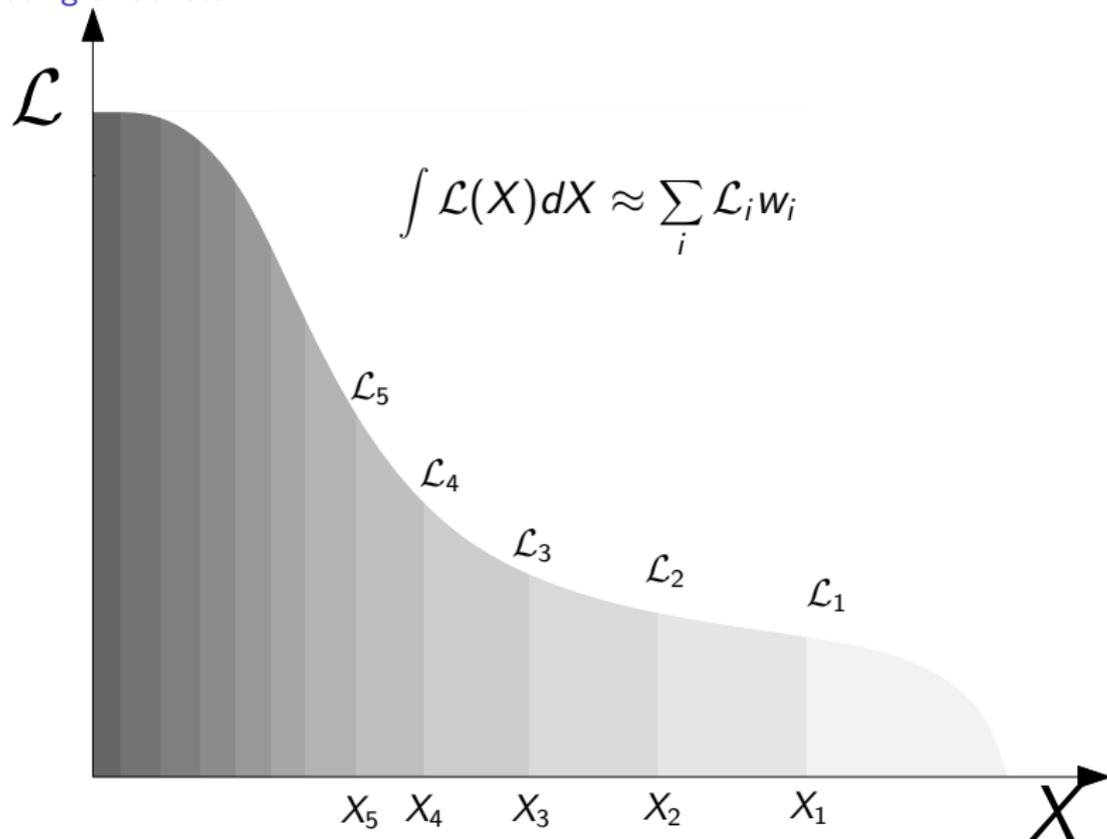
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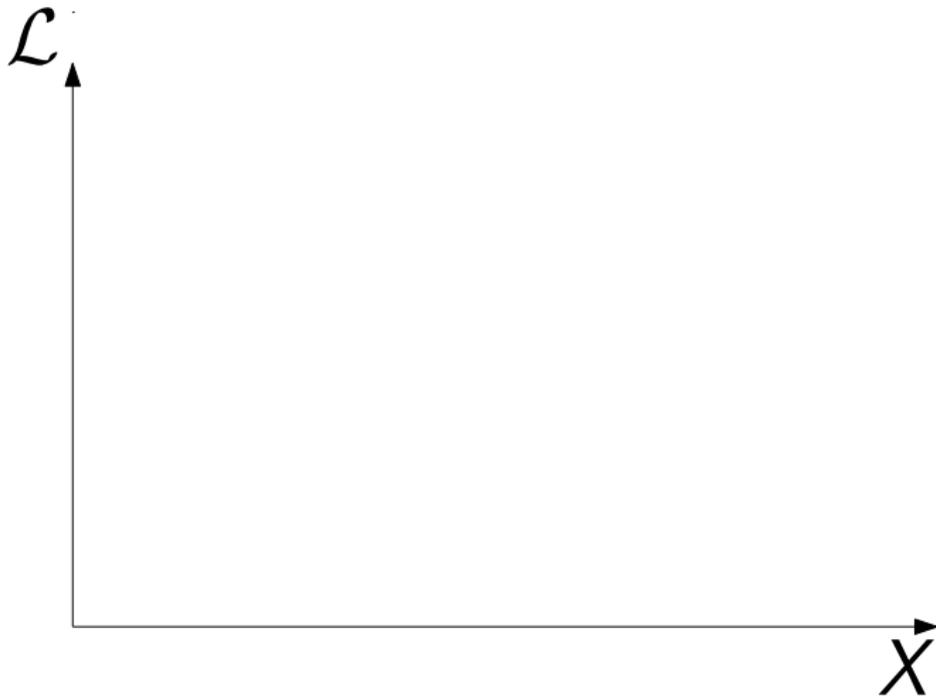
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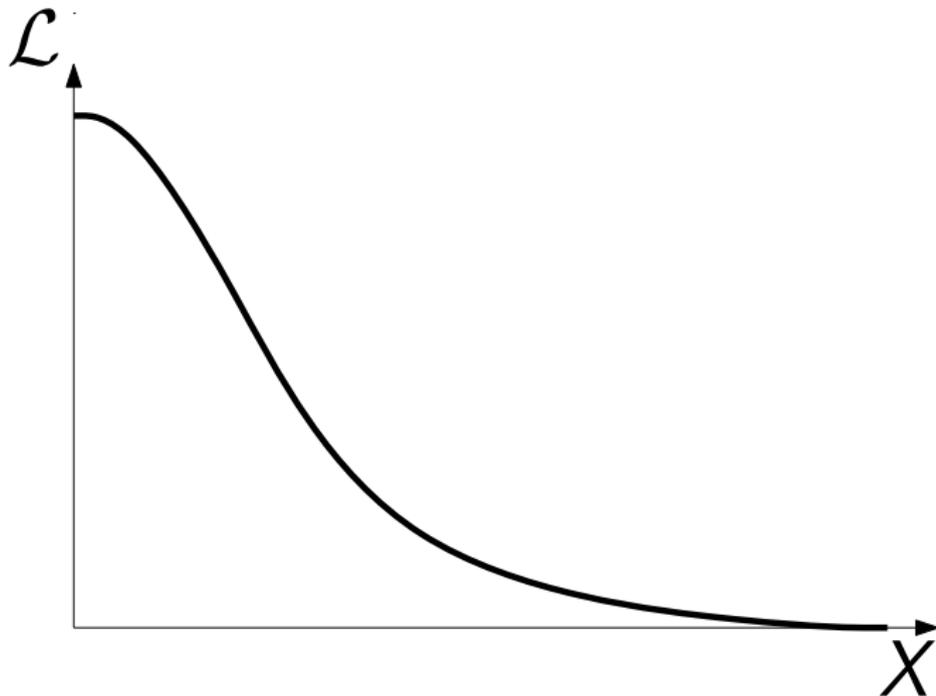
Estimating evidences

Evidence error



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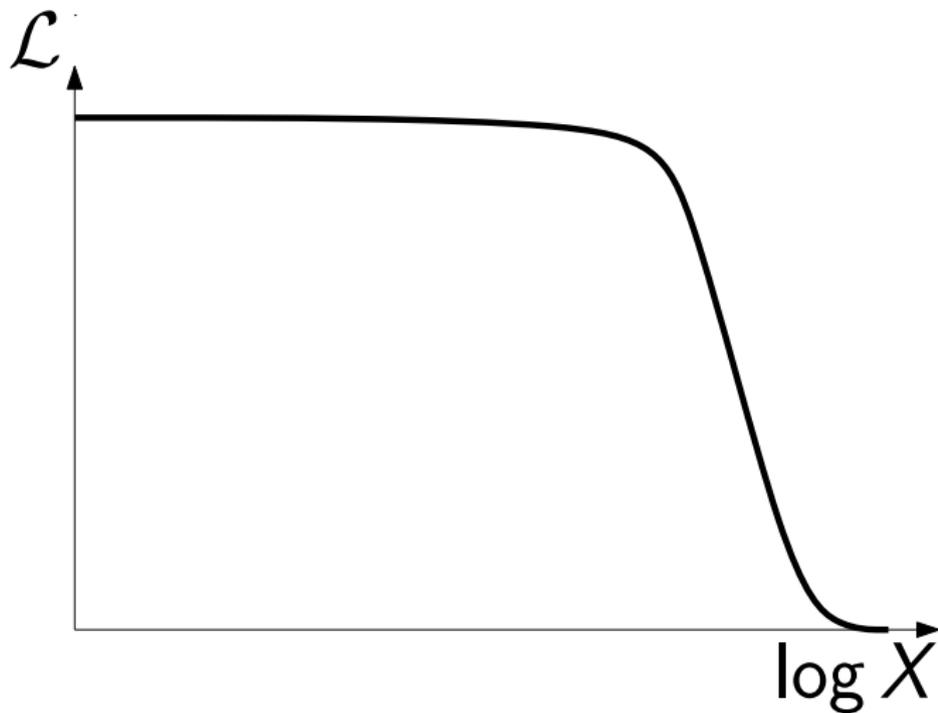
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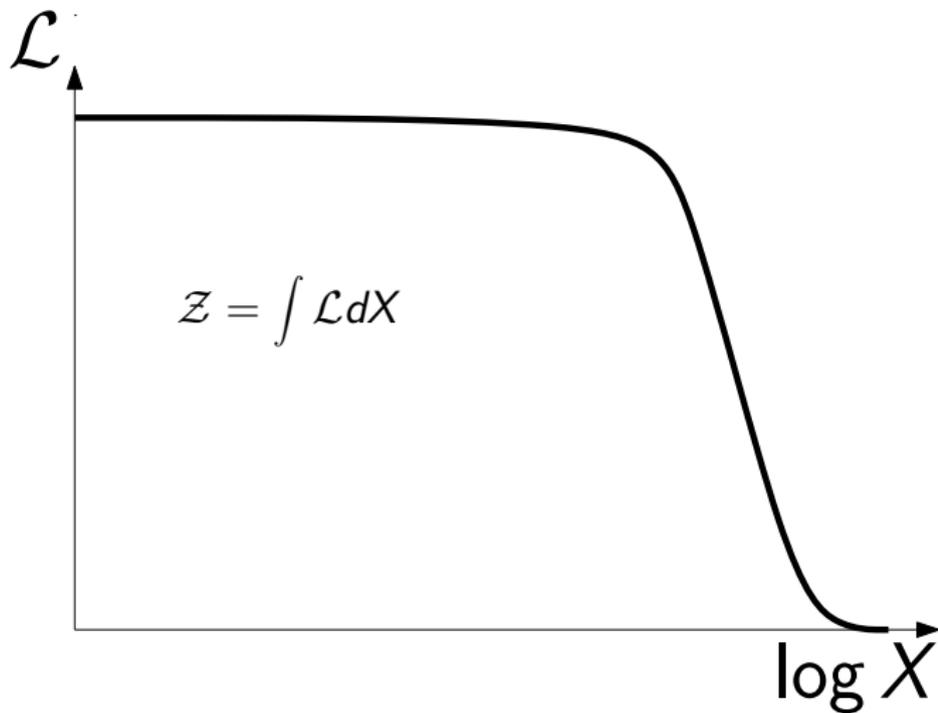
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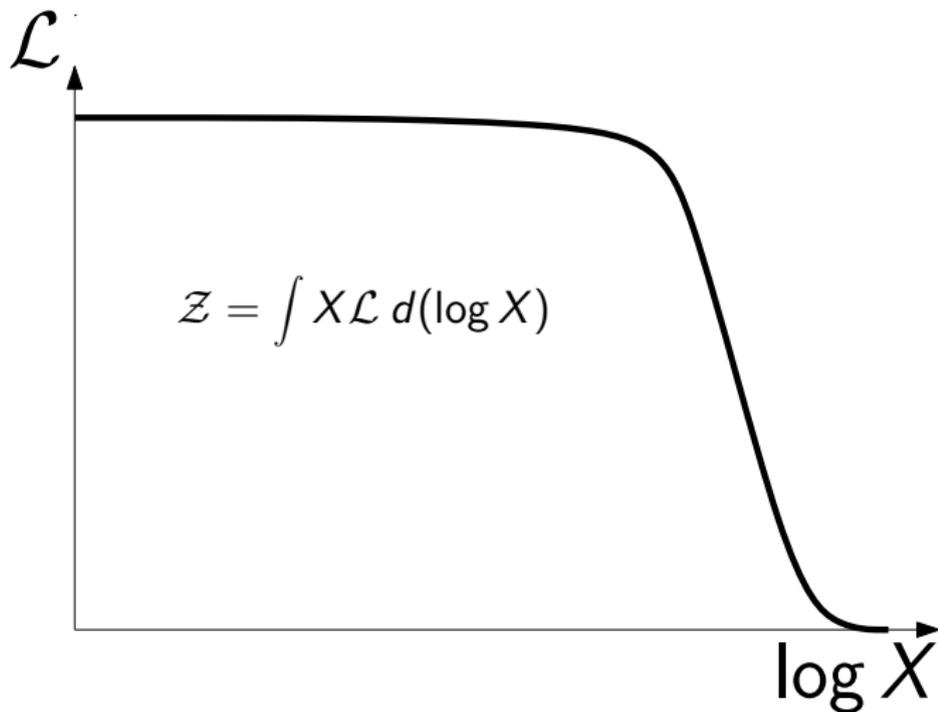
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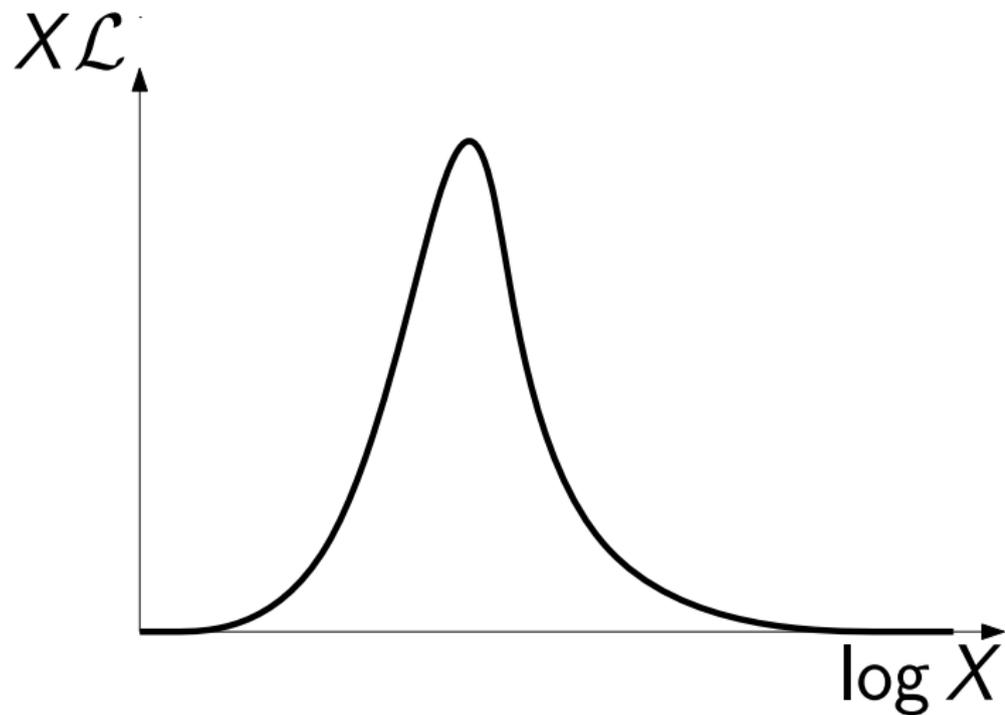
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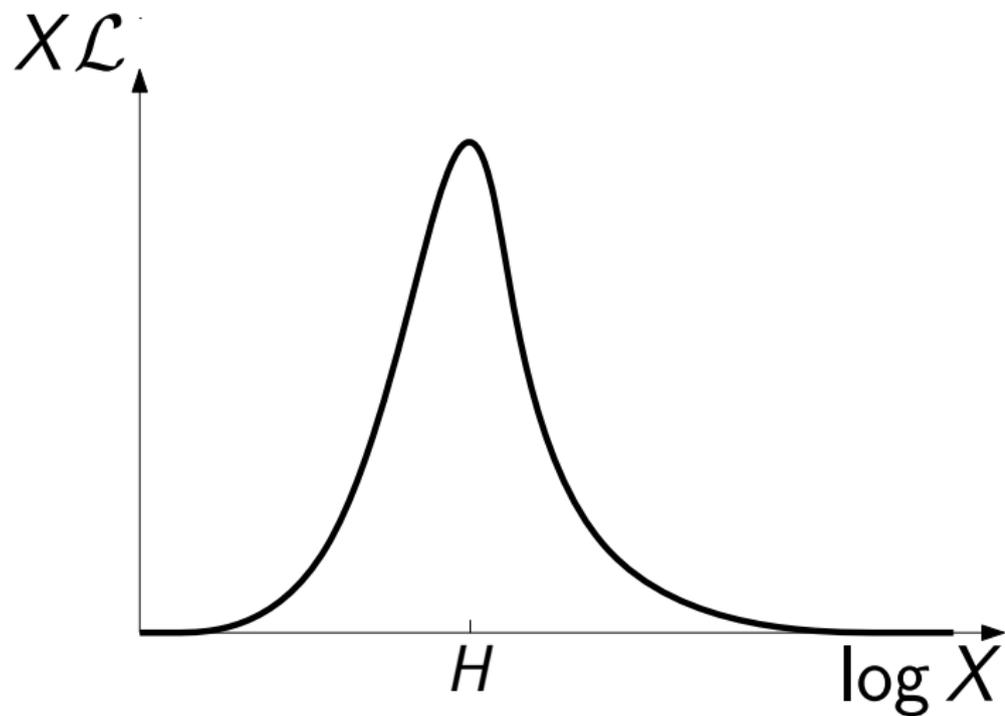
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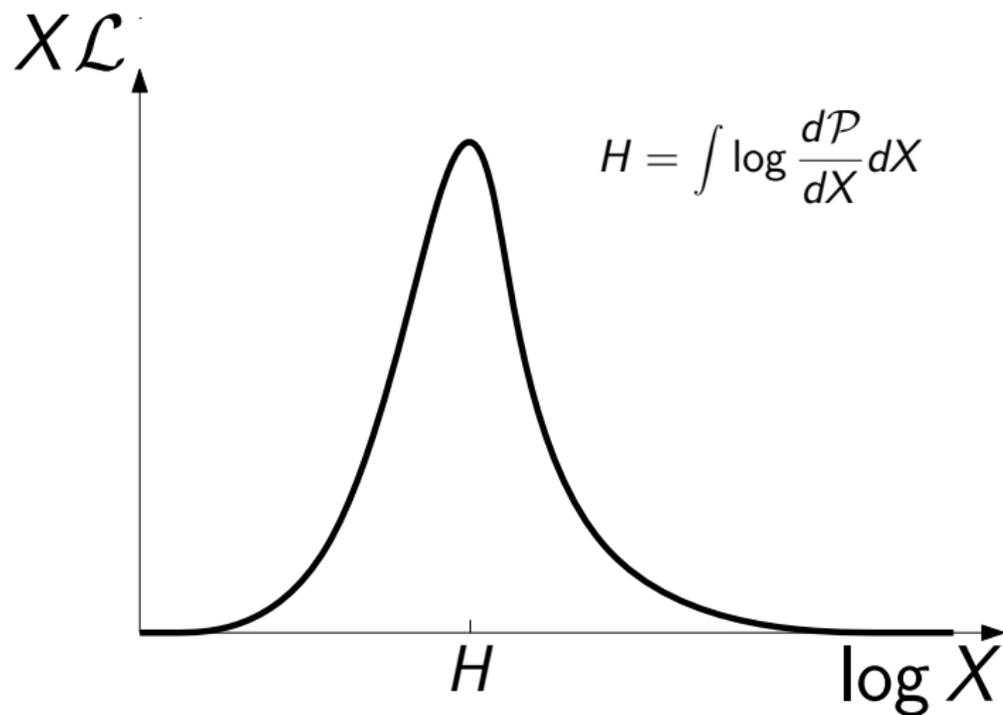
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- ▶ estimate of evidence error:

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

Nested sampling

Parameter estimation

Nested sampling

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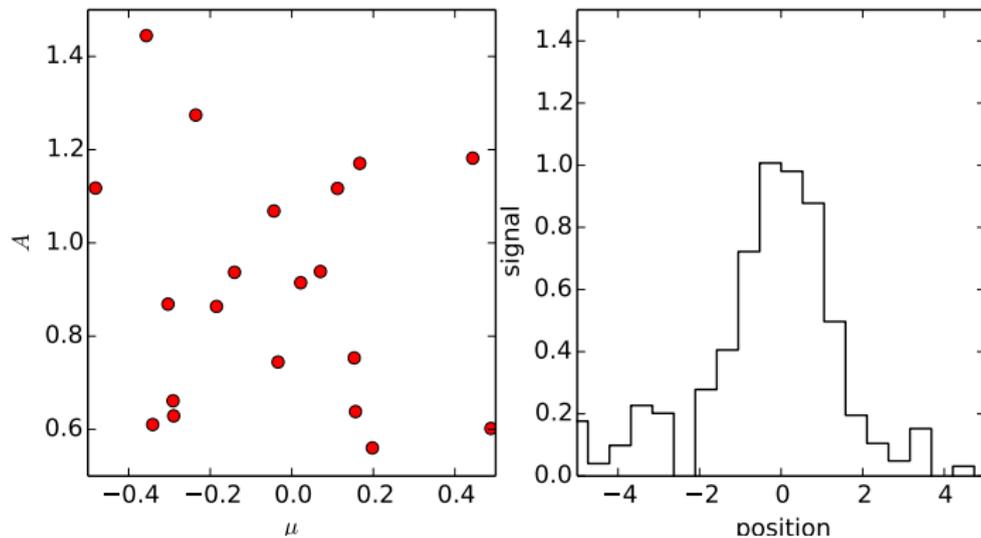
- ▶ NS can also be used to sample the posterior

Nested sampling

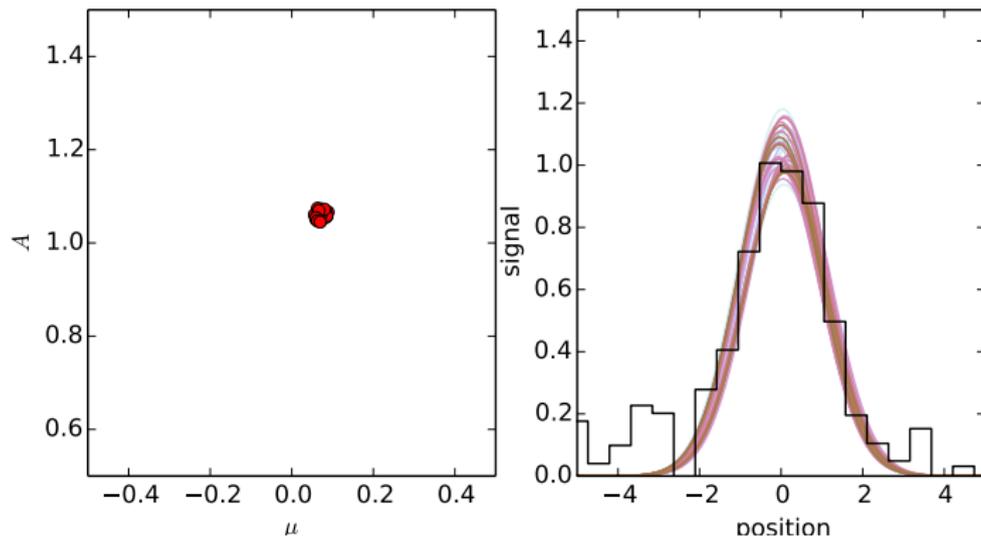
Parameter estimation

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

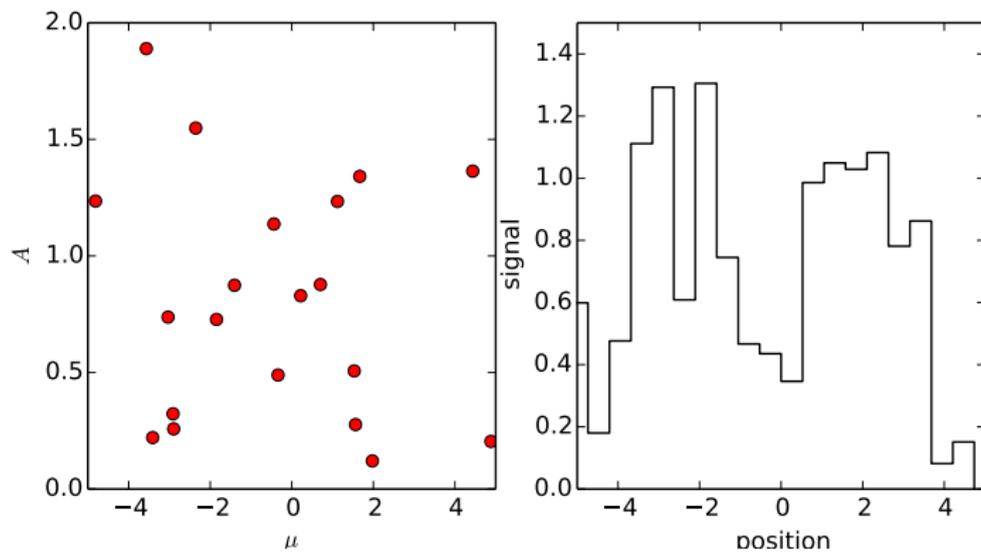
When NS succeeds



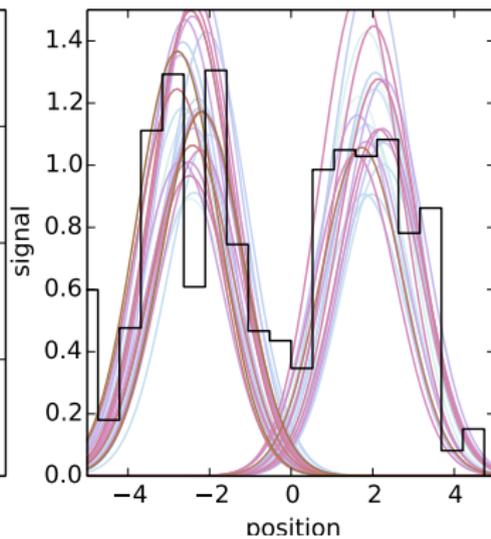
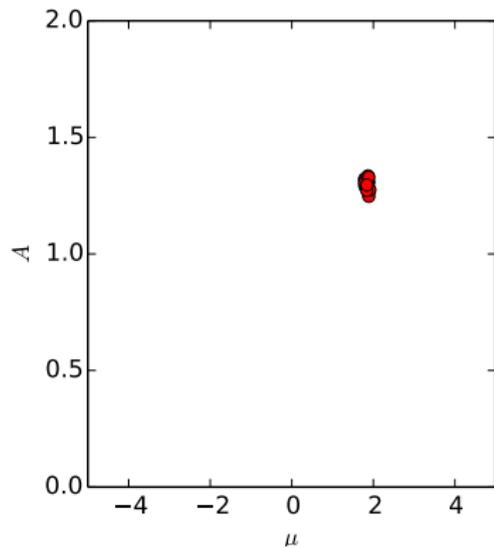
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Sampling from a hard likelihood constraint

Sampling from a hard likelihood constraint

“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

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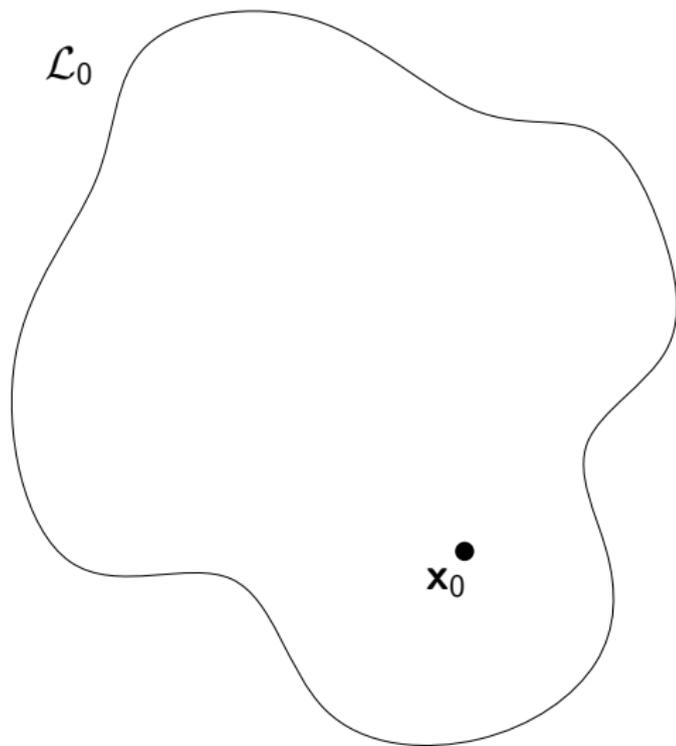
- ▶ Requires gradients and tuning

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- ▶ Too many tuning parameters

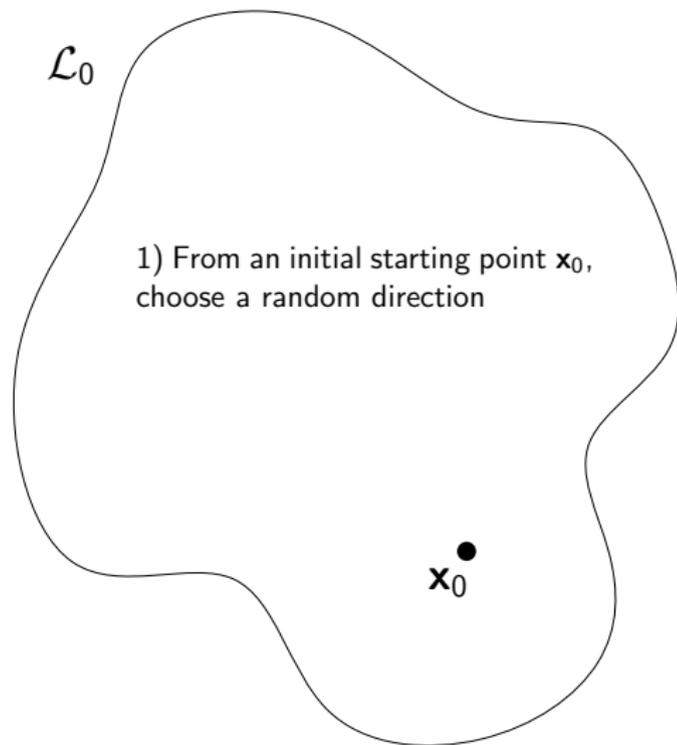
PolyChord

“Hit and run” slice sampling



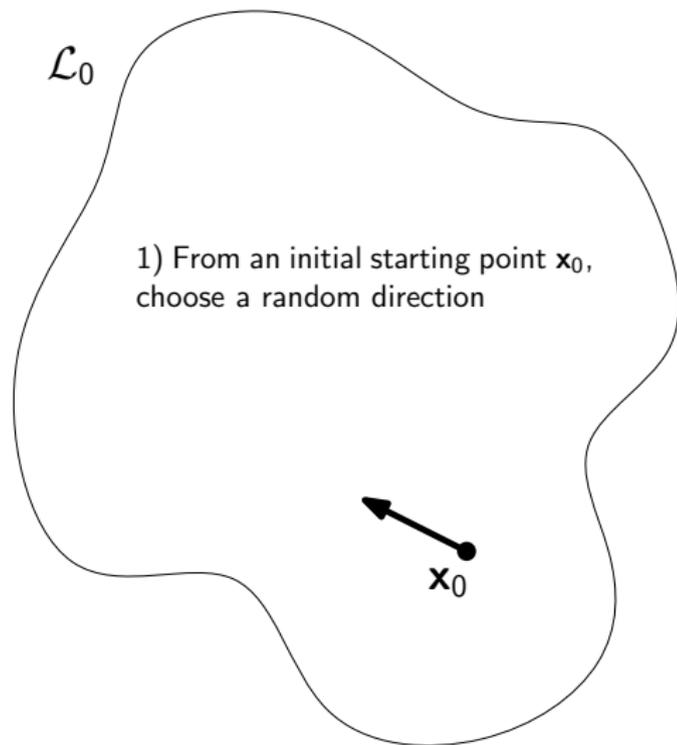
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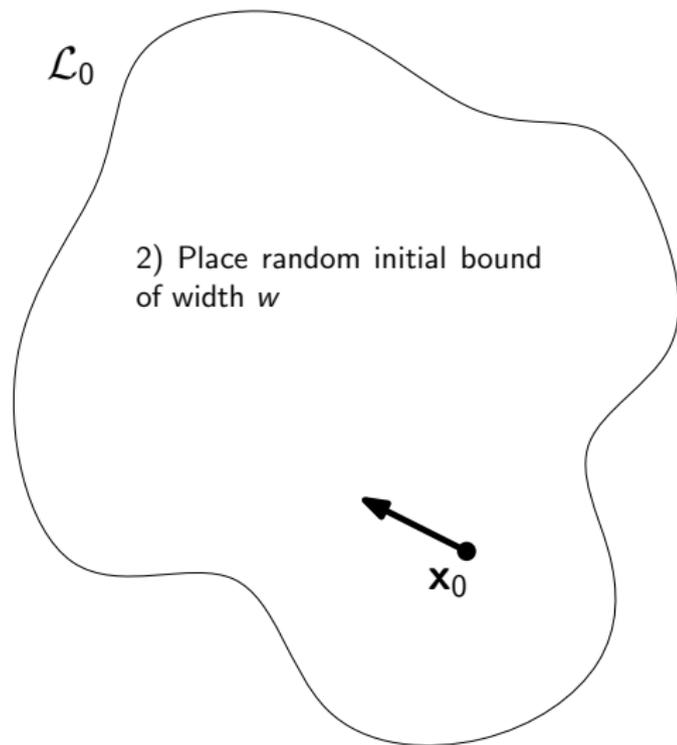
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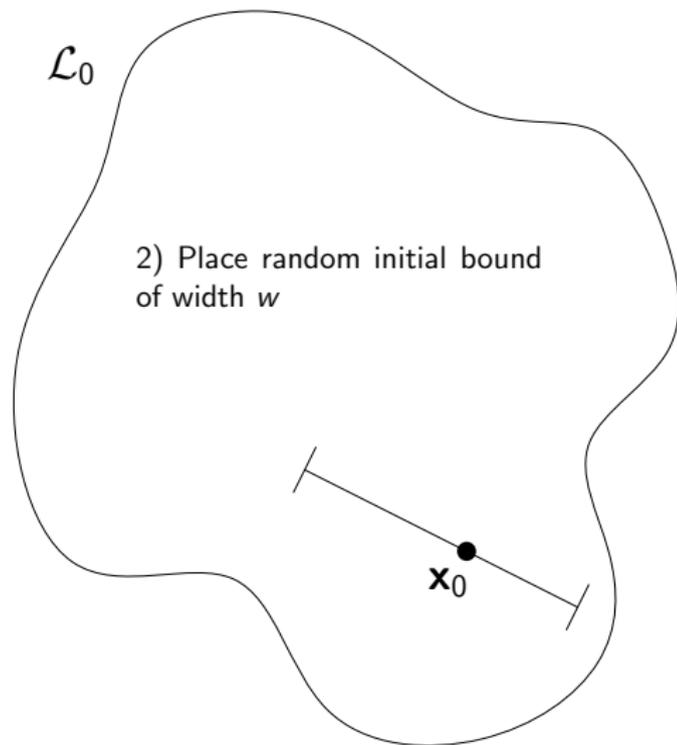
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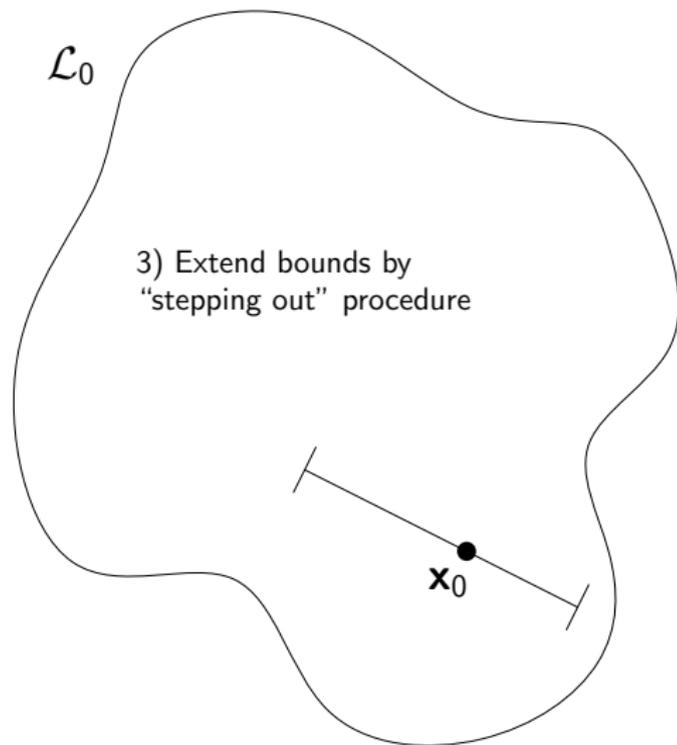
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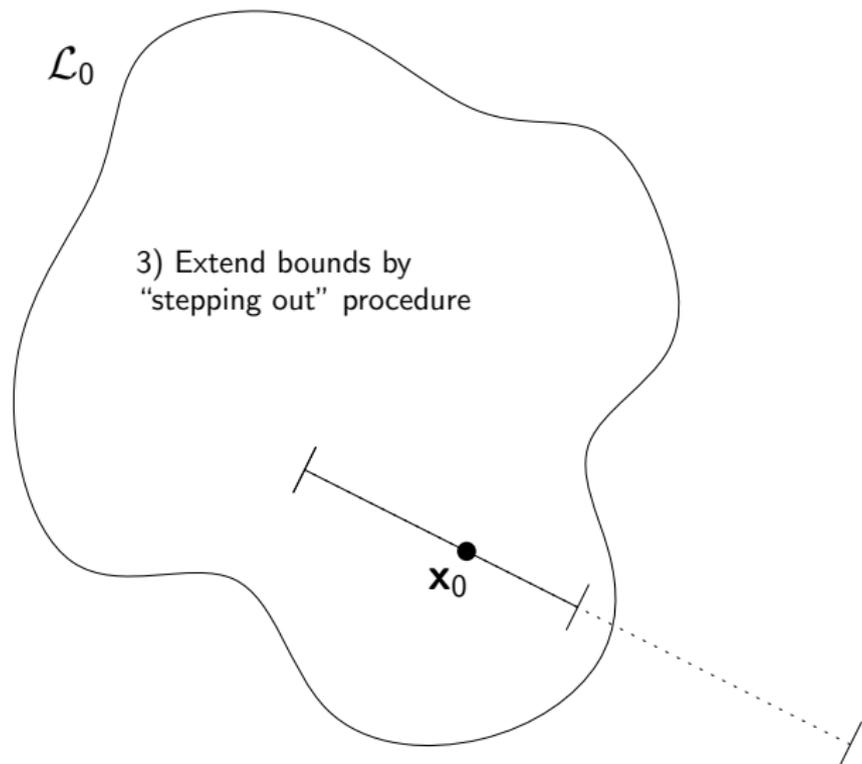
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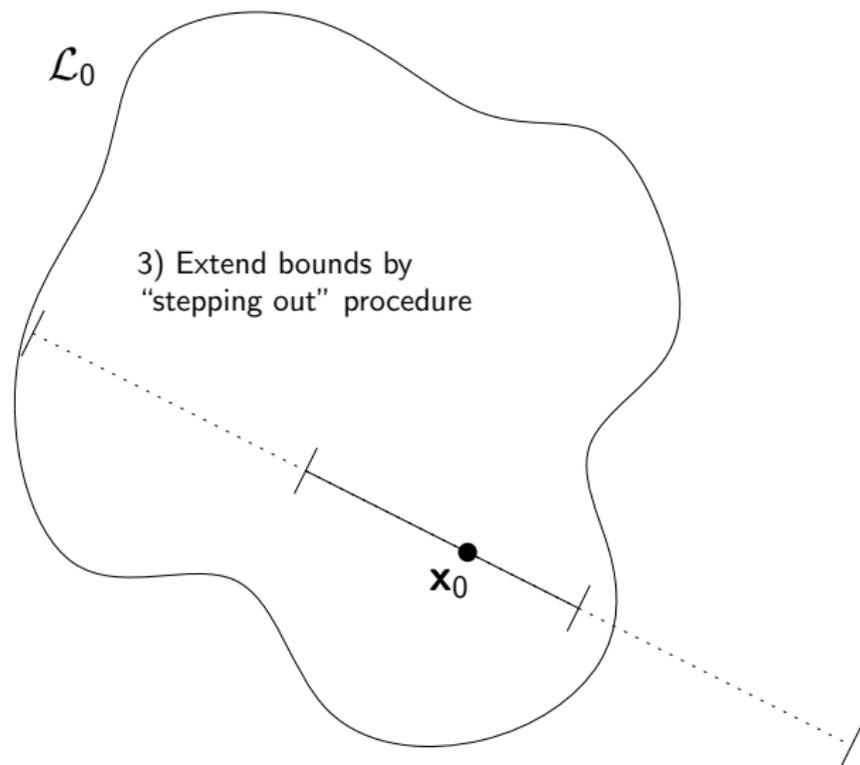
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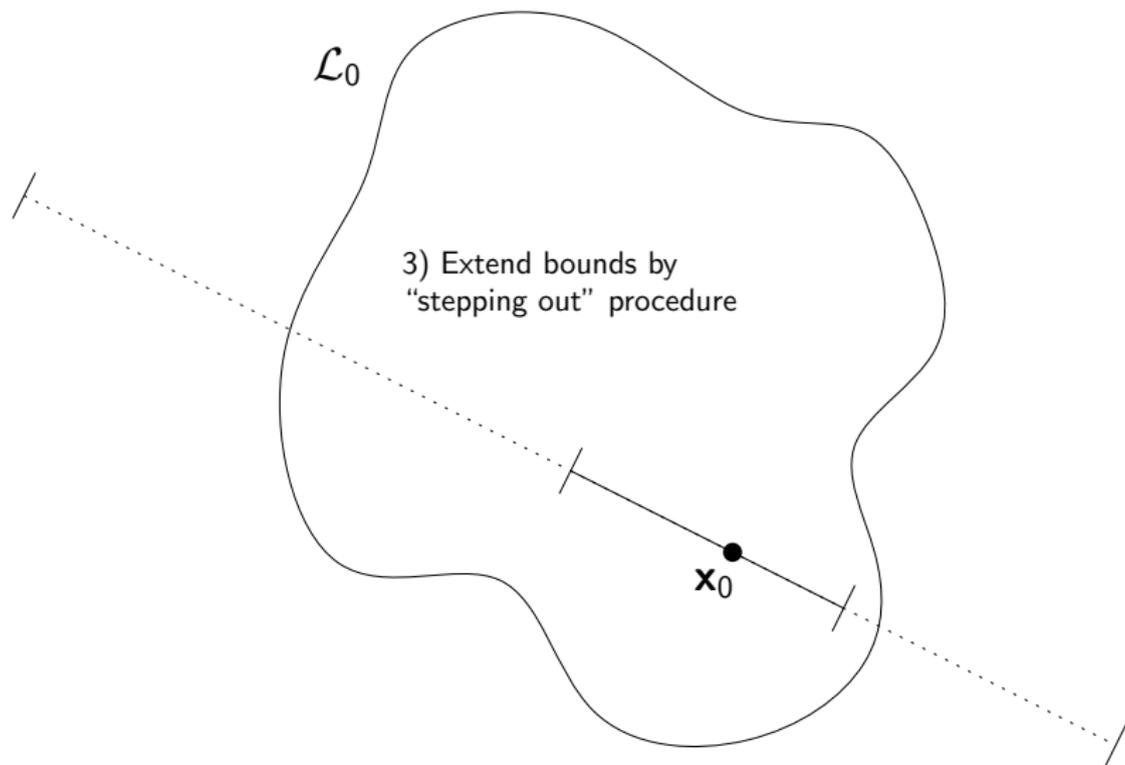
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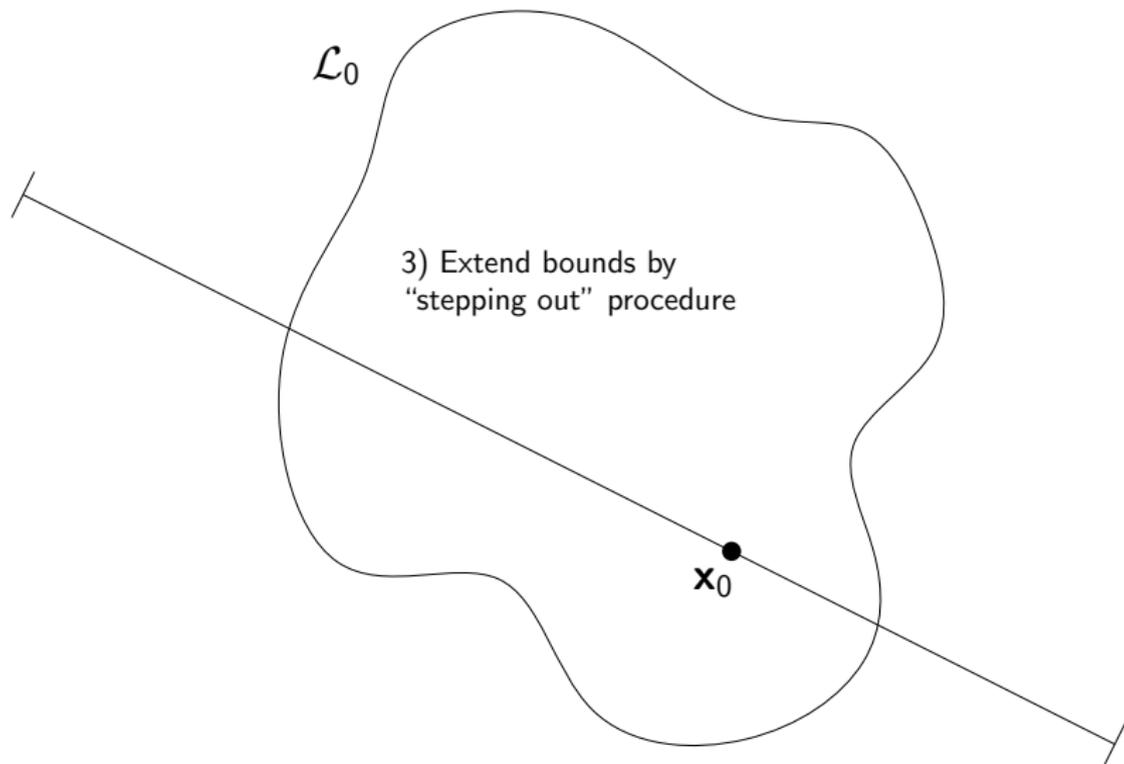
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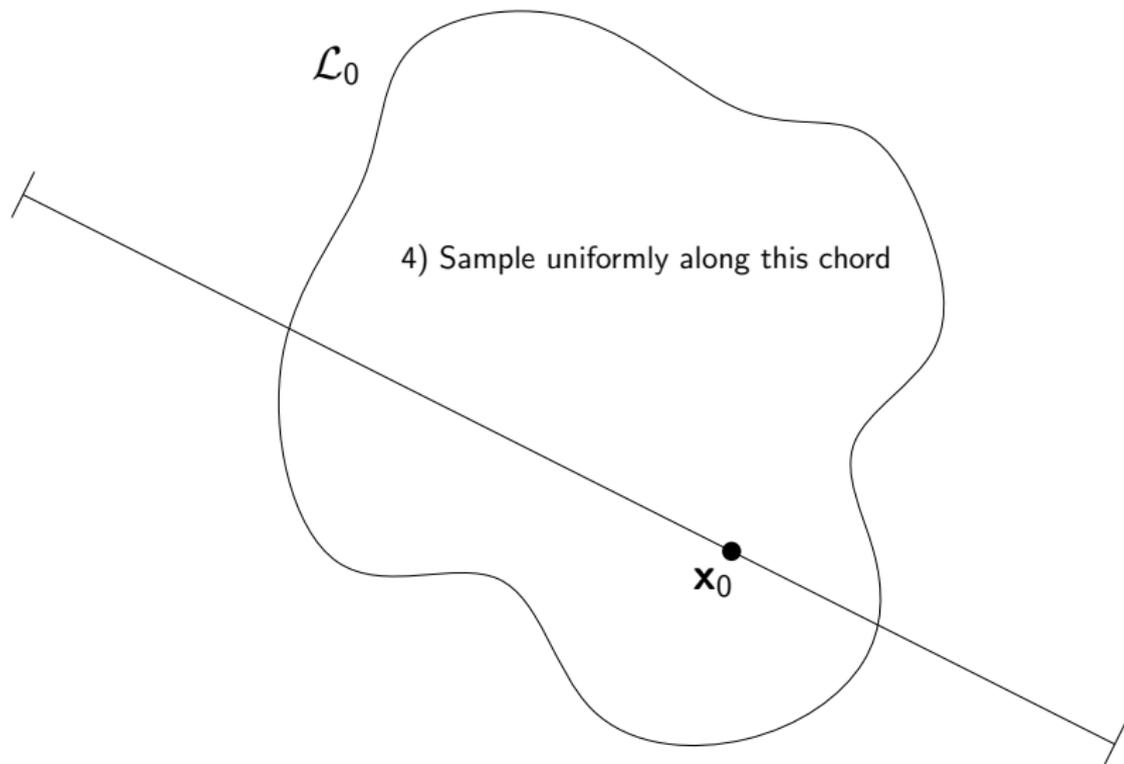
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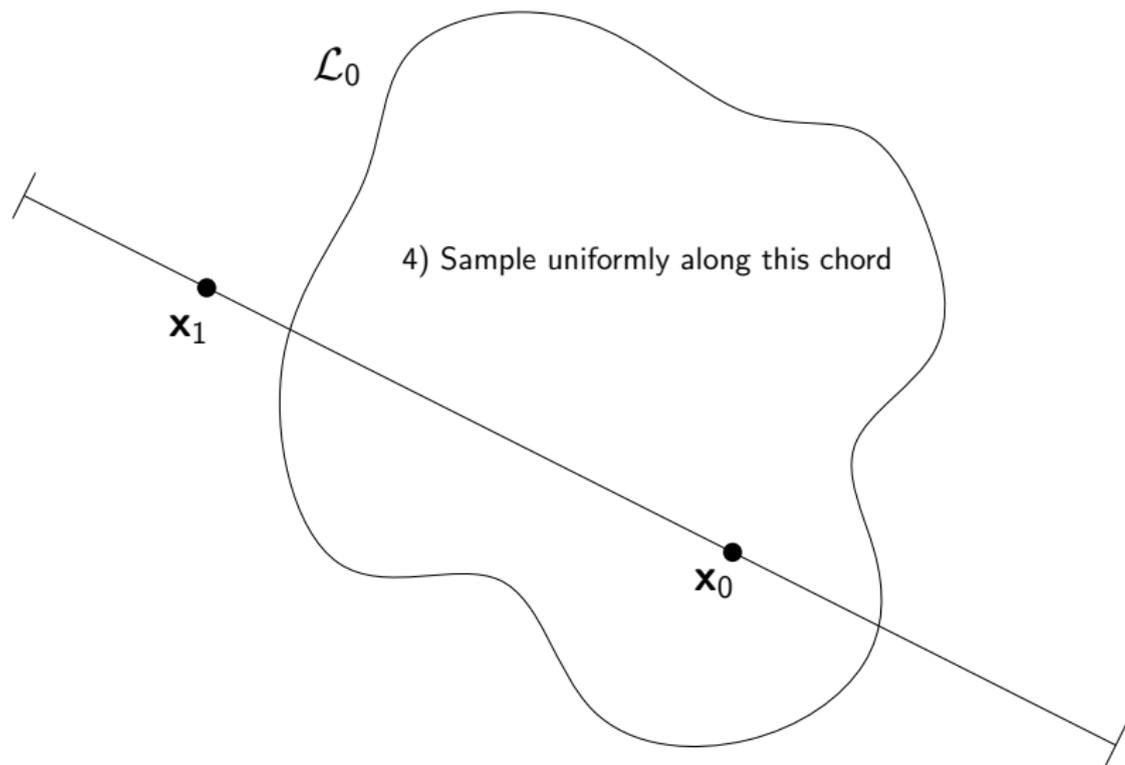
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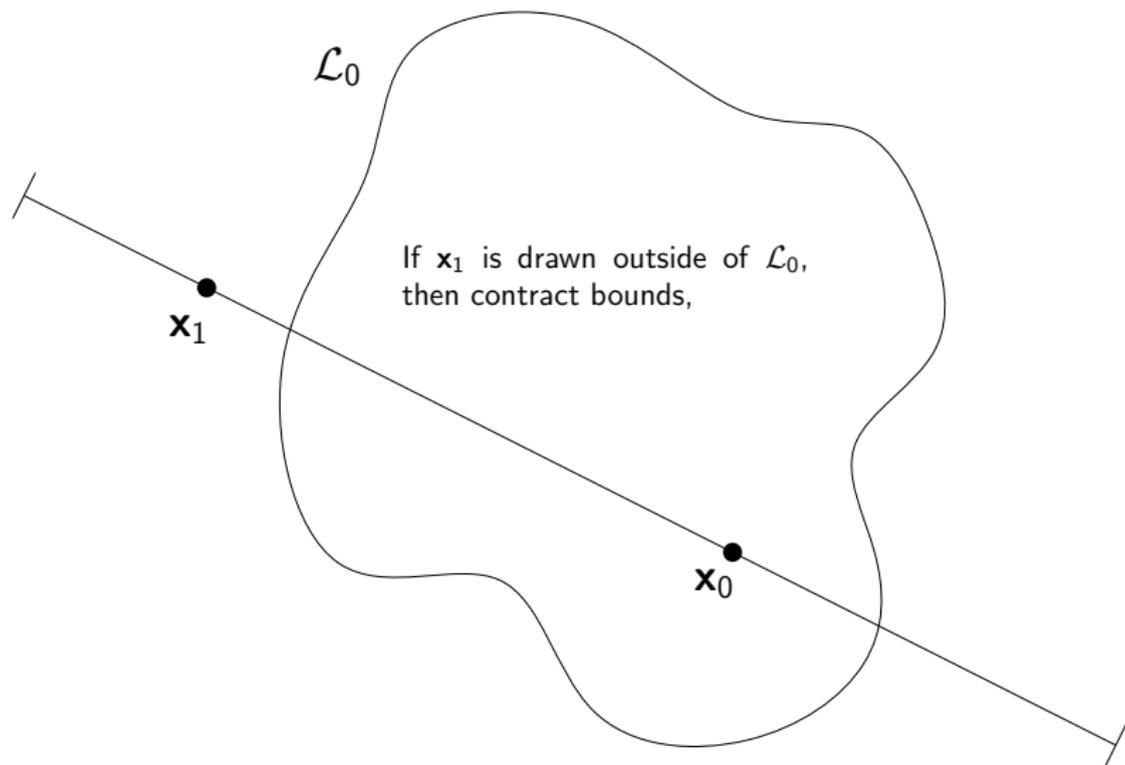
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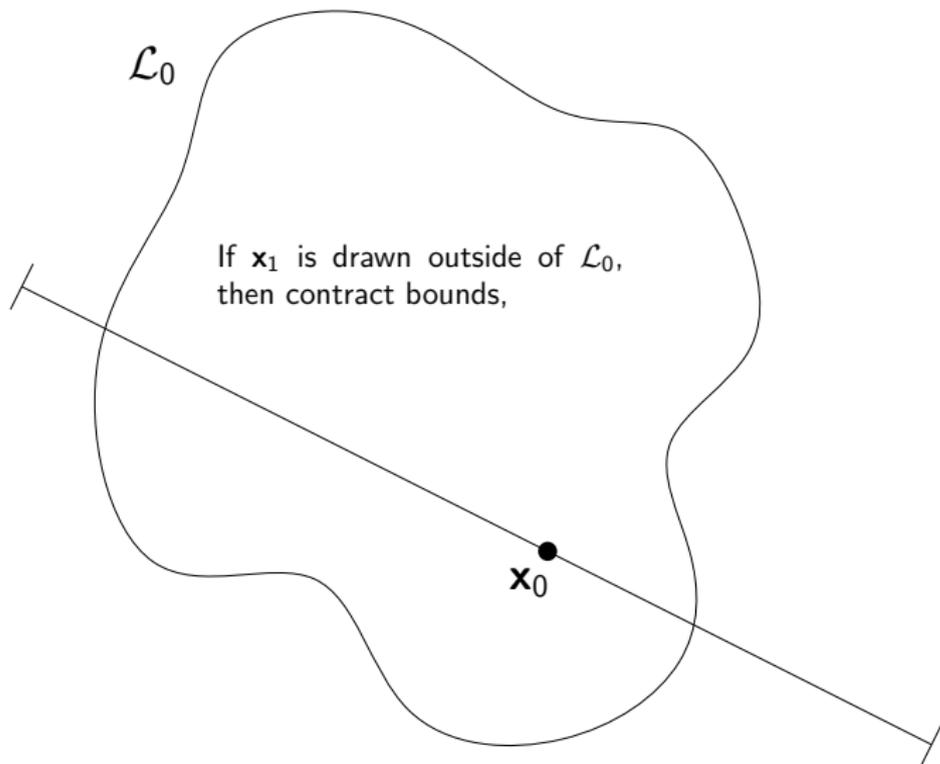
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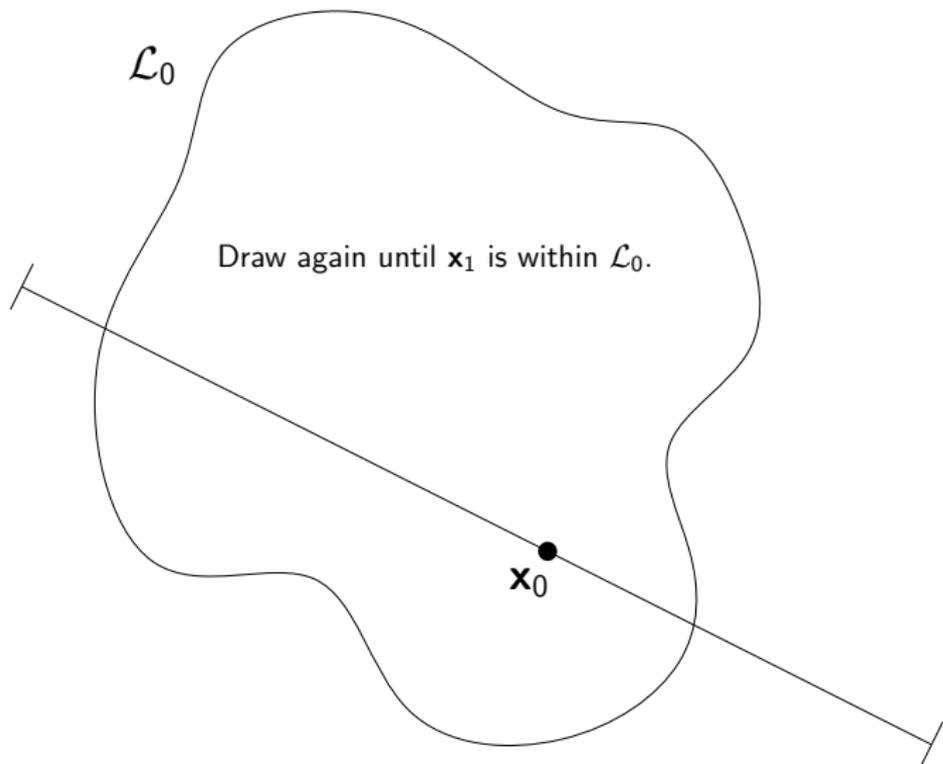
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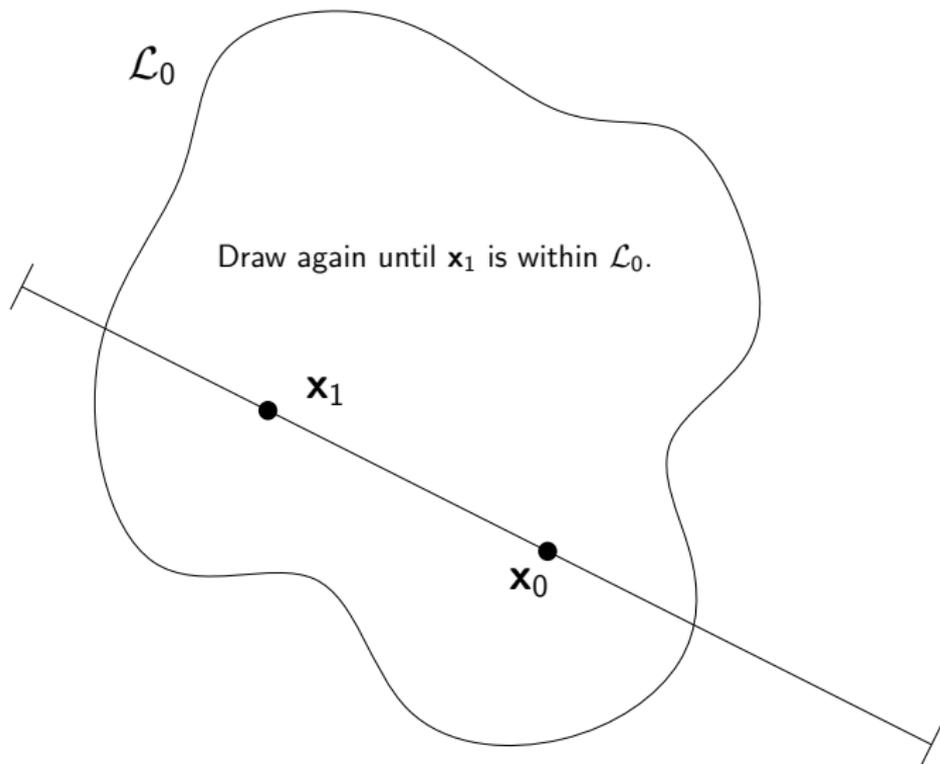
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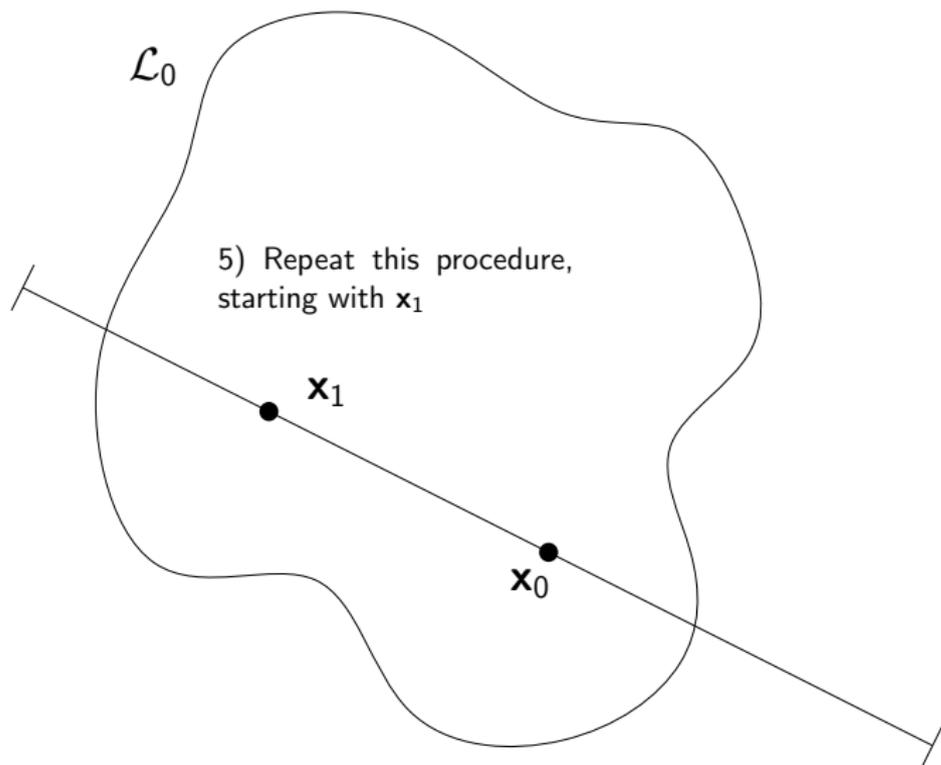
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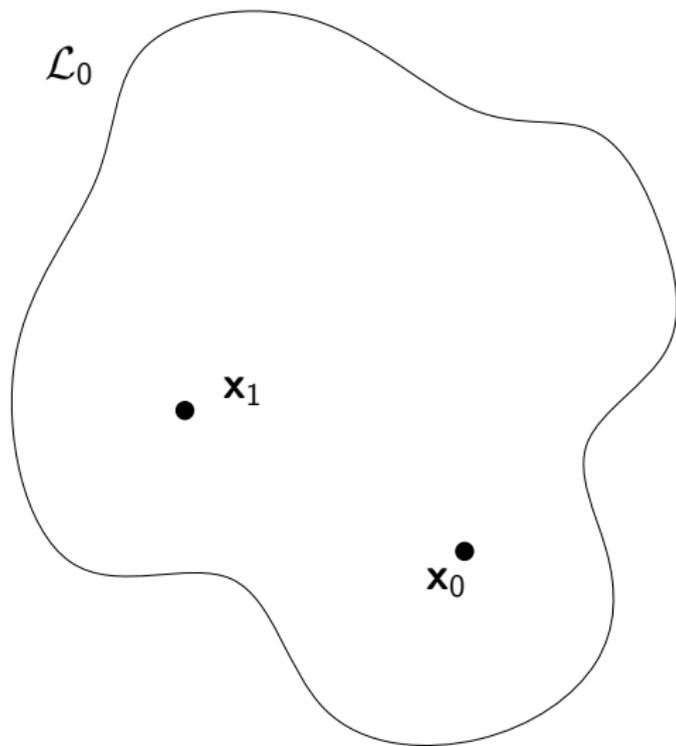
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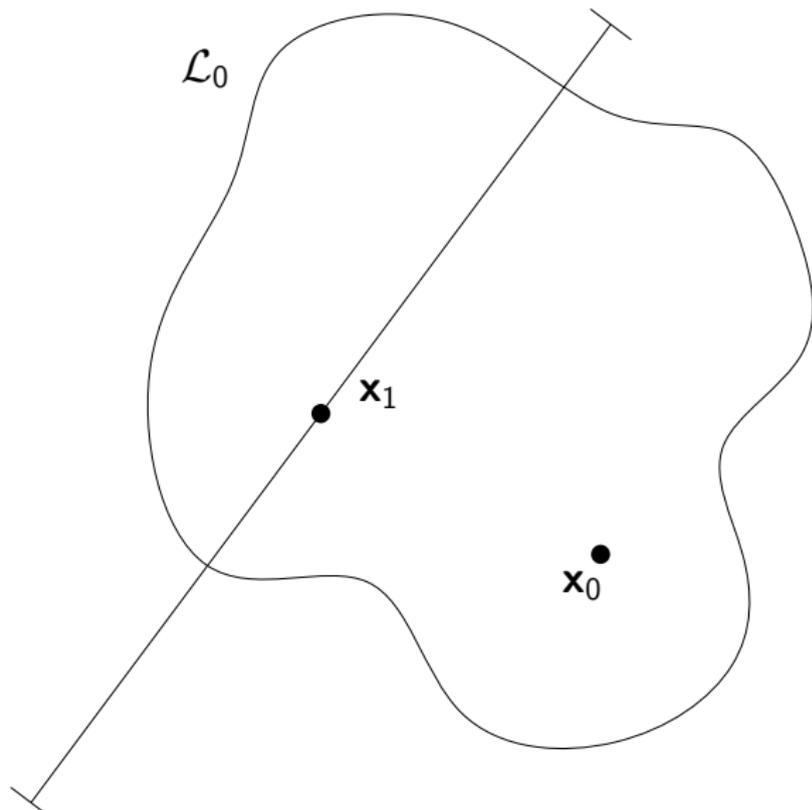
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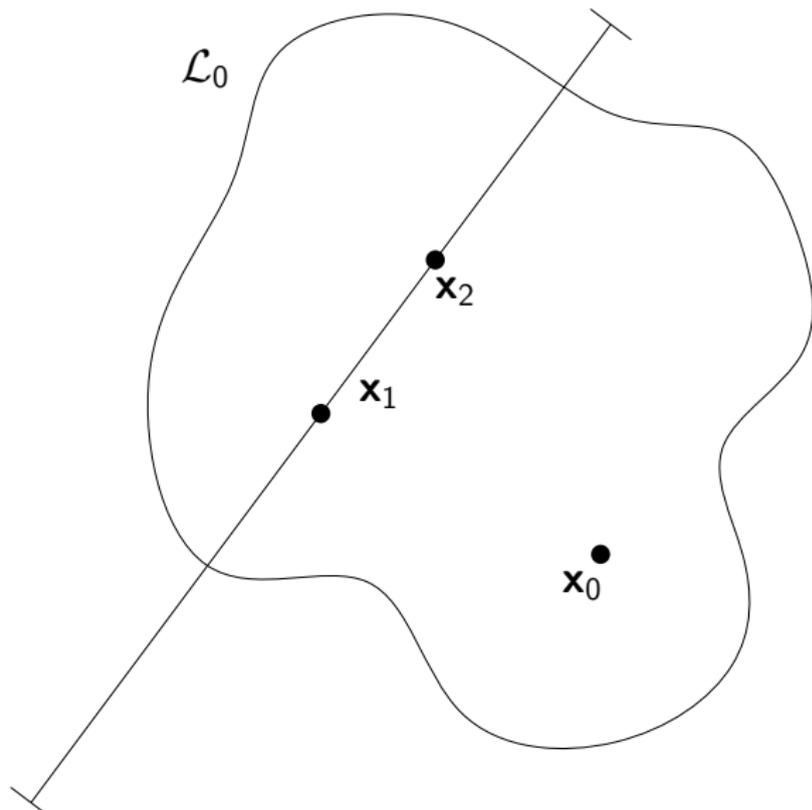
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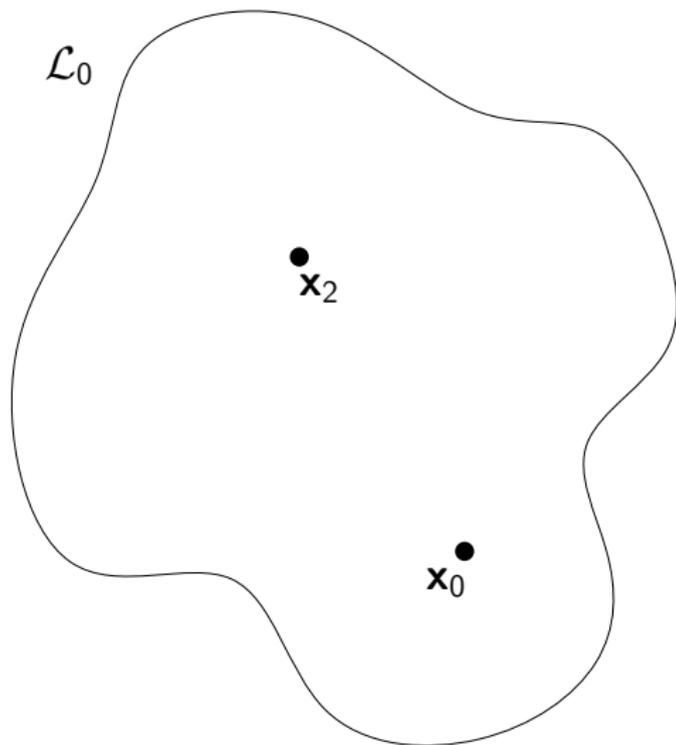
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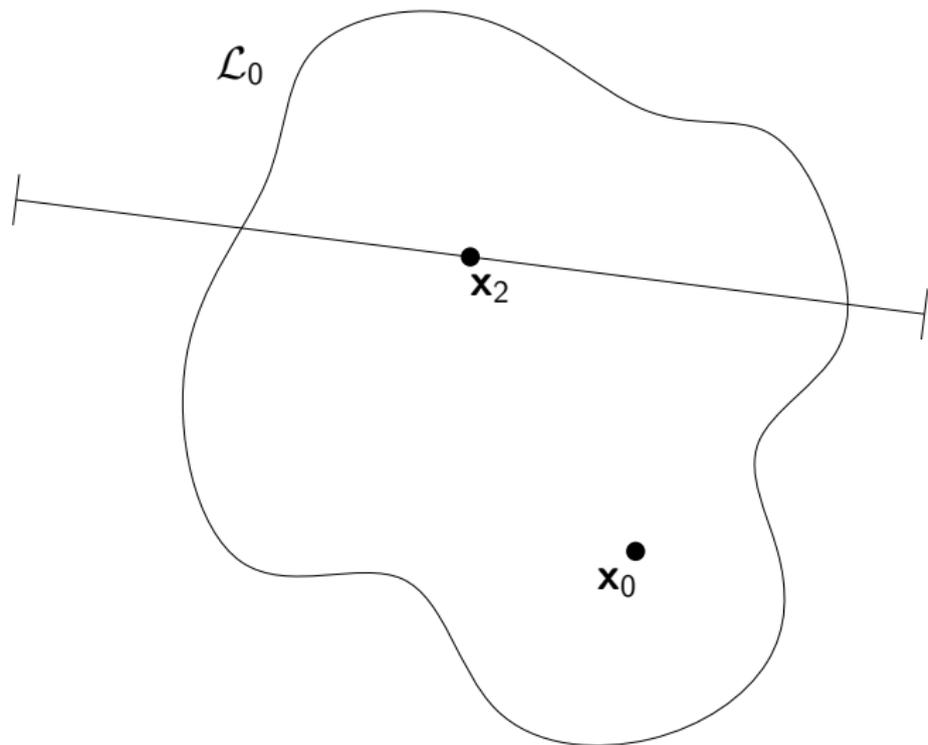
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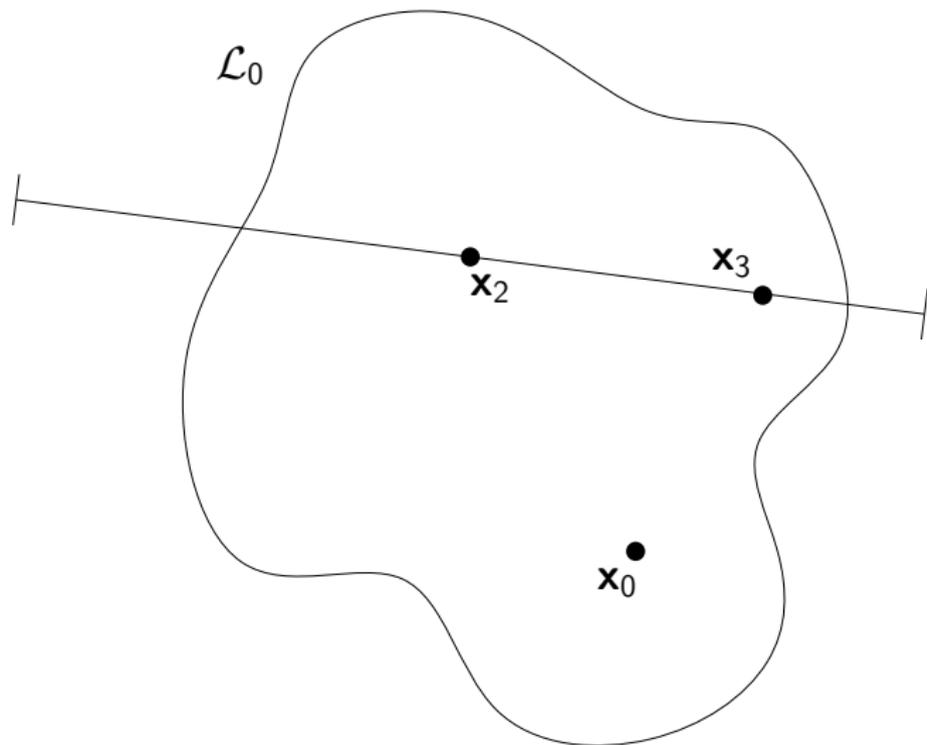
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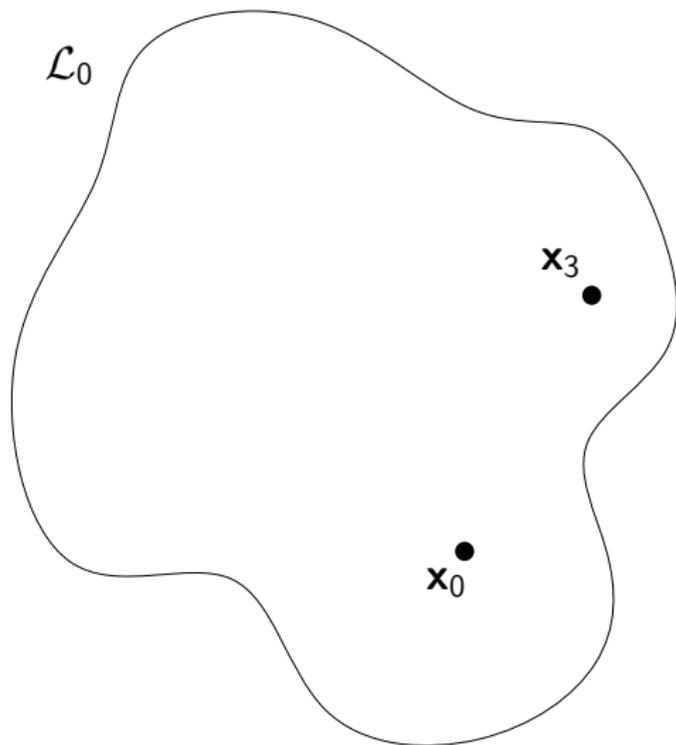
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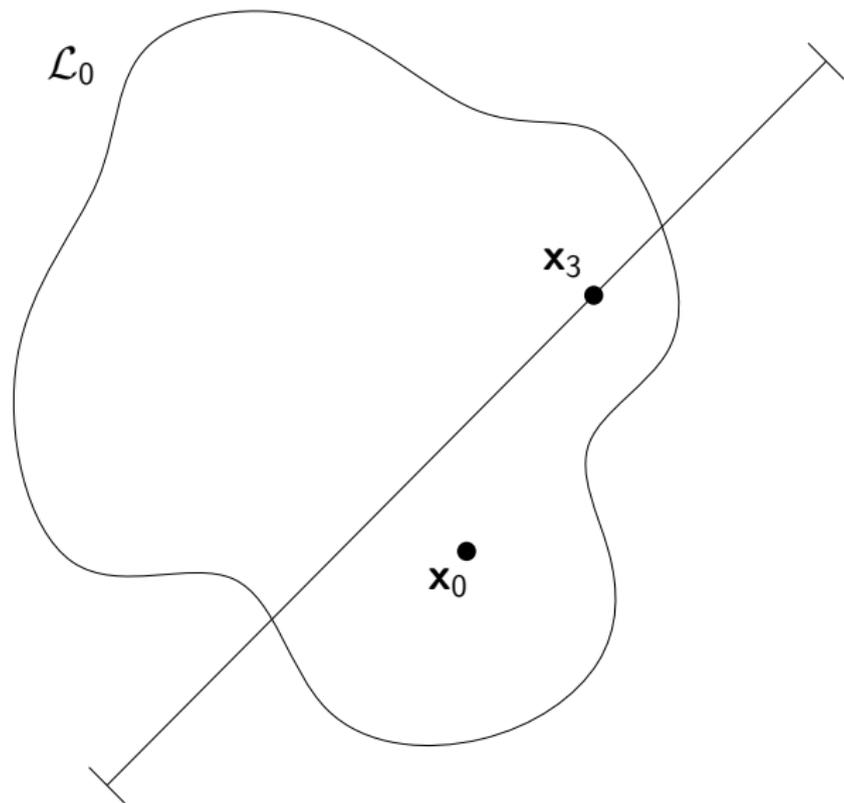
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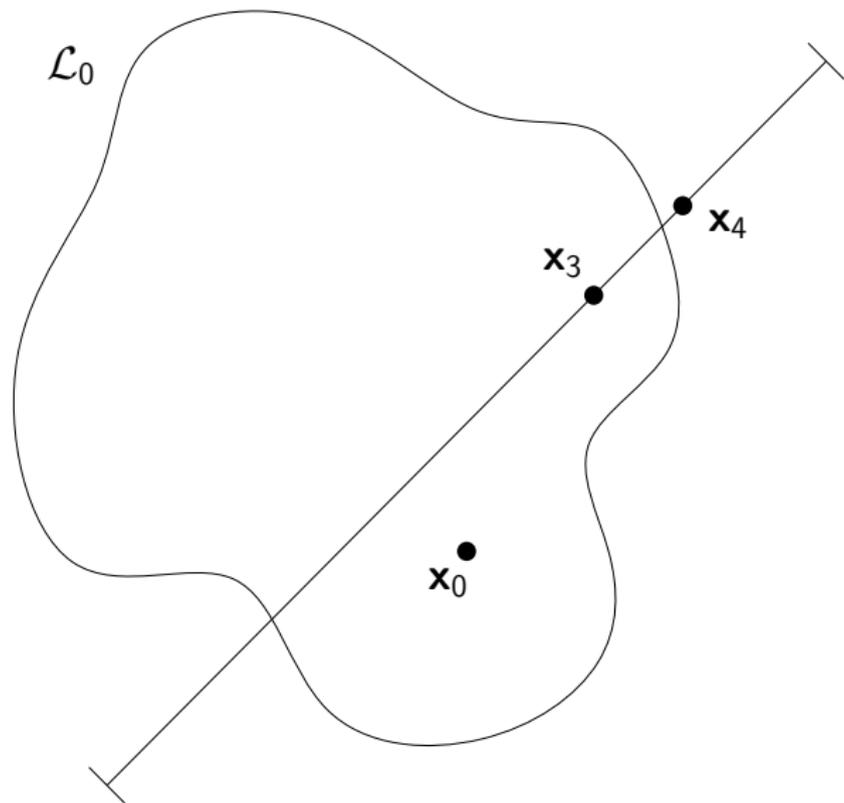
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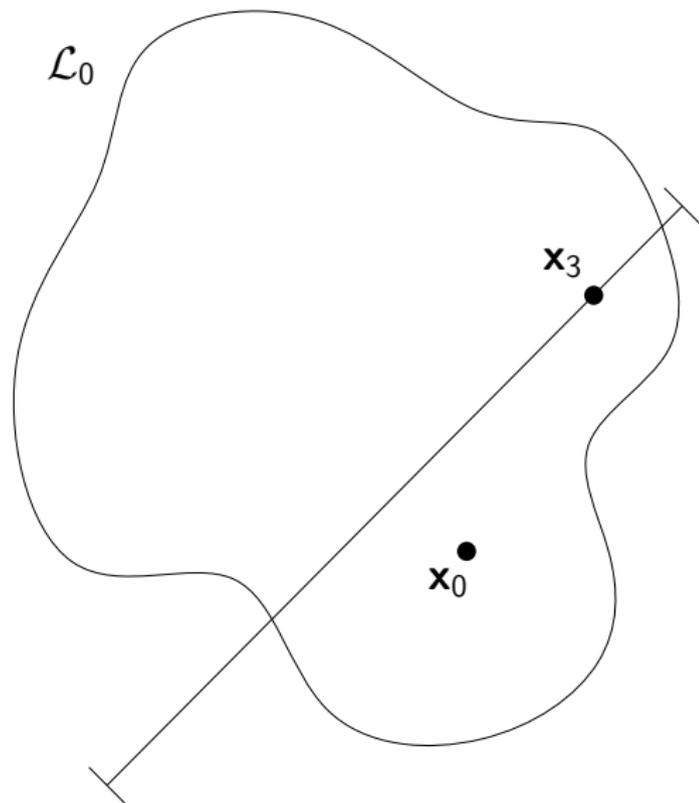
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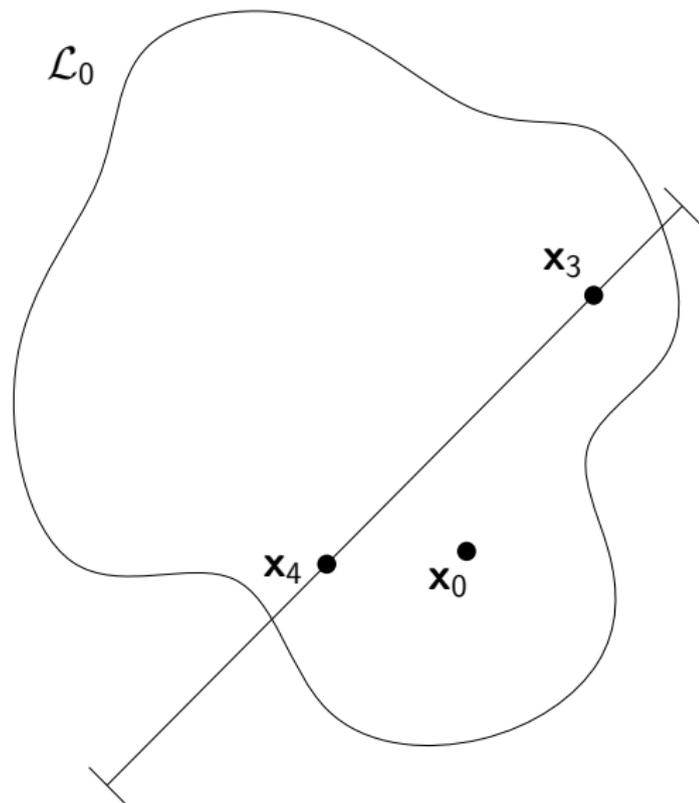
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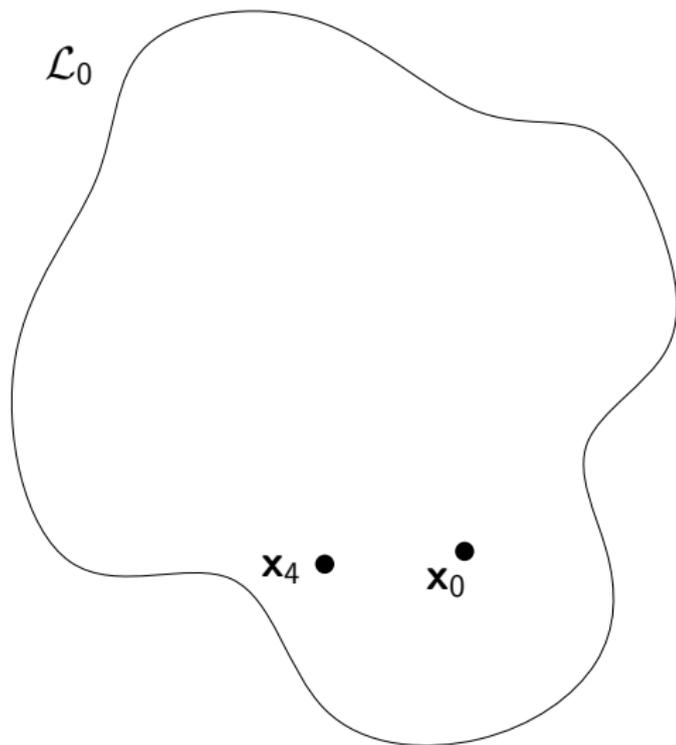
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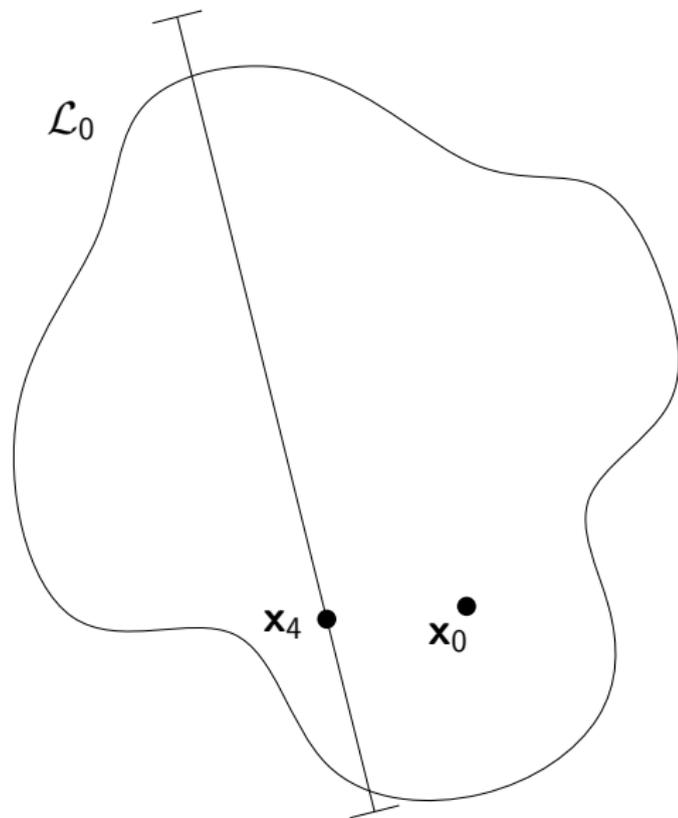
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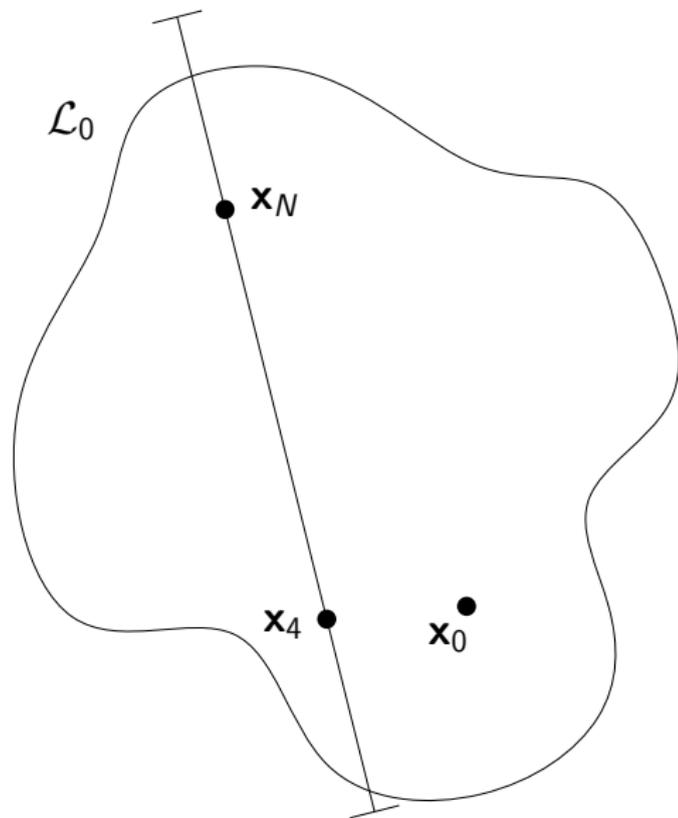
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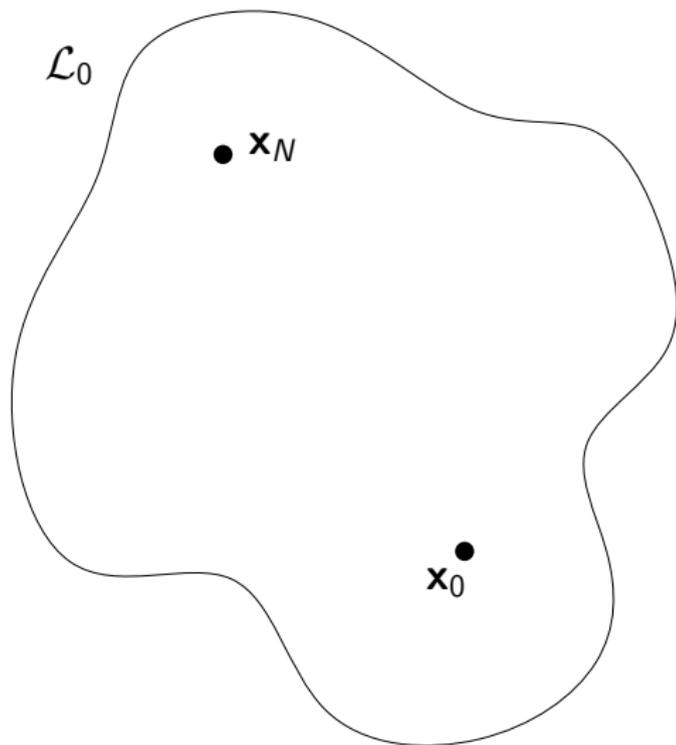
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“Hit and run” slice sampling



PolyChord

Key points

PolyChord

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- ▶ Works even if \mathcal{L}_0 contour is disjoint.
- ▶ Need N reasonably large $\sim \mathcal{O}(n_{\text{dims}})$ so that x_N is de-correlated from x_1 .

Issues with Slice Sampling

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1. Does not deal well with correlated distributions.

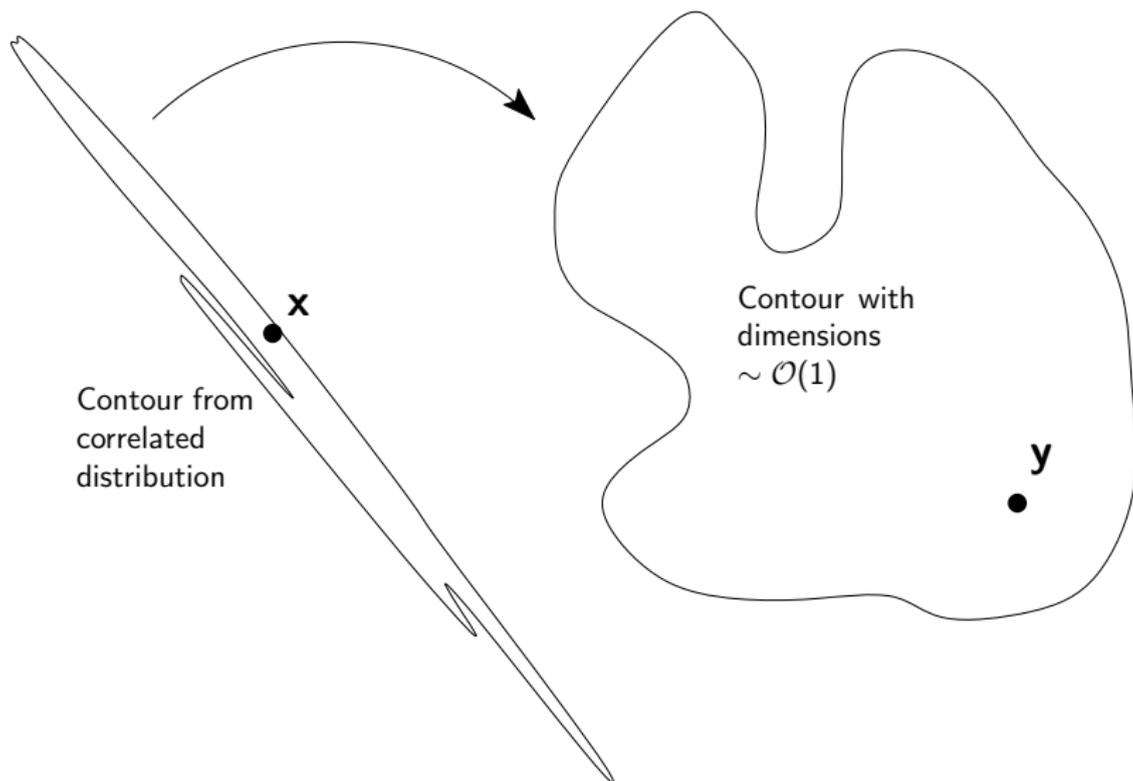
Issues with Slice Sampling

1. Does not deal well with correlated distributions.
2. Need to “tune” w parameter.

PolyChord's solutions

Correlated distributions

Affine transformation $\mathbf{y} = L\mathbf{x}$



PolyChord's solutions

Correlated distributions

PolyChord's solutions

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PolyChord's Additions

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- ▶ Parallelised up to number of live points with openMPI.

PolyChord's Additions

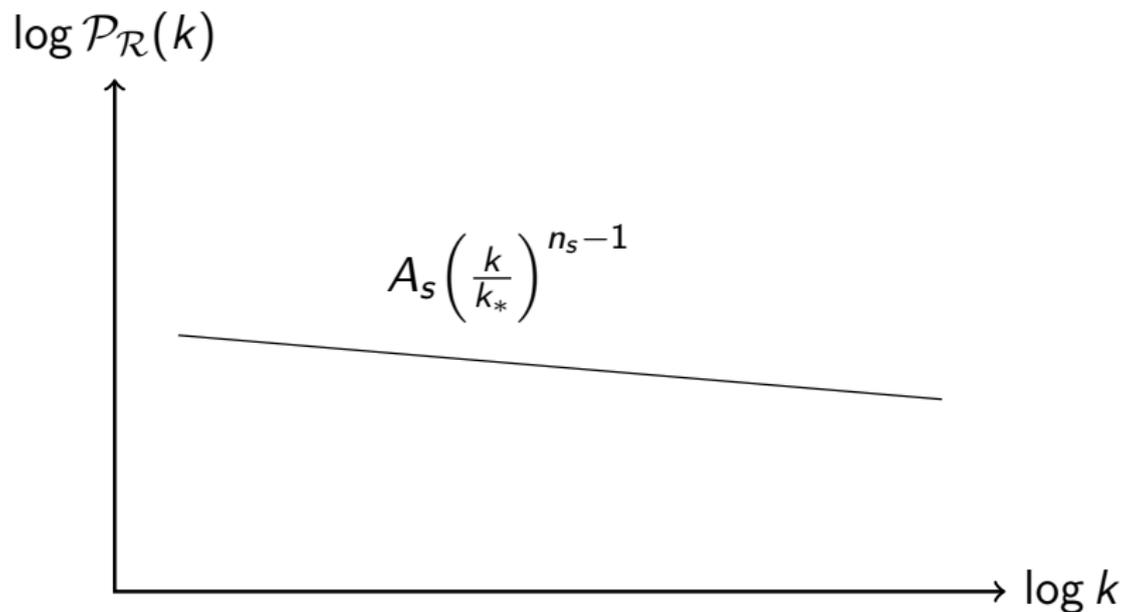
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PolyChord's Additions

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

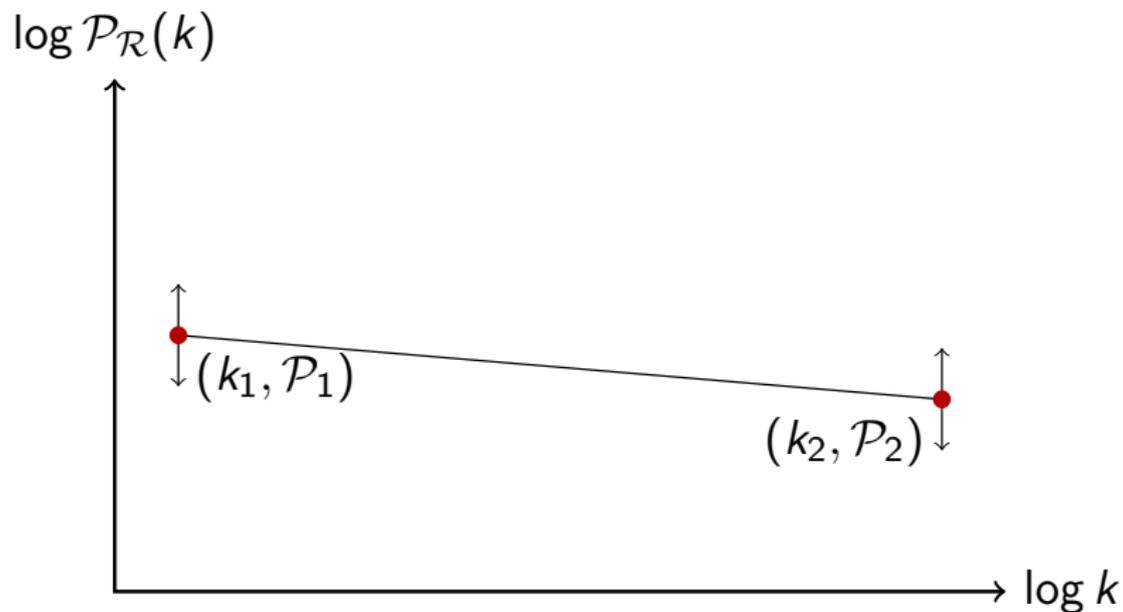
PolyChord in action

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



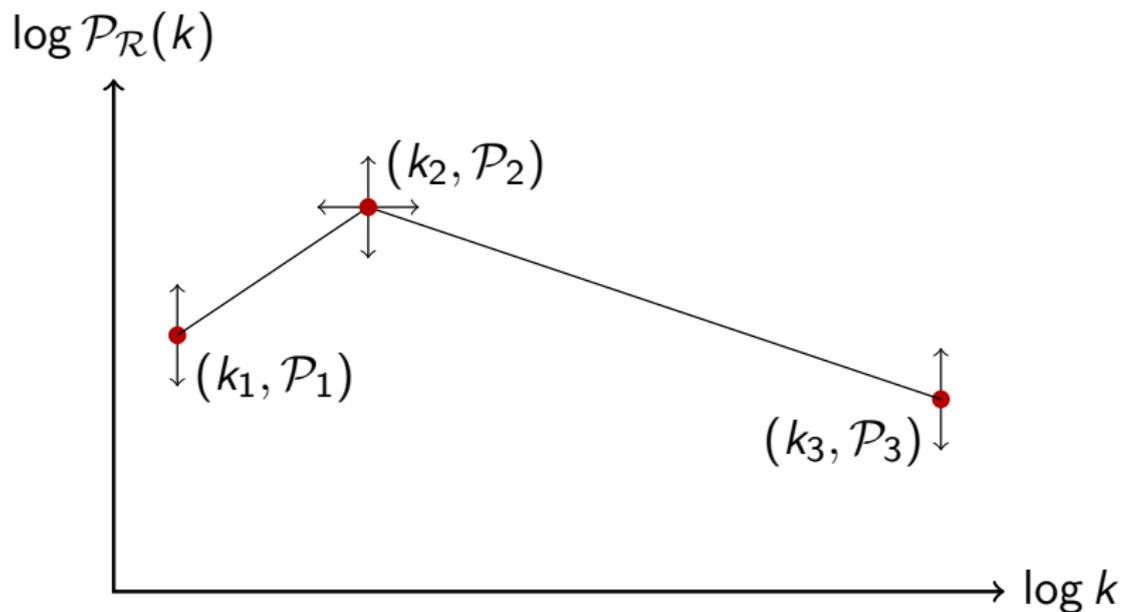
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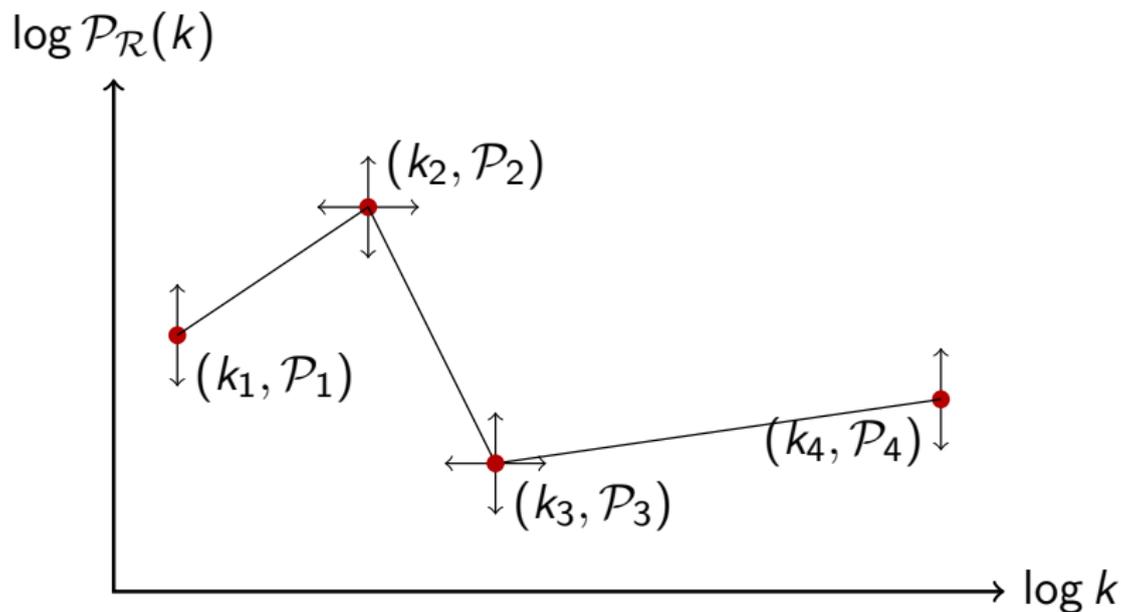
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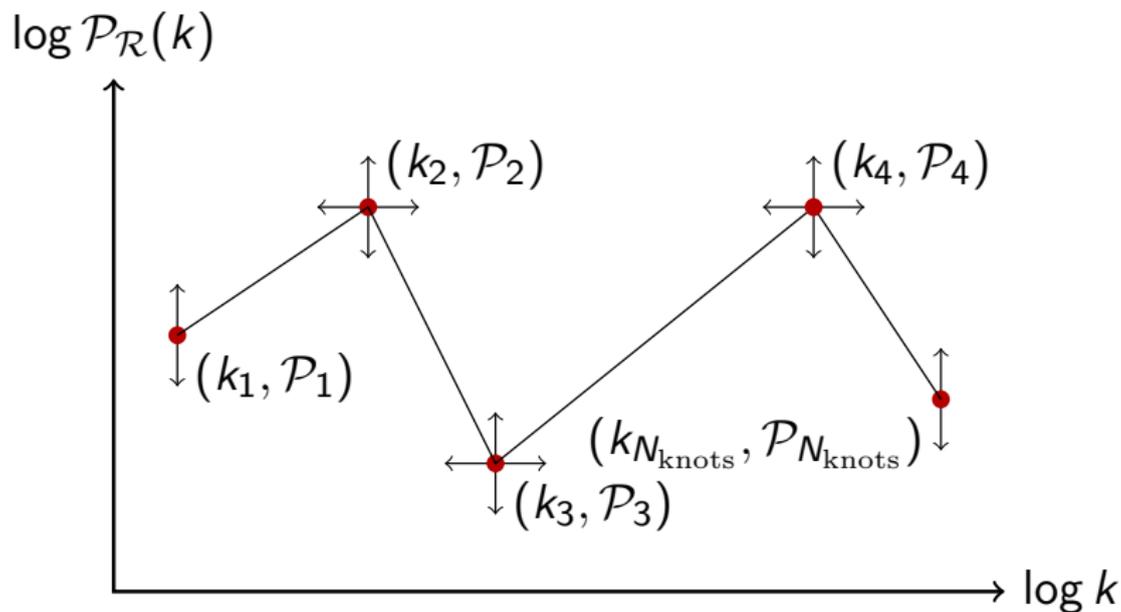
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Planck data

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

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- ▶ Temperature data TT+lowP

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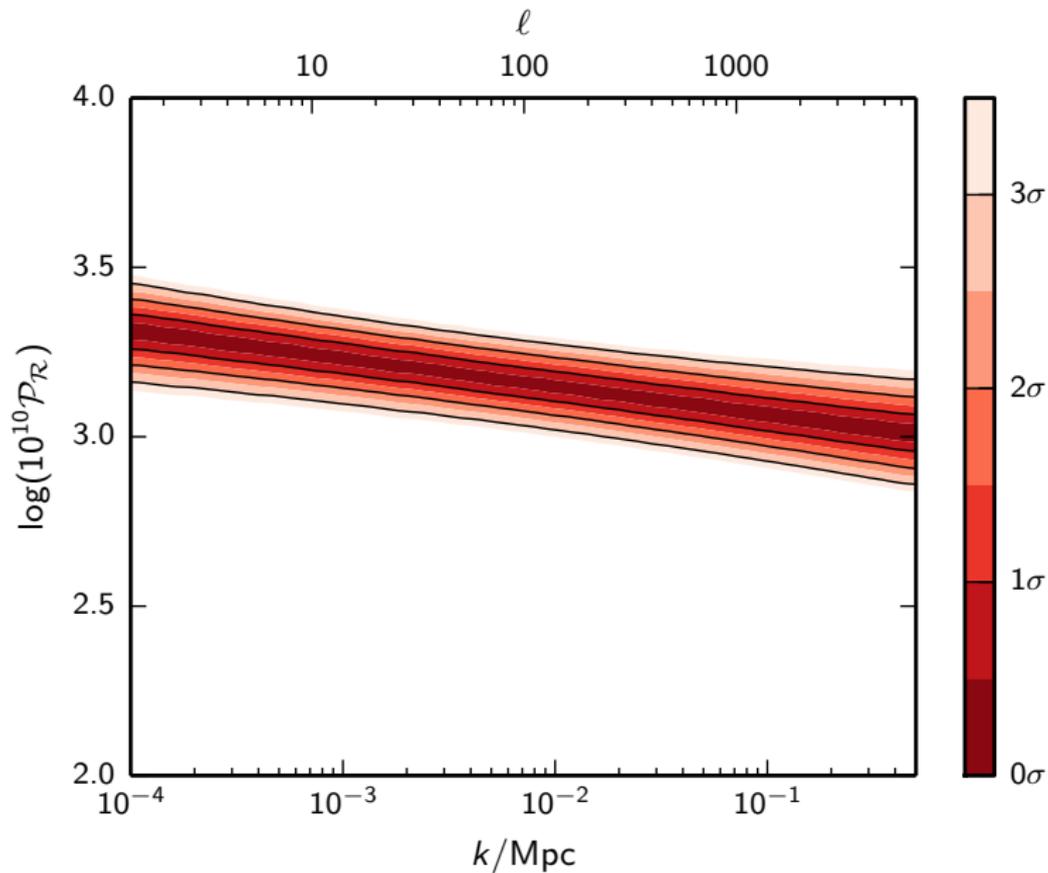
Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction

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- ▶

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

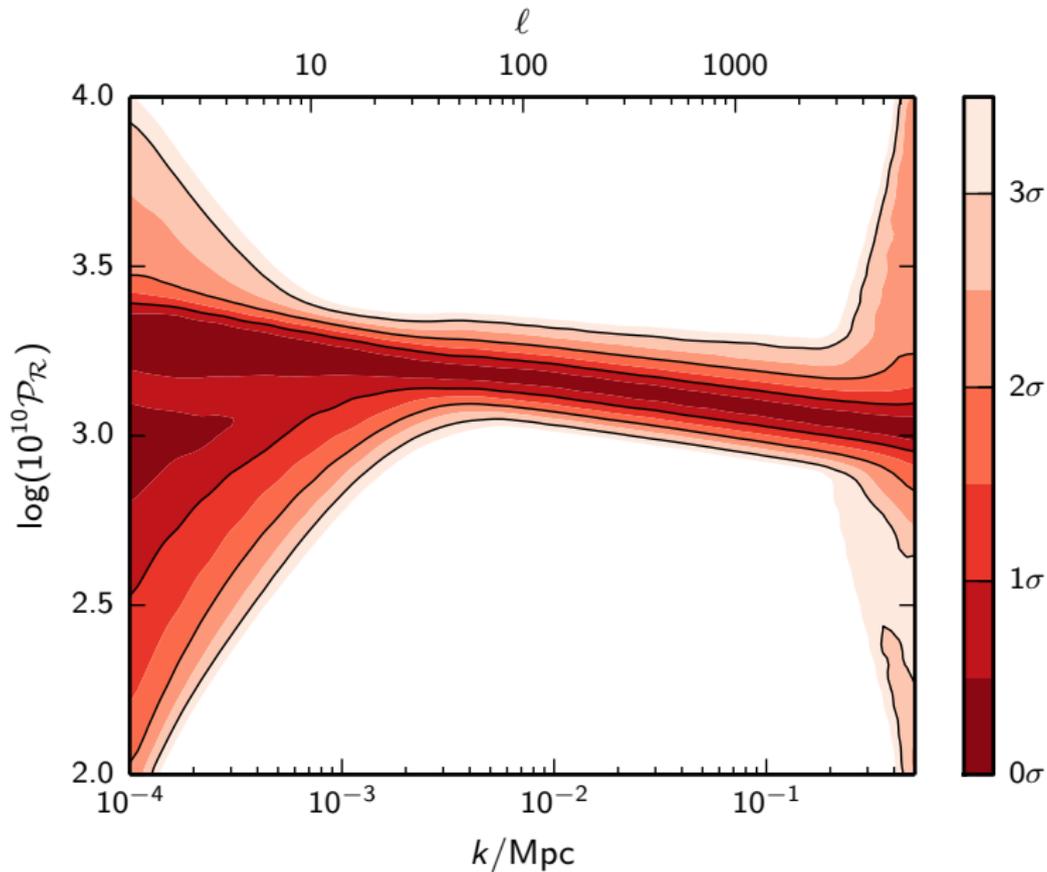
0 internal knots

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



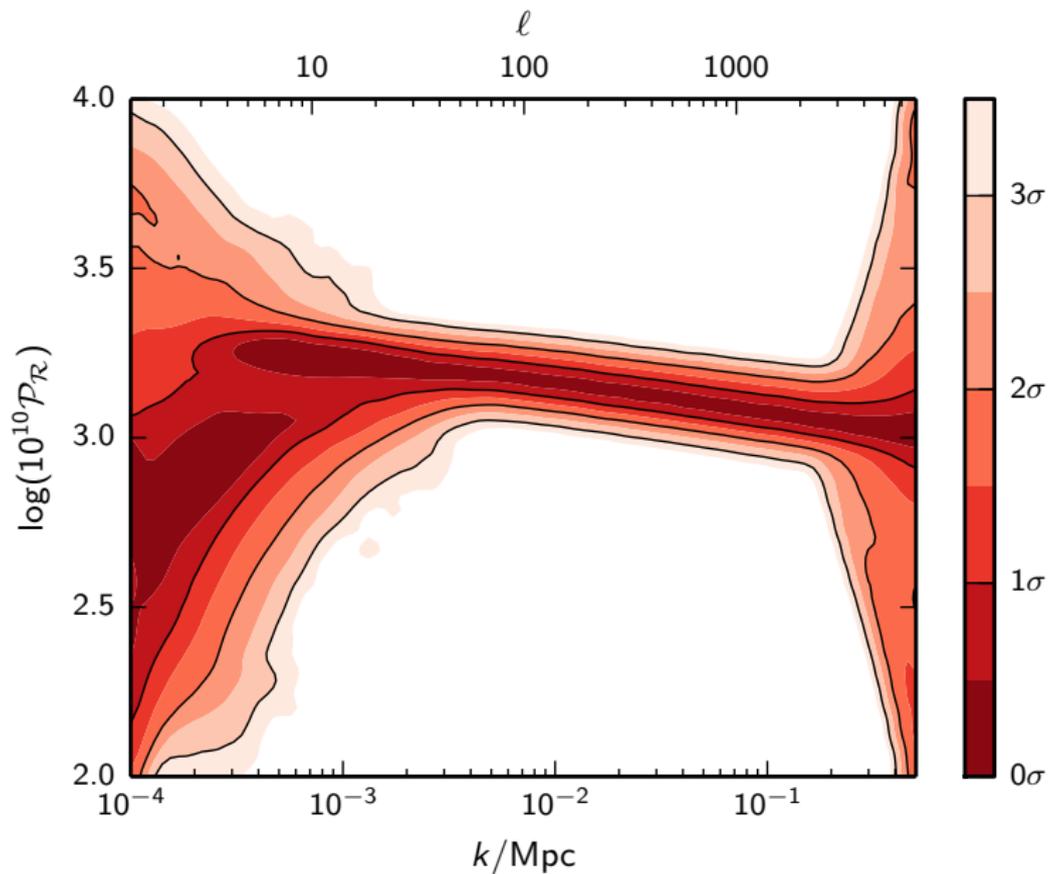
1 internal knots

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



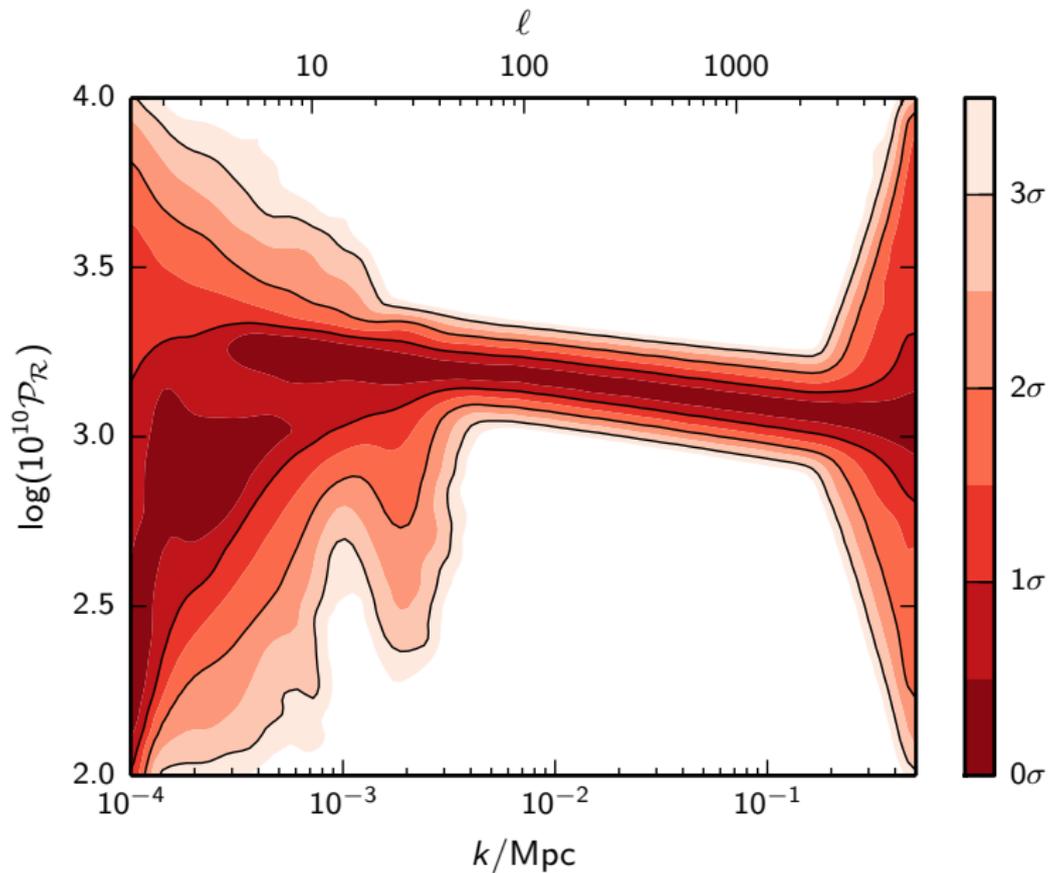
2 internal knots

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



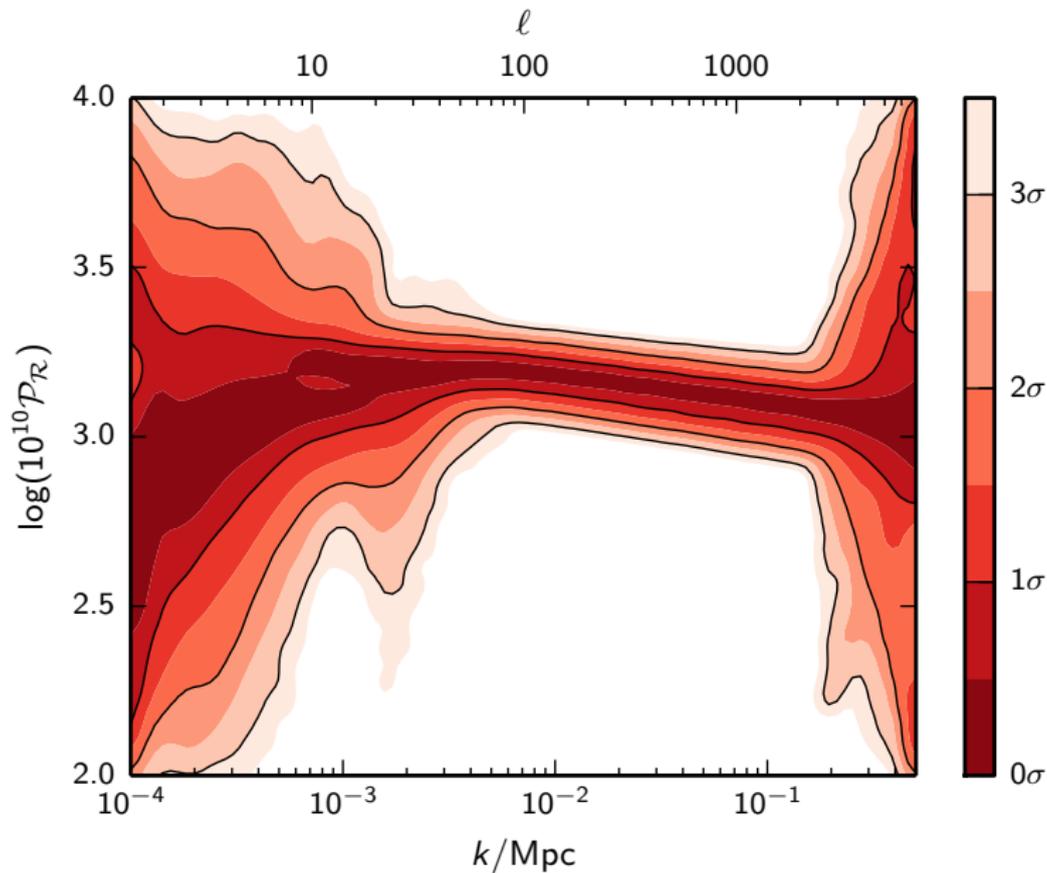
3 internal knots

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



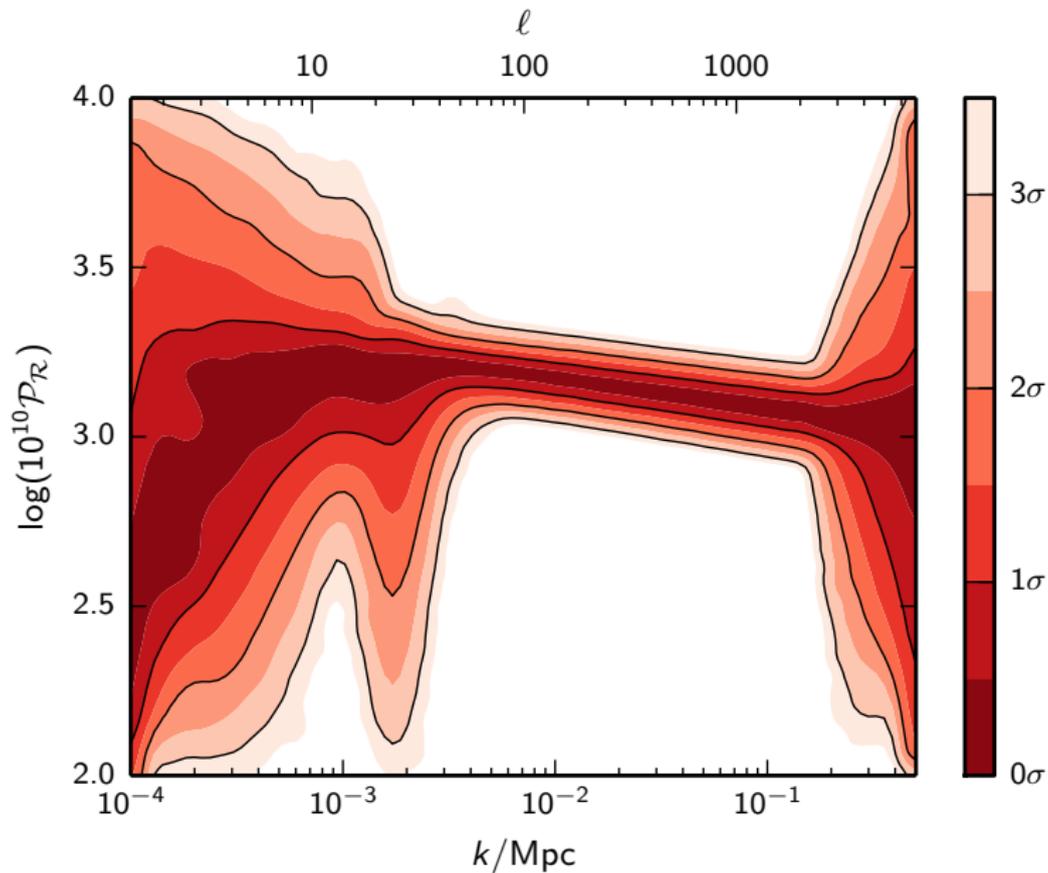
4 internal knots

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



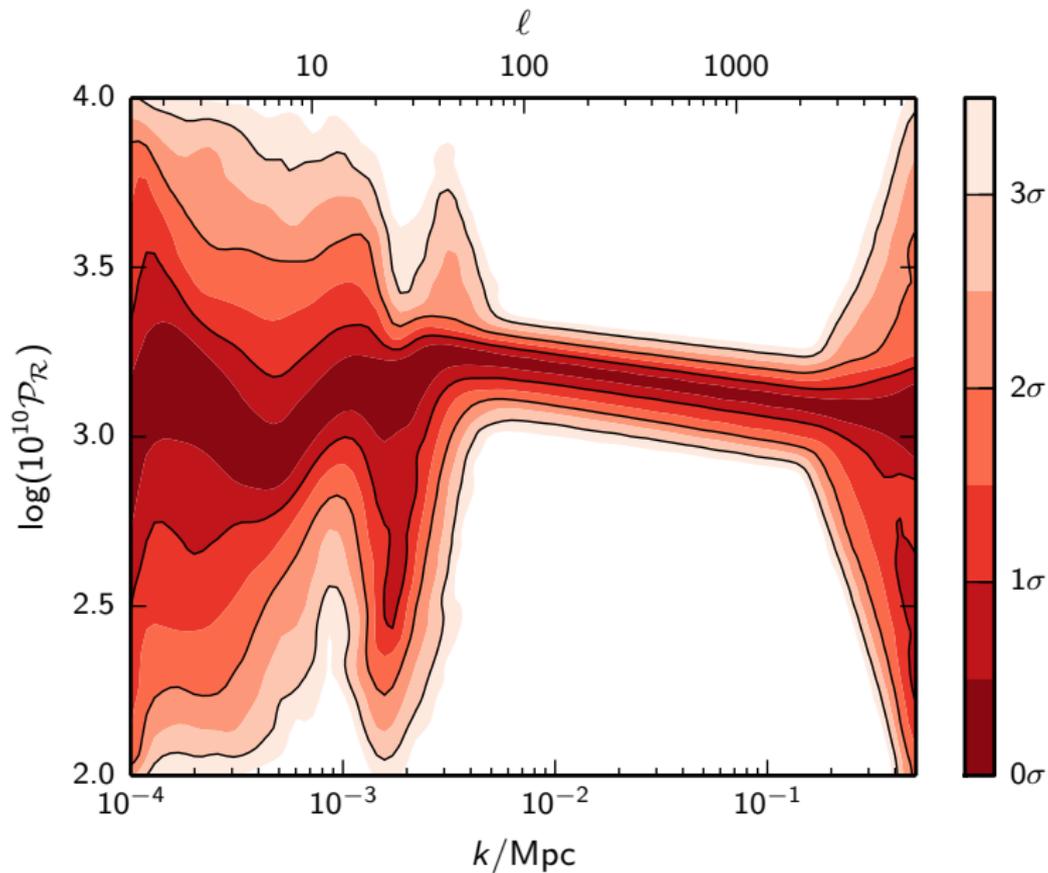
5 internal knots

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



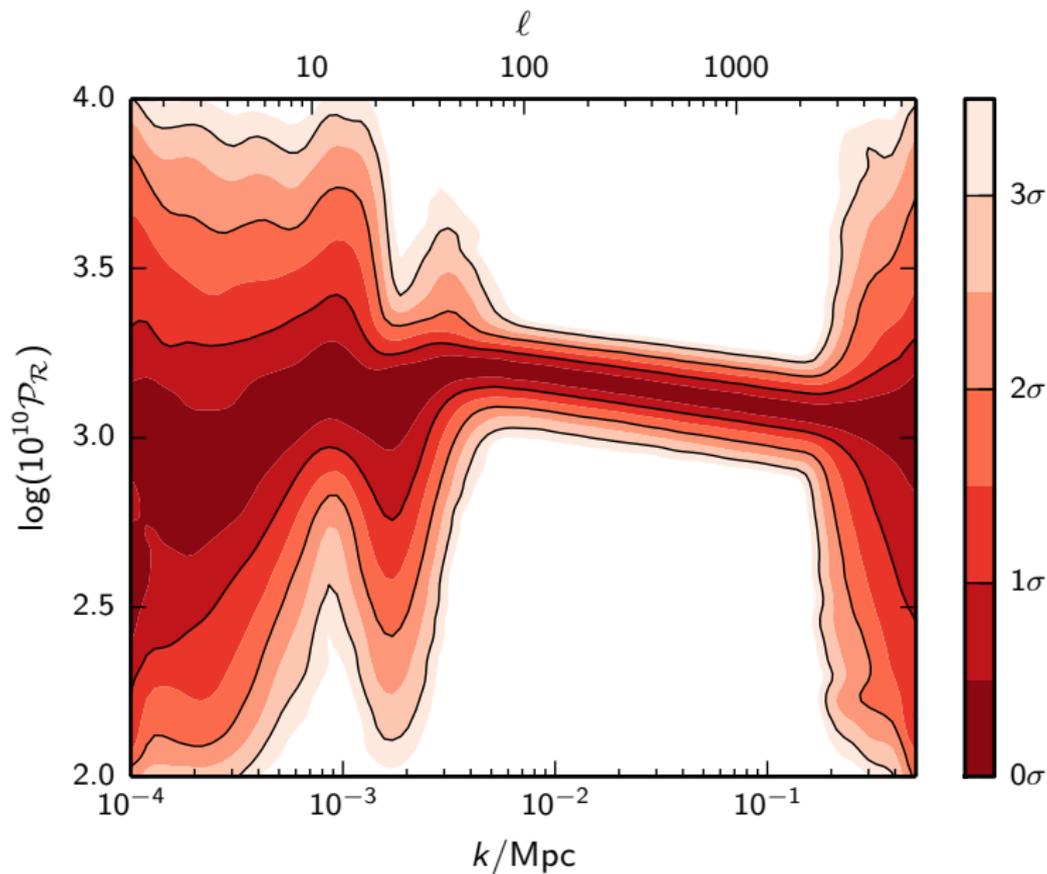
6 internal knots

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



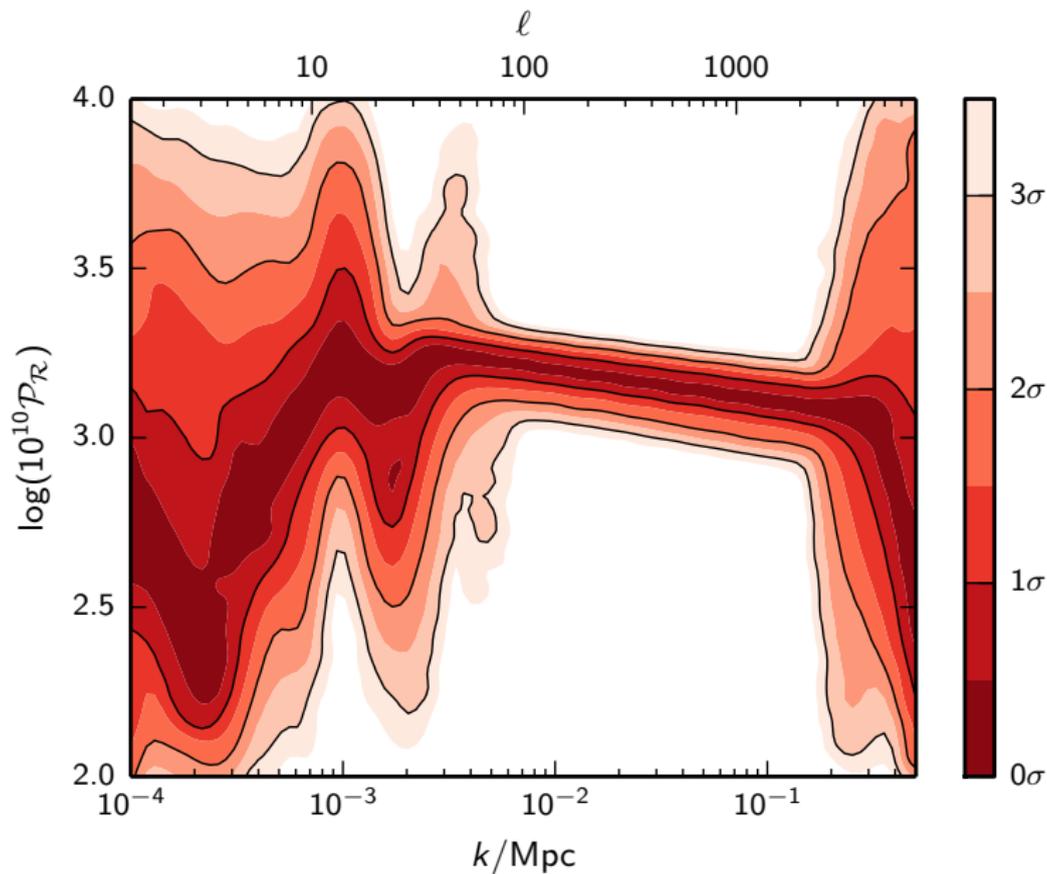
7 internal knots

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



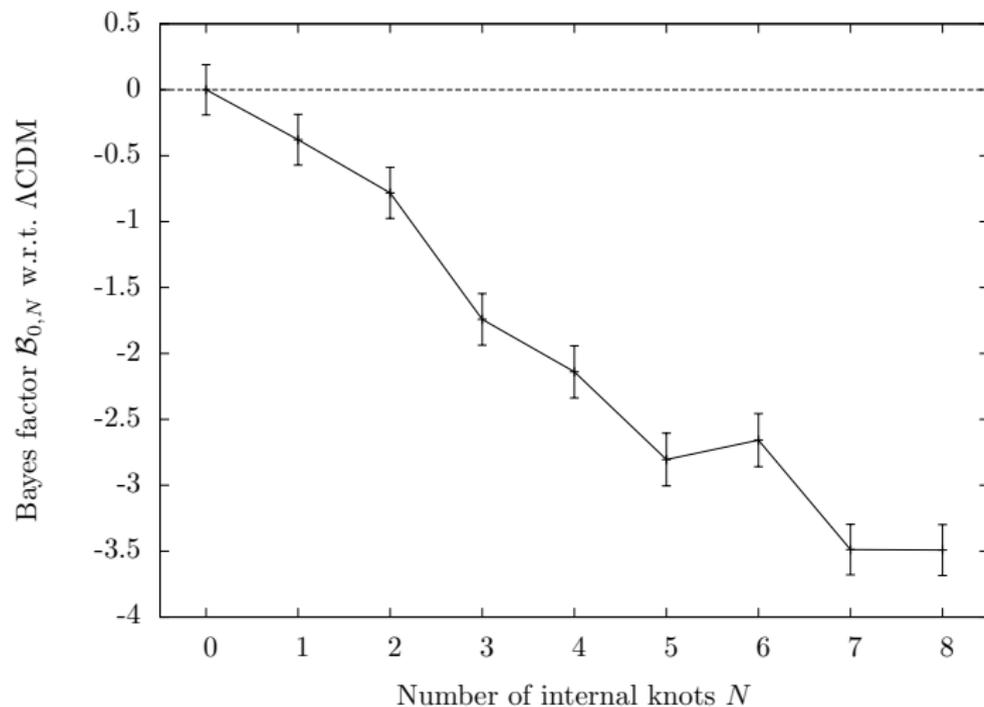
8 internal knots

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



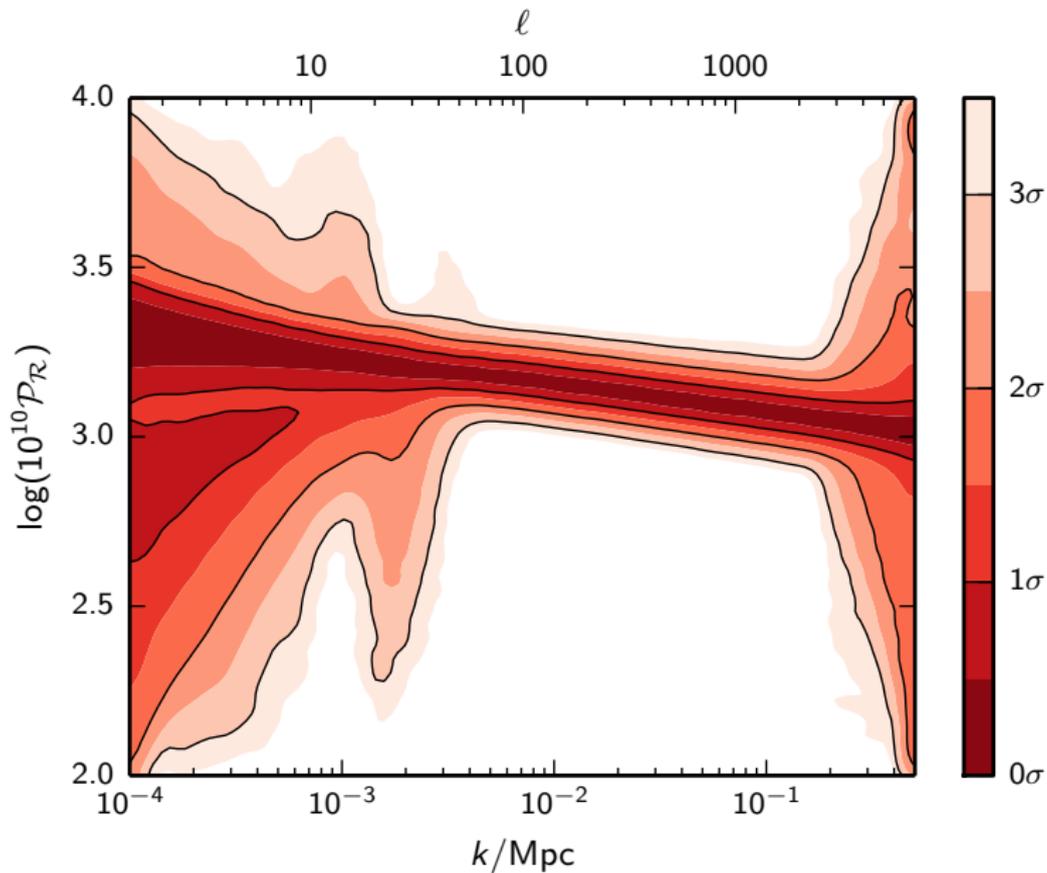
Bayes Factors

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



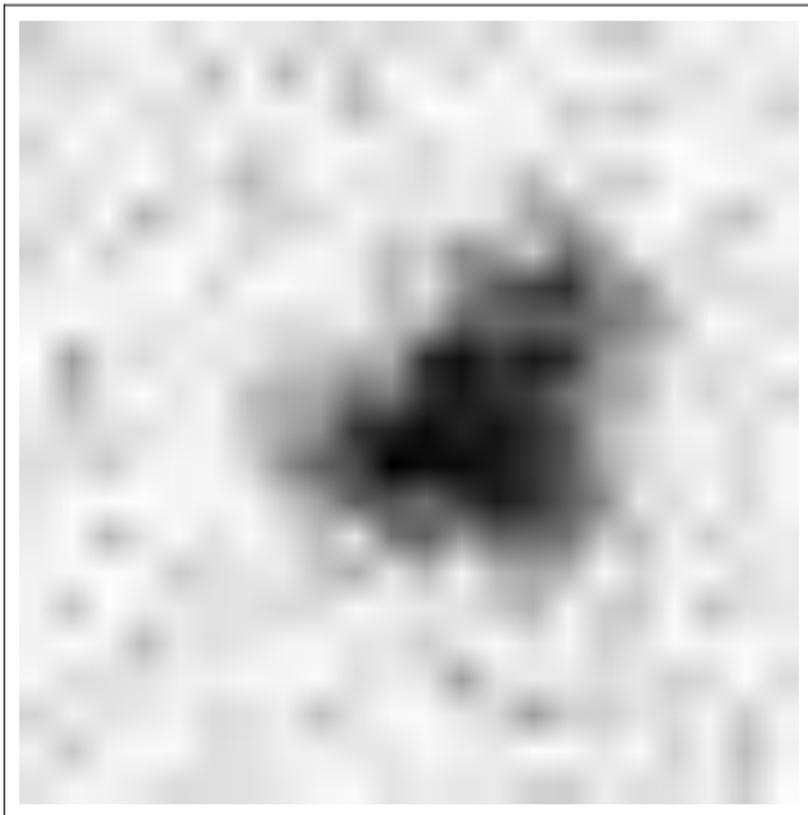
Marginalised plot

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



Object detection

Toy problem



Object detection

Evidences

Object detection

Evidences

- ▶ $\log \mathcal{Z}$ ratio: $-251 : -156 : -114 : -117 : -136$

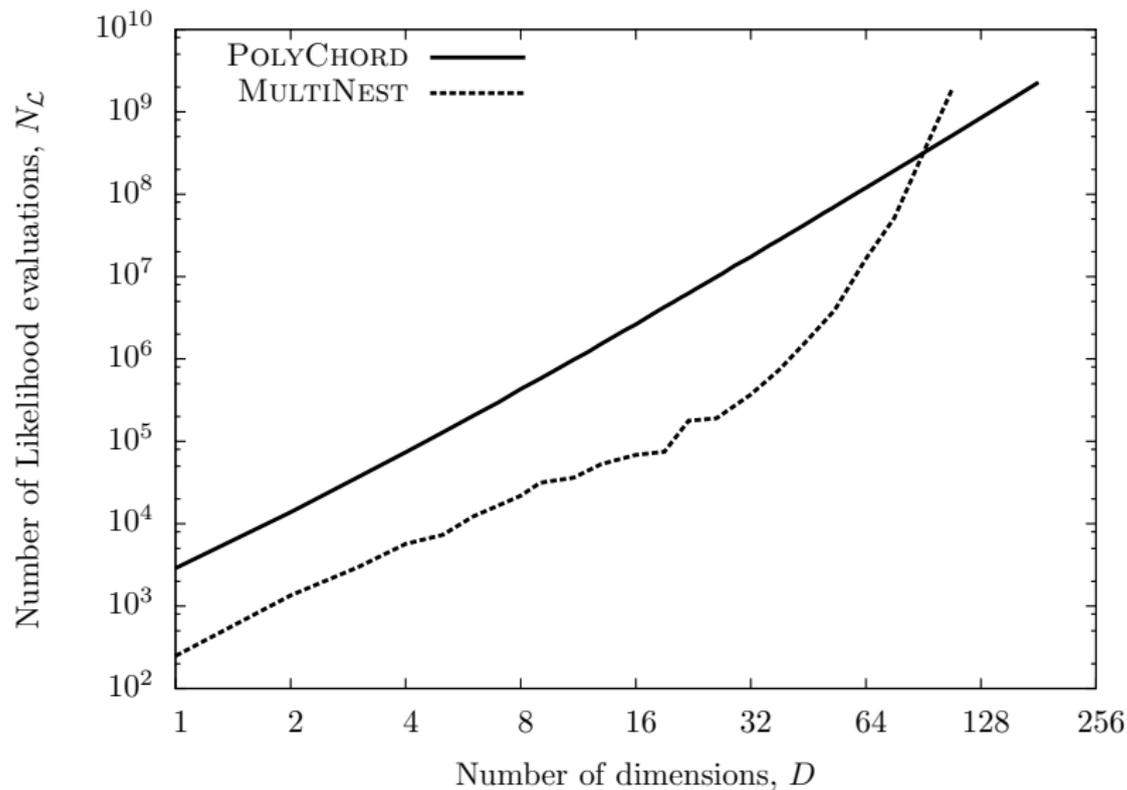
Object detection

Evidences

- ▶ $\log \mathcal{Z}$ ratio: $-251 : -156 : -114 : -117 : -136$
- ▶ odds ratio: $10^{-60} : 10^{-19} : 1 : 0.04 : 10^{-10}$

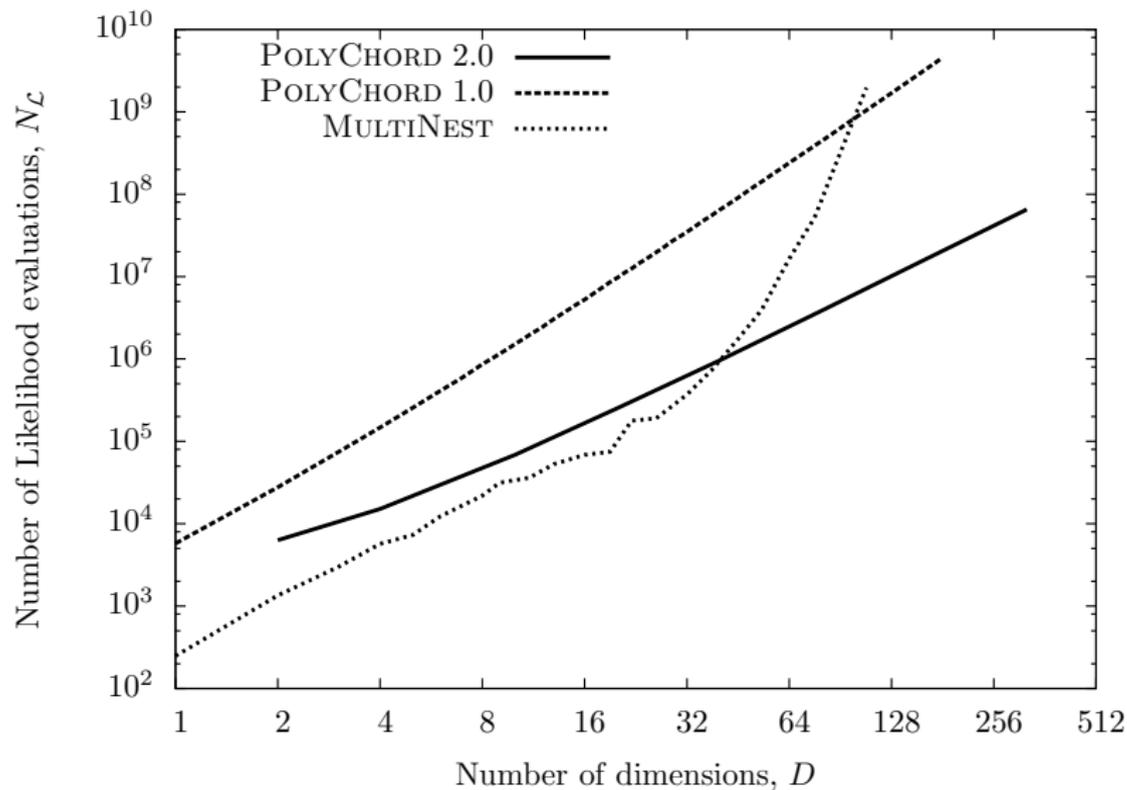
PolyChord vs. MultiNest

Gaussian likelihood



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Conclusions

The future of nested sampling

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