

# PolyChord & the future of nested sampling

## Sampling, Parameter Estimation and Bayesian Model Comparison

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Cavendish Laboratory  
University of Cambridge

March 8, 2016

Parameter estimation & model comparison

Metropolis Hastings

Nested Sampling

PolyChord

Applications

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- ▶ Nested sampling is an alternative sampling approach.
- ▶ Unlike traditional methods, it does not sample from the posterior directly.
- ▶ Instead it gradually compresses the prior onto the posterior.
- ▶ In doing so, it circumvents many issues (dimensionality, topology, geometry) that beset normal approaches.
- ▶ Similar to simulated annealing, but automatically picks the “correct” annealing schedule.

# Bayes' theorem

Parameter estimation



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## Parameter estimation

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$$P(M_i|D) = \frac{P(D|M_i)P(M_i)}{P(D)}$$

$$P(M_i|D) = \frac{\mathcal{Z}_i \mu_i}{\sum_k \mathcal{Z}_k \mu_k}$$

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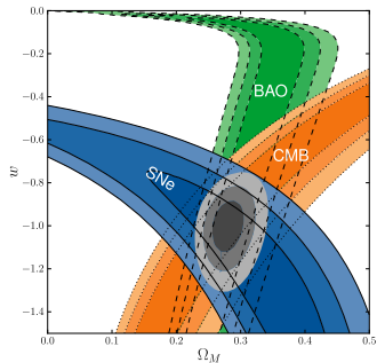
## The challenge

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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

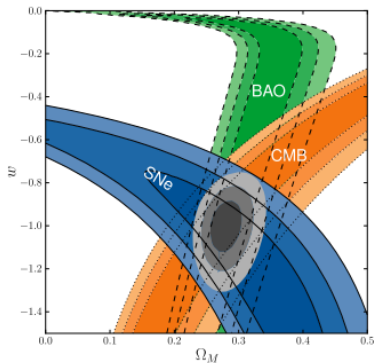
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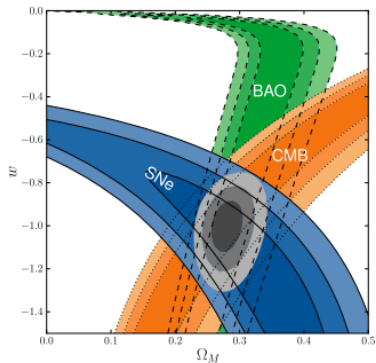
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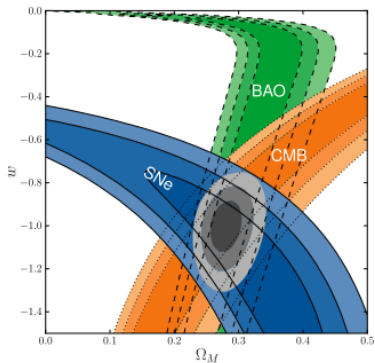
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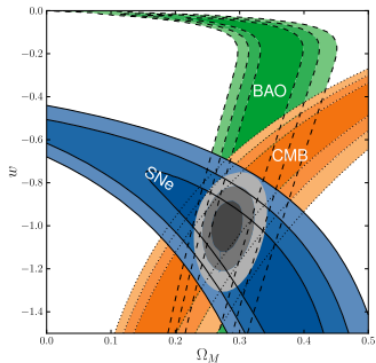


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- ▶ Describing an  $N$ -dimensional posterior fully is impossible.
- ▶ *Sampling* the posterior is an excellent compression scheme.



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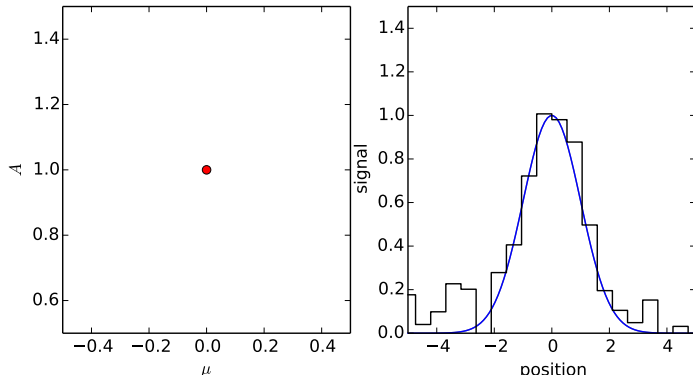
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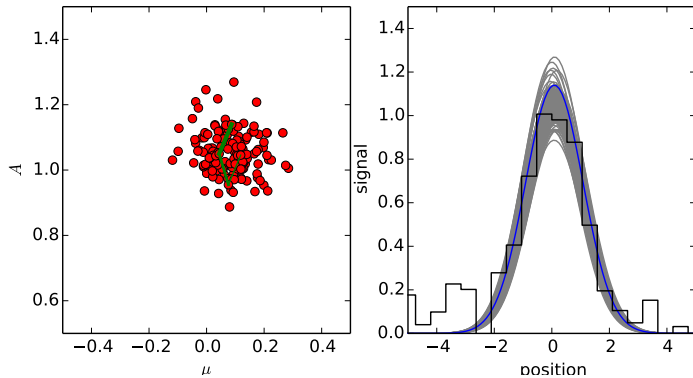
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  4. ...otherwise sometimes make step.

# MCMC in action



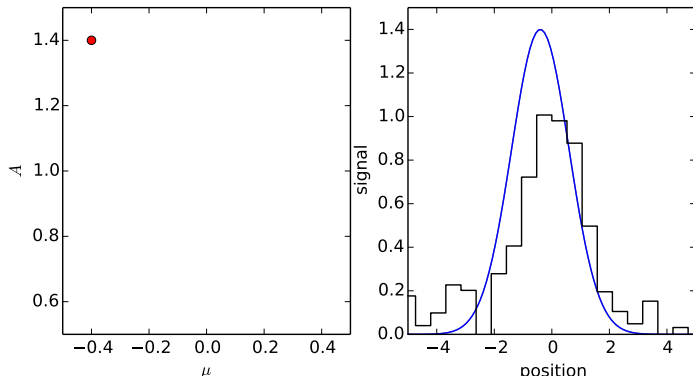


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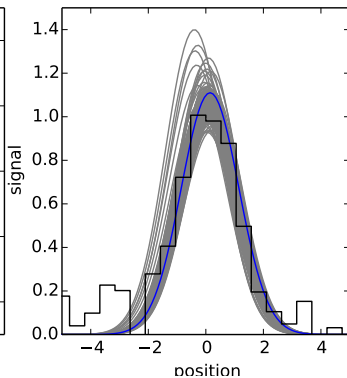
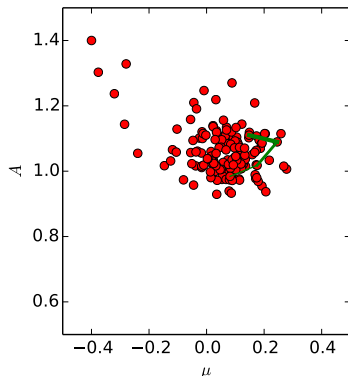
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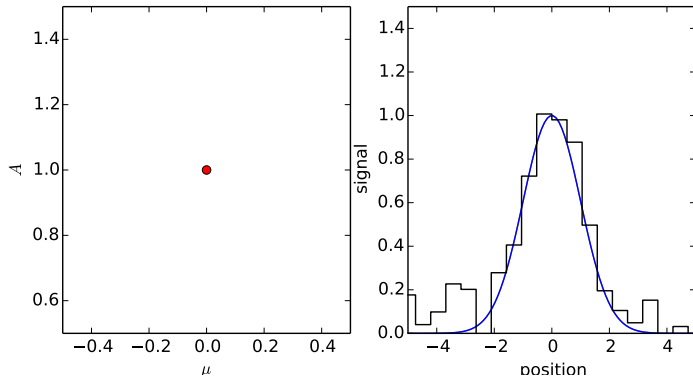
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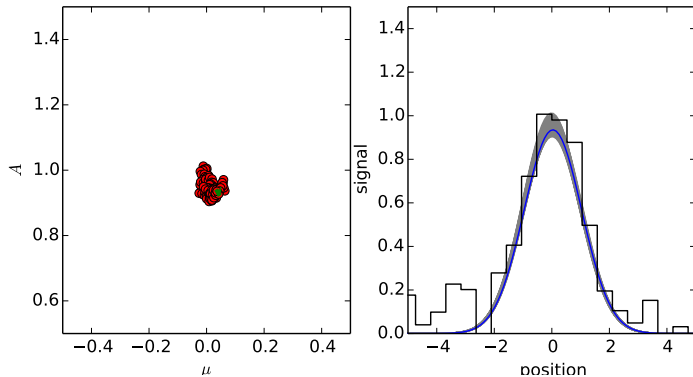
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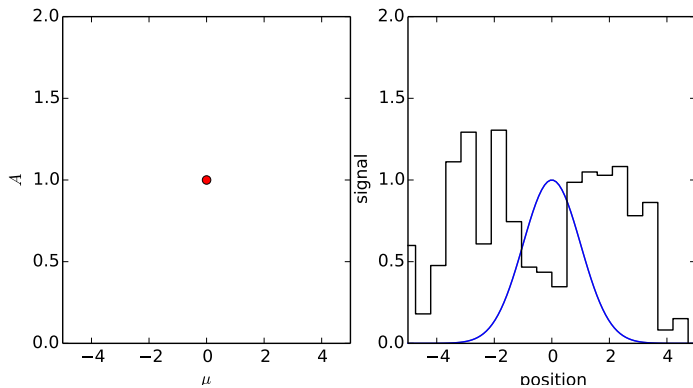
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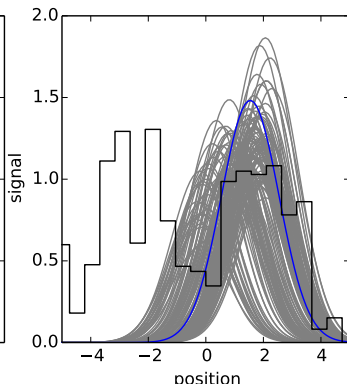
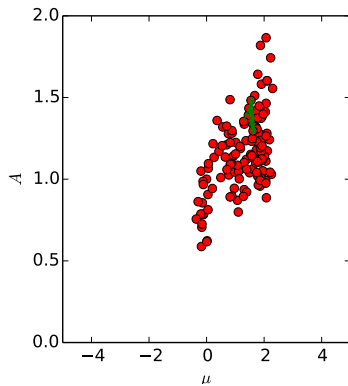
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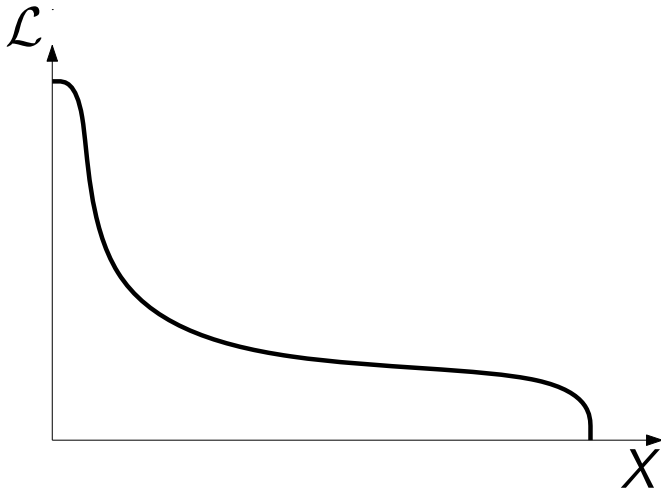
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## Multimodality



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Phase transitions





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- ▶ MCMC fundamentally explores the posterior, and cannot average over the prior.
- ▶ Simulated annealing gives one possibility for computing evidences.
  - ▶ Suffers from similar issues to MCMC, especially phase transitions

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John Skilling's alternative to MCMC!

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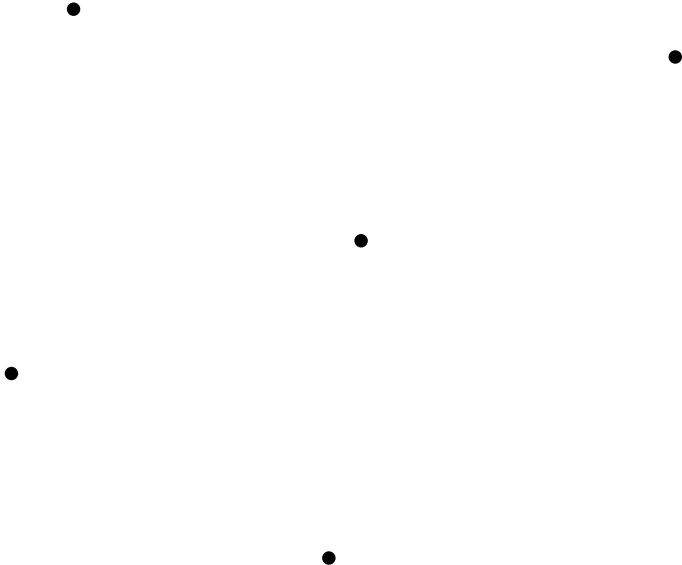
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Requires one to be able to sample from the prior, subject to a *hard likelihood constraint*.

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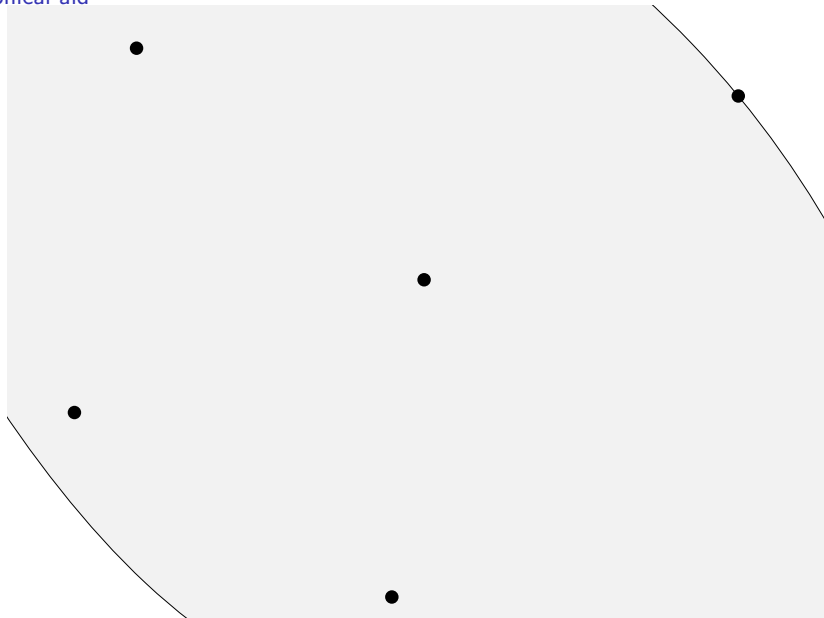
Graphical aid





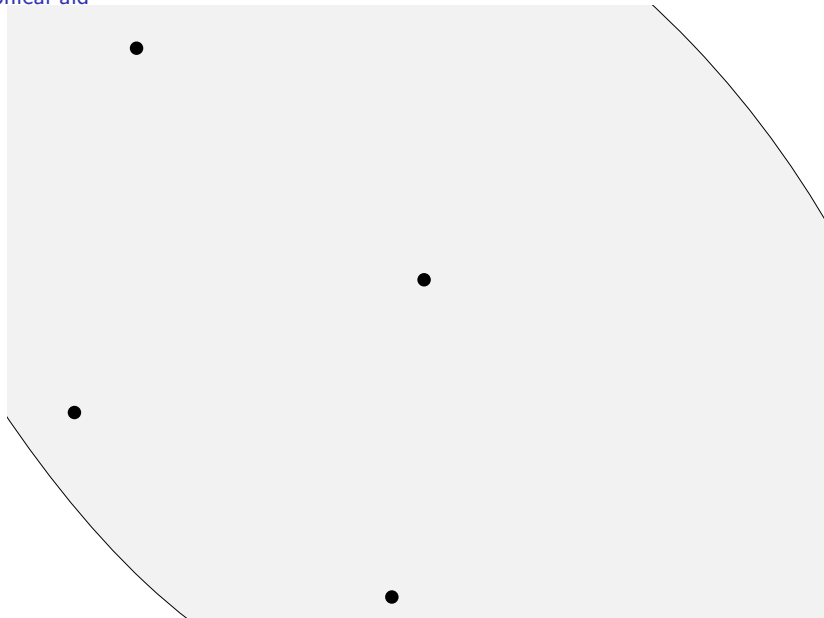
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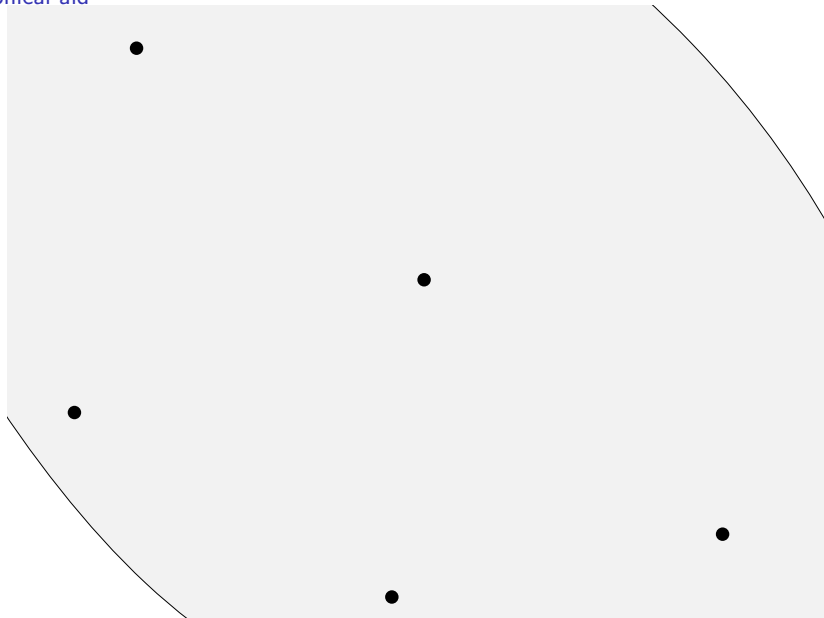
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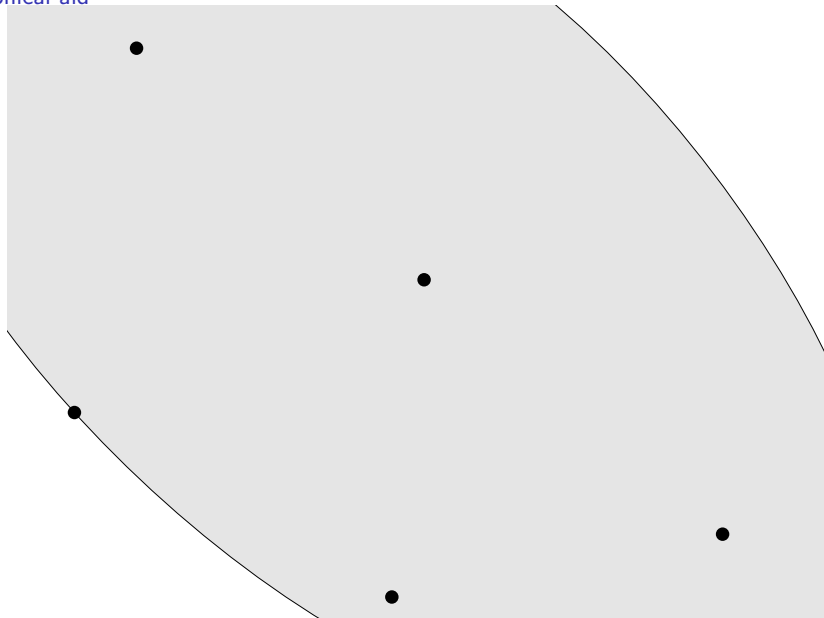
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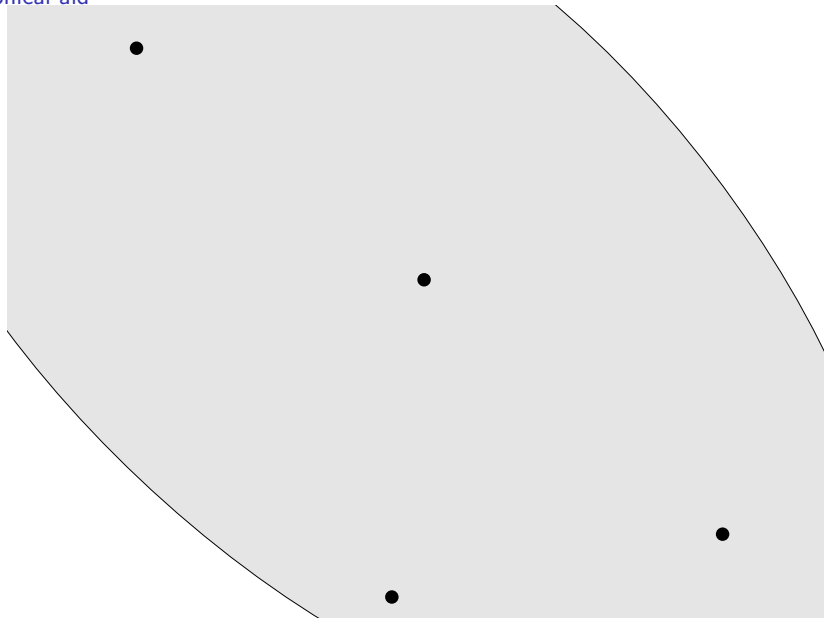
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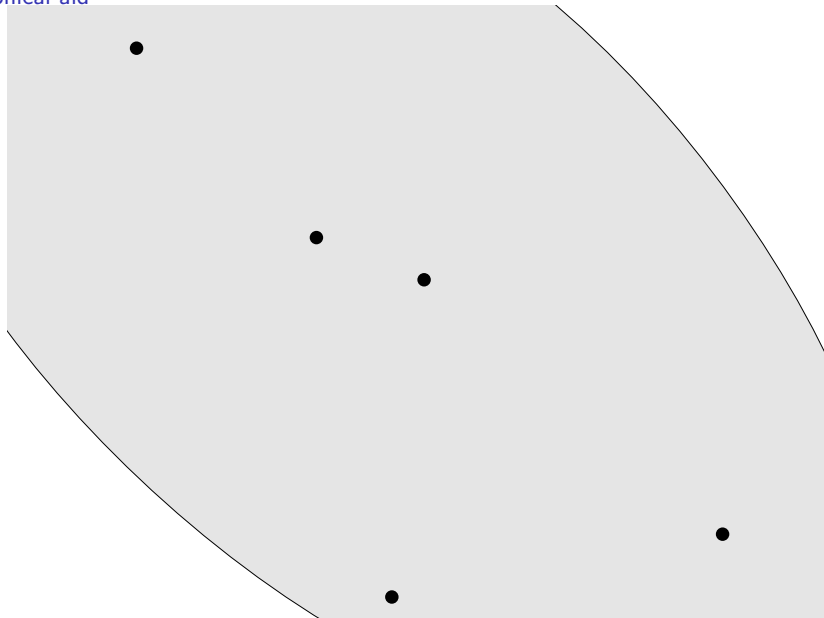
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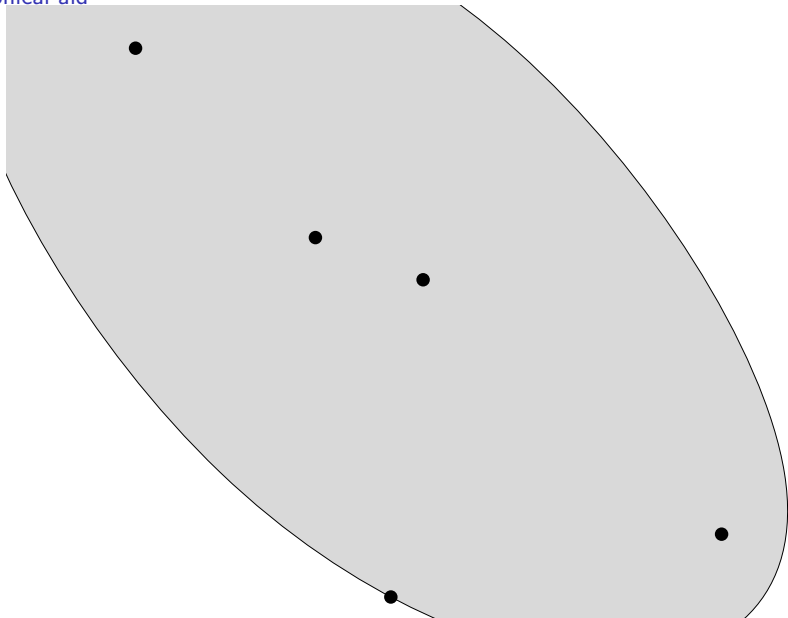
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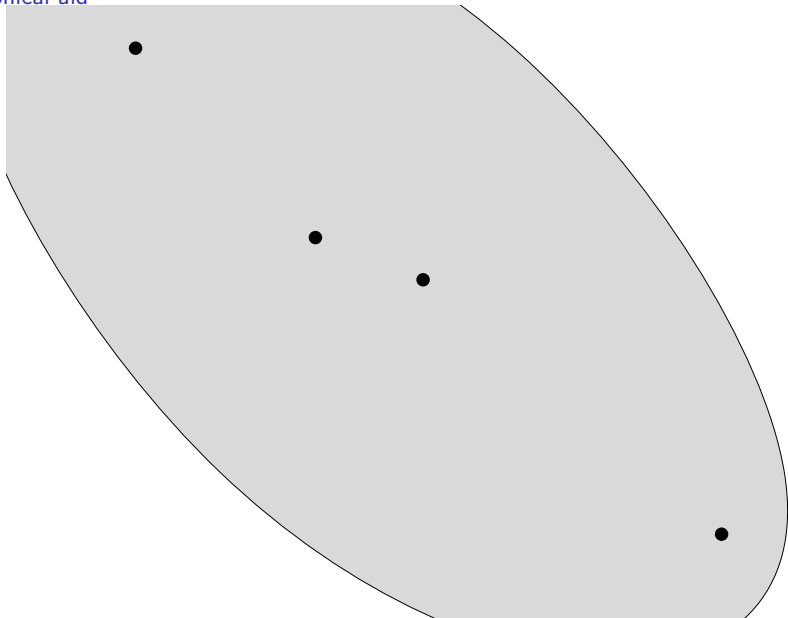
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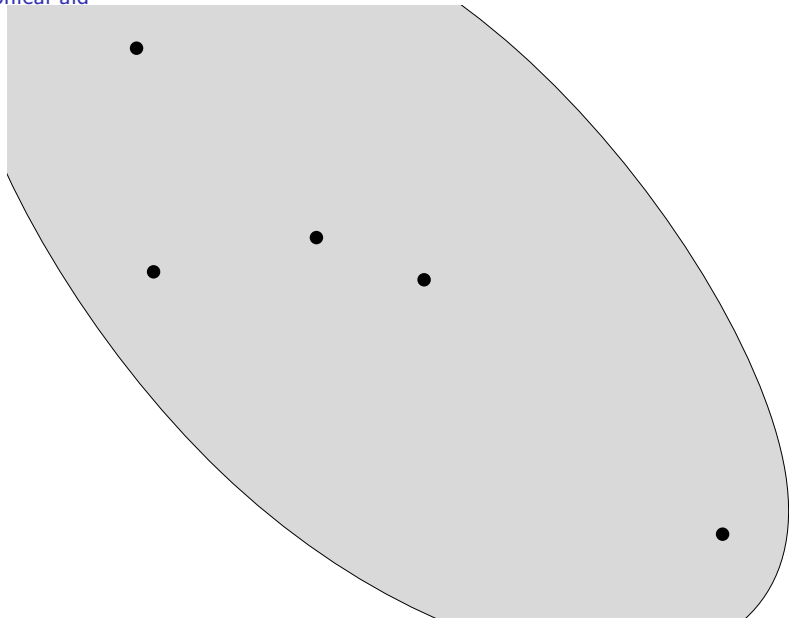
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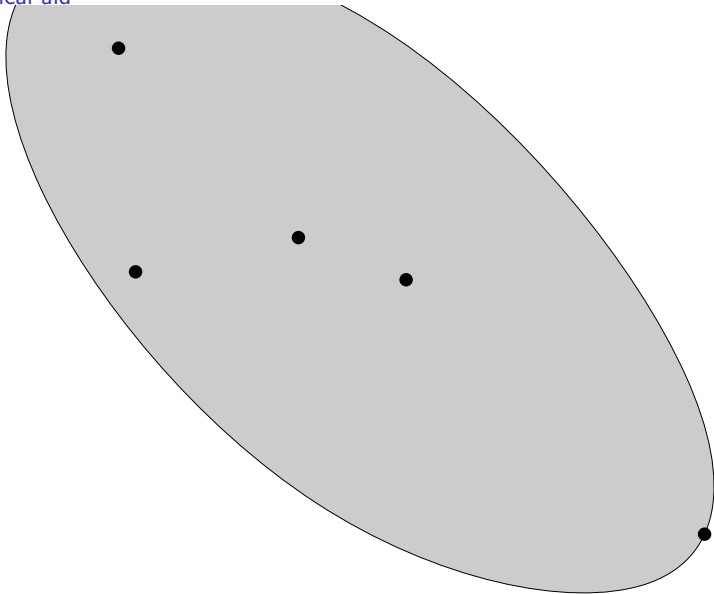
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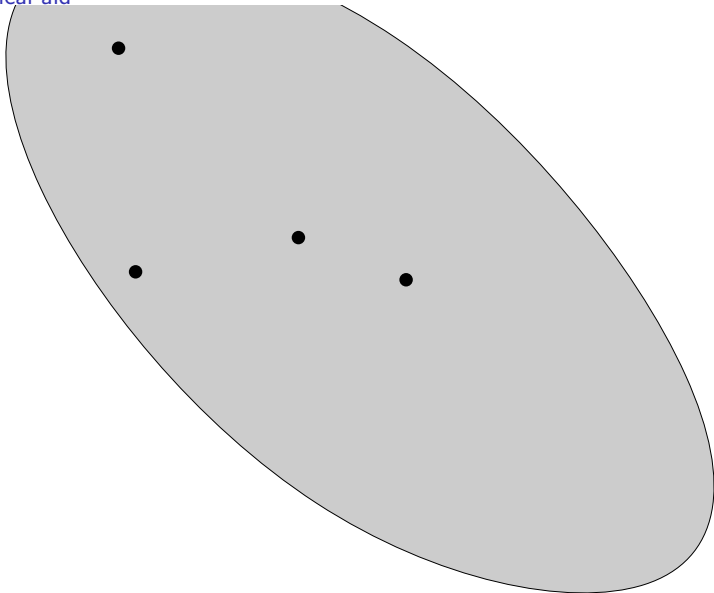
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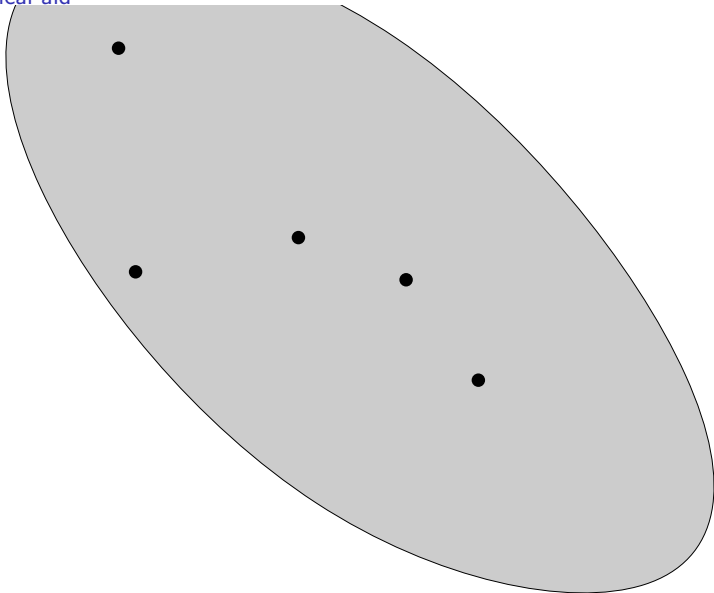
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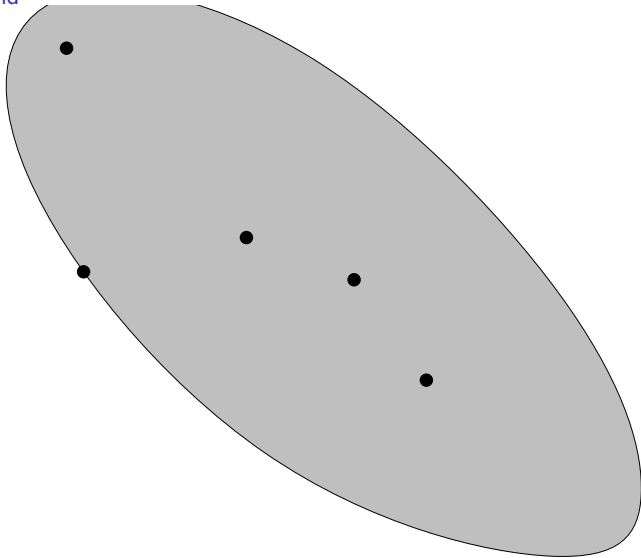
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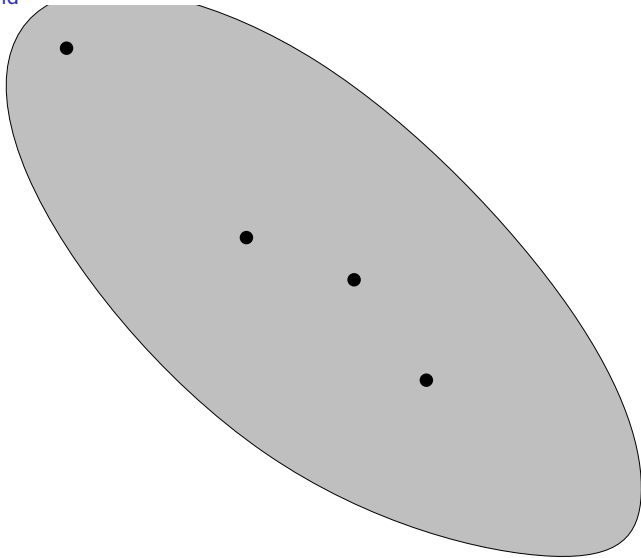
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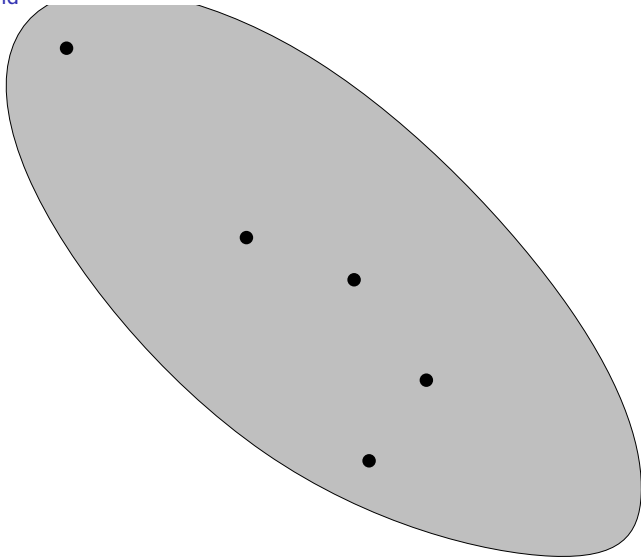
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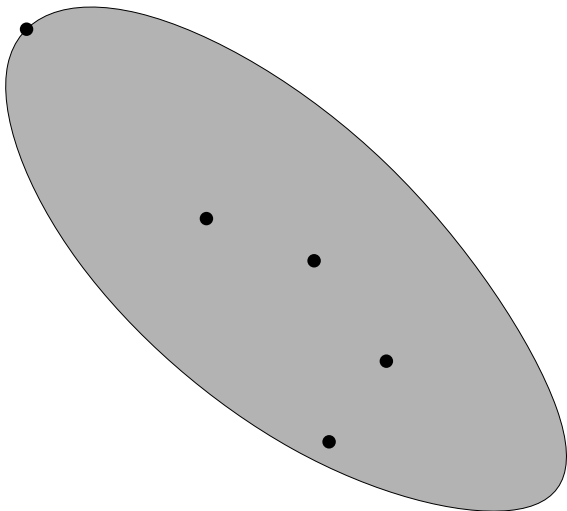
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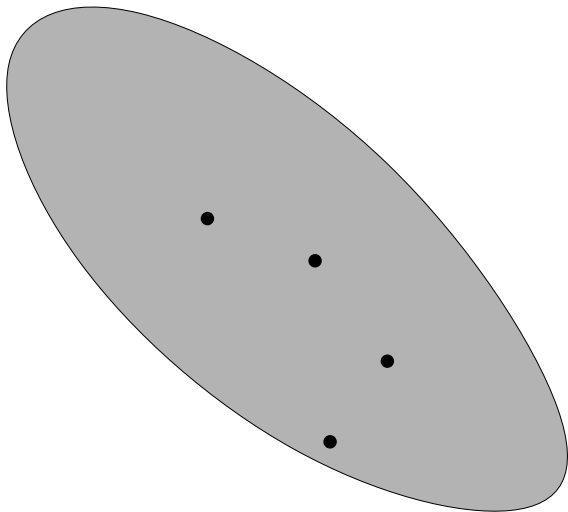
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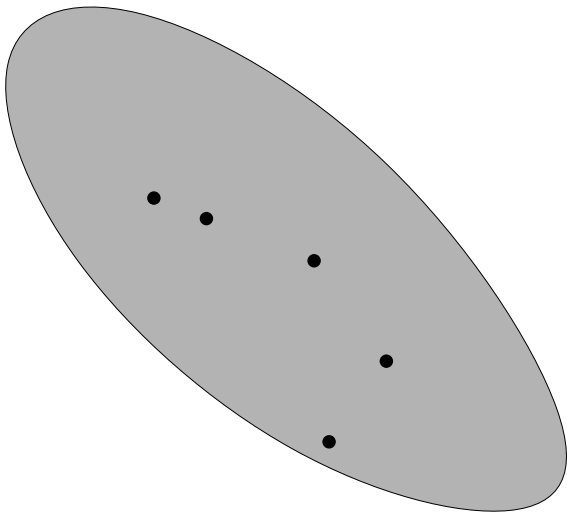
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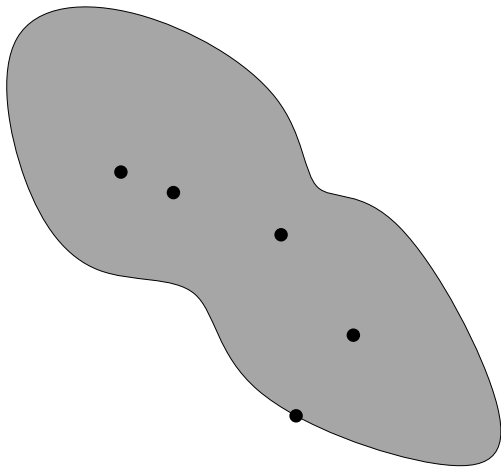
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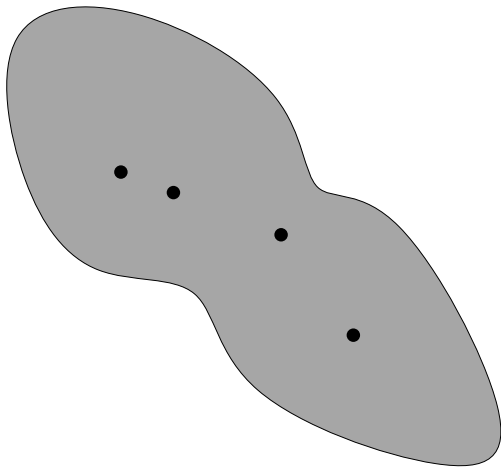
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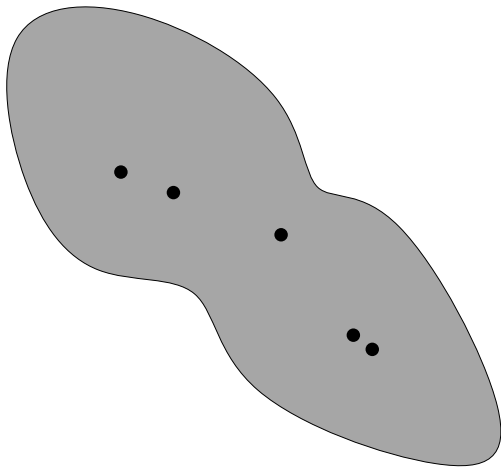
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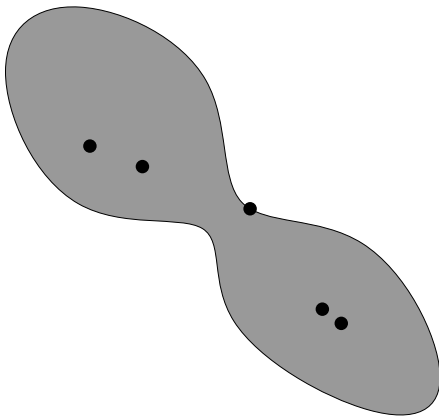
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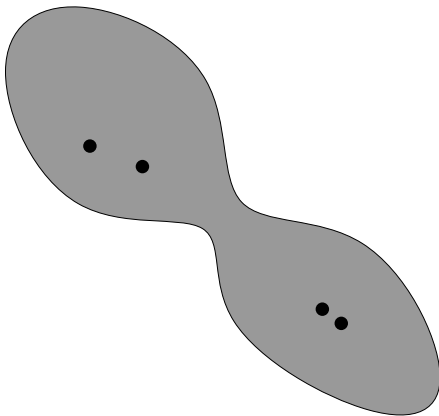
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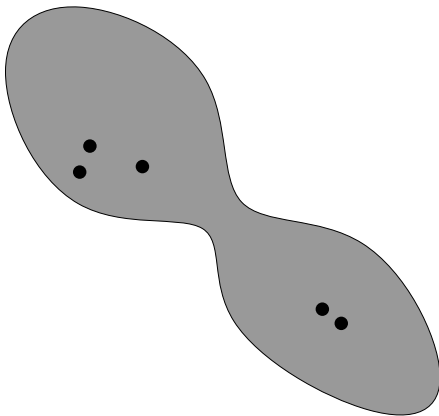
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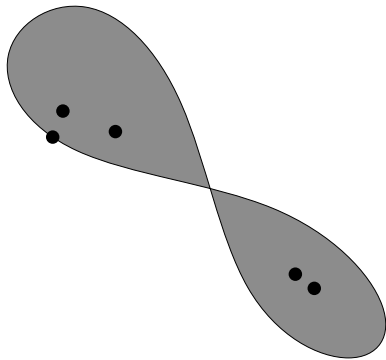
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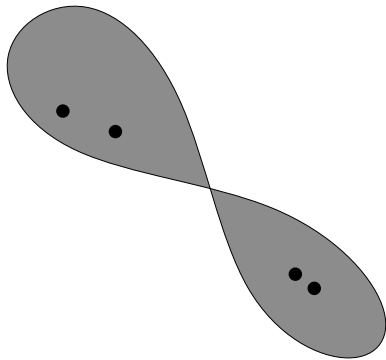
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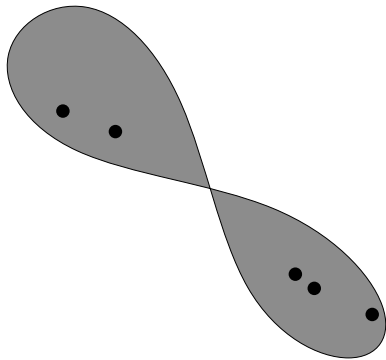
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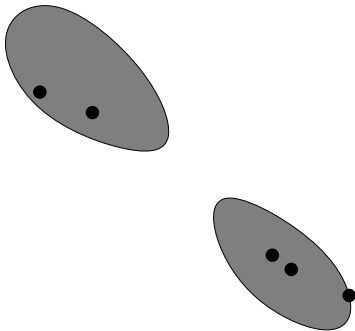
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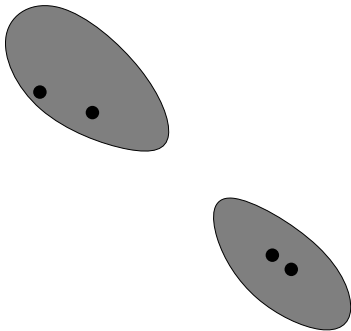
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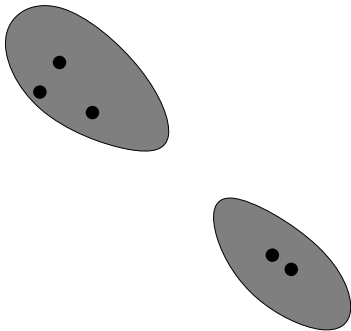
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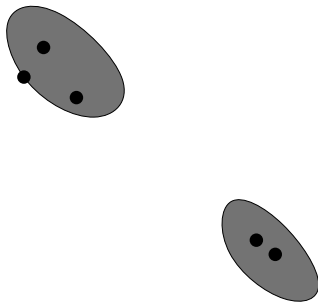
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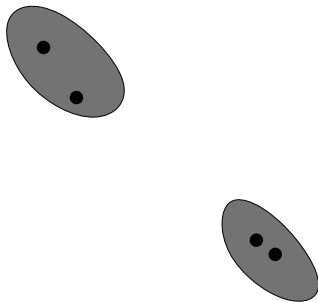
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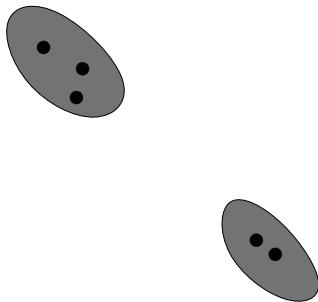
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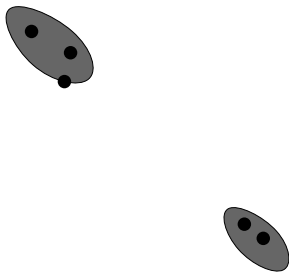
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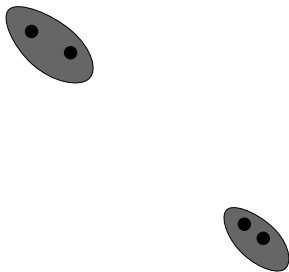
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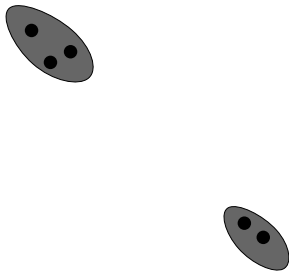
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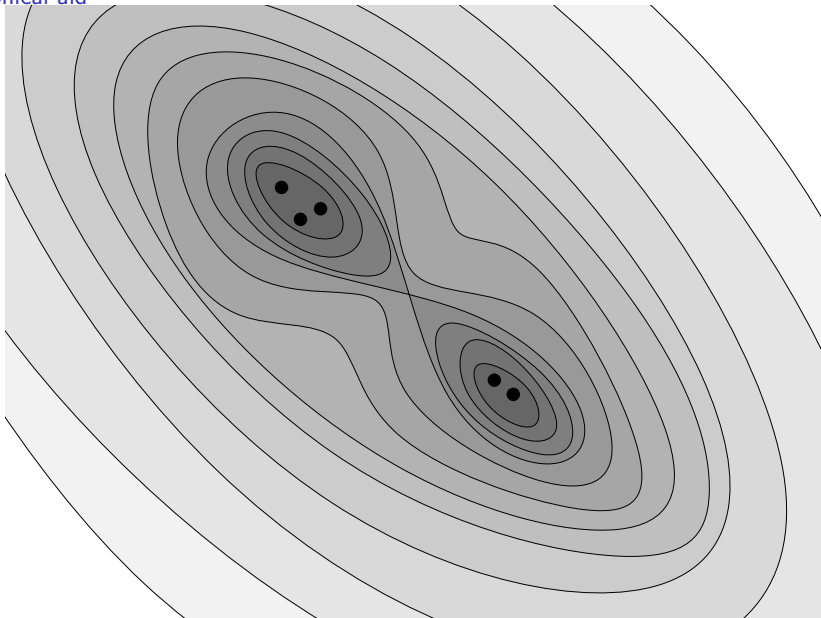
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## Calculating evidences

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- Transform to 1 dimensional integral

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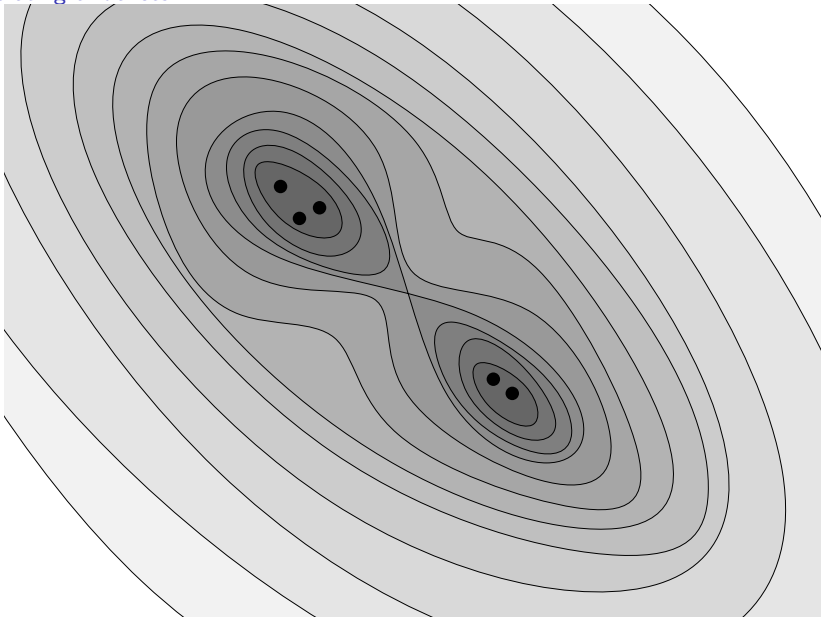
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- ▶ i.e. the fraction of the prior which the iso-likelihood contour  $\mathcal{L}$  encloses.

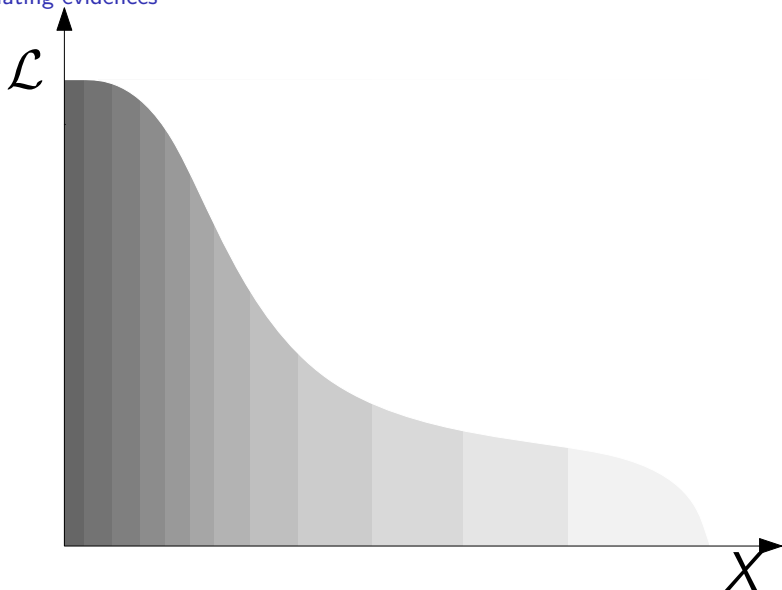
# Nested Sampling

Calculating evidences



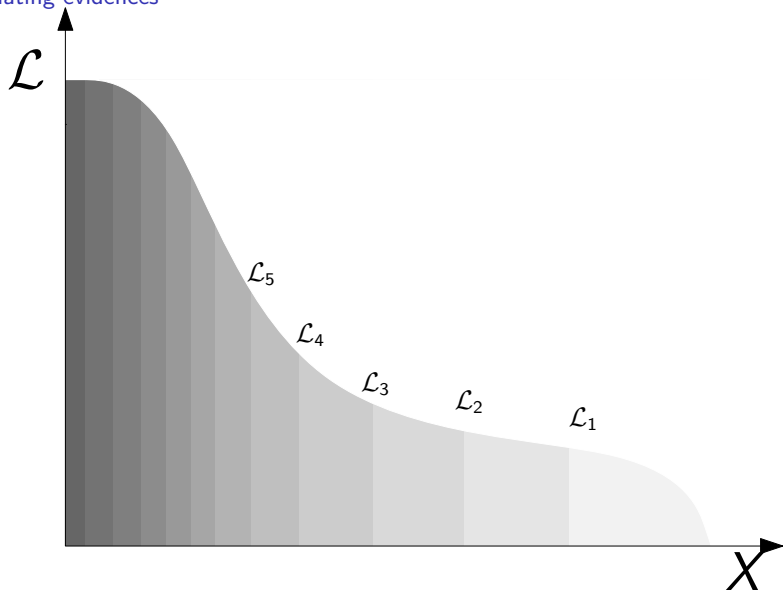
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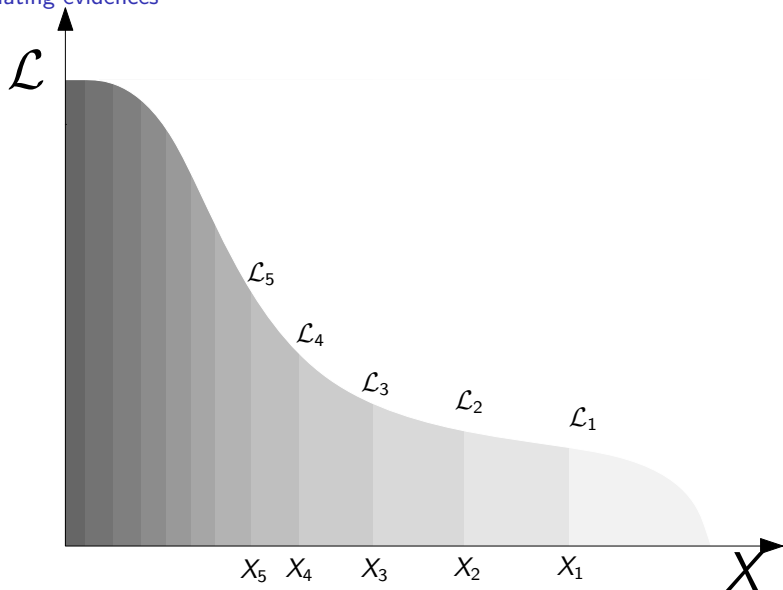
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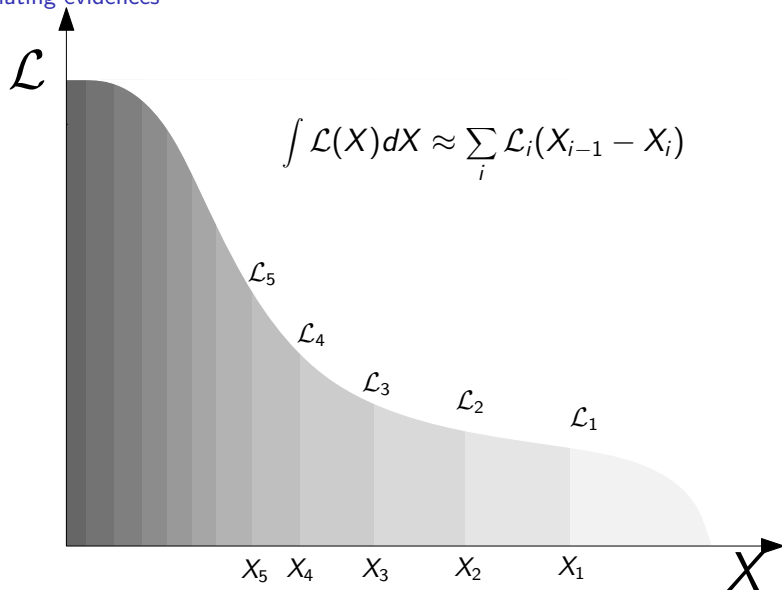
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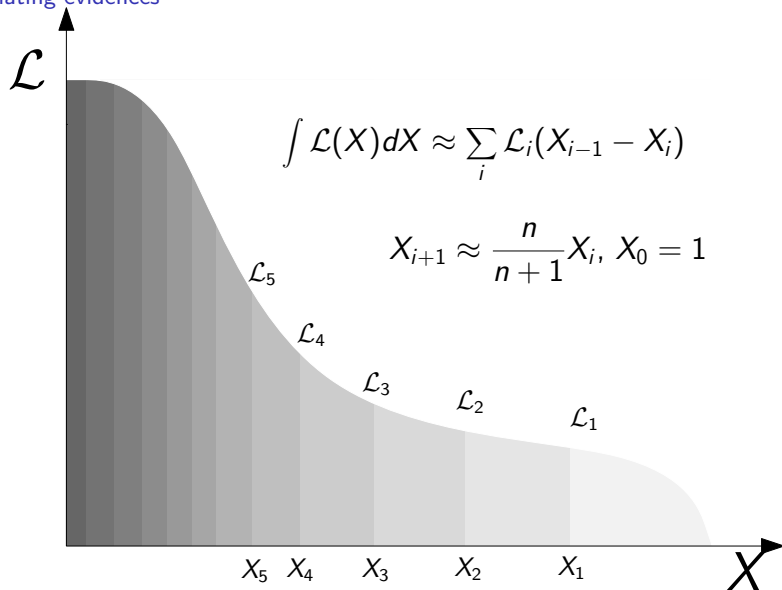
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$$X_{i+1} \approx \frac{n}{n+1} X_i, \quad X_0 = 1 \quad (2)$$



# Nested sampling

Parameter estimation

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## Parameter estimation

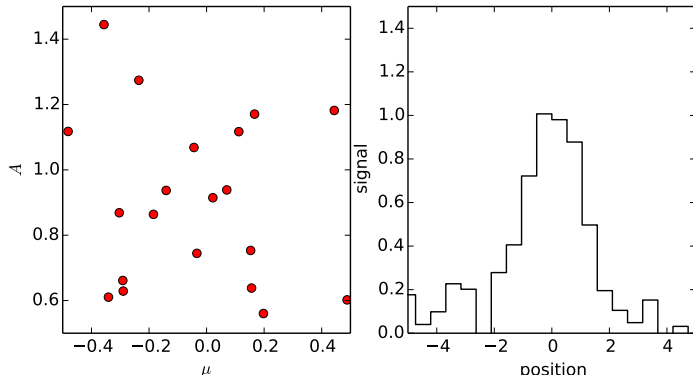
- ▶ NS can also be used to sample the posterior

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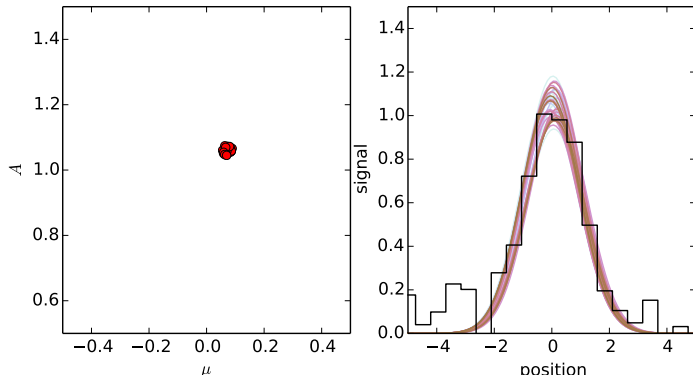
## Parameter estimation

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

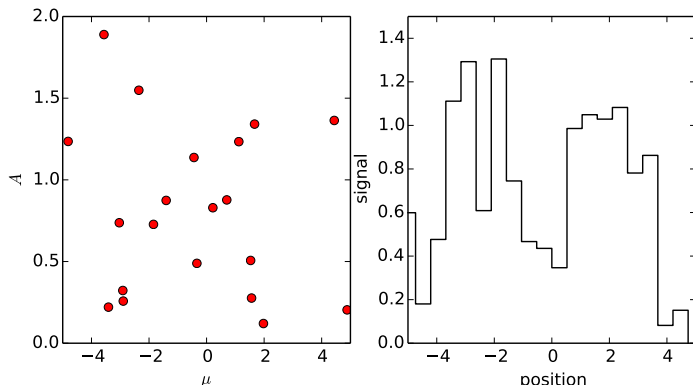
## When NS succeeds



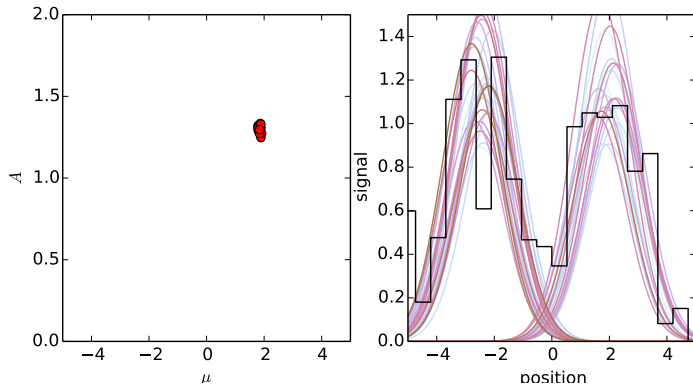
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## Sampling from a hard likelihood constraint



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- ▶ Most of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm.

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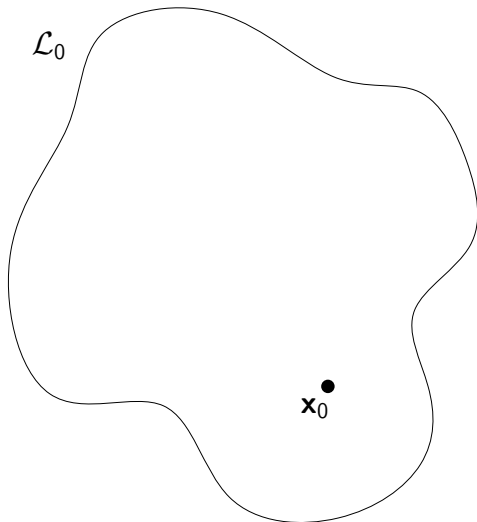
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Diffusion Nested Sampling B. Brewer et al. (2009).

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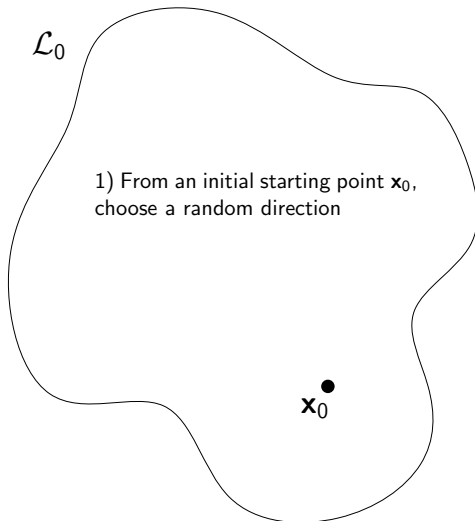
# PolyChord

“Hit and run” slice sampling



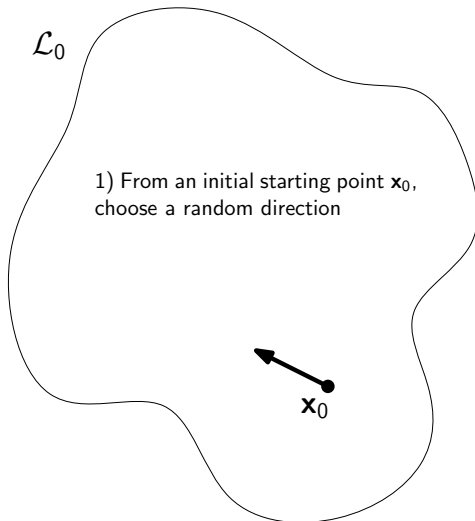
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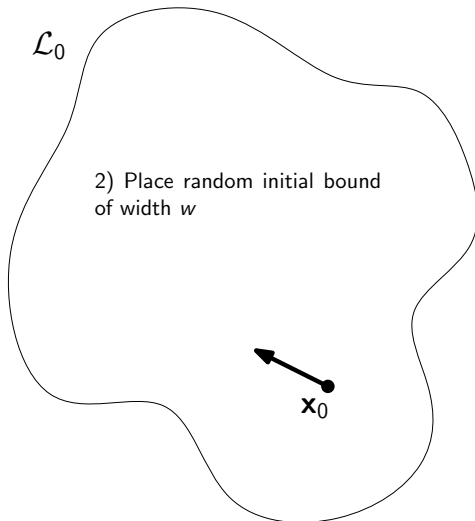
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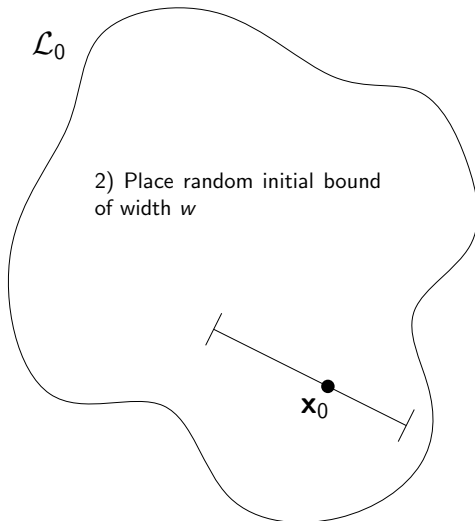
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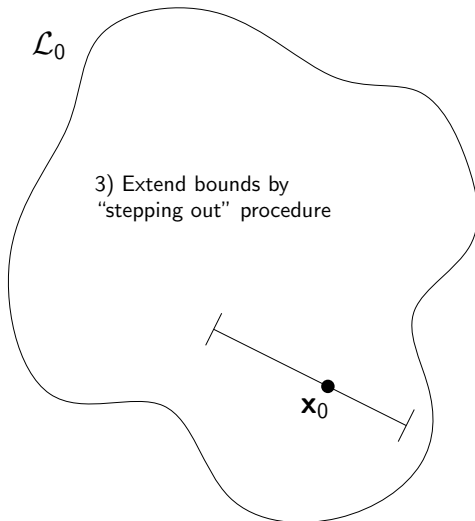
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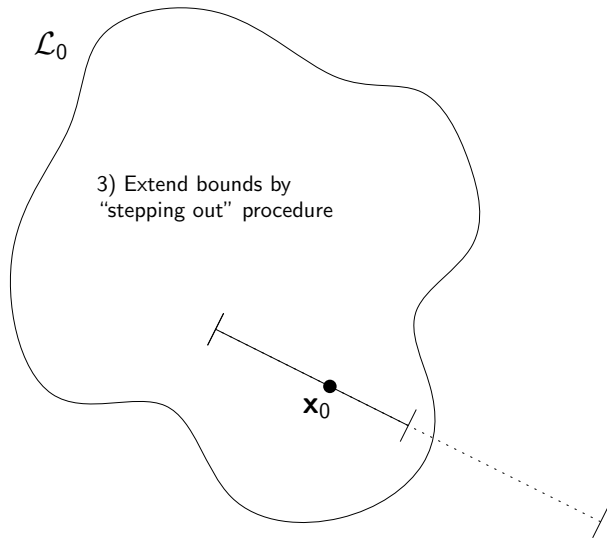
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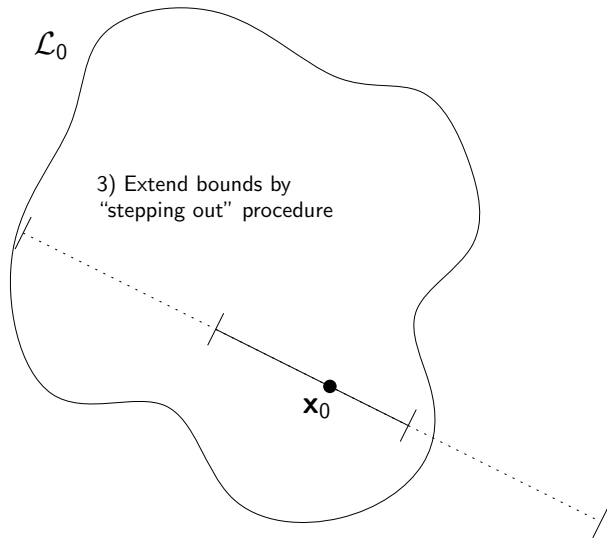
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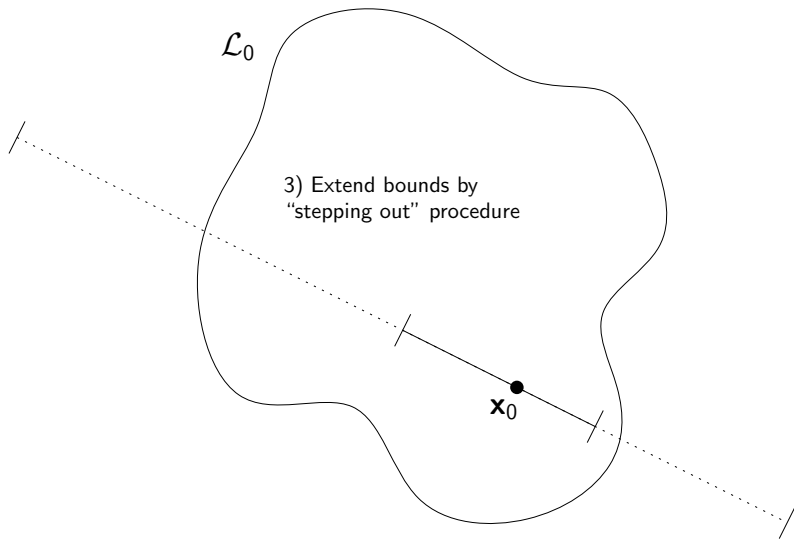
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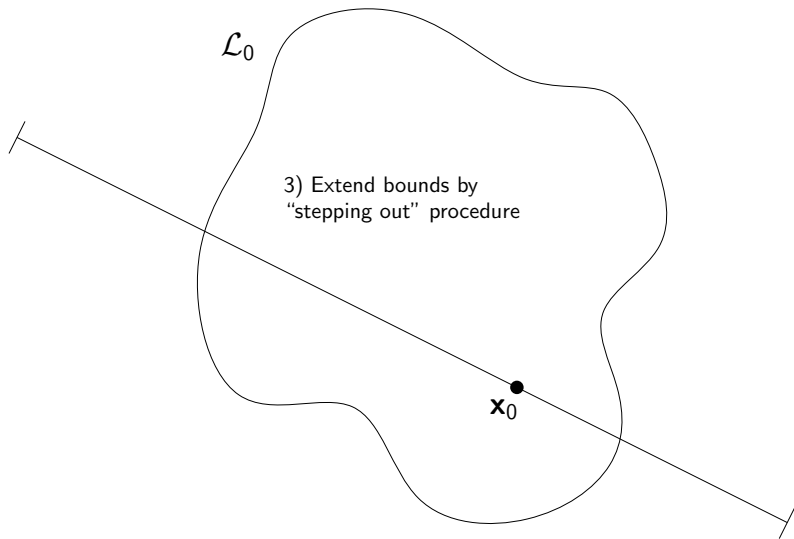
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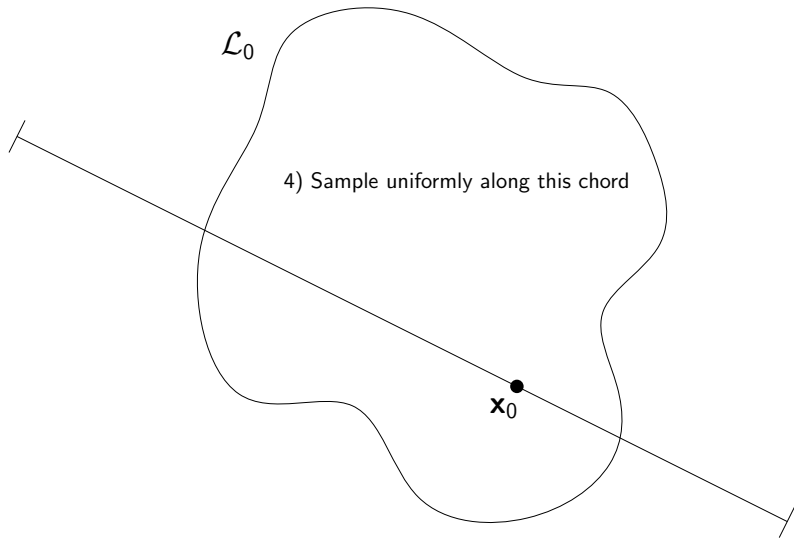
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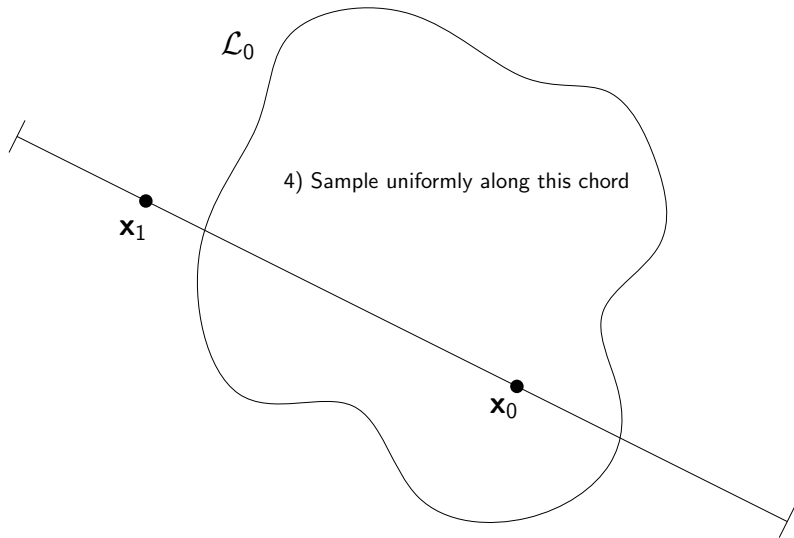
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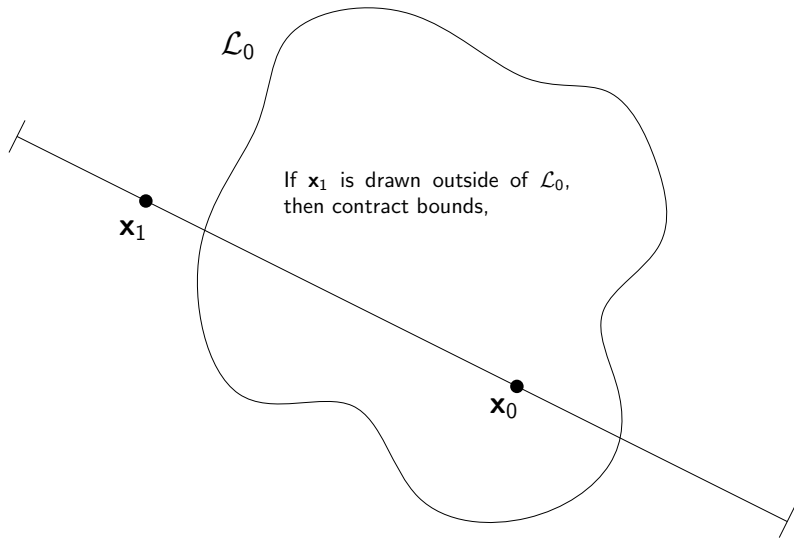
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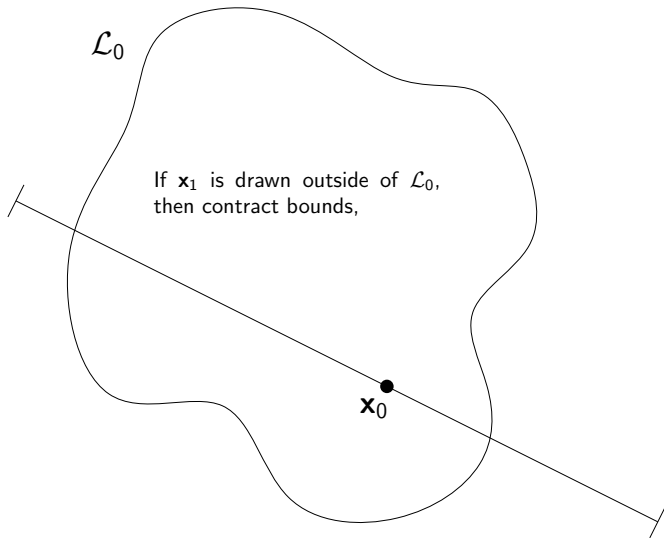
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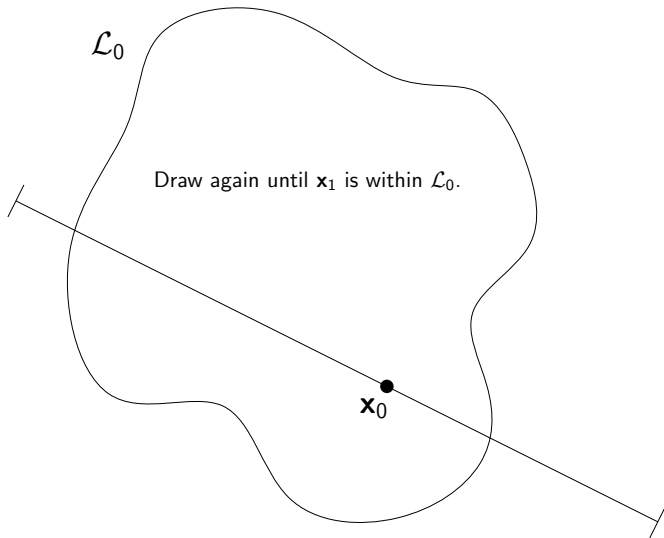
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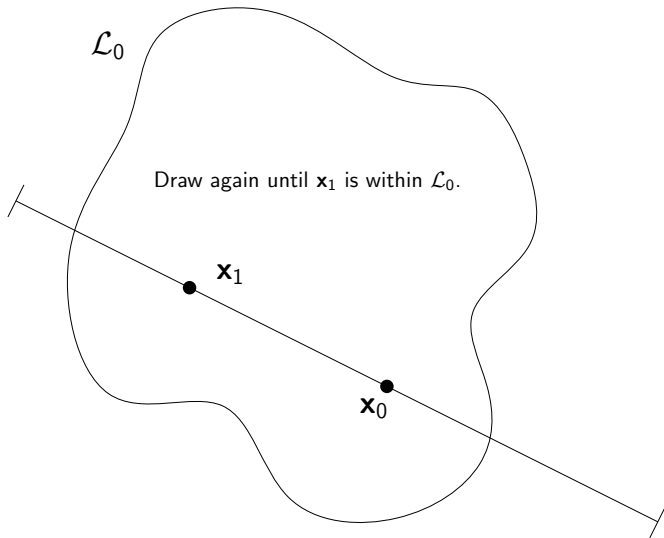
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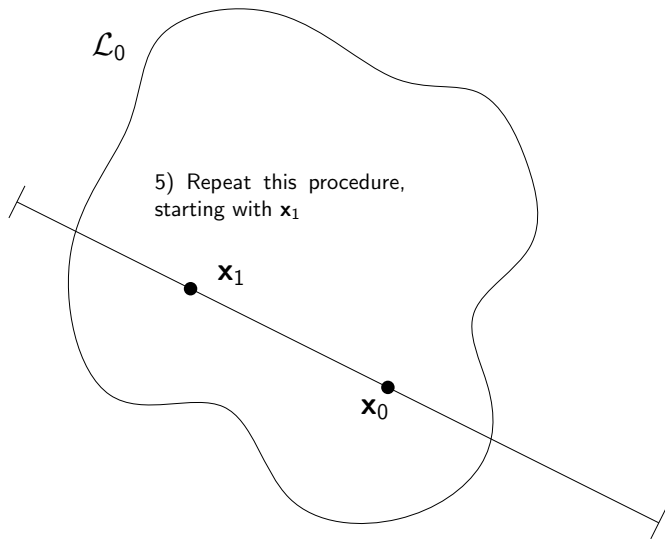
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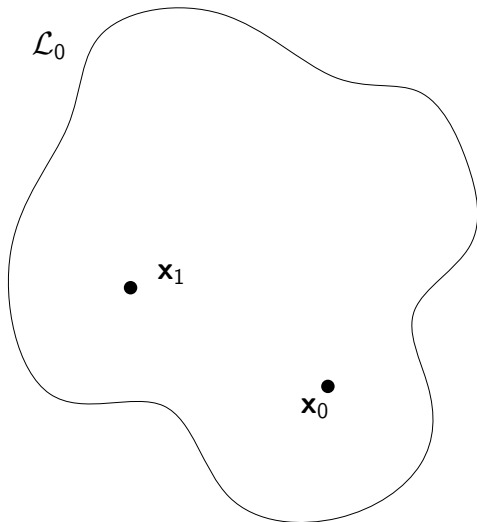
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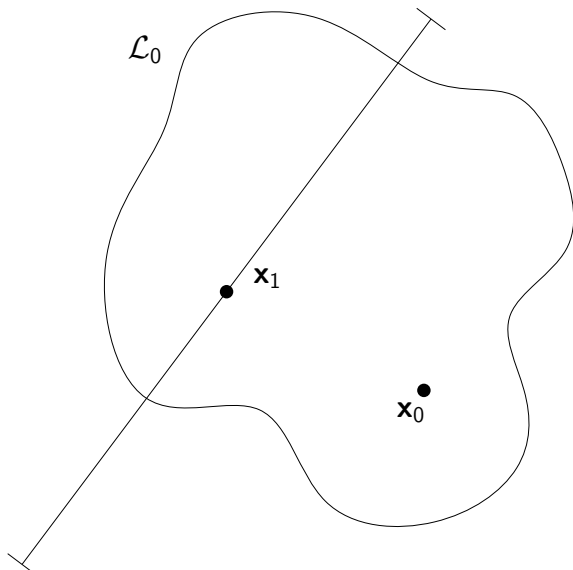
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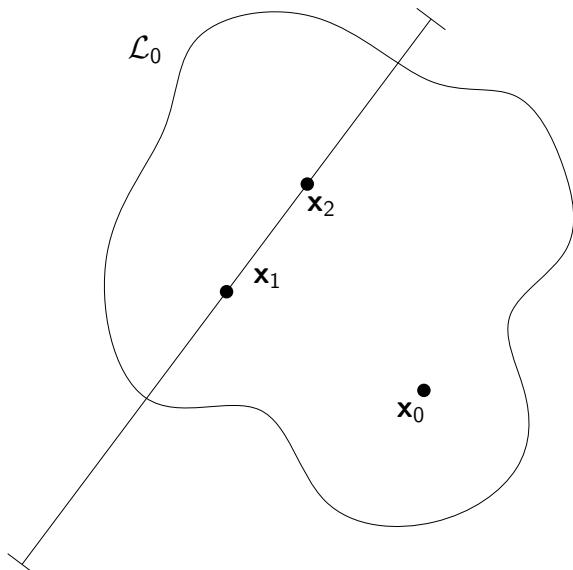
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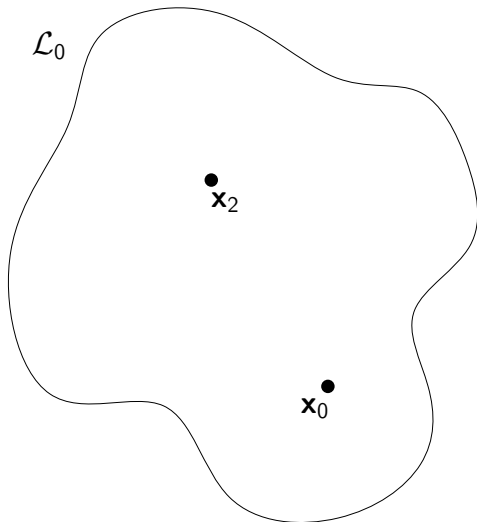
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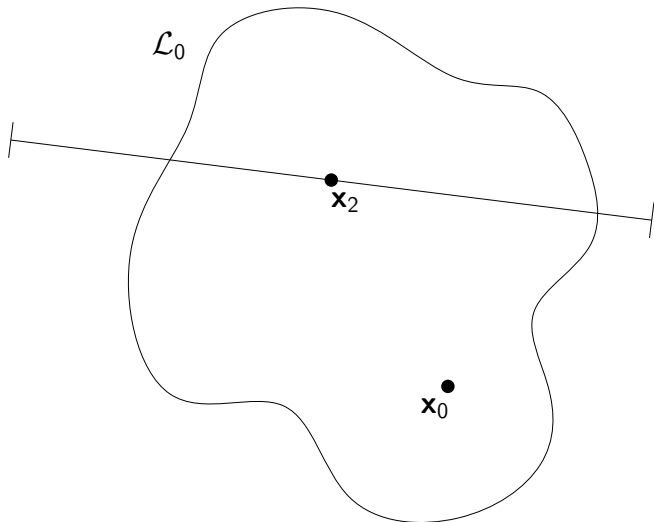
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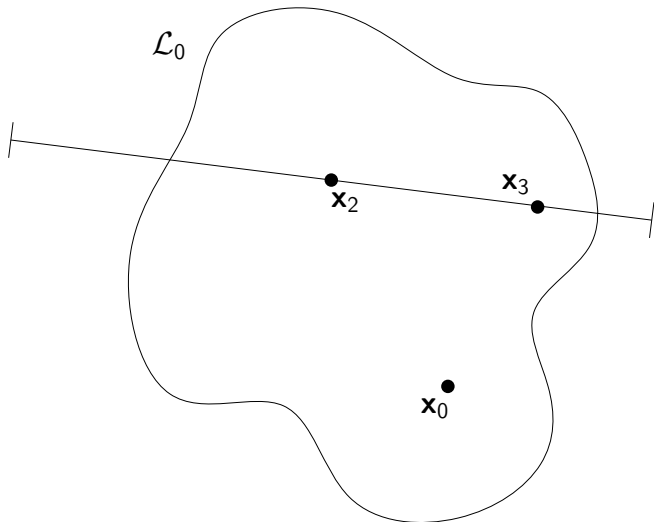
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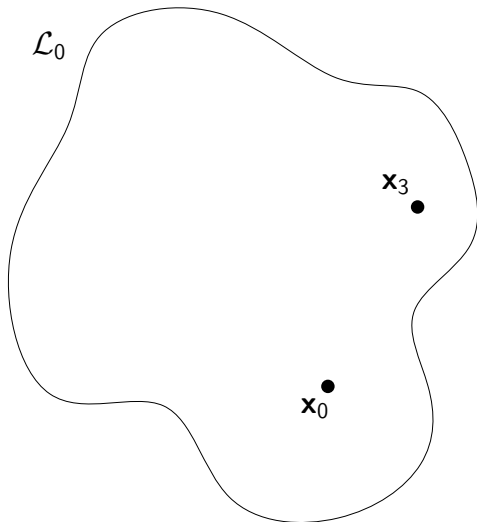
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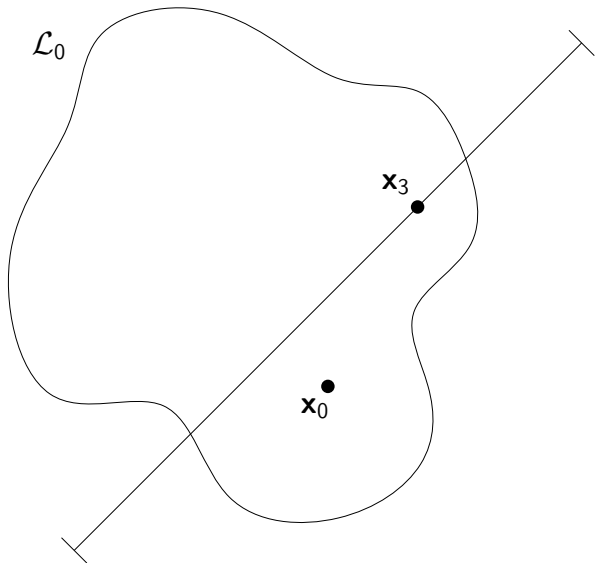
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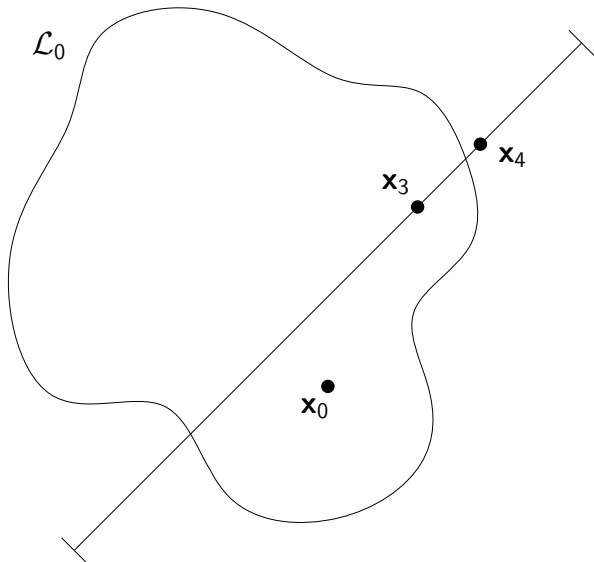
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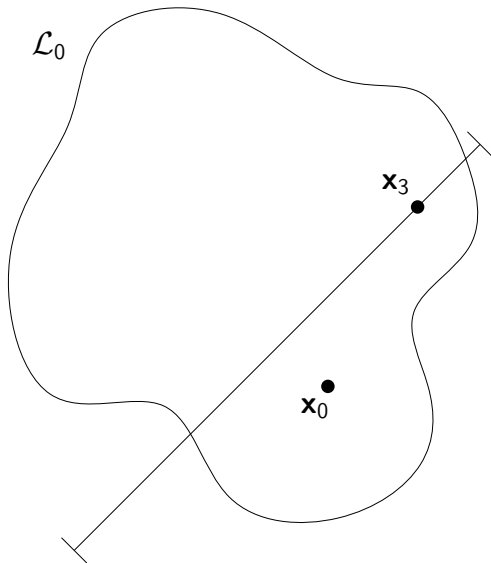
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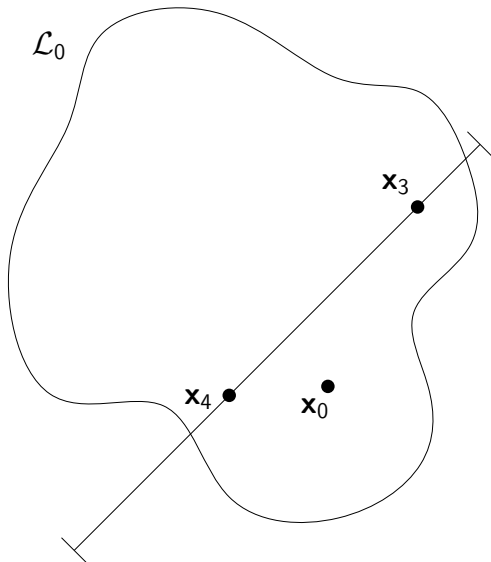
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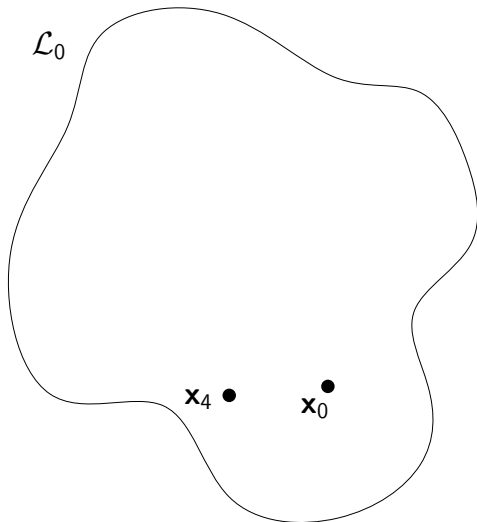
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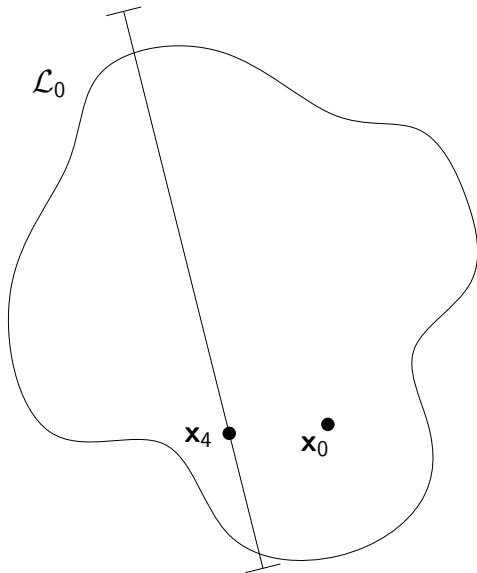
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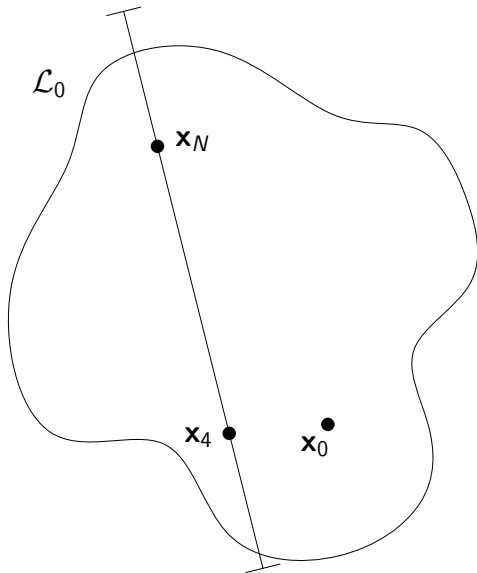
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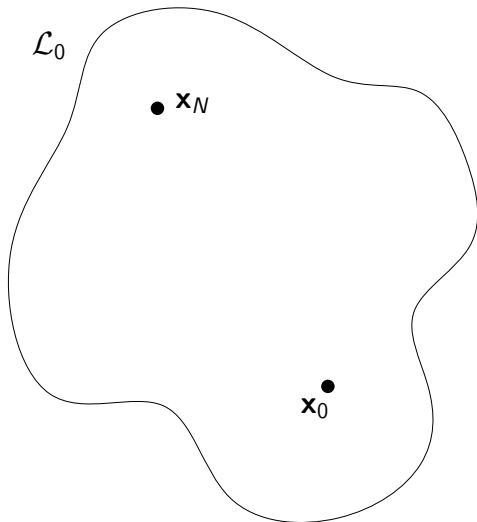
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1. Does not deal well with correlated distributions.



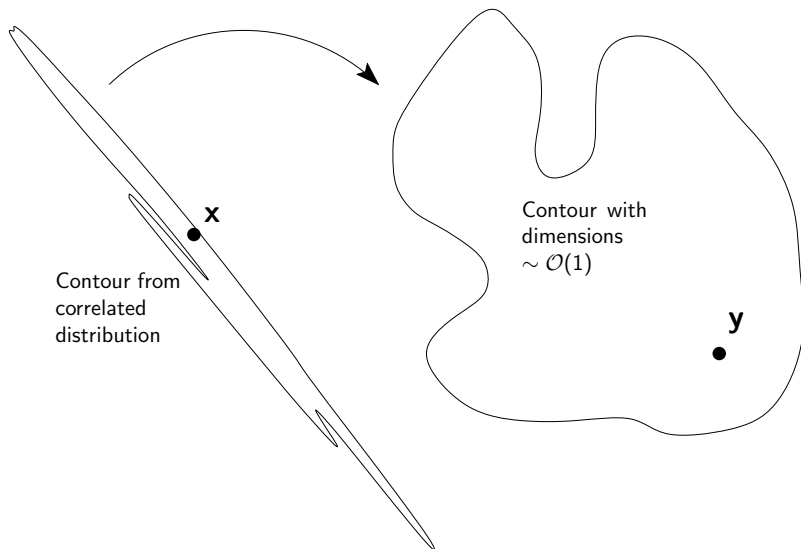
# Issues with Slice Sampling

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2. Need to “tune”  $w$  parameter.

# PolyChord's solutions

## Correlated distributions

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



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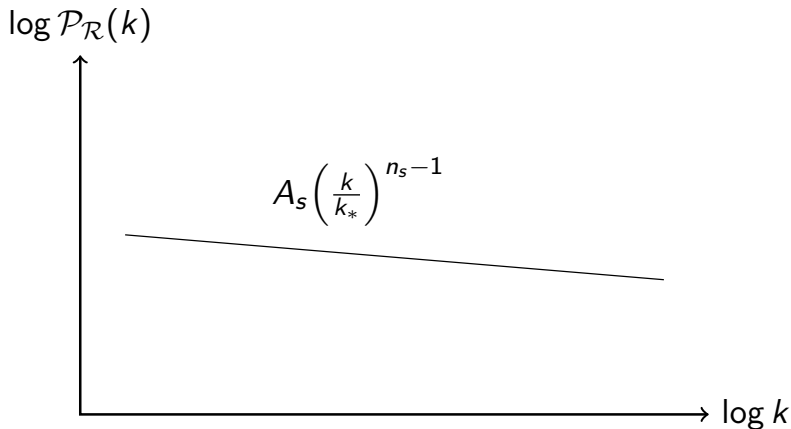
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- ▶ Novel method for identifying and evolving modes separately.
- ▶ Implemented in CosmoMC, as “CosmoChord”, with fast-slow parameters.

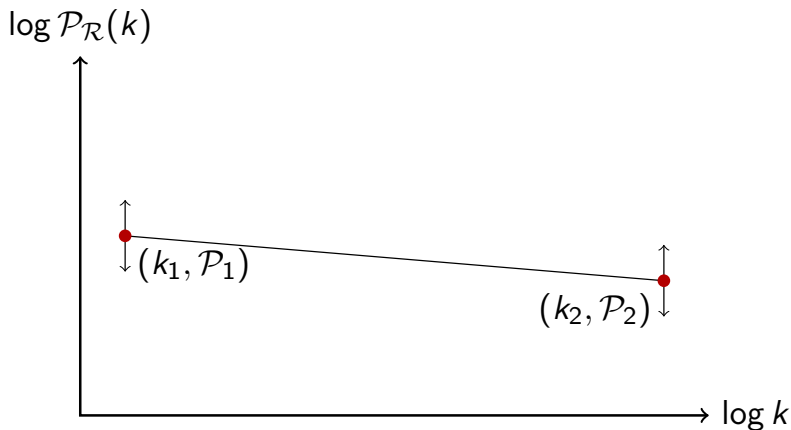
# PolyChord in action

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



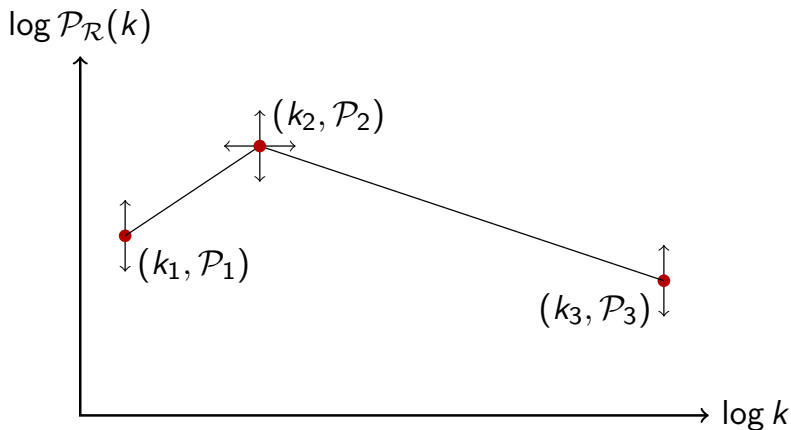
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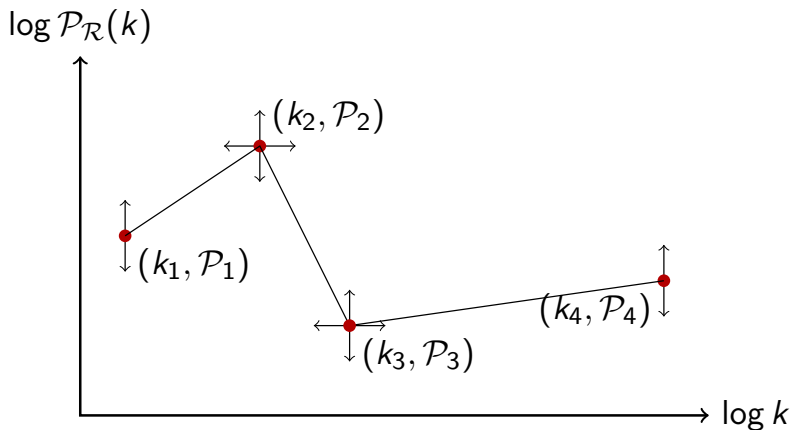
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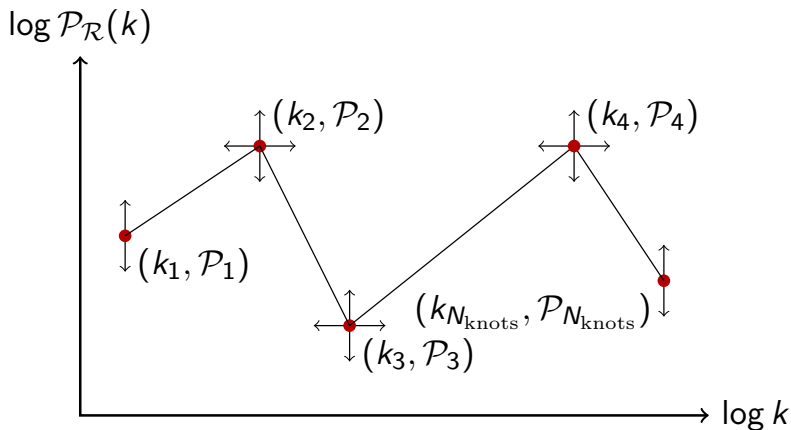
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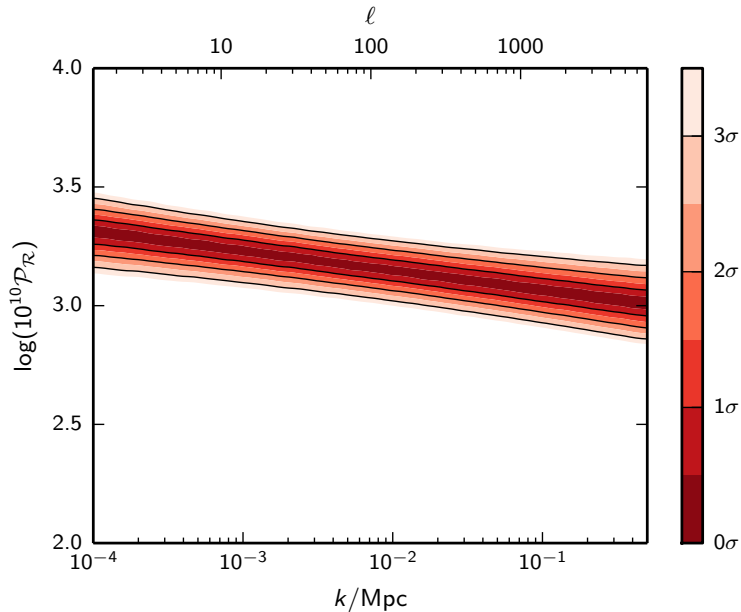
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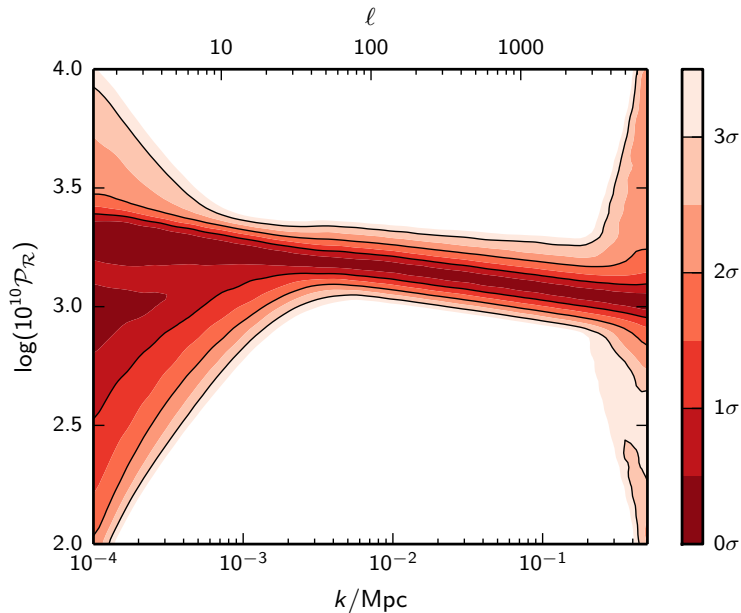
# 0 internal knots

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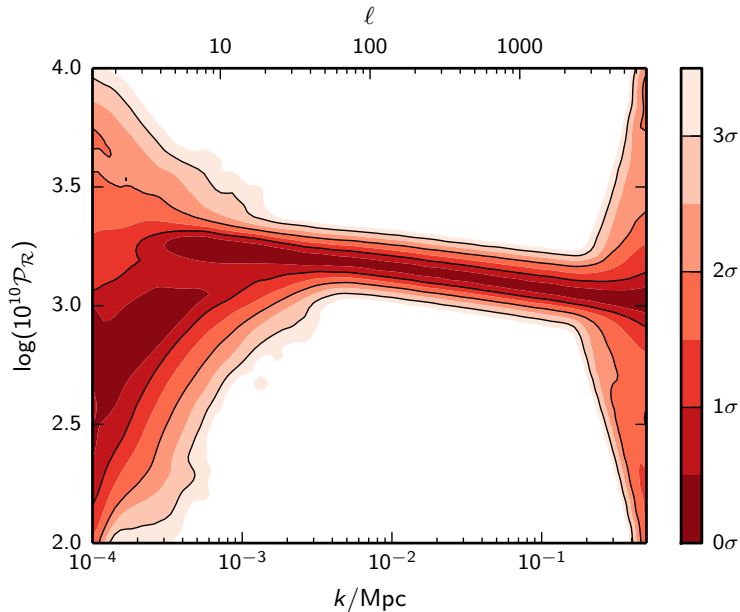
# 1 internal knots

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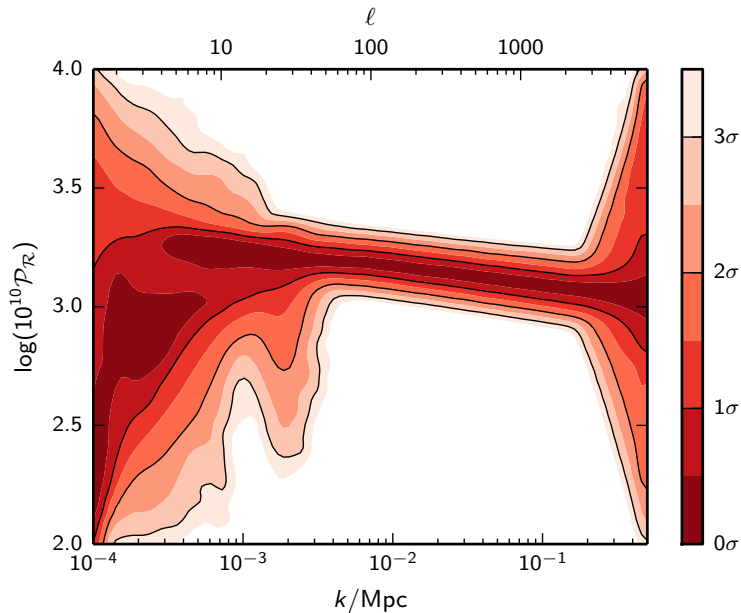
## 2 internal knots

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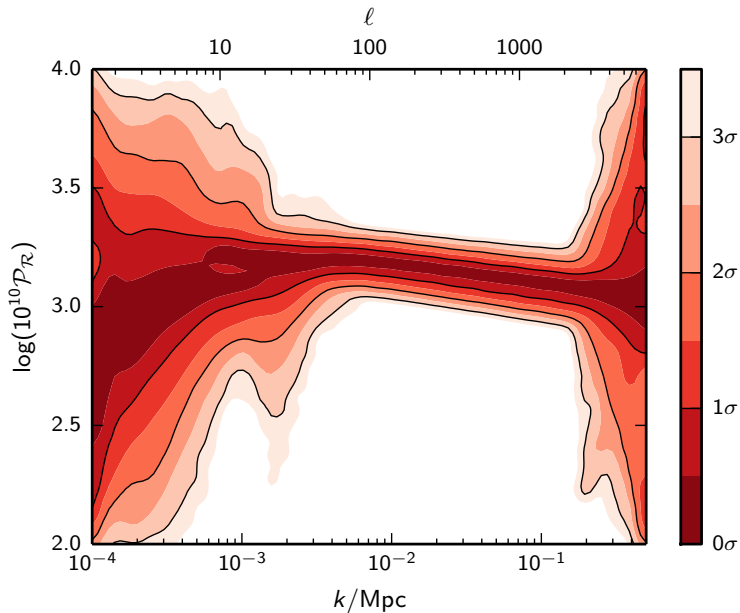
### 3 internal knots

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



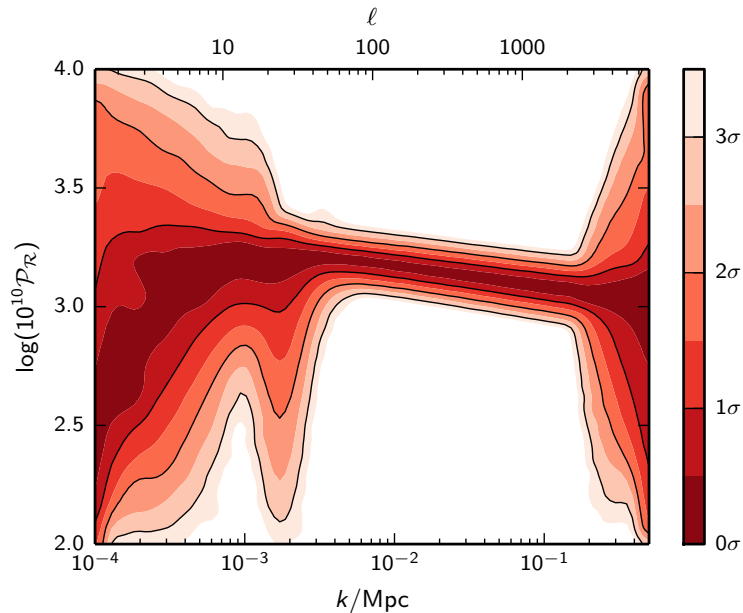
## 4 internal knots

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



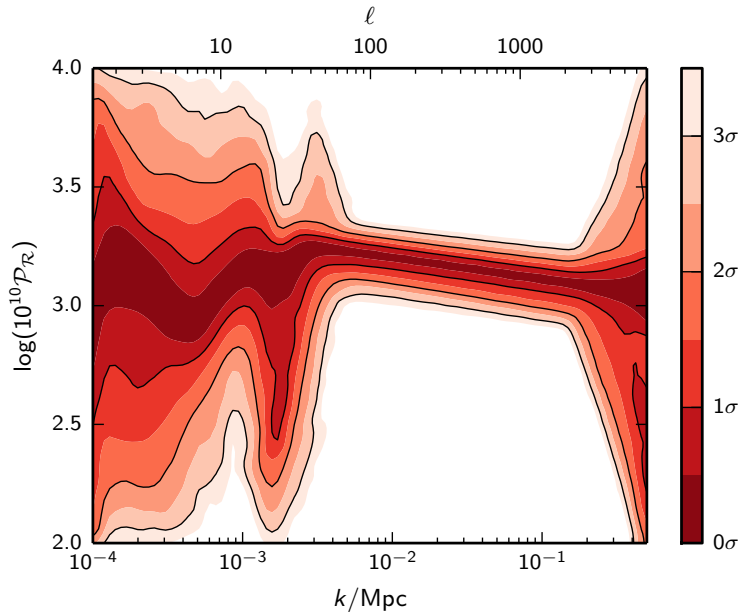
## 5 internal knots

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



## 6 internal knots

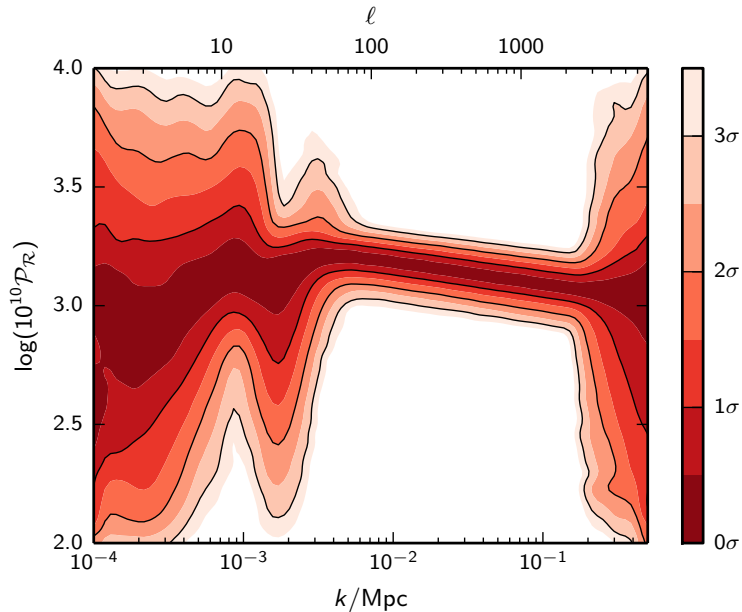
Primordial power spectrum  $\mathcal{P}_{\mathcal{R}}(k)$  reconstruction





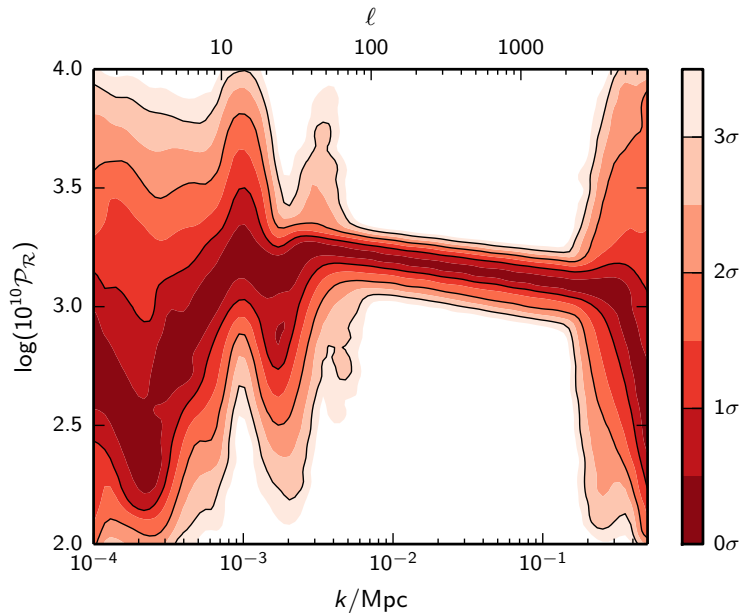
## 7 internal knots

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



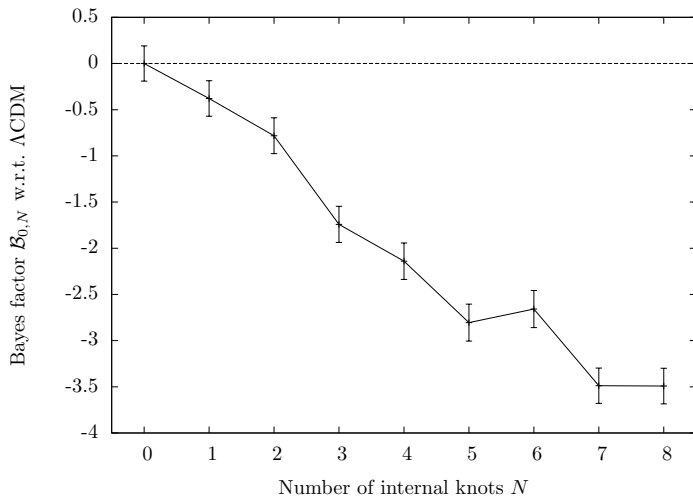
## 8 internal knots

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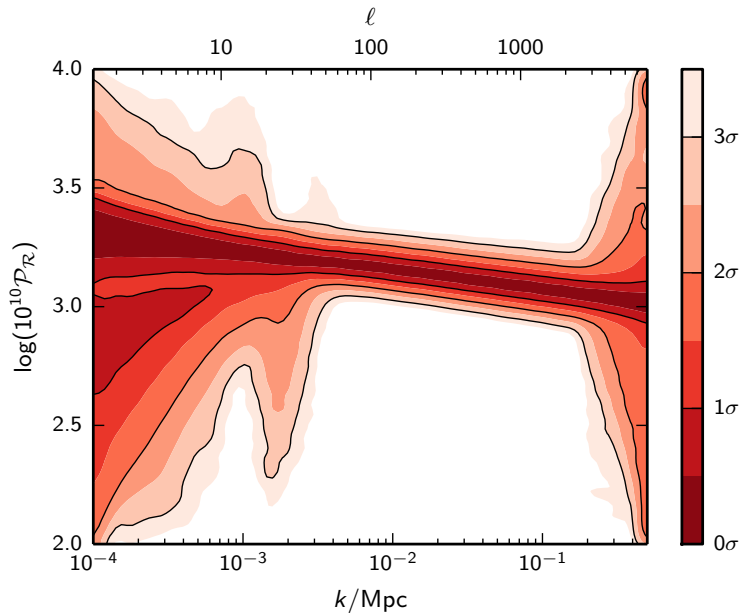
# Bayes Factors

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



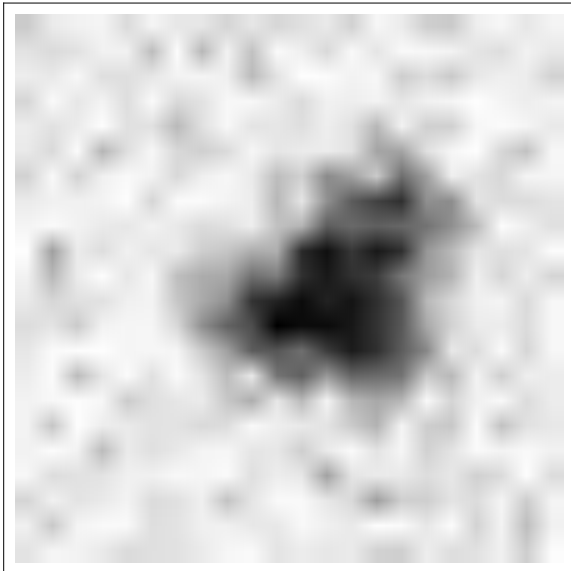
# Marginalised plot

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

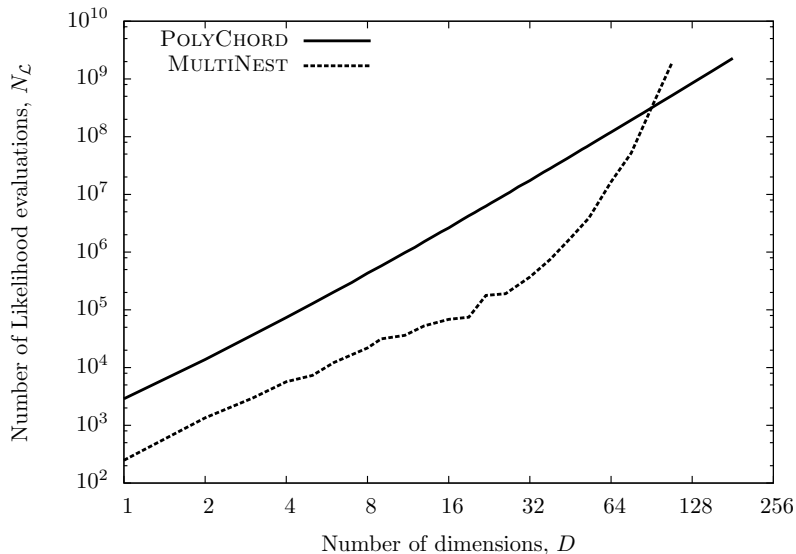
## Evidences

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



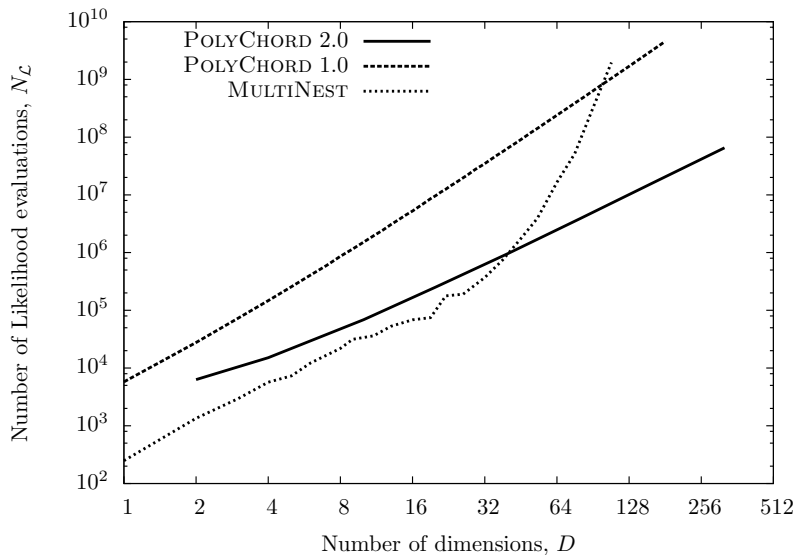
# PolyChord vs. MultiNest

Gaussian likelihood



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# The future of nested sampling

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- ▶ Nested sampling is really the first in a new class of “probabilistic integration” algorithms.

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