# PolyChord & the future of nested sampling

## Tools for sampling, Parameter Estimation and Bayesian Model Comparison


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Parameter estimation & model comparison

Metropolis Hastings

Nested Sampling

PolyChord

PolyChord 2.0

Examples

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- Similar to simulated annealing, but automatically picks the "correct" annealing schedule.

# Bayes' theorem

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Model averaging:

- Multiple models with posterior on the same parameter: $\mathrm{P}(y|M_i, D)$

$$\mathrm{P}(y|D) = \sum_i \mathrm{P}(y|M_i, D)\mathrm{P}(M_i|D)$$

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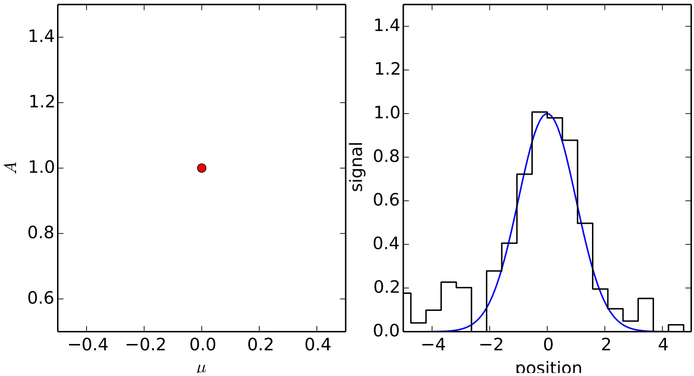
  4. ...otherwise sometimes make step.

# MCMC in action



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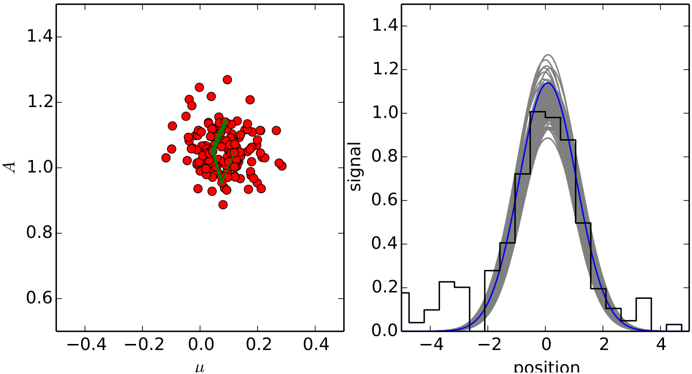

# When MCMC fails

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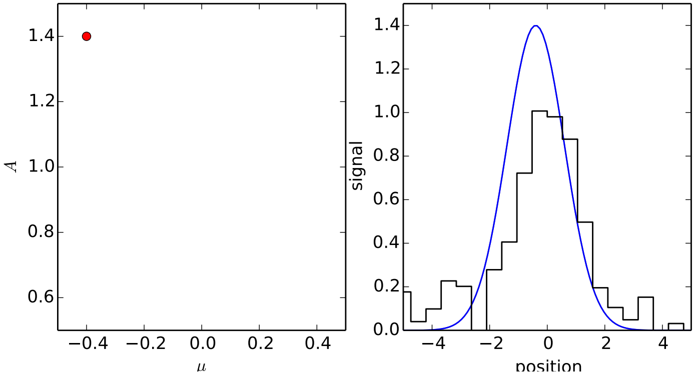

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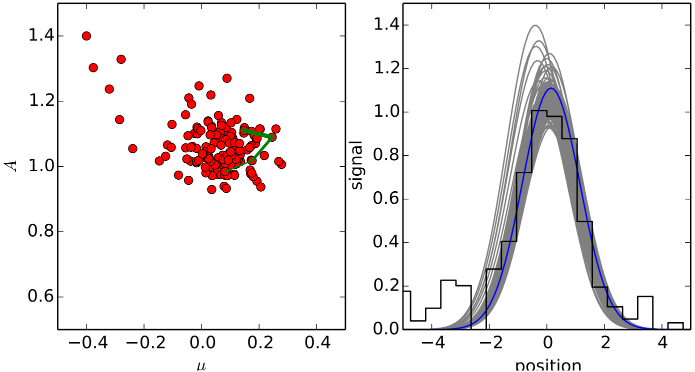

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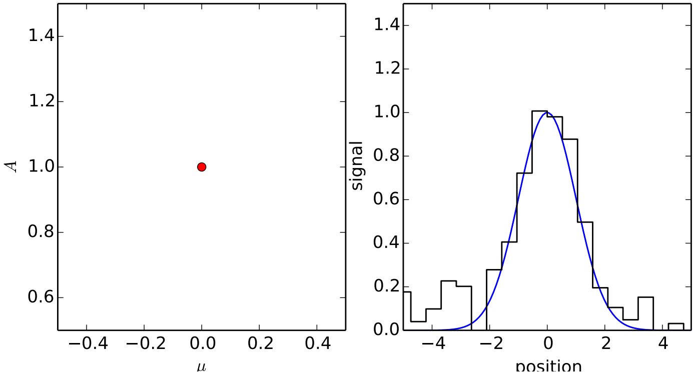

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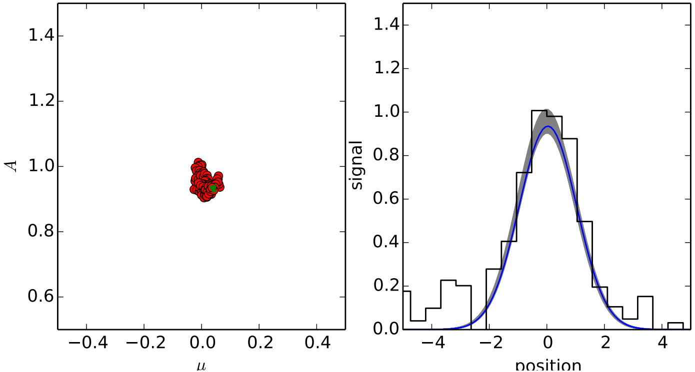

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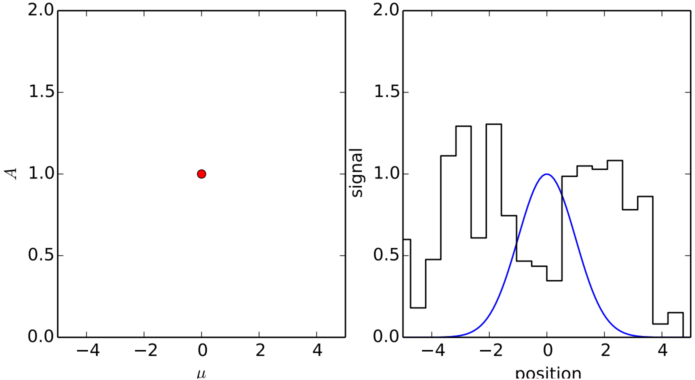

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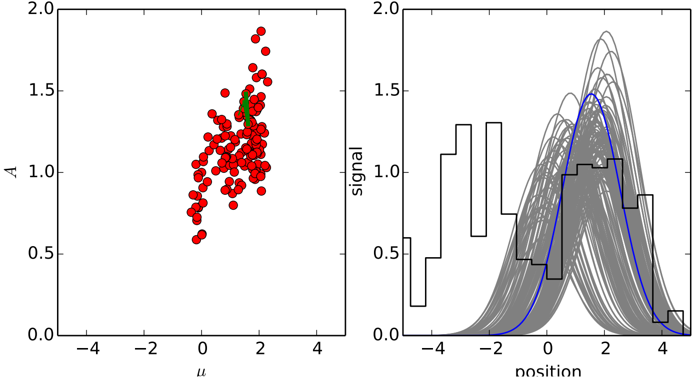

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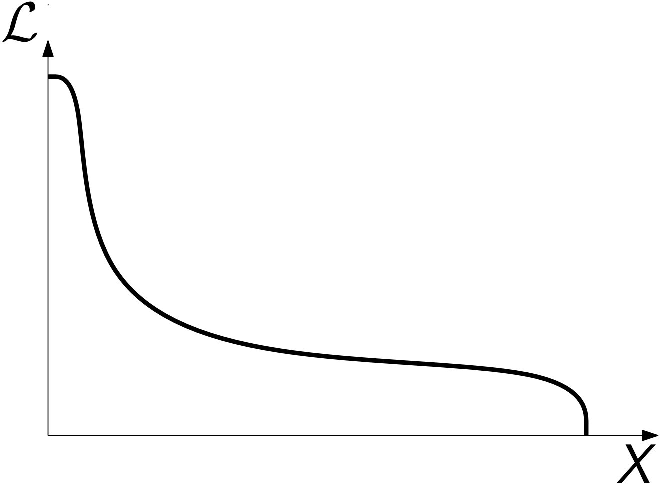
## Phase transitions



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Requires one to be able to uniformly within a region, subject to a *hard likelihood constraint*.

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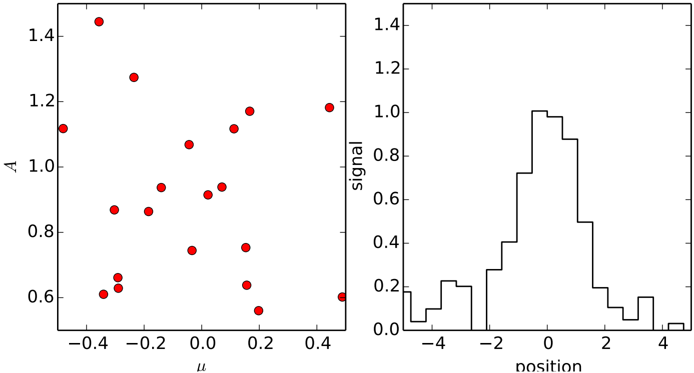

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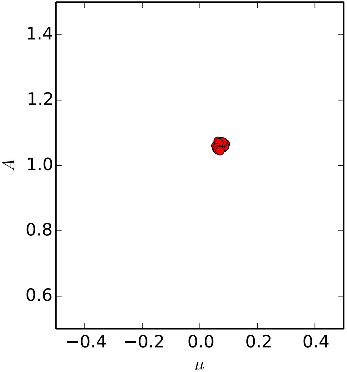


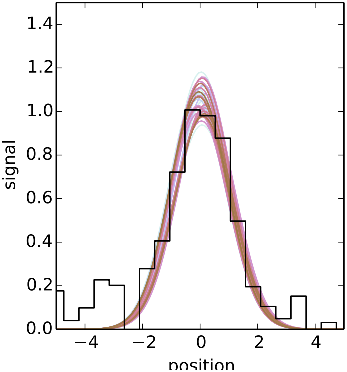

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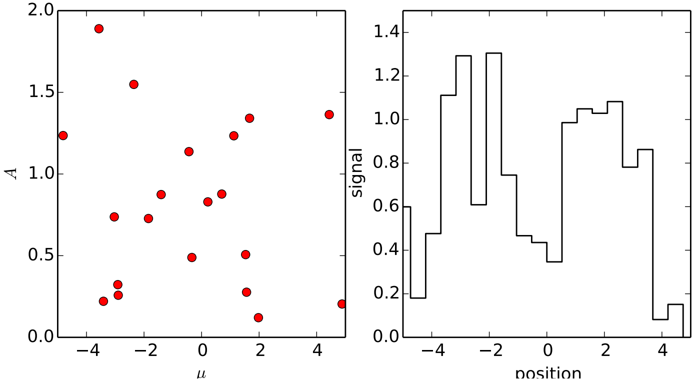
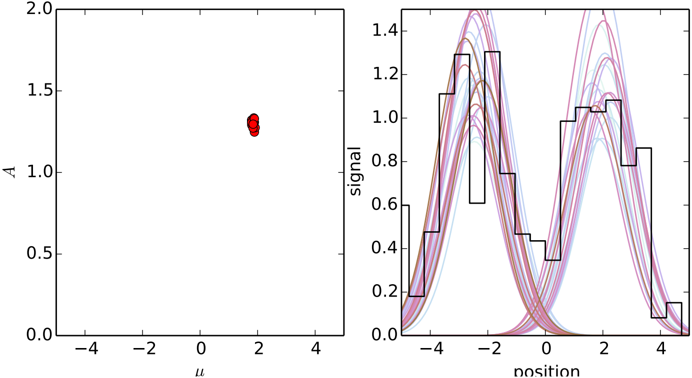


# When NS suceeds

## Multimodal



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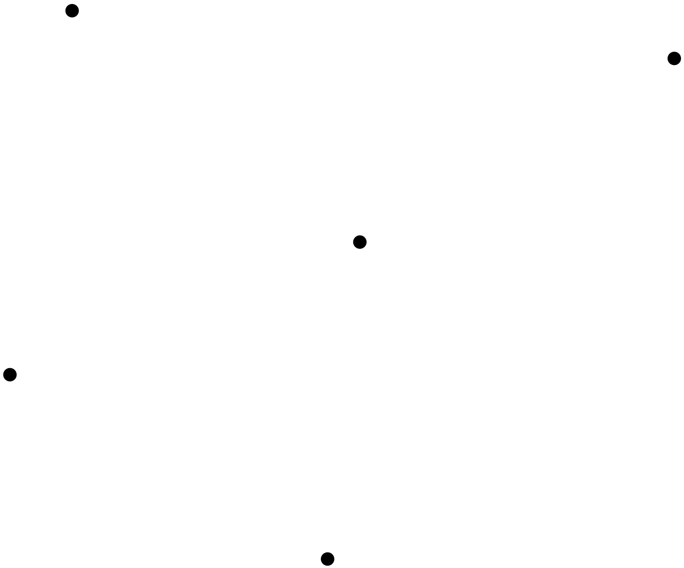

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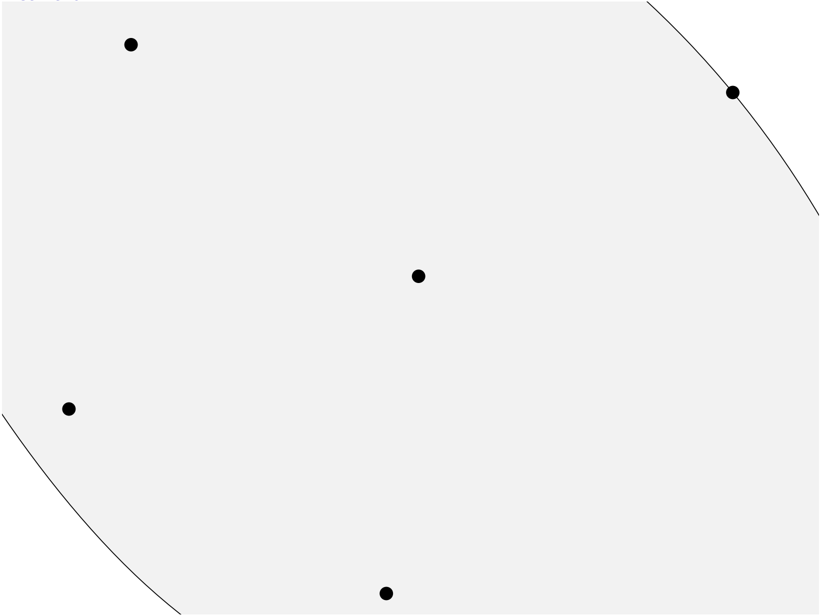

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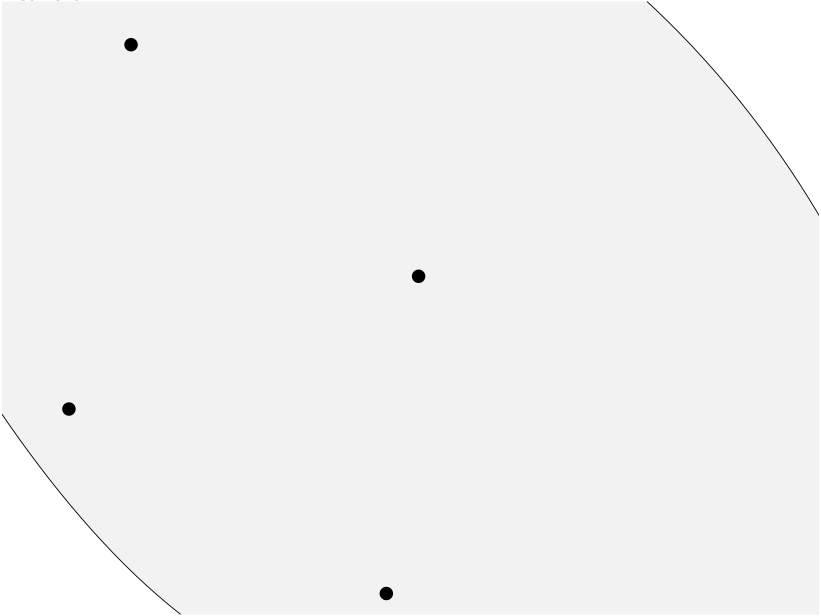

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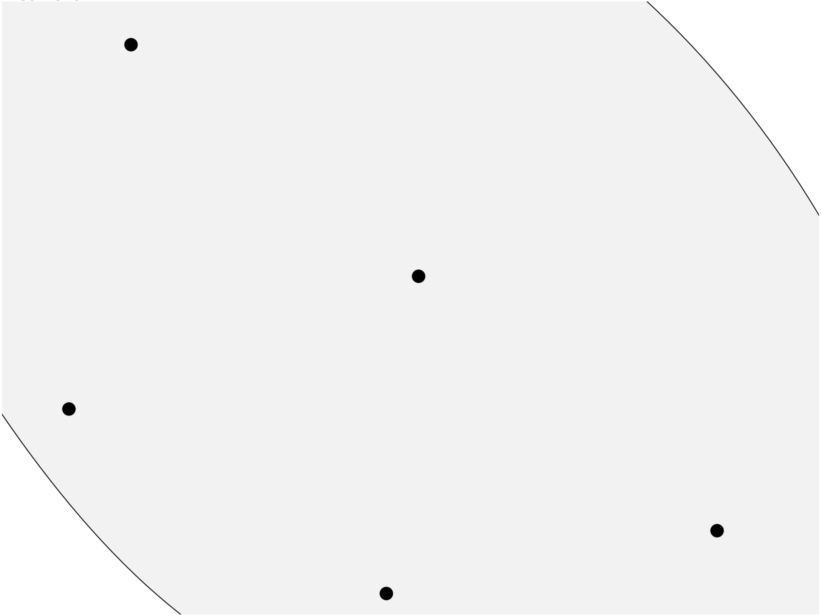

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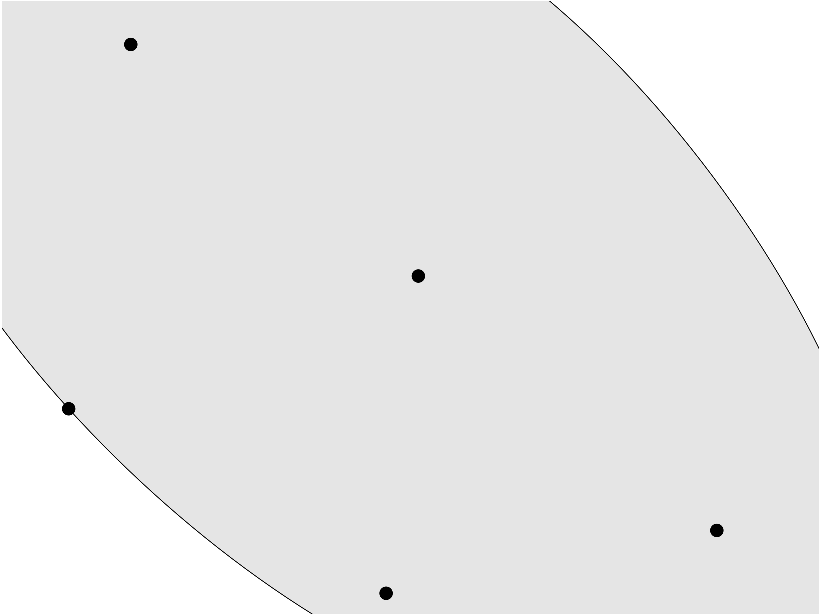

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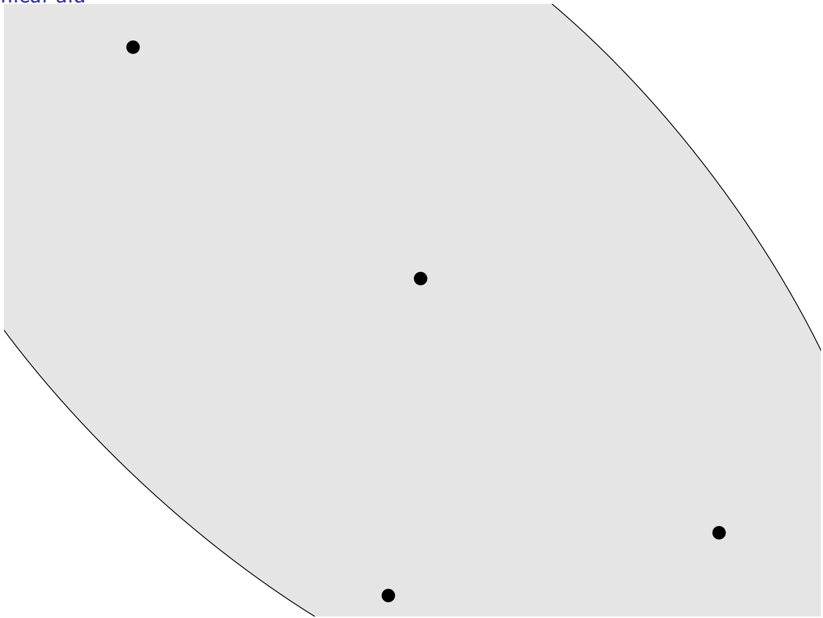

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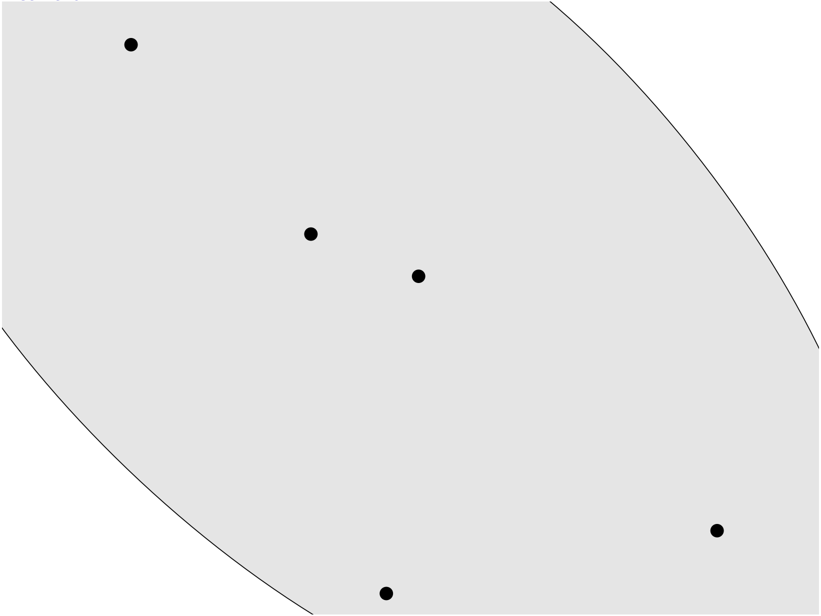

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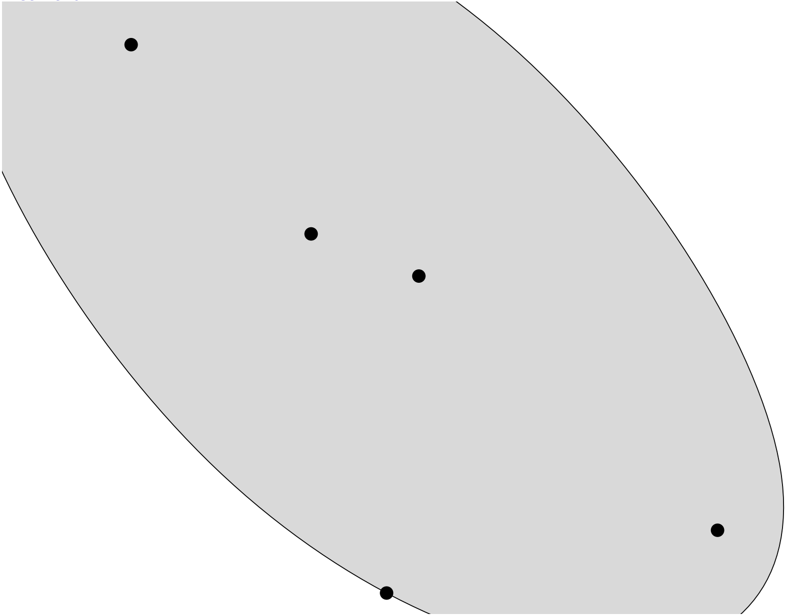

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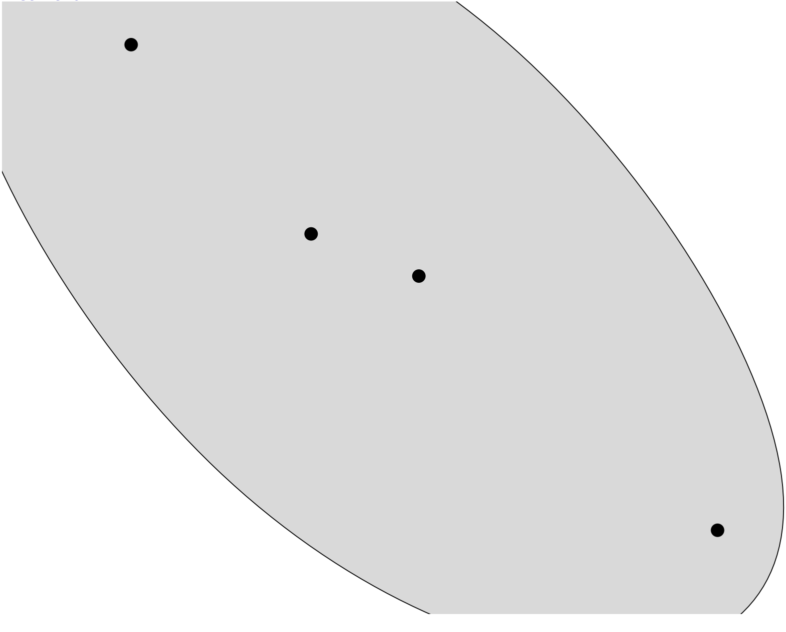

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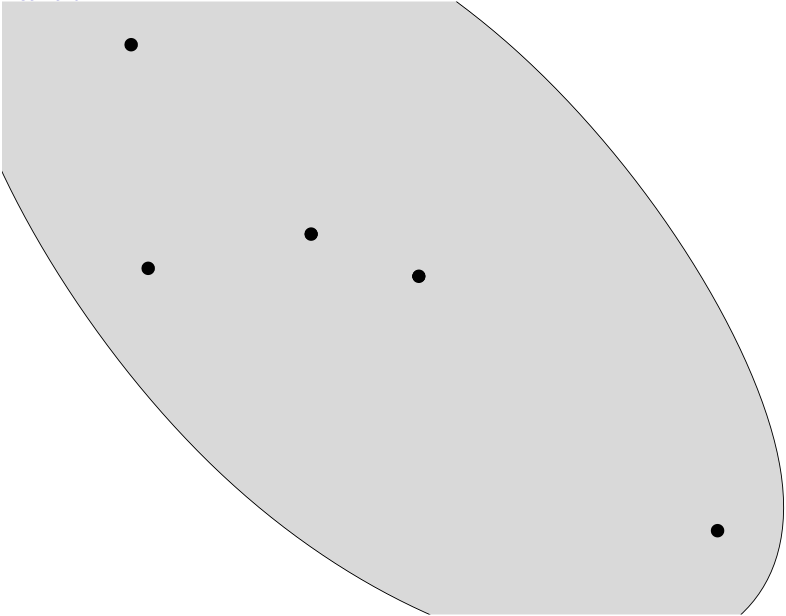

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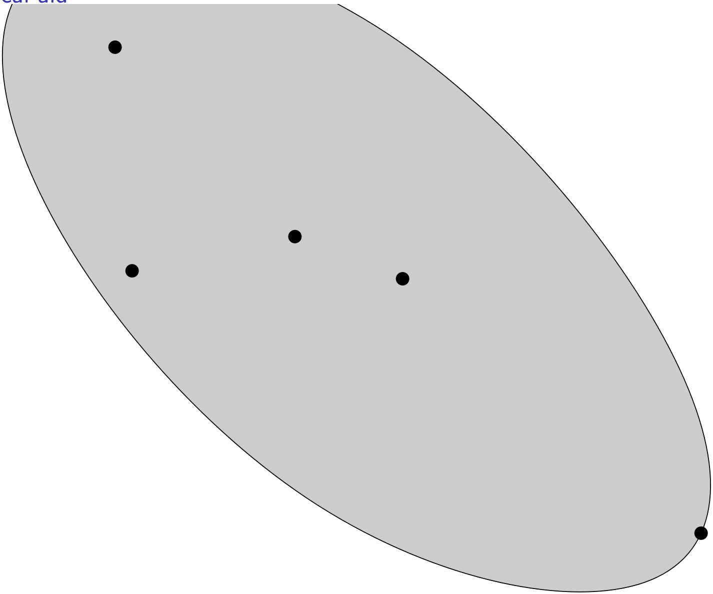

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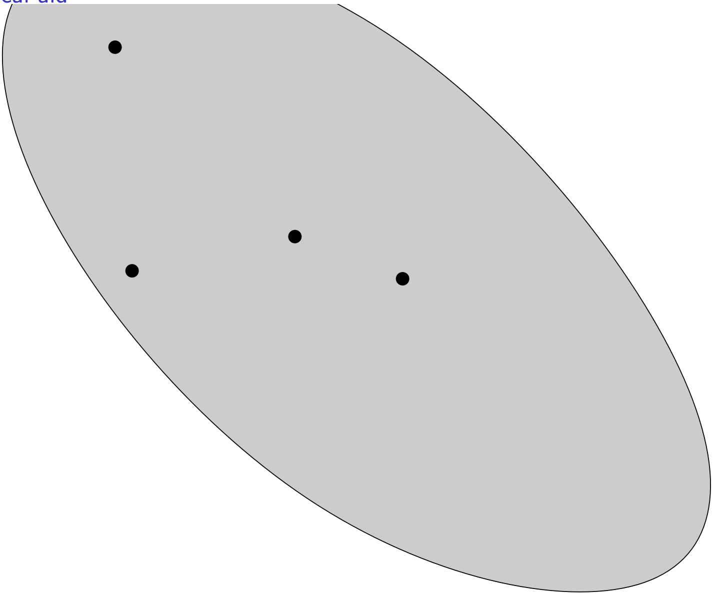

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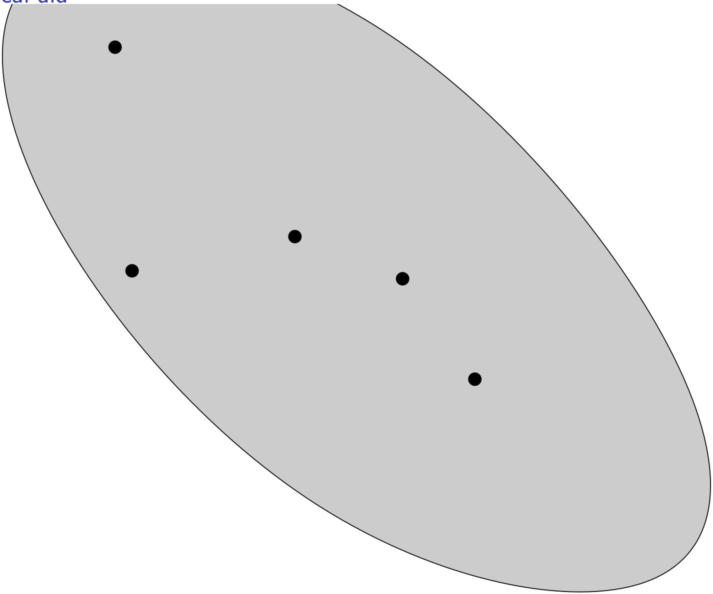

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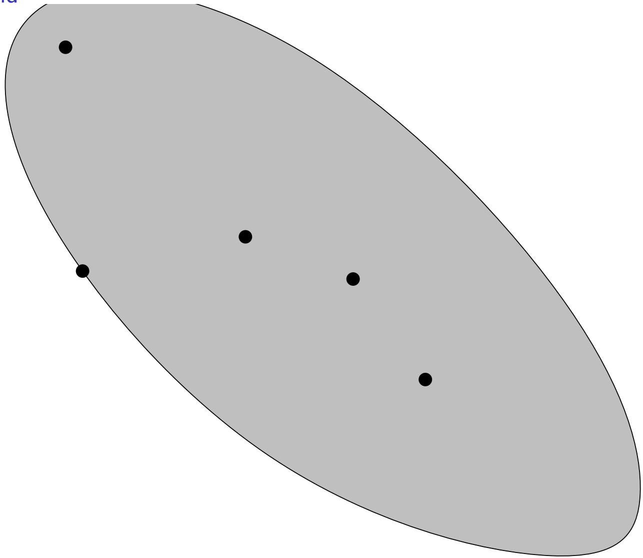

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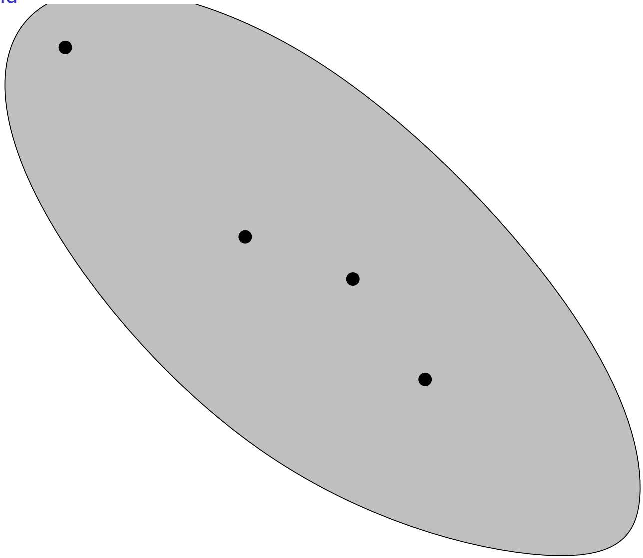

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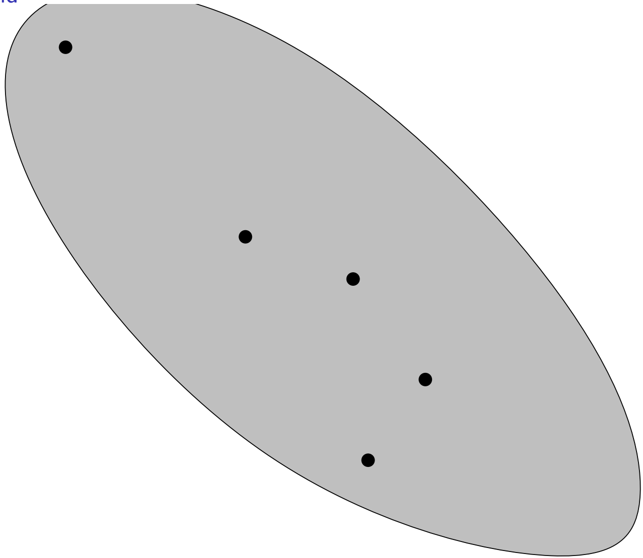

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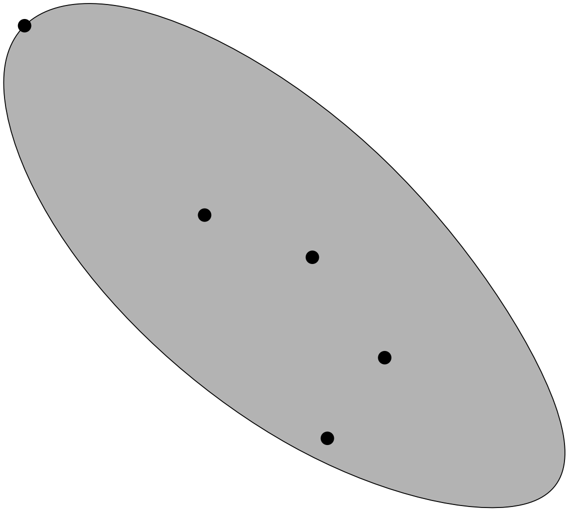

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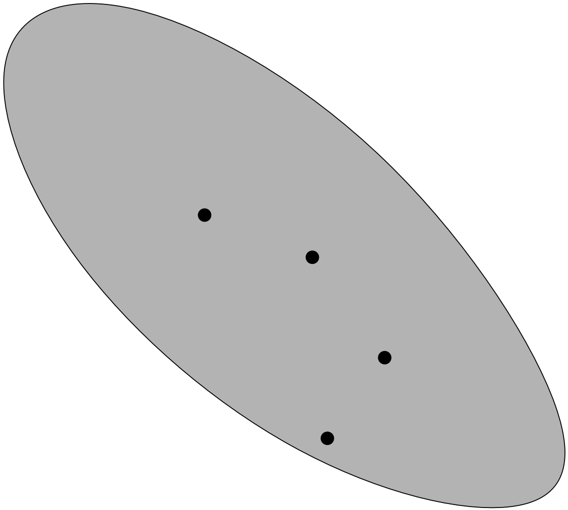

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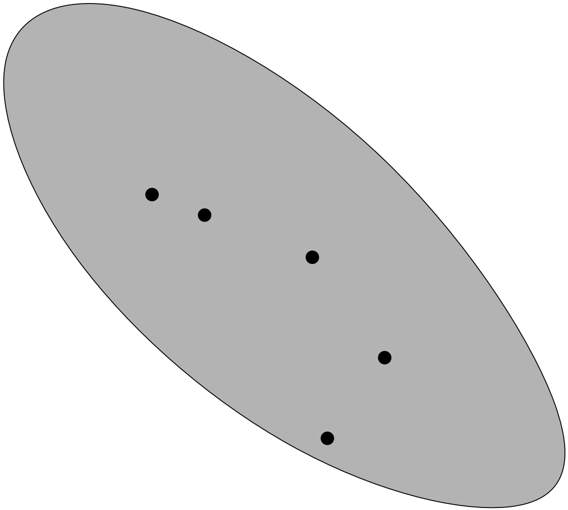

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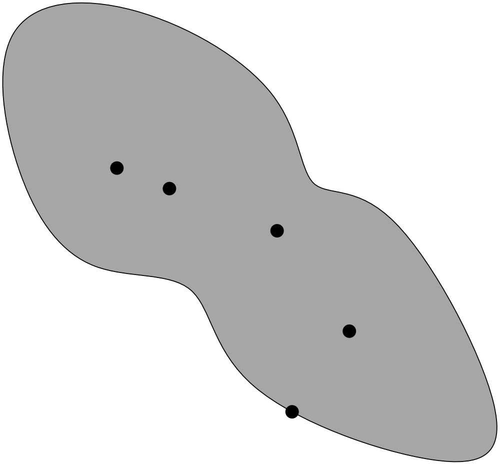

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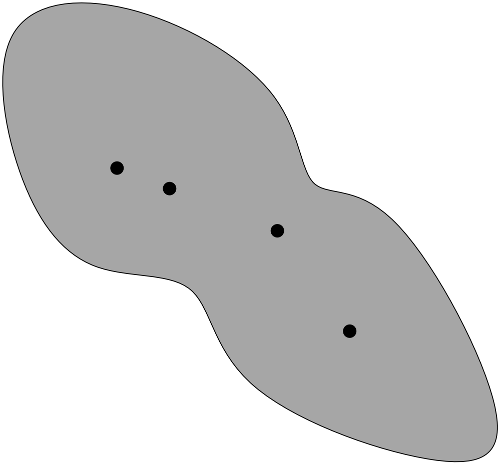

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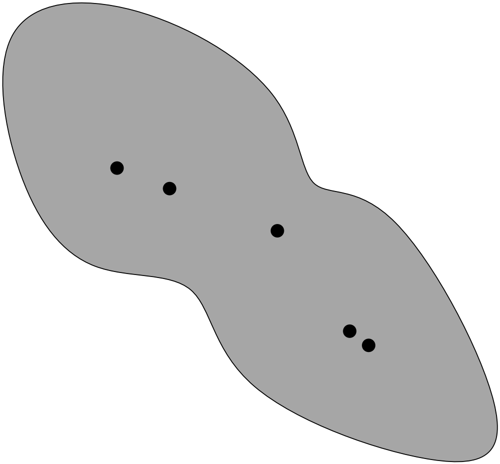

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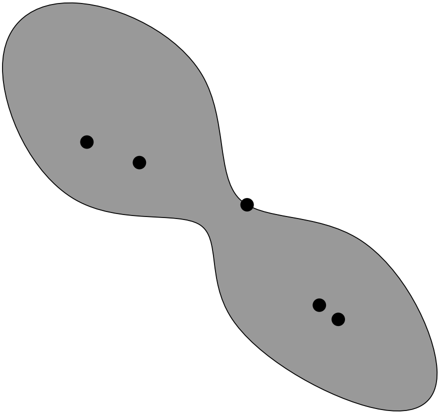

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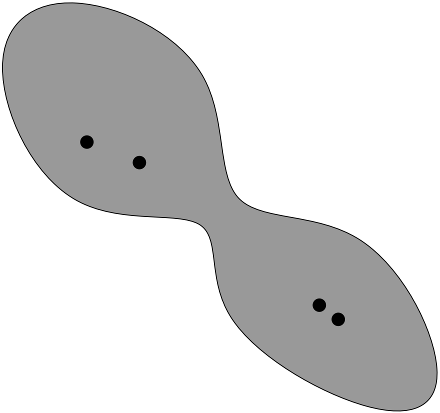

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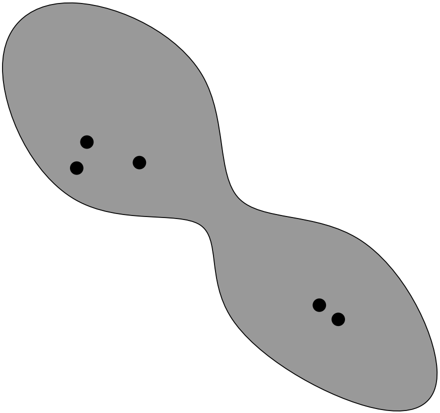

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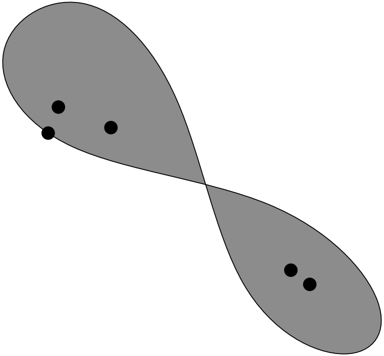

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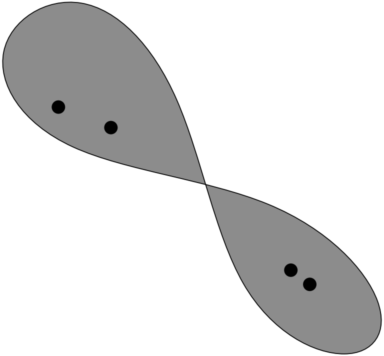

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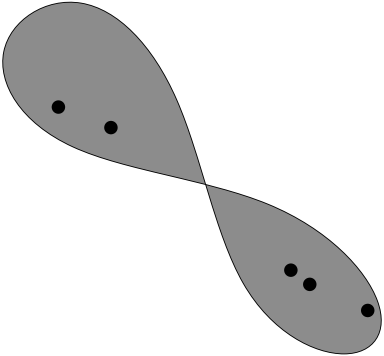

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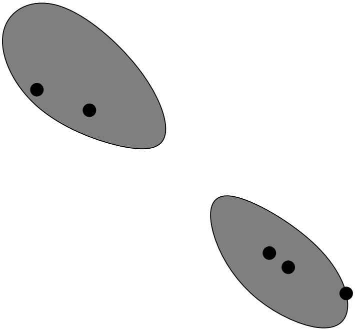

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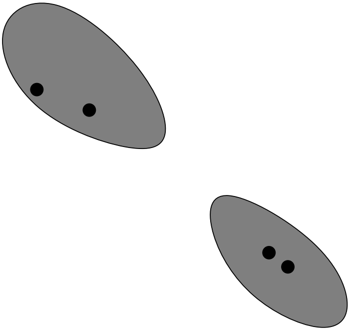

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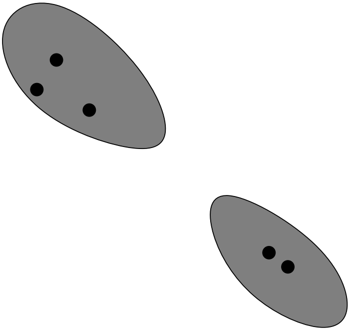

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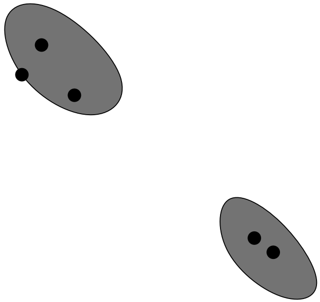

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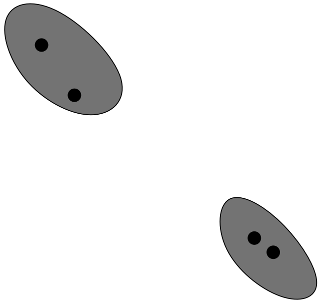

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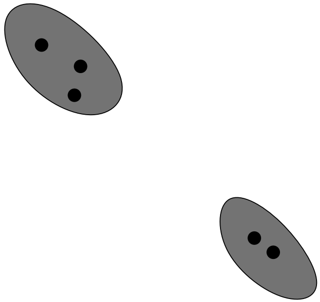

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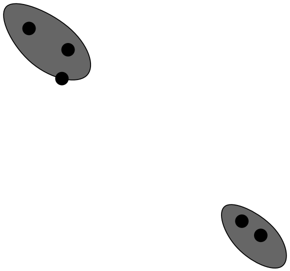

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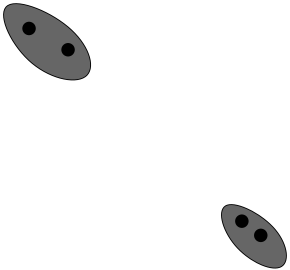

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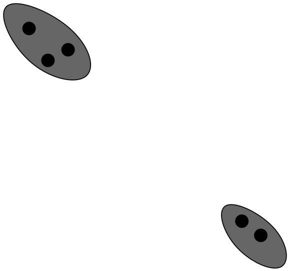

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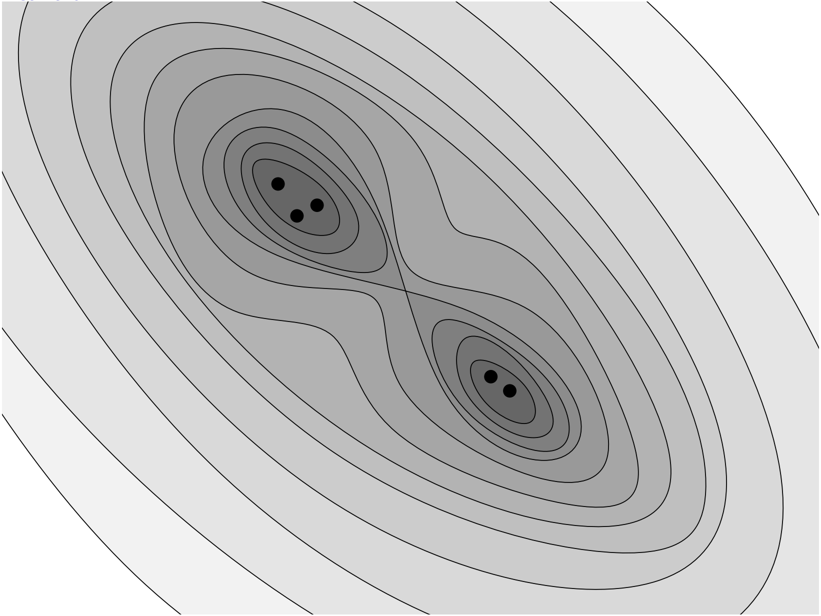

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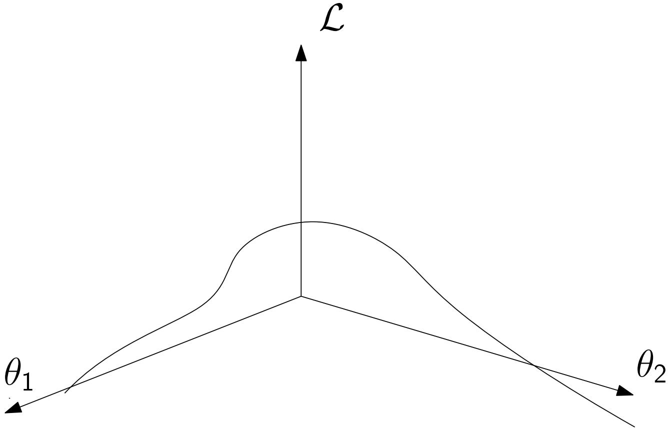

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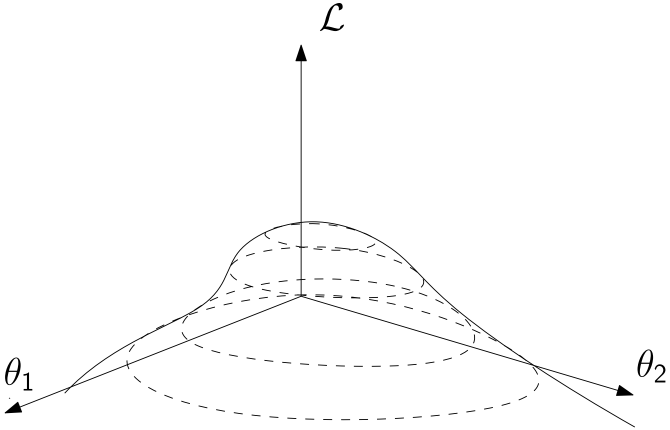

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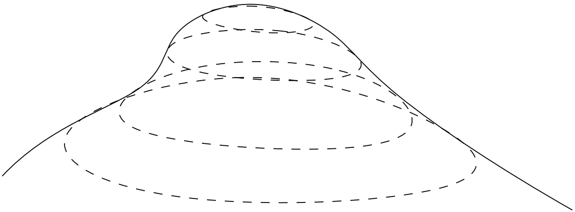

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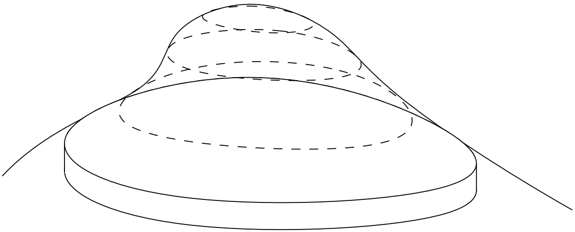

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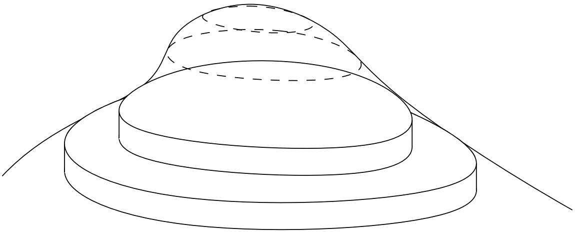

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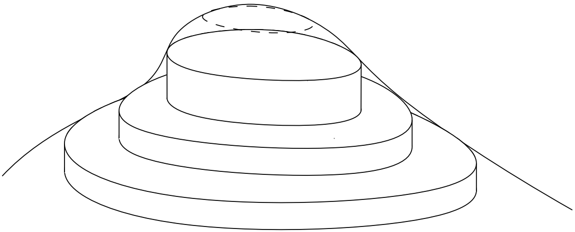

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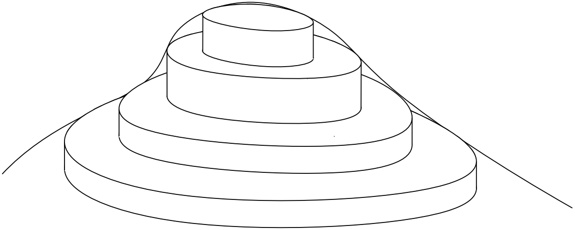

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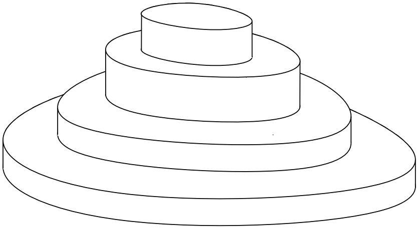

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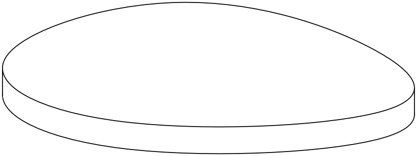

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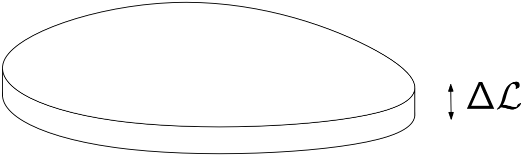

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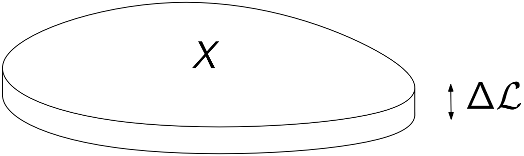

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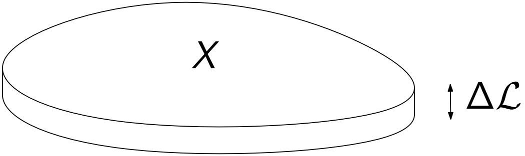


$$\text{Volume} = X\Delta\mathcal{L}$$

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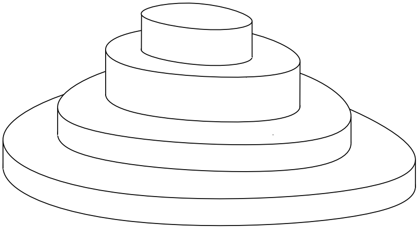

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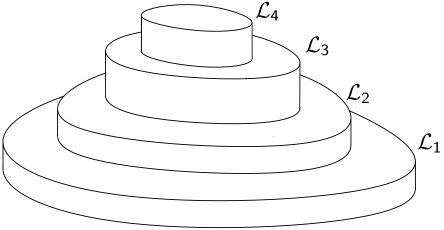

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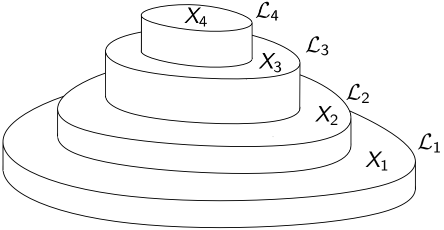

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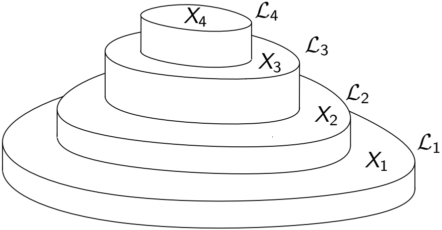
## Calculating evidences

$$\mathcal{Z} \approx \sum_i X_i \Delta \mathcal{L}_i$$



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- The set of dead points are posterior samples with an appropriate weighting factor

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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.

# Sampling within an iso-likelihood contour

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- Too many tuning parameters

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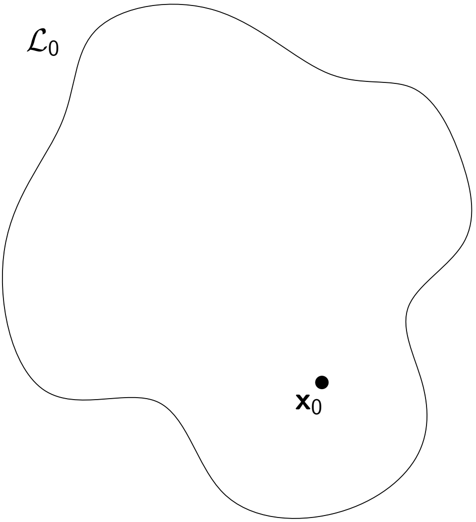

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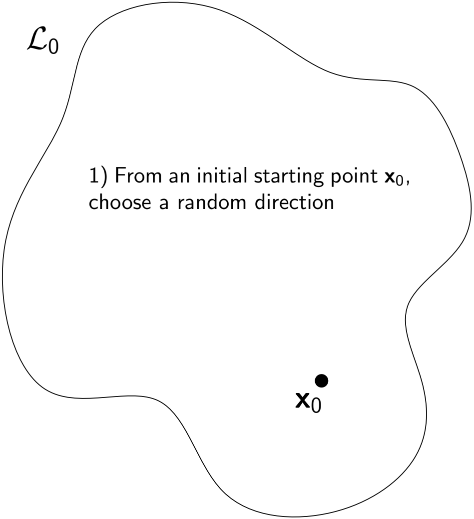

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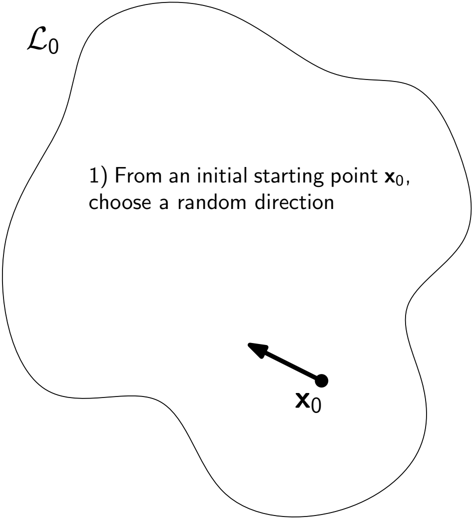

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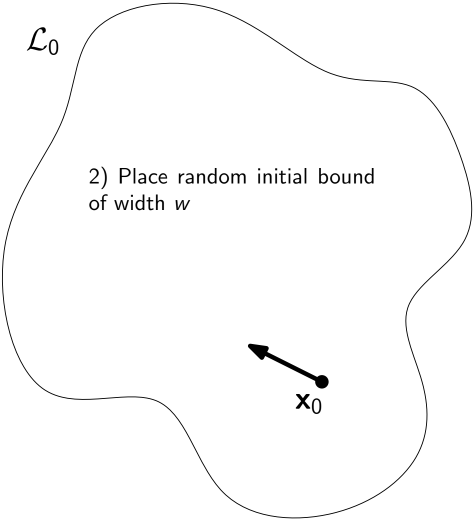

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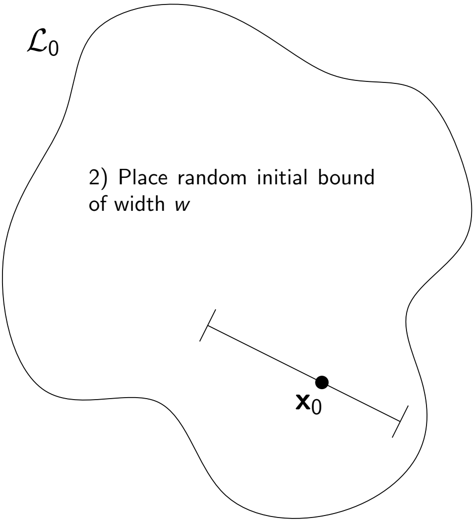

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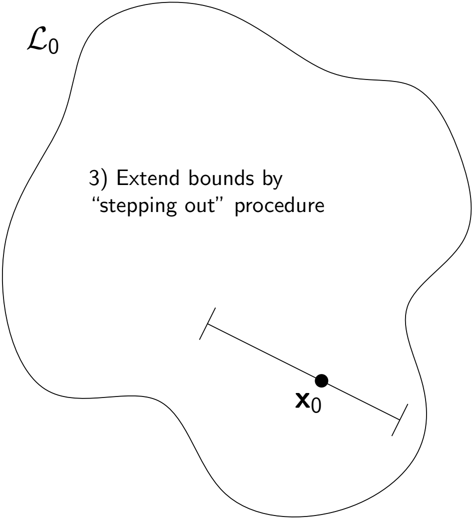

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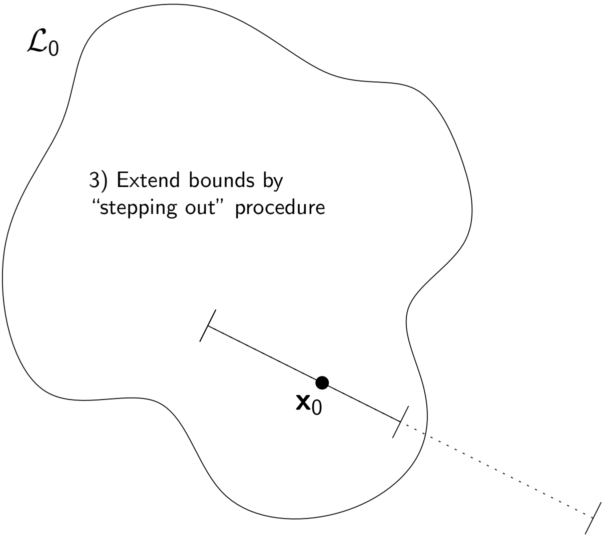

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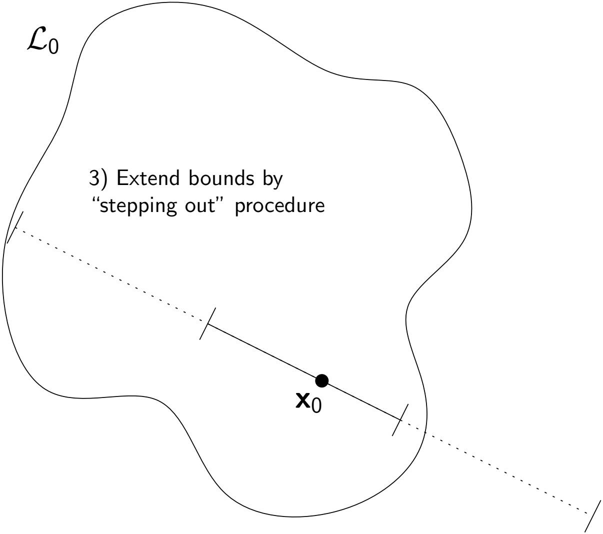

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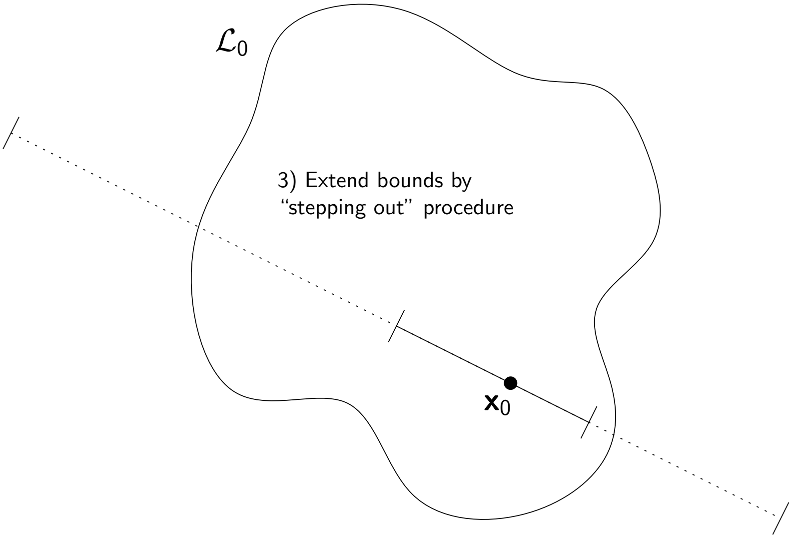

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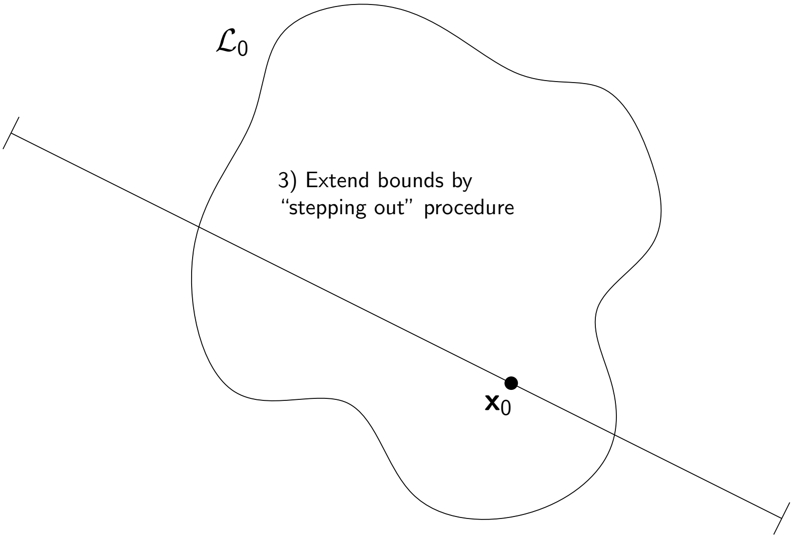

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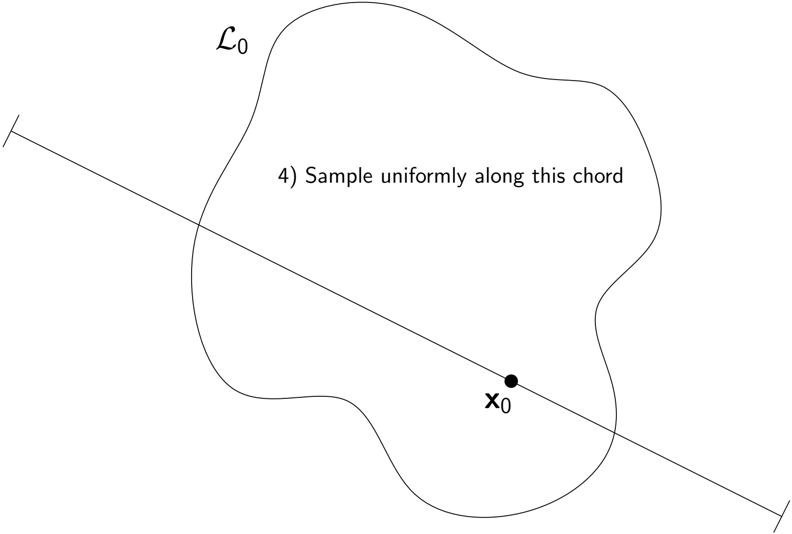

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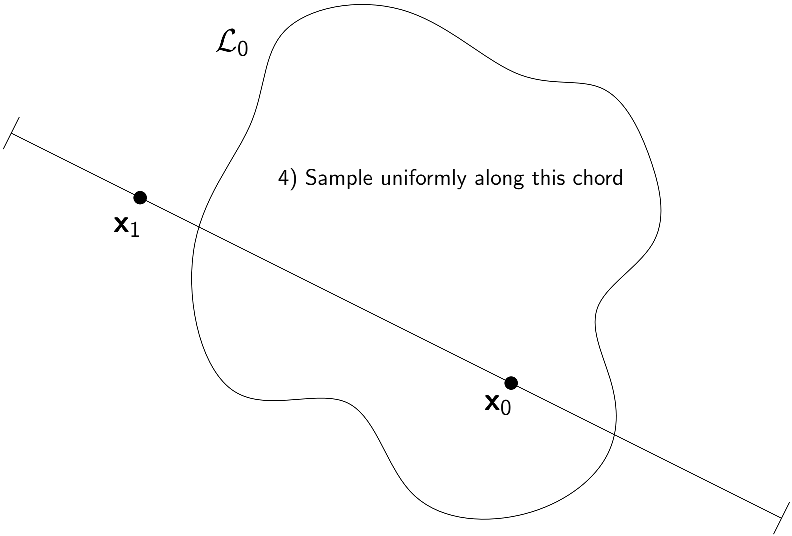

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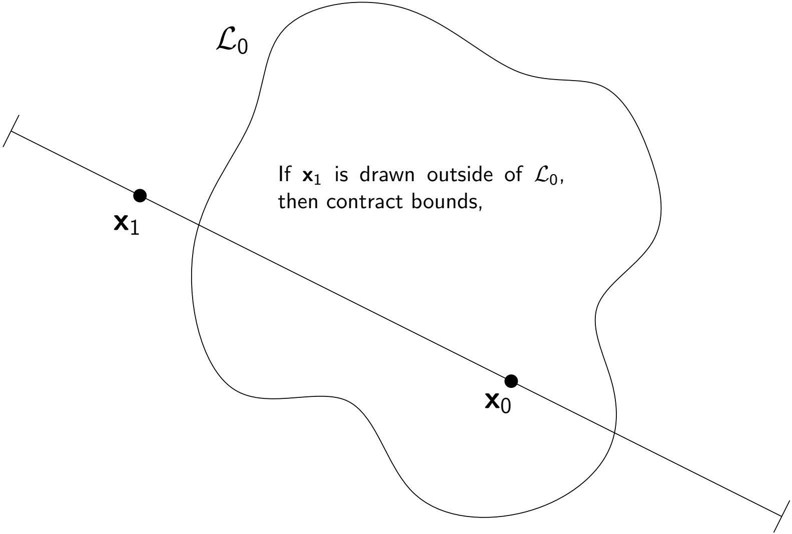

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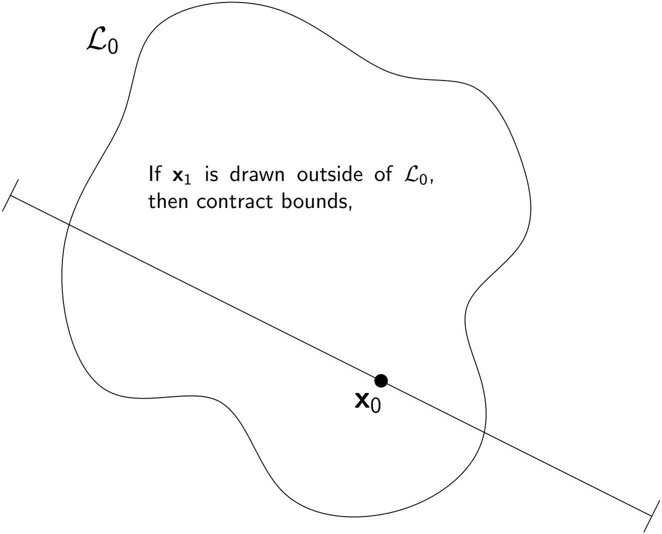

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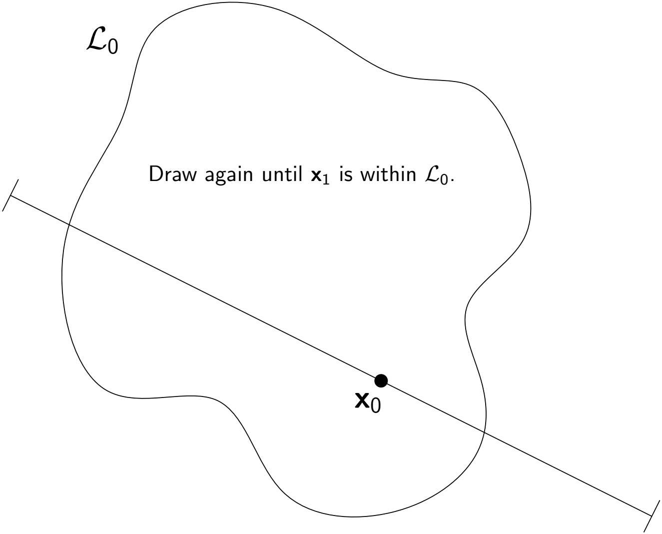

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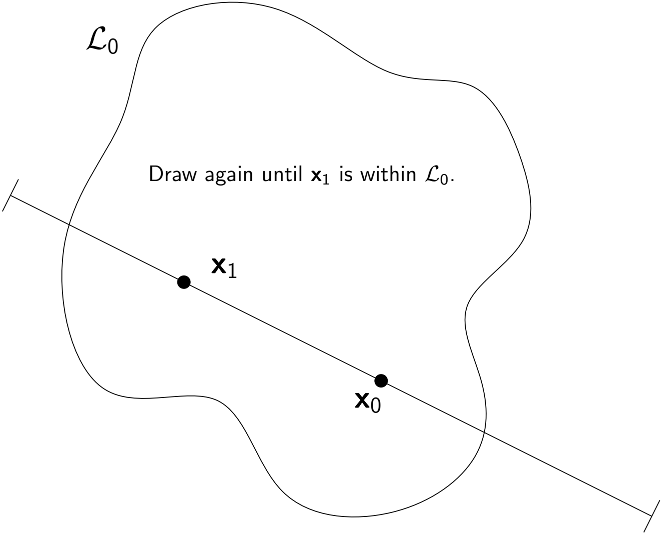

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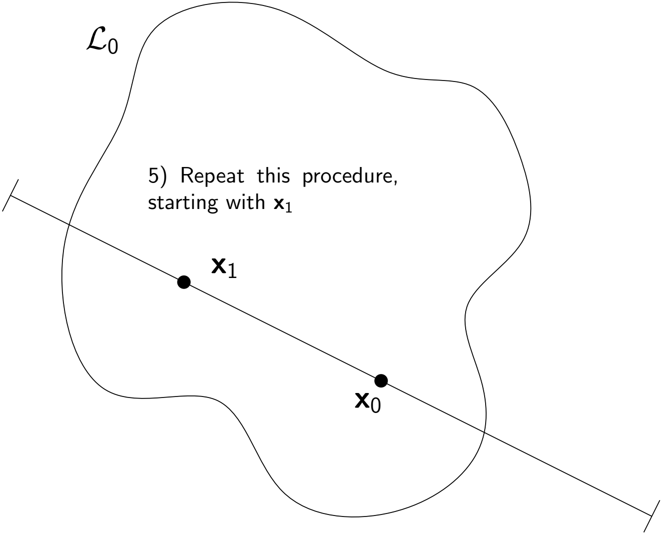

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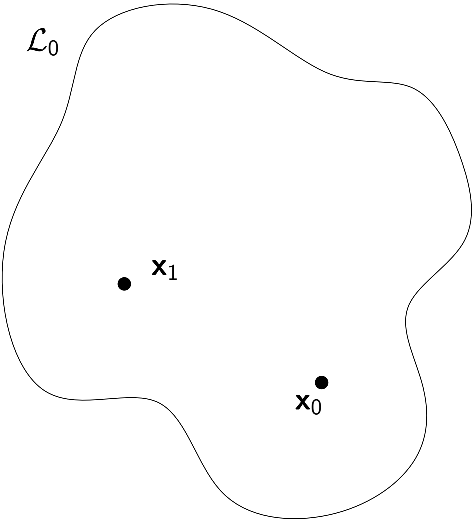

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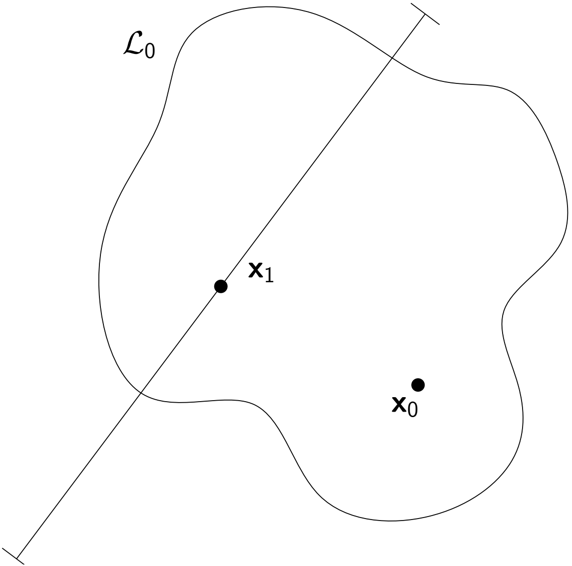

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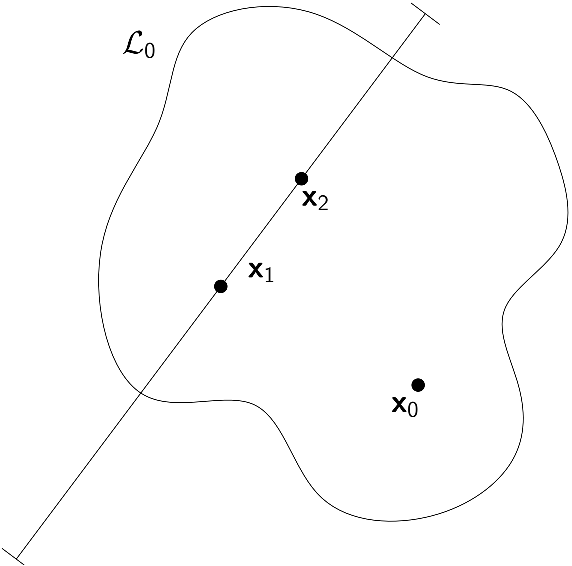

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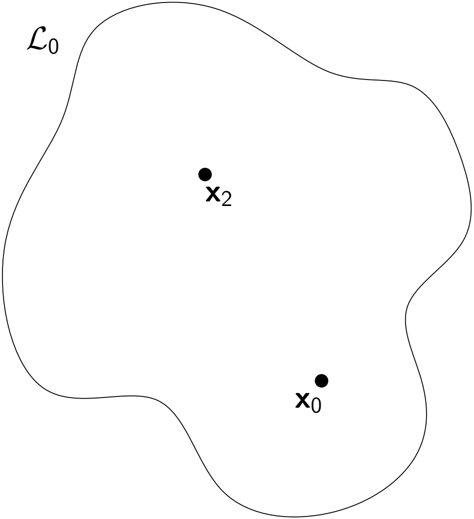

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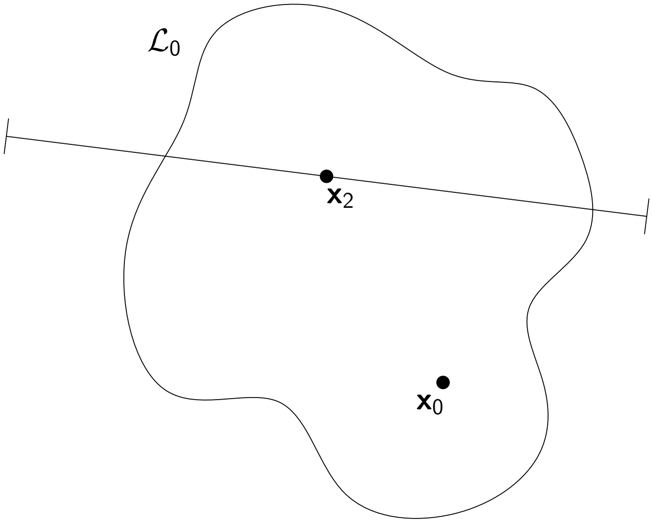

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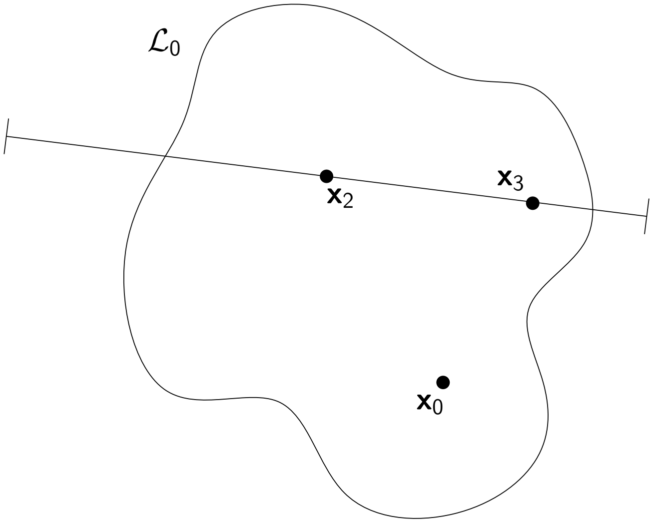

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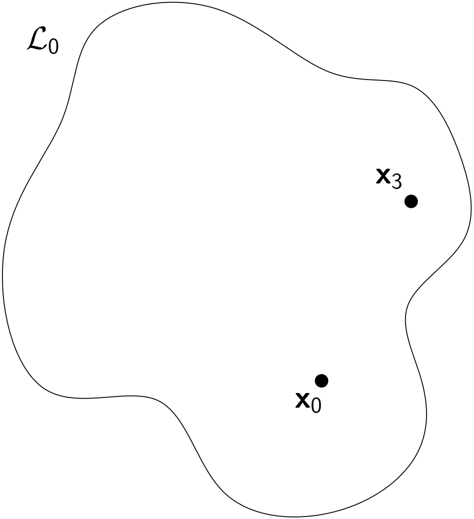

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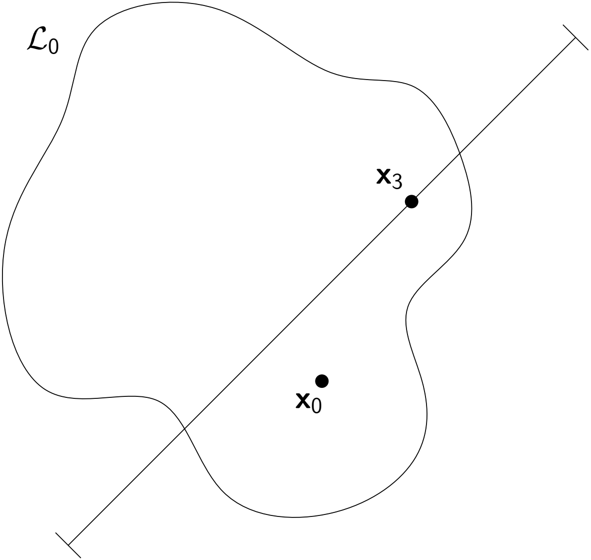

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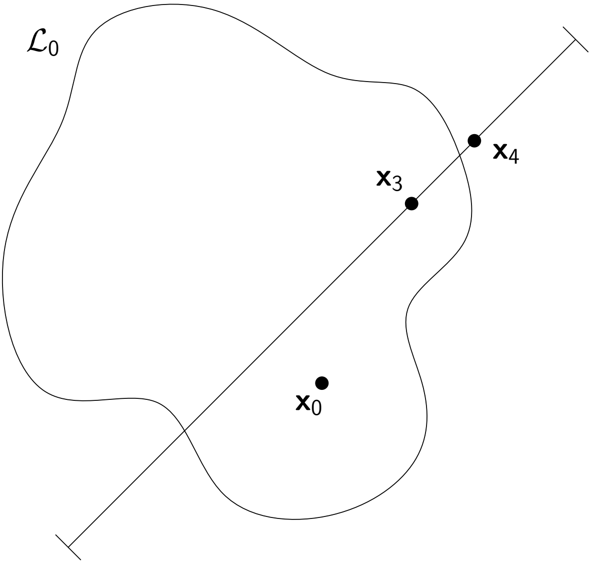

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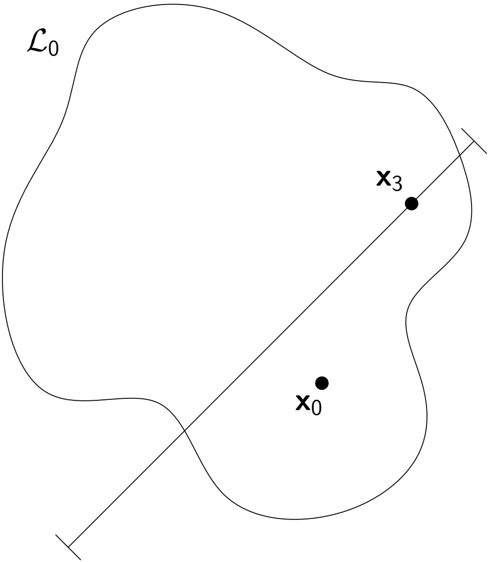

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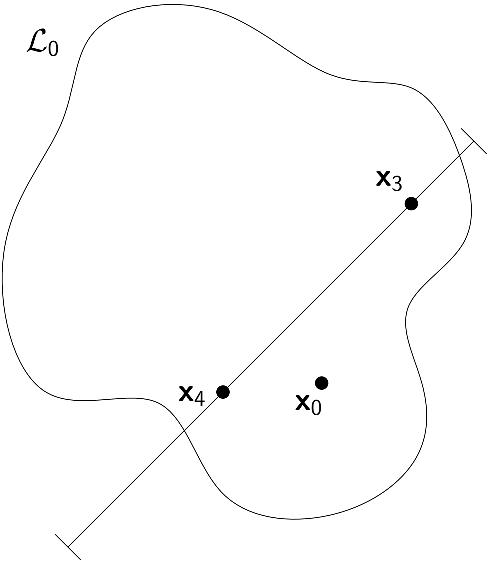

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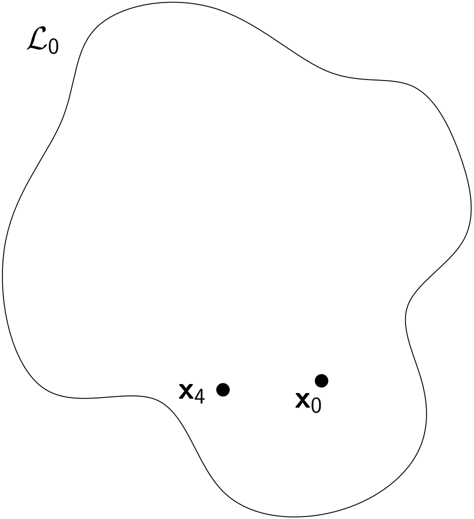

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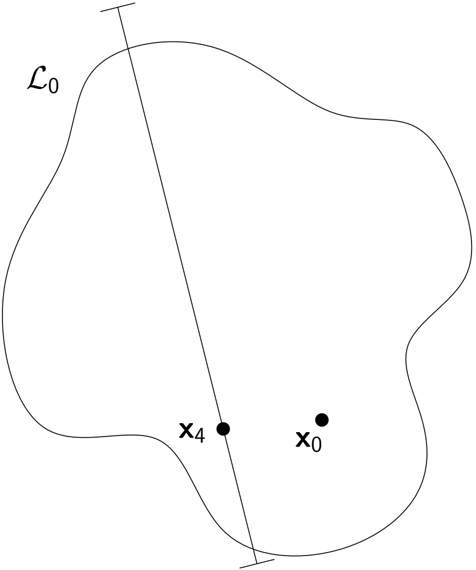

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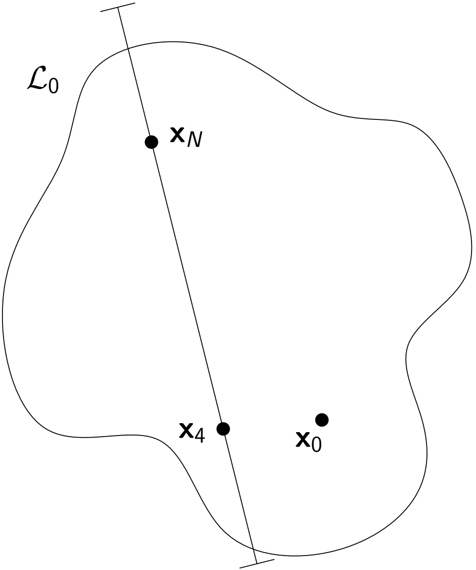

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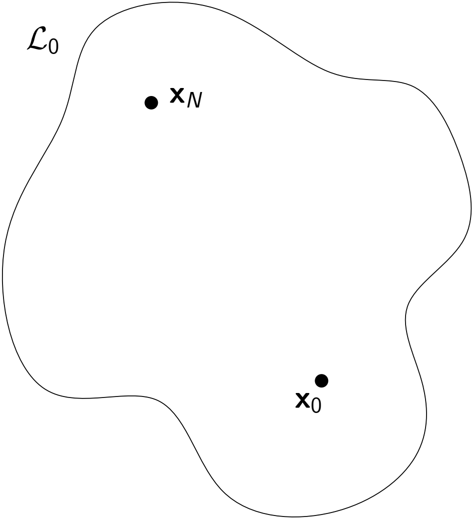

# “Hit and run” slice sampling

## Key points

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- This procedure satisfies detailed balance.

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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

## Correlated distributions

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1. Does not deal well with correlated distributions.

# Issues with Slice Sampling

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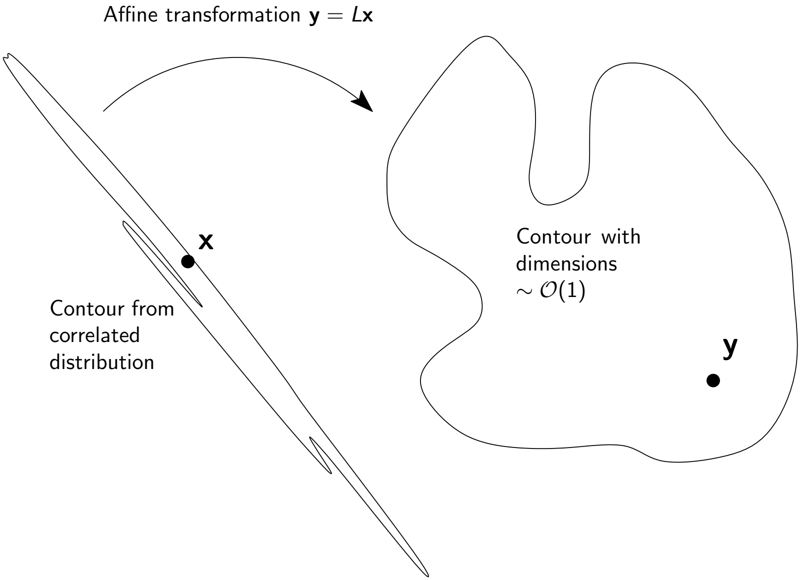
2. Need to “tune” $w$ parameter.

# PolyChord's solutions

## Correlated distributions



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2. Affine transformation is useless.

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1. Identifies separate modes via clustering algorithm on live points.
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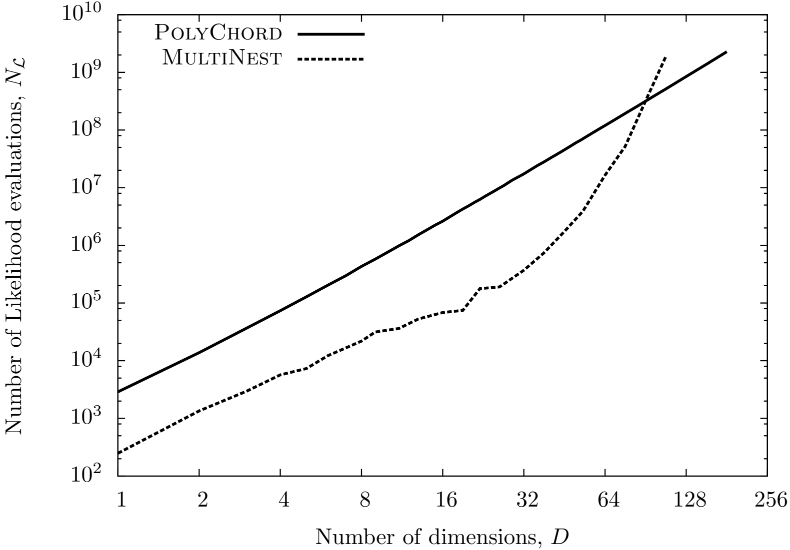
- Implemented in CosmoMC, as "CosmoChord", with fast-slow parameters.

# PolyChord vs. MultiNest

## Gaussian likelihood



# PolyChord 1.0

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- `ccpforge.cse.rl.ac.uk/gf/project/polychord/`

# PolyChord

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  - Need $\sim \mathcal{O}(D)$ to de-correlate at each step
  - Forced to throw $\sim \mathcal{O}(D)$ inter-chain points away.

# PolyChord 2.0

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- If $n_{\mathrm{chain}} \sim \mathcal{O}(D)$ (as required), then overall $\sim \mathcal{O}(D^3) \to \sim \mathcal{O}(D^2)$.
- Need to be able to quantify degree of correlation for correct inference.

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- In his original paper, John Skilling noted that nested sampling runs can be merged.
- Take two complete nested sampling runs generated by $n_{\rm live}^{(1)}$ and $n_{\rm live}^{(2)}$ live points.
- Combining the two runs in likelihood order gives a new run generated by $n_{\rm live}^{(1)} + n_{\rm live}^{(2)}$ live points.

# Aside: Unweaving nested sampling runs

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- The reverse is also true.
- Given a nested sampling run with $n_{\rm live}$ points, there is a unique way of separating it into $n_{\rm live}$ single-point runs (threads).

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- Each thread is a "true" nested sampling run, although threads are correlated.
- Can use traditional techniques on threads to quantify correlation
    - Batch means
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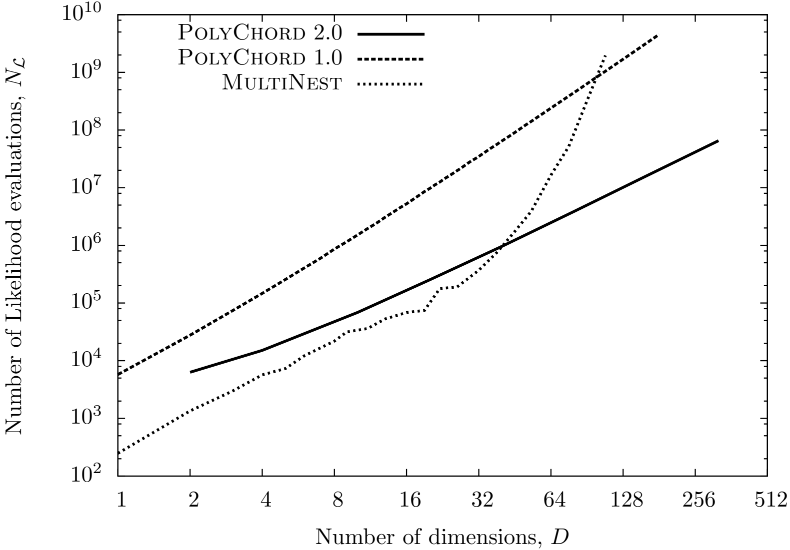
- With this in hand, can produce correct inferences from correlated runs.

# PolyChord 2.0 vs. MultiNest

## Gaussian likelihood



# Correlated distributions

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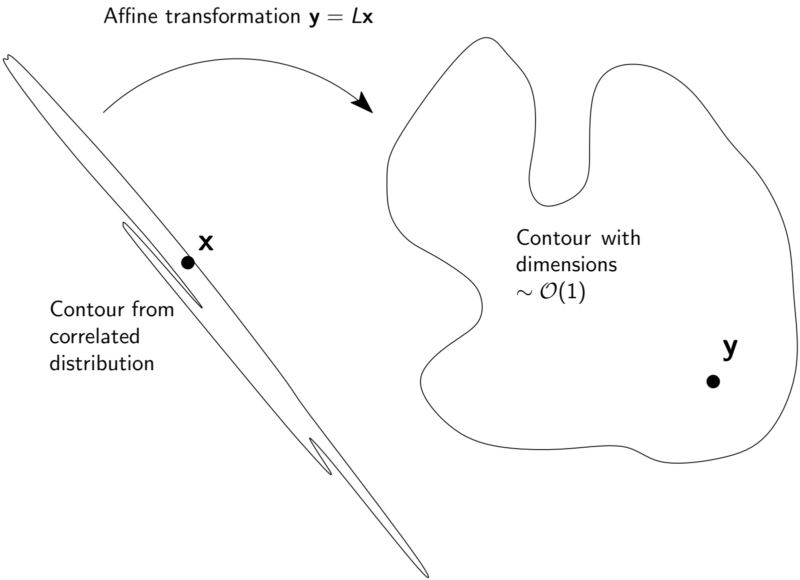
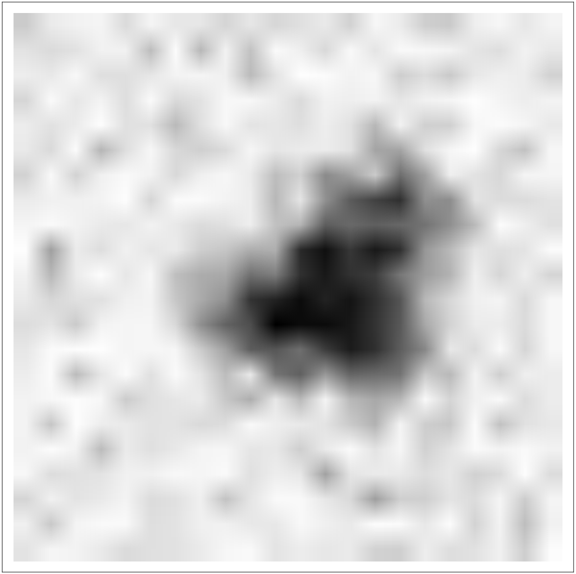
- Correlated distributions are hard

# Correlated distributions



# Object detection

## Toy problem



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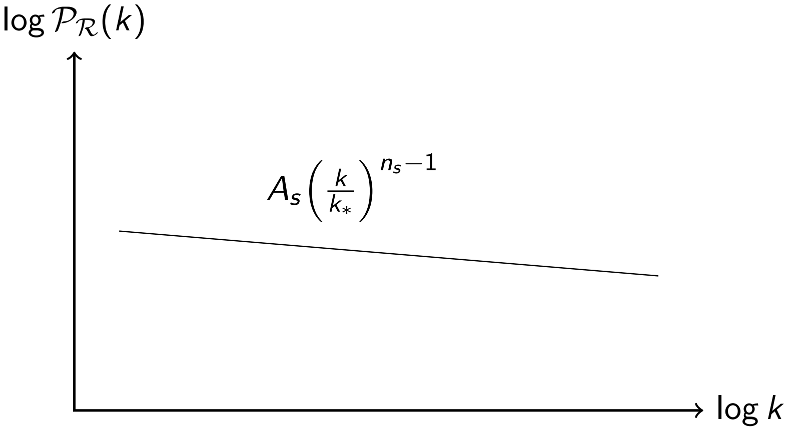
- $\log \mathcal{Z}$ ratio: $-251 : -156 : -114 : -117 : -136$
- odds ratio: $10^{-60} : 10^{-19} : 1 : 0.04 : 10^{-10}$

# PolyChord in action

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



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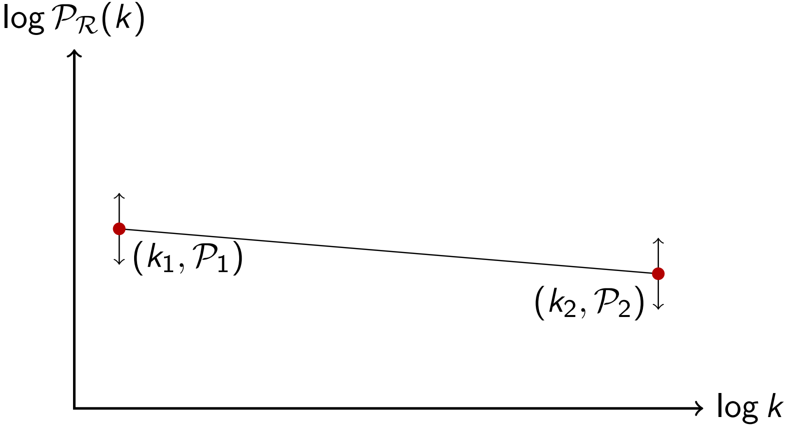

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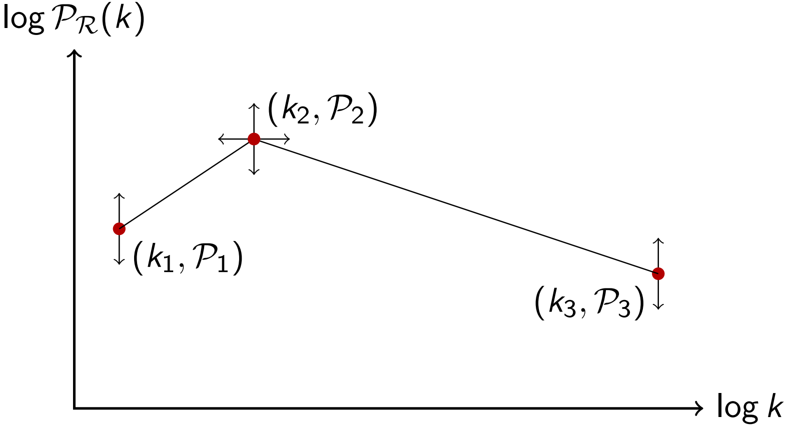

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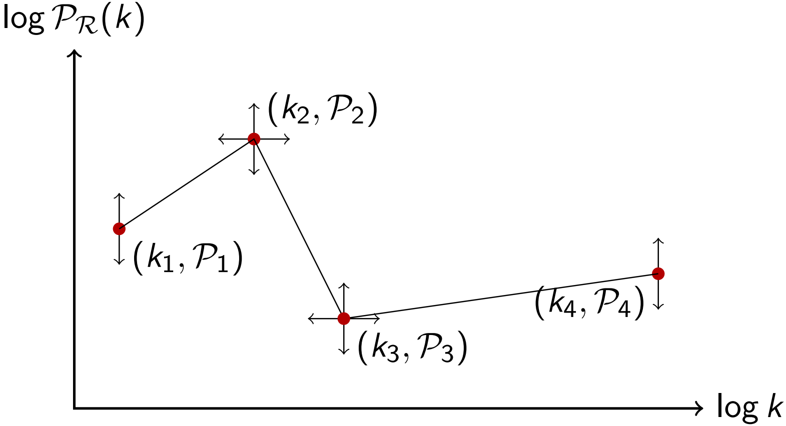

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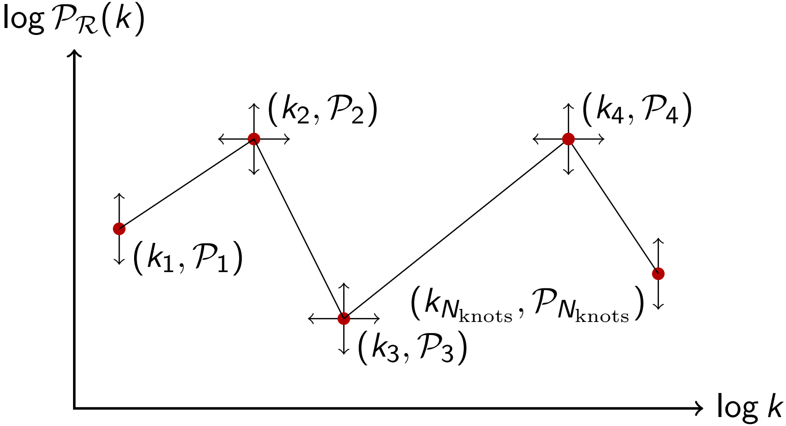
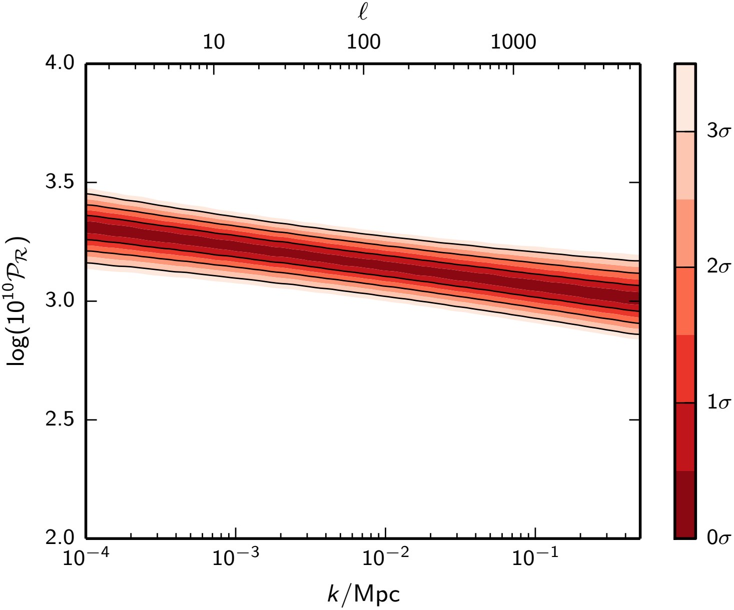


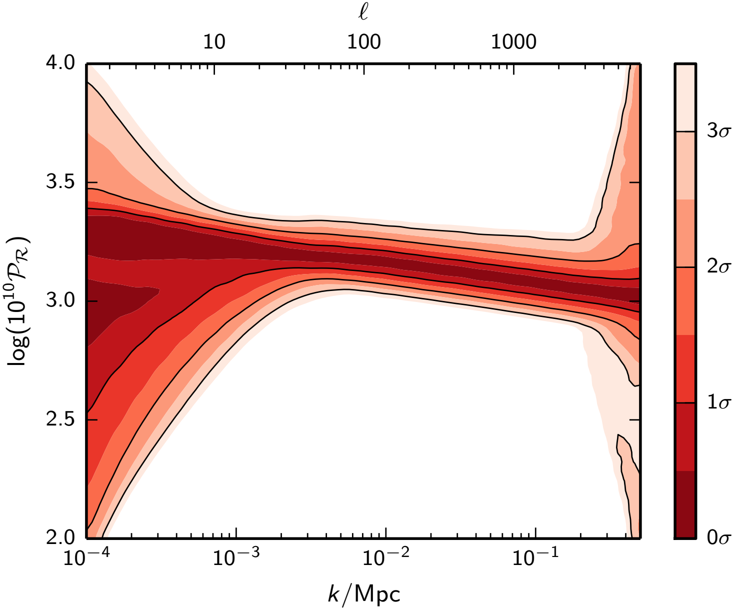
# 0 internal knots

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



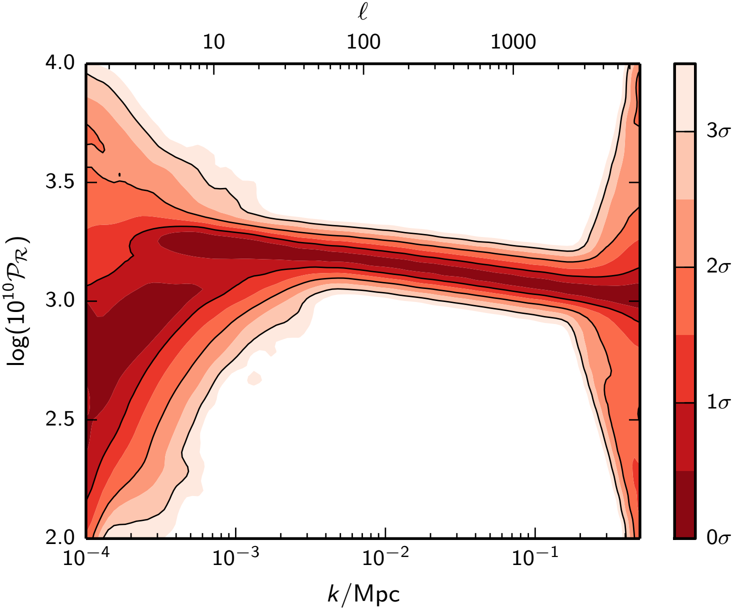
# 1 internal knots

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



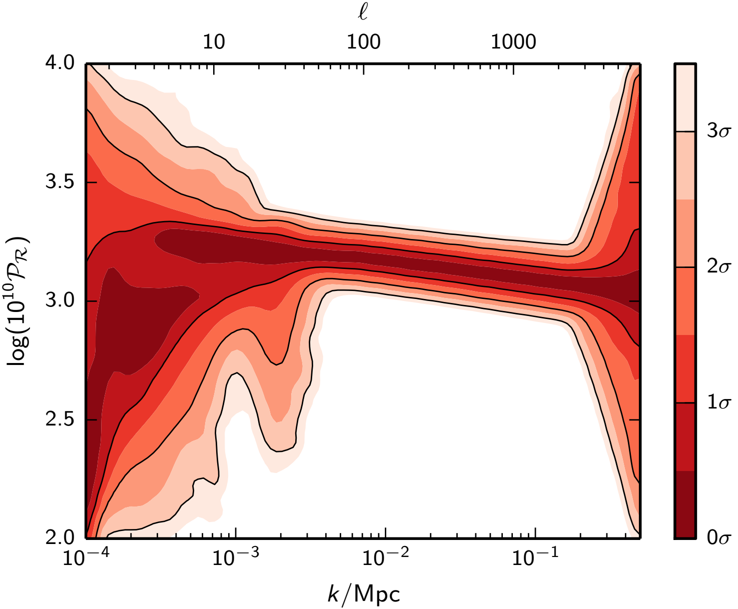
# 2 internal knots

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



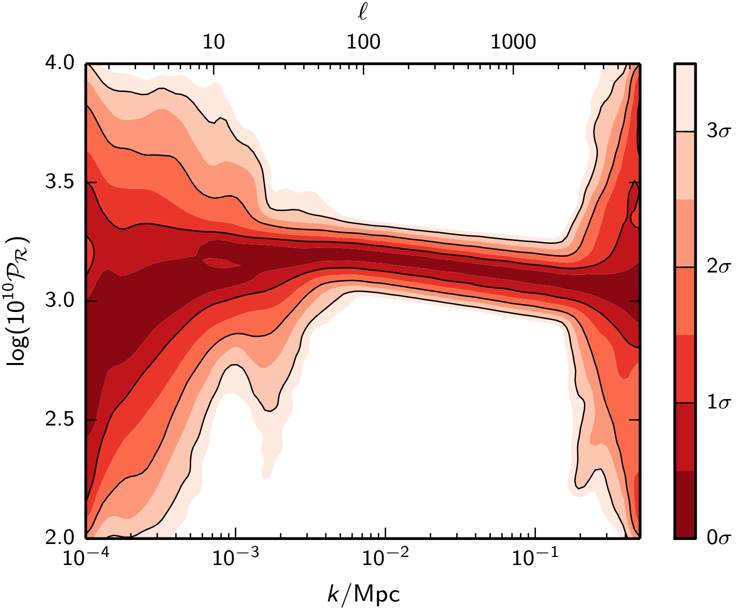
# 3 internal knots

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



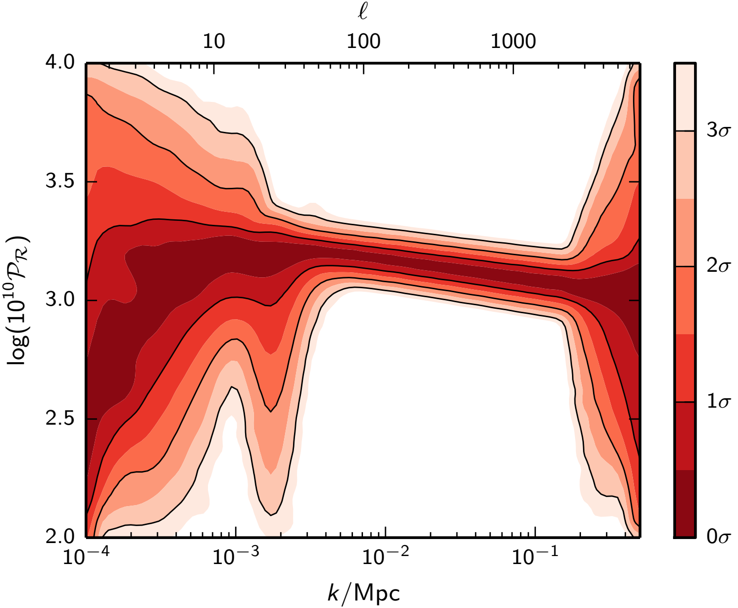
# 4 internal knots

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



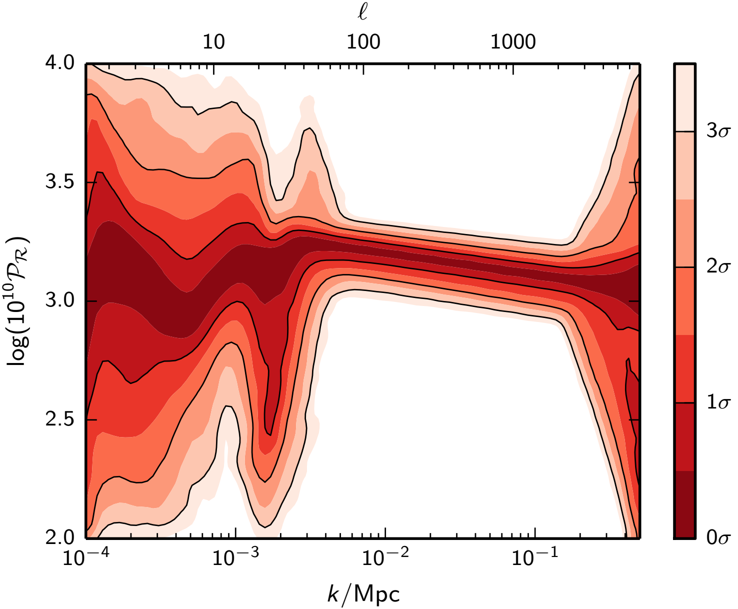
# 5 internal knots

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



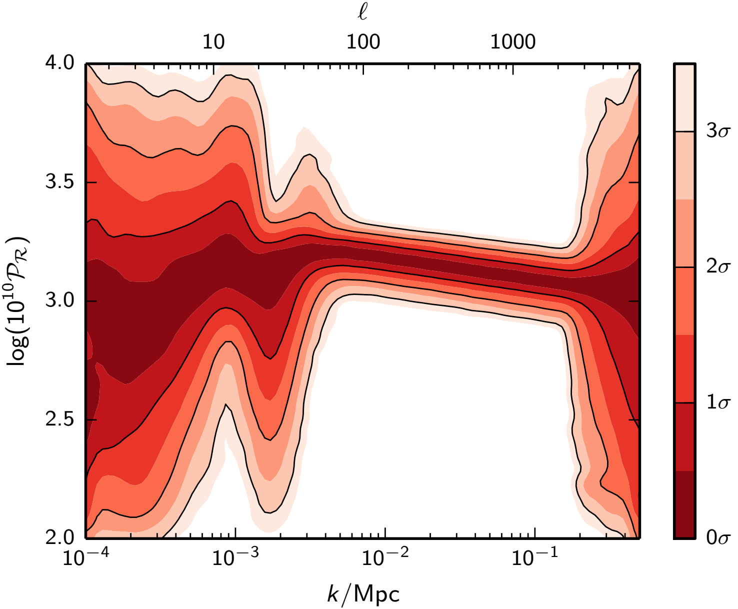
# 6 internal knots

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



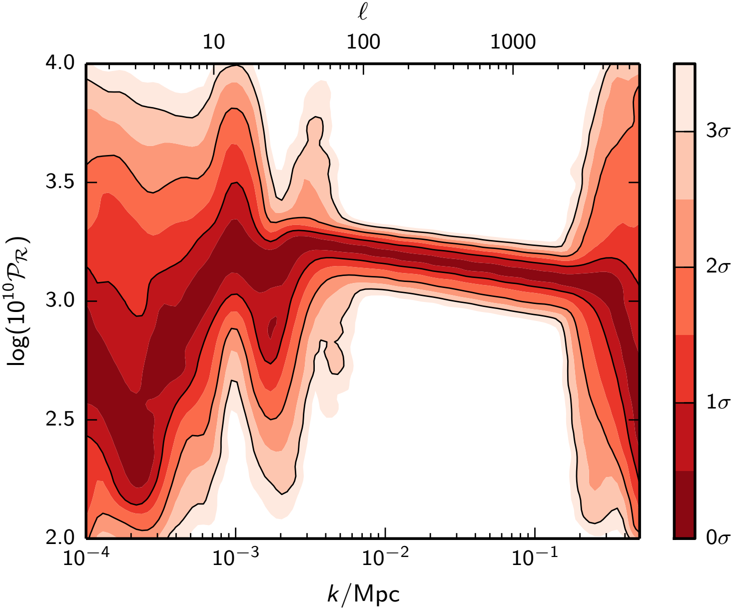
# 7 internal knots

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



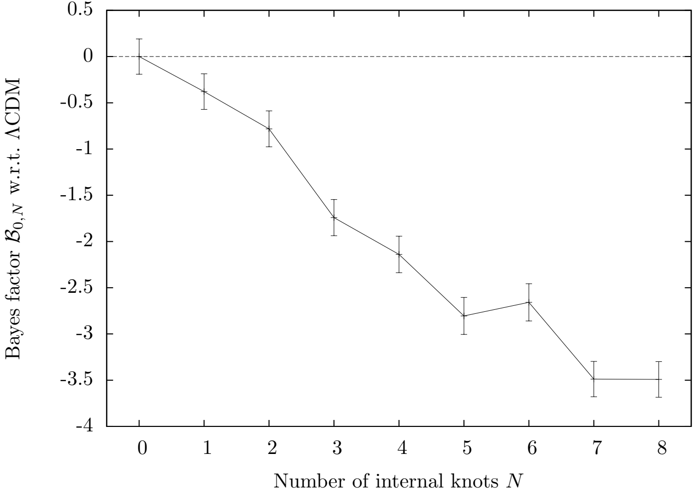
# 8 internal knots

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



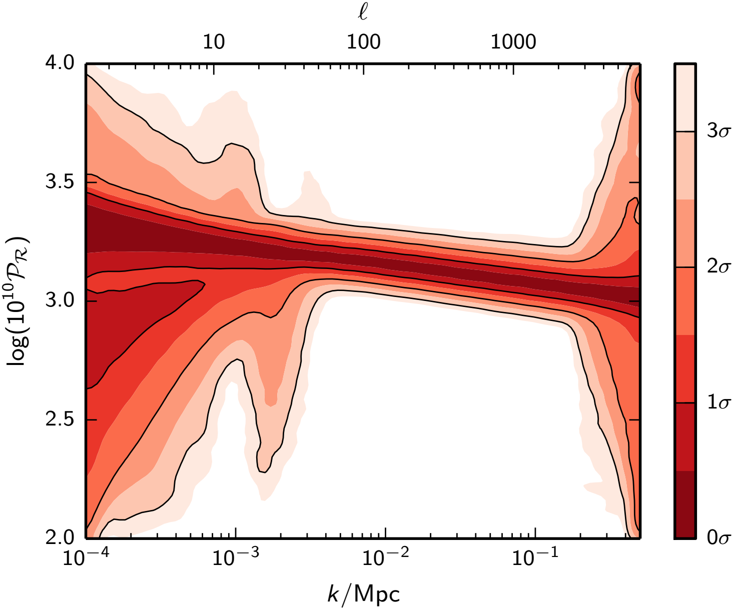
# Bayes Factors

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



# Marginalised plot

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



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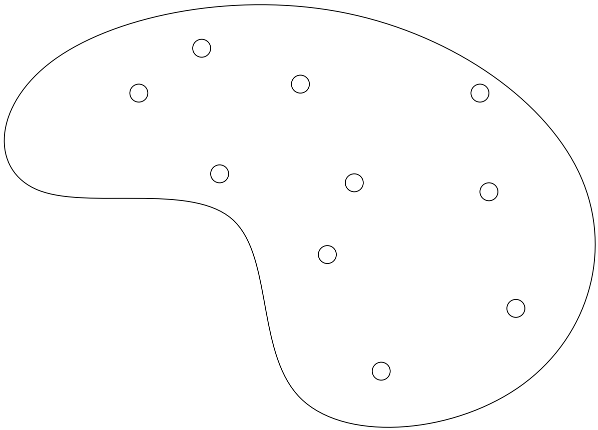
- Good example: Now highly successful emcee (MCMC hammer).
  - Important: emcee is not unique (or necessarily best)

# Skillings affine invariant ideas

## Leapfrog



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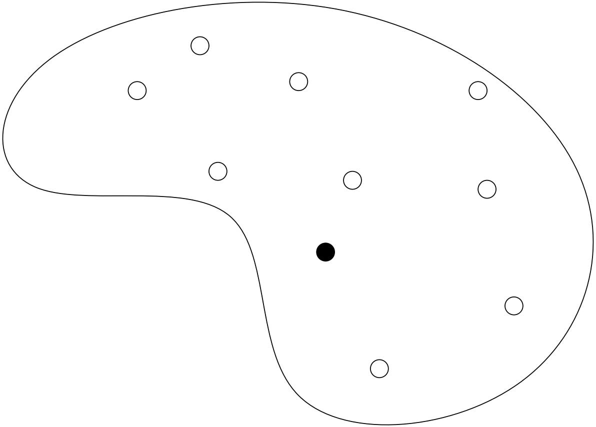

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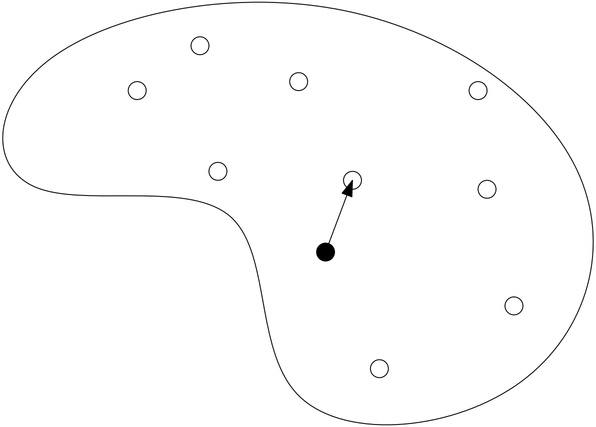

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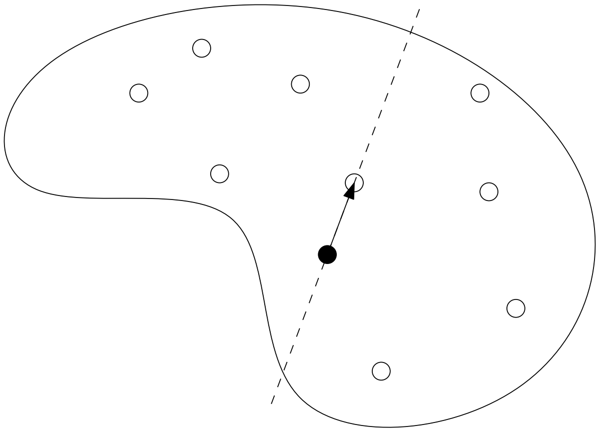

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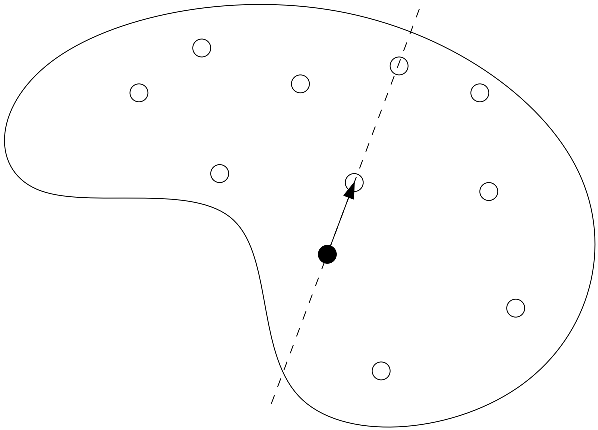

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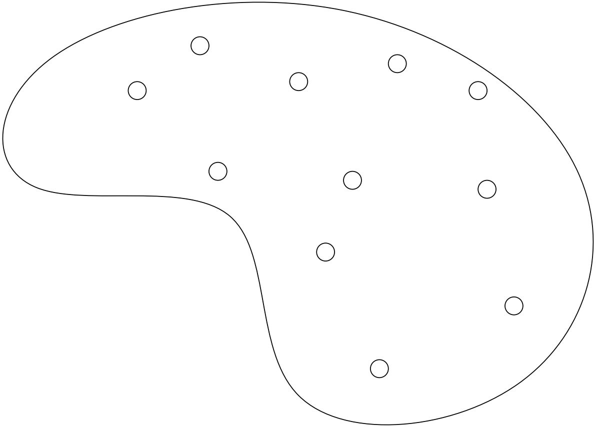
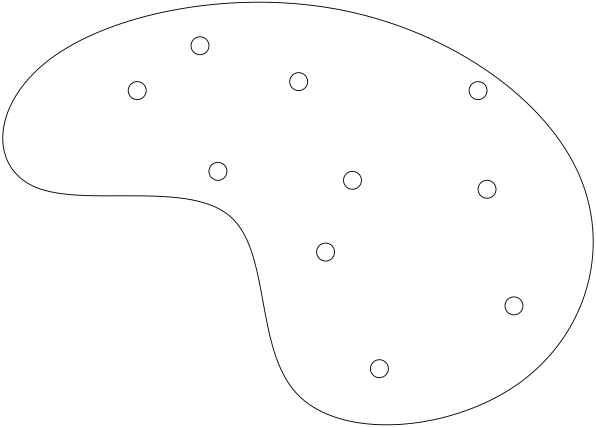


# Skillings affine invariant ideas

## Parallel walk



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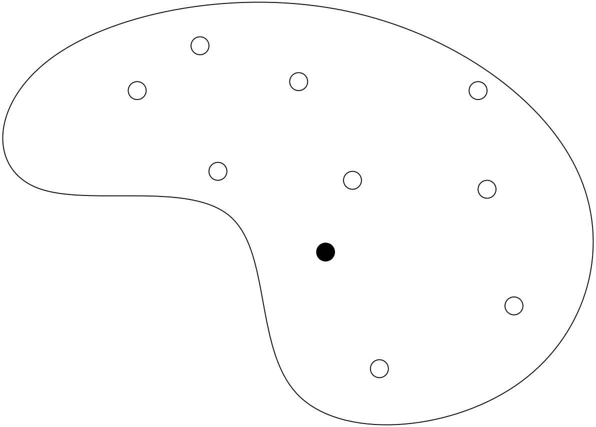

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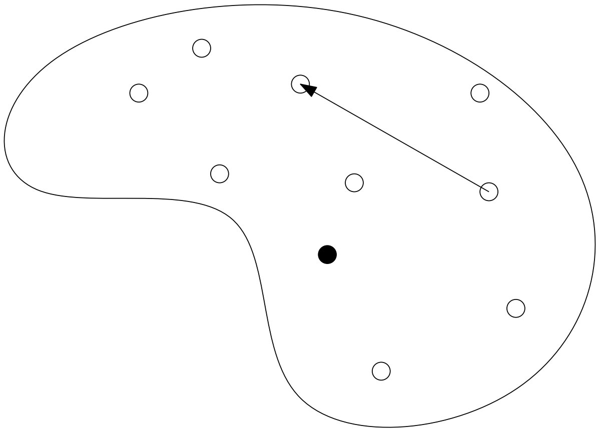

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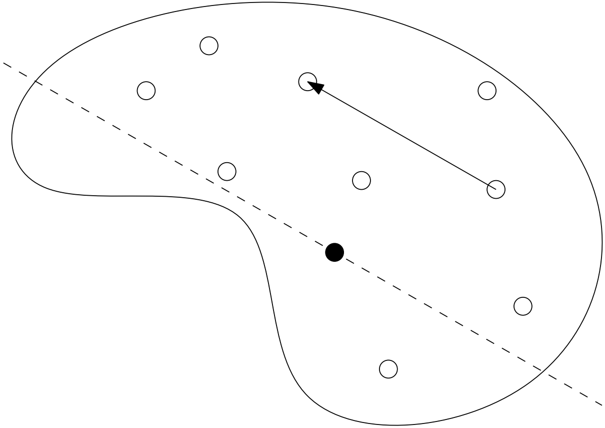

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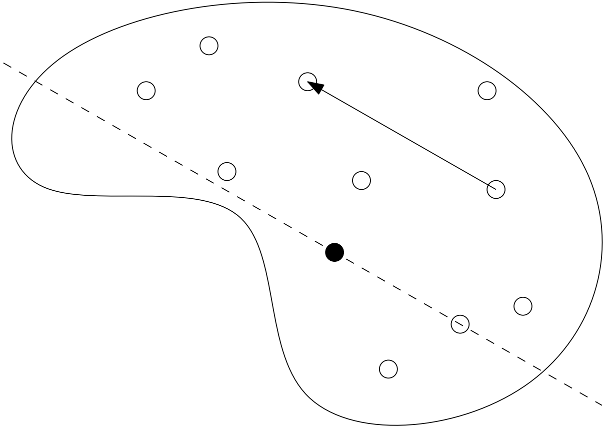

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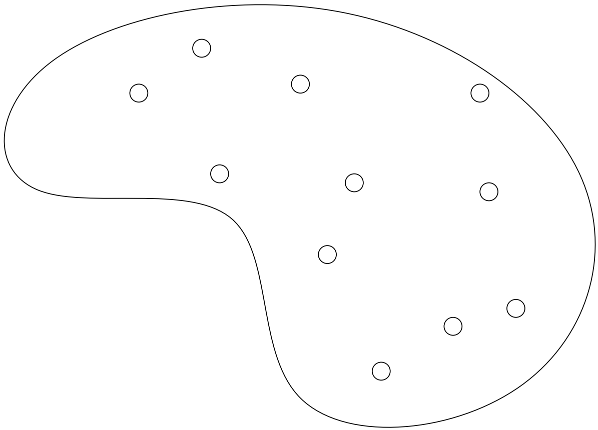

# Affine invariance

## Subspace collapse

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- The main problem that besets these techniques is "subspace collapse".

# Subspace collapse

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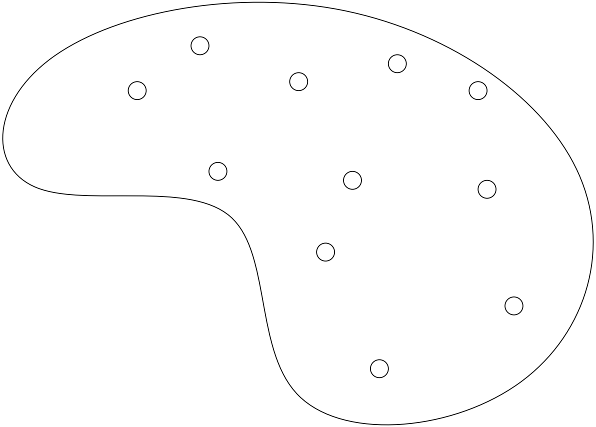

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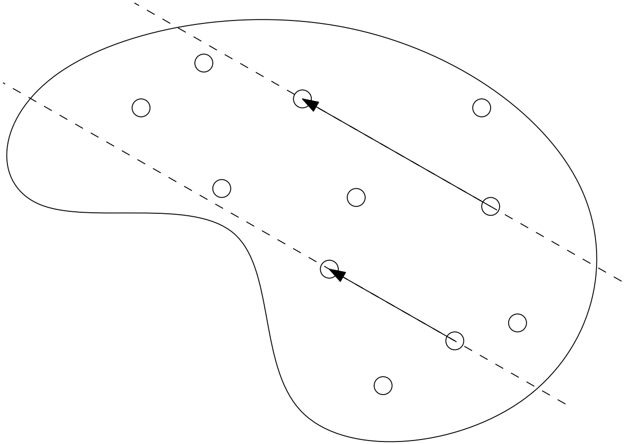

# Subspace collapse

## Solution

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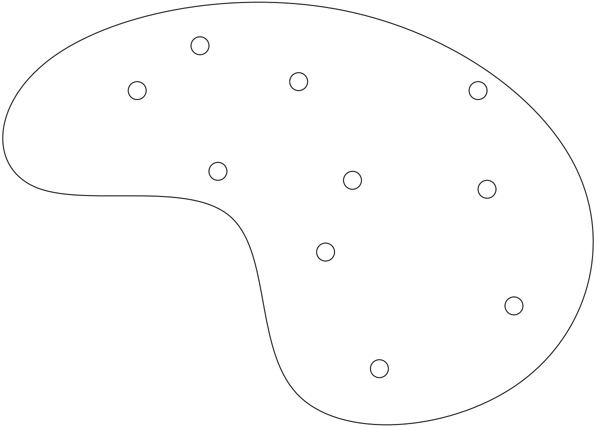
- Need to use $\sim \mathcal{O}(D)$ points to avoid this.

# Skillings affine invariant ideas

## Guided walk



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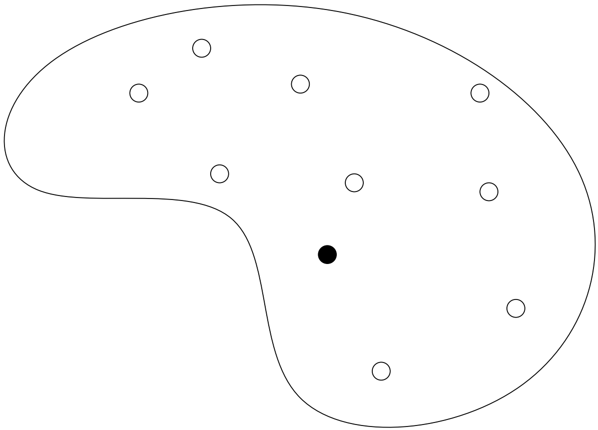

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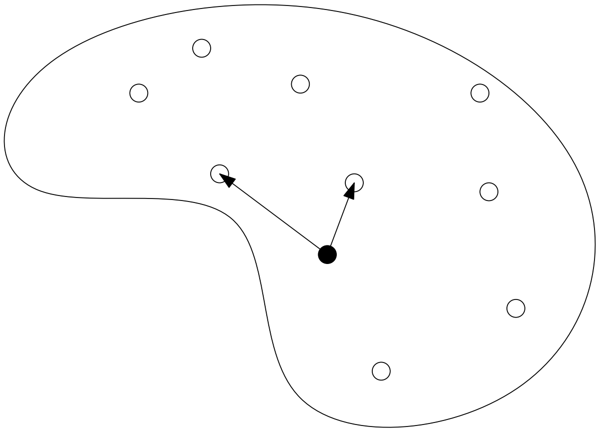

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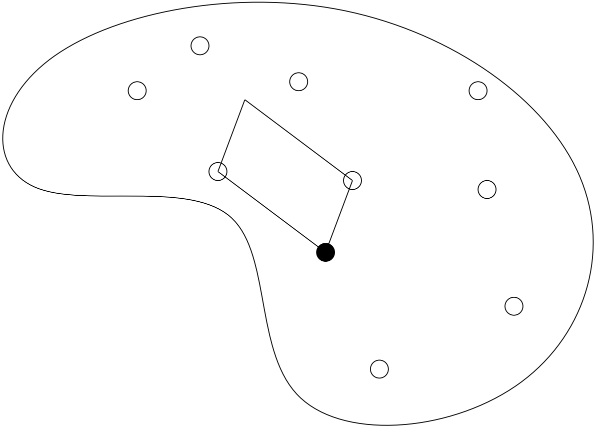

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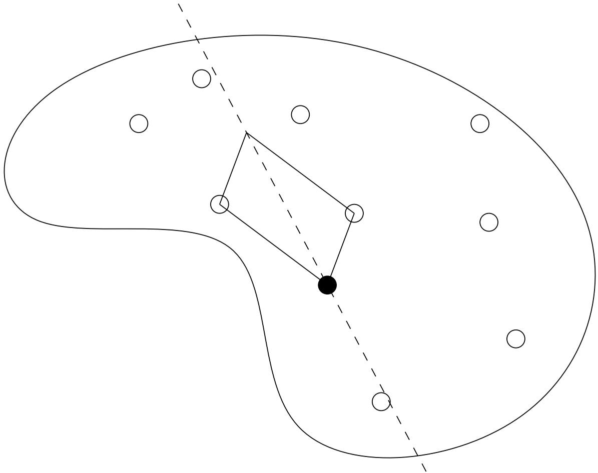

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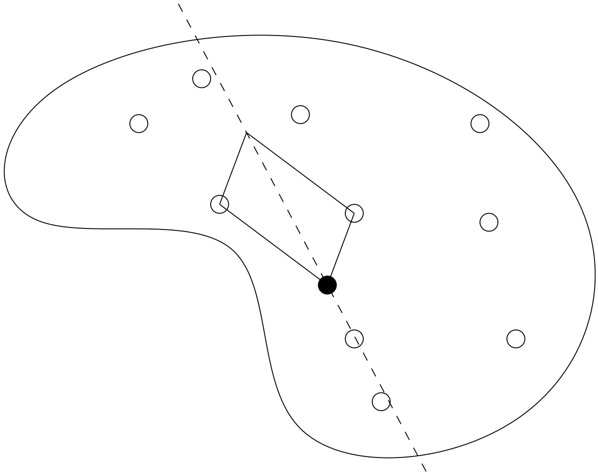

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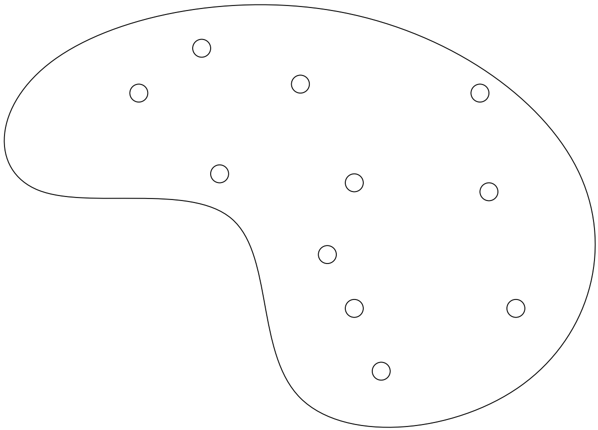

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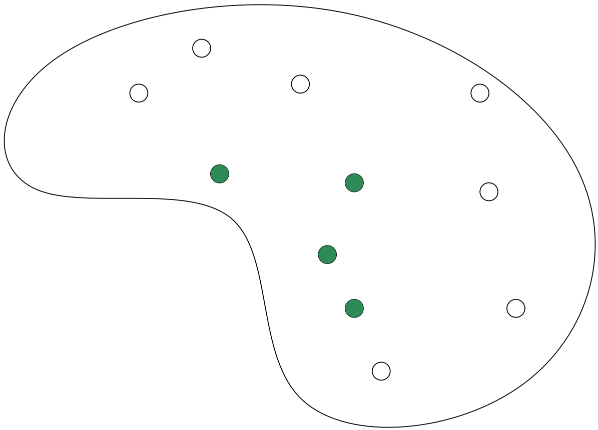

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# Affine invariant

## Other variations

- Generalise guided walk to $D$ dimensions (slice through the mean of $D$ other points).
- Slice through a “random” linear combination of $D$ points.
- Slice through a “random” linear combination of all points
- There are lots of variations: This is an underused area of the field.

# PolyChord 2.0

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- Using intermediate points so $\sim \mathcal{O}(D^3) \to \sim \mathcal{O}(D^2)$.

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- Unweaving runs to quantify correlations

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- Unweaving runs to quantify correlations
- Affine invariant sampling