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

Parameter estimation

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Model averaging:

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

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

Markov-Chain Monte-Carlo (MCMC)

Metropolis-Hastings, Gibbs, Hamiltonian...

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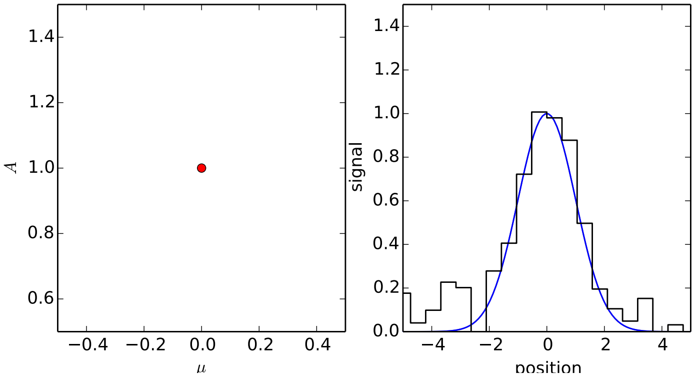
  4. ...otherwise sometimes make step.

MCMC in action



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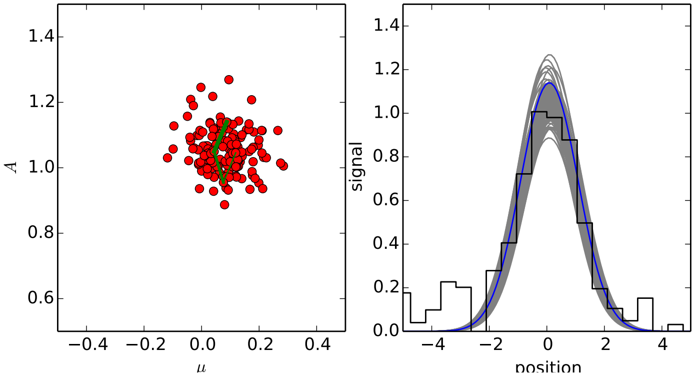
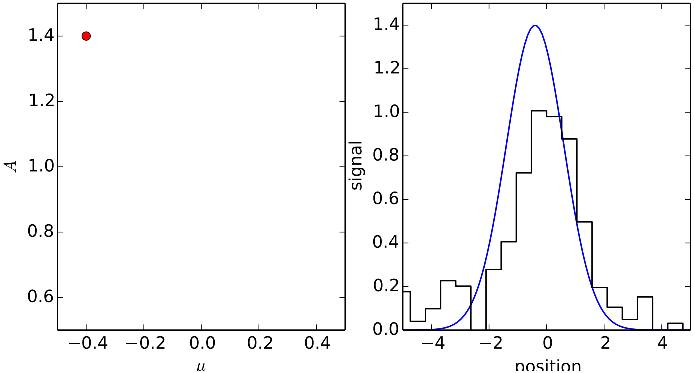


When MCMC fails

Burn in



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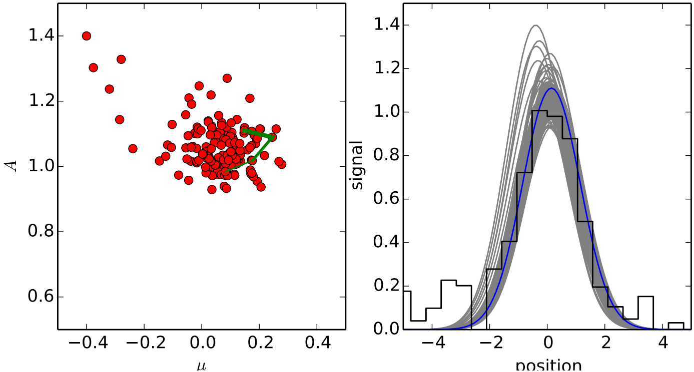

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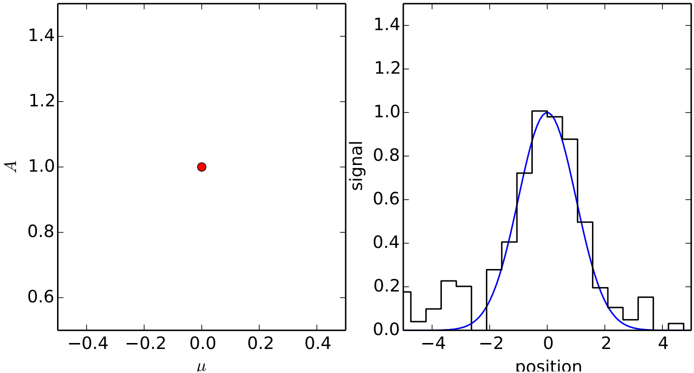

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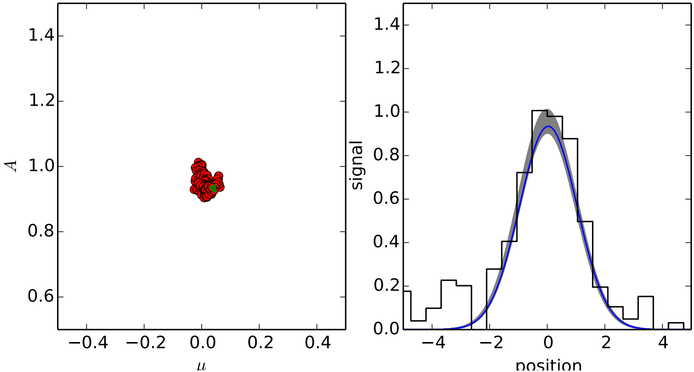
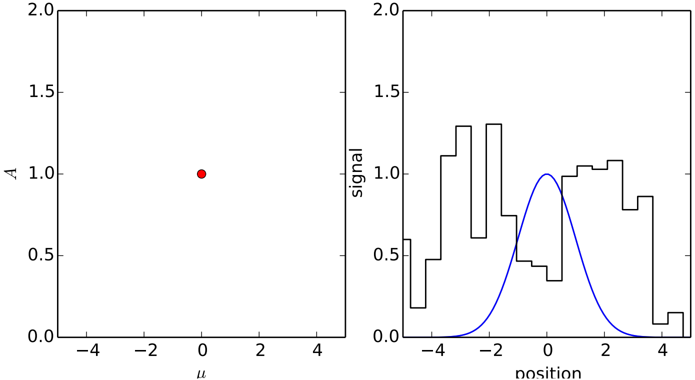


When MCMC fails

Multimodality



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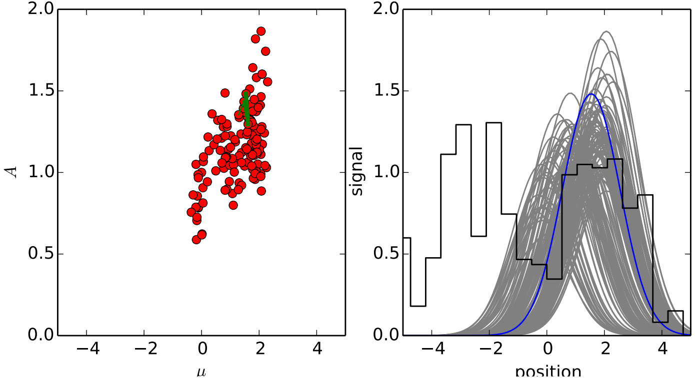

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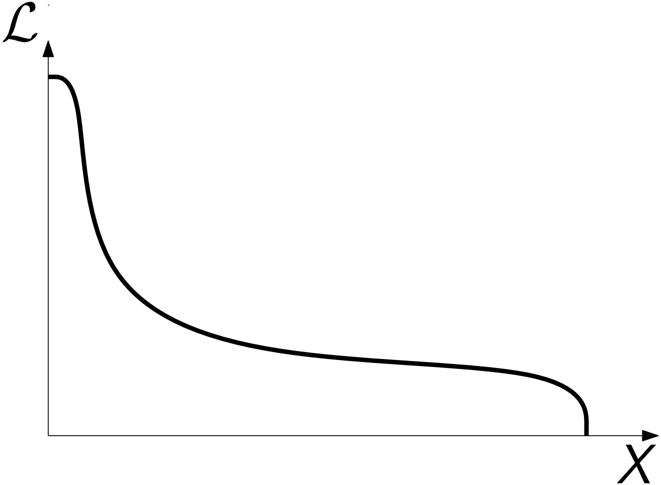
Phase transitions



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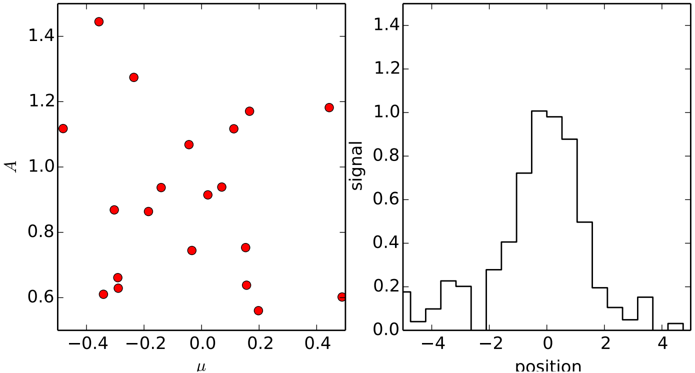
Requires one to be able to uniformly within a region, subject to a *hard likelihood constraint*.

Nested sampling

Unimodal



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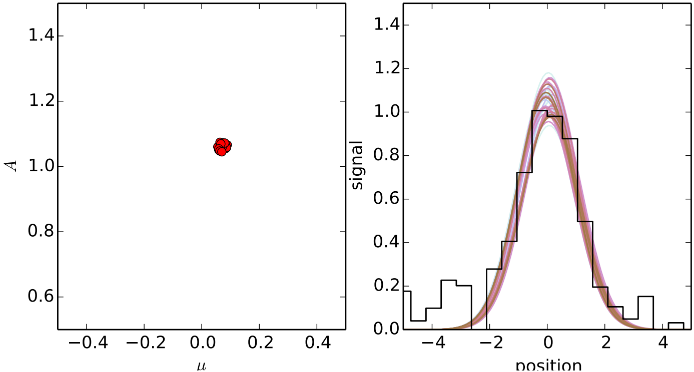

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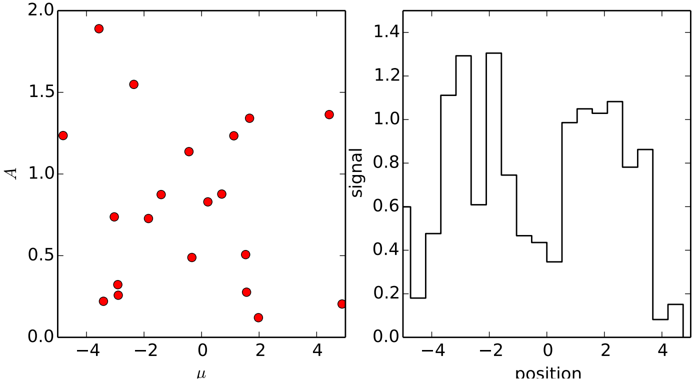

When NS suceeds

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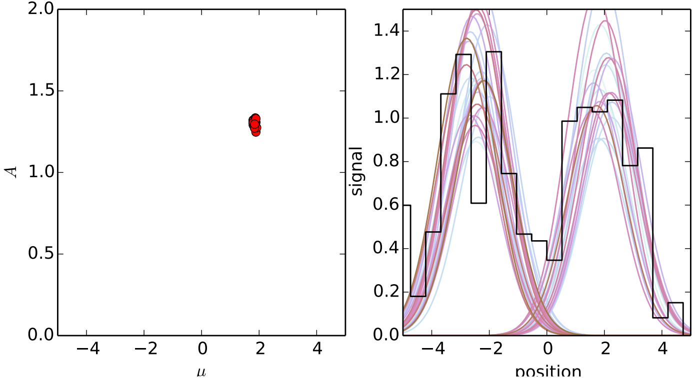
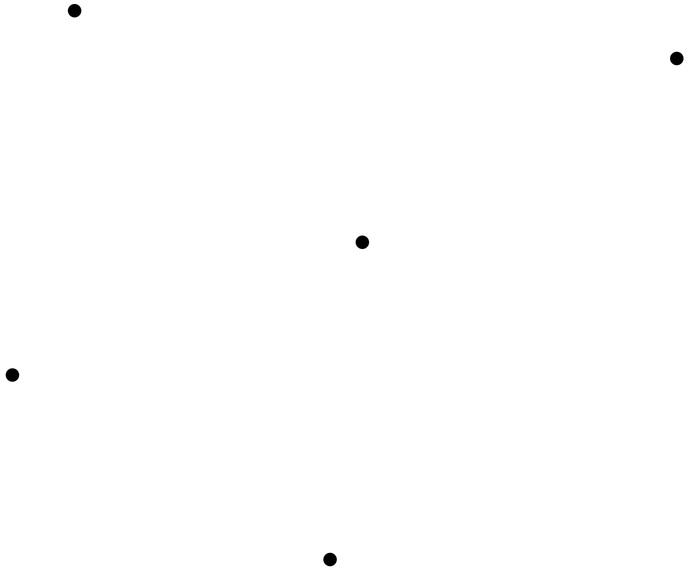


Nested Sampling

Graphical aid



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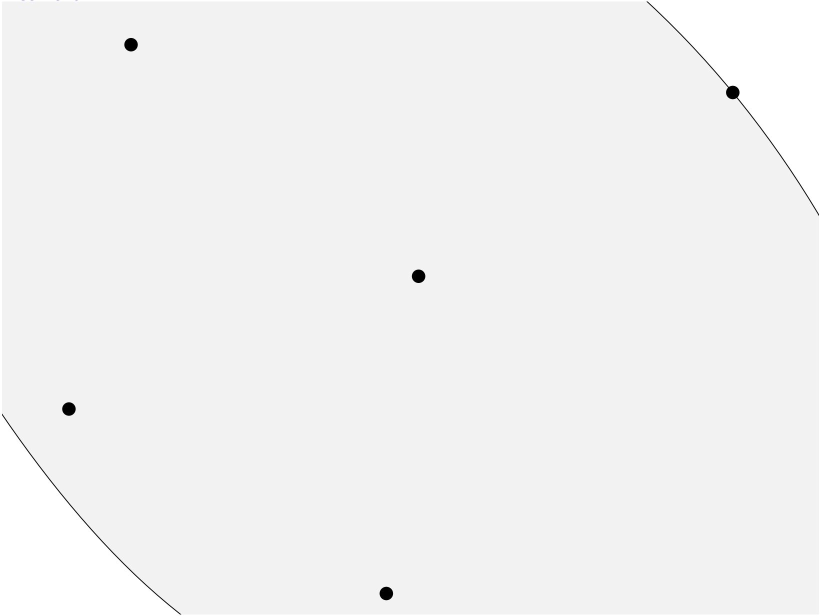

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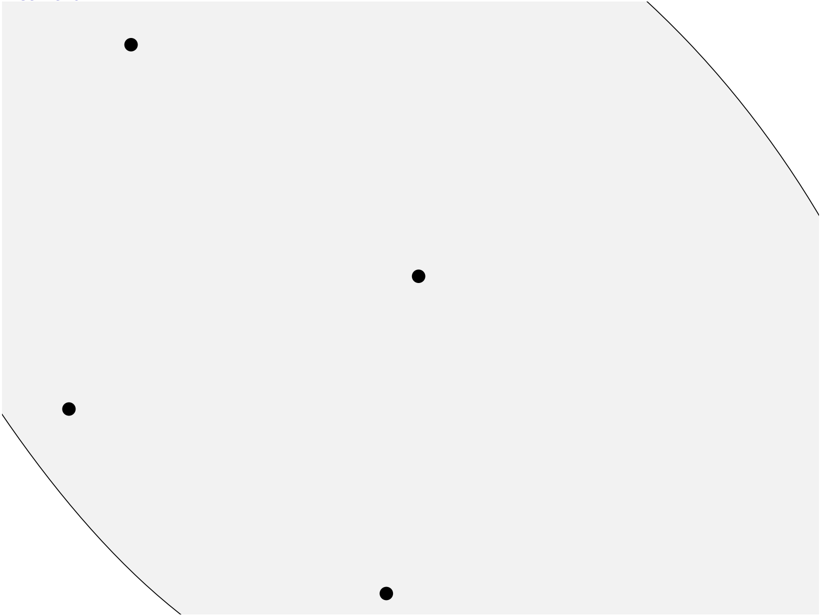

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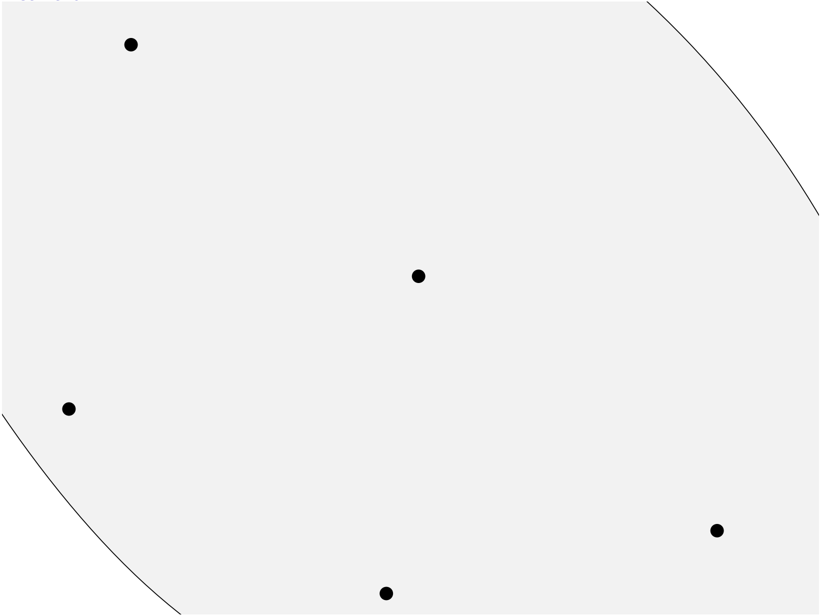

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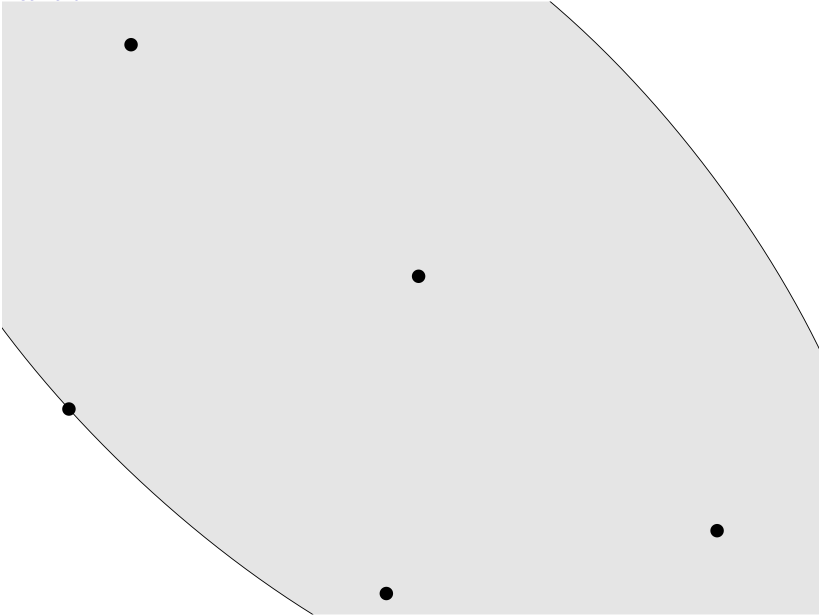

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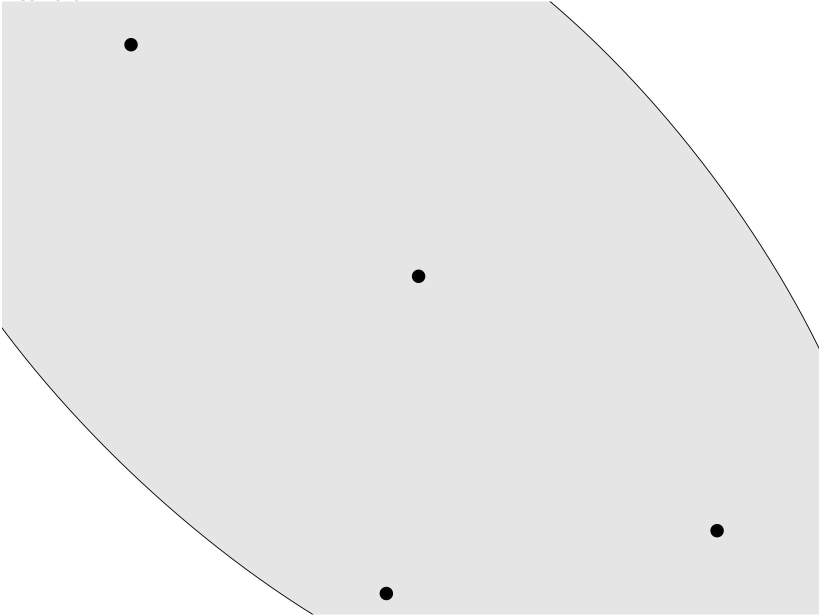

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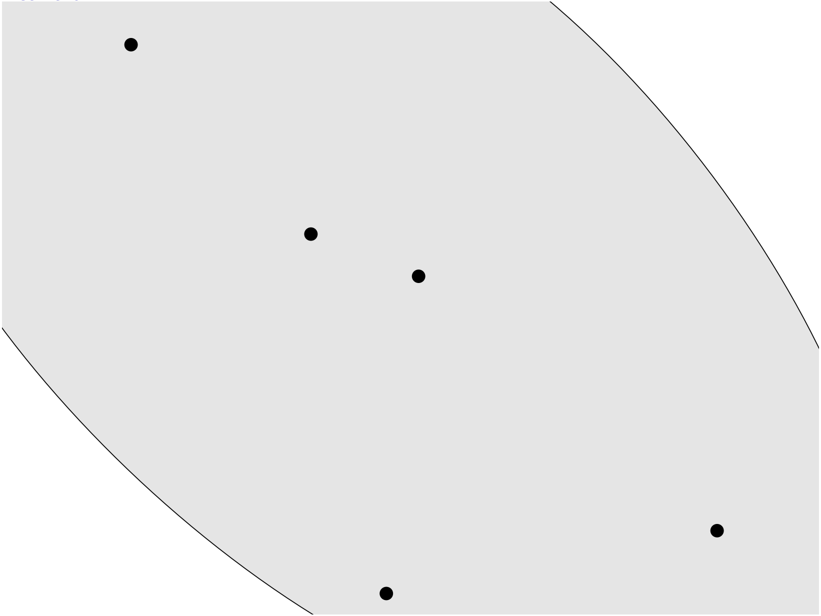

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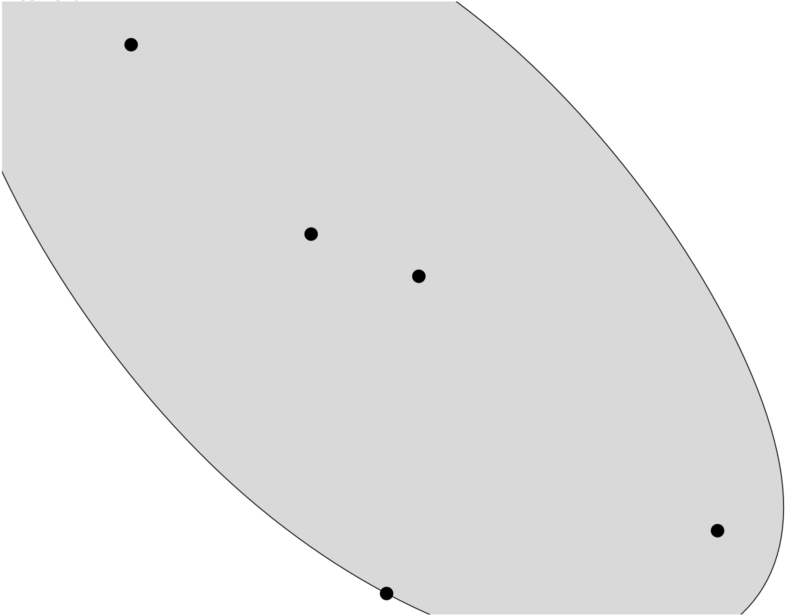

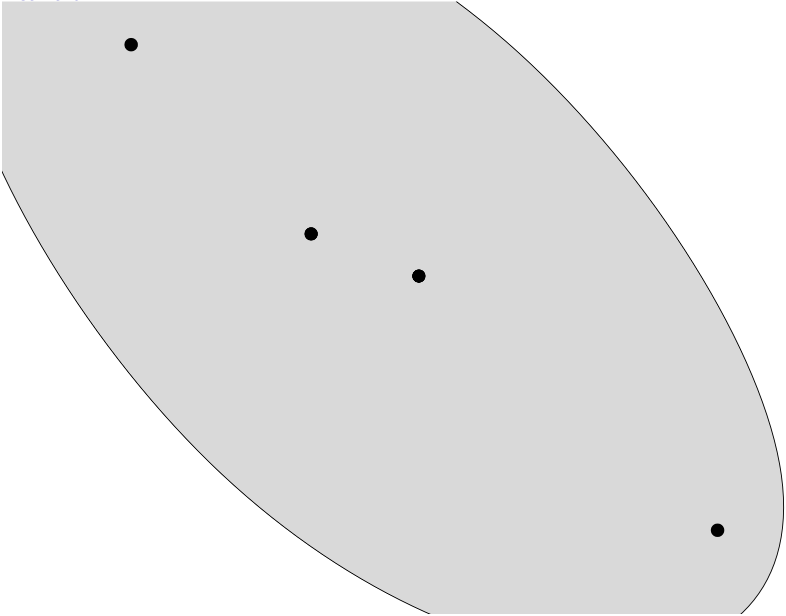

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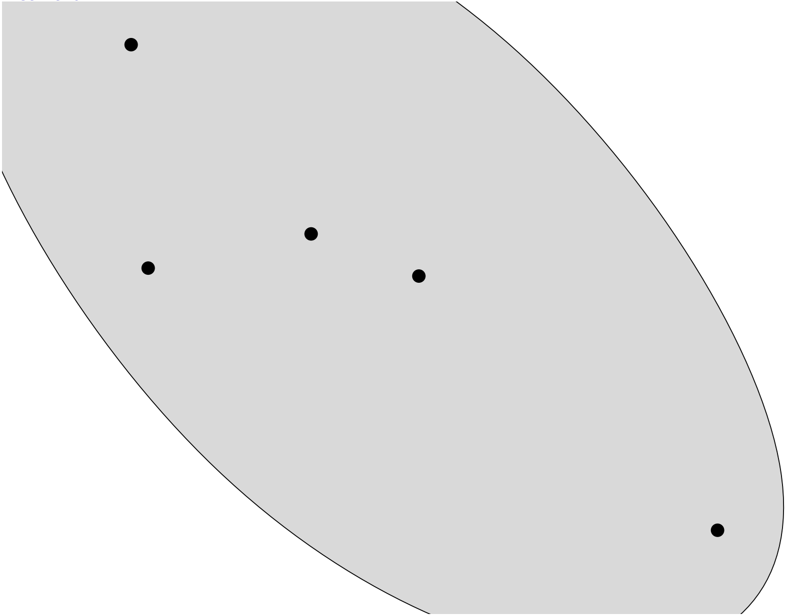

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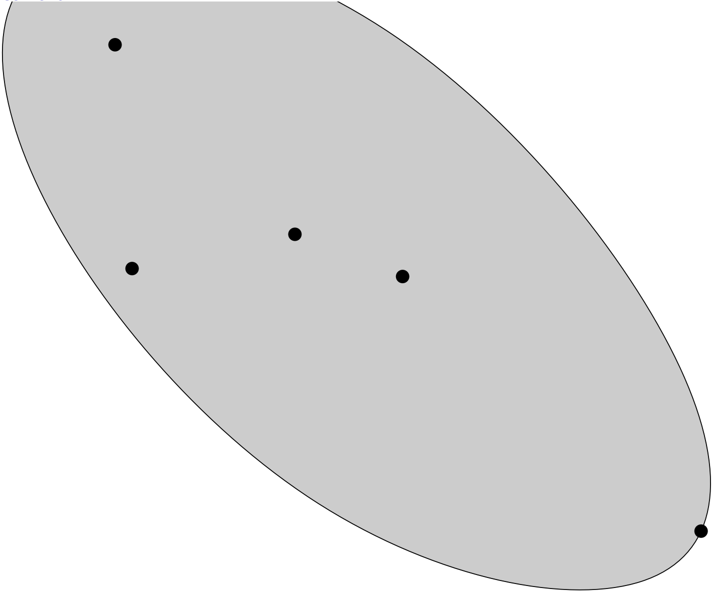

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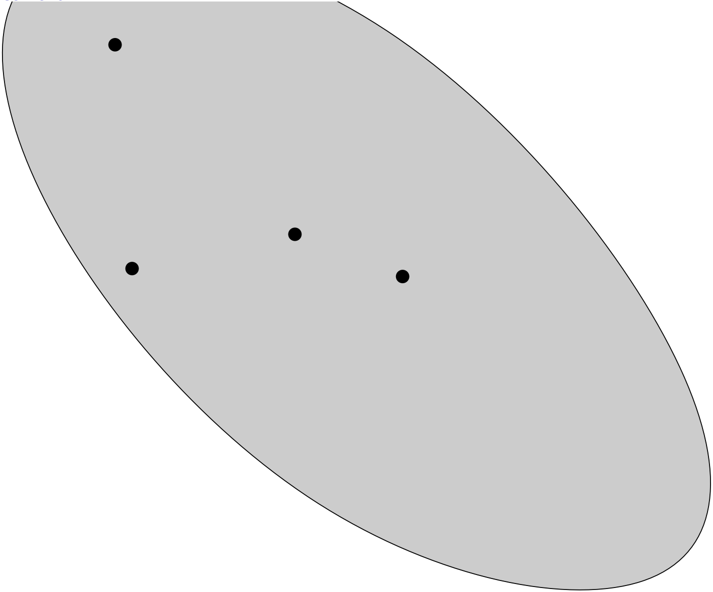

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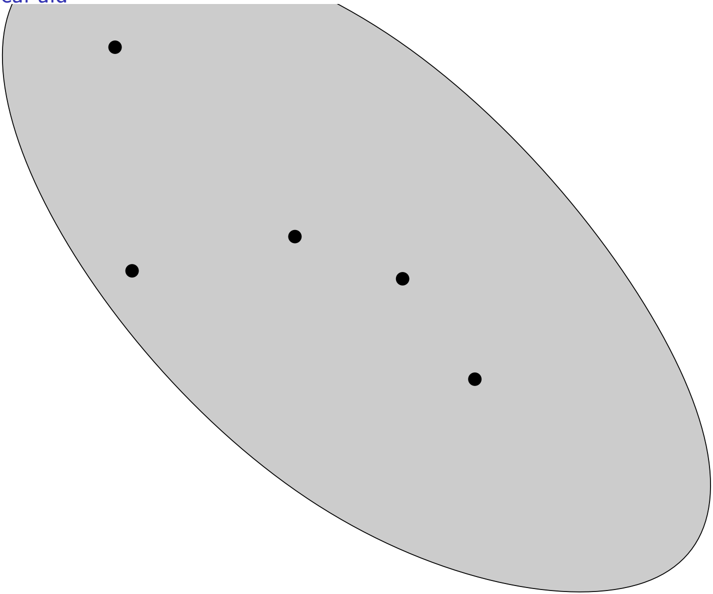

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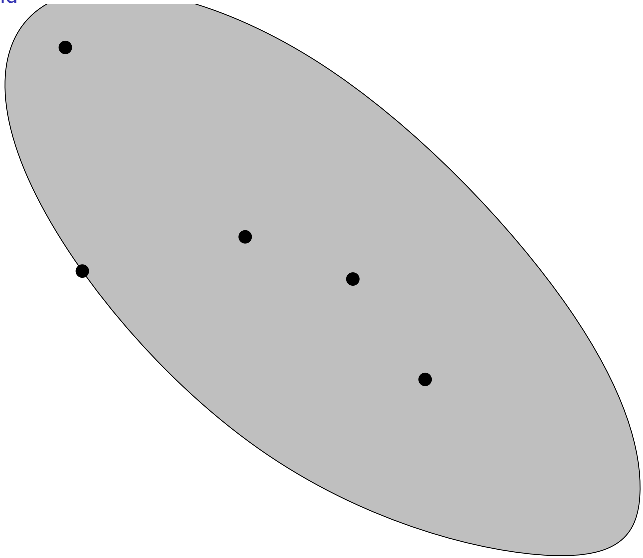

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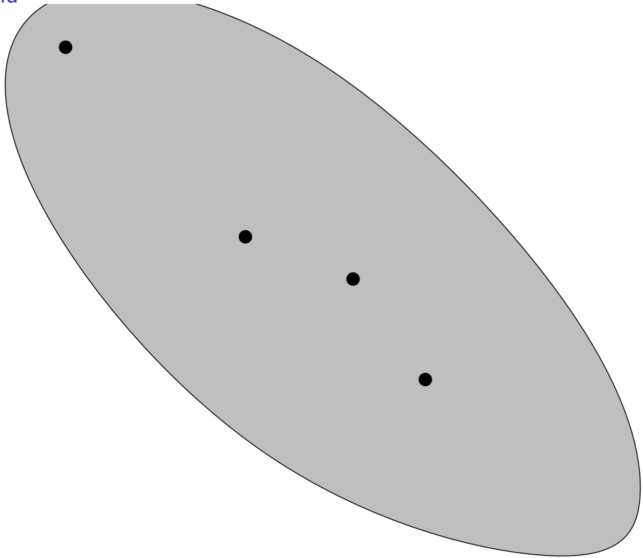

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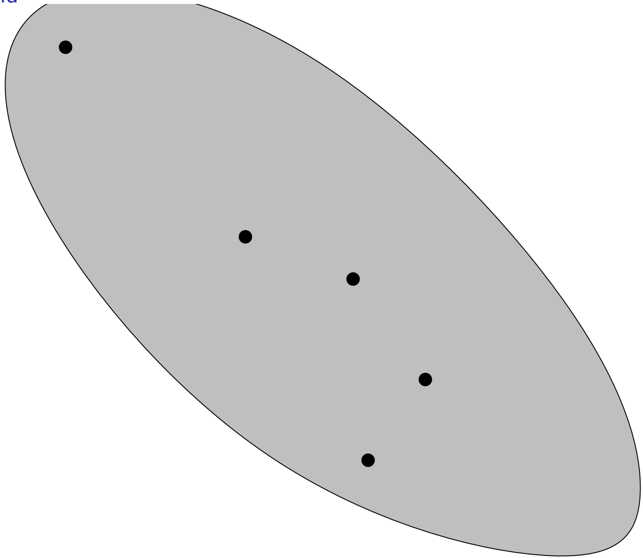

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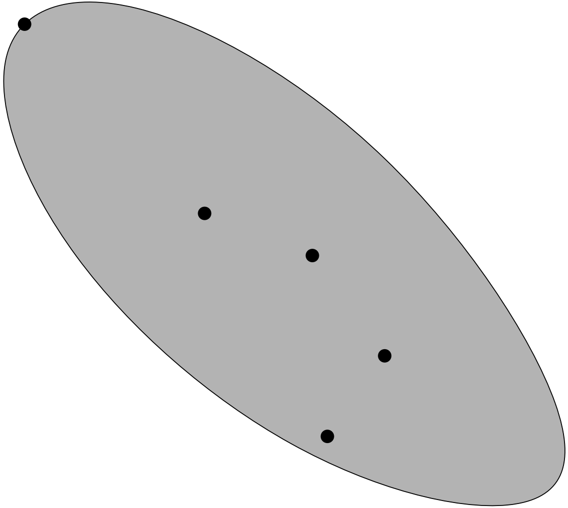

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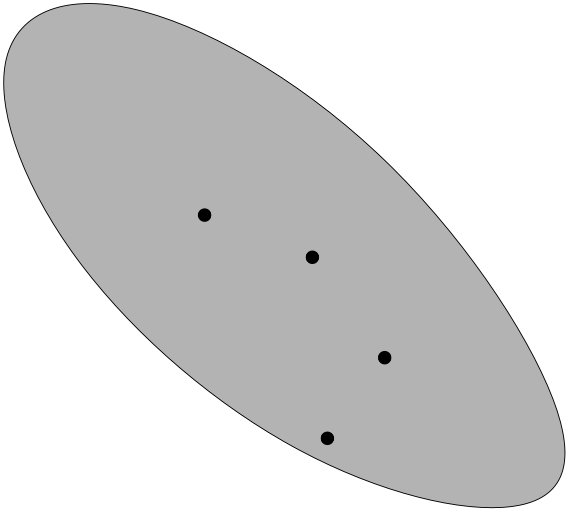

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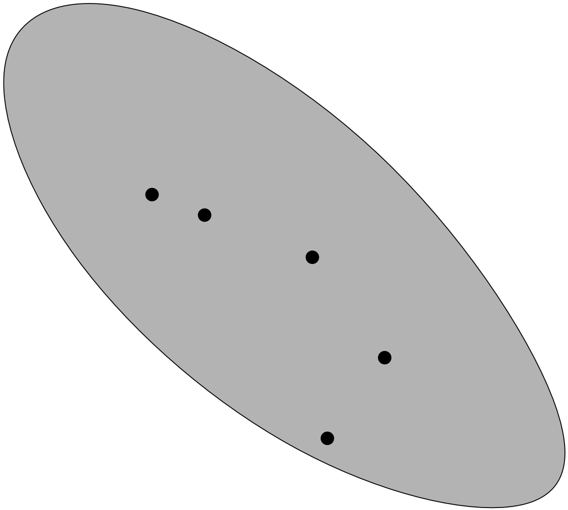

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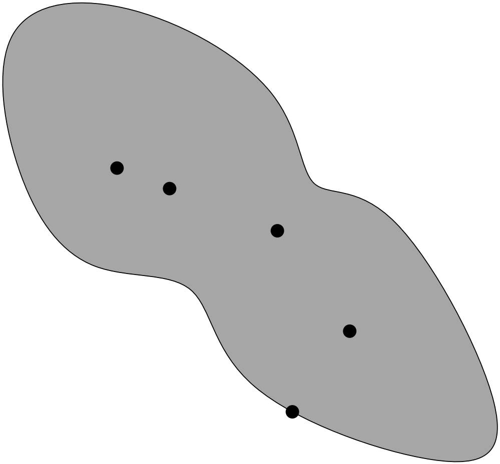

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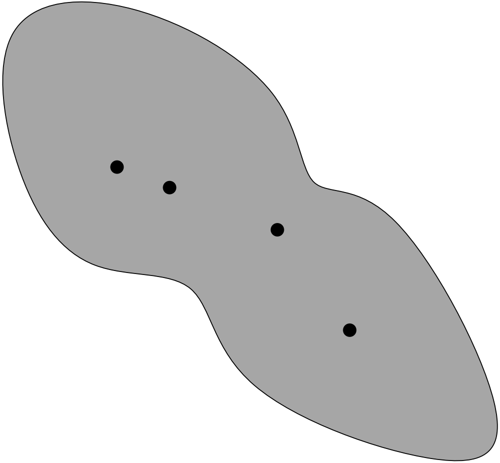

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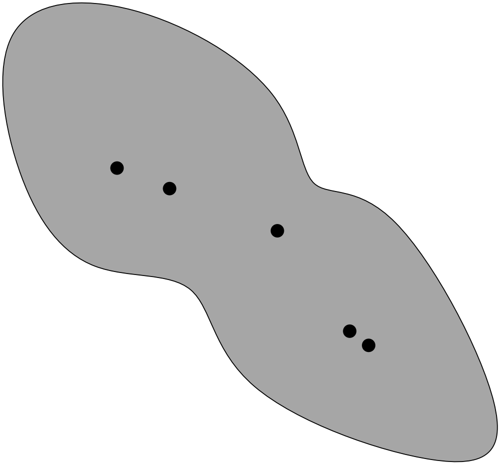

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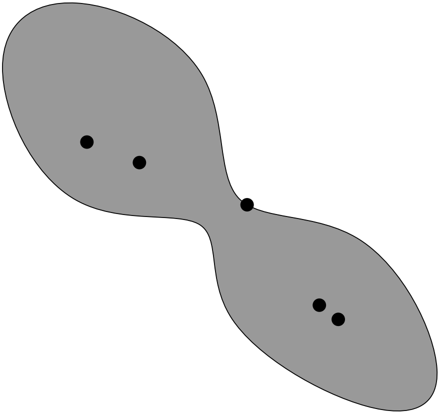

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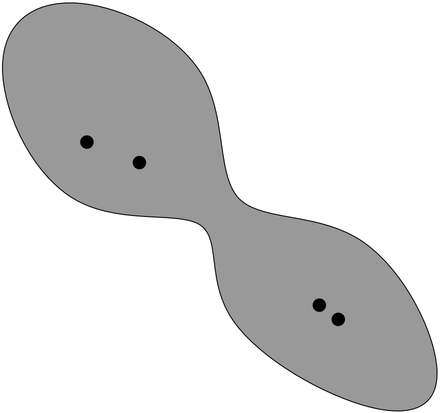

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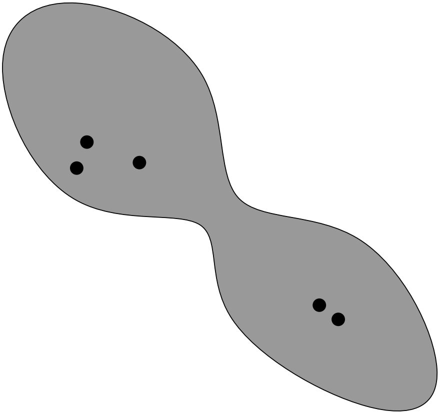

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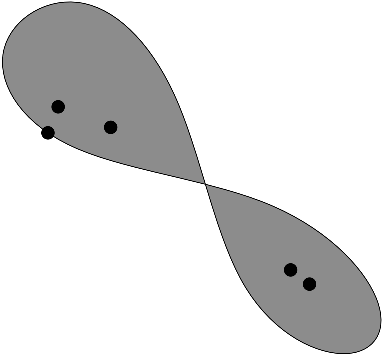

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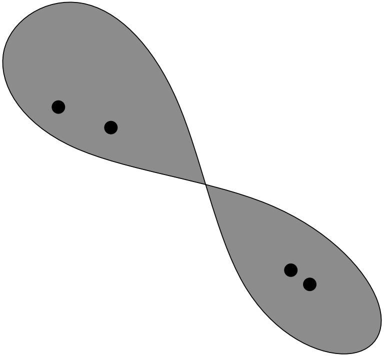

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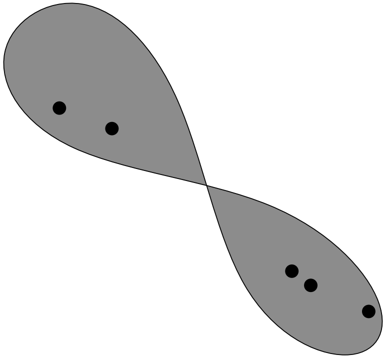

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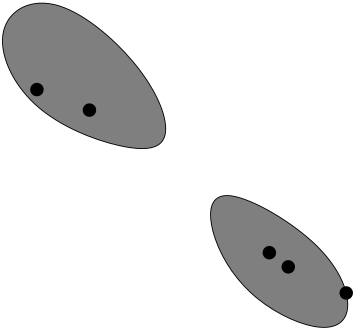

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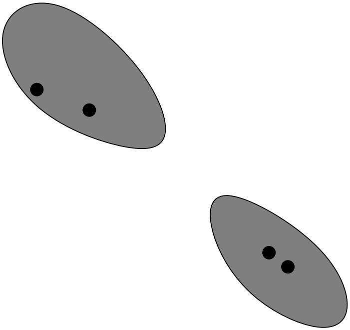

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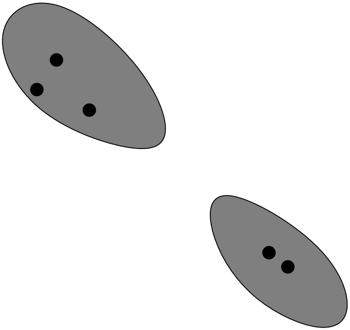

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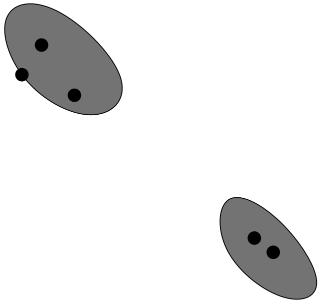

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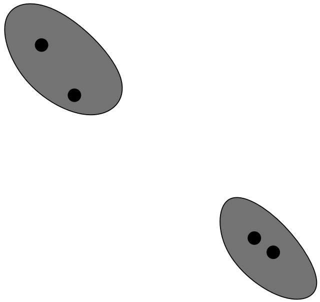

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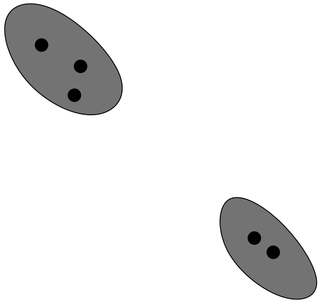

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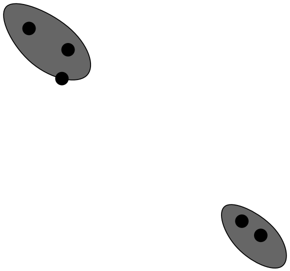

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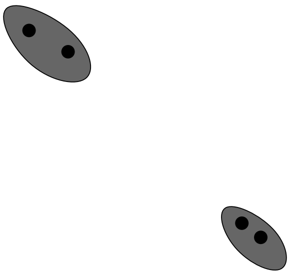

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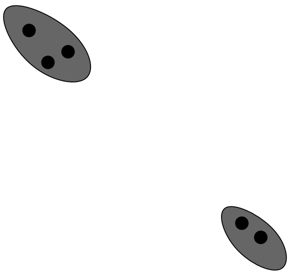
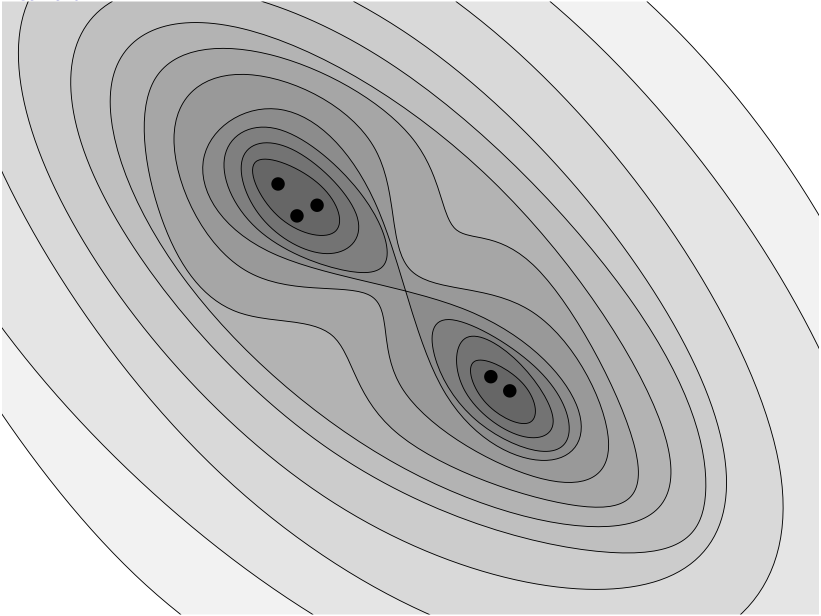


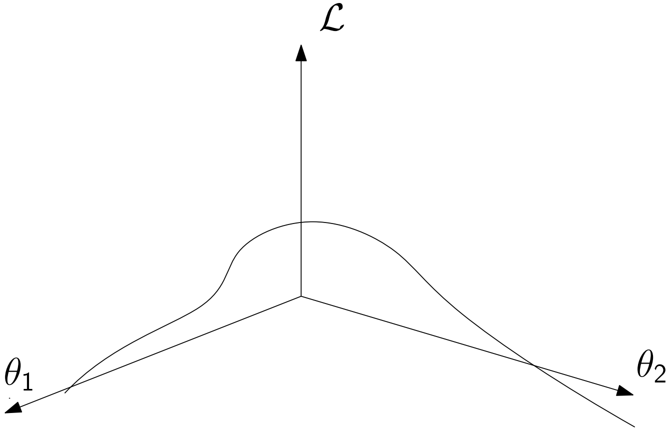
Nested Sampling

Graphical aid



Nested Sampling

Calculating evidences



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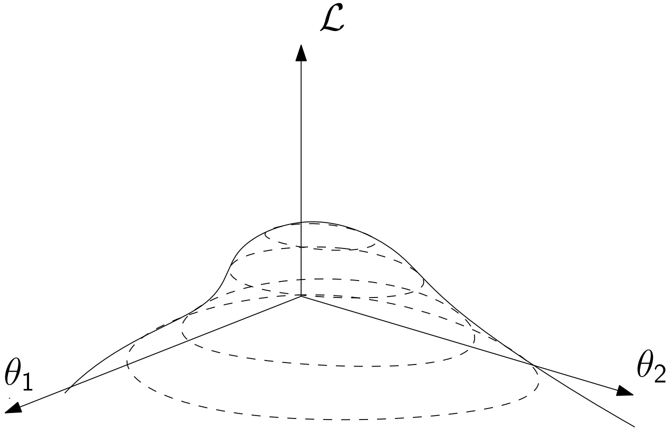

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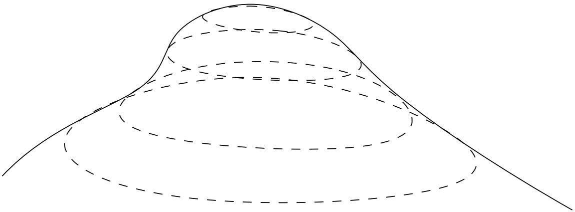

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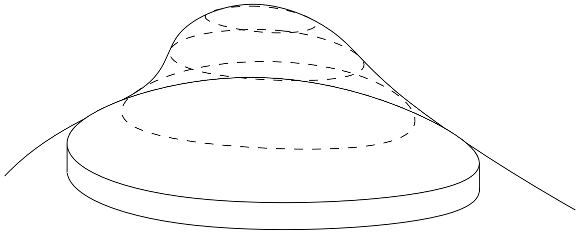

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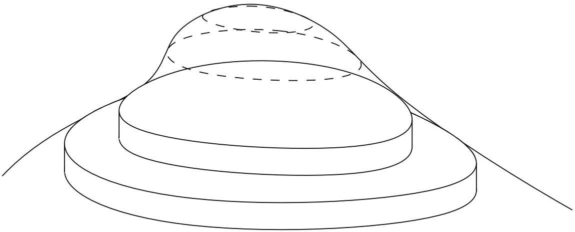

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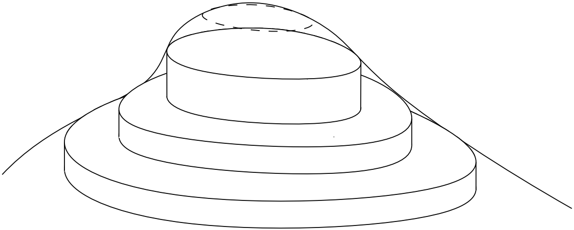

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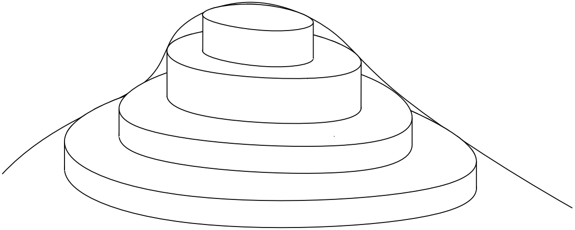

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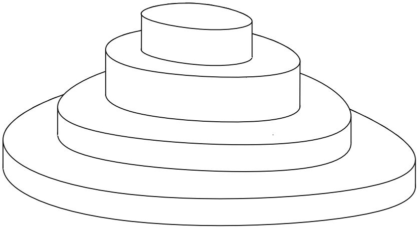

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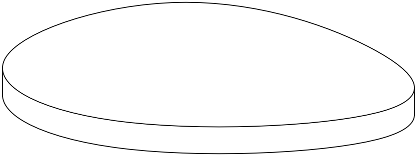

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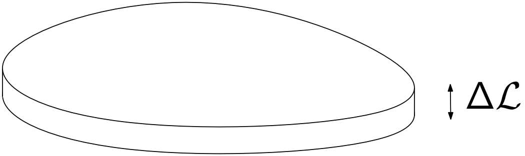

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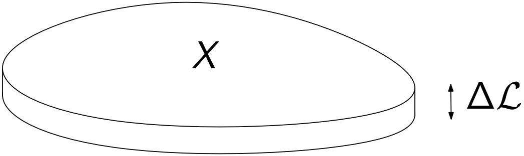

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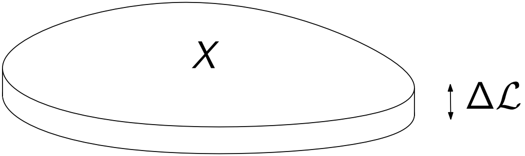

Volume $= X\Delta\mathcal{L}$

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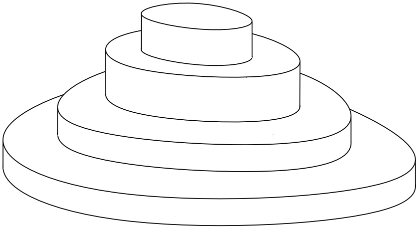

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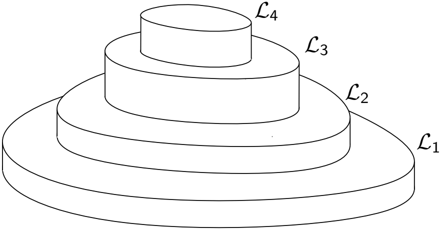

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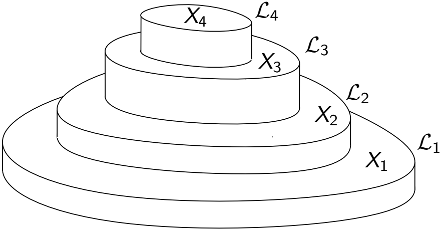
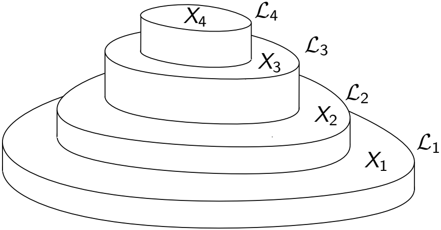


Nested Sampling

Calculating evidences

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



Nested Sampling

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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

Sampling from a hard likelihood constraint

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

— *John Skilling*

Sampling 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.

Sampling within an iso-likelihood contour

Previous attempts

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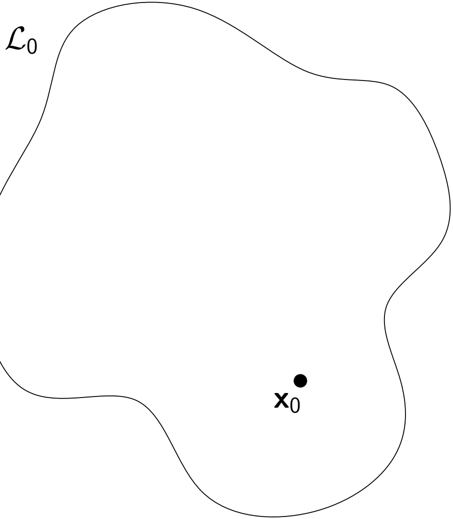
Diffusion Nested Sampling B. Brewer et al. (2009).

- Very promising
- Too many tuning parameters

"Hit and run" slice sampling



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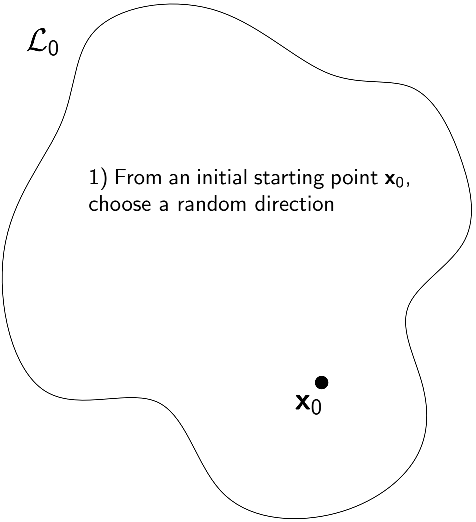

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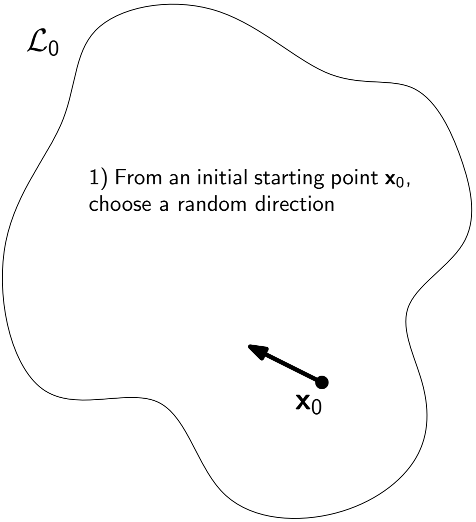

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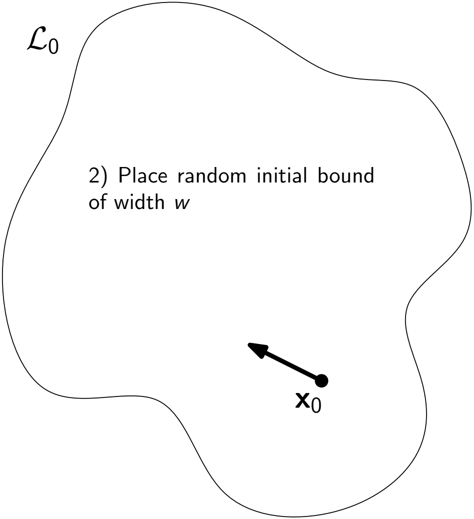

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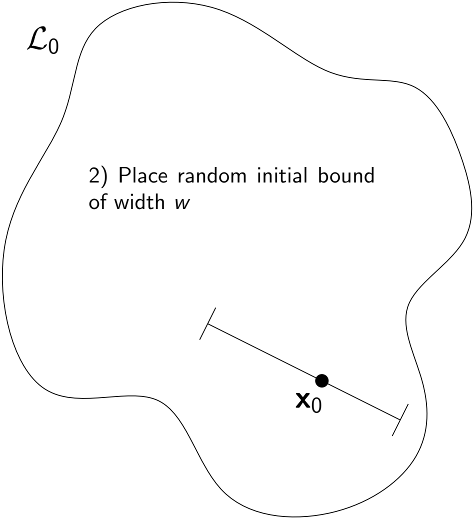

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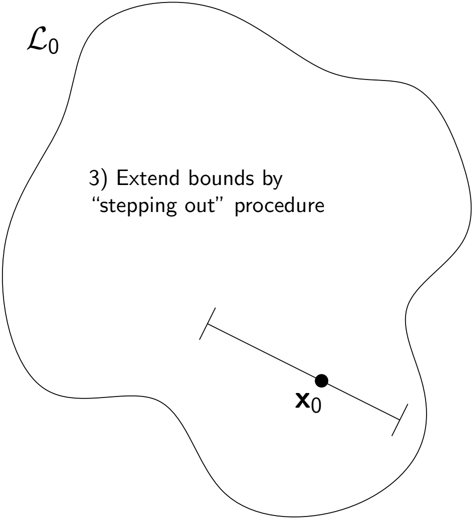

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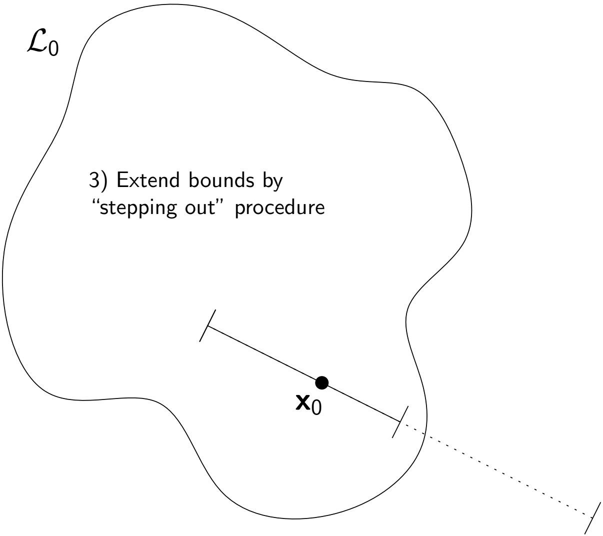

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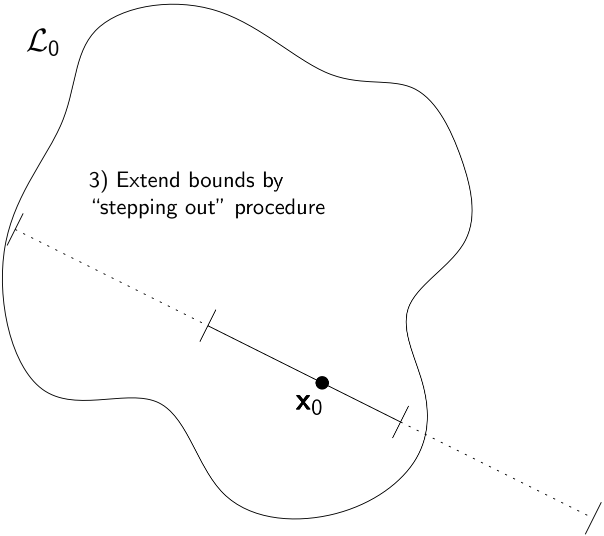

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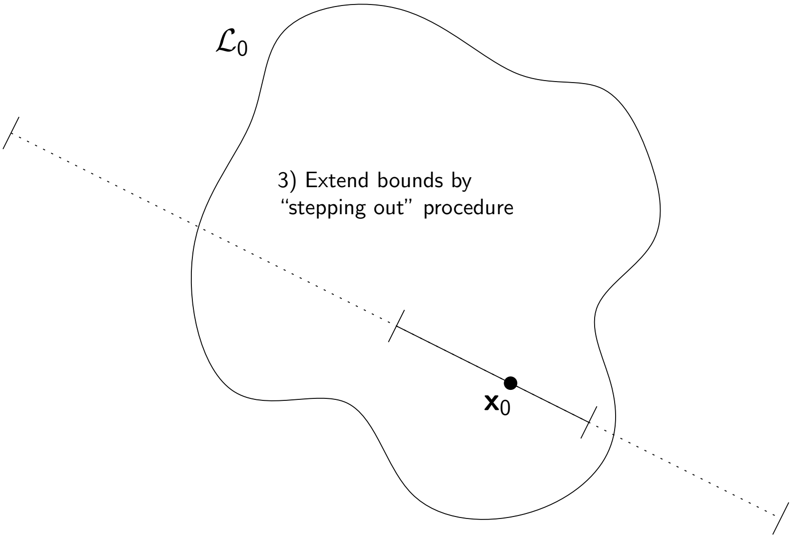

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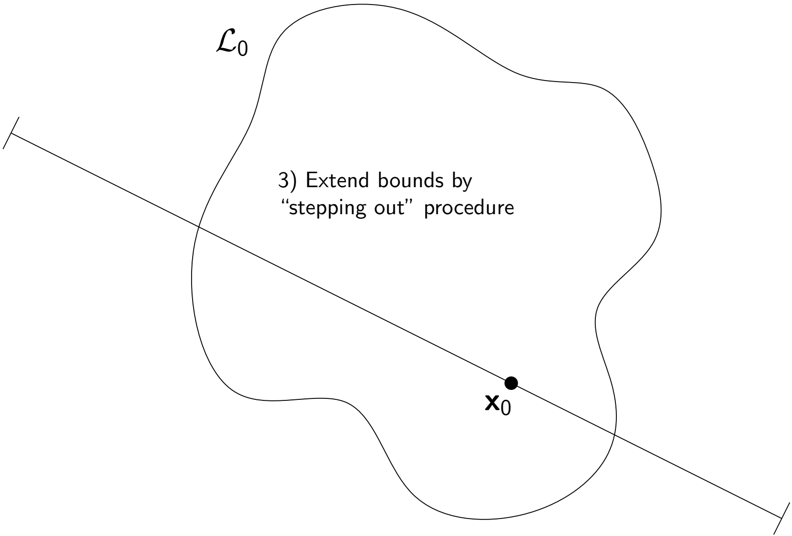

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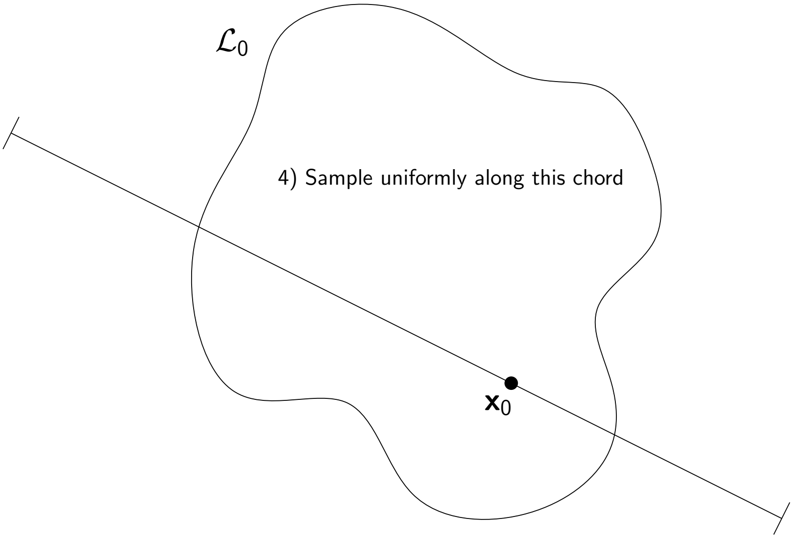

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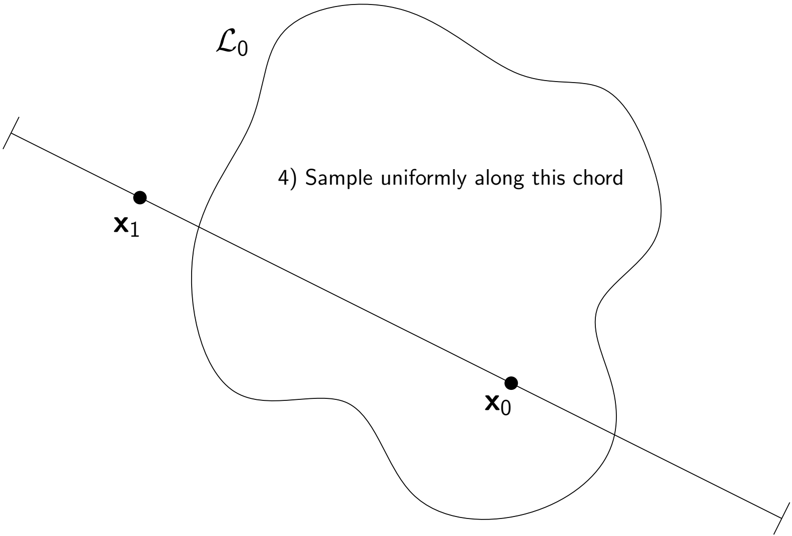

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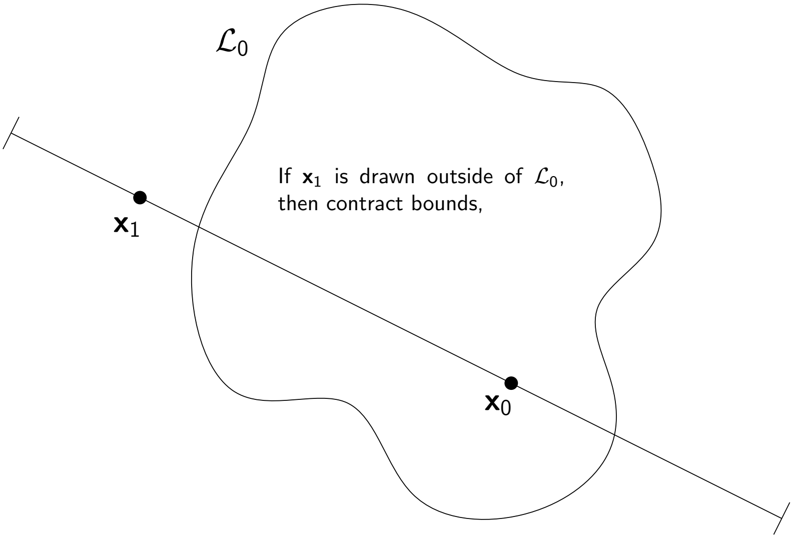

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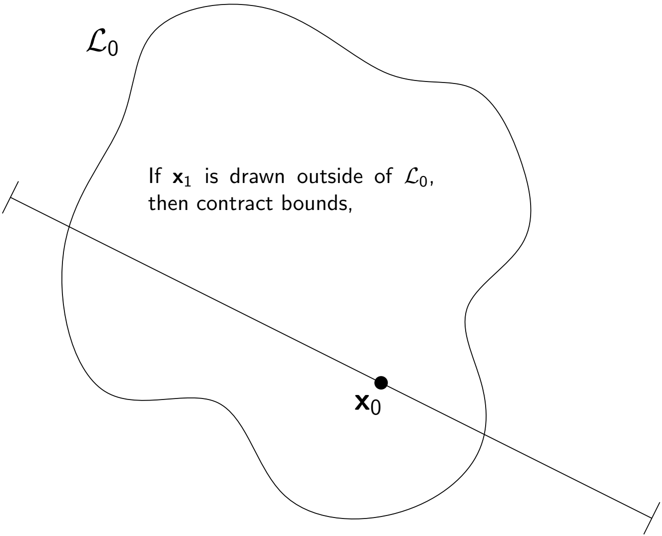

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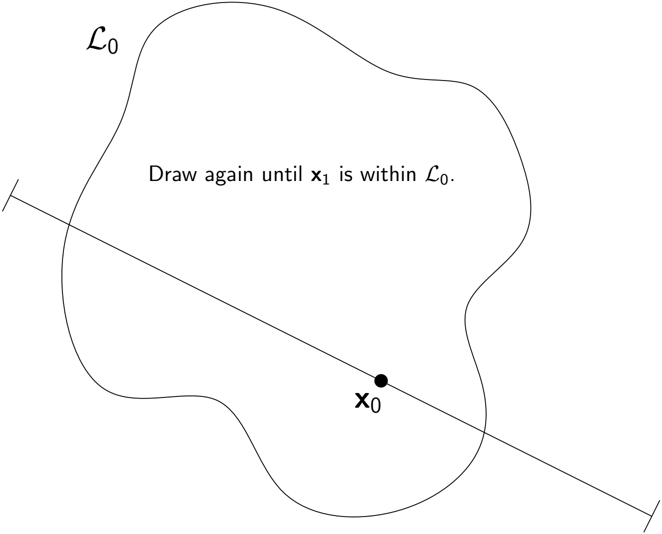

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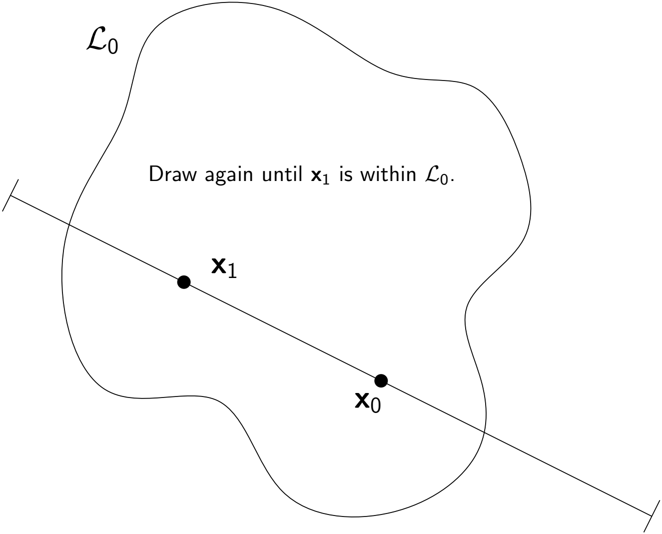

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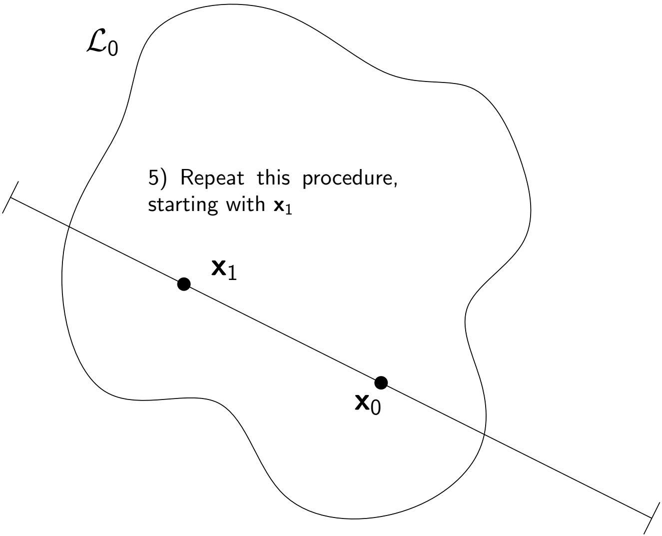

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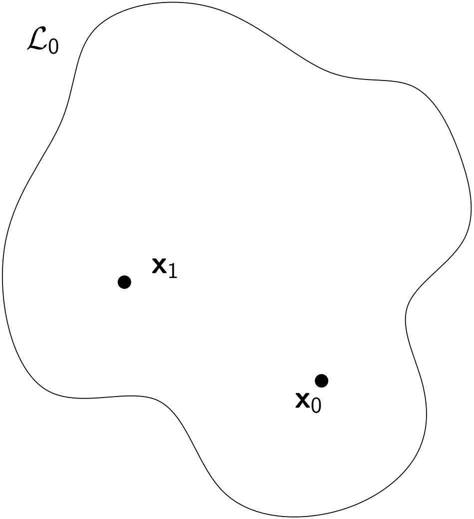

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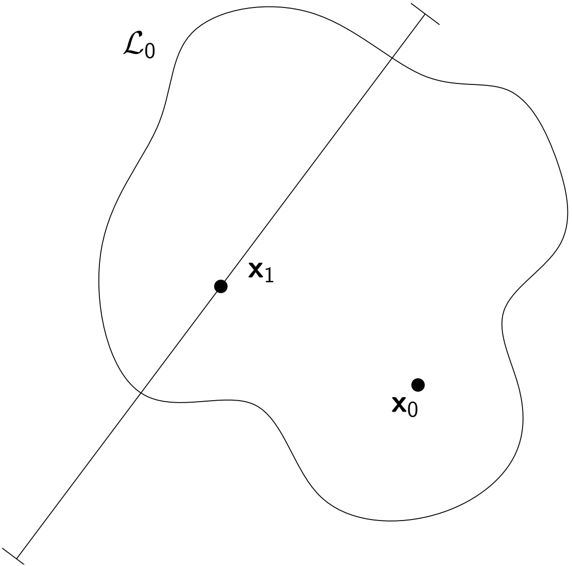

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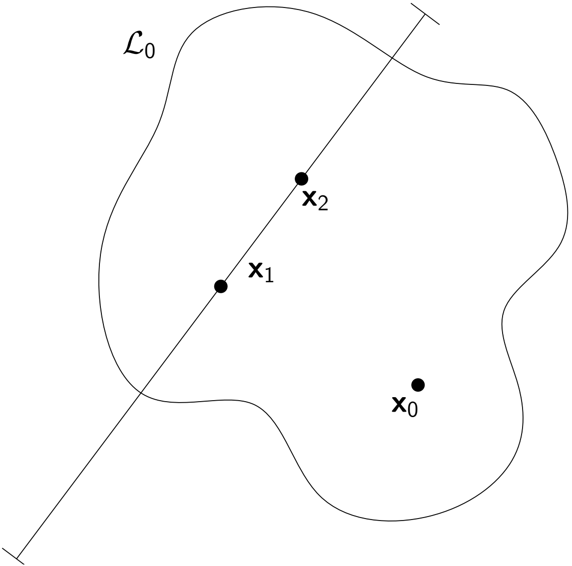

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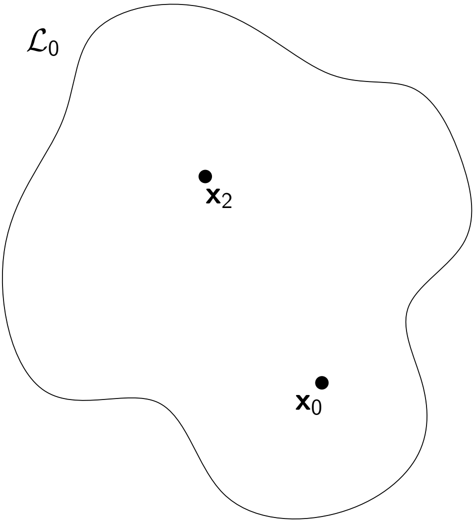

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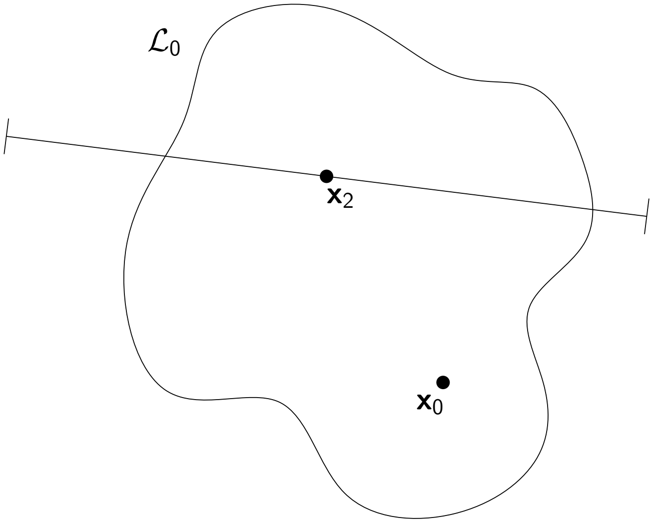

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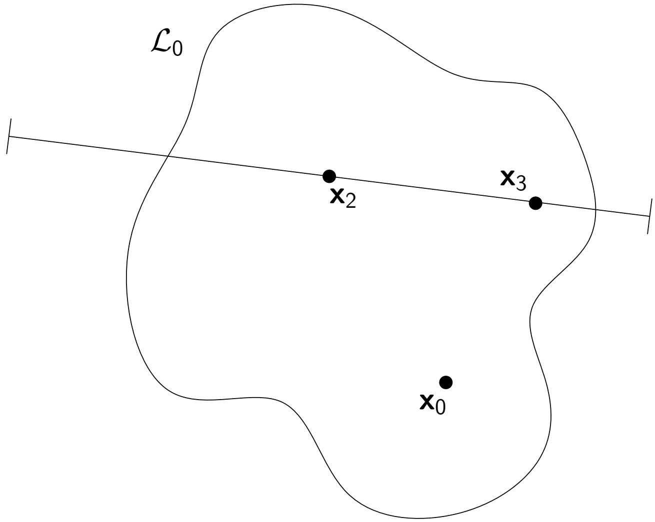

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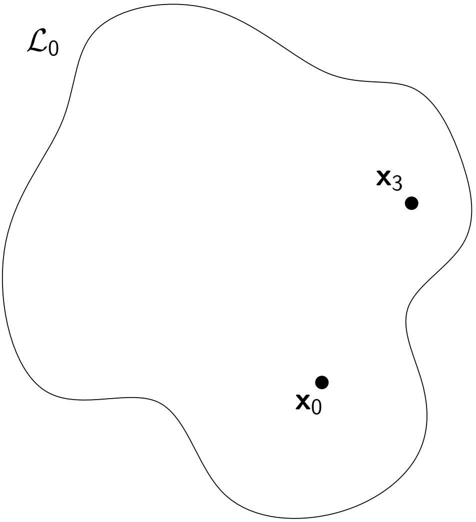

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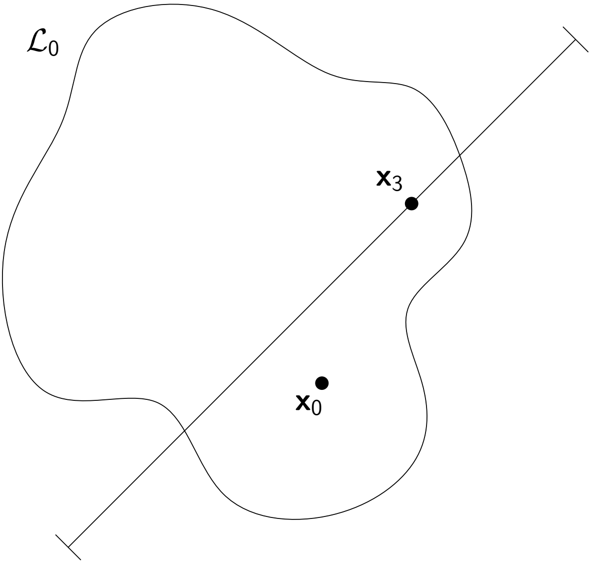

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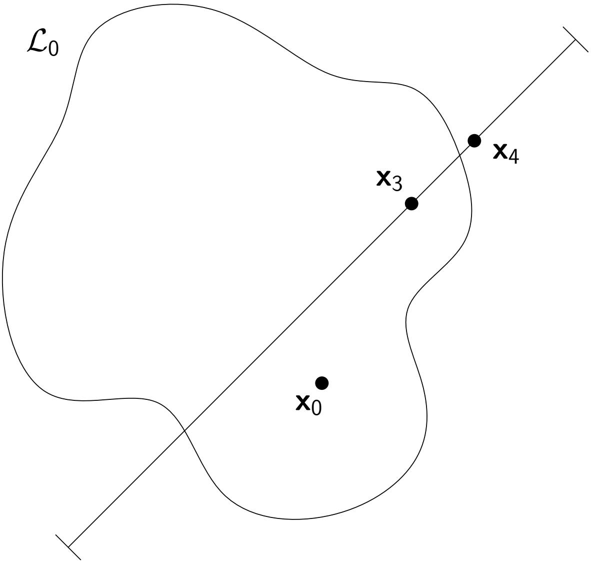

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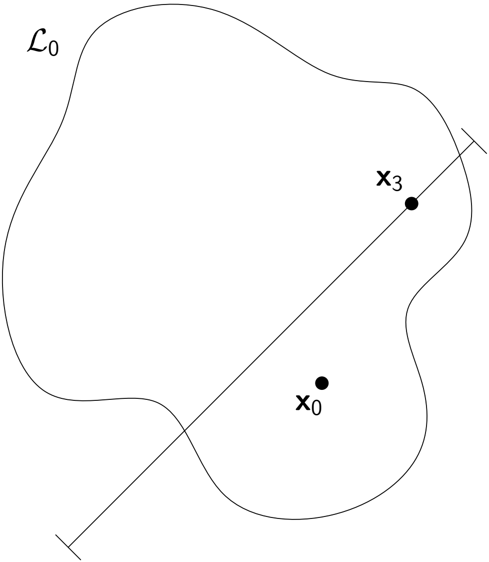

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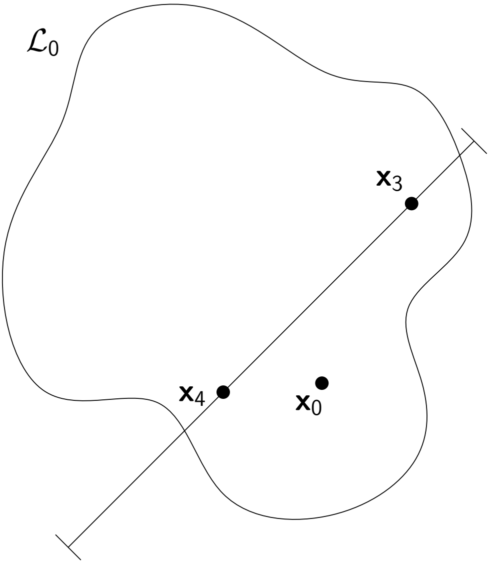

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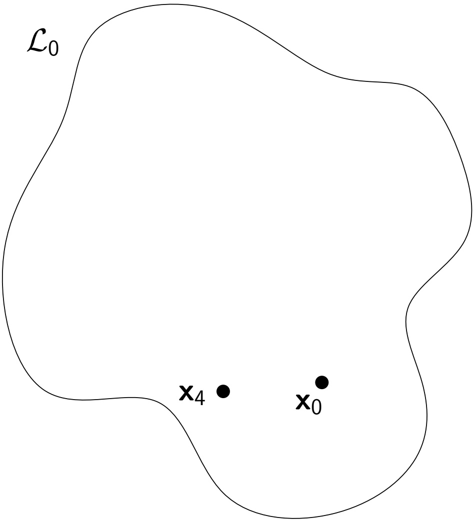

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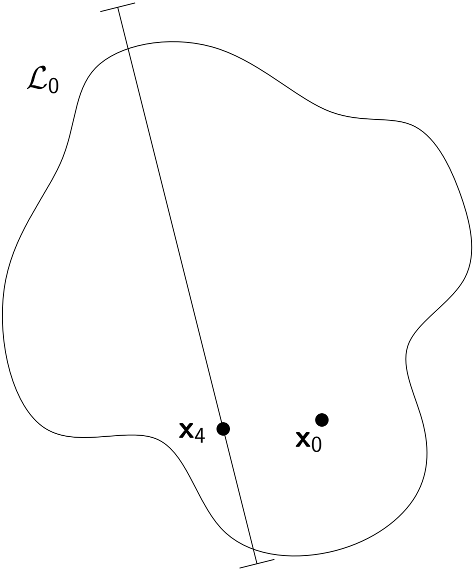

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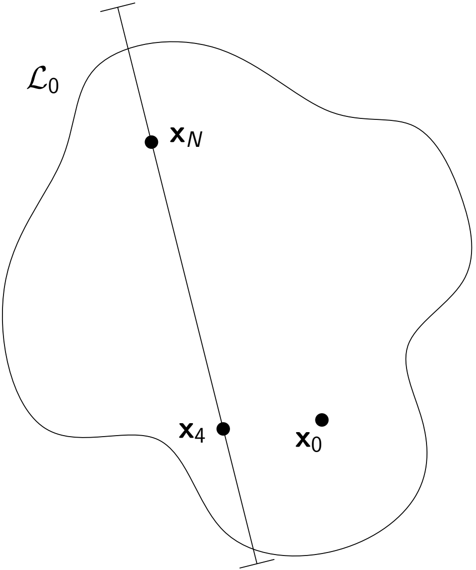

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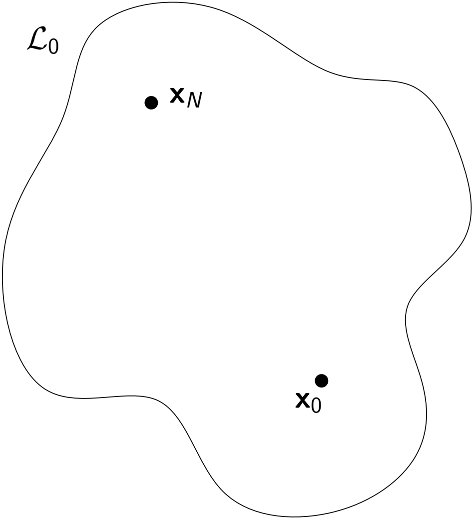

“Hit and run” slice sampling

Key points

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- This procedure satisfies detailed balance.

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- This procedure satisfies detailed balance.
- 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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Correlated distributions

1. Does not deal well with correlated distributions.

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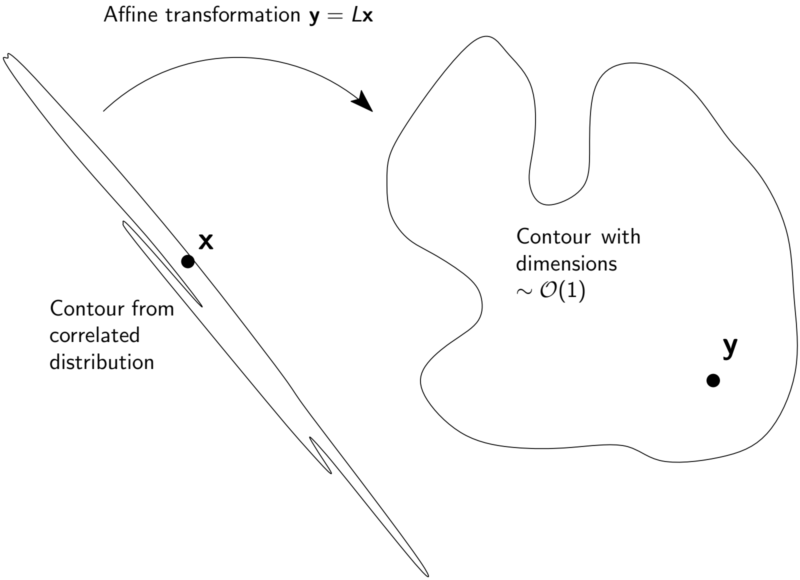
Correlated distributions

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

PolyChord's solutions

Correlated distributions



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- Cholesky decomposition is the required skew transformation
- $w = 1$ in this transformed space

Issues with Slice Sampling

Multimodality

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Issues with Slice Sampling

Multimodality

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2. Affine transformation is useless.

PolyChord's solutions

Multimodality

PolyChord's solutions

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1. Identifies separate modes via clustering algorithm on live points.

PolyChord's solutions

Multimodality

1. Identifies separate modes via clustering algorithm on live points.
2. Evolves these modes "semi-independently"

PolyChord's Additions

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- Parallelised up to number of live points with openMPI.

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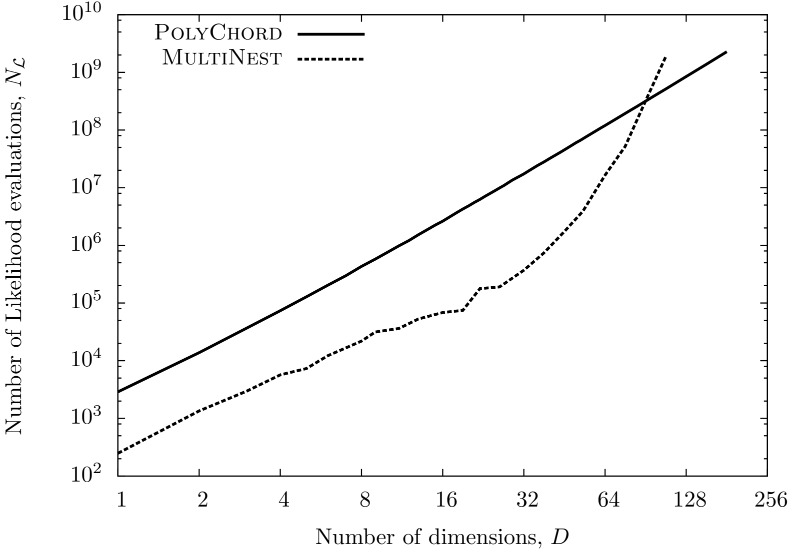
- Implemented in CosmoMC, as "CosmoChord", with fast-slow parameters.

PolyChord vs. MultiNest

Gaussian likelihood



PolyChord 1.0

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

PolyChord

Scaling with dimensionality

PolyChord

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PolyChord

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PolyChord

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PolyChord

Scaling with dimensionality

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- PolyChord 1.0 has $N_{\mathcal{L}} \sim \mathcal{O}(D^3)$
  - 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

Inter-chain evaluations

PolyChord 2.0

Inter-chain evaluations

- Traditional nested sampling requires the ability to easily generate a single sample at each iteration.

PolyChord 2.0

Inter-chain evaluations

- Traditional nested sampling requires the ability to easily generate a single sample at each iteration.
- MCMC-like approaches generate many (correlated) samples

PolyChord 2.0

Inter-chain evaluations

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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.

Aside: Merging nested sampling runs

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- Take two complete nested sampling runs generated by $n_{\mathrm{live}}^{(1)}$ and $n_{\mathrm{live}}^{(2)}$ live points.
- Combining the two runs in likelihood order gives a new run generated by $n_{\mathrm{live}}^{(1)} + n_{\mathrm{live}}^{(2)}$ live points.

Aside: Unweaving nested sampling runs

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- The reverse is also true.

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

PolyChord 2.0

Handling correlations

PolyChord 2.0

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PolyChord 2.0
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PolyChord 2.0

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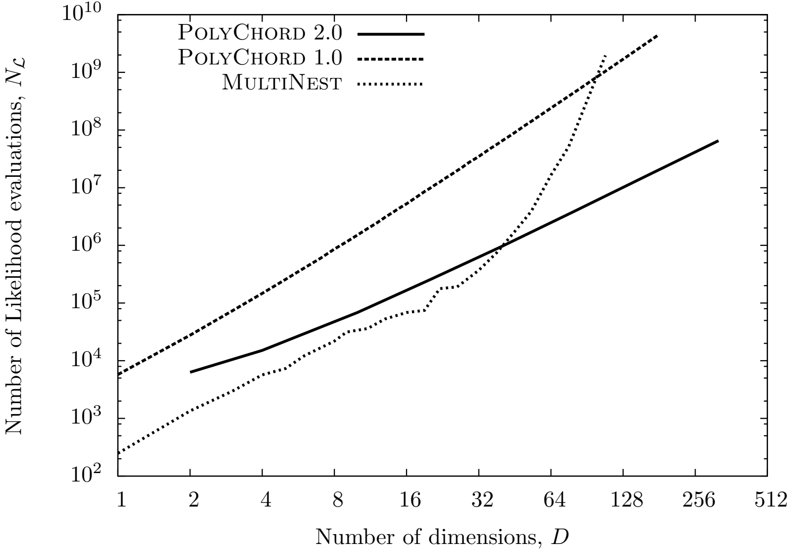
- With this in hand, can produce correct inferences from correlated runs.

PolyChord 2.0 vs. MultiNest

Gaussian likelihood

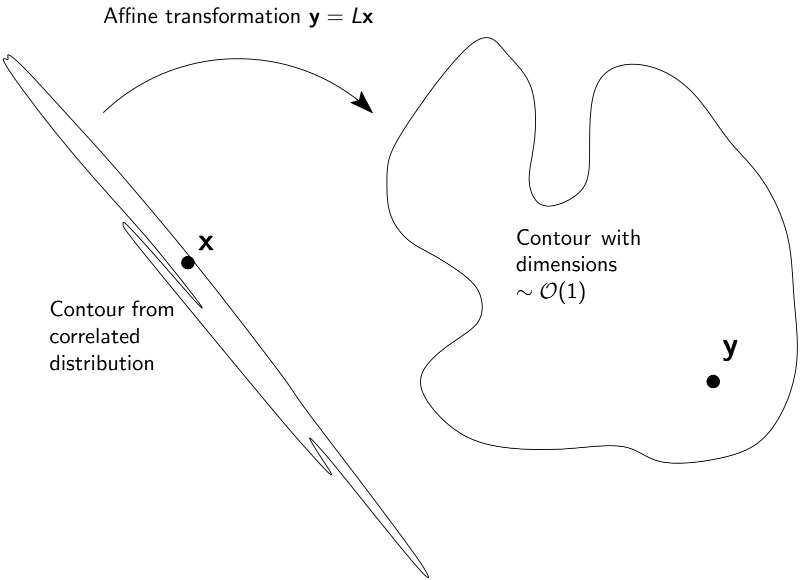


Correlated distributions

Correlated distributions

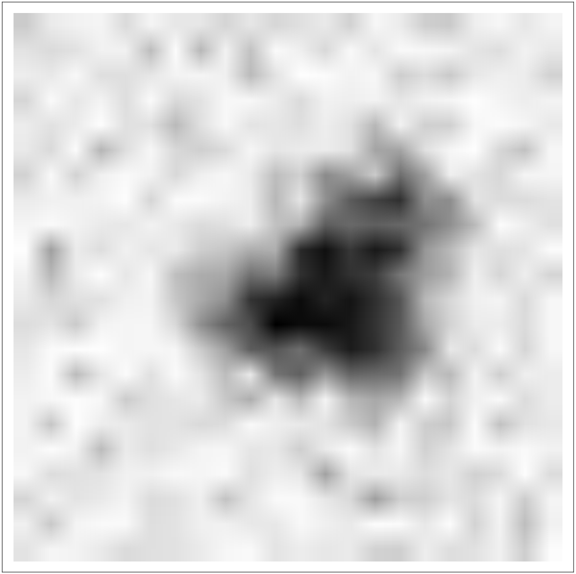
- Correlated distributions are hard

Correlated distributions



Object detection

Toy problem



Object detection

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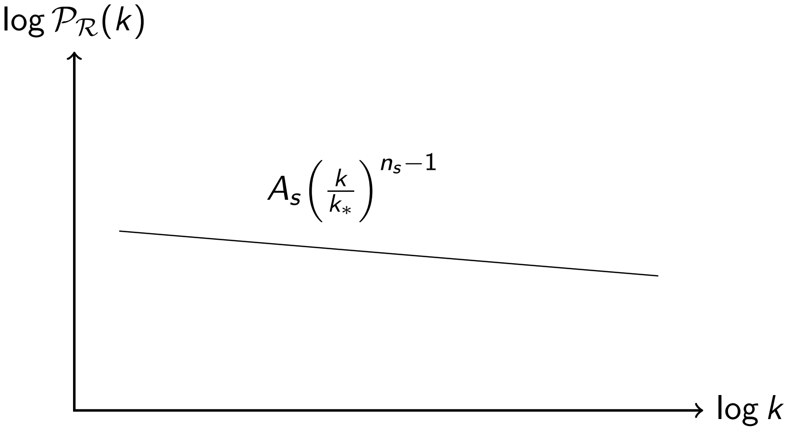
Object detection

Evidences

- $\log \mathcal{Z}$ 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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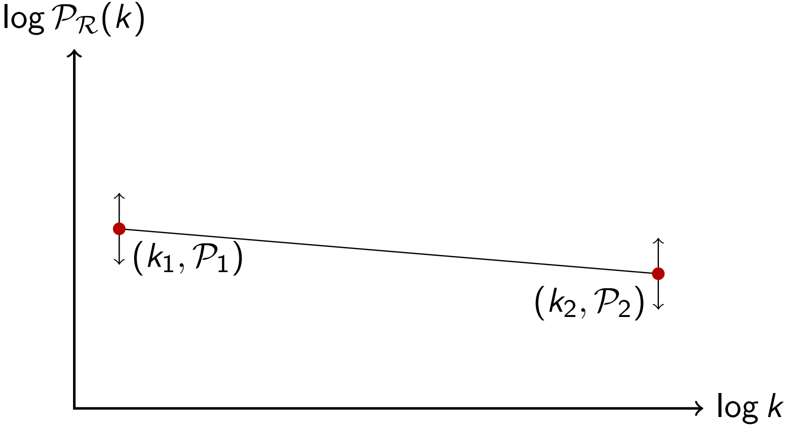

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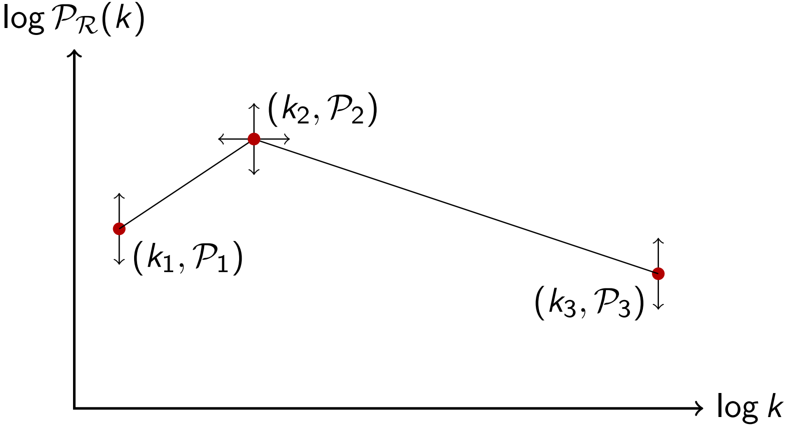

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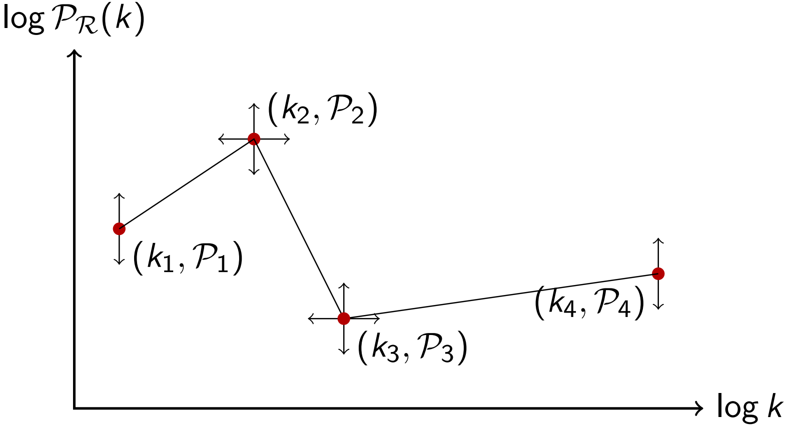

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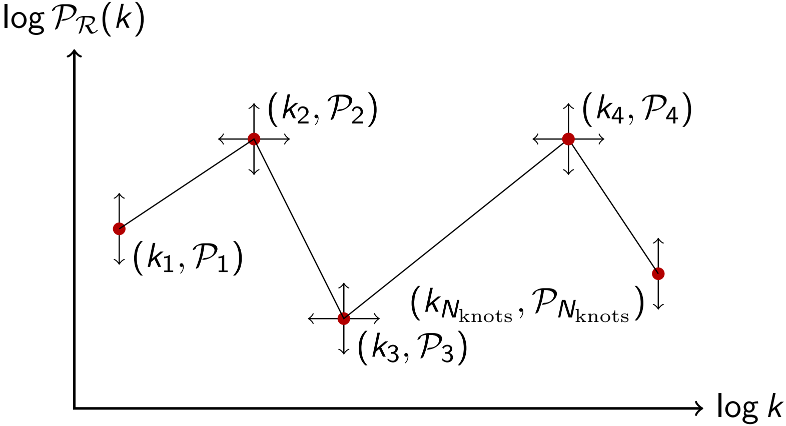
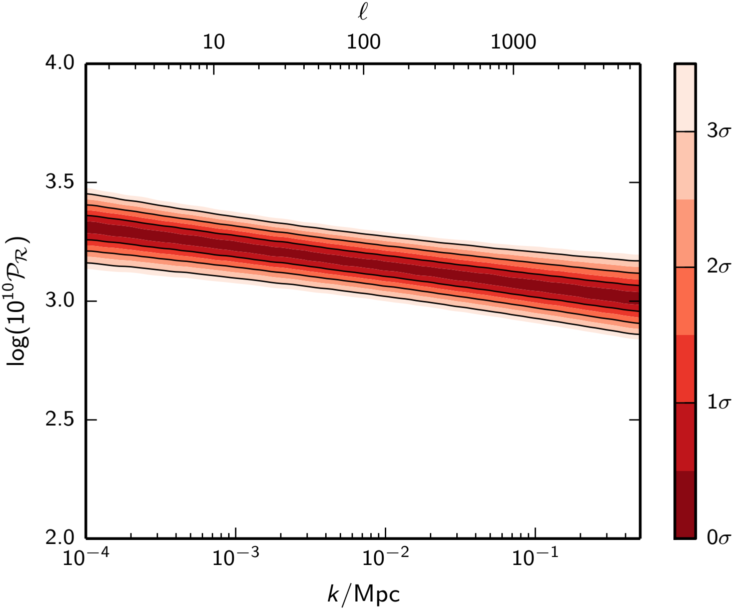


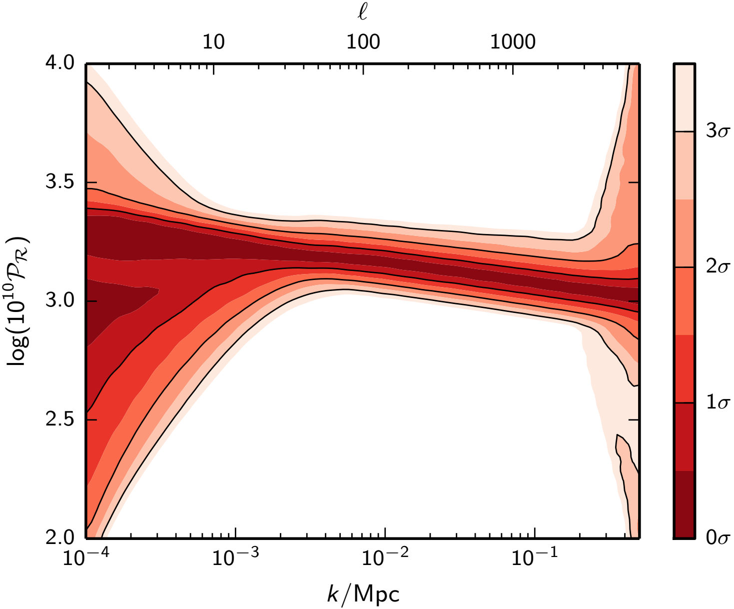
0 internal knots

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



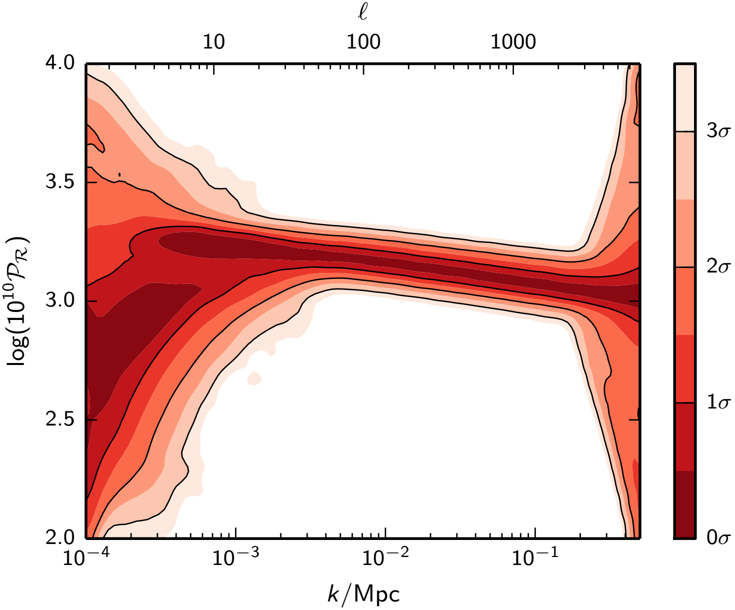
1 internal knots

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



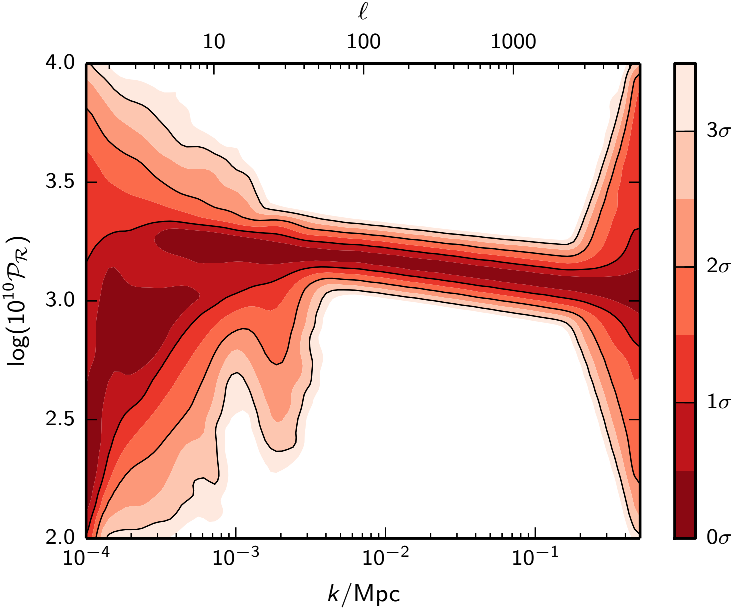
2 internal knots

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



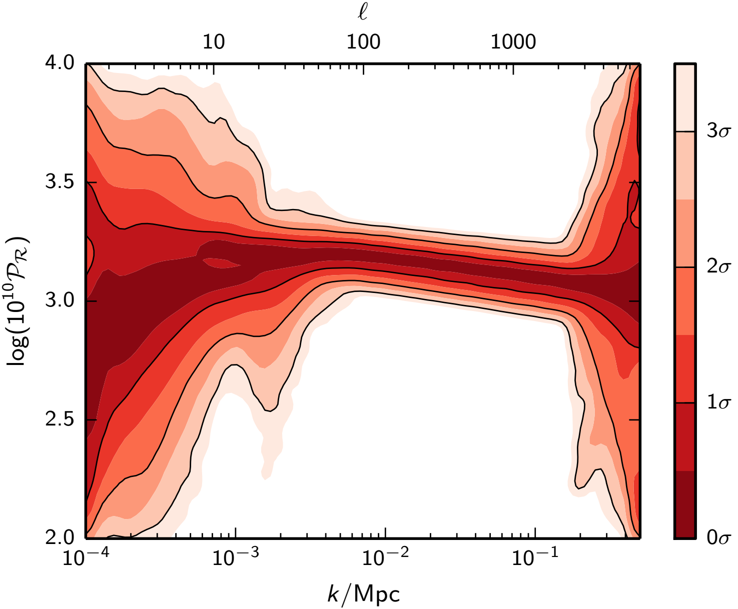
3 internal knots

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



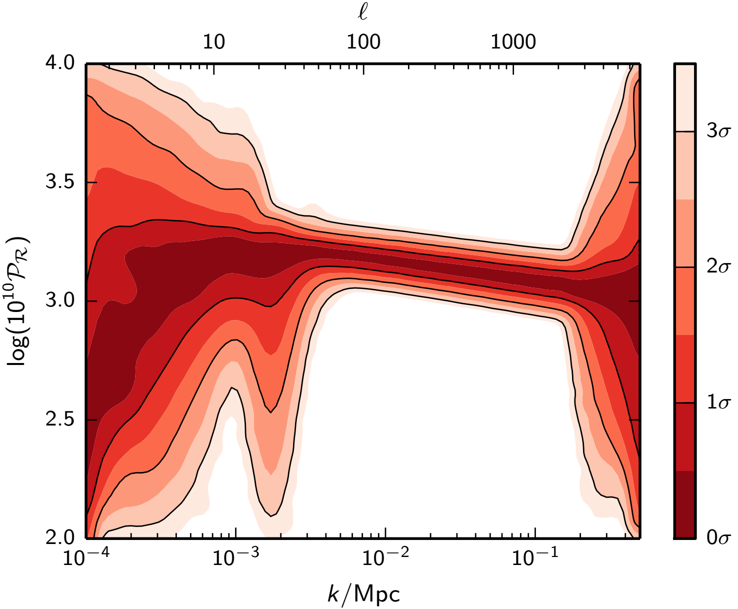
4 internal knots

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



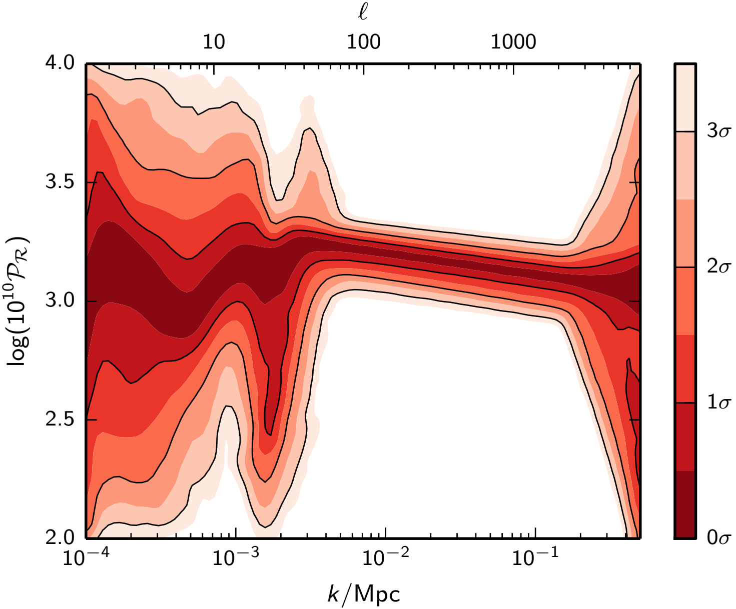
5 internal knots

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



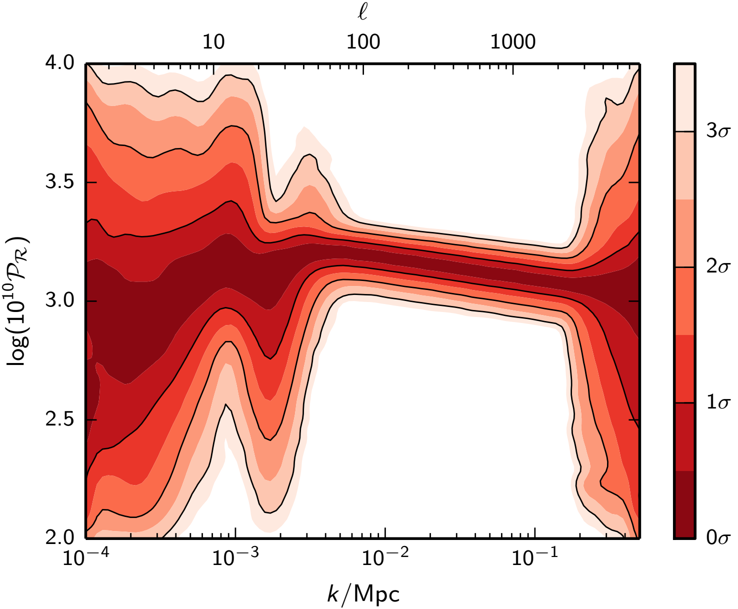
6 internal knots

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



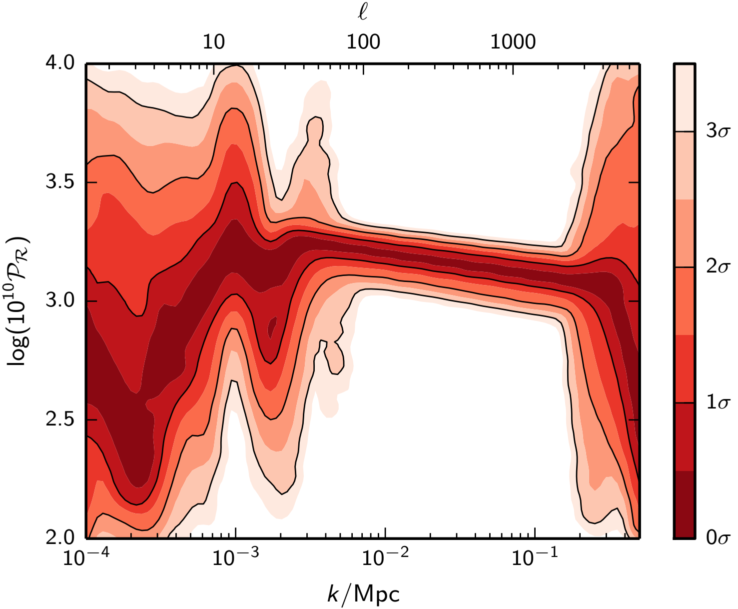
7 internal knots

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



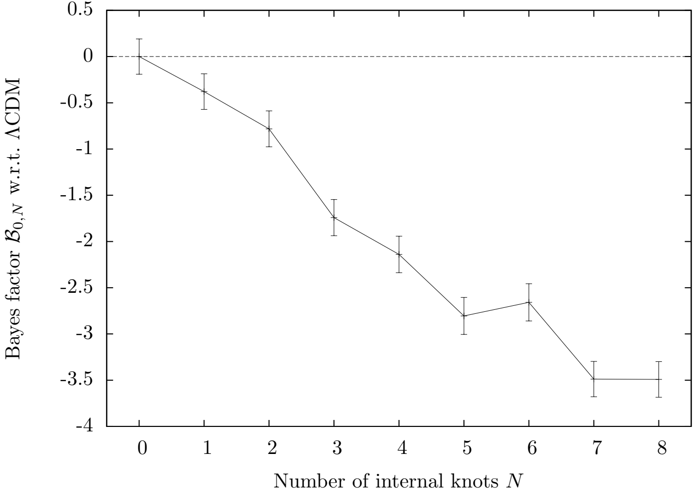
8 internal knots

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



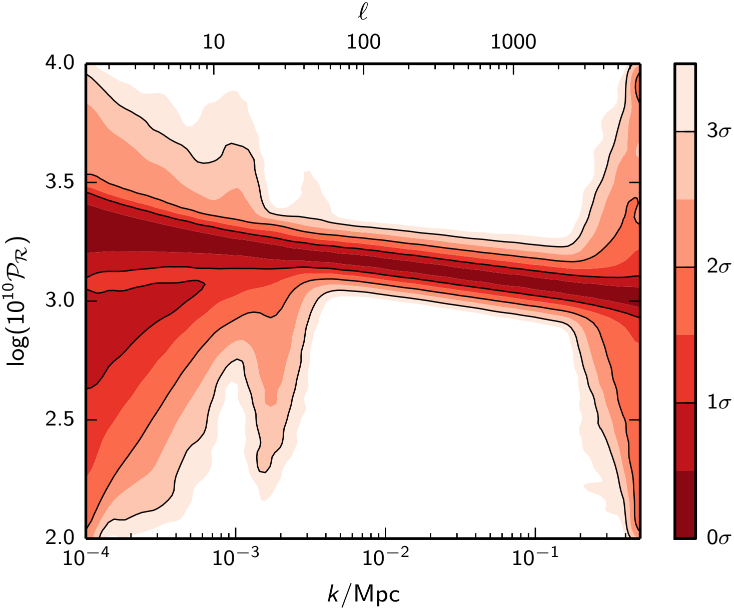
Bayes Factors

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



Marginalised plot

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



Affine invariance

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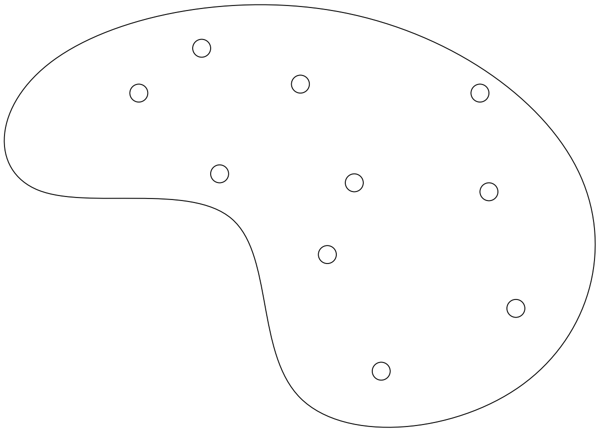
- Good example: Now highly successful emcee (MCMC hammer).
  - Important: emcee is not unique (or necessarily best)

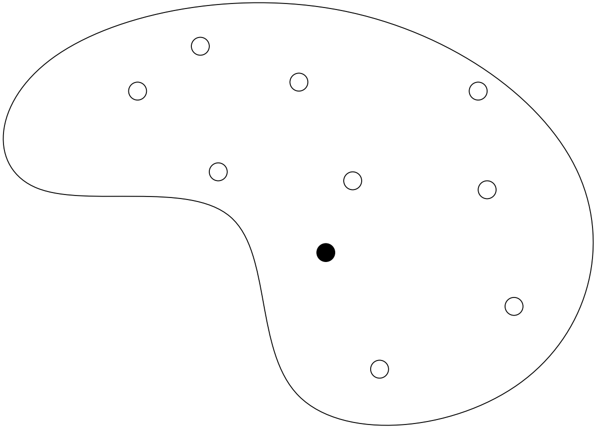
Skillings affine invariant ideas

Leapfrog



Skillings affine invariant ideas

Leapfrog



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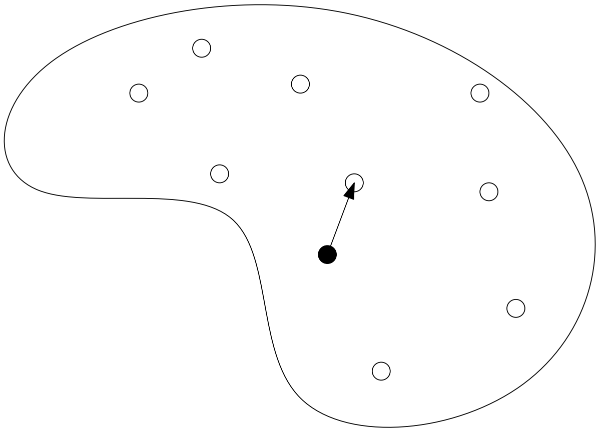

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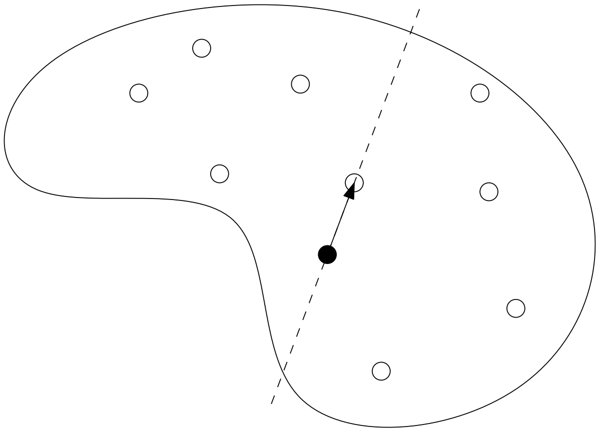

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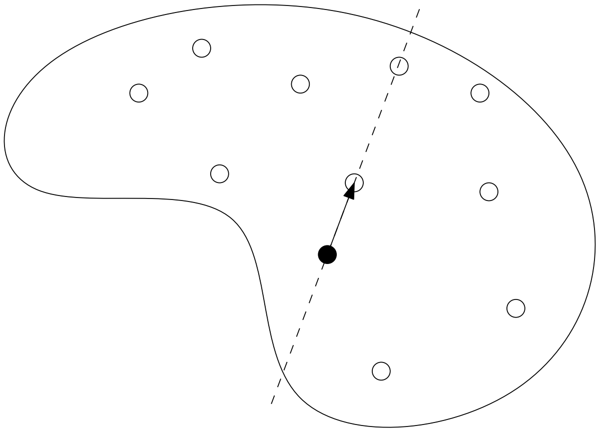

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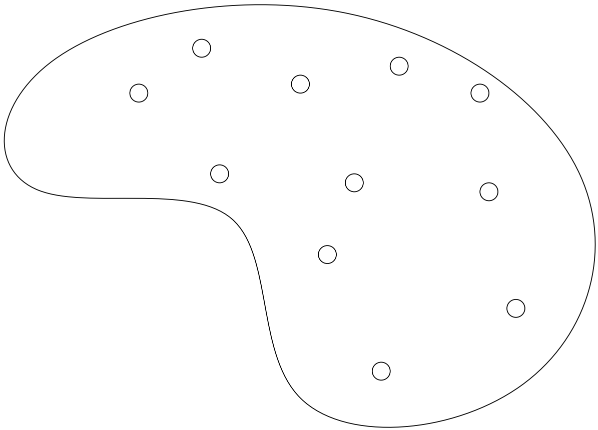
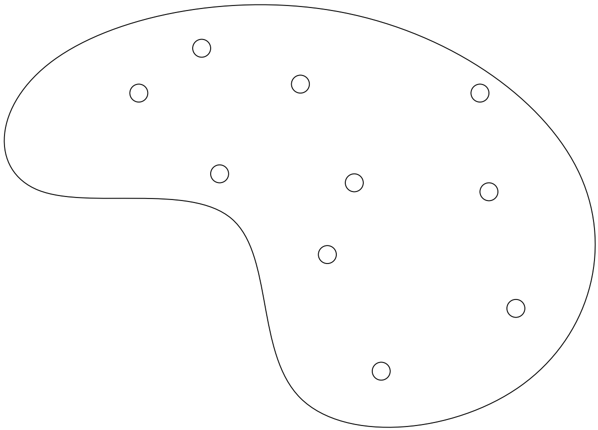


Skillings affine invariant ideas

Parallel walk



Skillings affine invariant ideas

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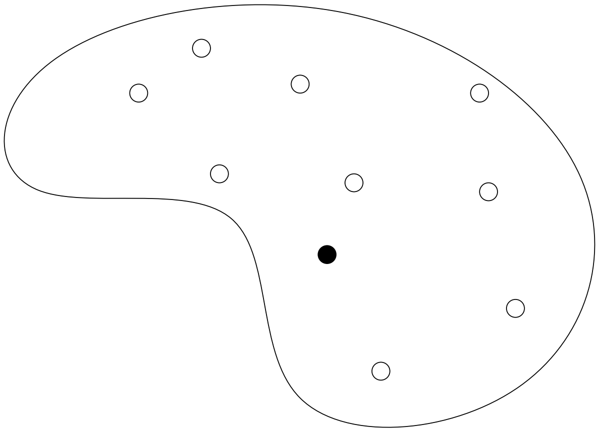

Skillings affine invariant ideas

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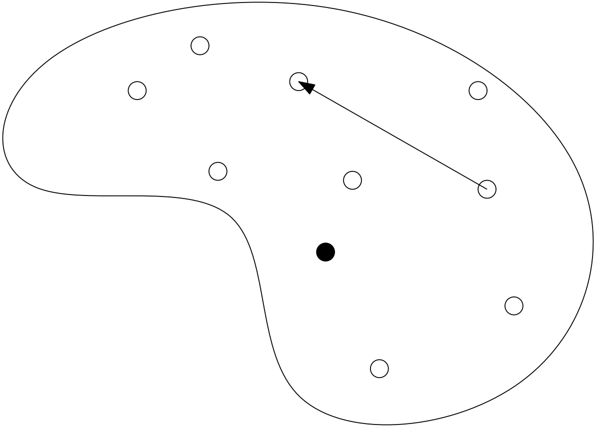

Skillings affine invariant ideas

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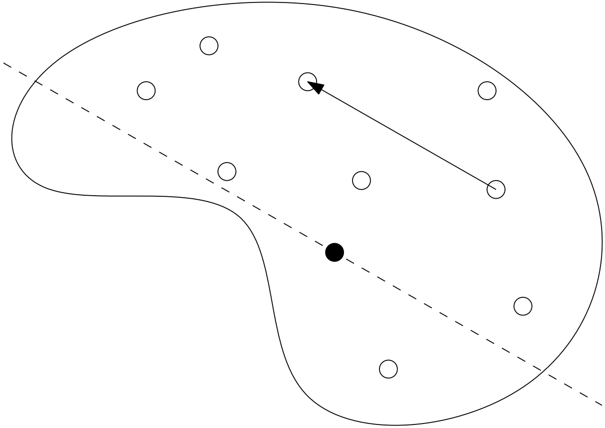

Skillings affine invariant ideas

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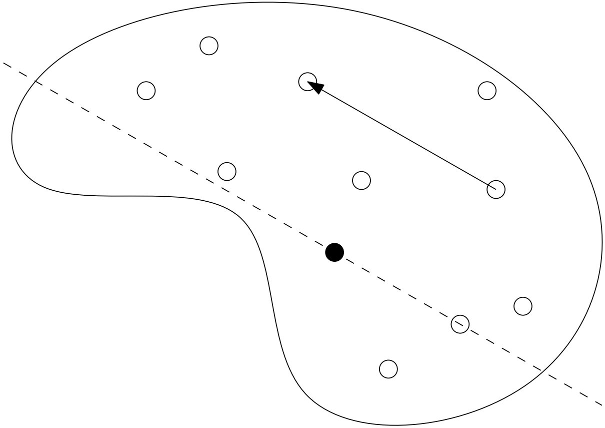

Skillings affine invariant ideas

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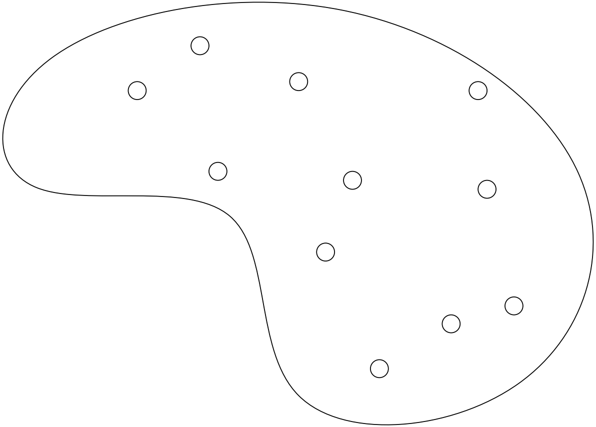


Affine invariance

Subspace collapse

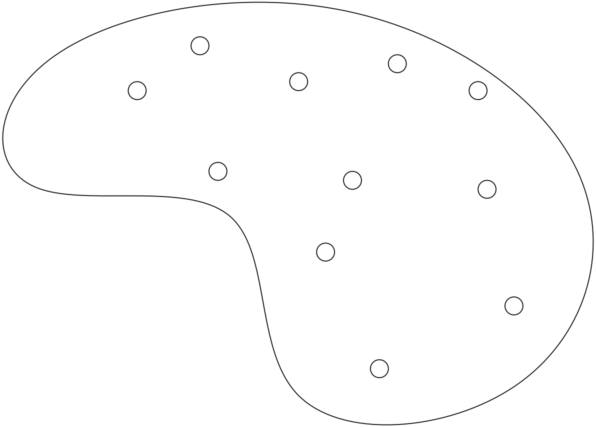
Affine invariance

Subspace collapse

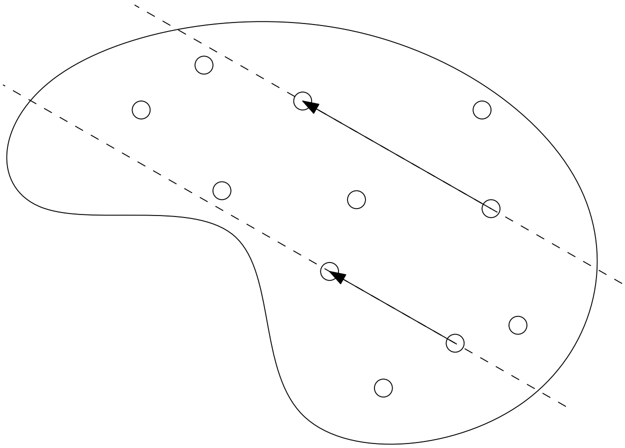
- The main problem that besets these techniques is "subspace collapse".

Subspace collapse

Leapfrog



Subspace collapse



Subspace collapse

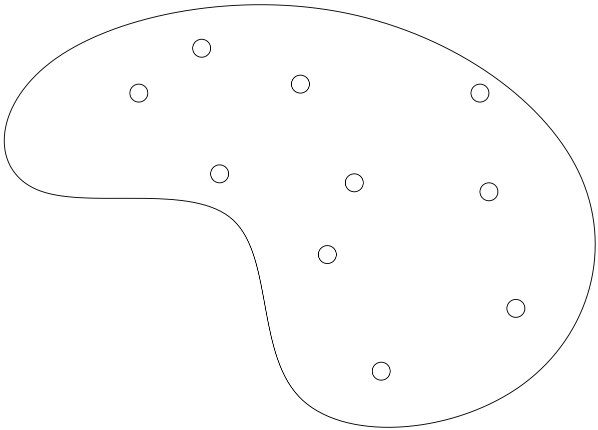
Solution

Subspace collapse
Solution

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

Skillings affine invariant ideas

Guided walk



Skillings affine invariant ideas

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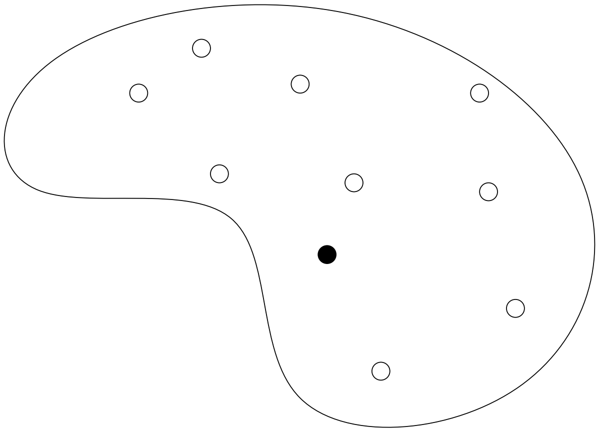
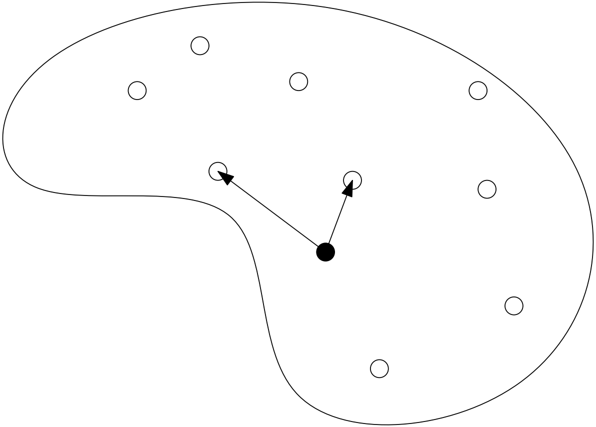


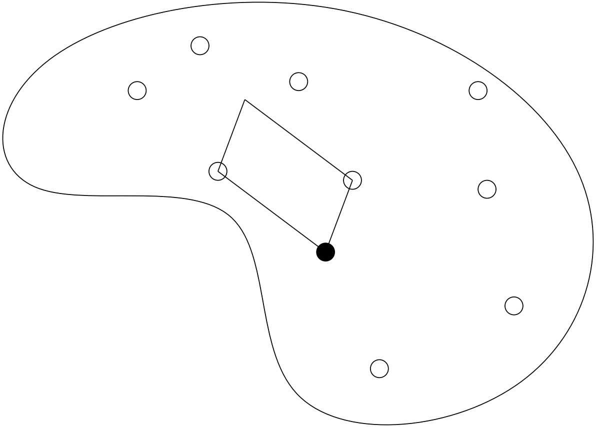
Skillings affine invariant ideas

Guided walk



Skillings affine invariant ideas

Guided walk



Skillings affine invariant ideas

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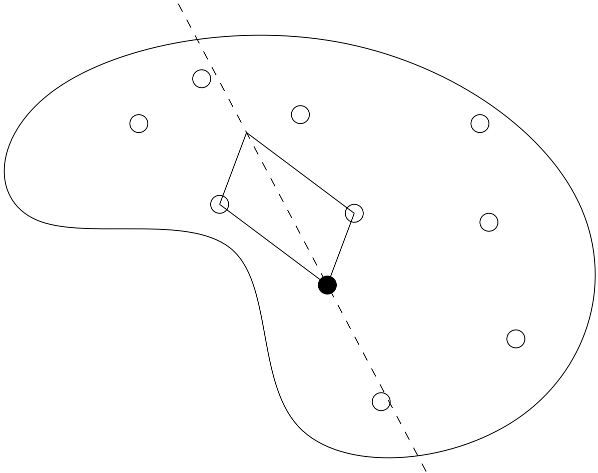

Skillings affine invariant ideas

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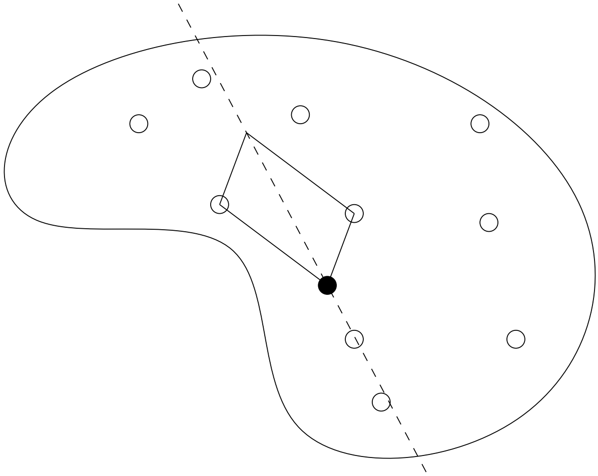

Skillings affine invariant ideas

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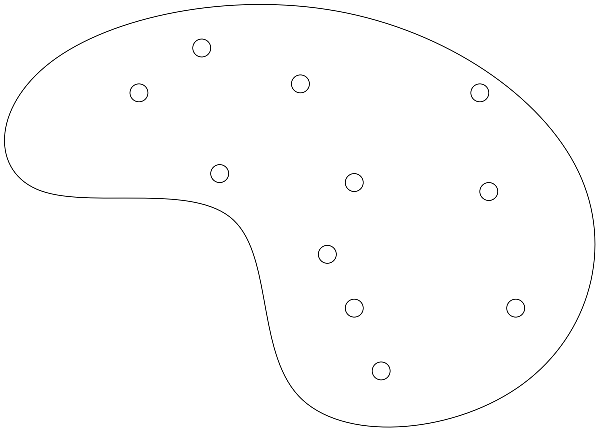

Skillings affine invariant ideas

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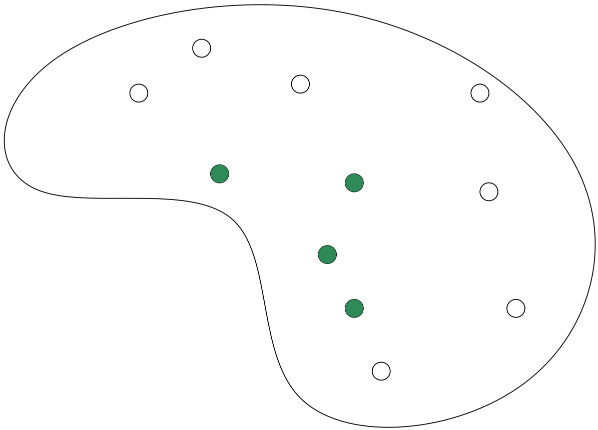

Affine invariant

Other variations

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- Generalise guided walk to D dimensions (slice through the mean of D other points).

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Affine invariant

Other variations

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- There are lots of variations: This is an underused area of the field.

PolyChord 2.0

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PolyChord 2.0

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- Unweaving runs to quantify correlations

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- Unweaving runs to quantify correlations
- Affine invariant sampling