

PolyChord 2.0

Advances in nested sampling with astrophysical applications

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What is nested sampling?

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- ▶ Uses ensemble sampling to compress prior to posterior.
- ▶ In doing so, it circumvents many issues (dimensionality, topology, geometry) that beset standard approaches.

Outline

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1. Background theory

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2. Review existing sampling approaches

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3. Nested Sampling & Historical implementations.

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4. PolyChord
5. Applications

Bayes' theorem

Parameter estimation

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A concrete example.

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- ▶ Likelihoods can be quite complicated!
- ▶ We need advanced sampling approaches.

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Model averaging:

- ▶ Multiple models with posterior on the same parameter:

$$P(y|M_i, D)$$

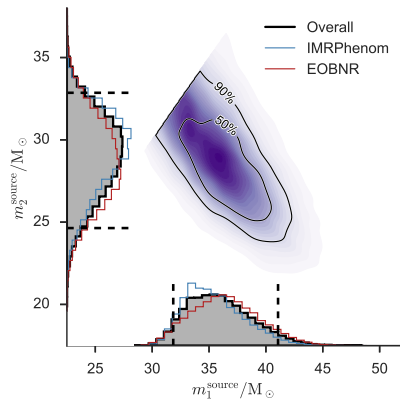
$$P(y|D) = \sum_i P(y|M_i, D)P(M_i|D)$$

Parameter estimation

Why do sampling?

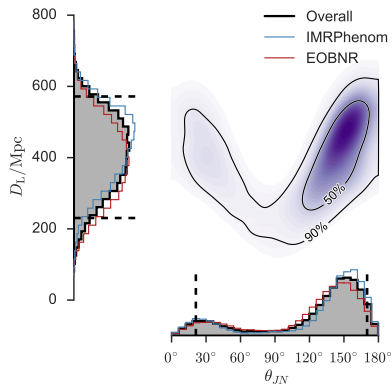
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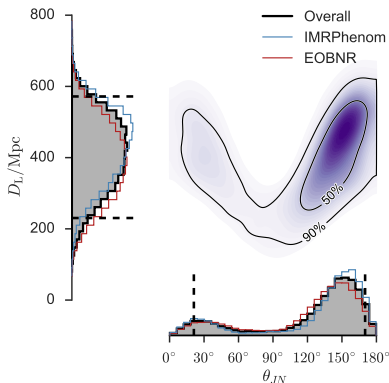
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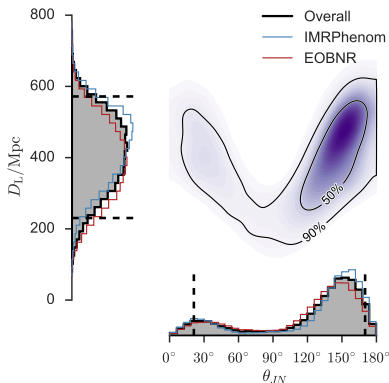
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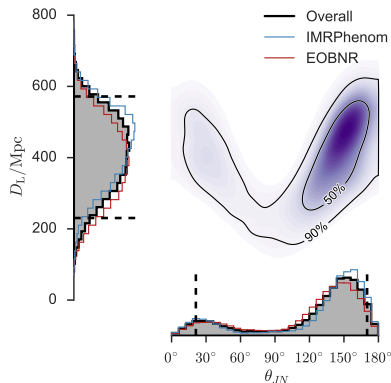
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- ▶ Describing an N -dimensional posterior fully is impossible.



Parameter estimation

Why do sampling?

- ▶ In high dimensions, posterior \mathcal{P} occupies a vanishingly small region of the prior π .
- ▶ Describing an N -dimensional posterior fully is impossible.
- ▶ *Sampling* the posterior is an excellent compression scheme.



Current sampling approaches

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2. Hamiltonian Monte-Carlo (HMC).

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1. Metropolis Hastings.
2. Hamiltonian Monte-Carlo (HMC).
3. Ensemble sampling (e.g. emcee).

Metropolis Hastings

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- ▶ Turn the N -dimensional problem into a one-dimensional one.

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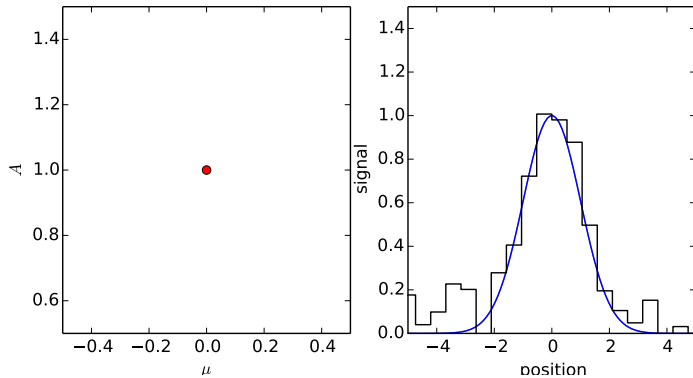
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- ▶ Turn the N -dimensional problem into a one-dimensional one.
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Metropolis Hastings

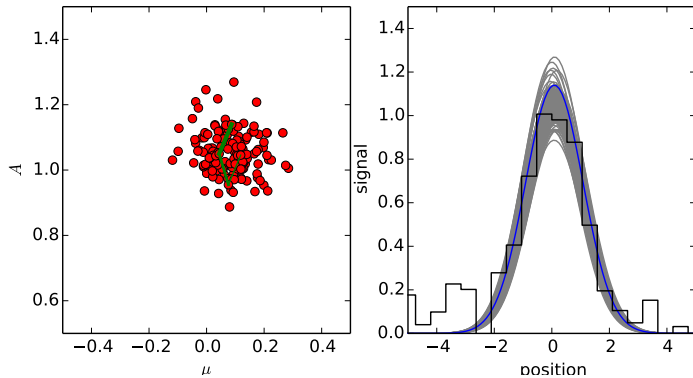
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 4. . . . otherwise sometimes make step.

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Struggles with...

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1. Burn in

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- ▶ Walker is naturally “guided” uphill
- ▶ Conserved quantities mean efficient acceptance ratios.

Hamiltonian Monte-Carlo

Problems

Hamiltonian Monte-Carlo

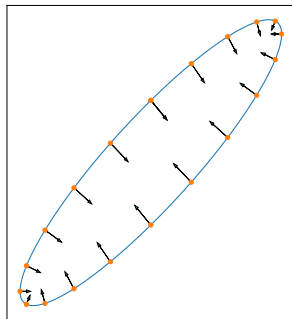
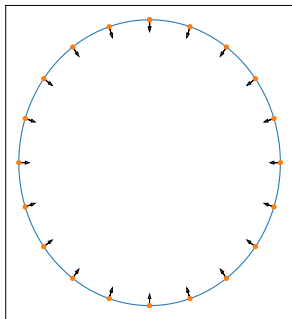
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- ▶ “Uphill” is not covariant.

Hamiltonian Monte-Carlo

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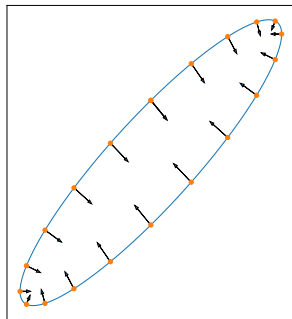
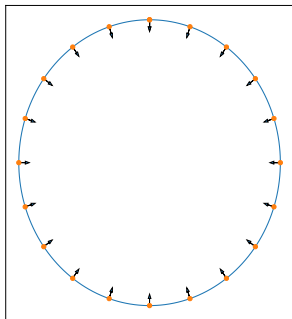
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- Requires gradients (autograd – python)

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- ▶ Can use information present in ensemble to guide proposals.
- ▶ emcee: affine invariant proposals.
- ▶ emcee is not the only (or even best) affine invariant approach.

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The real reason these all fail

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$$\begin{aligned} \mathcal{Z} &= P(D|M) \\ &= \int P(D|\Theta, M)P(\Theta|M)d\Theta \end{aligned}$$

The real reason these all fail

- ▶ MCMC does not give you evidences!

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- ▶ MCMC fundamentally explores the posterior, and cannot average over the prior.
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 - ▶ Inspired by thermodynamics.
 - ▶ Suffers from similar issues to MCMC.
 - ▶ Unclear how to choose correct annealing schedule

Nested Sampling

John Skilling's alternative to traditional MCMC!

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New procedure:

Nested Sampling

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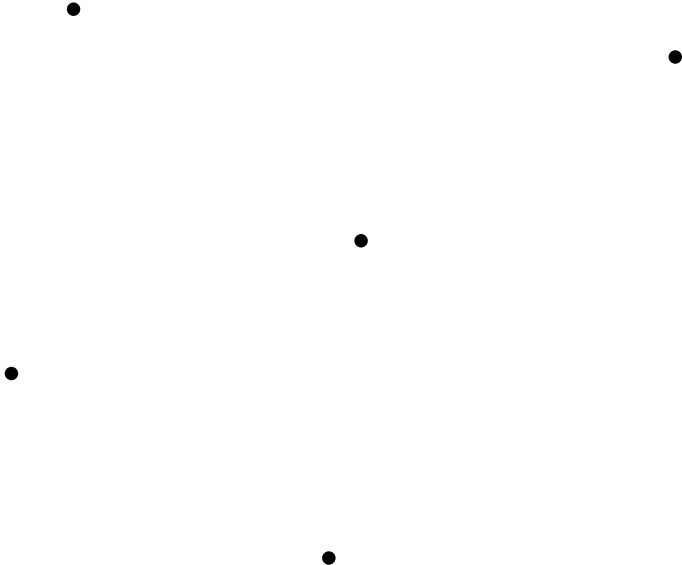
S_0 : Generate n samples uniformly over the space (from the prior π).

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

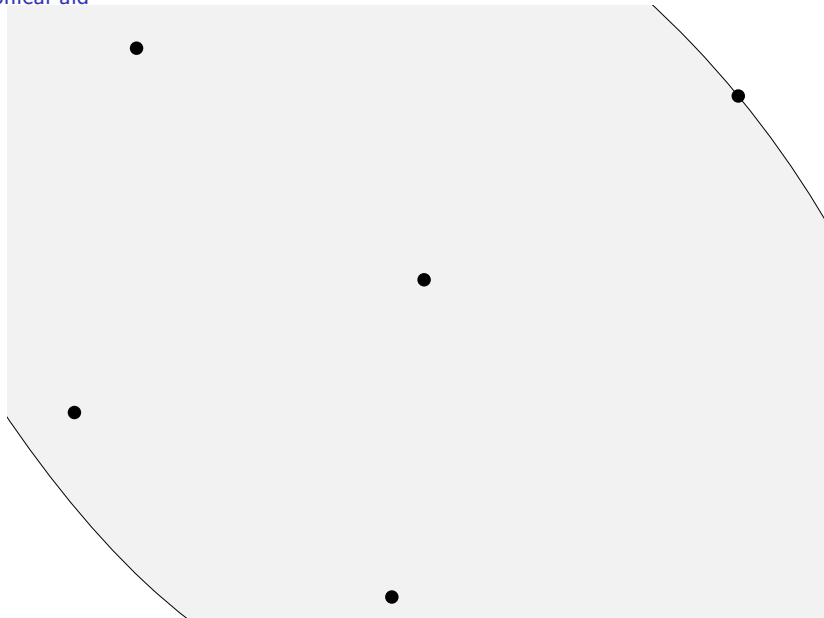
Nested Sampling

Graphical aid



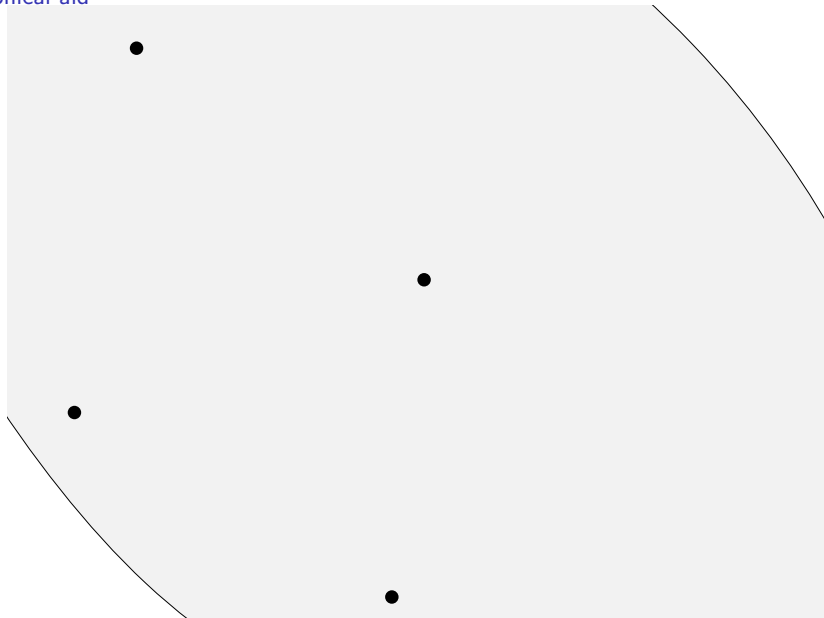
Nested Sampling

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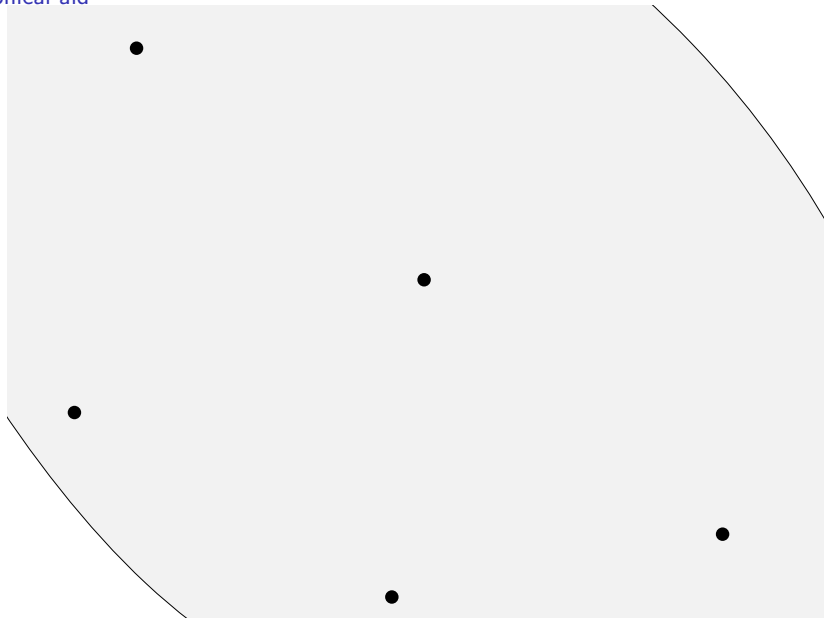
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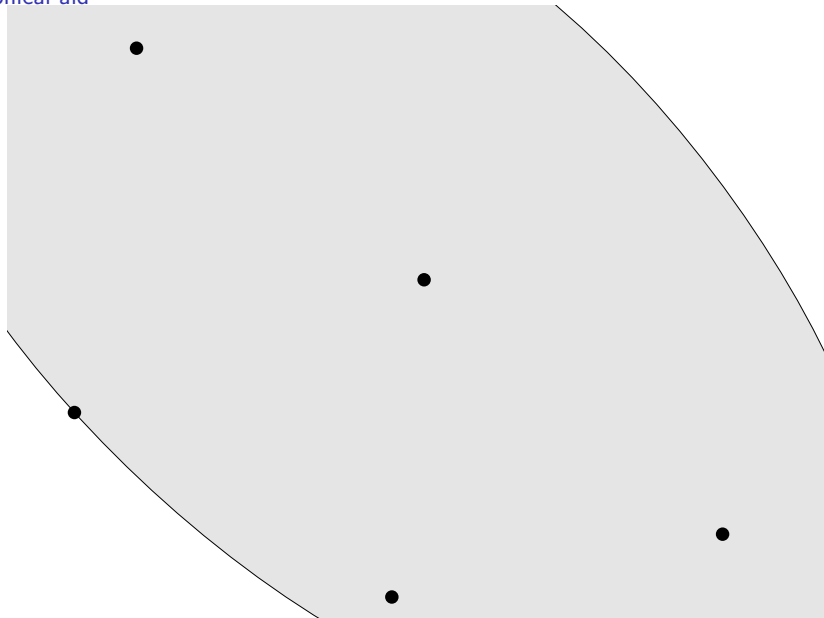
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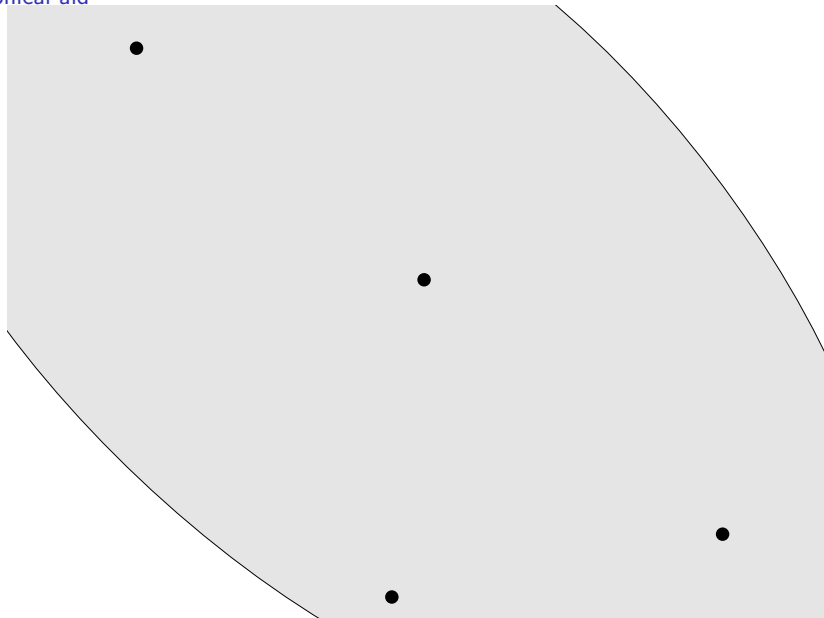
Nested Sampling

Graphical aid



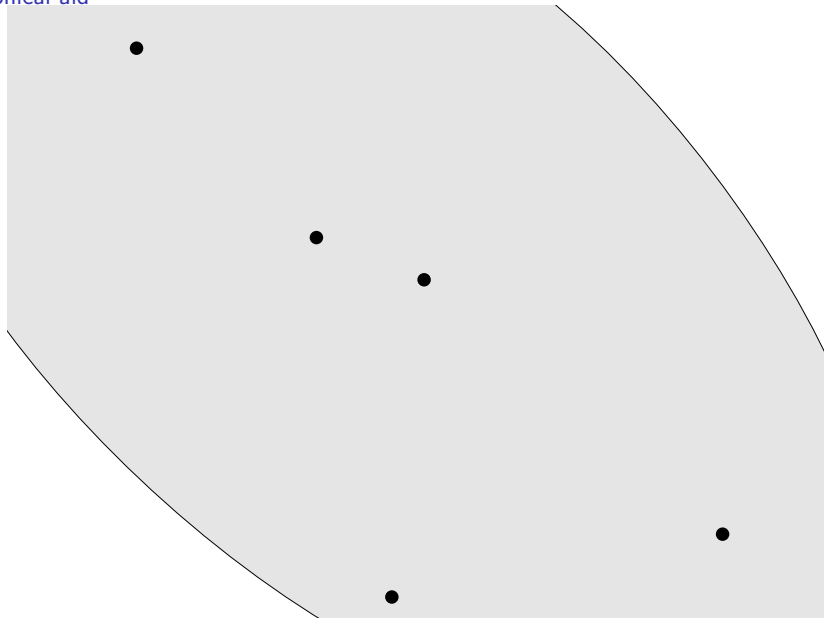
Nested Sampling

Graphical aid



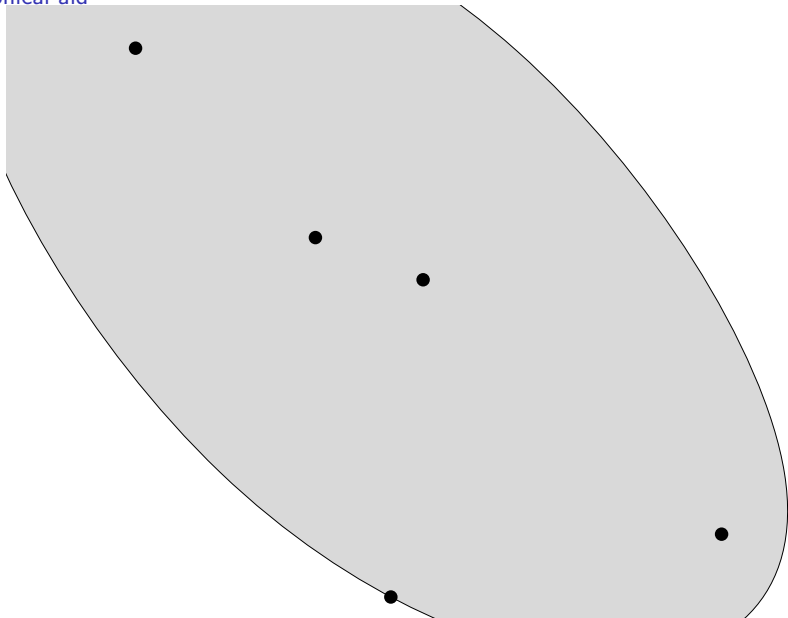
Nested Sampling

Graphical aid



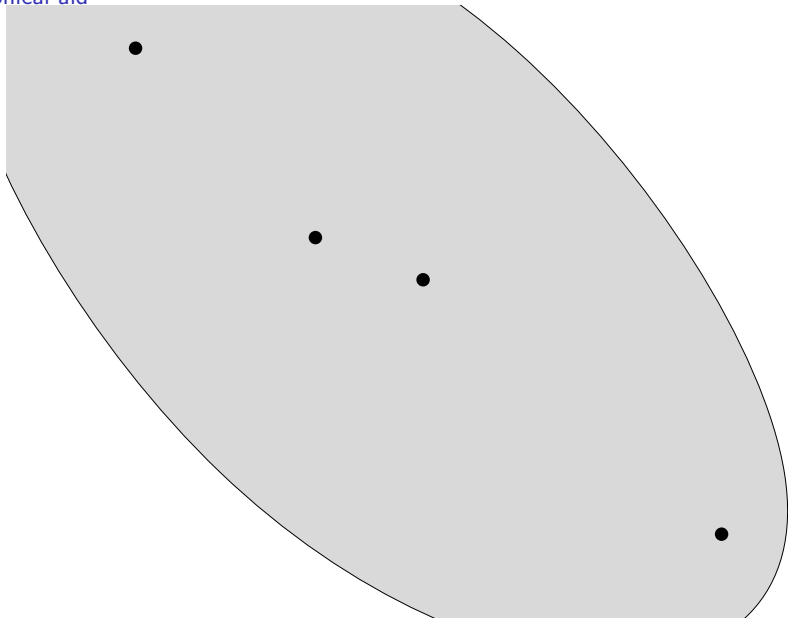
Nested Sampling

Graphical aid



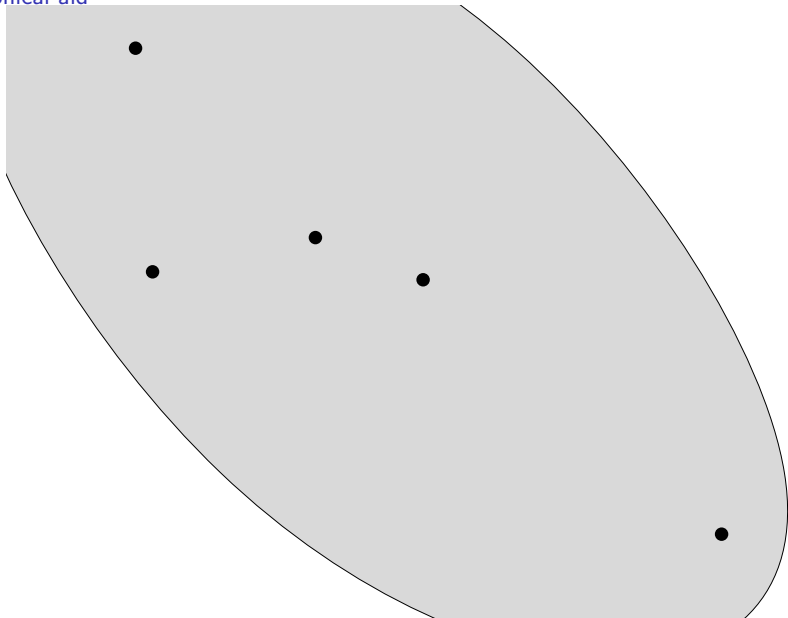
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Graphical aid



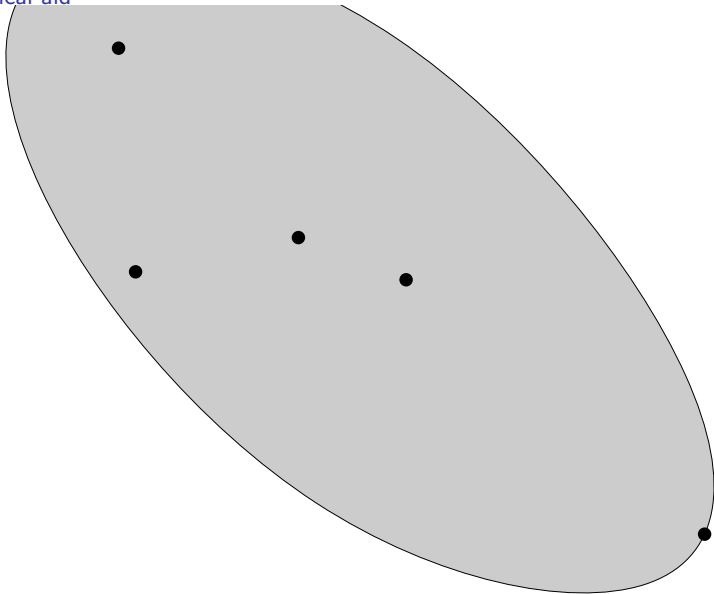
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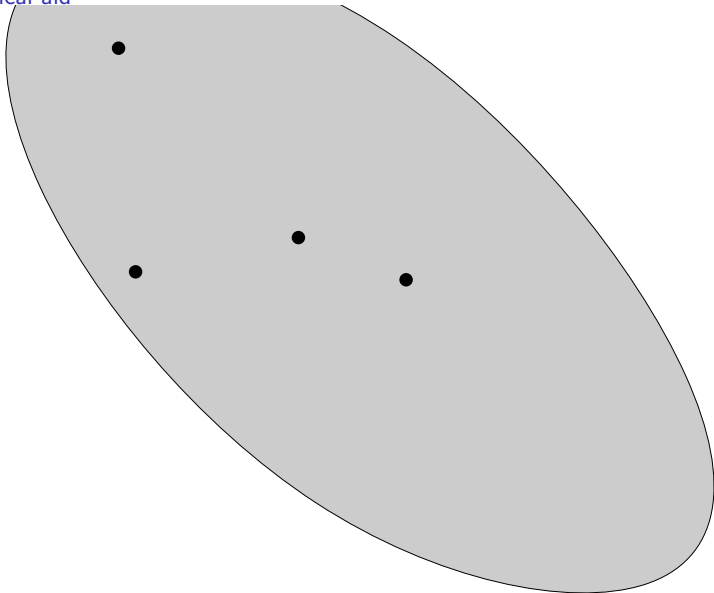
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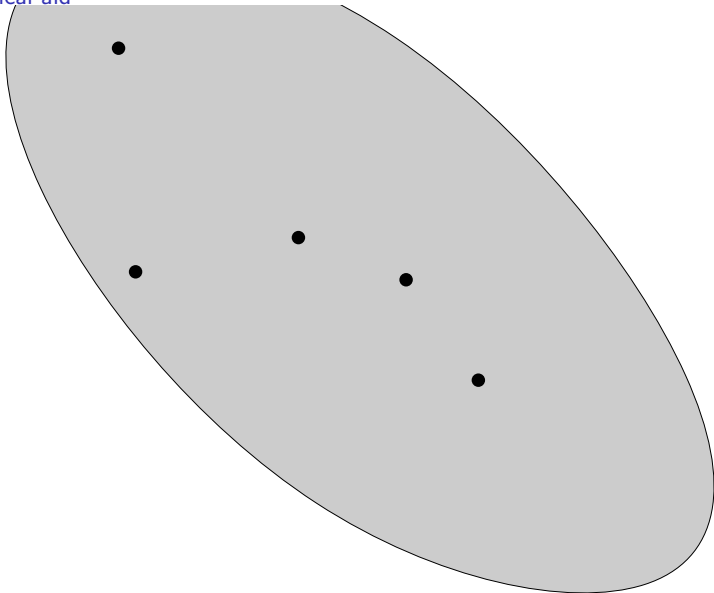
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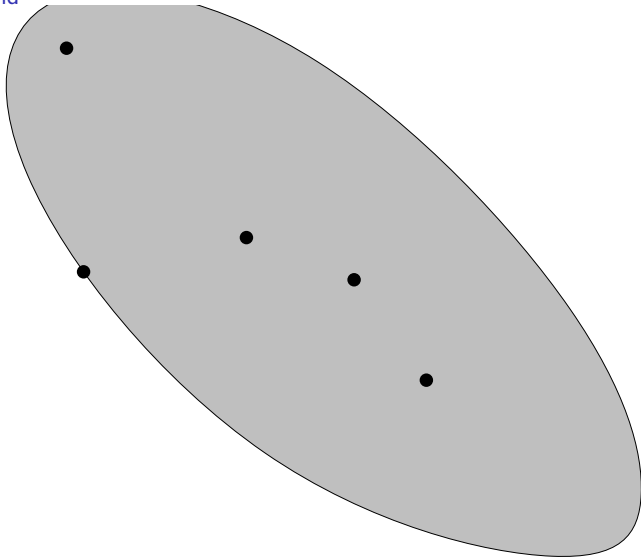
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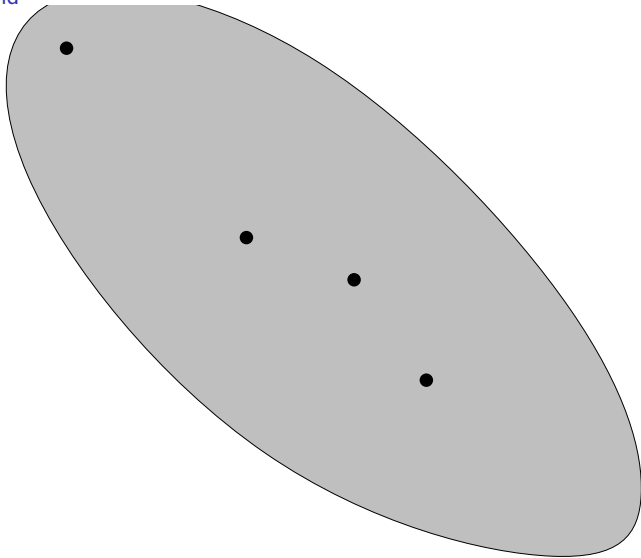
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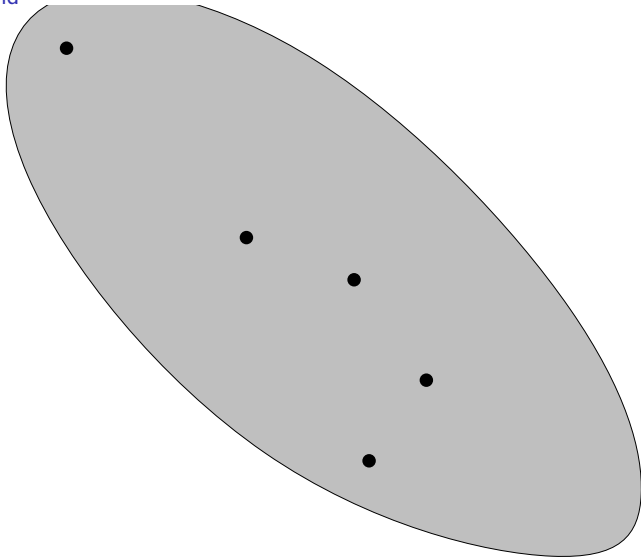
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Graphical aid



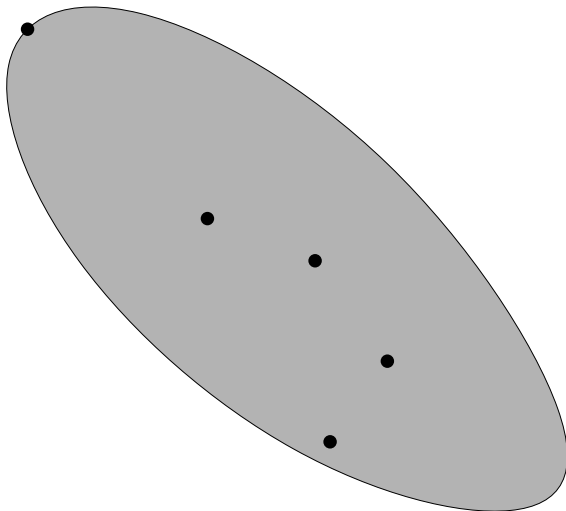
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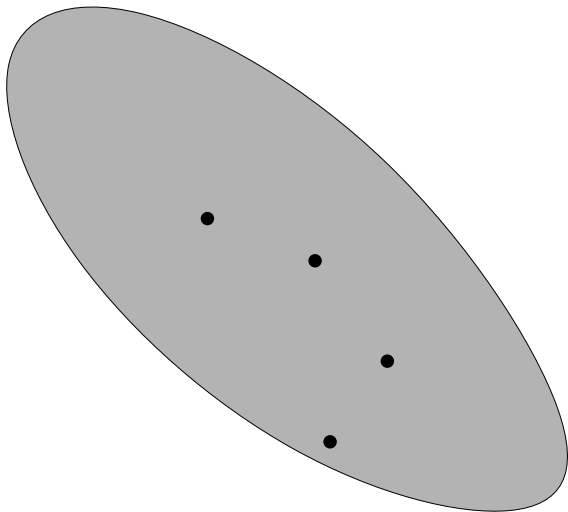
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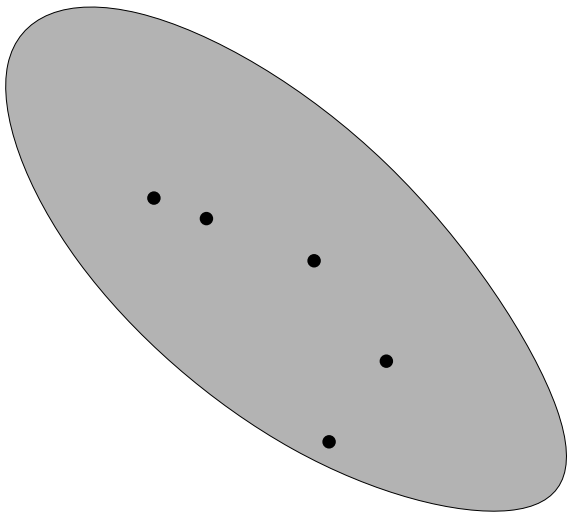
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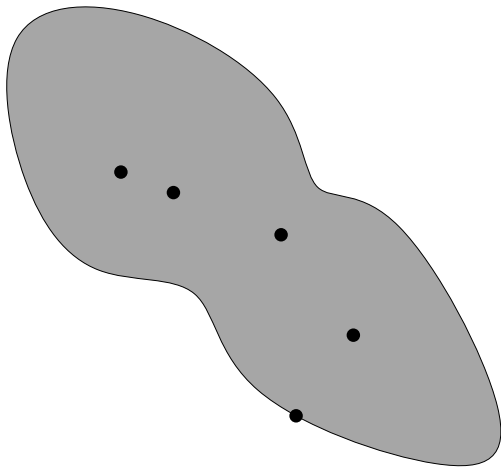
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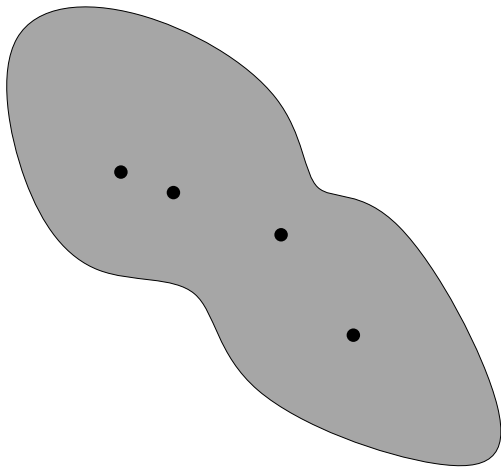
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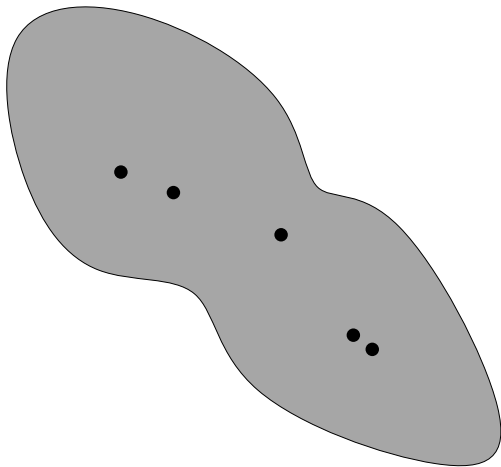
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Graphical aid



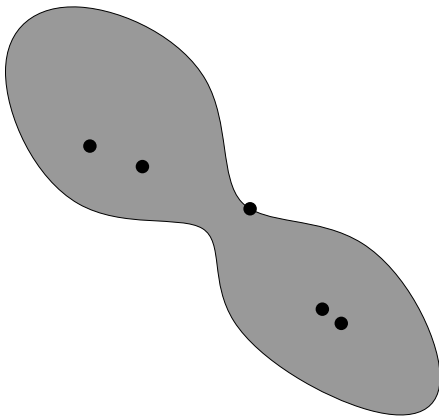
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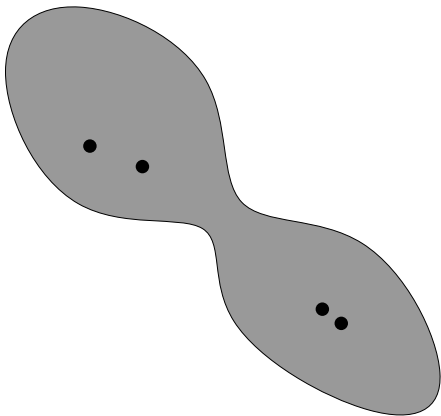
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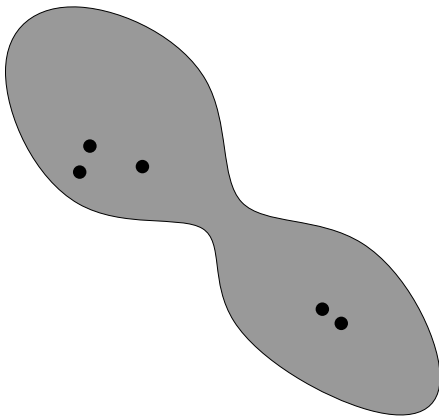
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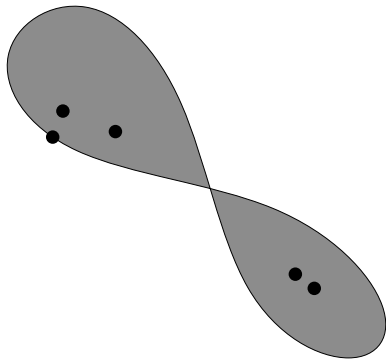
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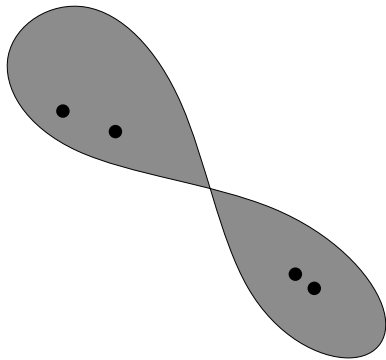
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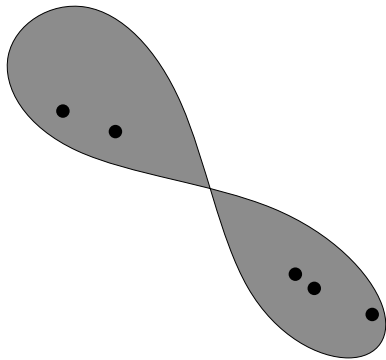
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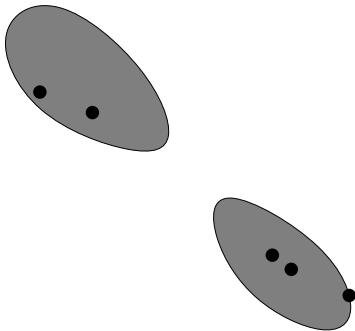
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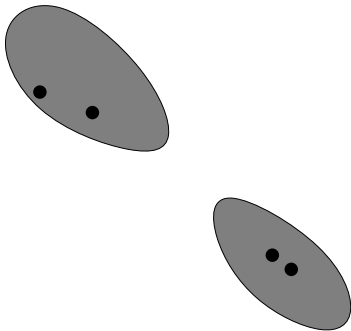
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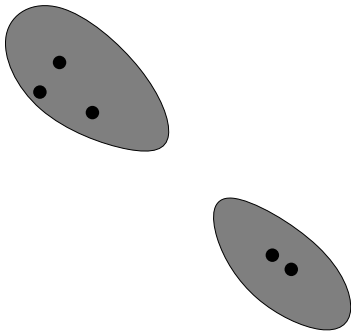
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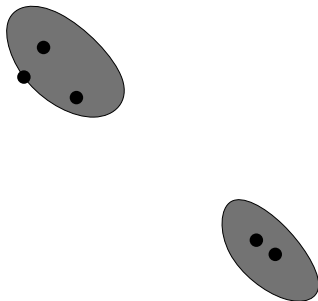
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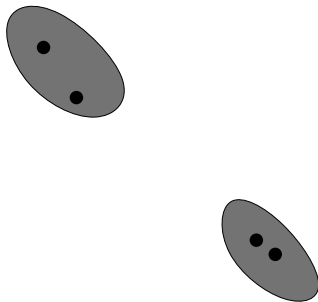
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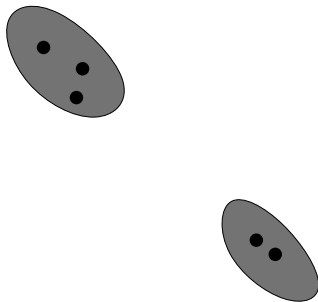
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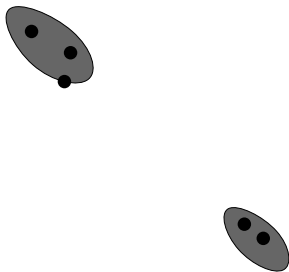
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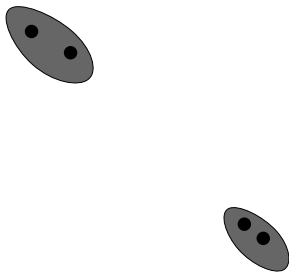
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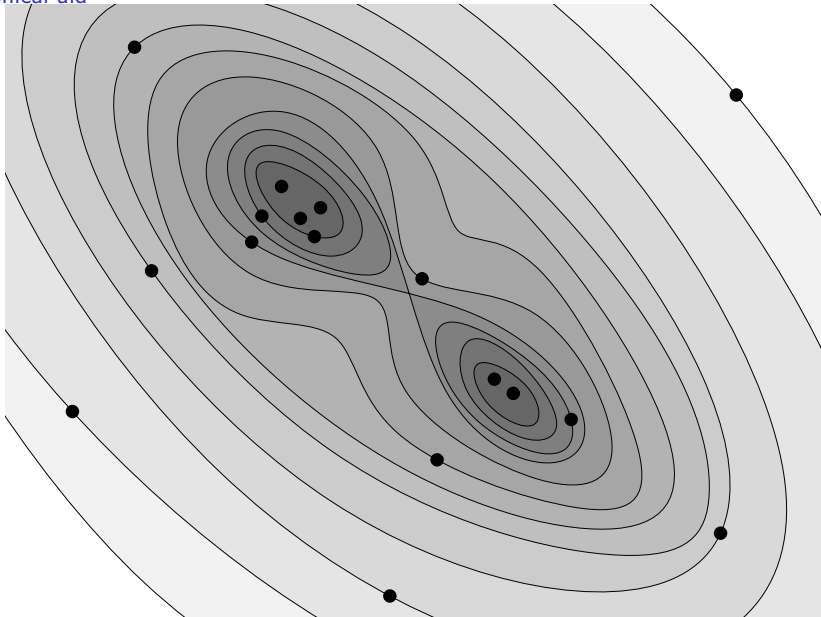
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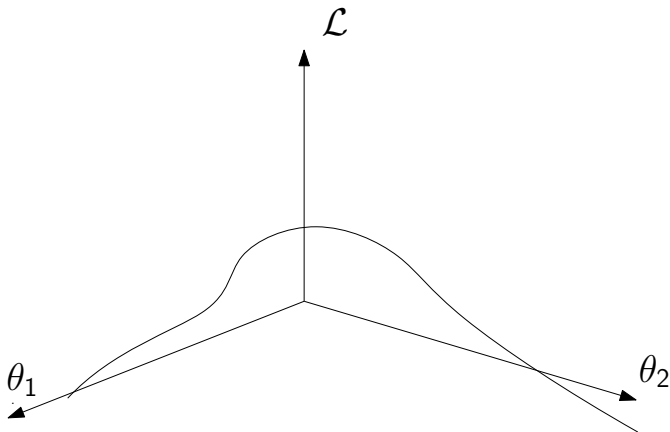
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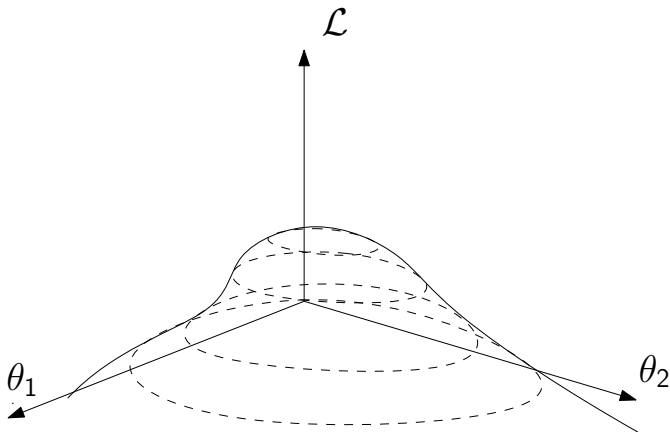
Nested Sampling

Calculating evidences



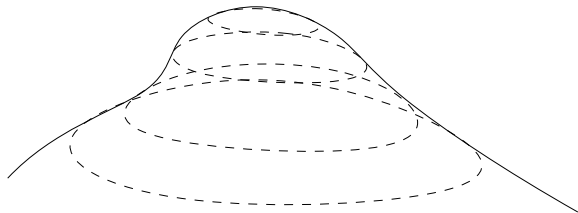
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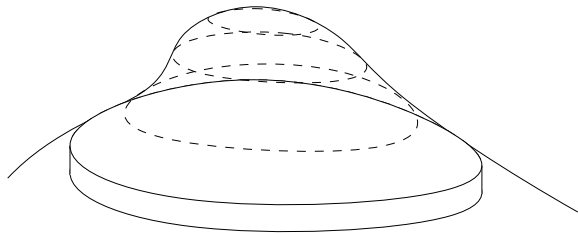
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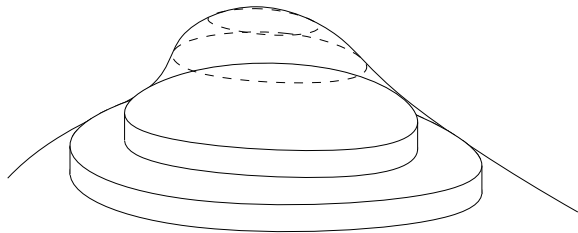
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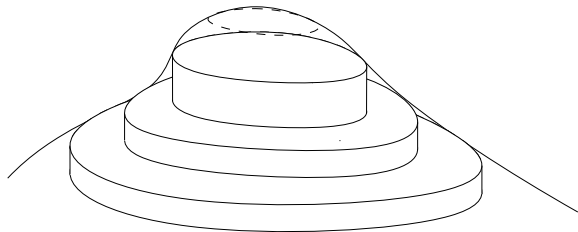
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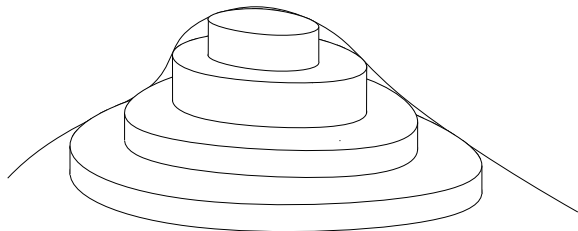
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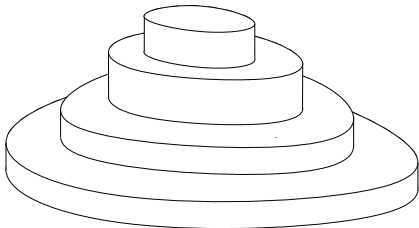
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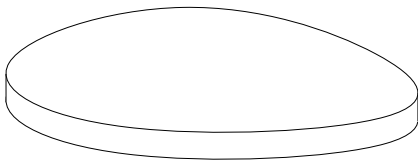
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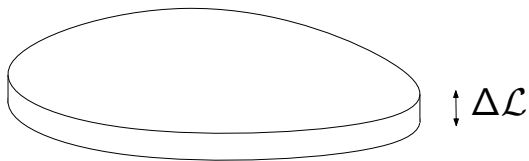
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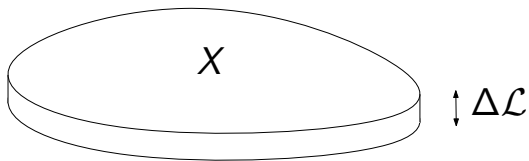
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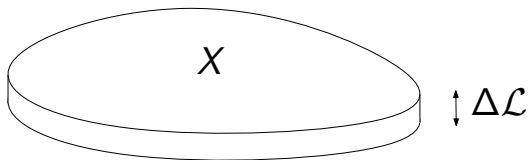
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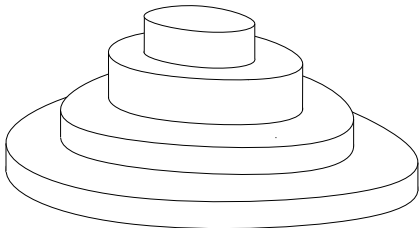
Calculating evidences



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

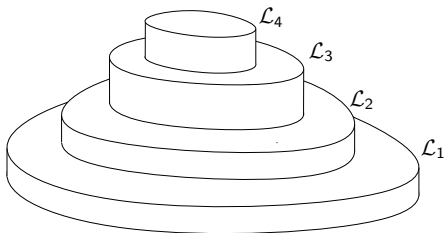
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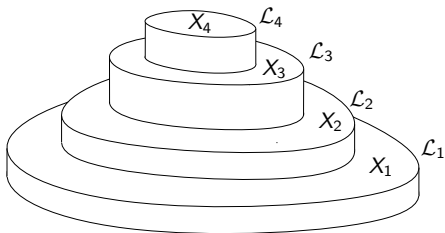
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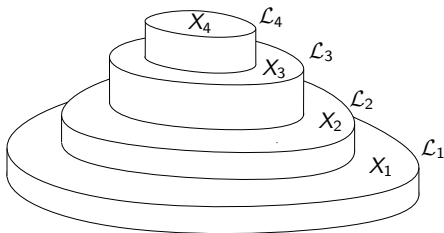
Calculating evidences



Nested Sampling

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



Nested Sampling

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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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- ▶ NS can also be used to sample the posterior

Nested sampling

Parameter estimation

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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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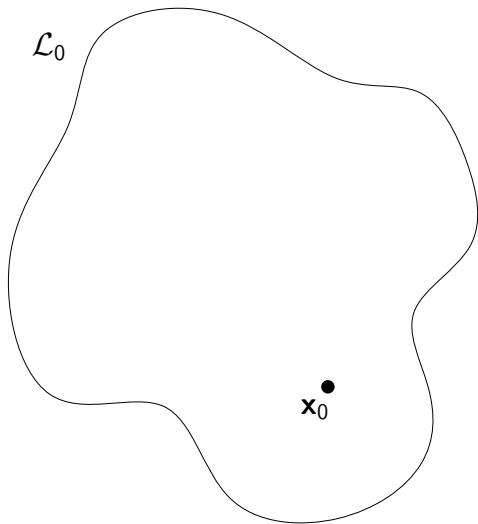
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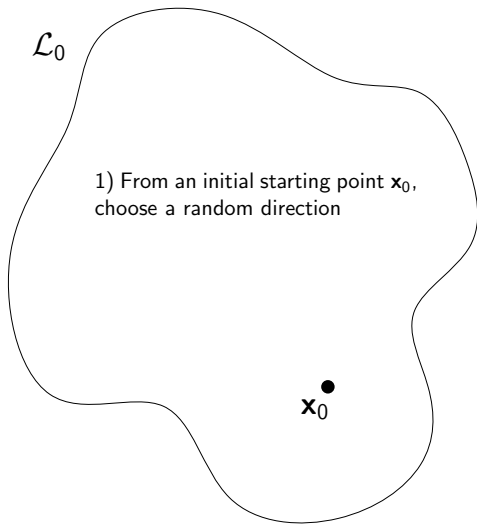
Diffusive Nested Sampling B. Brewer et al. (2009,2016).

- ▶ Very promising
- ▶ Still needs tuning.

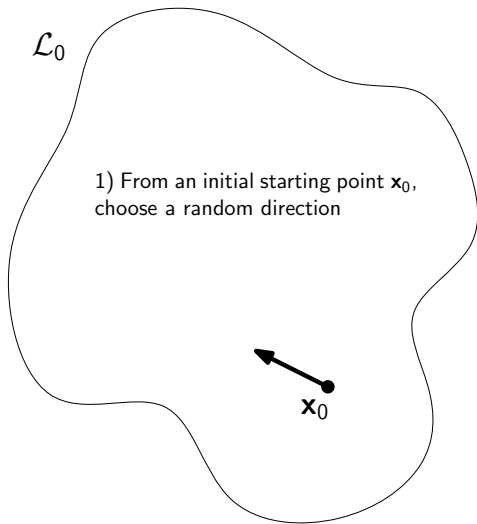
“Hit and run” slice sampling



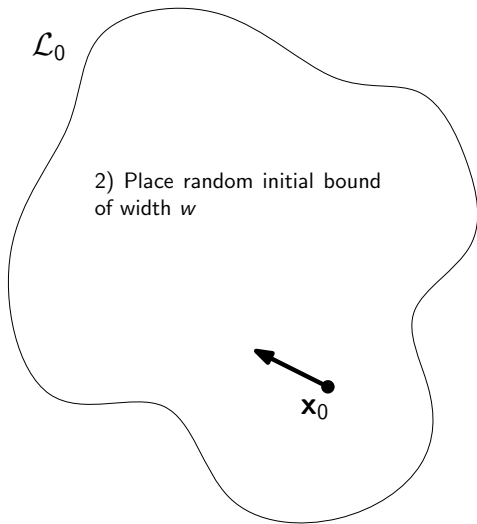
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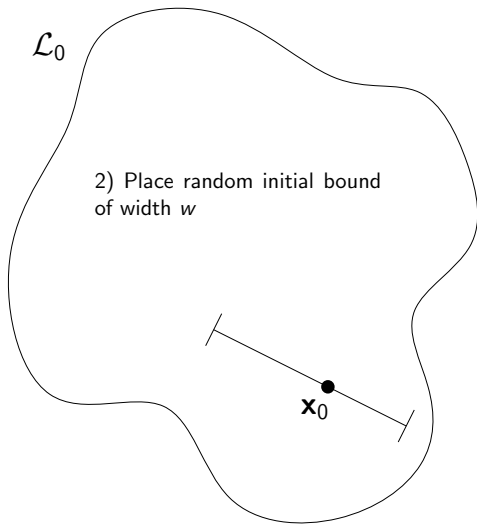
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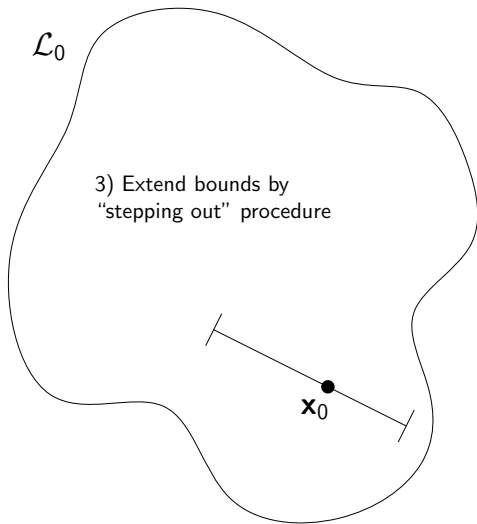
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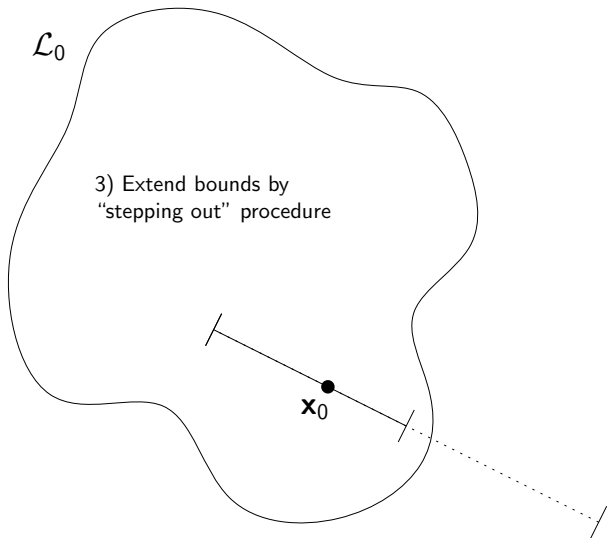
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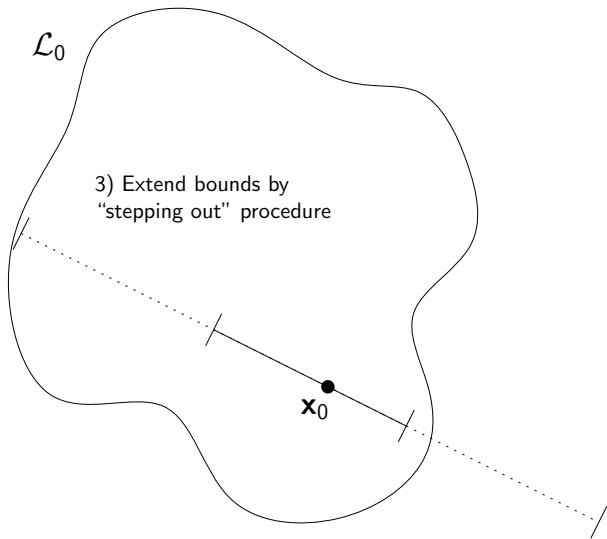
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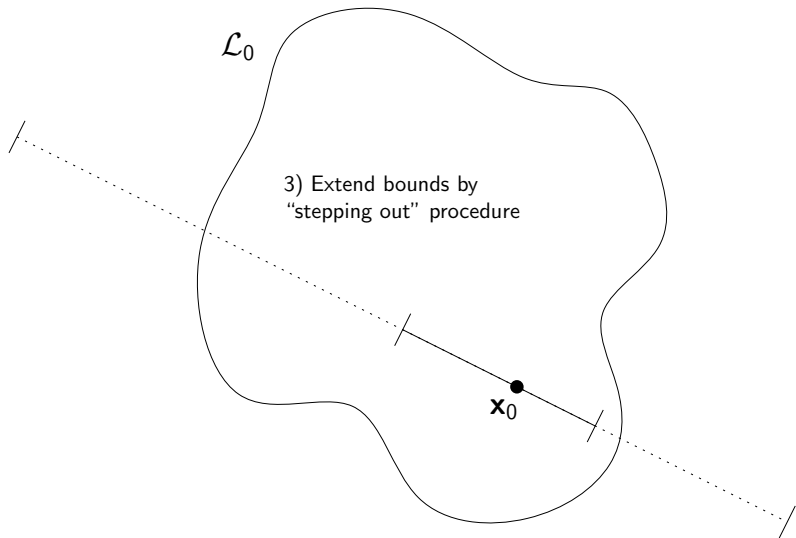
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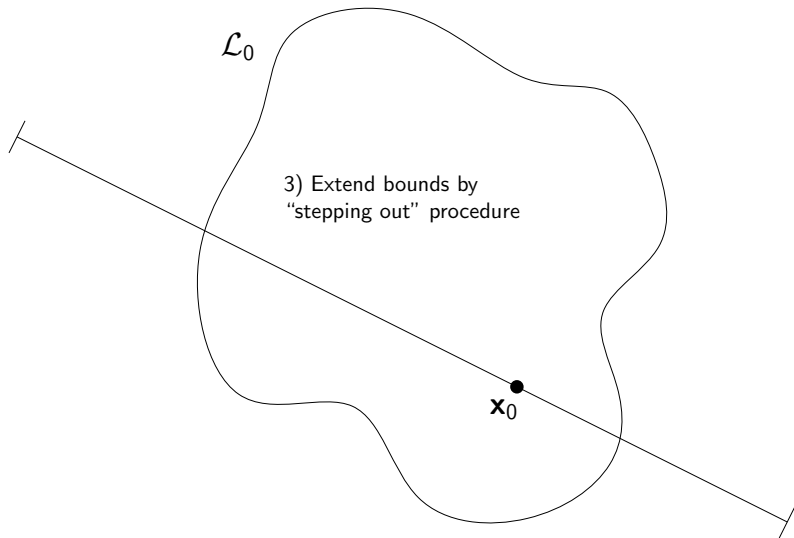
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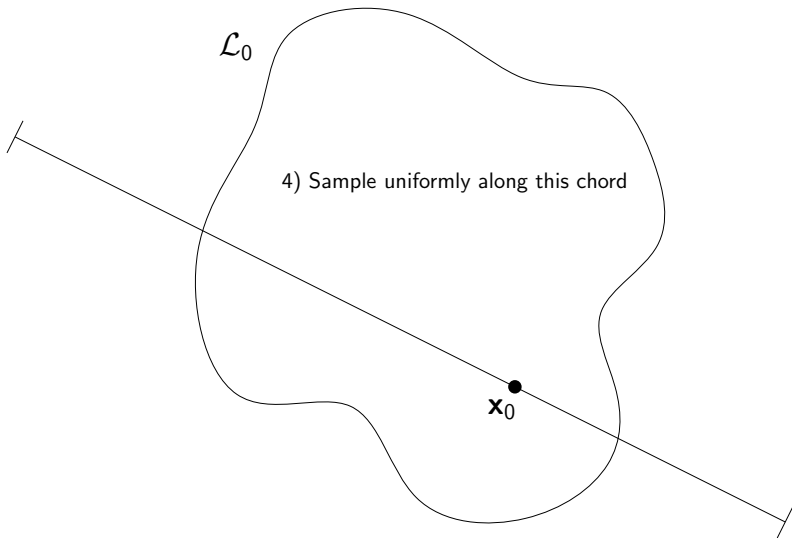
“Hit and run” slice sampling



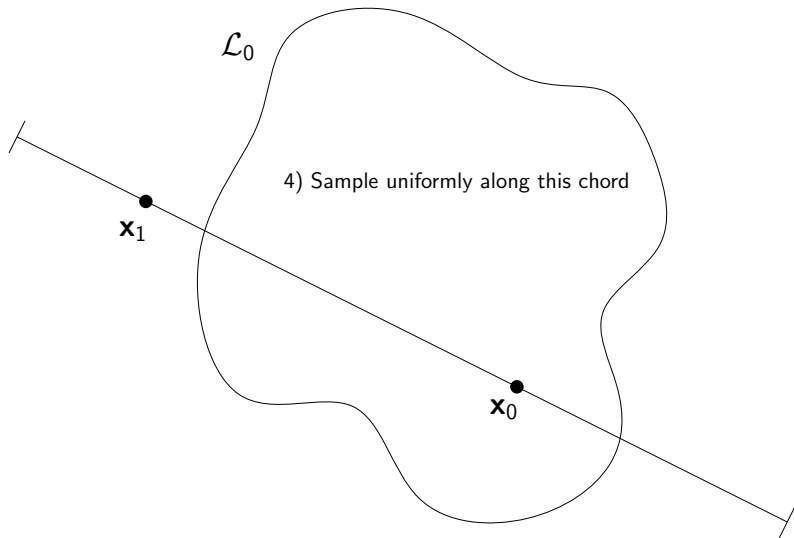
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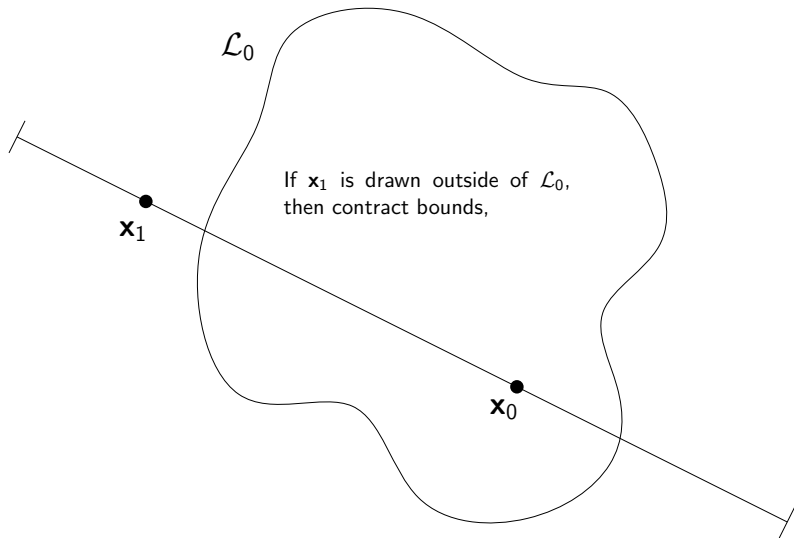
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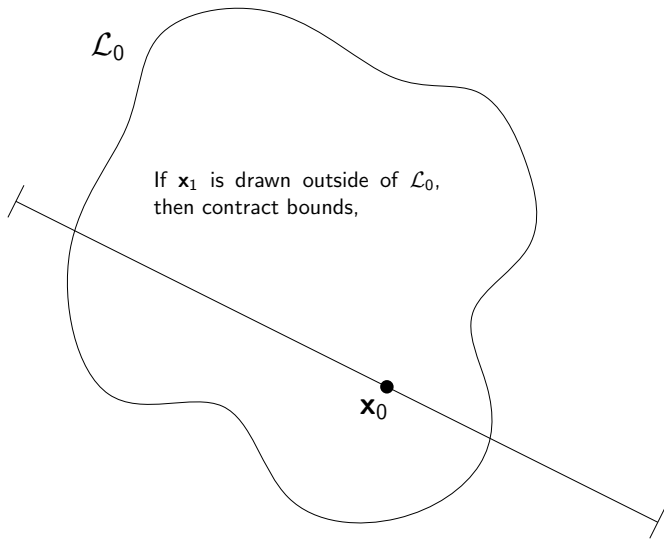
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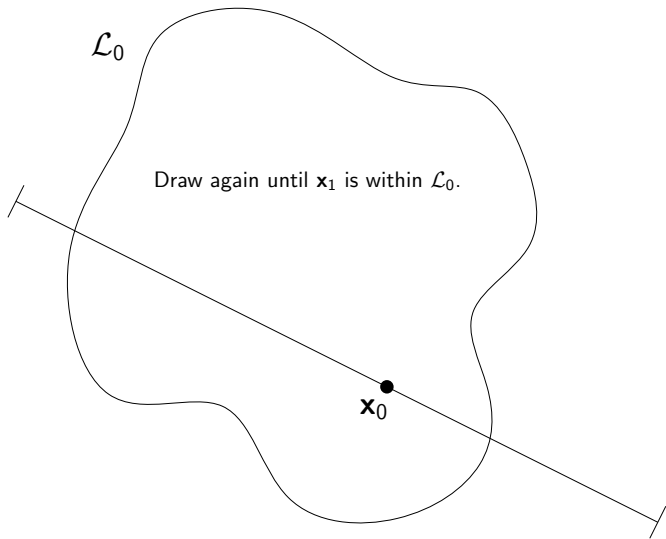
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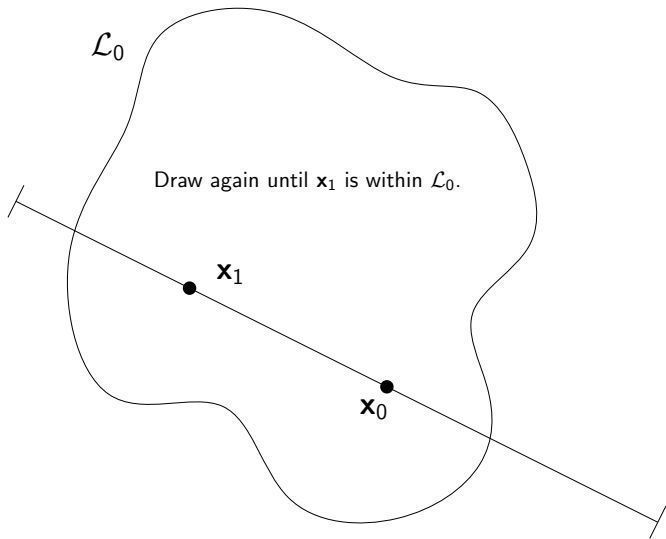
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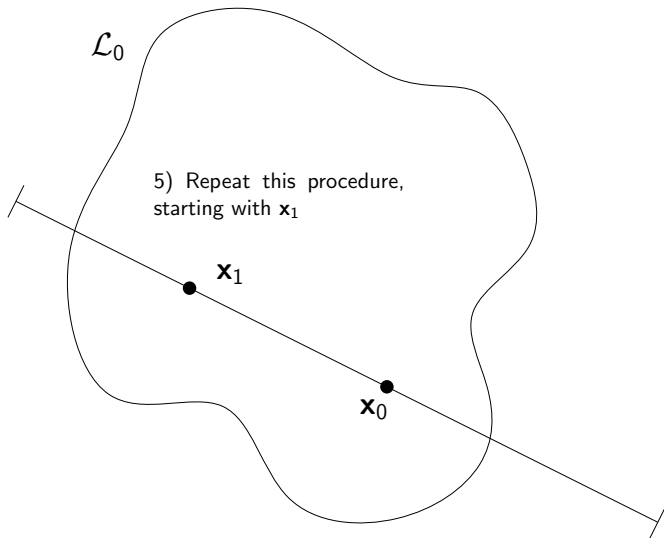
“Hit and run” slice sampling



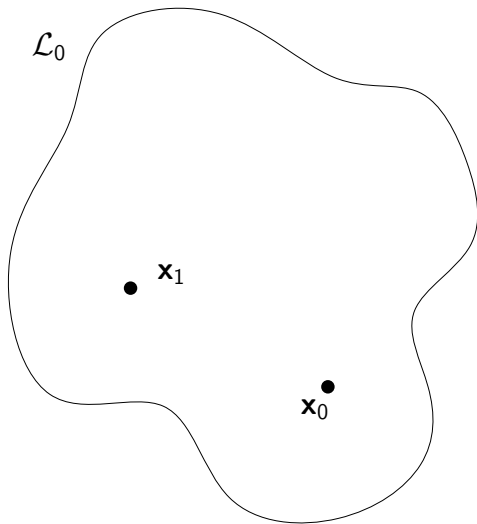
“Hit and run” slice sampling



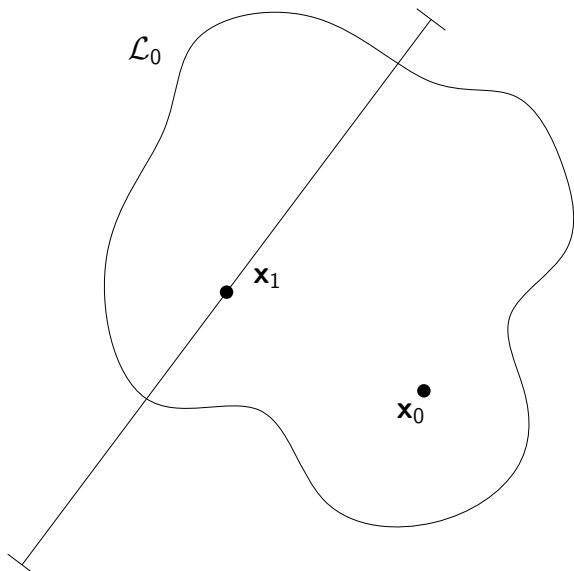
“Hit and run” slice sampling



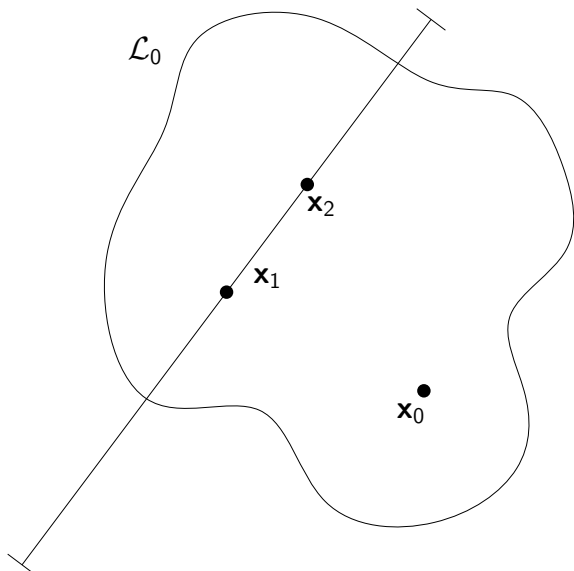
“Hit and run” slice sampling



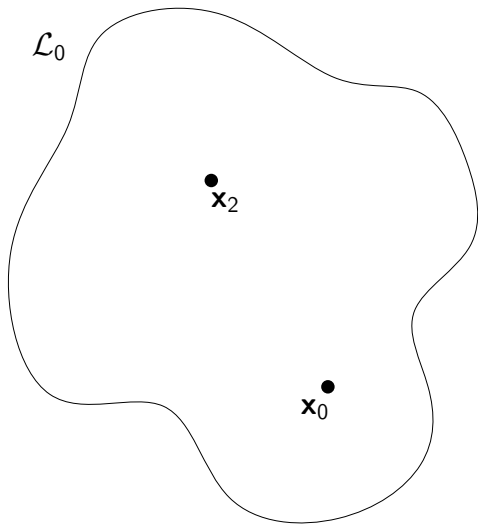
“Hit and run” slice sampling



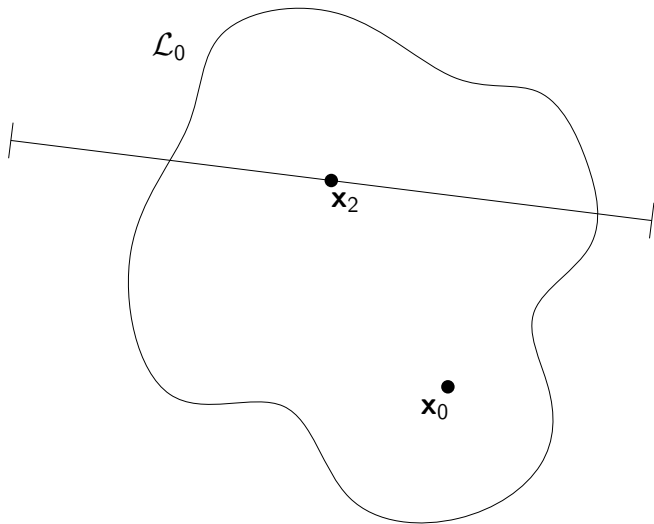
“Hit and run” slice sampling



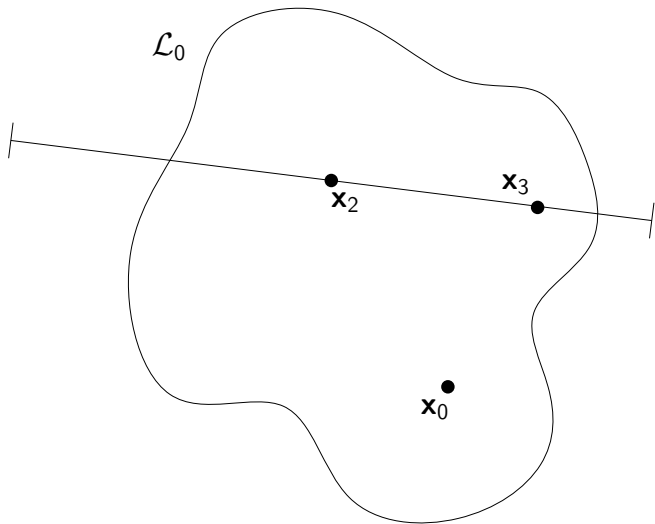
“Hit and run” slice sampling



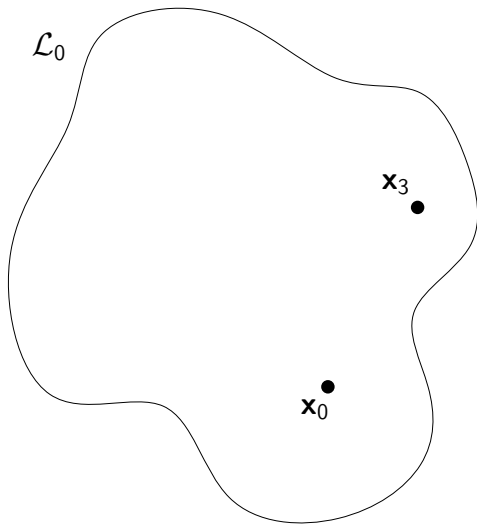
“Hit and run” slice sampling



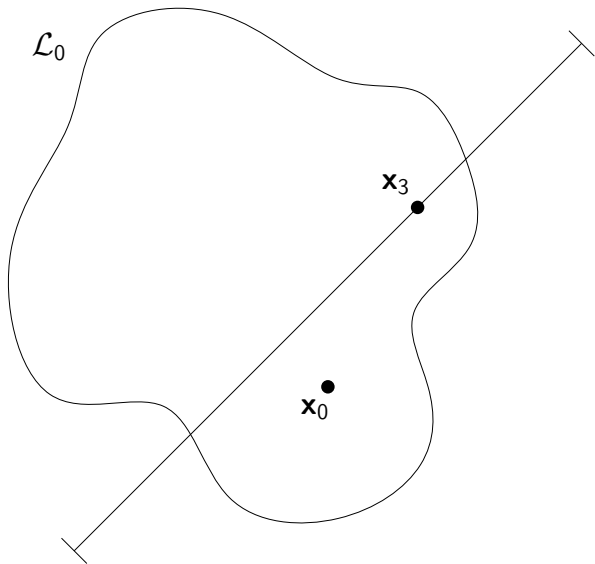
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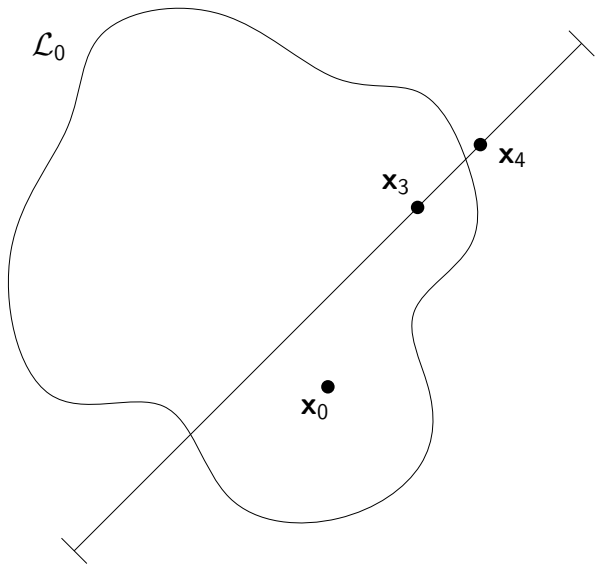
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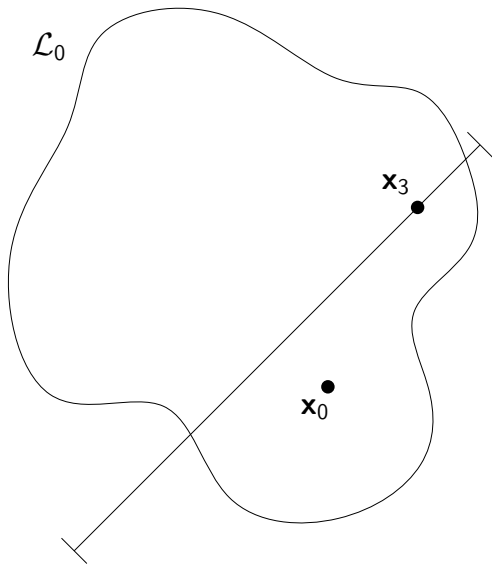
“Hit and run” slice sampling



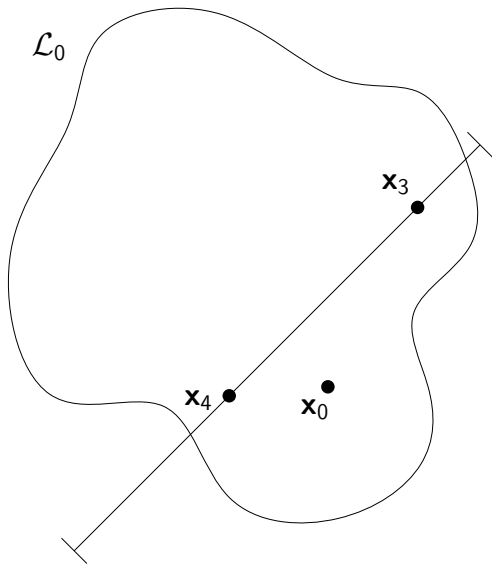
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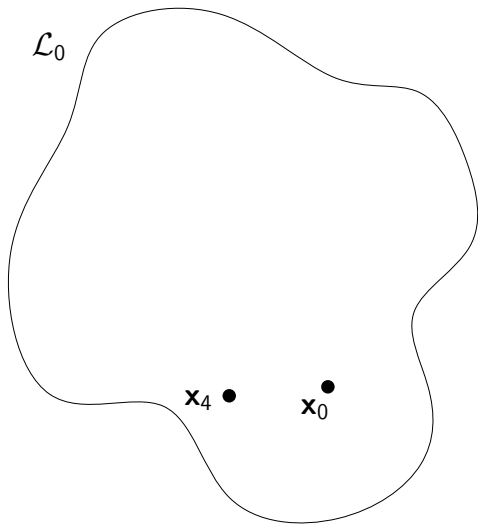
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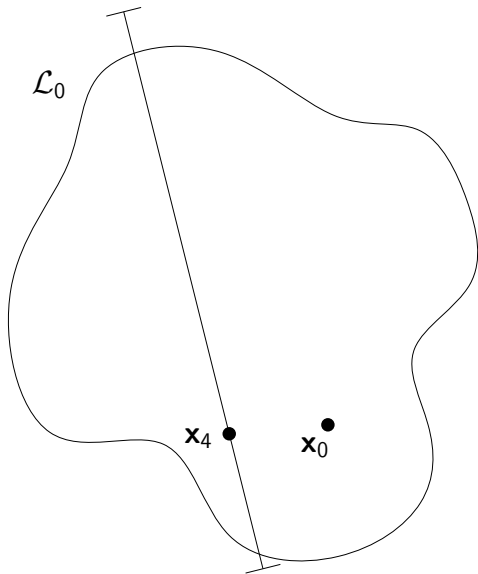
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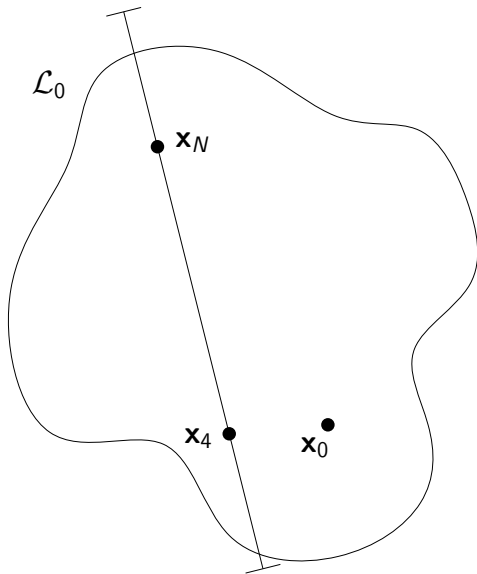
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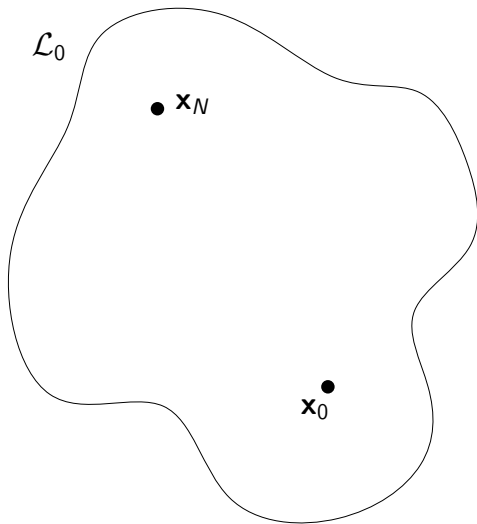
“Hit and run” slice sampling



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Issues with Slice Sampling

Correlated distributions

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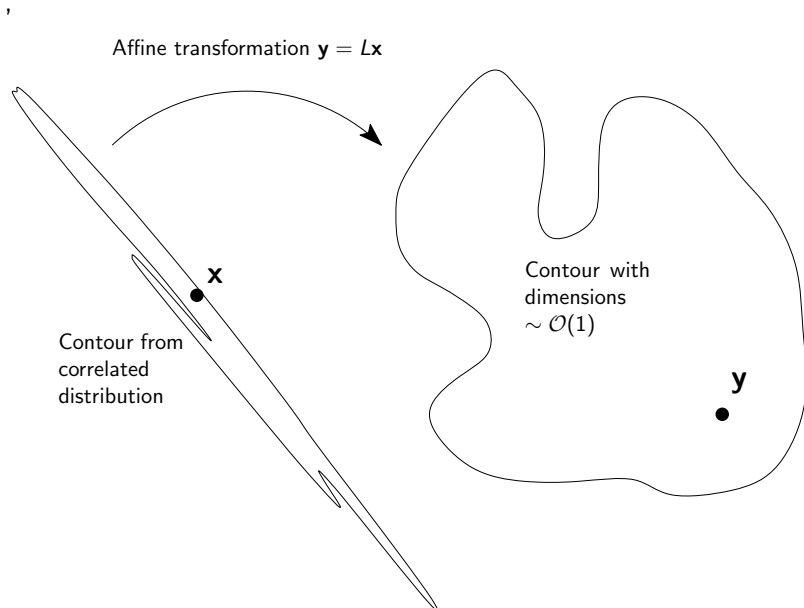
Issues with Slice Sampling

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- ▶ Need to “tune” w parameter.

PolyChord 1.0's solution

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- ▶ $w = 1$ in this transformed space

Issues with Slice Sampling

Multimodality

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Issues with Slice Sampling

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2. Affine transformation is useless.

PolyChord 1.0's solutions

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

PolyChord 1.0's solutions

Multimodality

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PolyChord 1.0's Additions

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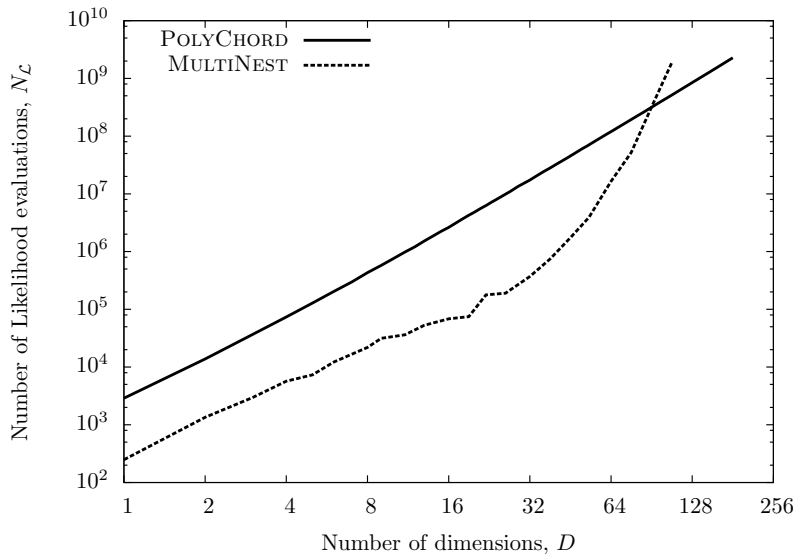
- ▶ Parallelised up to number of live points with openMPI.

PolyChord 1.0's Additions

- ▶ Parallelised up to number of live points with openMPI.
- ▶ Implemented in CosmoMC, as “CosmoChord”, with fast-slow parameters.

PolyChord vs. MultiNest

Gaussian likelihood



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PolyChord

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PolyChord

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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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PolyChord 2.0

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- ▶ Need to be able to quantify degree of correlation for correct inference.

Aside: Merging nested sampling runs

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Aside: Merging nested sampling runs

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

Aside: Unweaving nested sampling runs

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- ▶ The reverse is also true.

Aside: Unweaving nested sampling runs

- ▶ The reverse is also true.
- ▶ 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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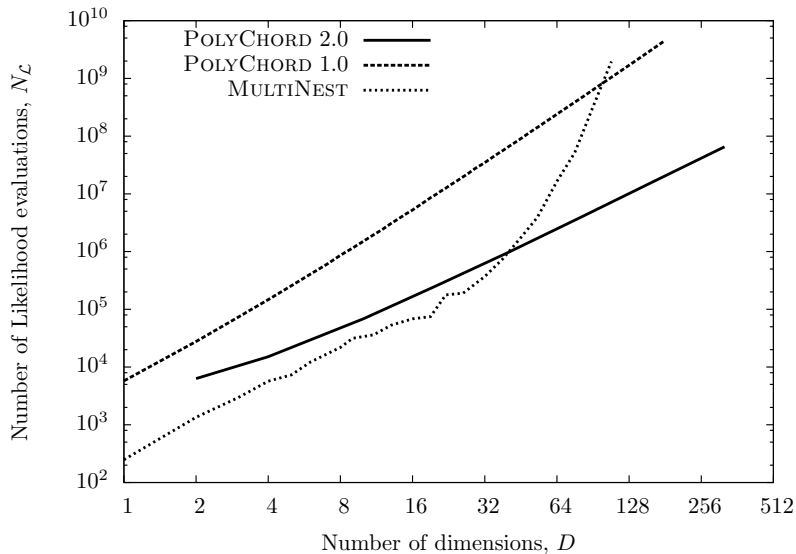
PolyChord 2.0

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- ▶ Unweave the run into n_{live} threads.
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- ▶ Can use traditional techniques on threads to quantify correlation
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 - ▶ Jackknifing
 - ▶ Bootstrapping
- ▶ With this in hand, can produce correct inferences from correlated runs.

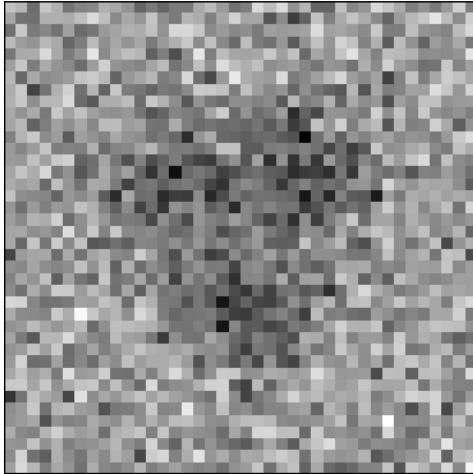
PolyChord 2.0 vs. MultiNest

Gaussian likelihood



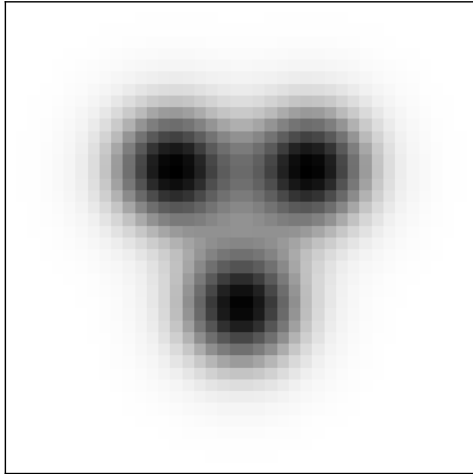
Object detection

Toy problem



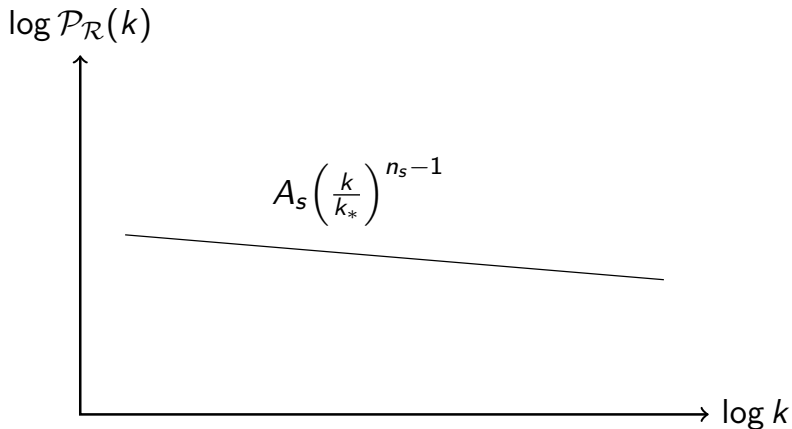
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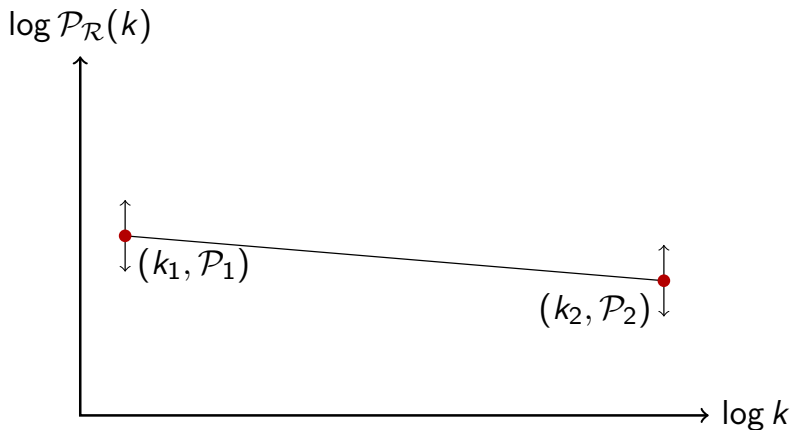
PolyChord in action

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



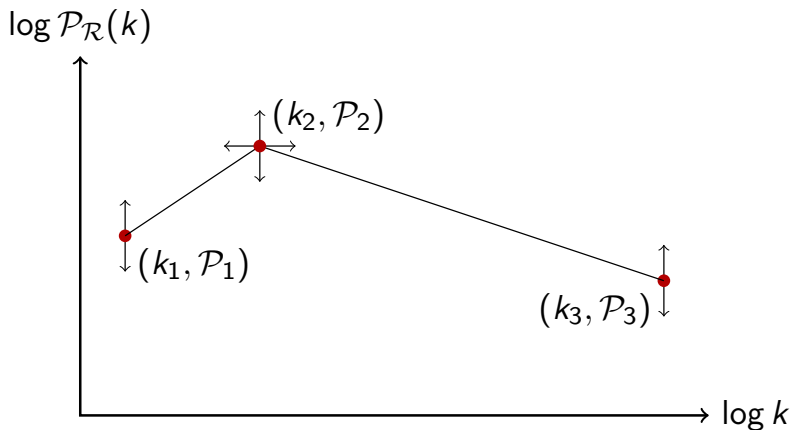
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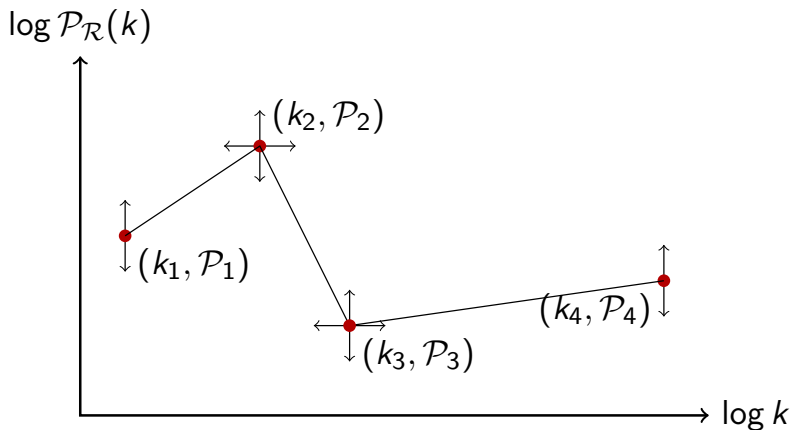
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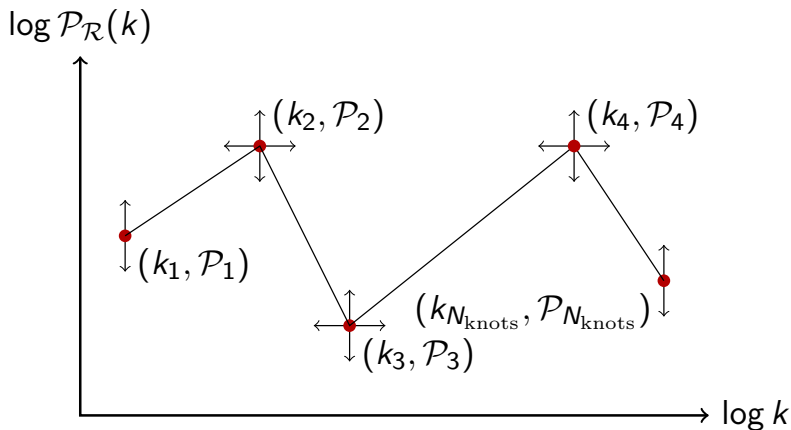
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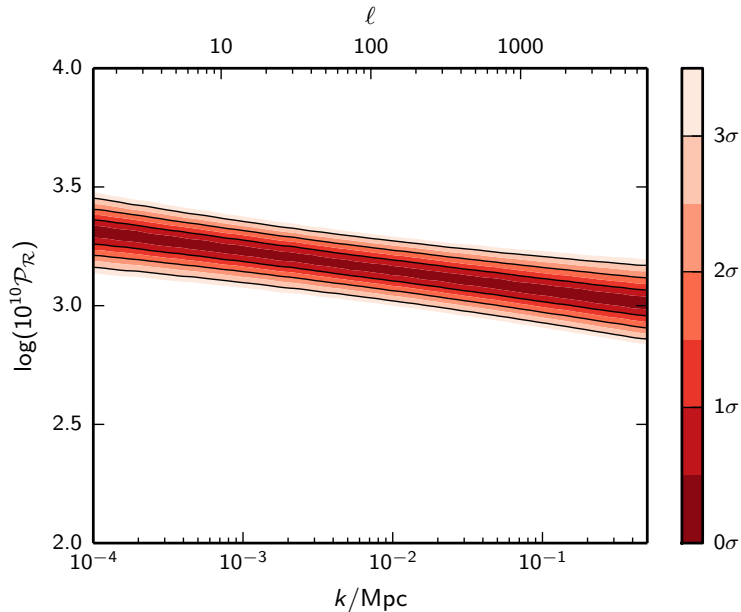
PolyChord in action

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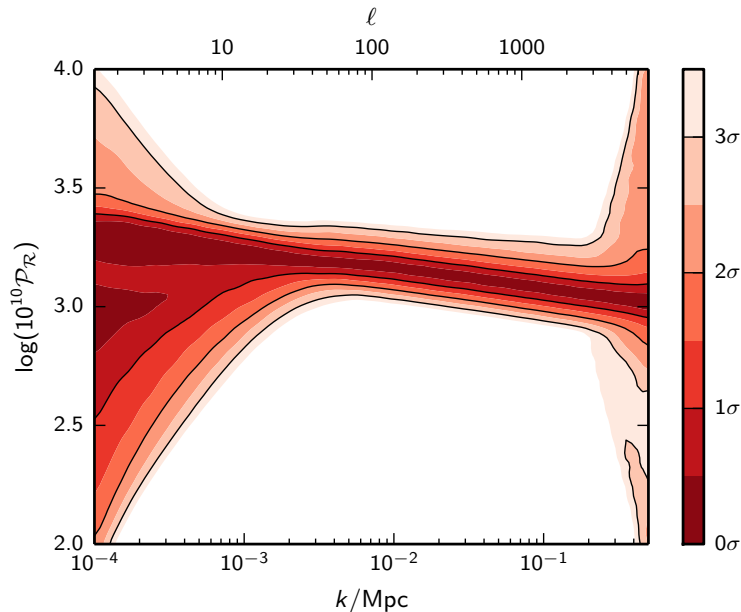
0 internal knots

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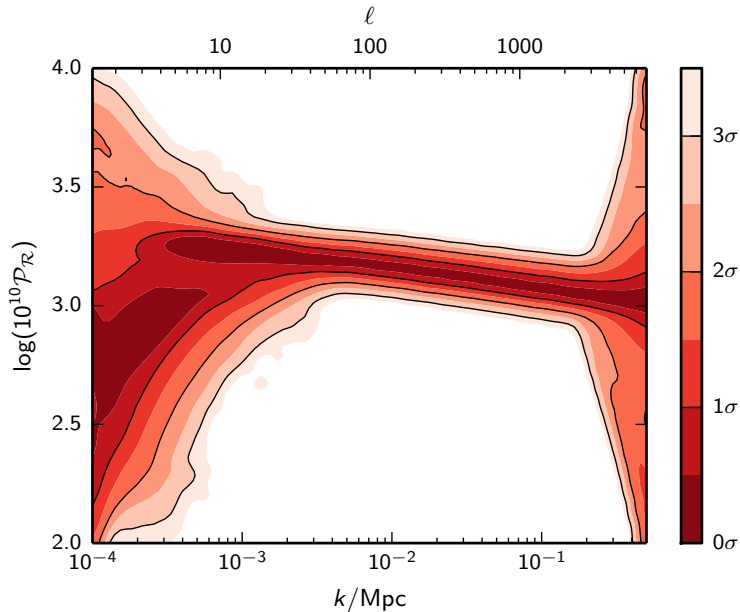
1 internal knots

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



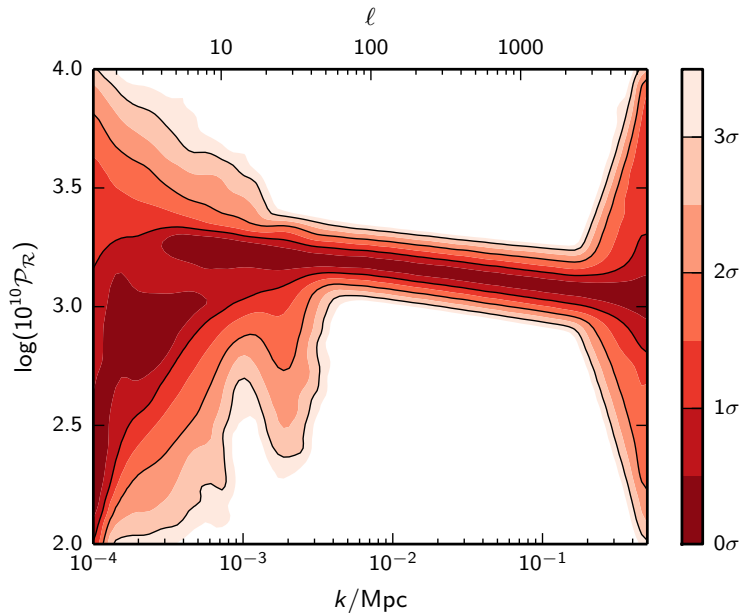
2 internal knots

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



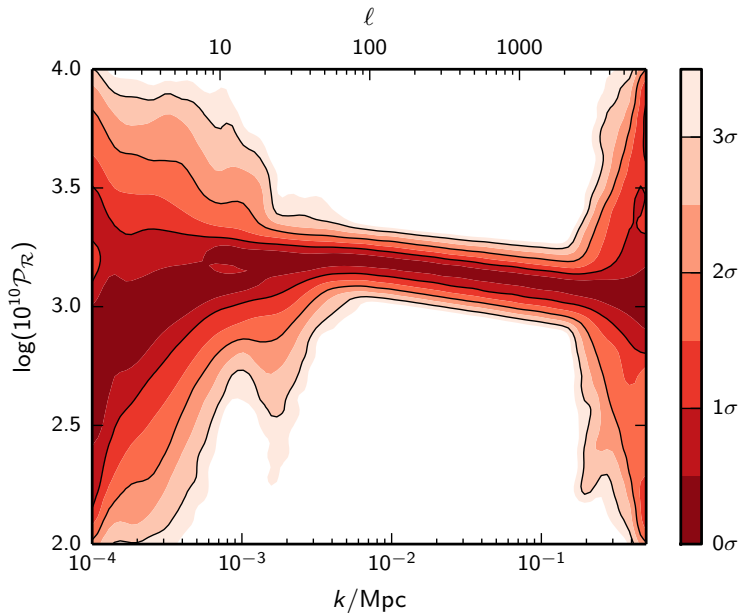
3 internal knots

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



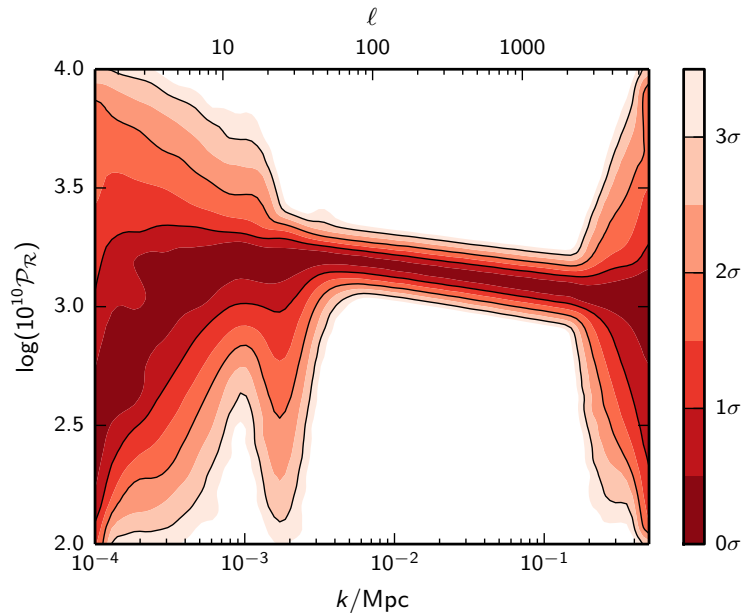
4 internal knots

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



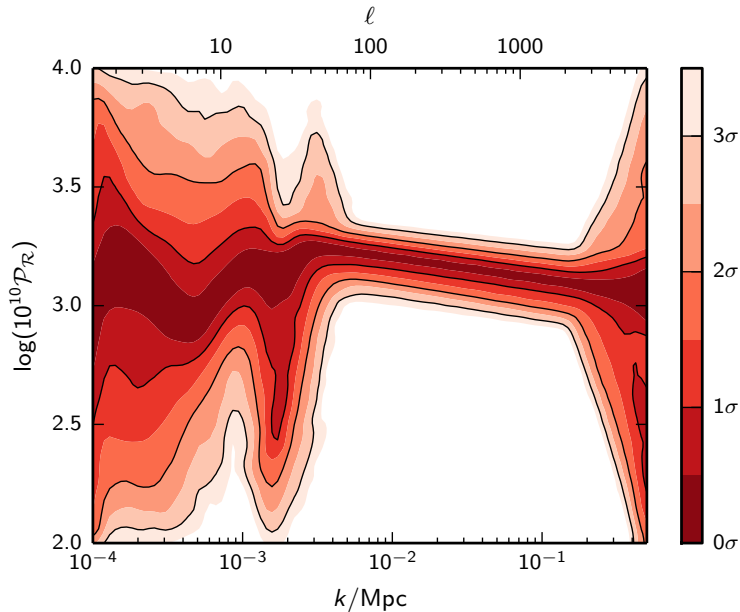
5 internal knots

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



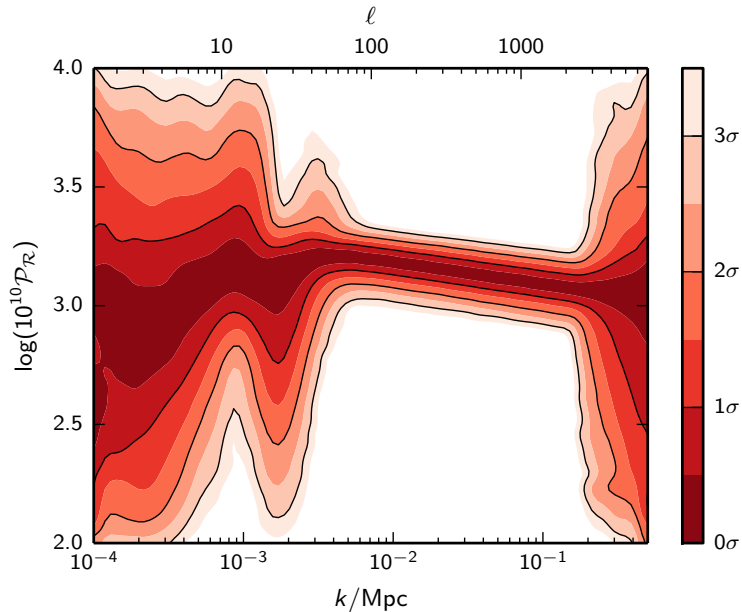
6 internal knots

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



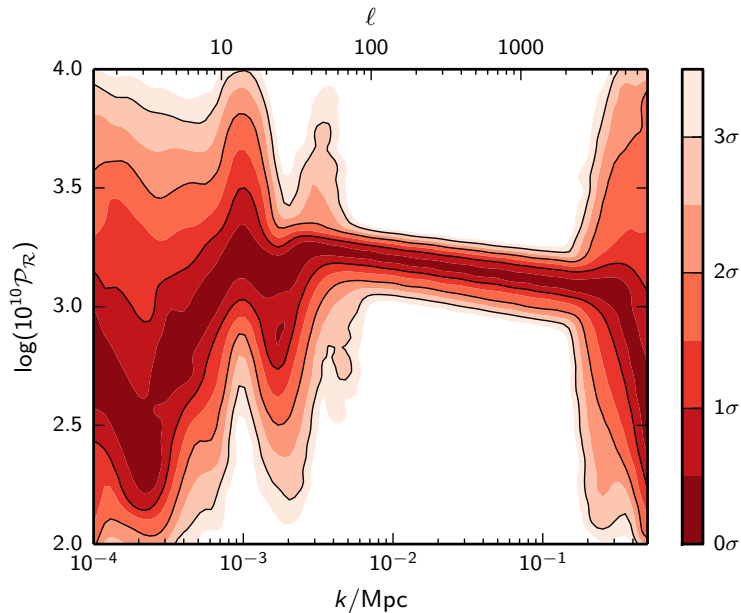
7 internal knots

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



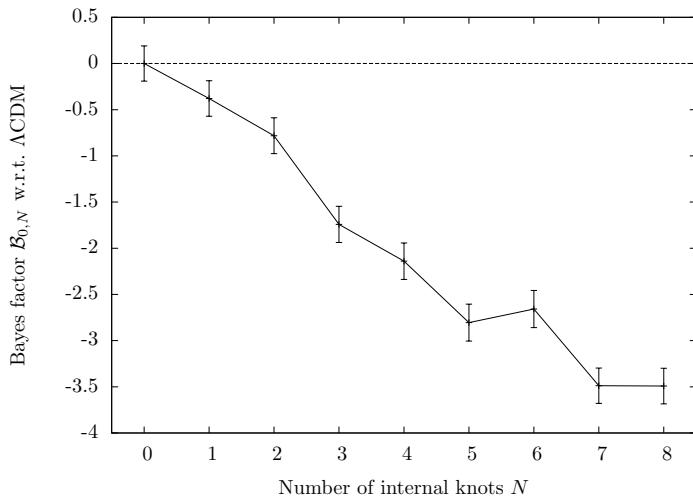
8 internal knots

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



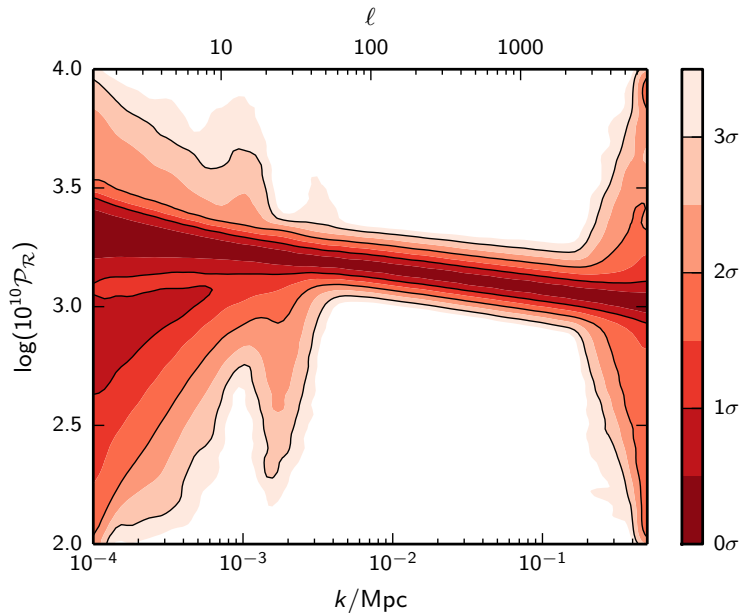
Bayes Factors

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



Marginalised plot

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



Dark energy equation of state reconstruction

Dark energy equation of state reconstruction

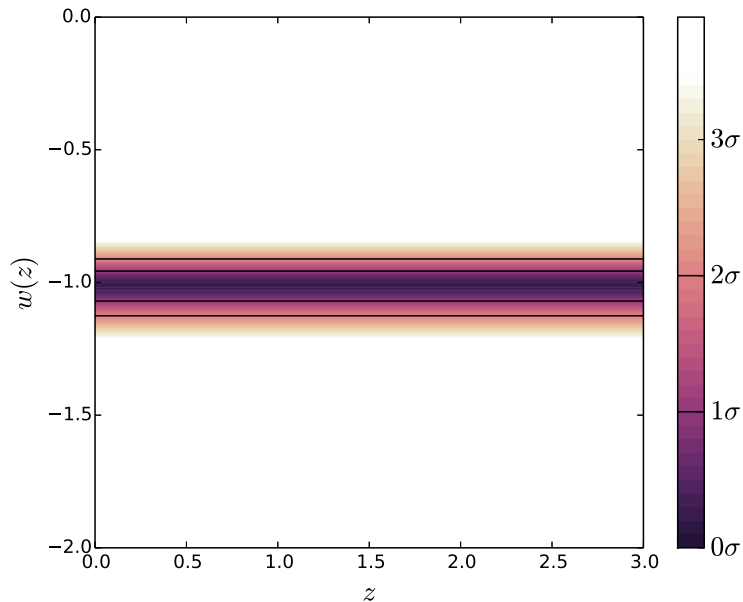
- ▶ Same thing, but for Dark energy equation of state $w(z)$ (quintessence).

Dark energy equation of state reconstruction

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- ▶ Data used is Planck 2015, BOSS DR 11, JLA supernovae and BOSS Ly α data

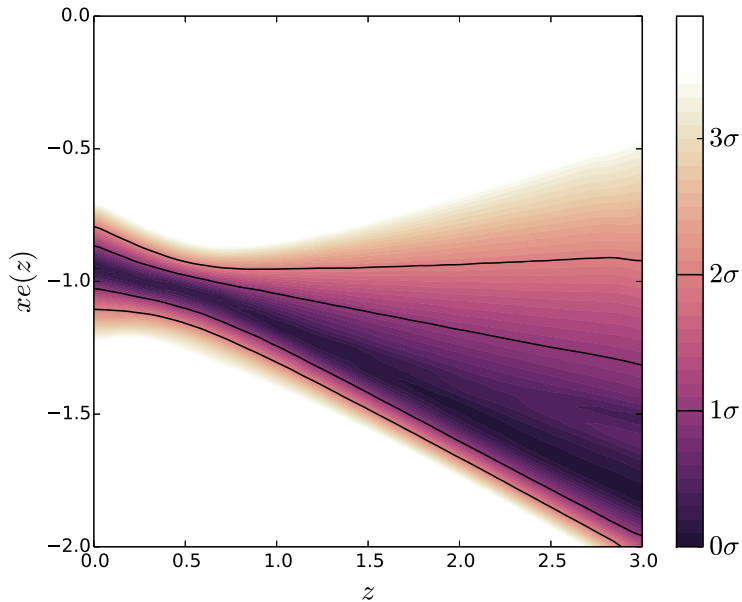
Flat, variable w

Dark energy equation of state reconstruction



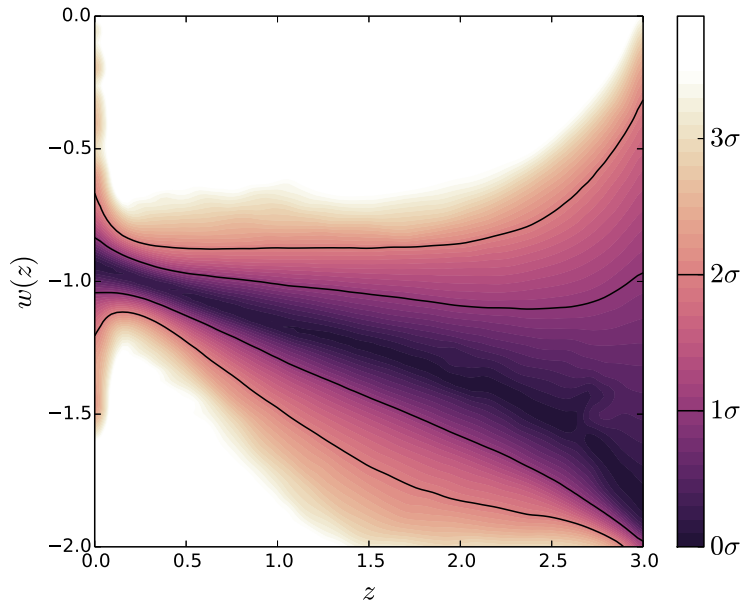
Tilted

Dark energy equation of state reconstruction



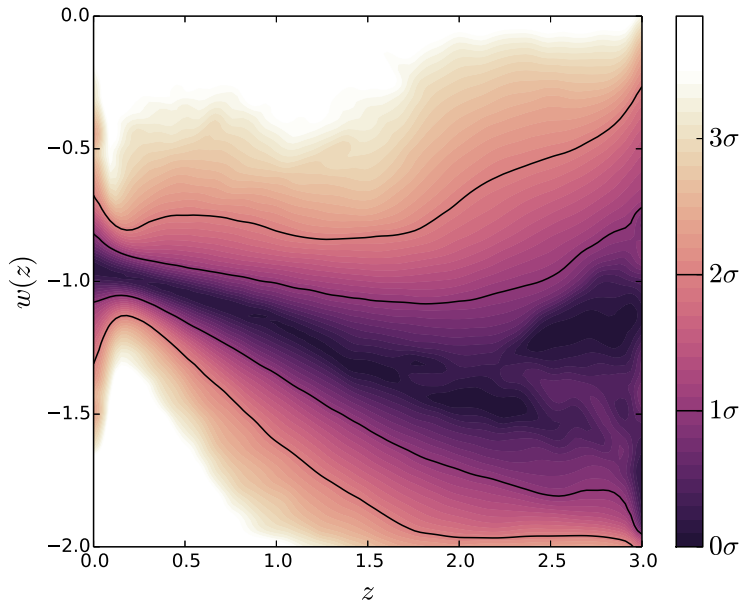
1 internal node

Dark energy equation of state reconstruction



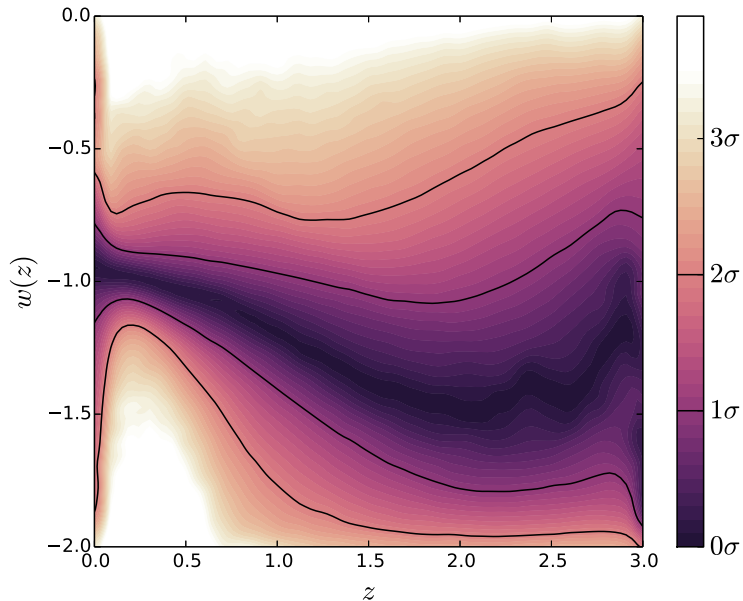
2 internal nodes

Dark energy equation of state reconstruction



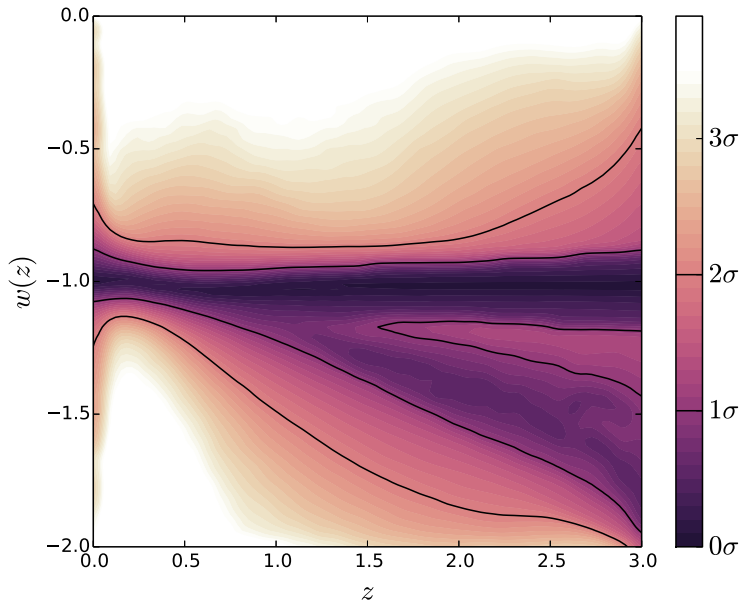
3 internal nodes

Dark energy equation of state reconstruction



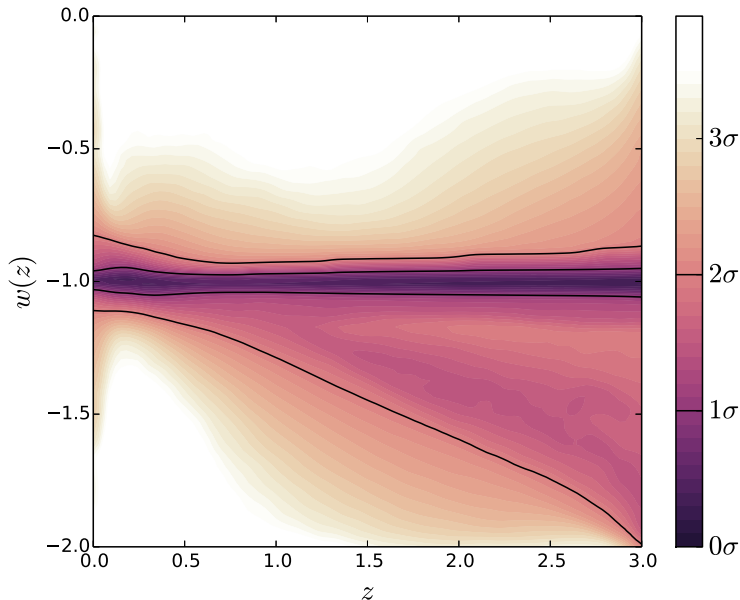
Marginalised plot - just extension models

Dark energy equation of state reconstruction



Marginalised plot - including LCDM

Dark energy equation of state reconstruction



PolyChord 2.0

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

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- ▶ Affine invariant sampling.

Future work

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1. Parallelisation

Future work

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2. Affine invariant mode detection.

Affine invariance

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- ▶ Treat distribution $P(x)$ and $P(Rx)$ the same.

Affine invariance

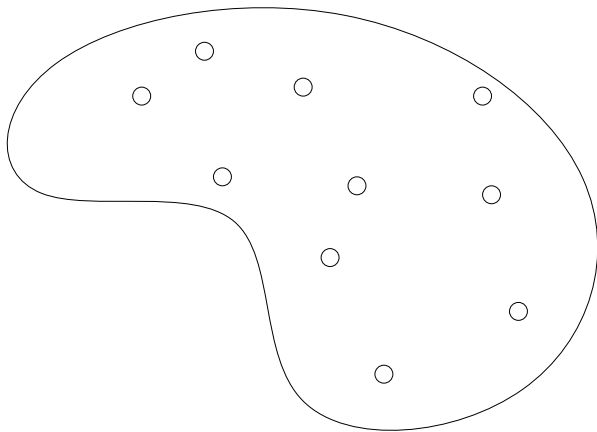
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- ▶ Treat distribution $P(x)$ and $P(Rx)$ the same.
- ▶ No need to worry about correlations.
- ▶ Good example: Now highly successful emcee (MCMC hammer).
 - ▶ Important: emcee is not unique (or necessarily best)

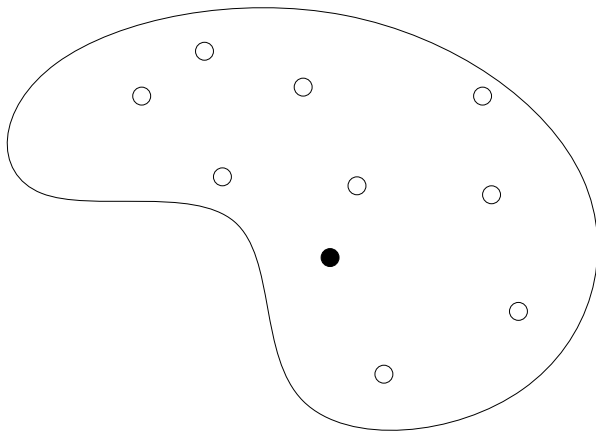
Skilling's affine invariant ideas

Leapfrog



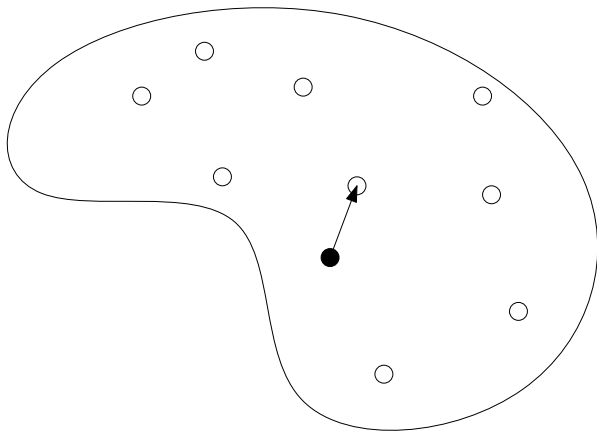
Skilling's affine invariant ideas

Leapfrog



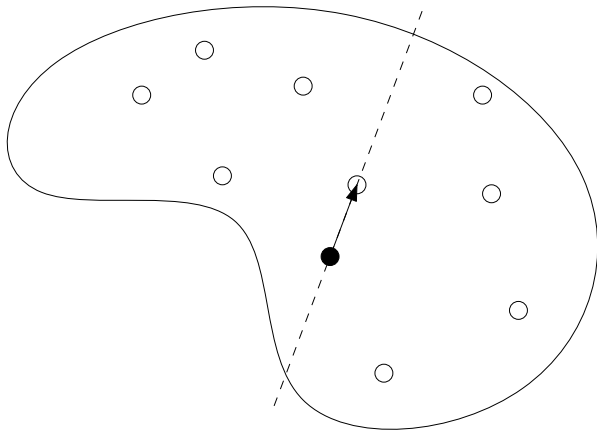
Skilling's affine invariant ideas

Leapfrog



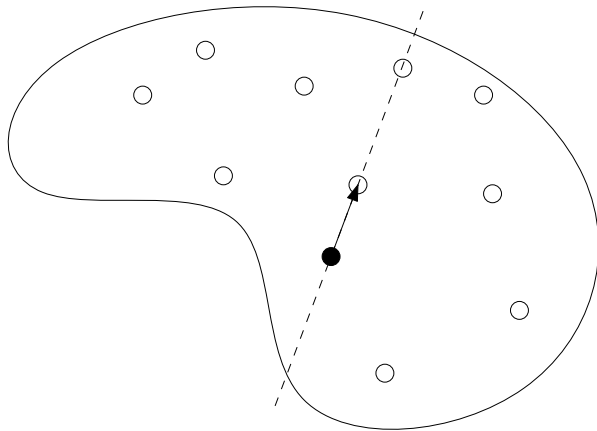
Skilling's affine invariant ideas

Leapfrog



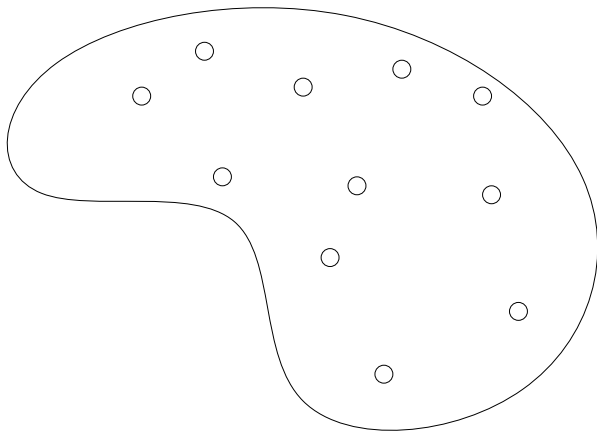
Skilling's affine invariant ideas

Leapfrog



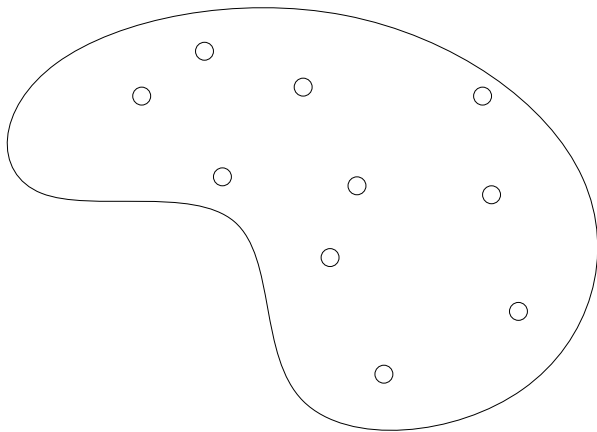
Skilling's affine invariant ideas

Leapfrog



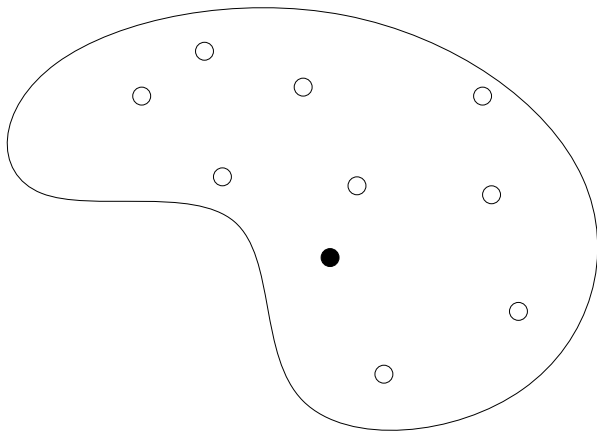
Skilling's affine invariant ideas

Parallel walk



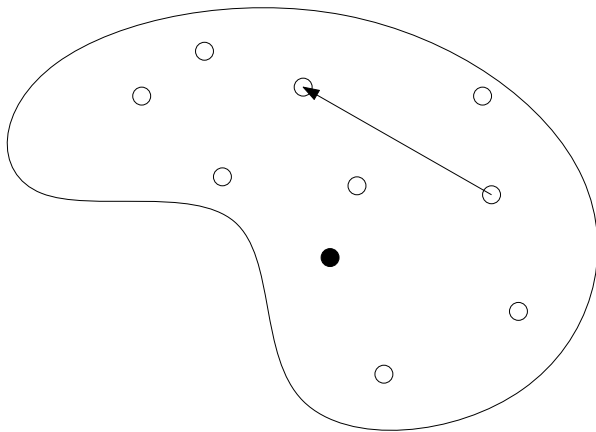
Skilling's affine invariant ideas

Parallel walk



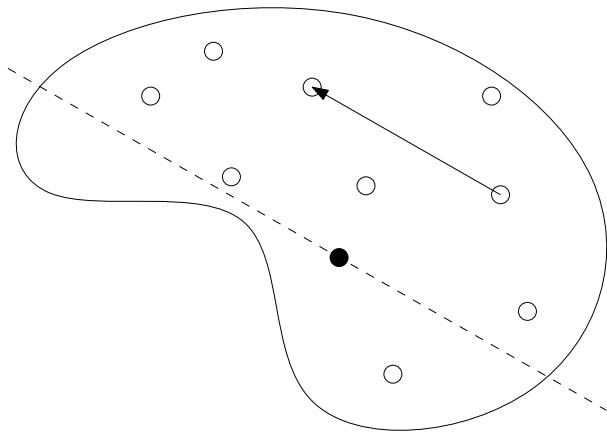
Skilling's affine invariant ideas

Parallel walk



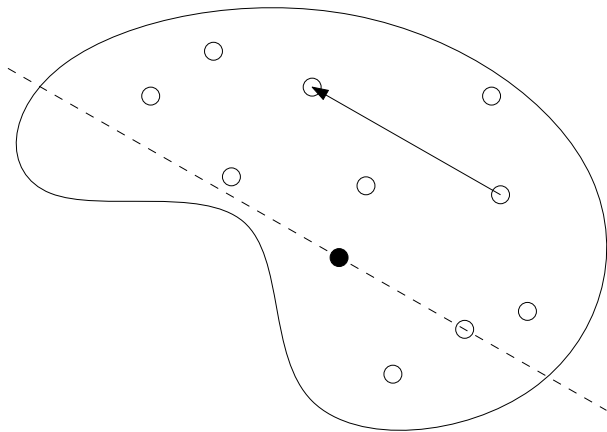
Skilling's affine invariant ideas

Parallel walk



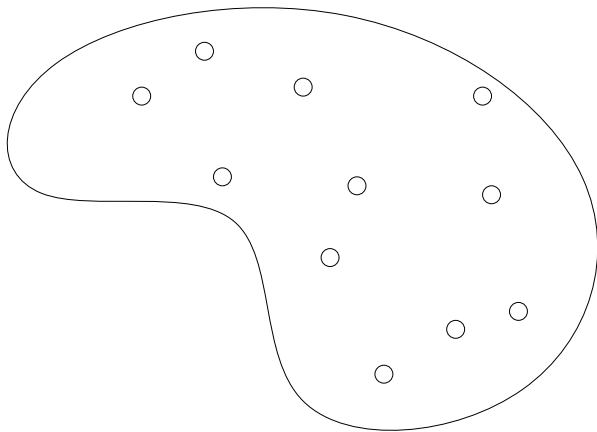
Skellings affine invariant ideas

Parallel walk



Skilling's affine invariant ideas

Parallel walk



Affine invariance

Subspace collapse

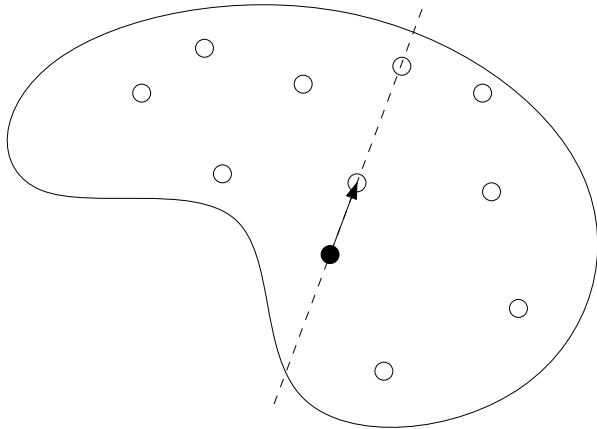
Affine invariance

Subspace collapse

- ▶ The main problem that besets these techniques is “subspace collapse”.

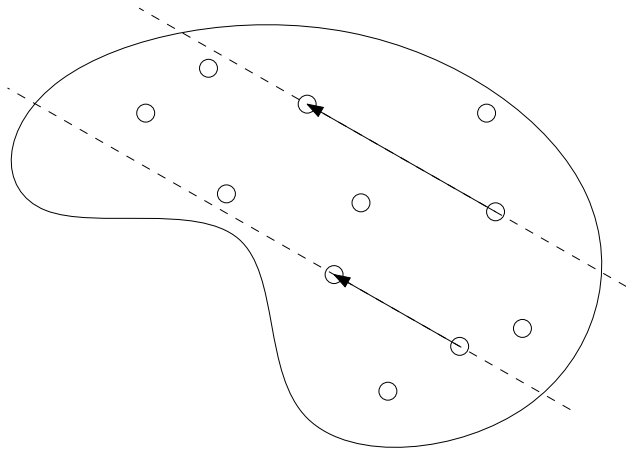
Subspace collapse

Leapfrog



Subspace collapse

Parallel walk



Subspace collapse

Solution

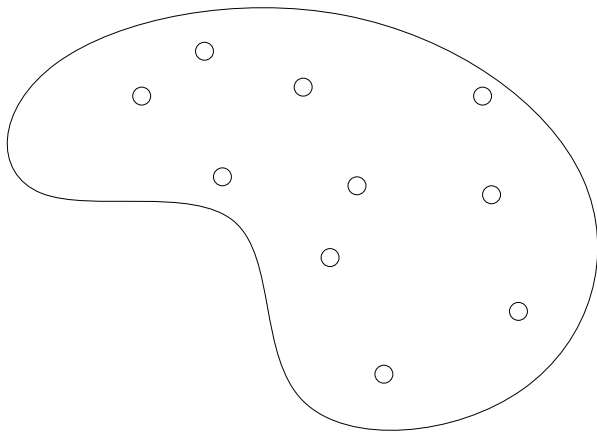
Subspace collapse

Solution

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

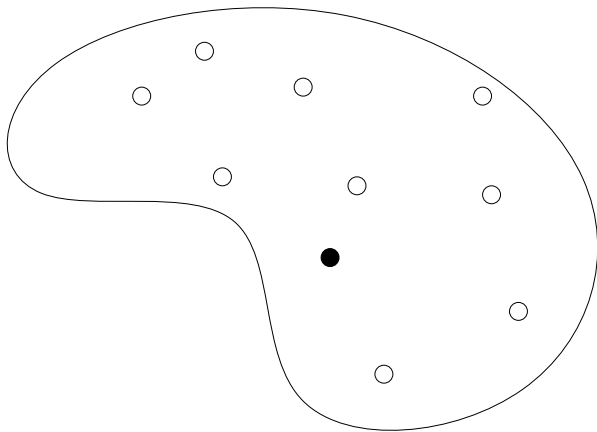
Skillings affine invariant ideas

Guided walk



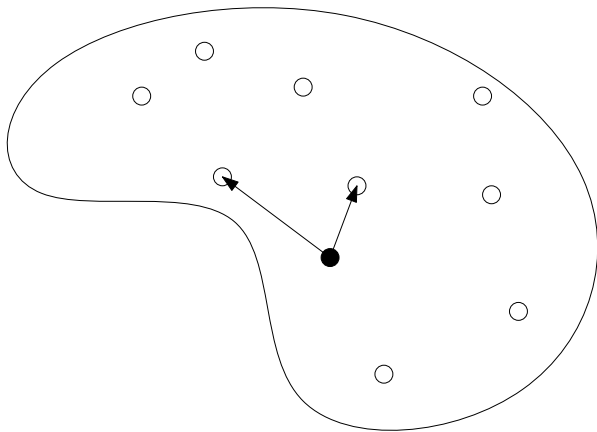
Skilling's affine invariant ideas

Guided walk



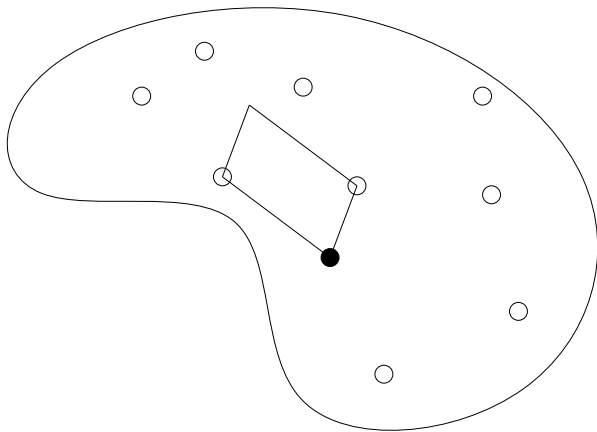
Skilling's affine invariant ideas

Guided walk



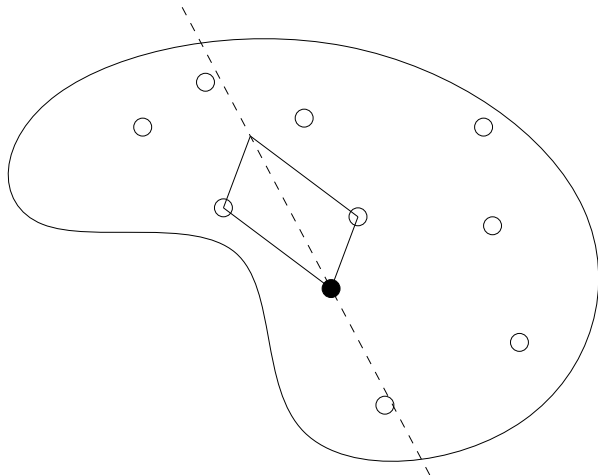
Skilling's affine invariant ideas

Guided walk



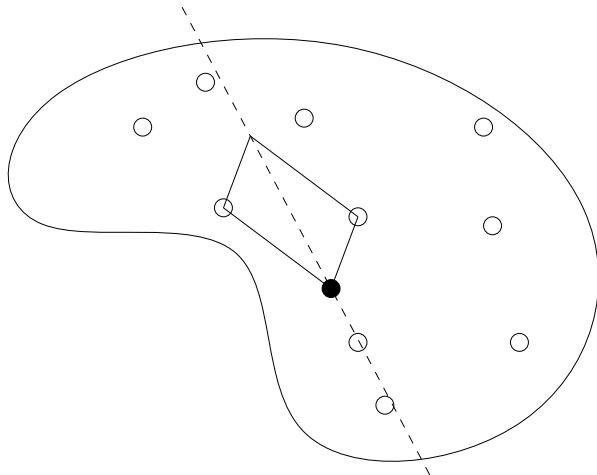
Skellings affine invariant ideas

Guided walk



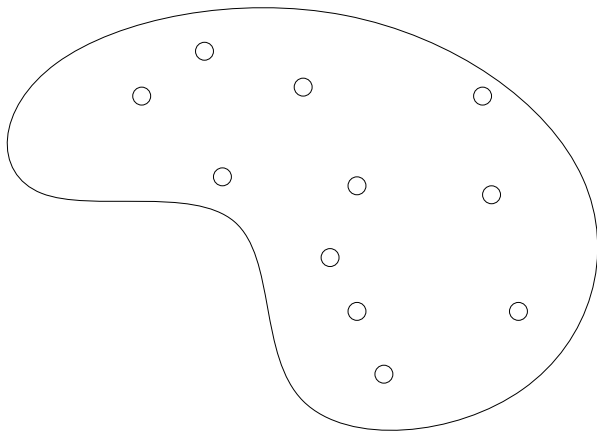
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Guided walk



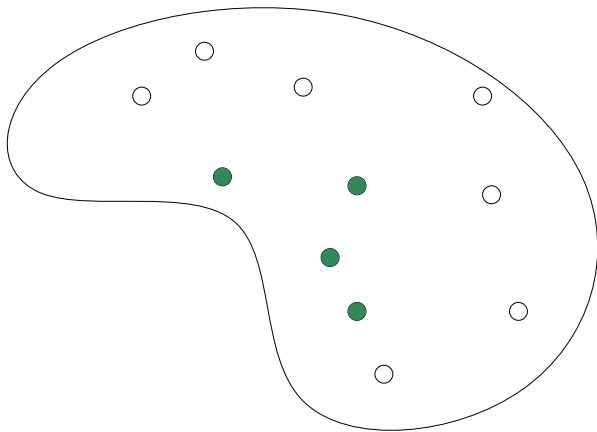
Skillings affine invariant ideas

Guided walk



Skilling's affine invariant ideas

Guided walk



Affine invariant

Other variations

Affine invariant

Other variations

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

Affine invariant

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- ▶ Slice through a “random” linear combination of D points.

Affine invariant

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- ▶ Generalise guided walk to D dimensions (slice through the mean of D other points).
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- ▶ Slice through a “random” linear combination of all points

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.