Nested Sampling

An efficient and robust Bayesian inference tool for physics and machine learning

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Motivating example

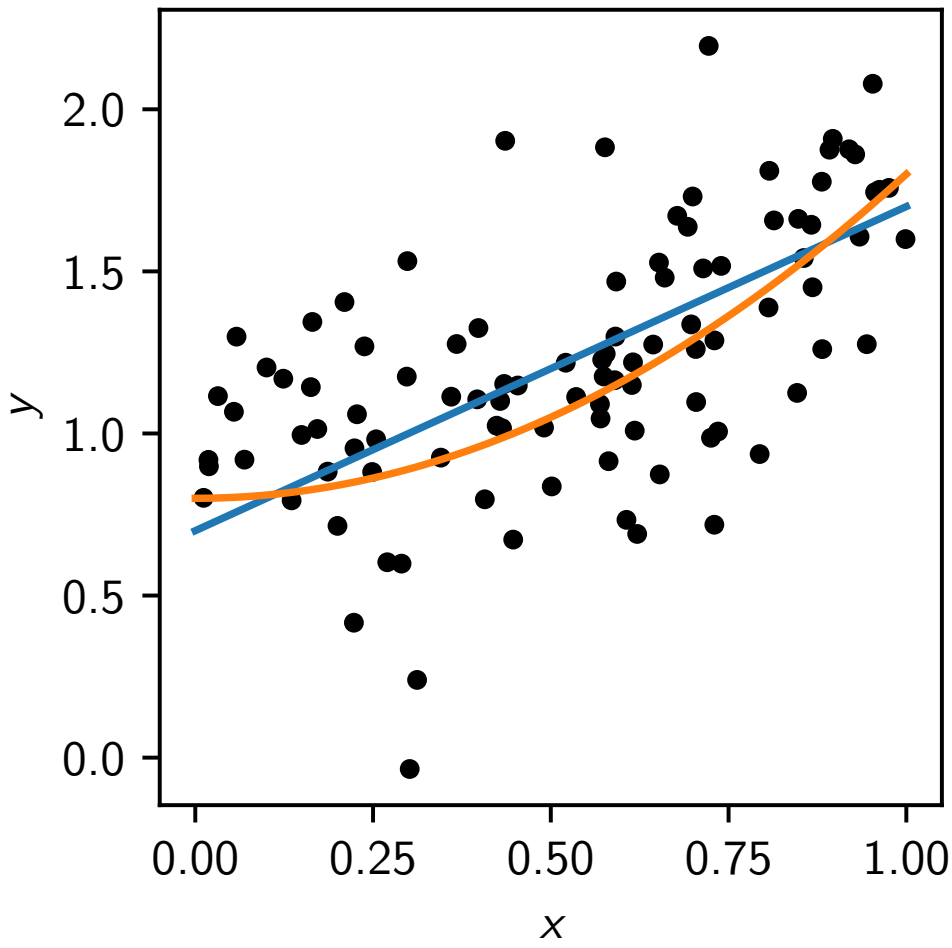
Fitting lines to data

- We have noisy data D
- We wish to fit a model M
- Functional form
  $y = f_M(x; \theta)$
- For example:

$$f_{\text{linear}}(x; \theta) = ax + b$$

$$f_{\text{quadratic}}(x; \theta) = ax^2 + b$$

- Model parameters
  $\theta = (a, b)$



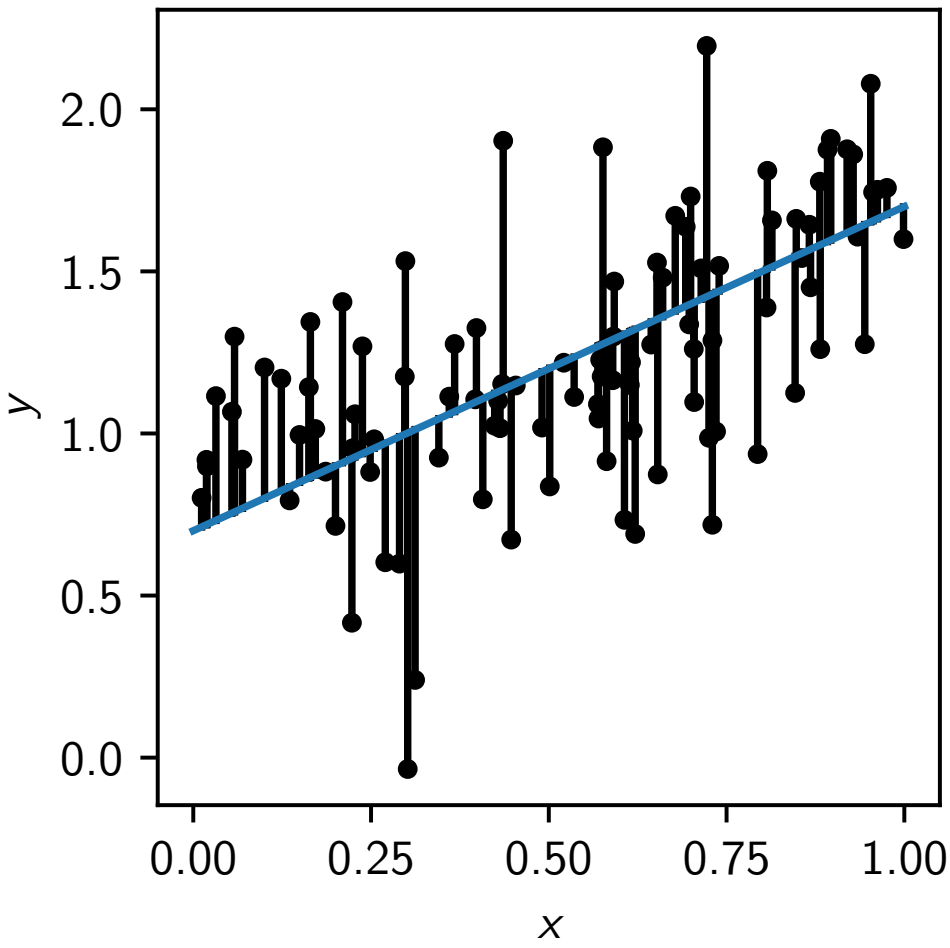
χ^2 best-fit

Fitting lines to data

- For each parameter set θ:

$$\chi^2(\theta) = \sum_i |y_i - f(x_i; \theta)|^2$$

- Minimise χ^2 wrt θ

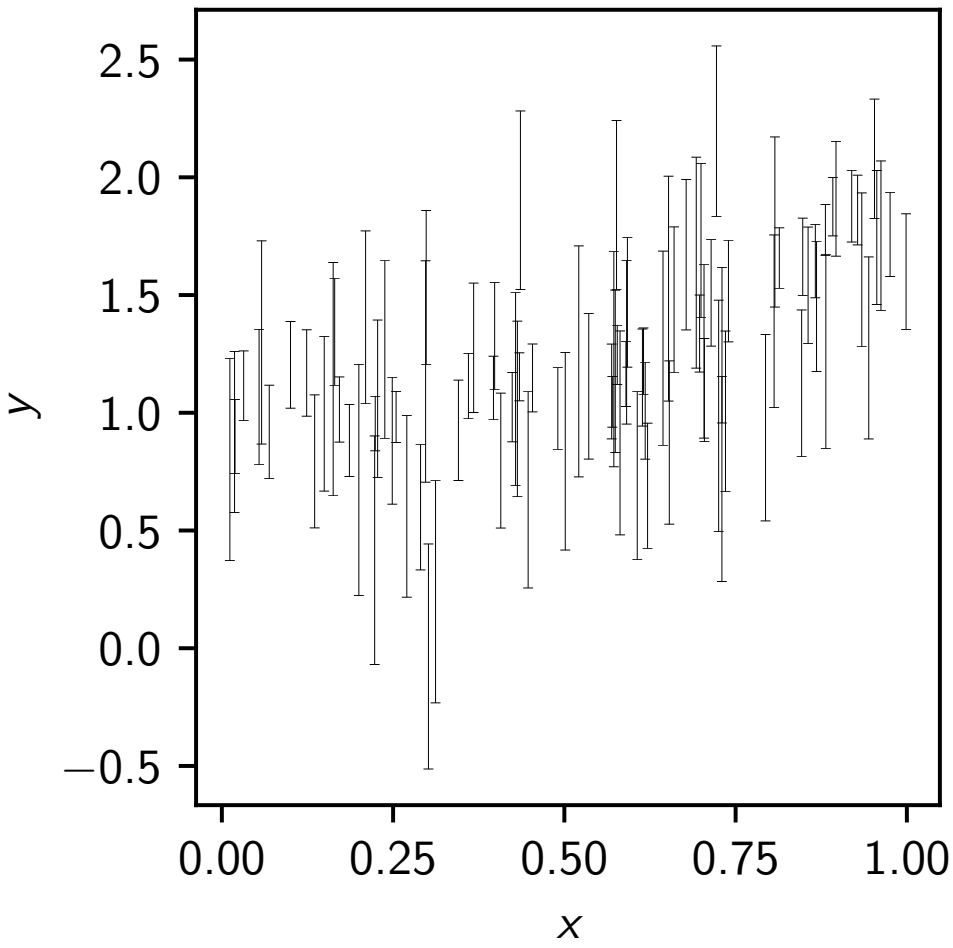


χ^2 with non-uniform data errors

Fitting lines to data

- If data have non-uniform errors:

$$\chi^2(\theta) = \sum_i \frac{|y_i - f(x_i;\theta)|^2}{\sigma_i^2}$$



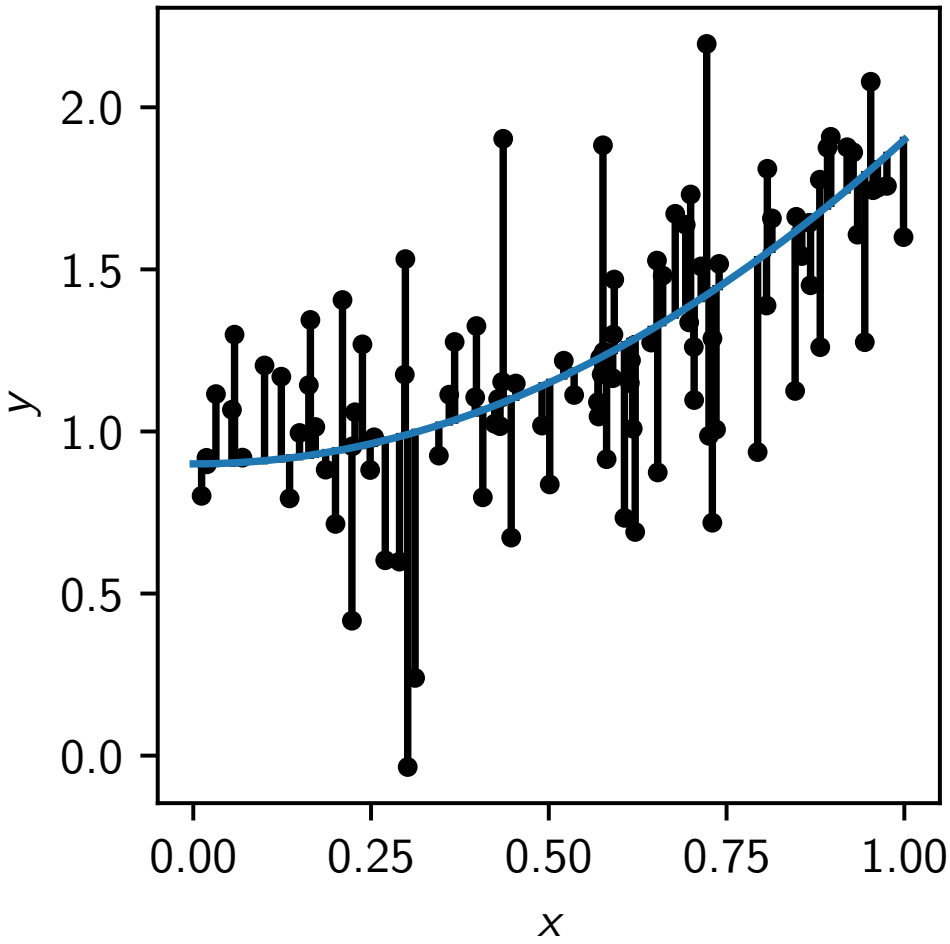
Problems with χ^2

Fitting lines to data

- How do we differentiate between models
- Why square the errors? – could take absolute:

$$\psi^2(\theta) = \sum_i \frac{|y_i - f(x_i;\theta)|}{\sigma_i}$$

- Where does this approach even come from?



Probability distributions

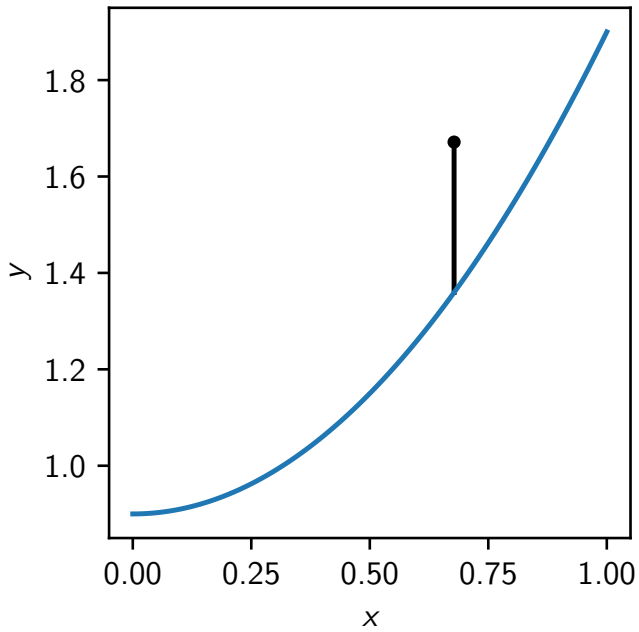
Fitting lines to data

The probability of observing a datum:

$$P(y_i|\theta, M) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{|y_i - f(x_i;\theta)|^2}{2\sigma_i^2}\right)$$

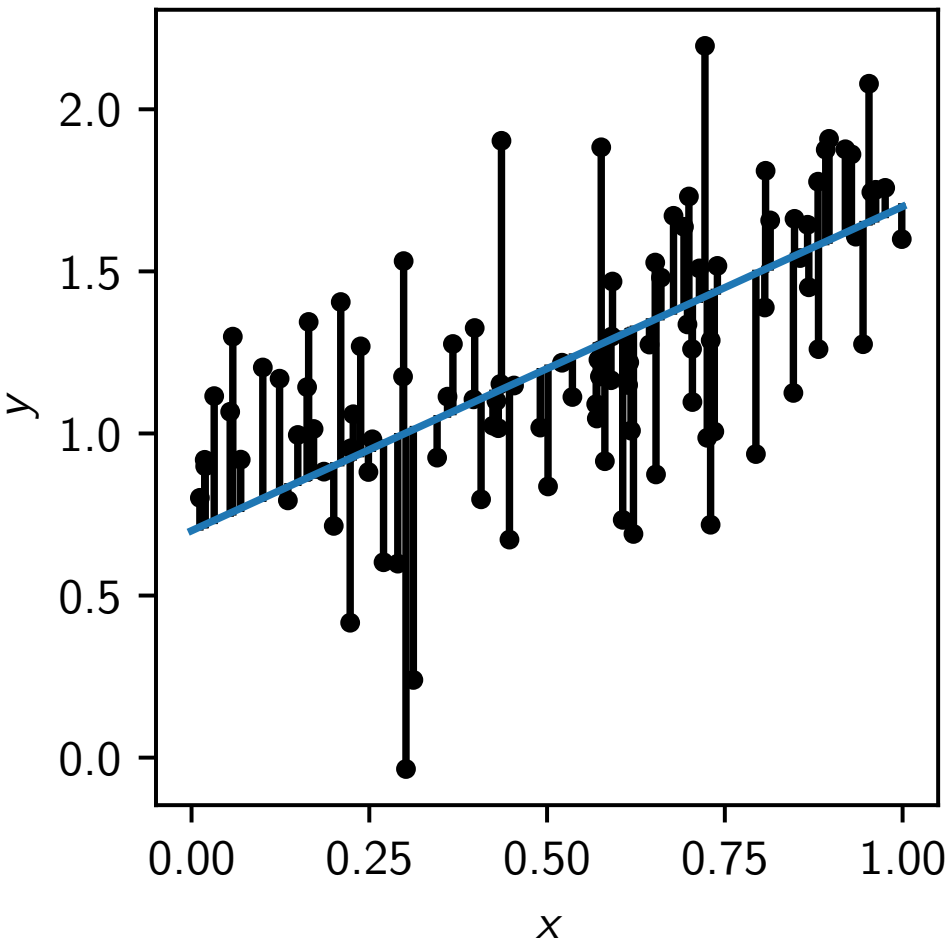
The probability of observing the data:

$$\begin{aligned} P(D|\theta, M) &= \prod_i \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{|y_i - f(x_i;\theta)|^2}{2\sigma_i^2}\right) \\ &= \frac{1}{\prod_i \sqrt{2\pi}\sigma_i} \exp \sum_i -\frac{|y_i - f(x_i;\theta)|^2}{2\sigma_i^2} \\ &\propto e^{-\chi^2(\theta)/2} \end{aligned}$$



Maximum likelihood

Fitting lines to data



- Minimising $\chi^2(\theta)$ is equivalent to maximising $P(D|\theta, M) \propto e^{-\chi^2(\theta)/2}$
- $P(D|\theta, M)$ is called the Likelihood $L = L(\theta)$ of the parameters θ
- "Least squares" $\equiv$ "maximum likelihood" (if data are gaussian).

Bayesian inference

- Likelihood $L = P(D|\theta, M)$ is undeniably correct.
- Frequentists construct inference techniques purely from this function.
- The trend is cosmology is to work with a Bayesian approach.
- What we want are things like $P(\theta|D, M)$ and $P(M|D)$.
- To invert the conditionals, we need Bayes theorems:

$$P(\theta|D, M) = \frac{P(D|\theta, M)P(\theta|M)}{P(D|M)}$$

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

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

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

$$\text{Model probability} = \frac{\text{Evidence} \times \text{Model Prior}}{\text{Normalisation}}$$

Multivariate probability

- Marginalisation:

$$P(x) = \int P(x, y) dy$$

- Conditioning:

$$P(y|x) = \frac{P(x, y)}{P(x)} = \frac{P(x, y)}{\int P(x, y) dy}$$

- De-Conditioning:

$$P(x|y)P(y) = P(x, y)$$

- Bayes theorem:

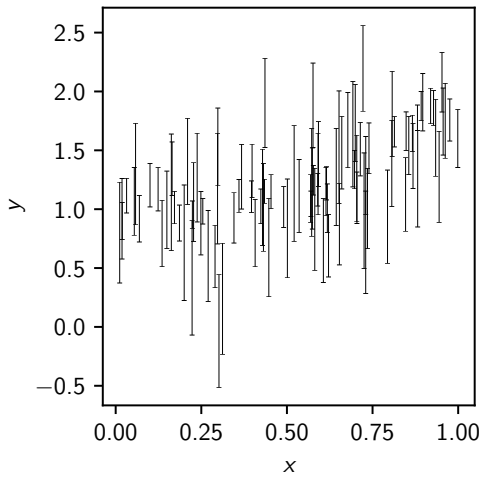
$$P(y|x) = \frac{P(x|y)P(y)}{P(x)}$$

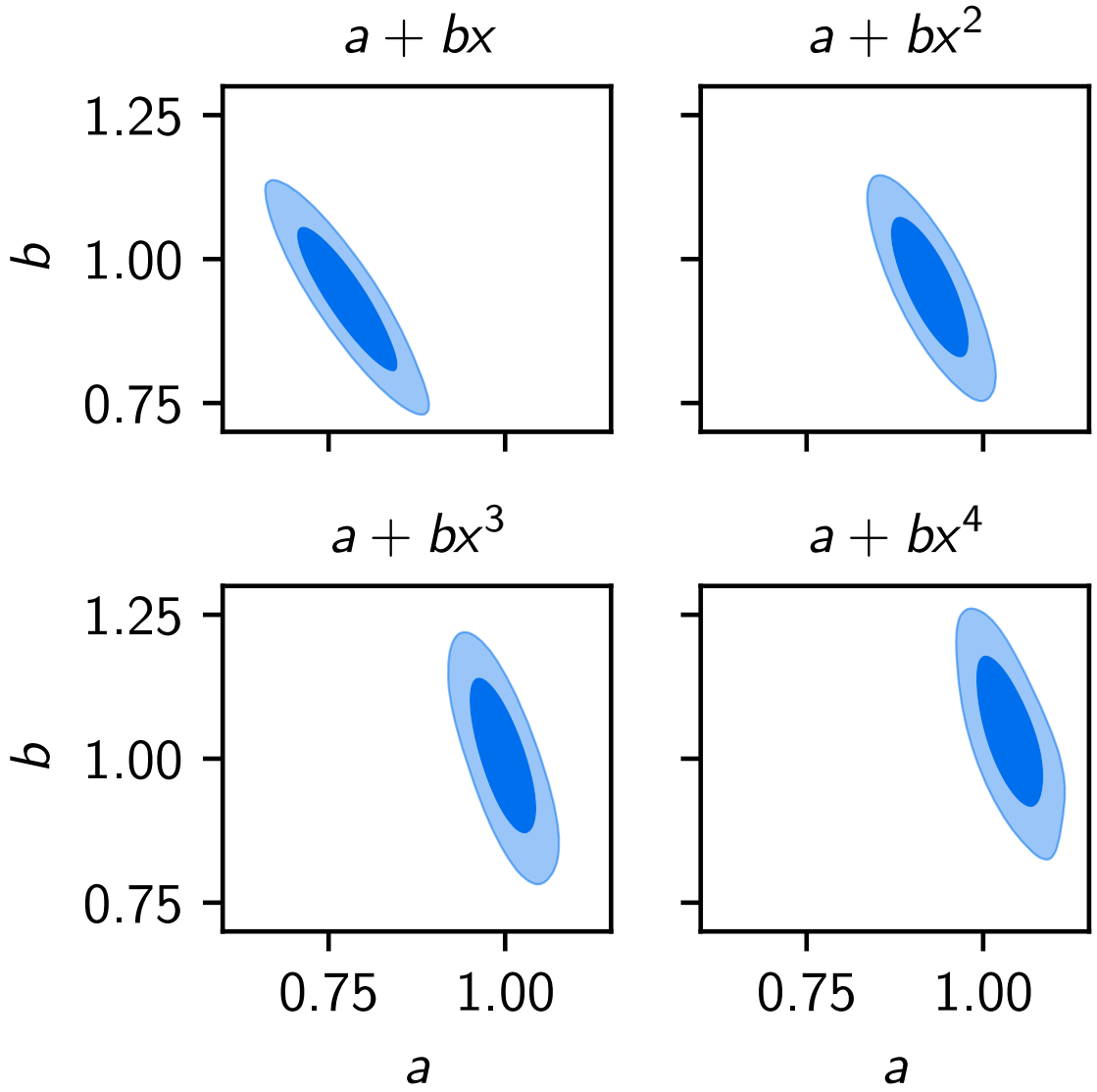
"To flip a conditional $P(x|y)$, you first de-condition on y, and then re-condition on x."

Parameter estimation

Bayesian inference

- We may use $P(\theta|D, M)$ to inspect whether a model looks reasonable



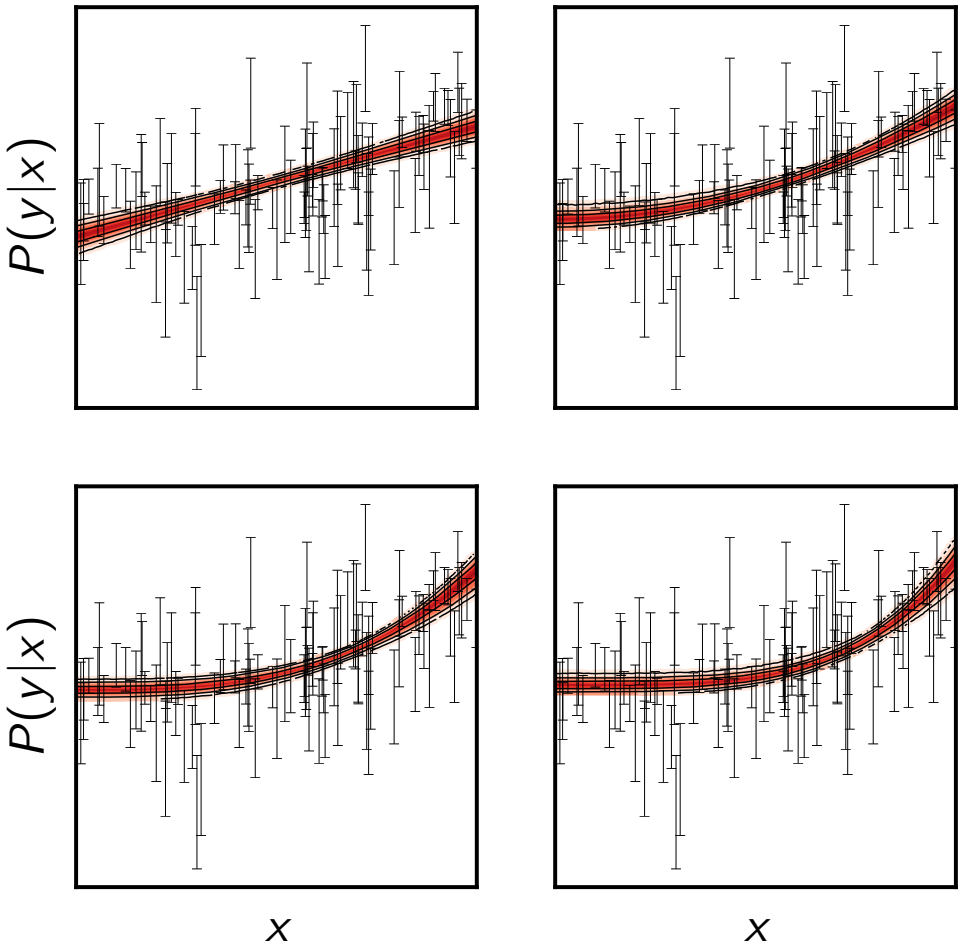


Predictive posterior

More useful to plot:

$$P(y|x) = \int P(y|x,\theta)P(\theta)d\theta$$

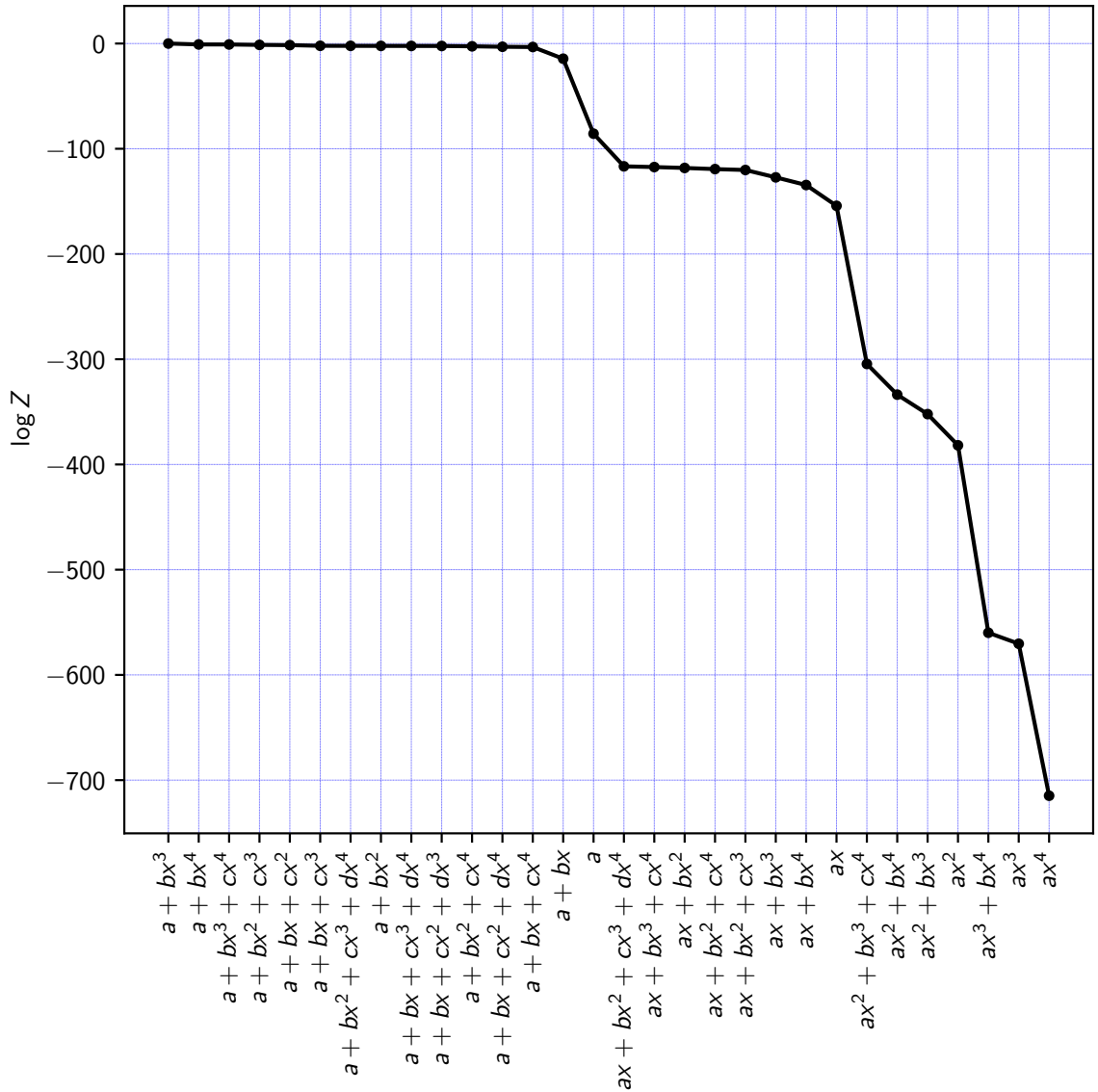
(all conditioned on D, M)



Model comparison

Bayesian inference

- We may use the Bayesian evidence Z to determine whether a model is reasonable.
- $Z = P(D|M) = \int P(D|M,\theta)P(\theta|M)d\theta$
- Normally assume uniform model priors $Z \propto P(M|D)P(M)$.



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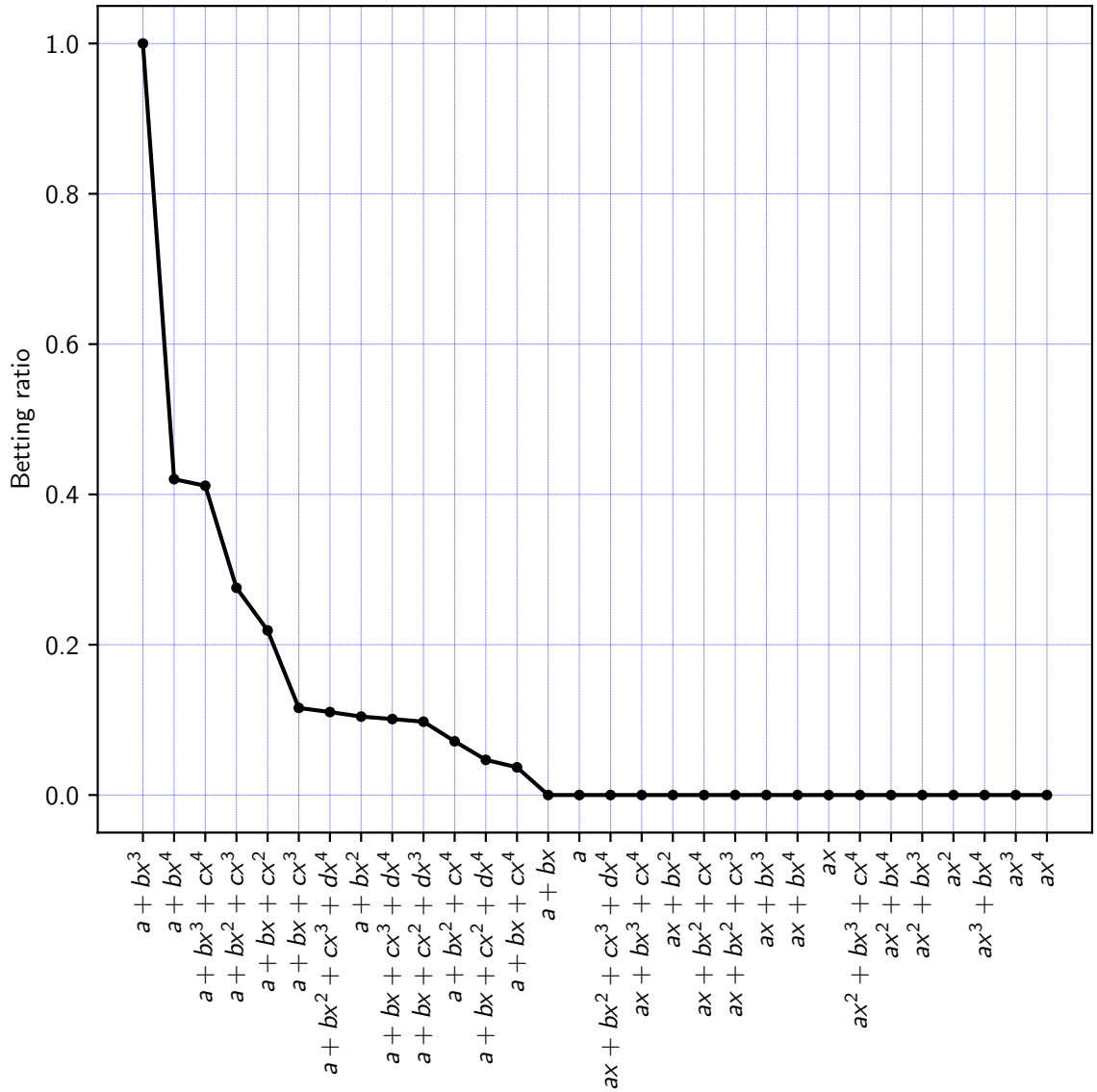
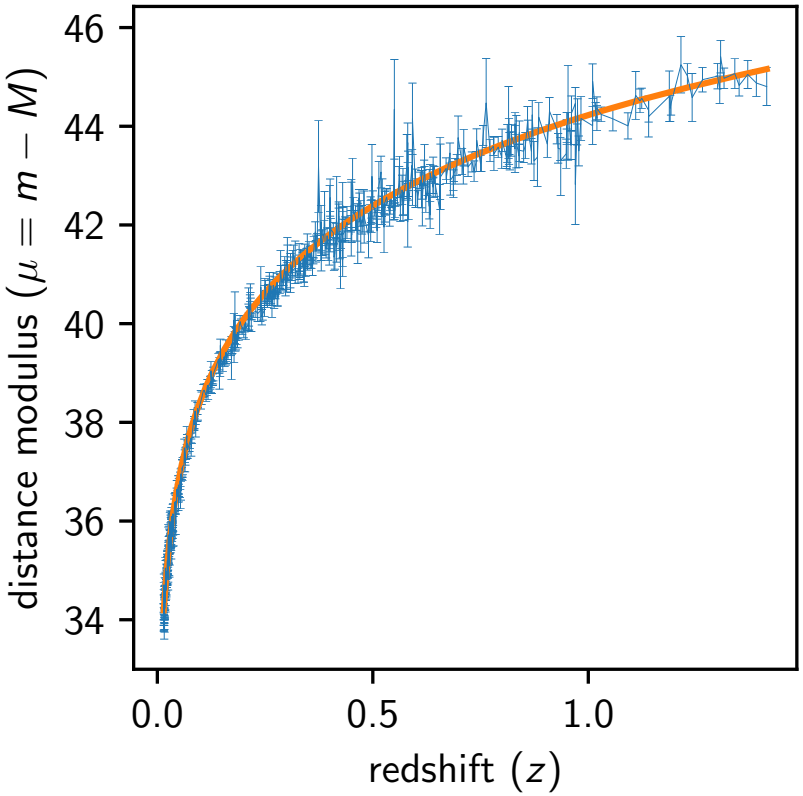


Line fitting (context)

- Whilst this model seems a little trite...
- ...determining polynomial indices $\equiv$ determining cosmological material content:

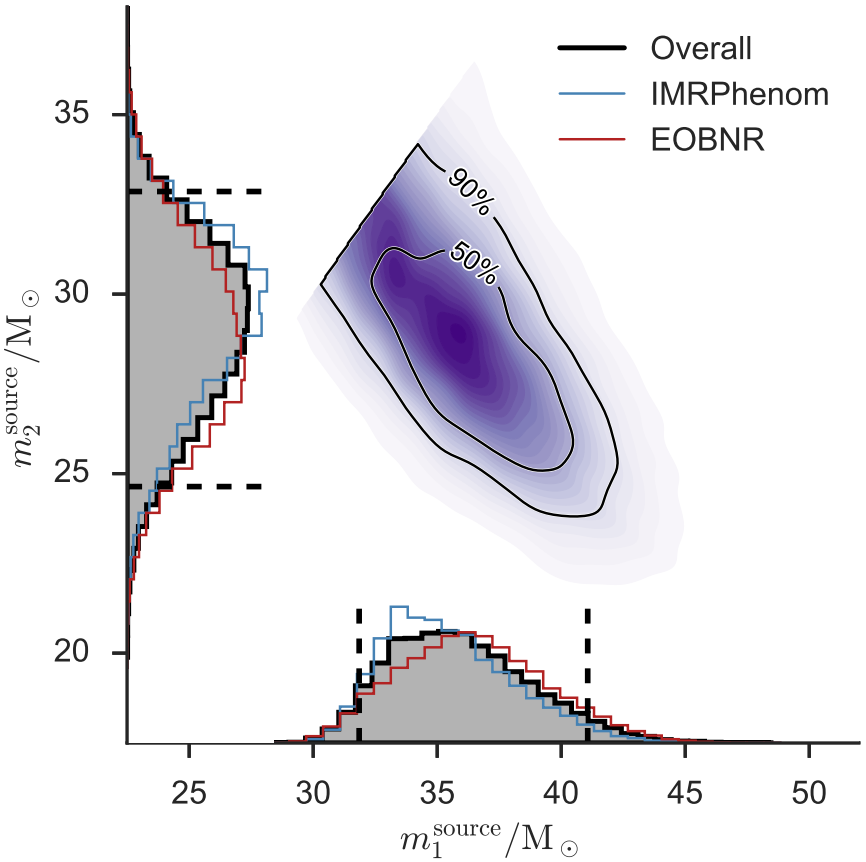


$$\left(\frac{H}{H_0}\right)^2 = \Omega_\mathrm{r}\left(\frac{a_0}{a}\right)^4 + \Omega_\mathrm{m}\left(\frac{a_0}{a}\right)^3 + \Omega_k\left(\frac{a_0}{a}\right)^2 + \Omega_\Lambda$$

Sampling

How to describe a high-dimensional posterior

- In high dimensions, posterior $\mathcal{P}$ occupies a vanishingly small region of the prior π.
- Gridding is doomed to failure for $D \gtrsim 4$.
- *Sampling* the posterior is an excellent compression scheme.



Sampling

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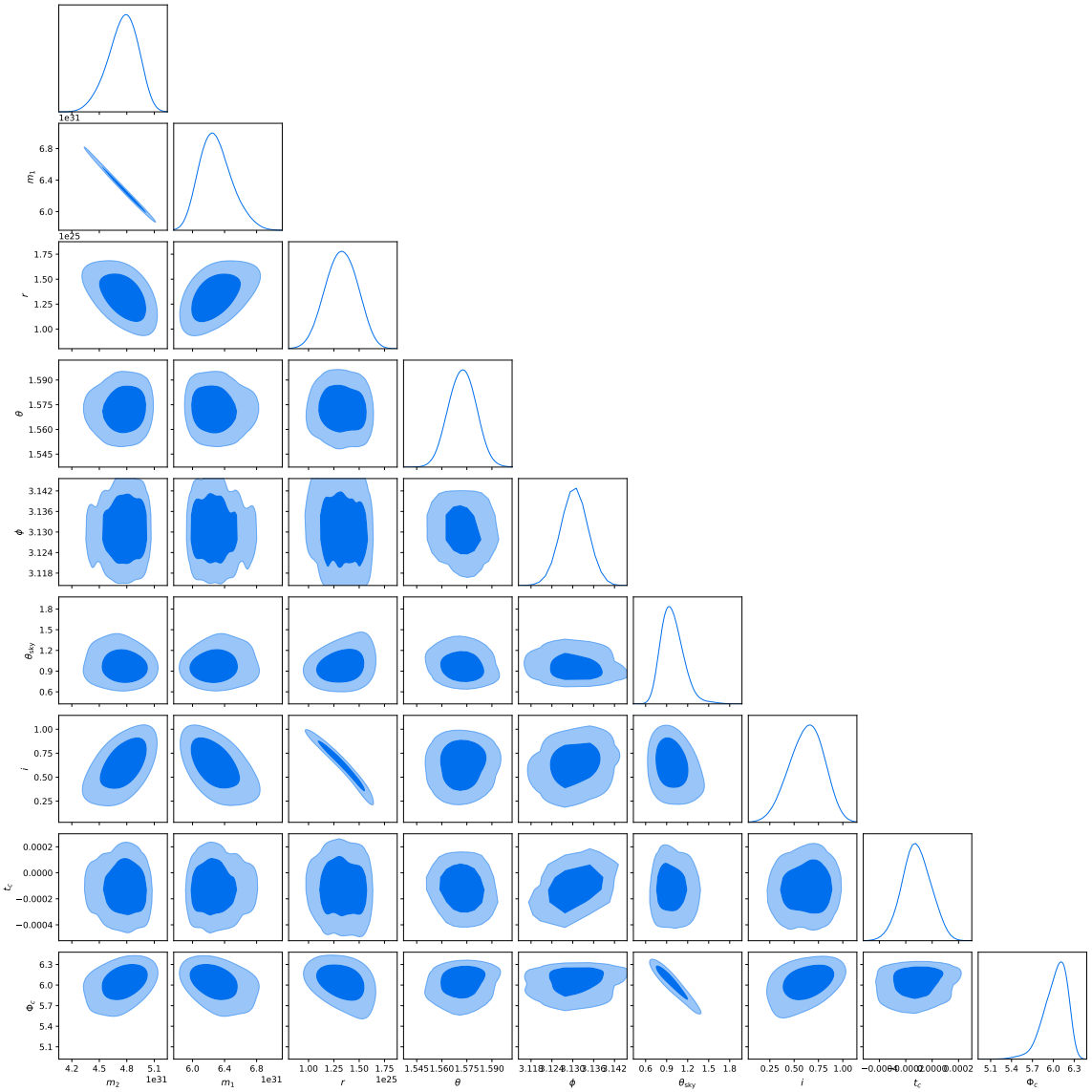

Cosmology in high dimensions

$$\mathcal{L}(\Theta) = P(D|\Theta, M)$$

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$$D = \{C_\ell\}$$
$$M = \Lambda\text{CDM}$$
$$\Theta = \Theta_{\Lambda\text{CDM}}$$

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Cosmology in high dimensions

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\Theta_{\text{extensions}} =& (n_{\text{run}}, n_{\text{run,run}}, w, \Sigma m_\nu, m_{\nu,\text{sterile}}^{\text{eff}})
\end{aligned}$$

- Parameter estimation: $L, \pi \to \mathcal{P}$: model parameters
- Model comparison: $L, \pi \to Z$: how good model is

Parameter estimation

- The name of the game is therefore drawing samples S from the posterior $\mathcal{P}$ with the minimum number of likelihood calls.
- Gridding is doomed to failure in high dimensions.
- Enter Metropolis Hastings.

Metropolis Hastings

- Turn the N-dimensional problem into a one-dimensional one.
  1. Propose random step
  2. If uphill, make step...
  3. ...otherwise sometimes make step.
- `chi-feng.github.io/mcmc-demo/`

Metropolis Hastings

Struggles with...

Metropolis Hastings

Struggles with...

1. Burn in
2. Multimodality
3. Correlated Peaks
4. Phase transitions

Hamiltonian Monte-Carlo

- Key idea: Treat $\log L(\Theta)$ as a potential energy
- Guide walker under "force":

$$F(\Theta) = \nabla \log L(\Theta)$$

- Walker is naturally "guided" uphill
- Conserved quantities mean efficient acceptance ratios.
- Mass matrix for kinetic term is a hidden tuning element.
- stan is a fully fledged, rapidly developing programming language with HMC as a default sampler.

Ensemble sampling

- Instead of one walker, evolve a set of n walkers.
- Can use information present in ensemble to guide proposals.
- emcee: affine invariant proposals.
- emcee is not the only (or even best) affine invariant approach.

The fundamental issue with all of the above

- They don't give you evidences!

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

- MCMC fundamentally explores the posterior, and cannot average over the prior.
- Thermodynamic annealing
  - Suffers from same tuning issues as MCMC
- Nearest neighbor volume estimation (Heavens arXiv:1704.03472)
  - Does not scale to high dimensions $D \gtrsim 10$.

Nested Sampling

John Skilling's alternative to traditional MCMC!

- Nested sampling is a completely different way of sampling.
- Uses ensemble sampling to compress prior to posterior.

New procedure:
Maintain a set S of n samples, which are sequentially updated:

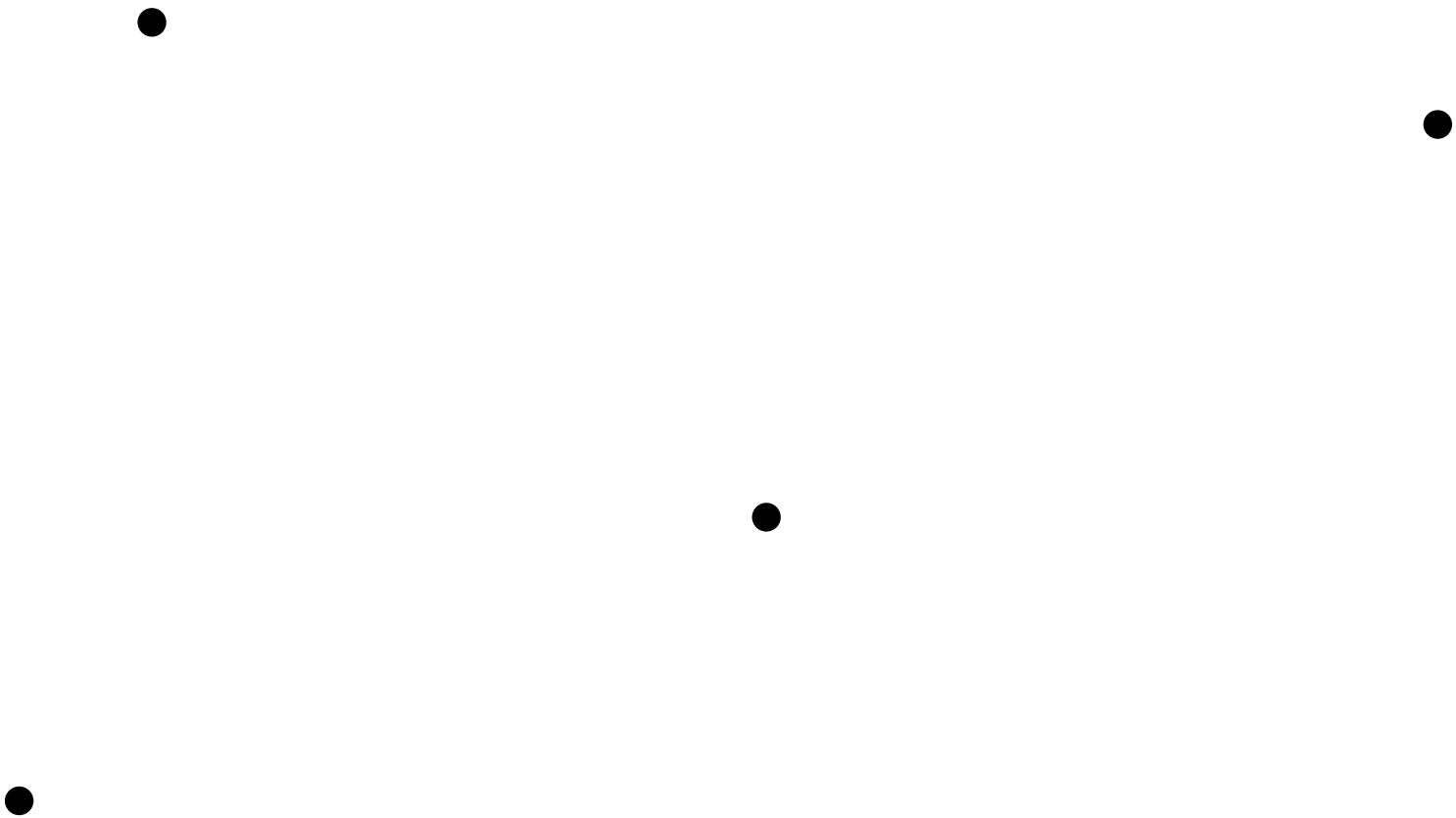
S_0: Generate n samples uniformly over the space (from the prior π).

S_{n+1}: Delete the lowest likelihood sample in S_n, and replace it with a new uniform sample with higher likelihood

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

Nested Sampling

Graphical aid



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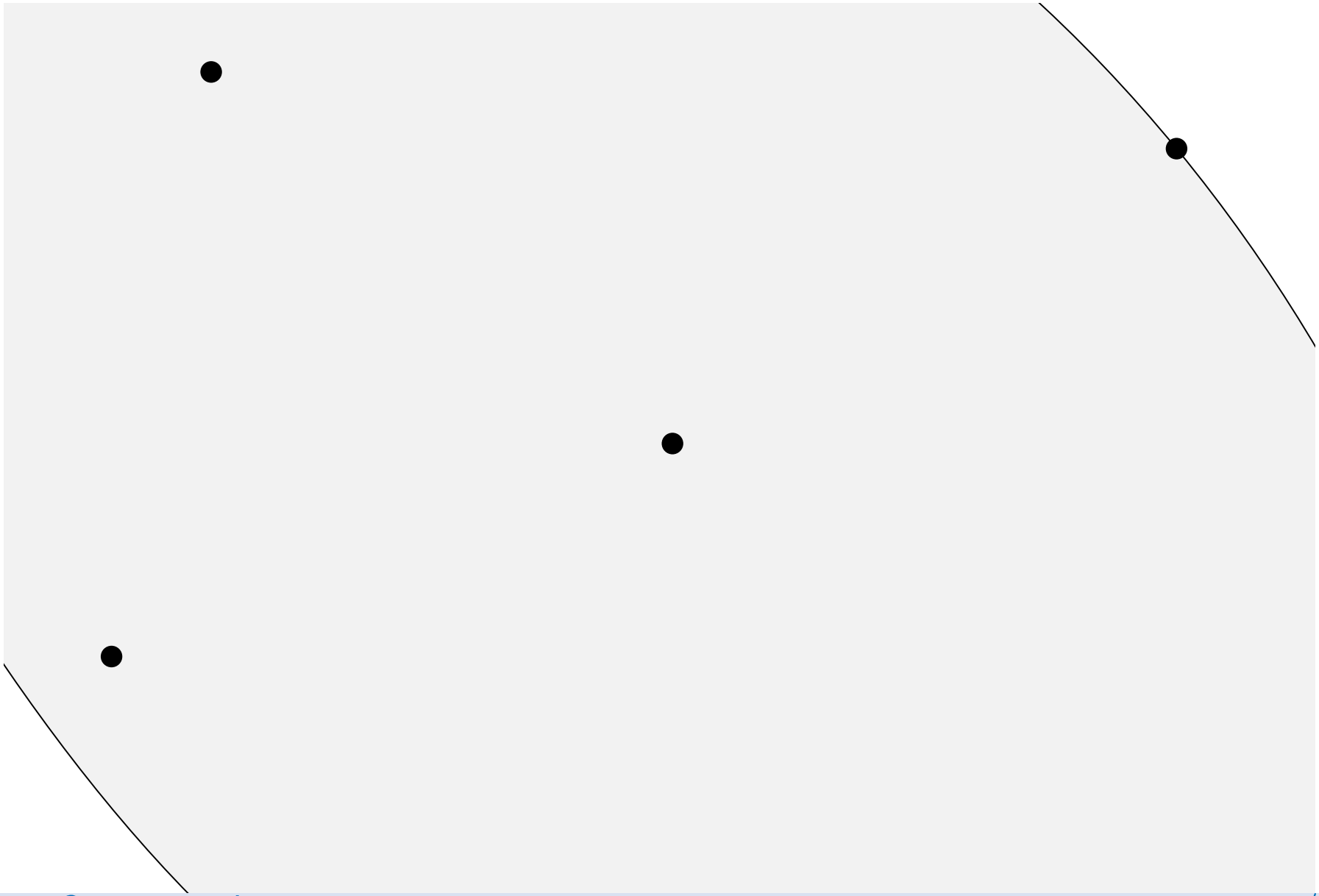

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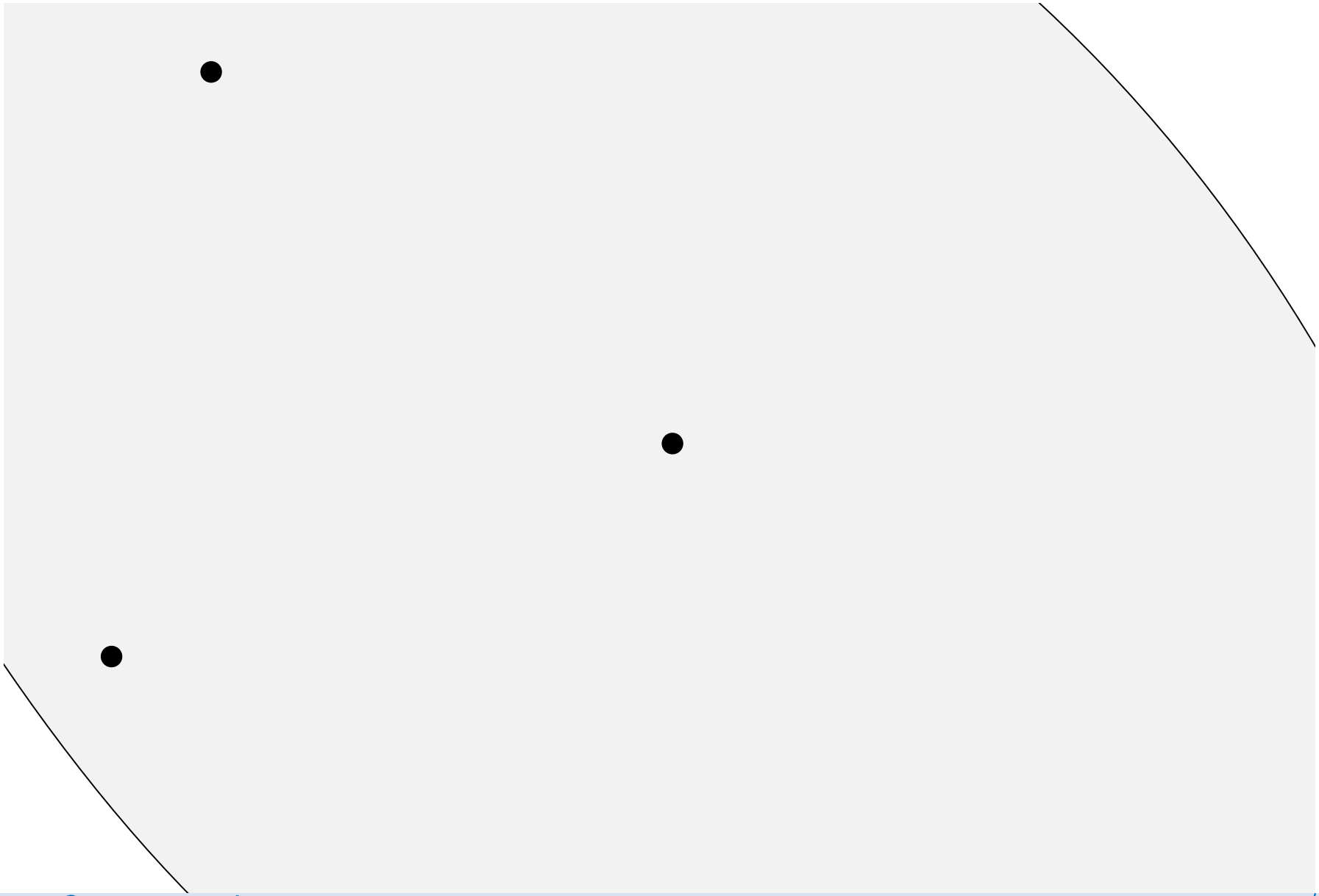

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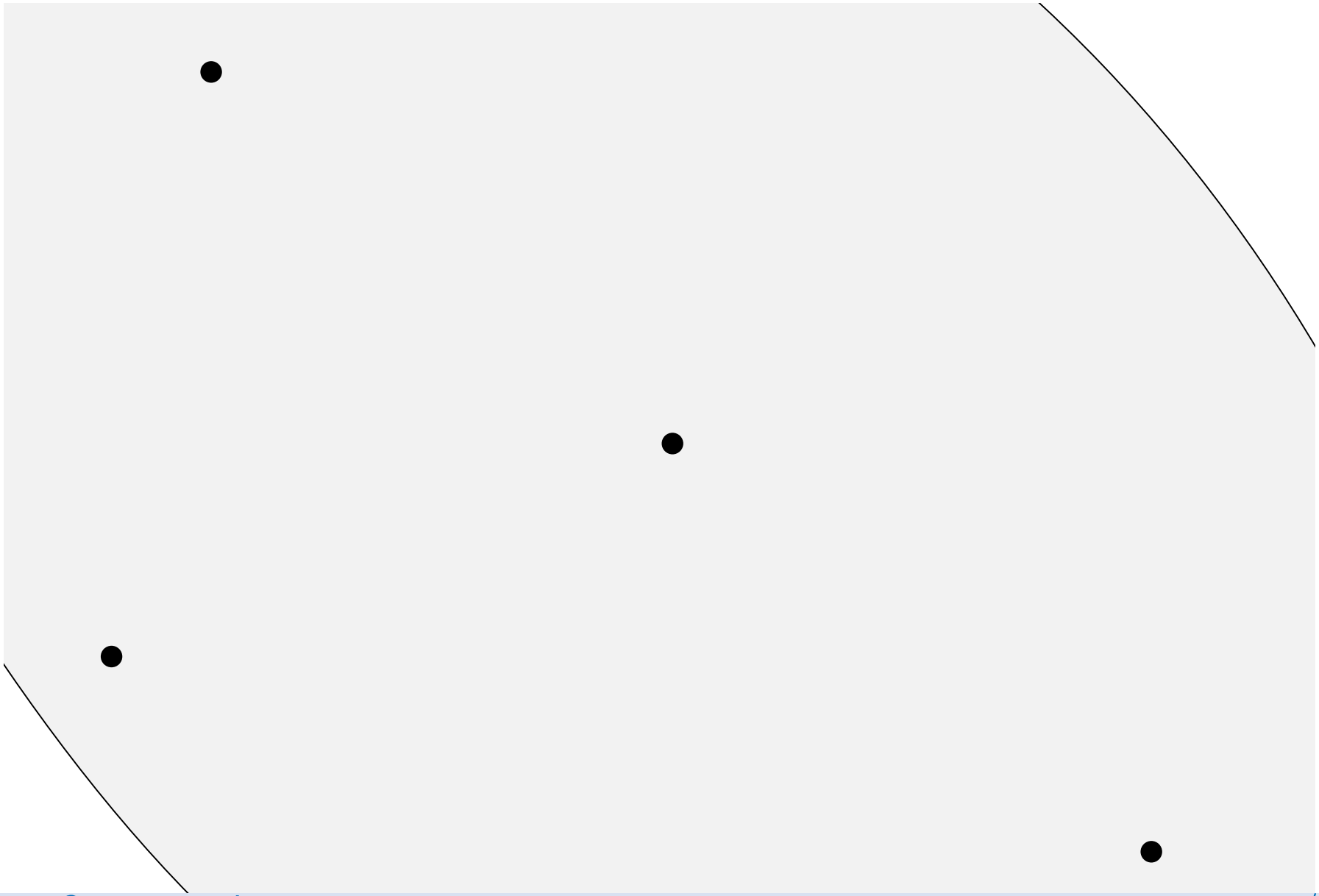

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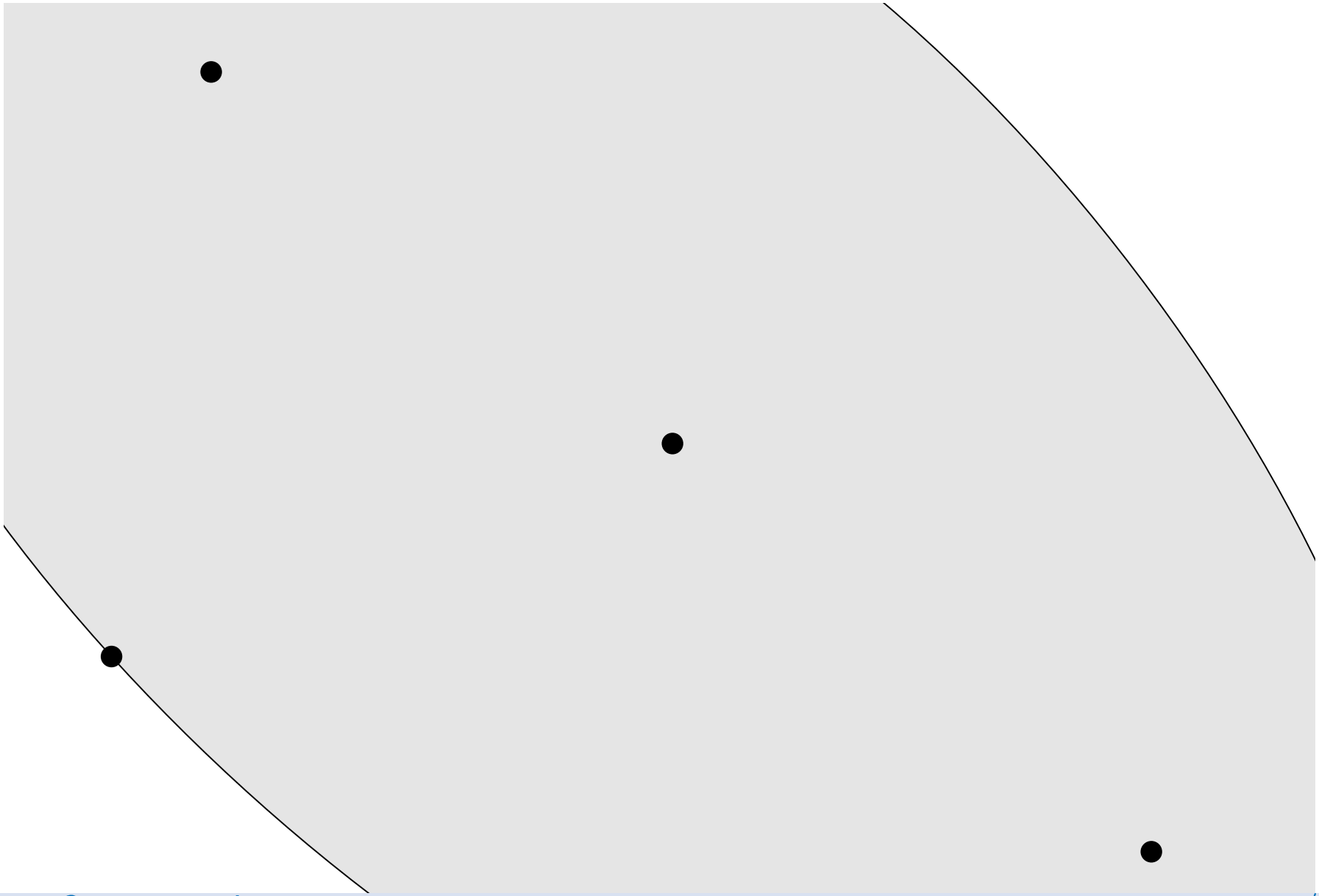

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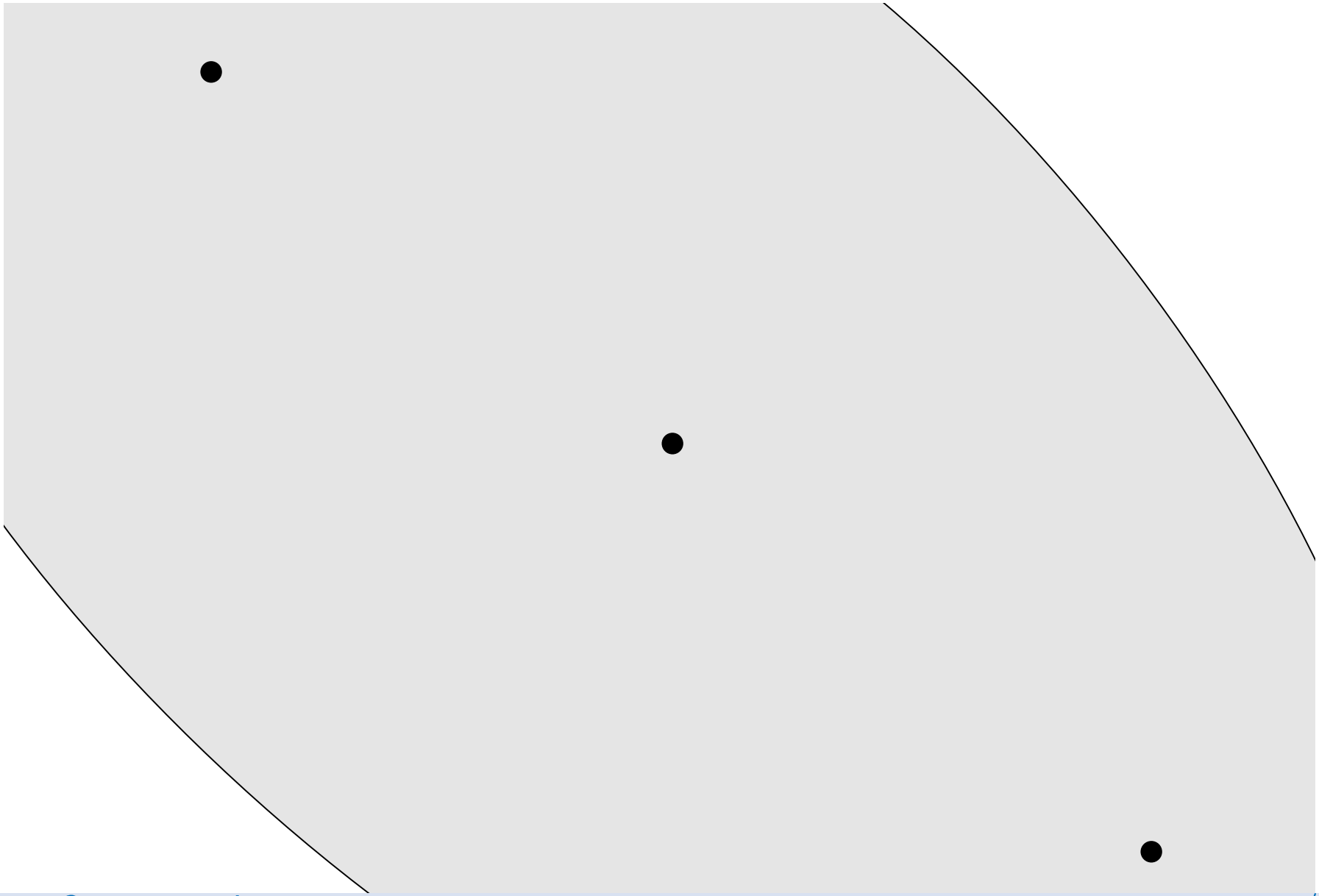

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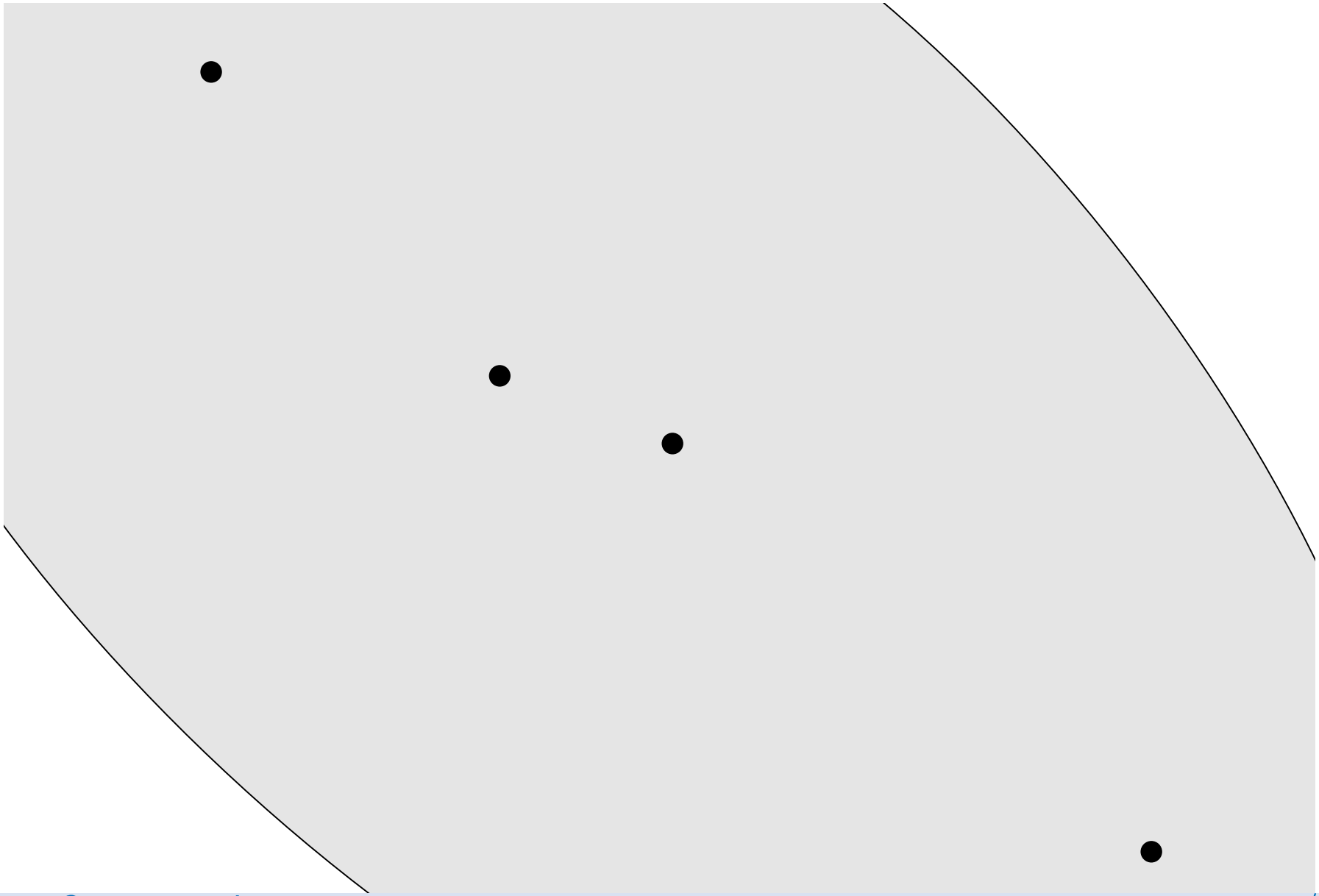

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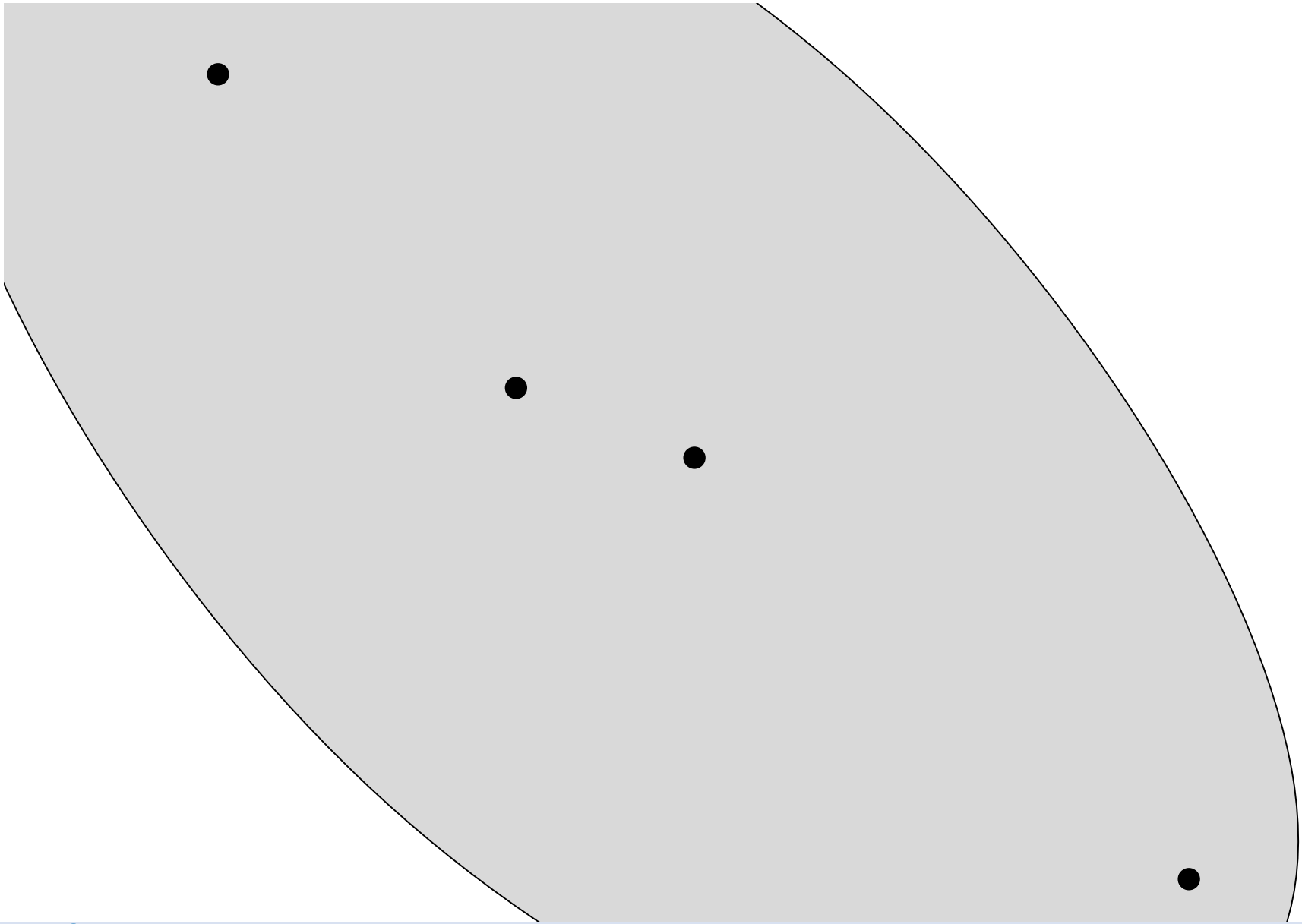

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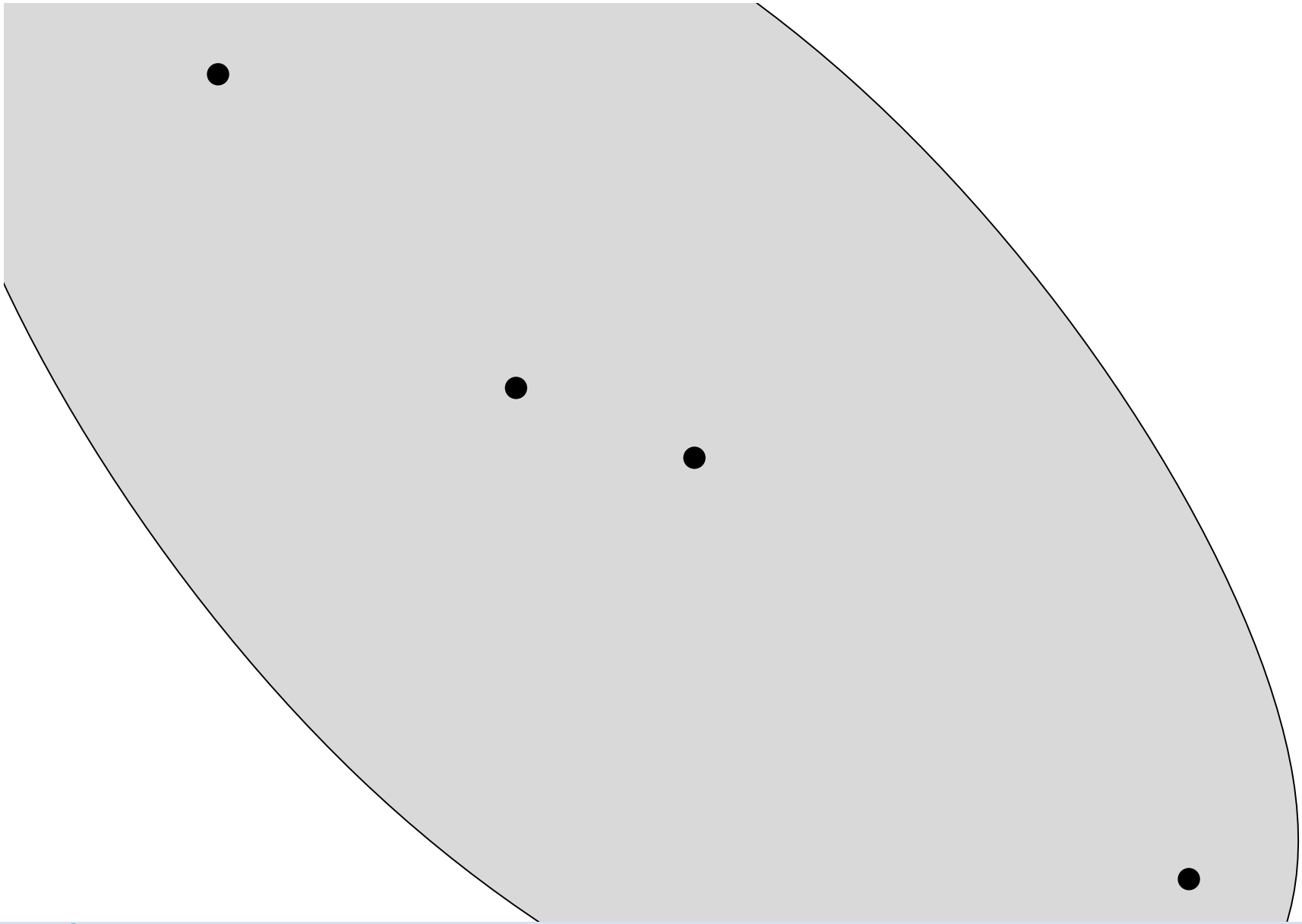

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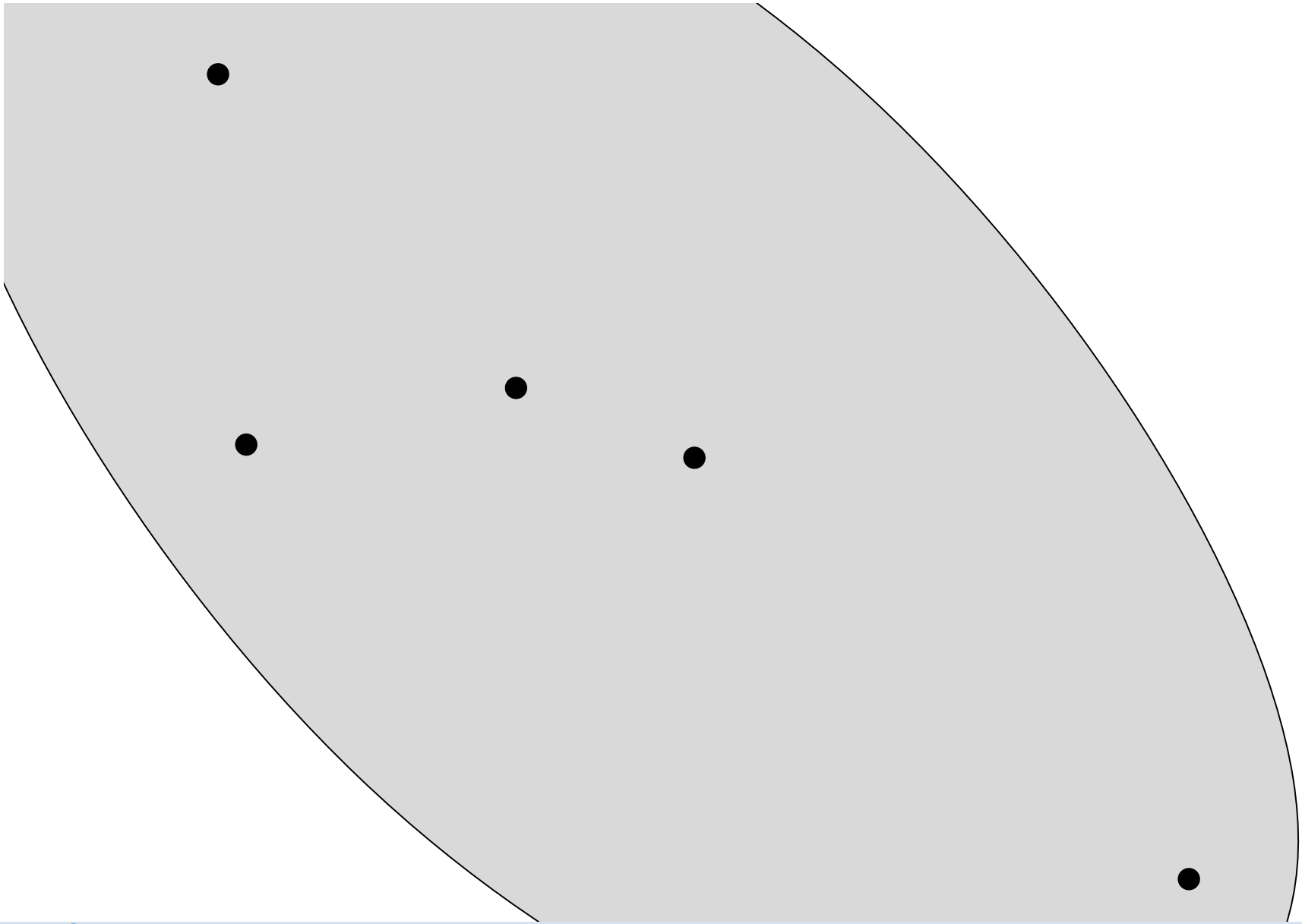

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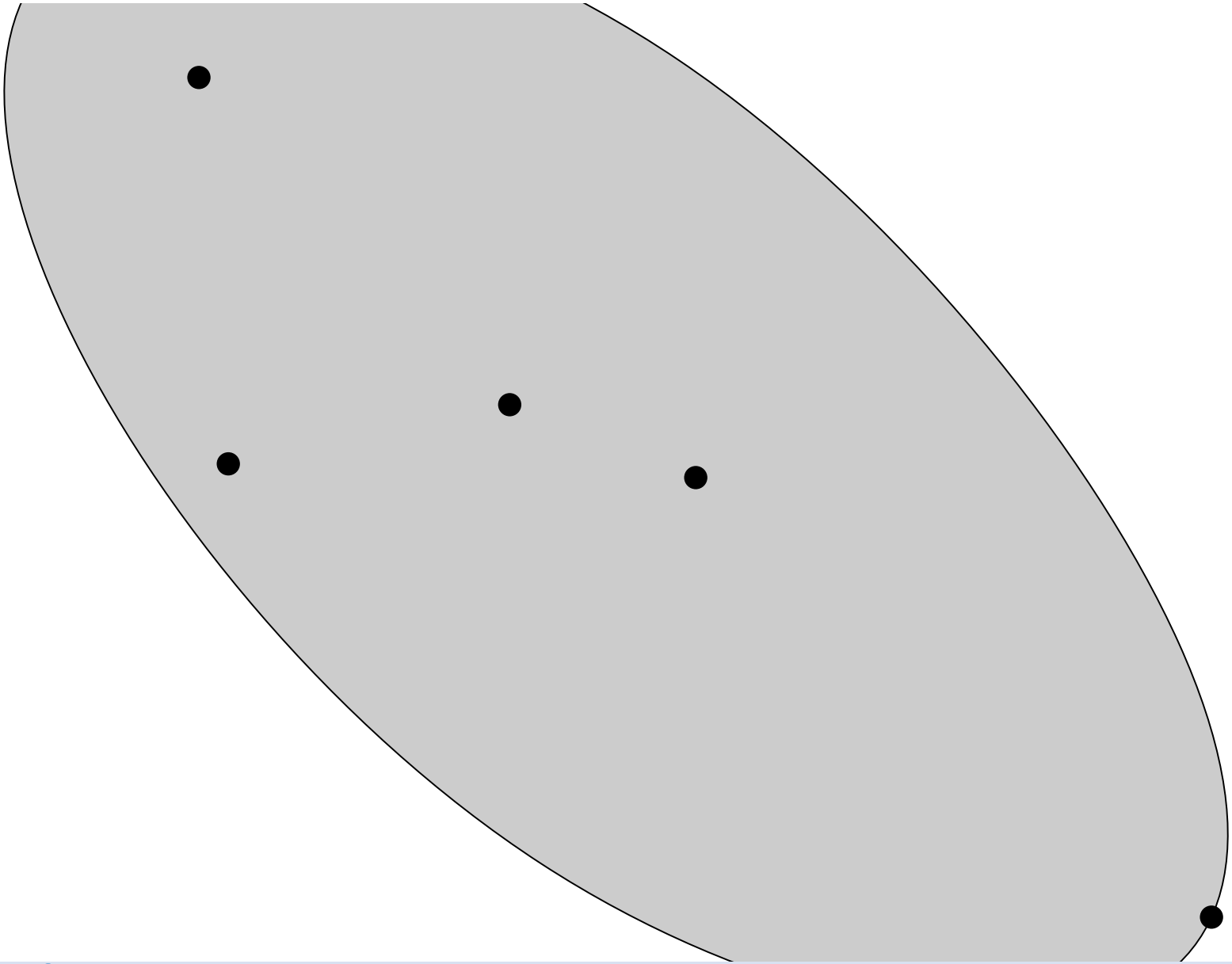

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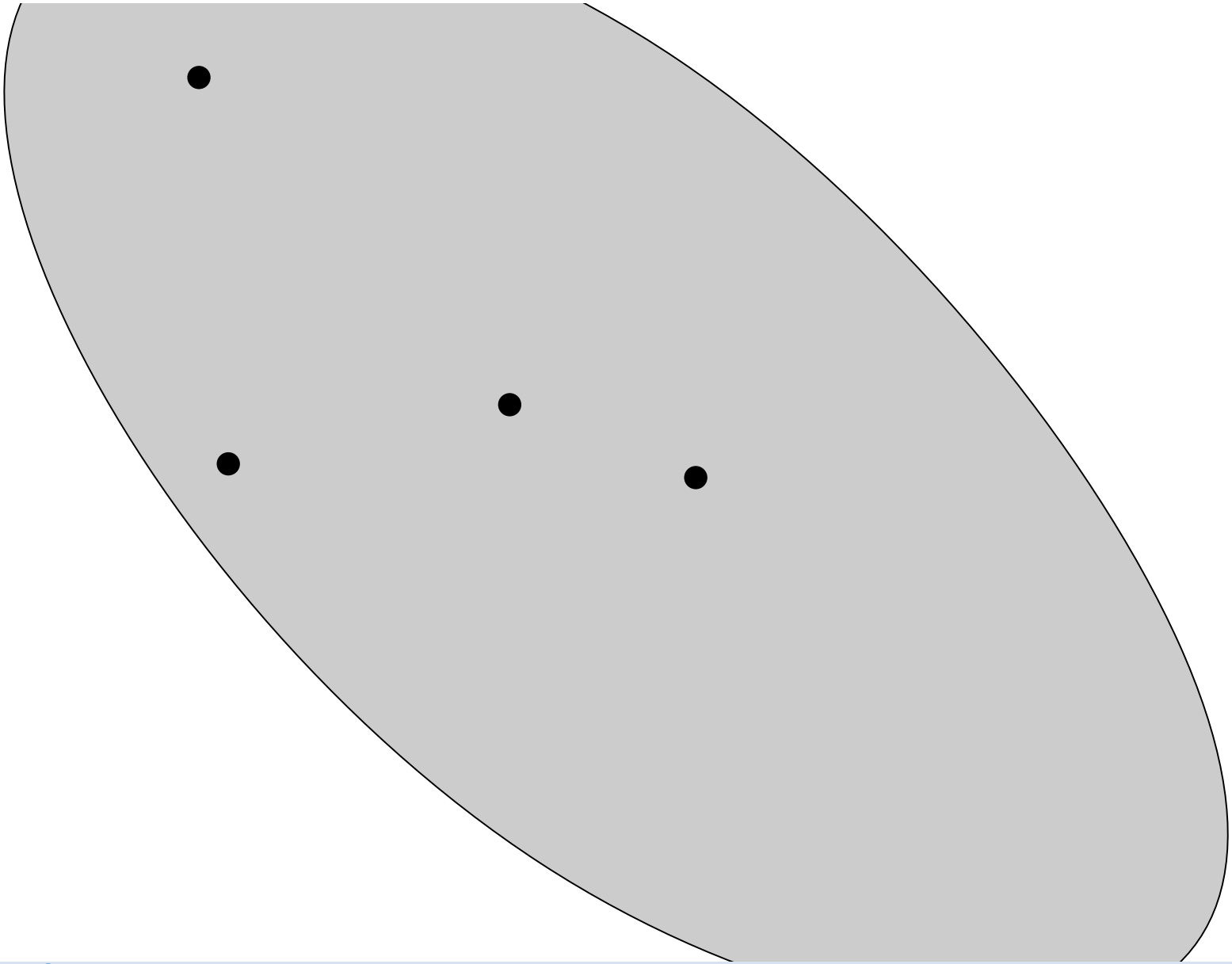

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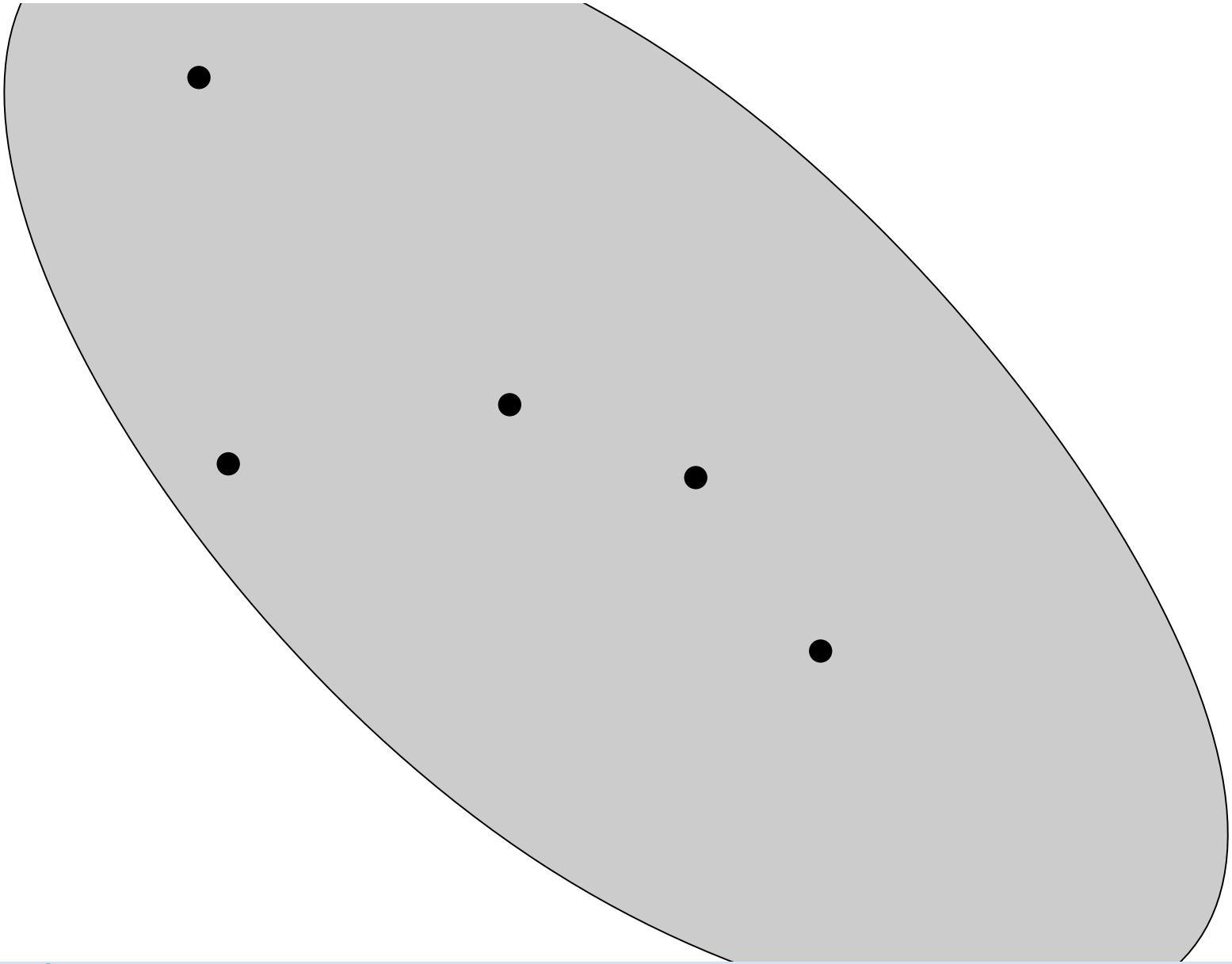

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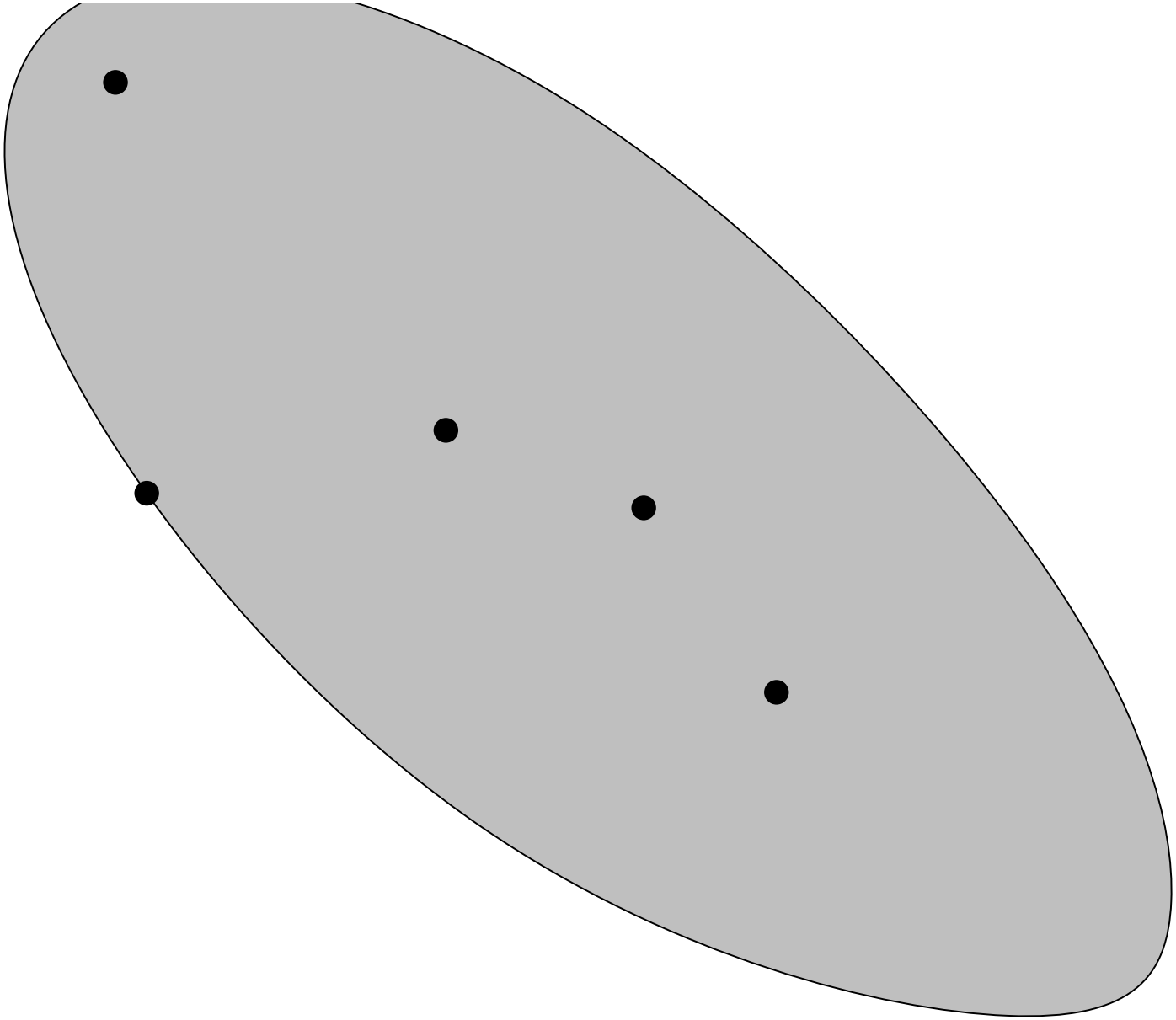

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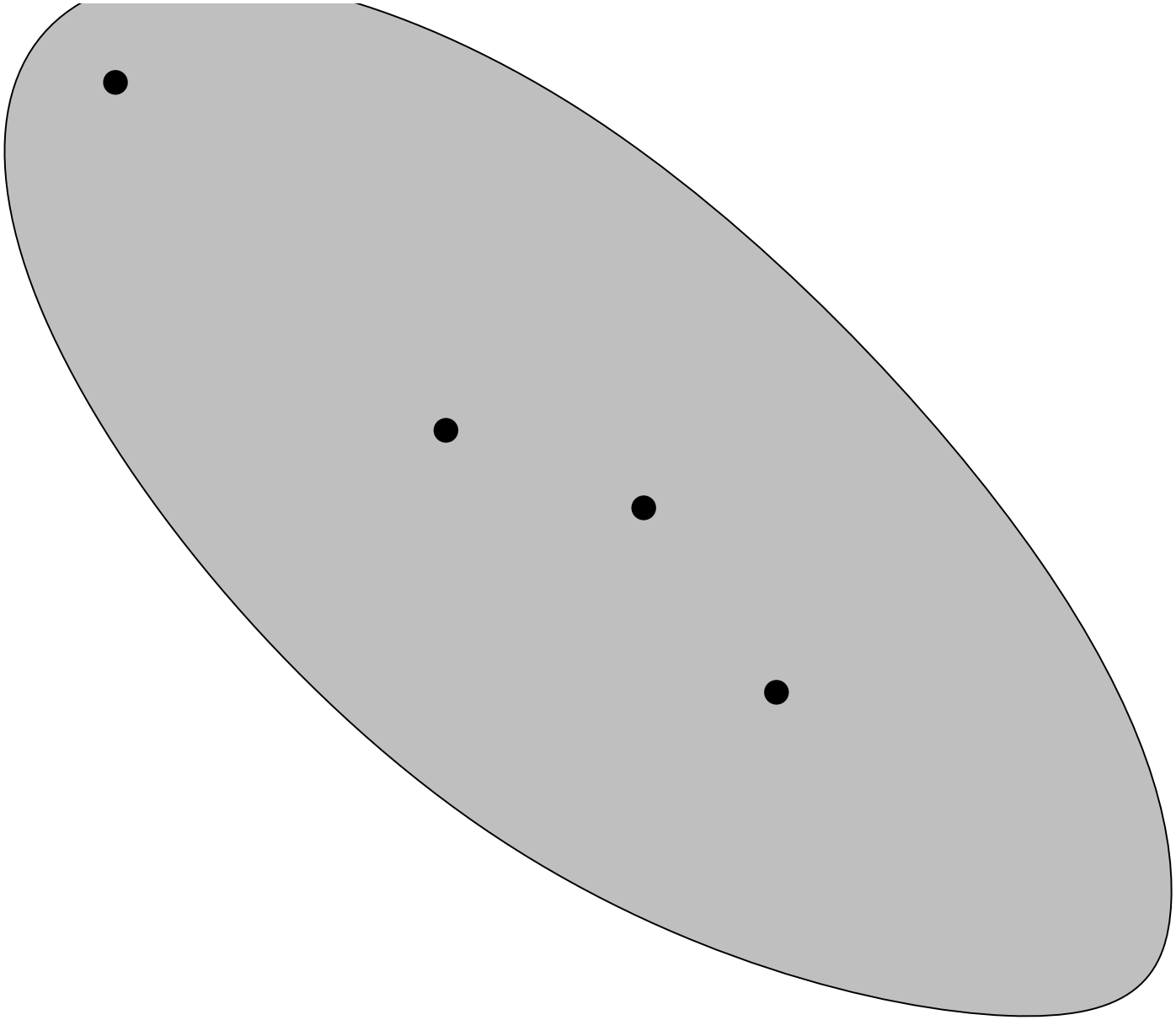

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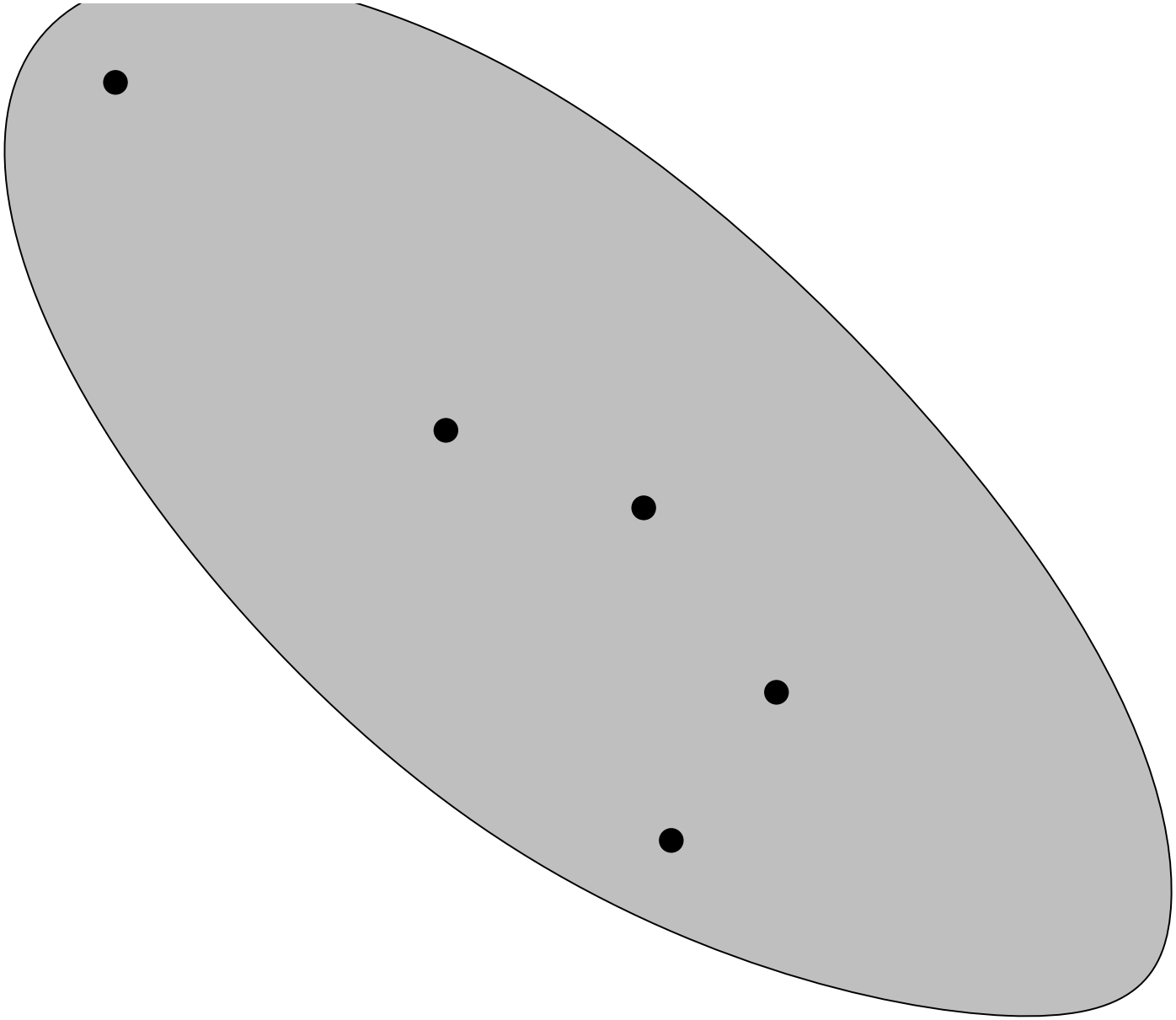

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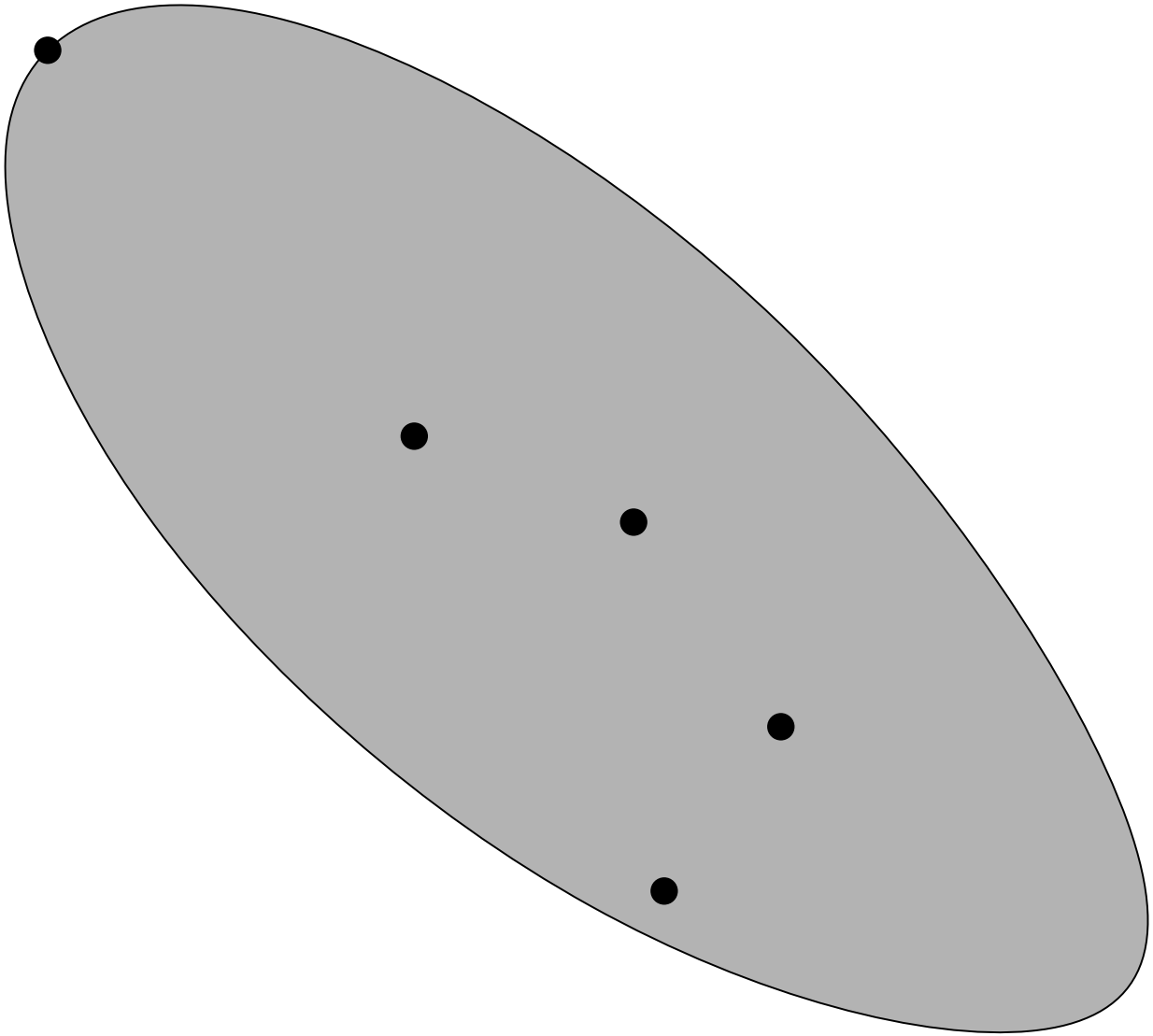

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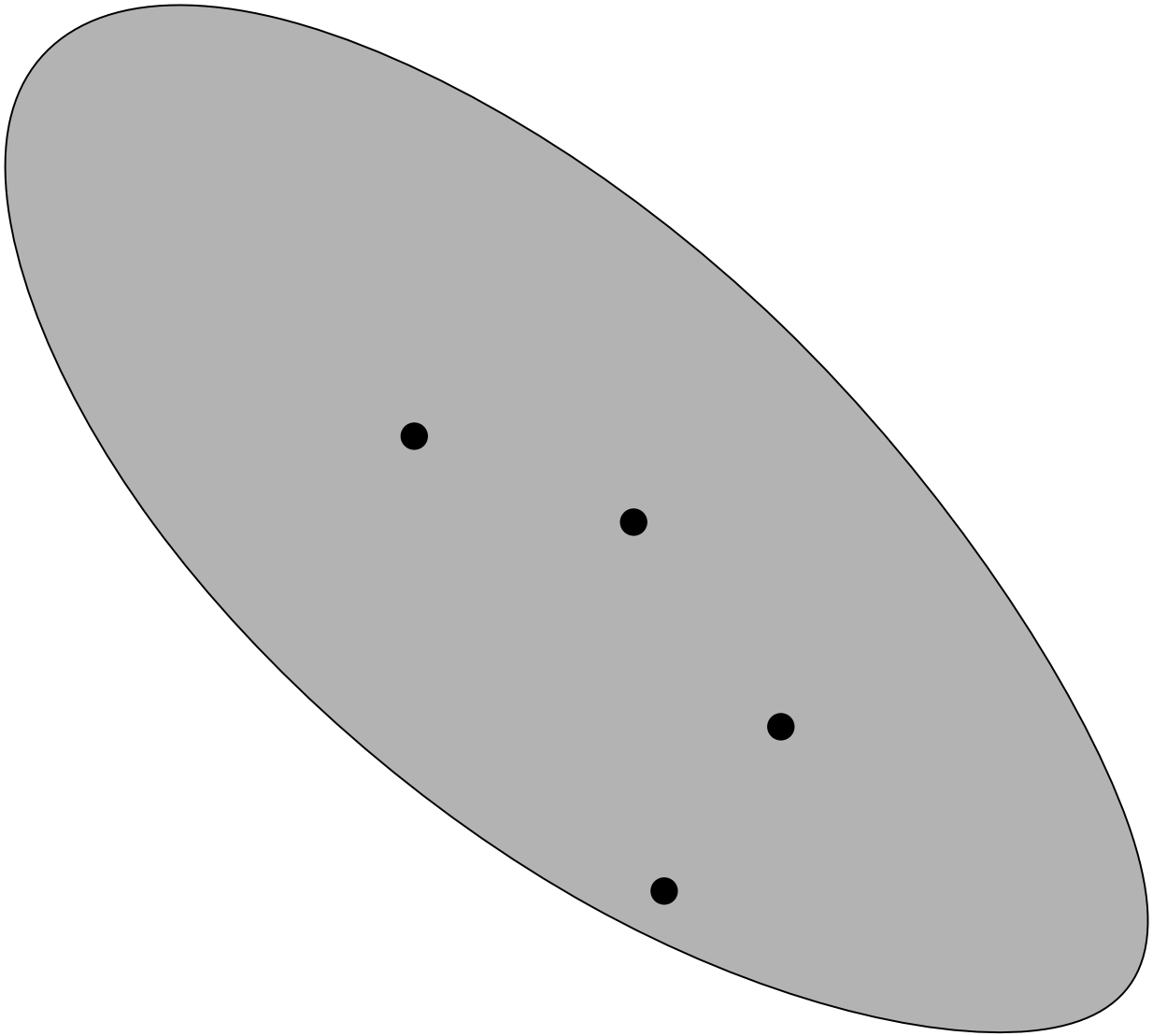

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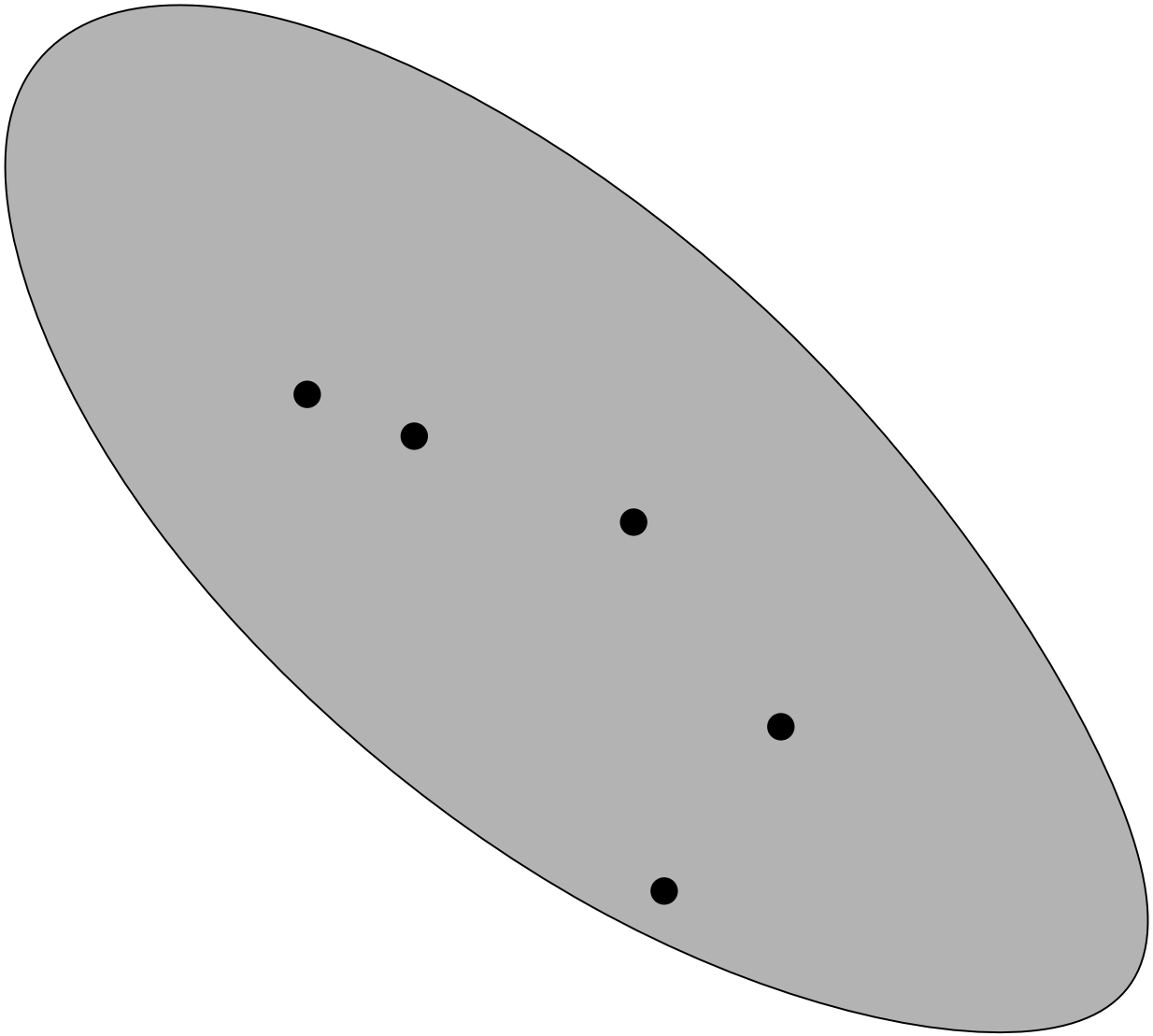

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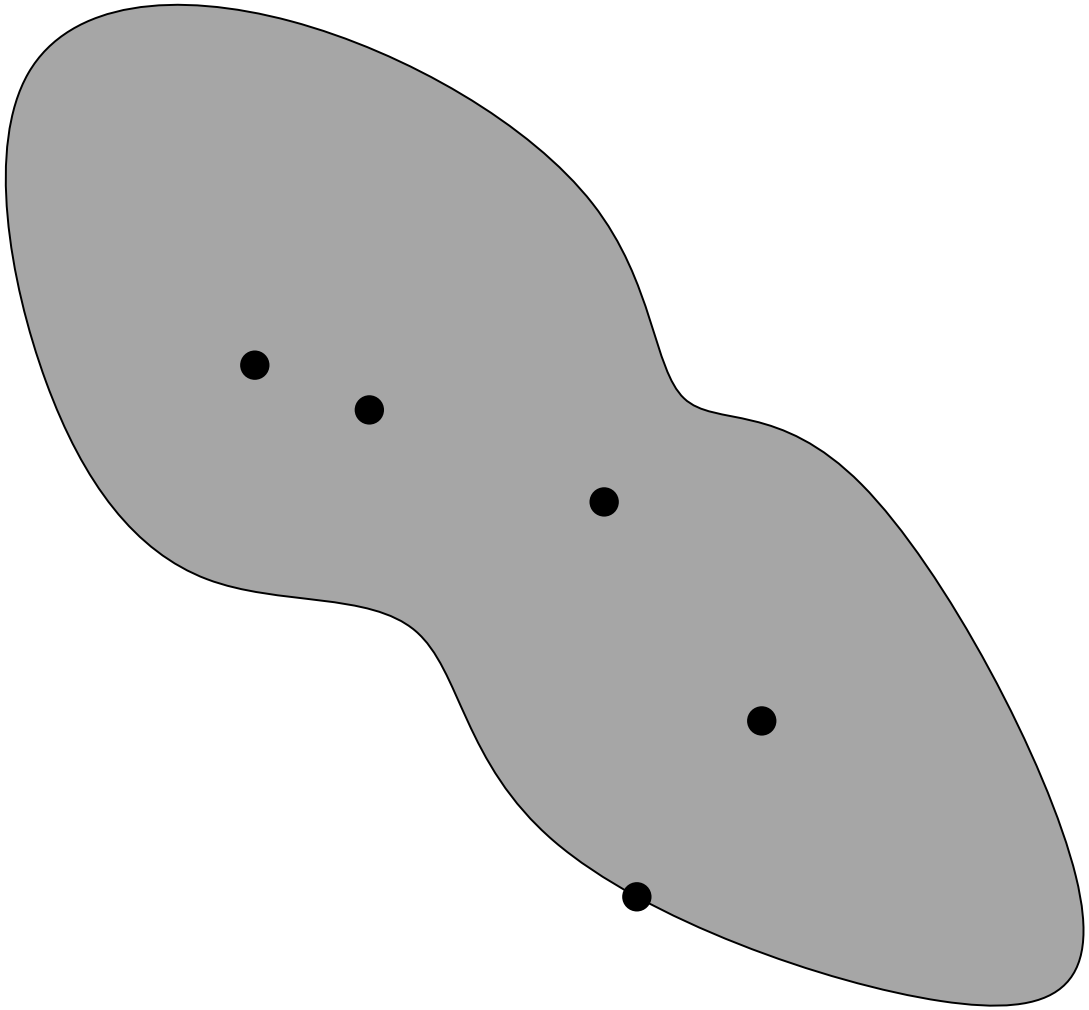

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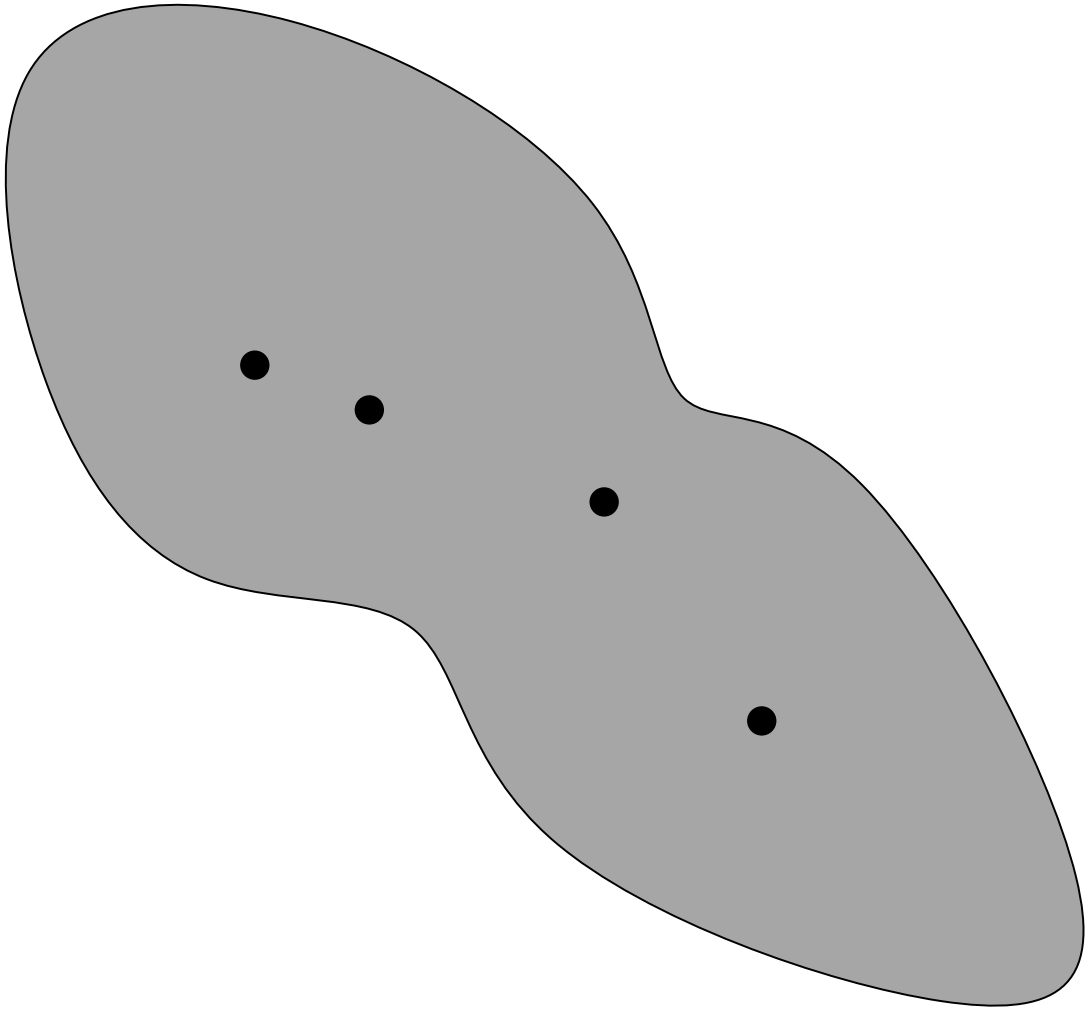

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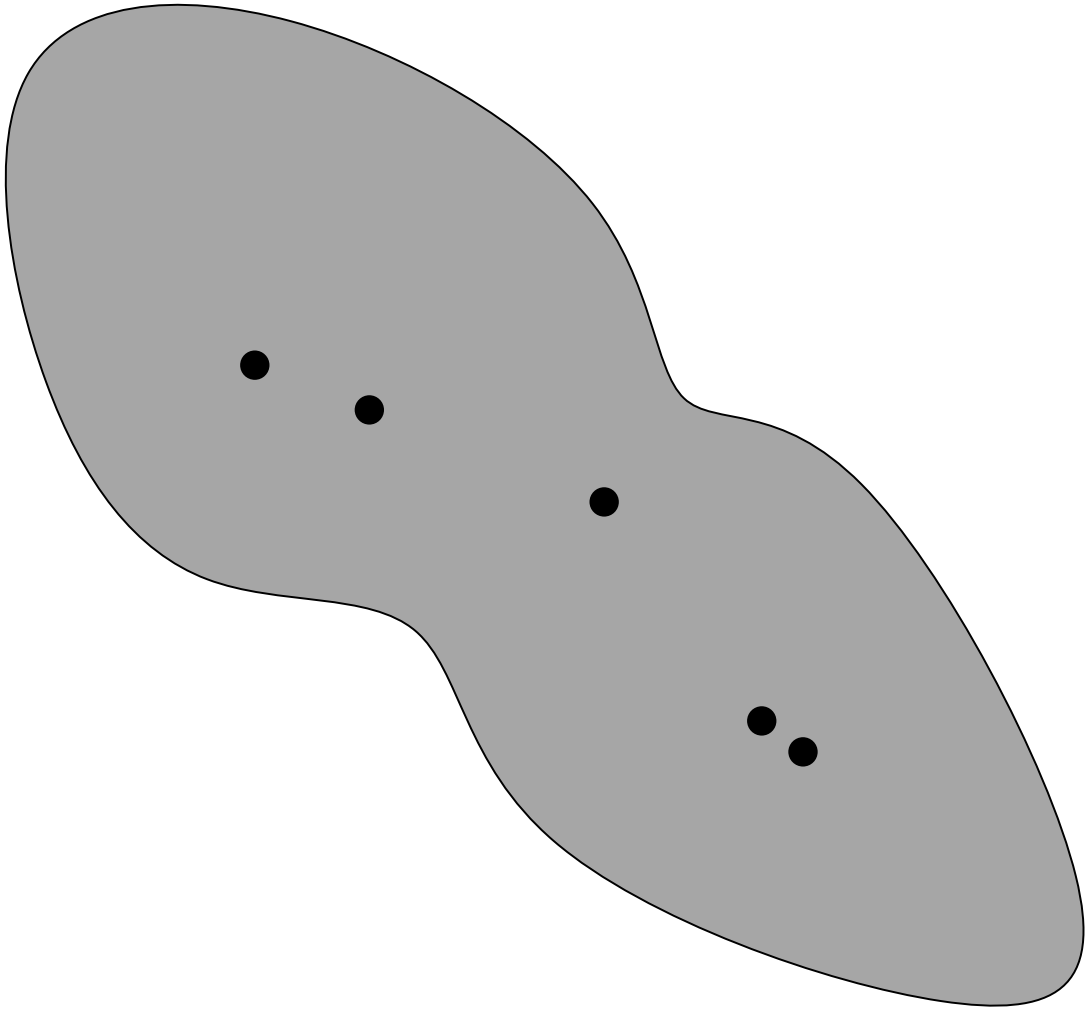

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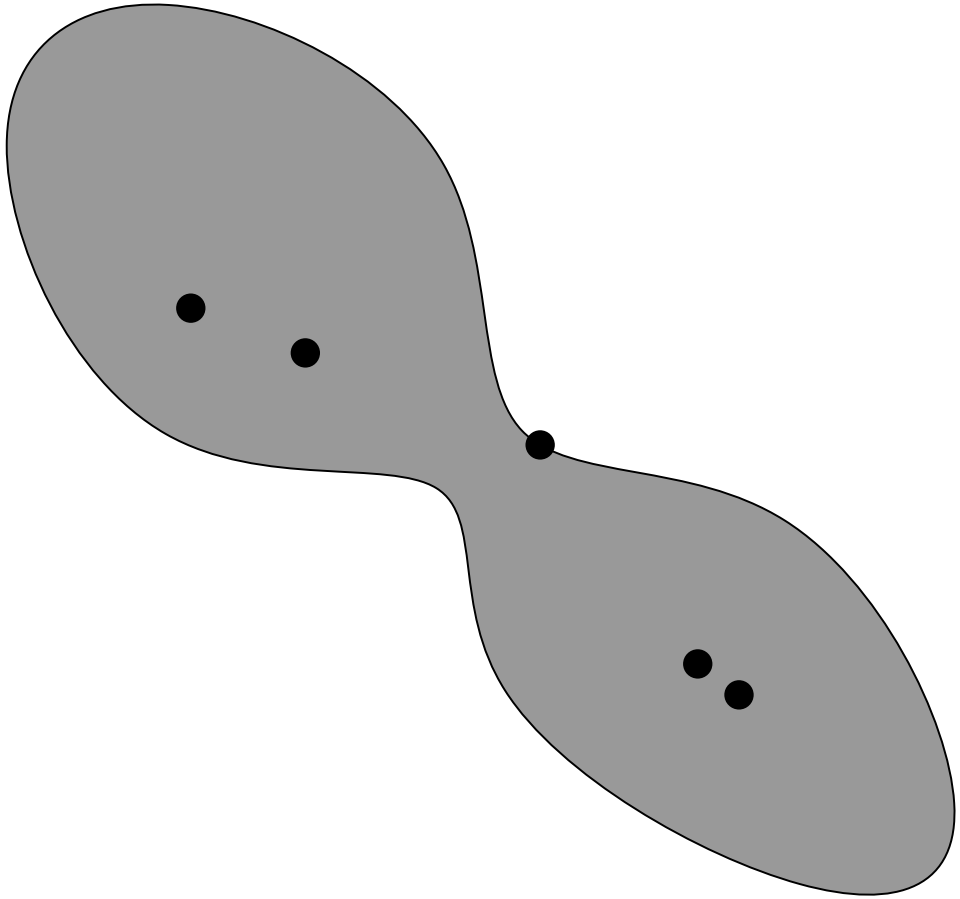

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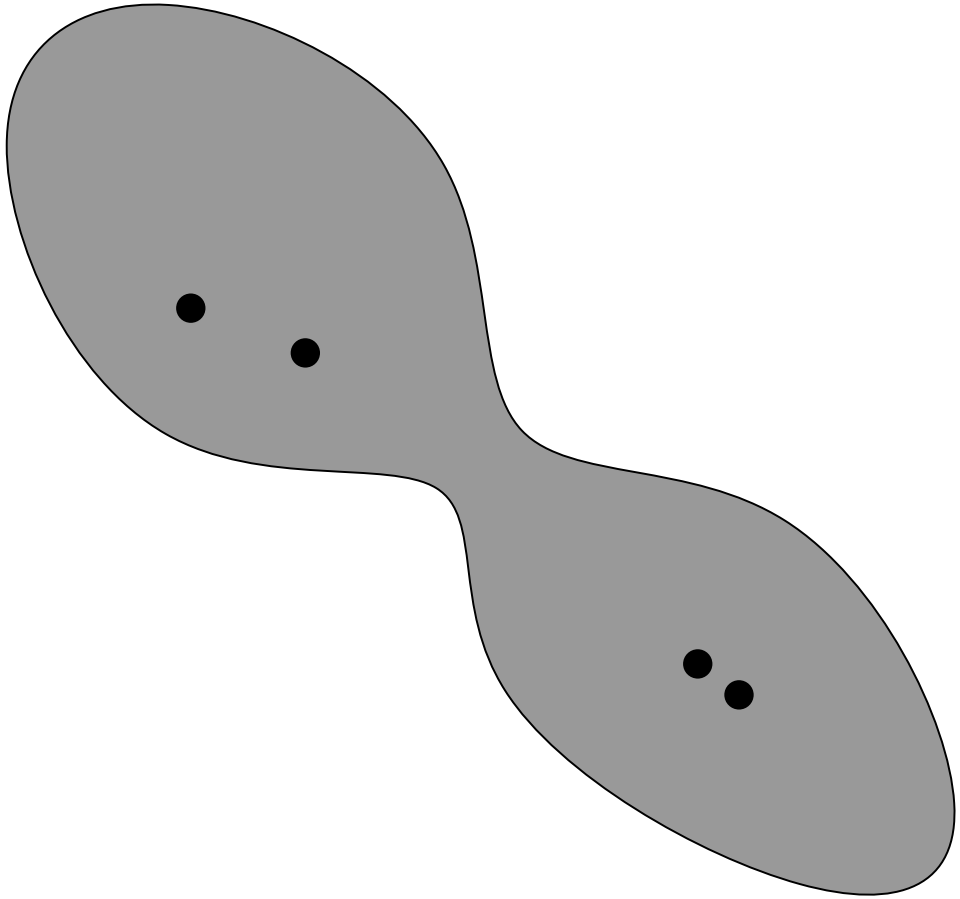

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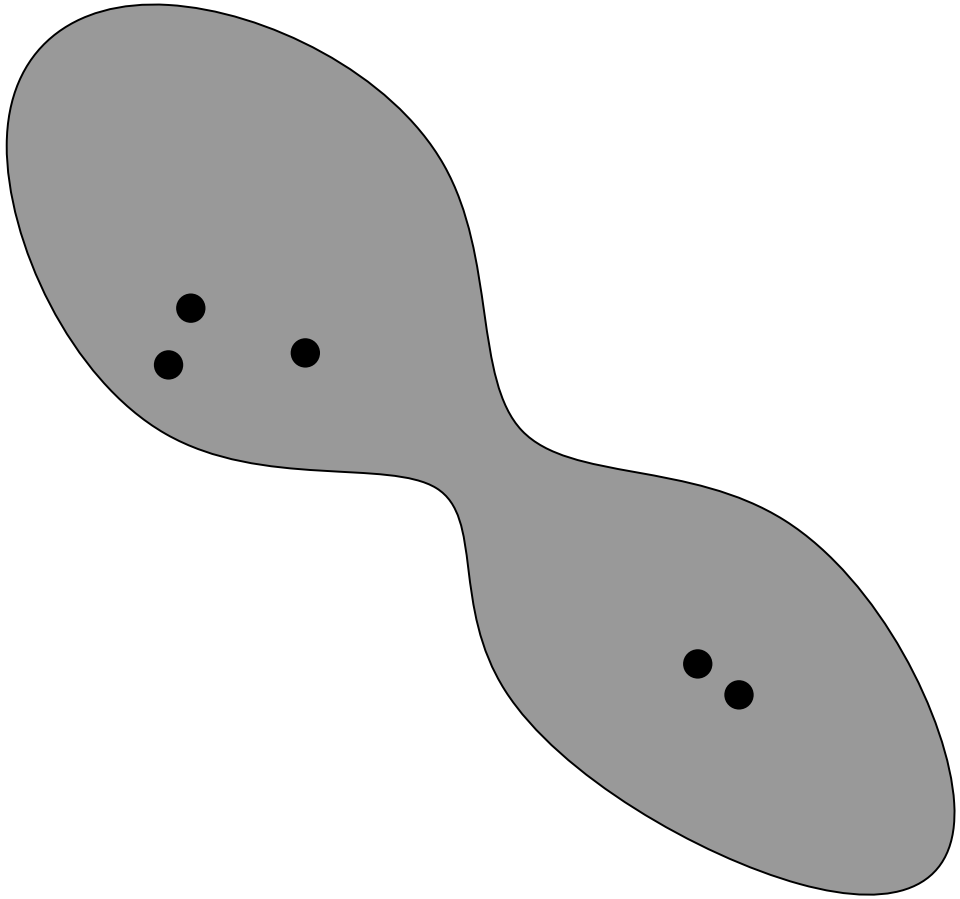

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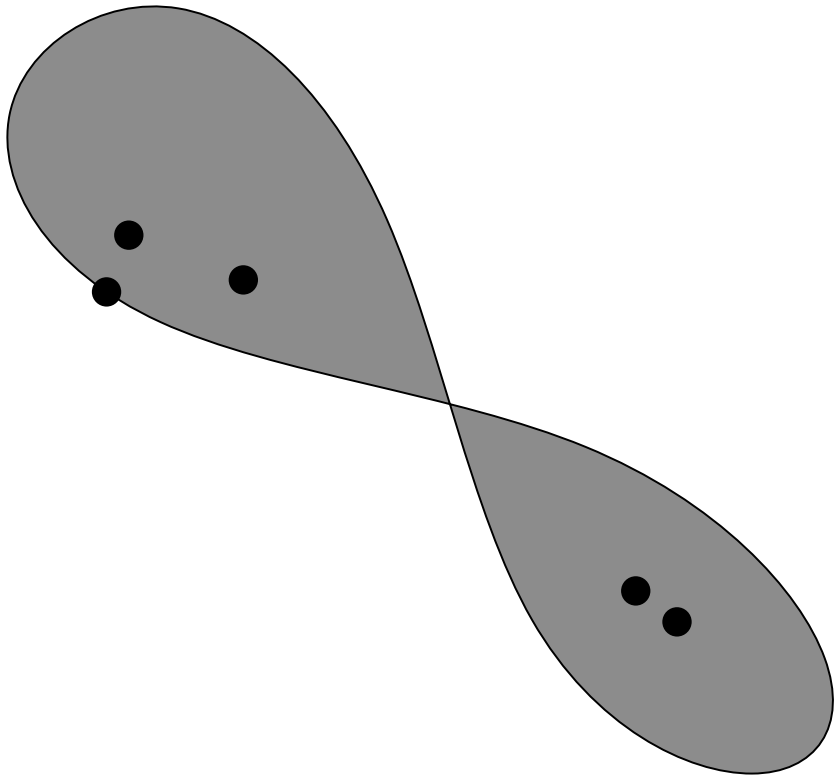

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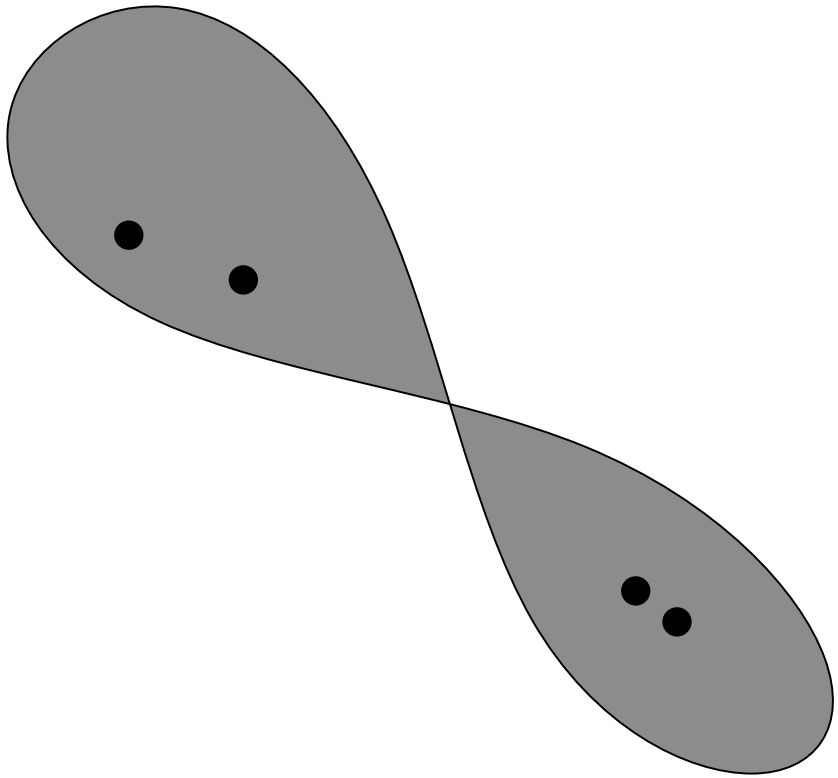

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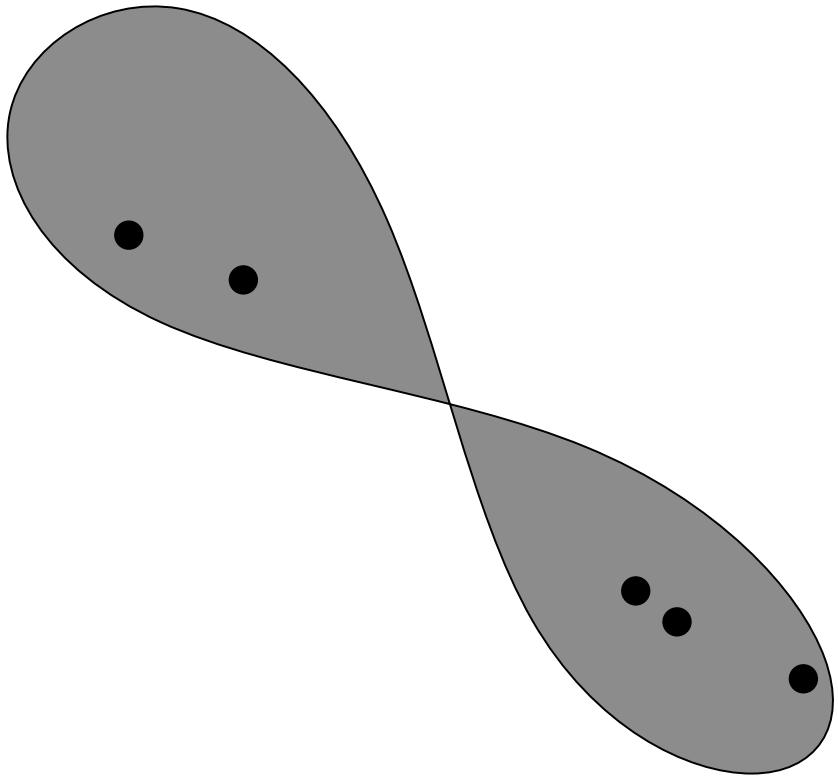

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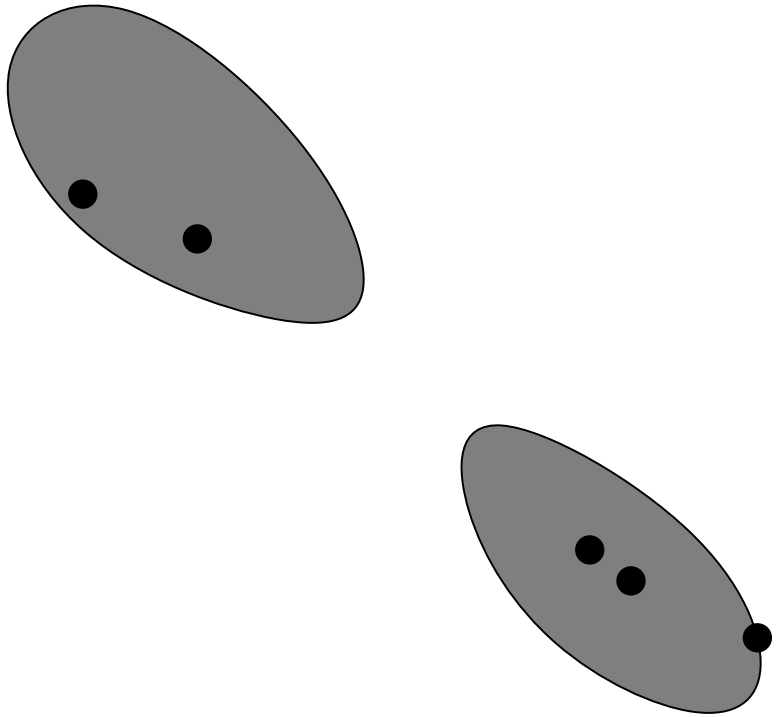

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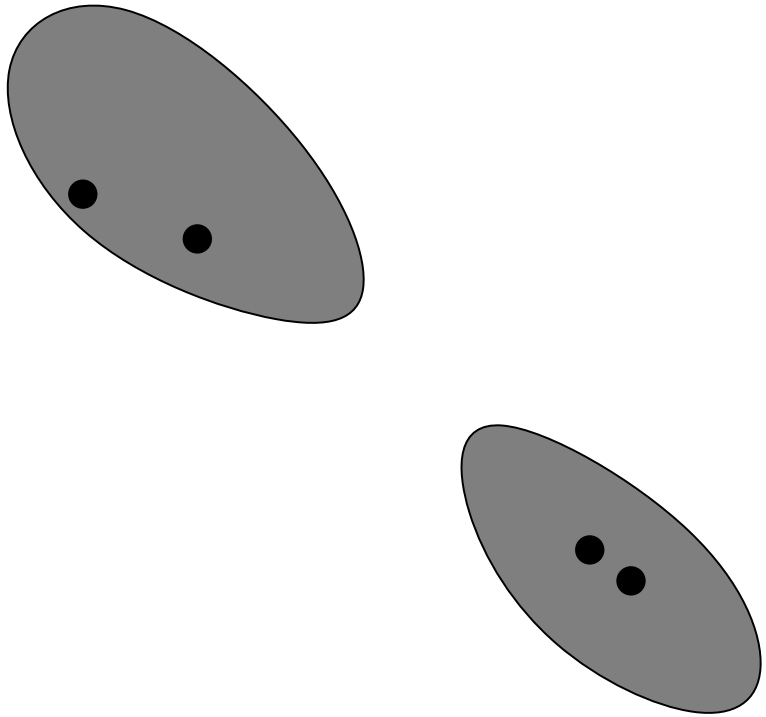

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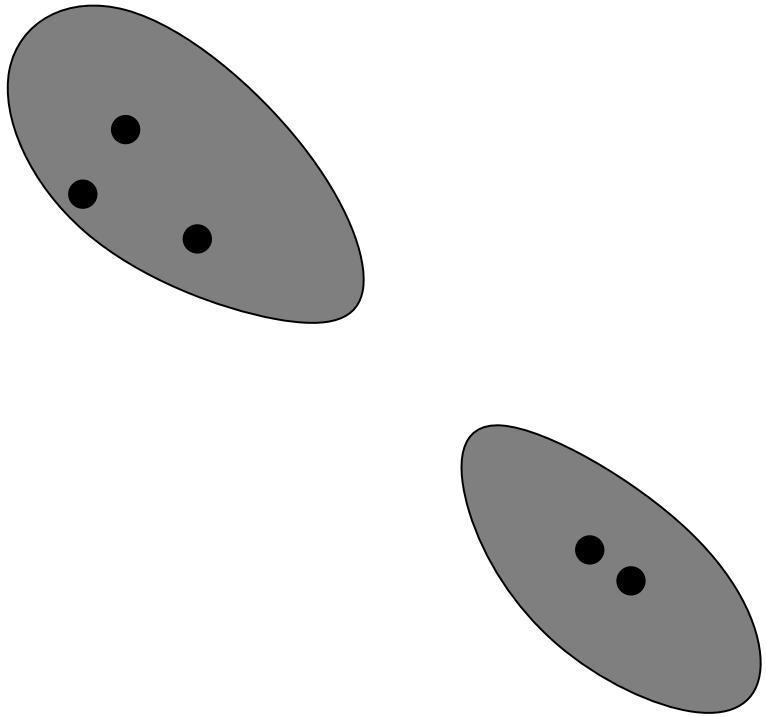

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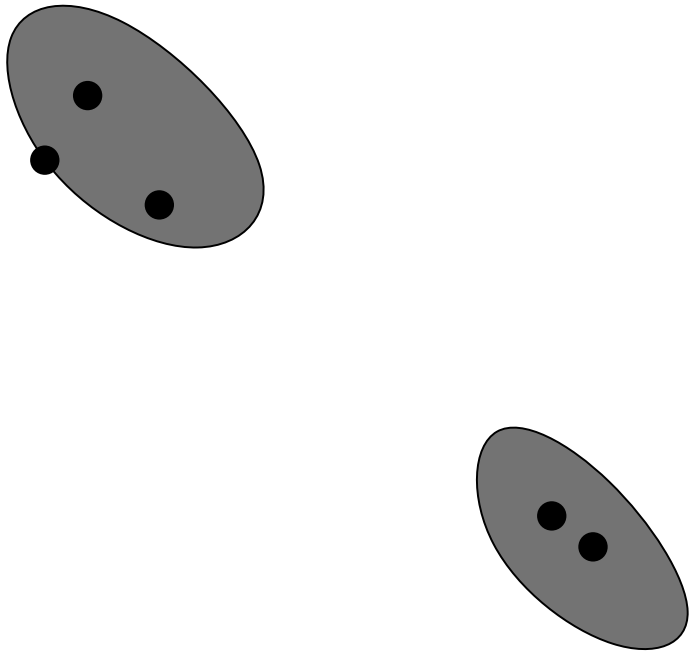

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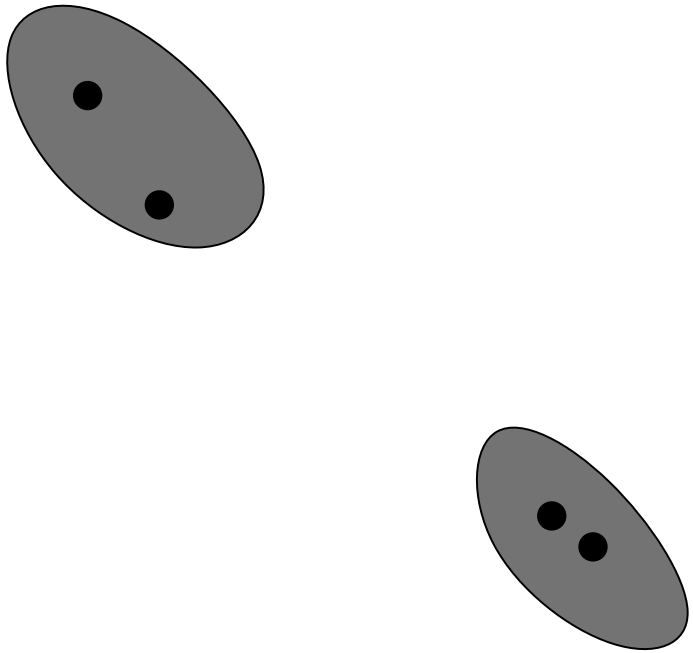

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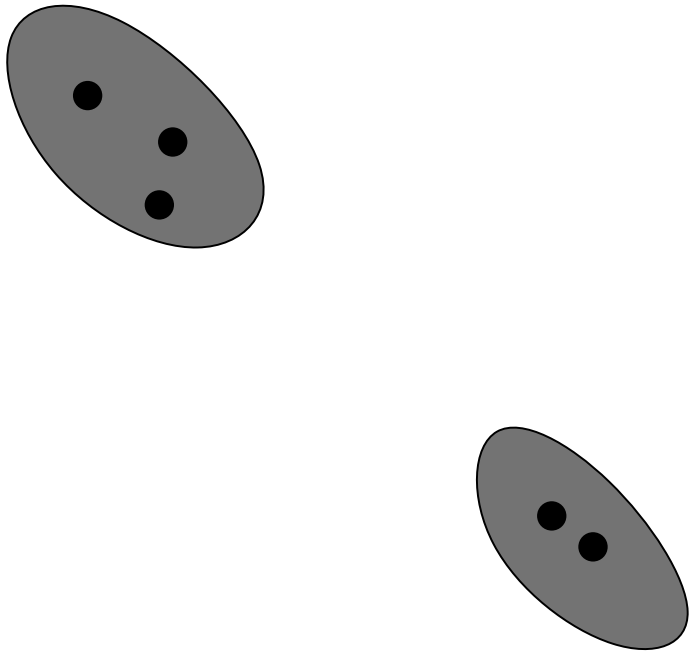

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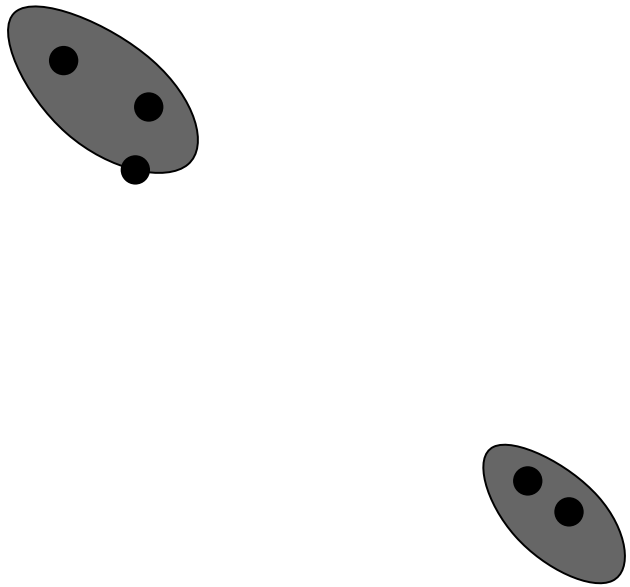

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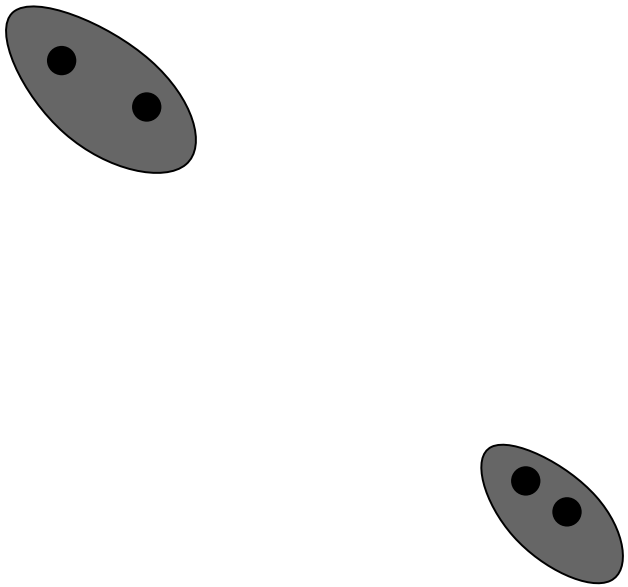

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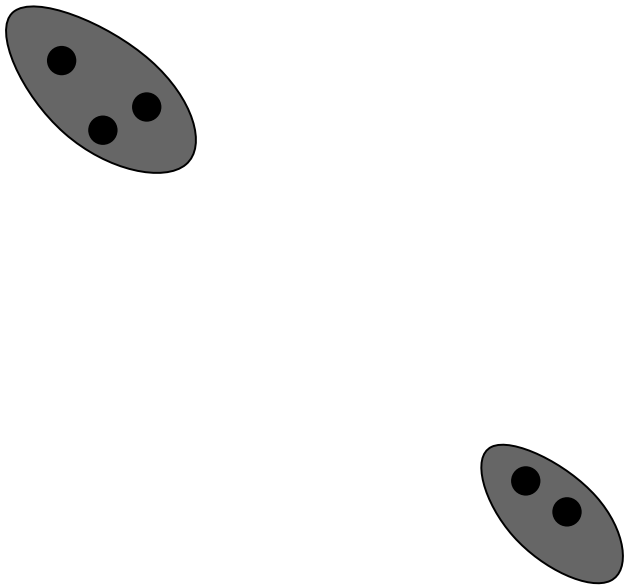

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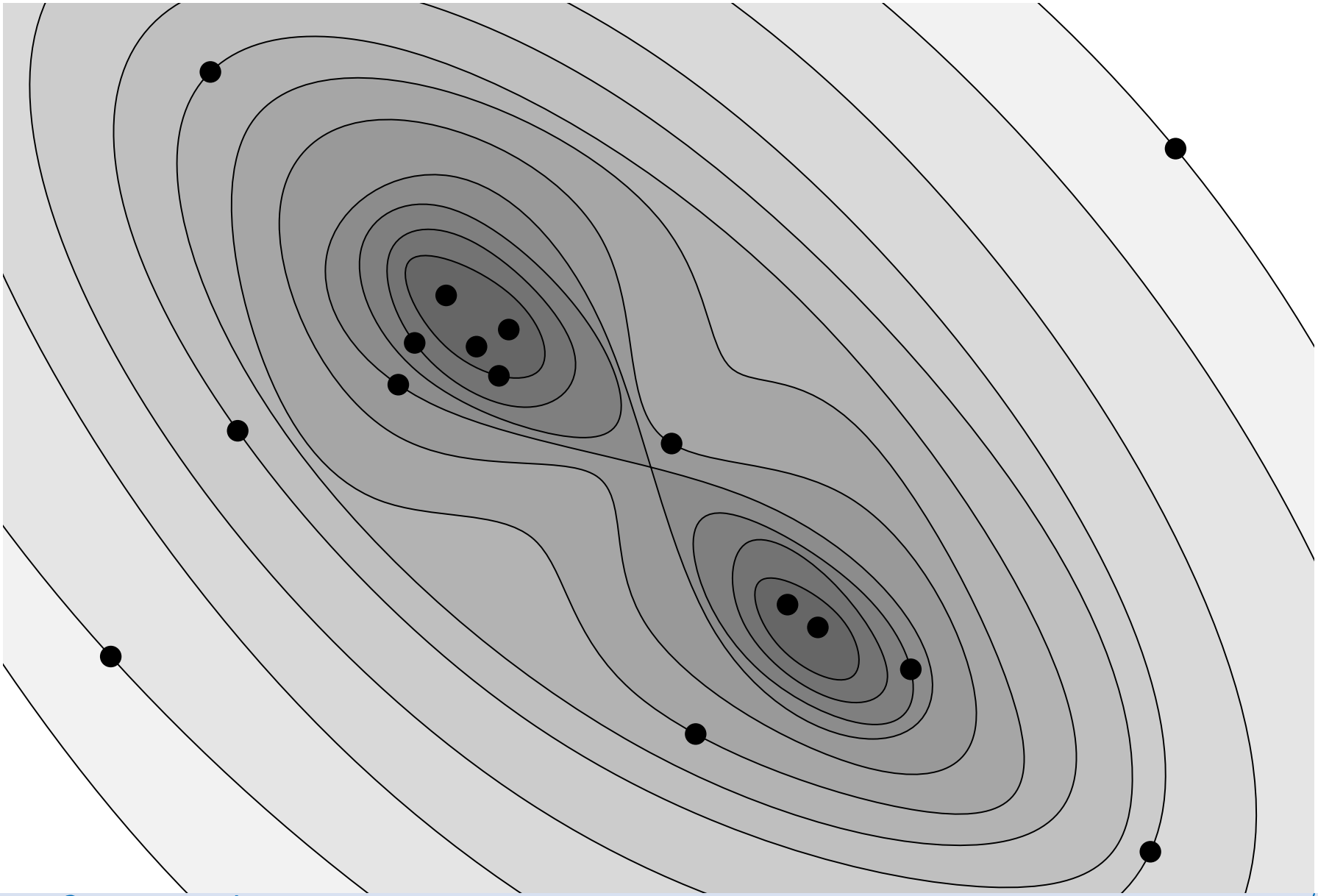
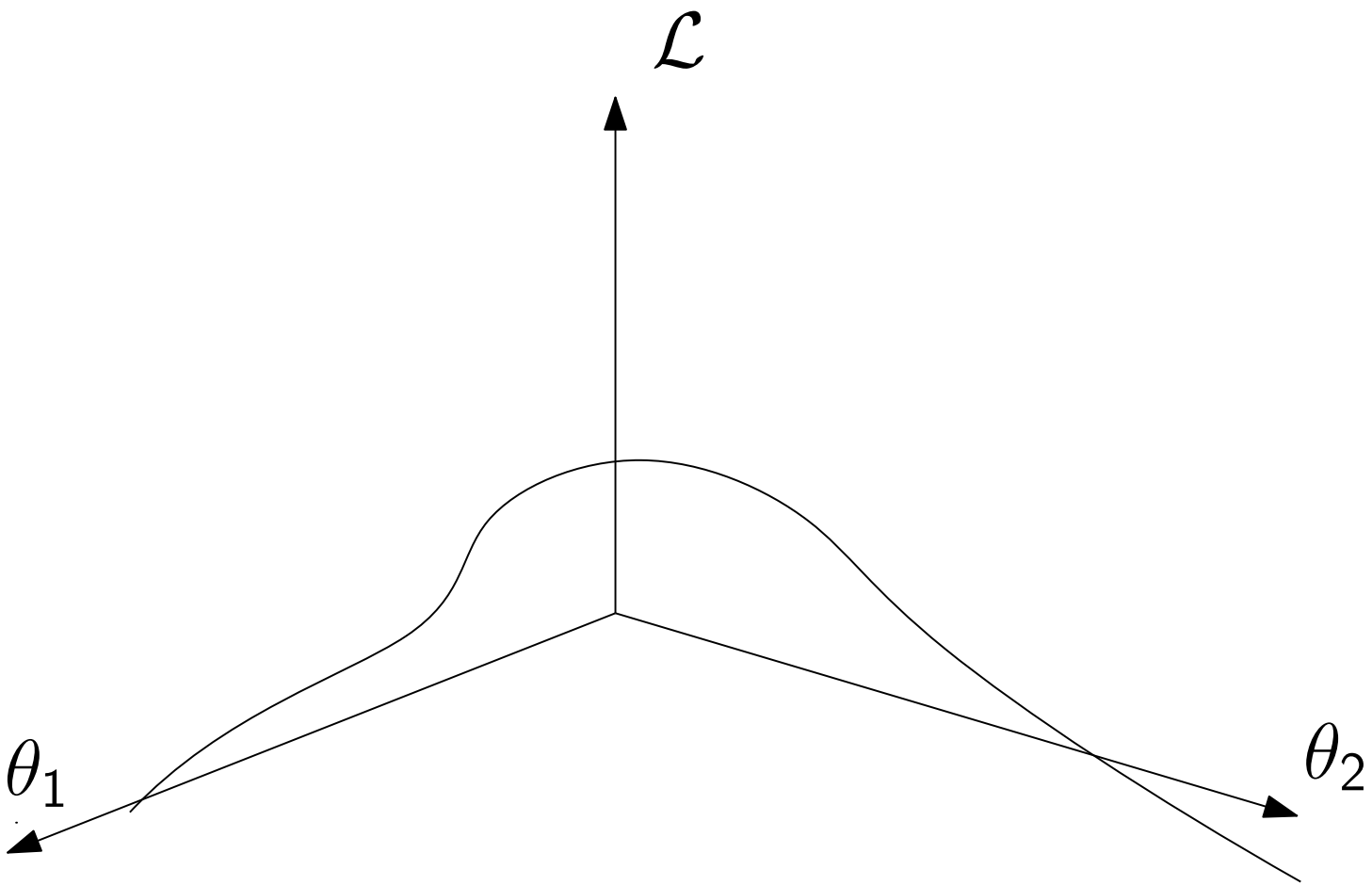


Nested sampling

- The set of dead points are posterior samples with an appropriate weighting factor
- They can also be used to calculate evidences, since it sequentially updates the priors.
- The current set of live points is useful for performing clustering and constructing new proposed points.
- Algorithm terminates when prior has been compressed onto (and past) the posterior bulk (typical set).

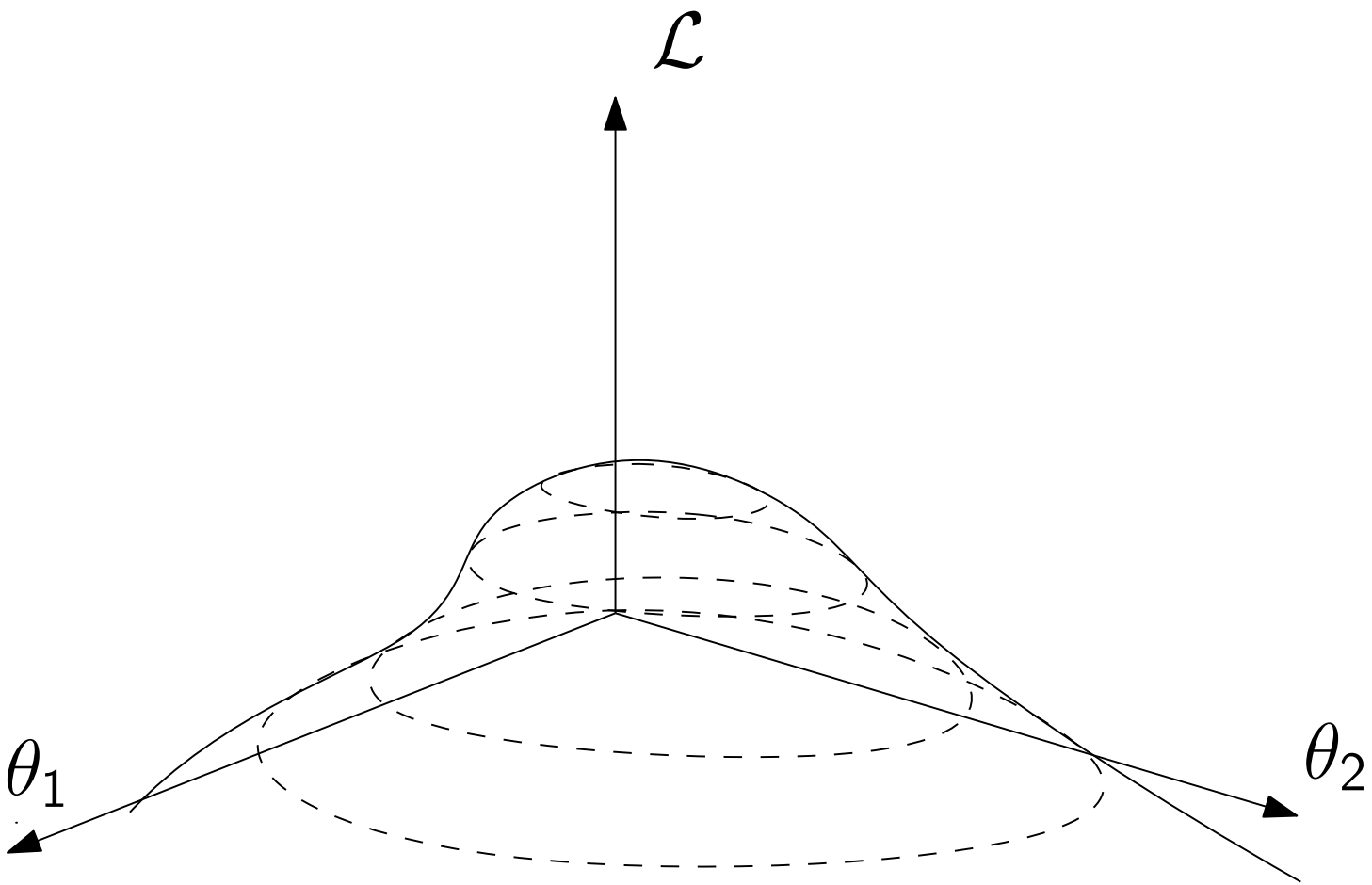
Nested Sampling

Calculating evidences



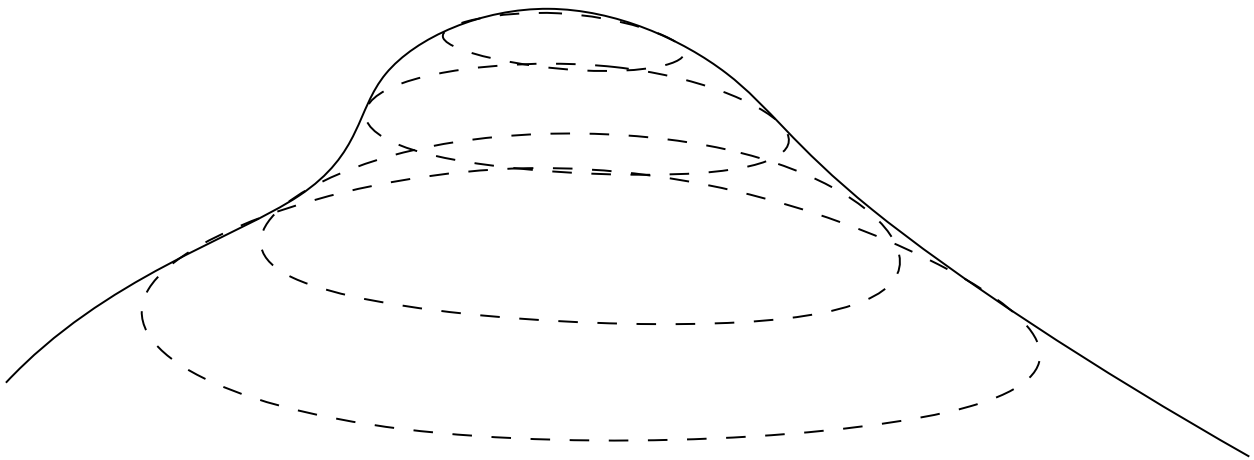
Nested Sampling

Calculating evidences



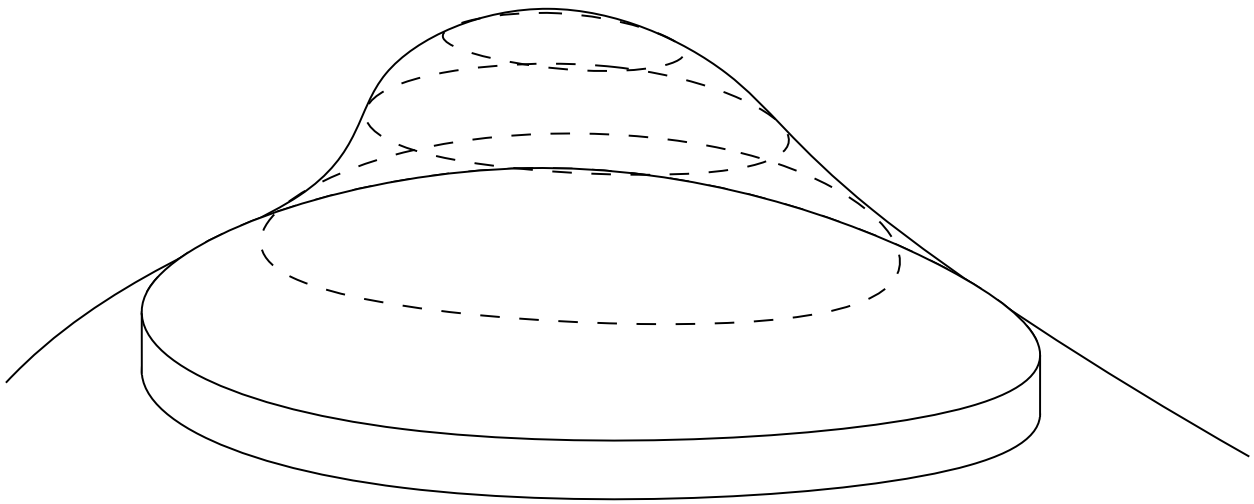
Nested Sampling

Calculating evidences



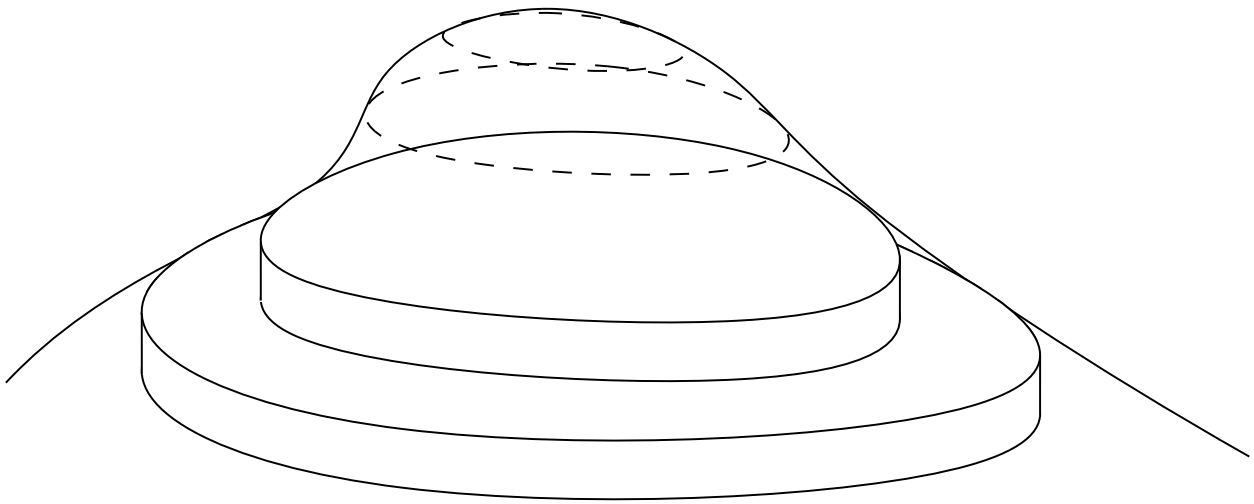
Nested Sampling

Calculating evidences



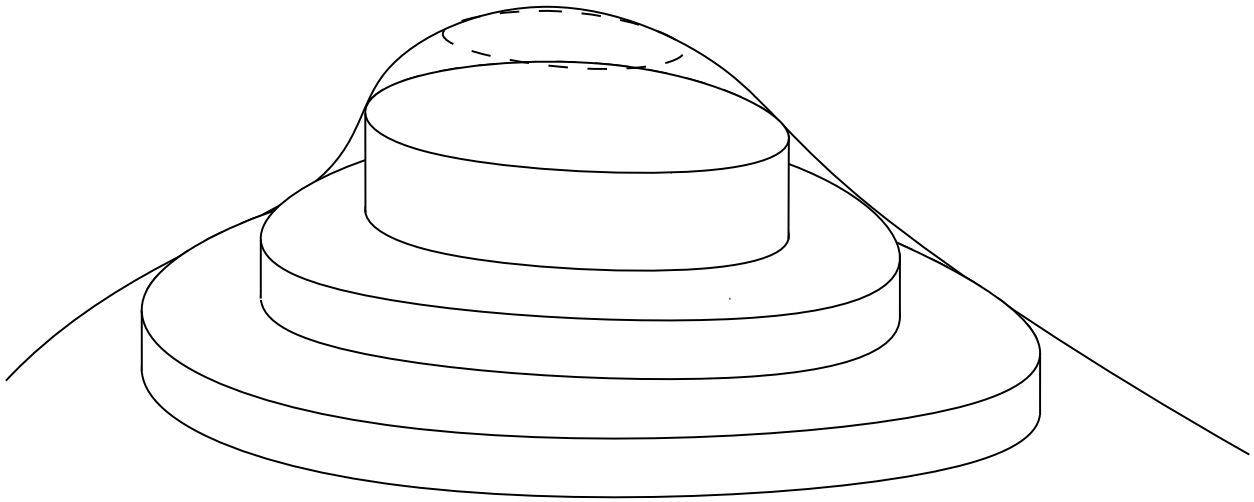
Nested Sampling

Calculating evidences



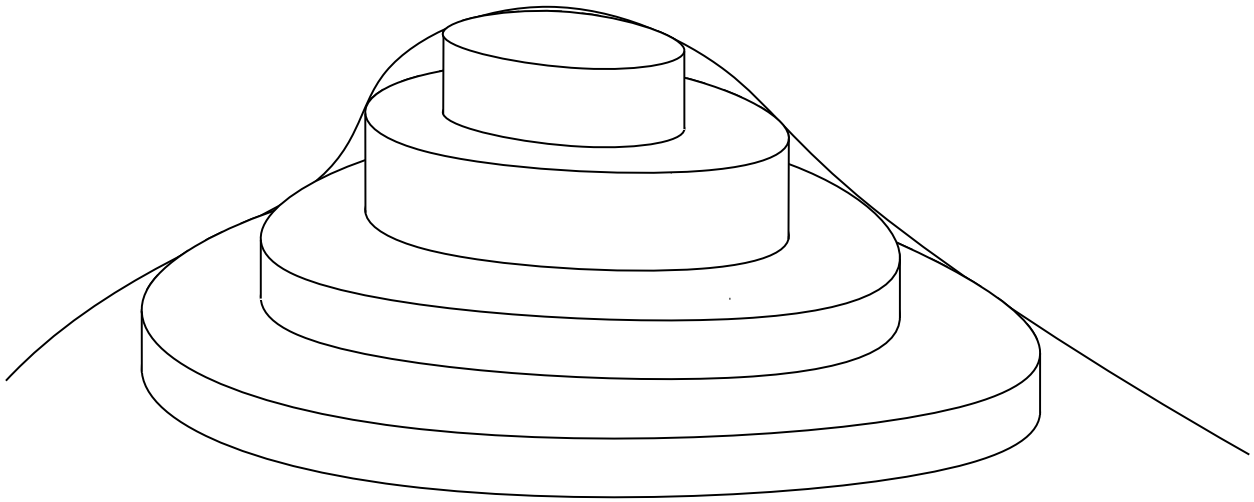
Nested Sampling

Calculating evidences



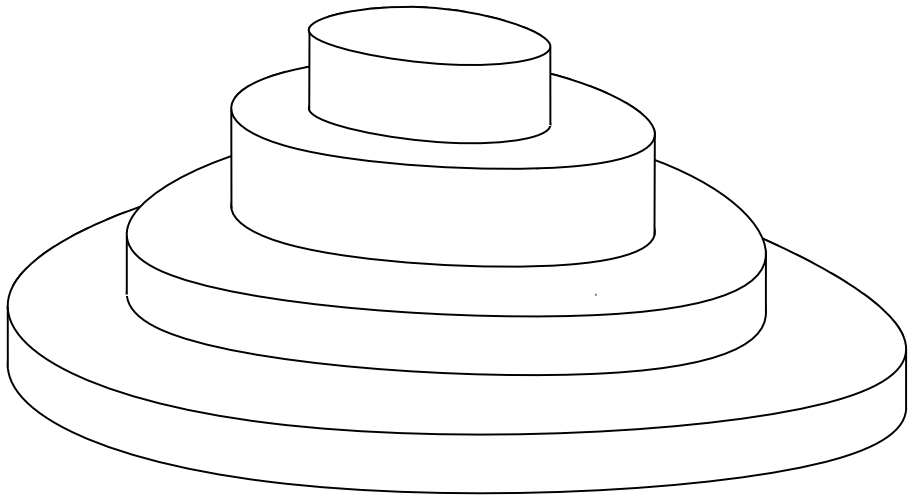
Nested Sampling

Calculating evidences



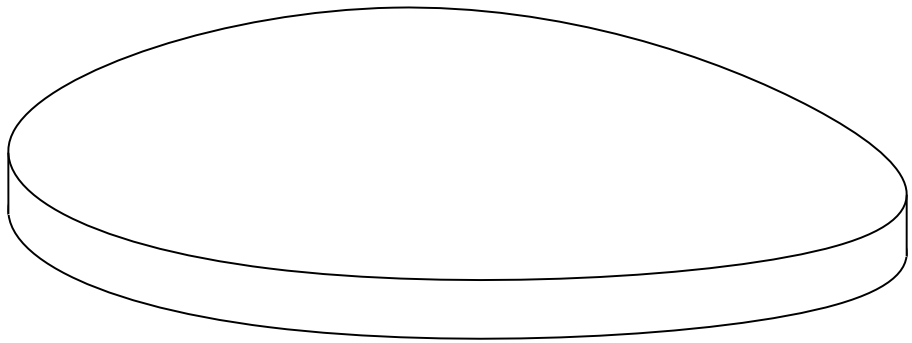
Nested Sampling

Calculating evidences



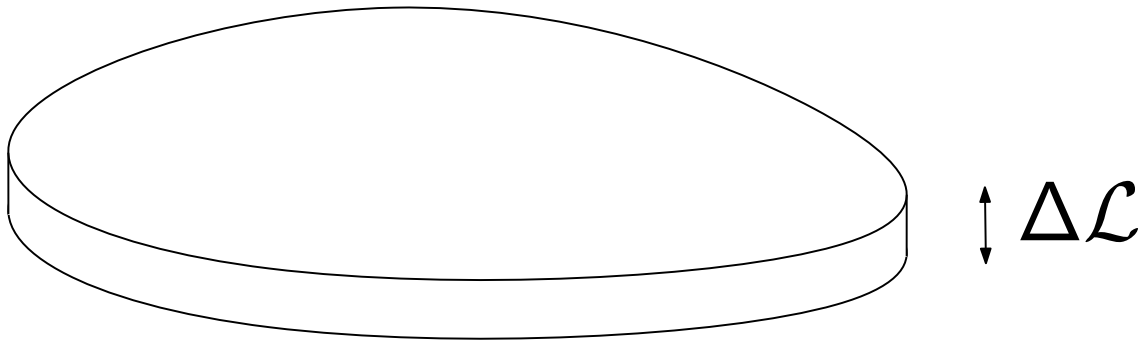
Nested Sampling

Calculating evidences



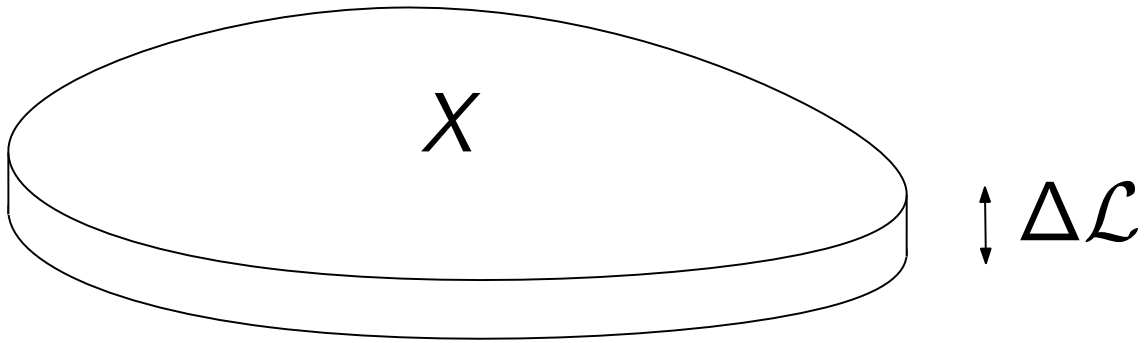
Nested Sampling

Calculating evidences



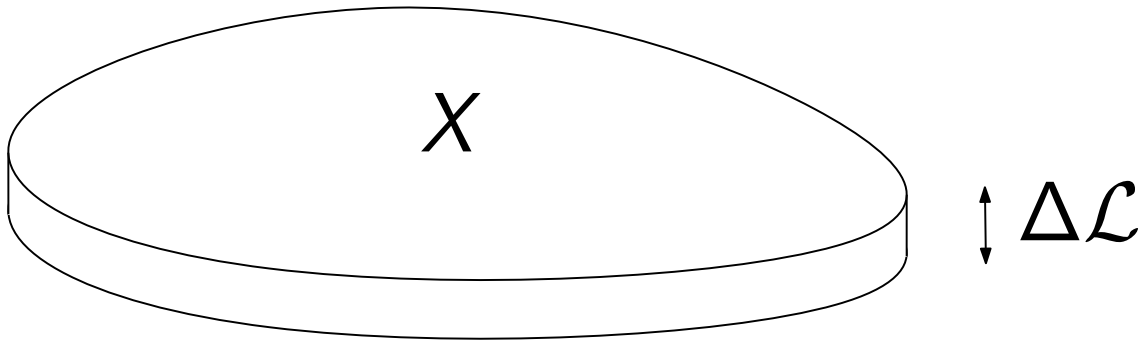
Nested Sampling

Calculating evidences



Nested Sampling

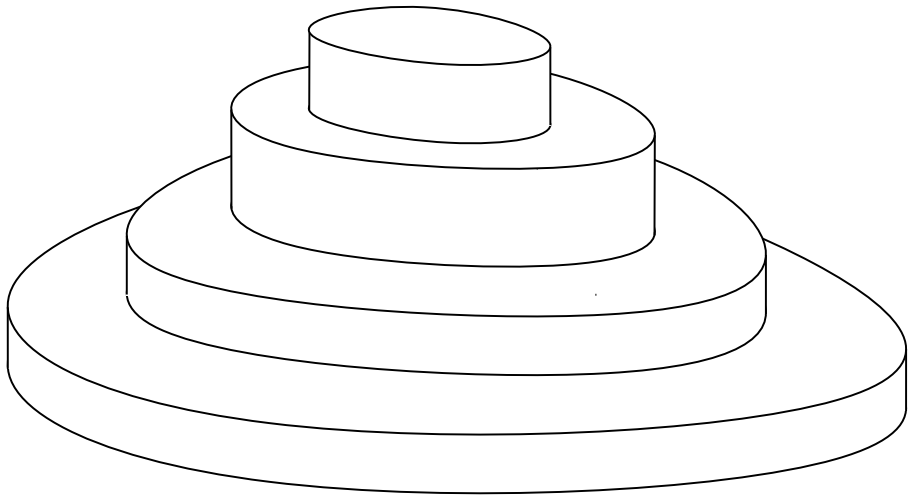
Calculating evidences



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

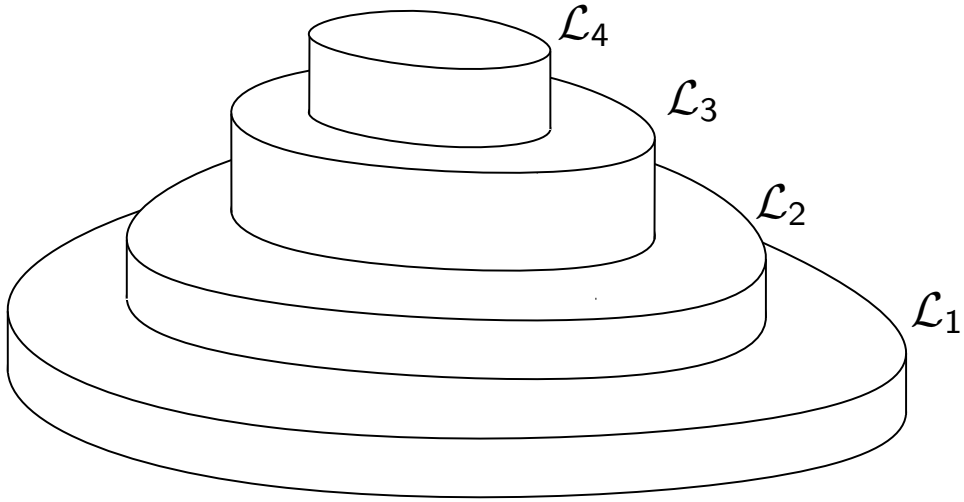
Nested Sampling

Calculating evidences



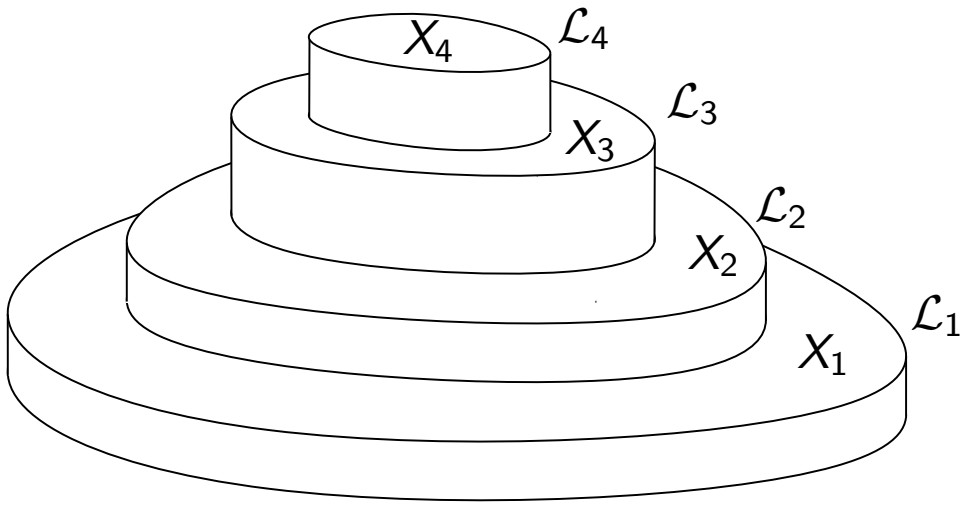
Nested Sampling

Calculating evidences



Nested Sampling

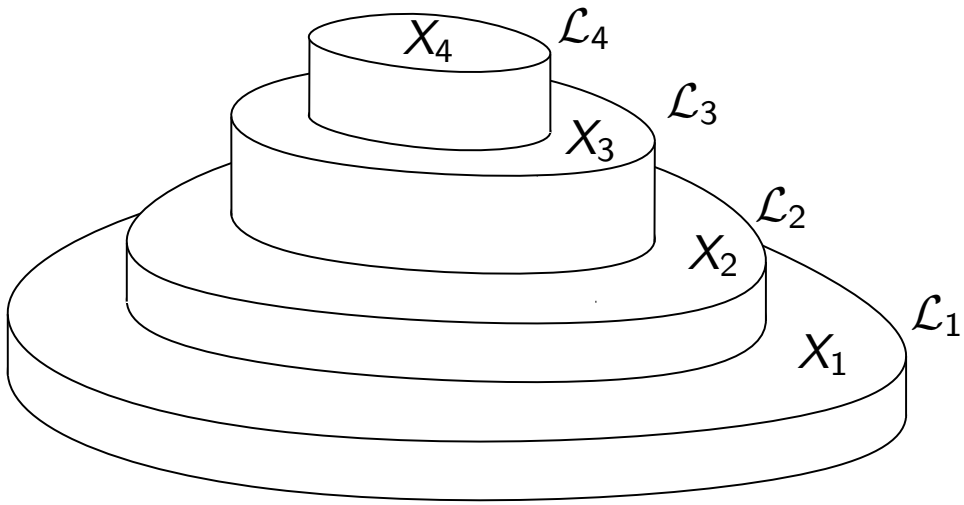
Calculating evidences



Nested Sampling

Calculating evidences

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



Nested Sampling

Exponential volume contraction

- At each iteration, the likelihood contour will shrink in volume by $\approx 1/n$.
- Nested sampling zooms in to the peak of the posterior *exponentially*.

$$\mathcal{Z} \approx \sum_i \Delta\mathcal{L}_i X_i, \qquad X_{i+1} \approx \frac{n}{n+1} X_i, \qquad X_0 = 1$$

- Although this is only approximate, we can quantify the error

$$P(X_{i+1}|X_i) = \frac{1}{nX_i}\left(\frac{X_{i+1}}{X_i}\right)^{n-1}[0 < X_i < X_{i+1}]$$

- Integral can be expressed in one of two ways

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

Sampling from a hard likelihood constraint

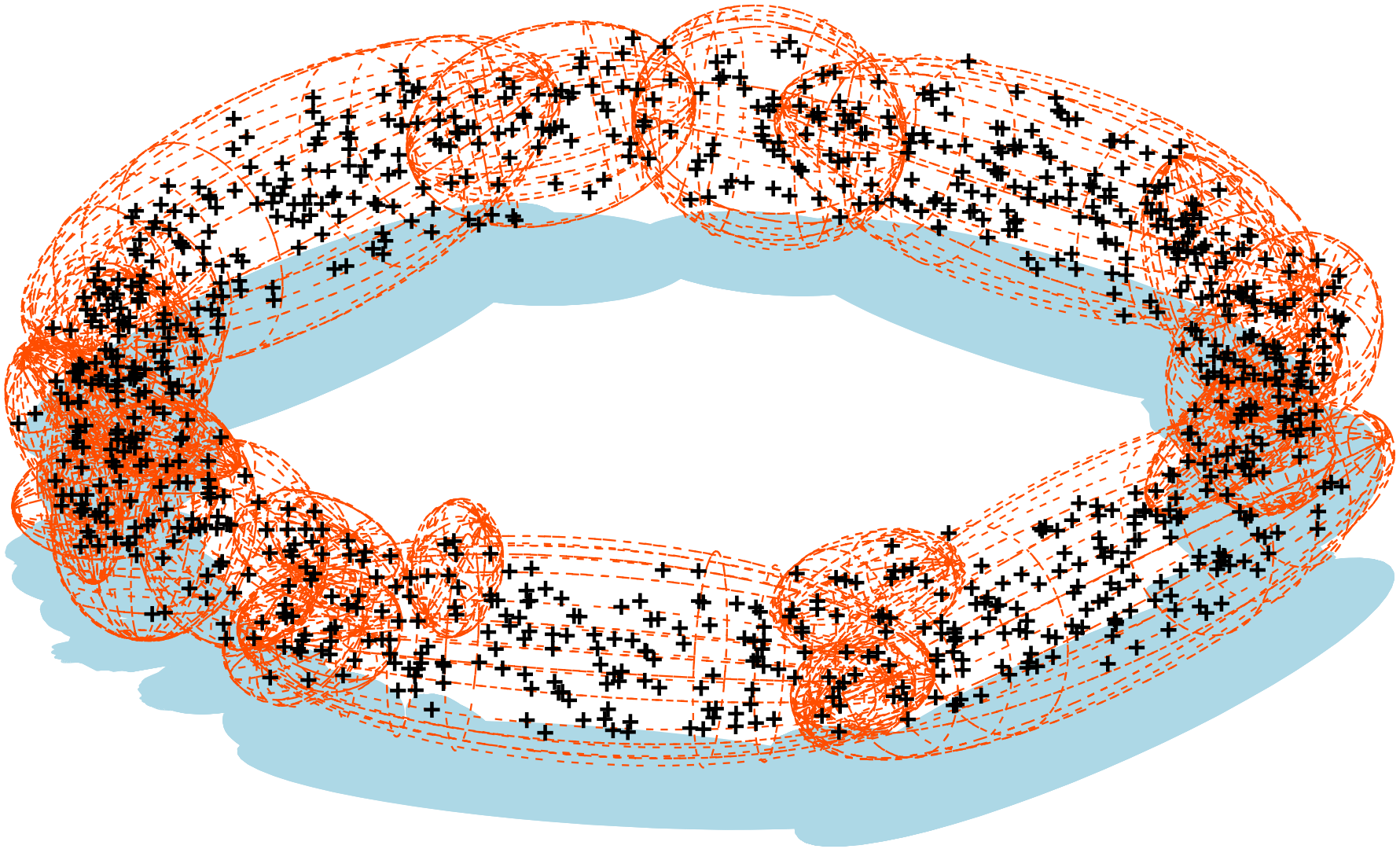
"It is not the purpose of this introductory paper to develop the technology of navigation within such a volume. We merely note that exploring a hard-edged likelihood-constrained domain should prove to be neither more nor less demanding than exploring a likelihood-weighted space."

— *John Skilling*

- Most of the work in NS to date has been in attempting to implement a hard-edged sampler in the NS meta-algorithm.
- `https://projecteuclid.org/euclid.ba/1340370944`

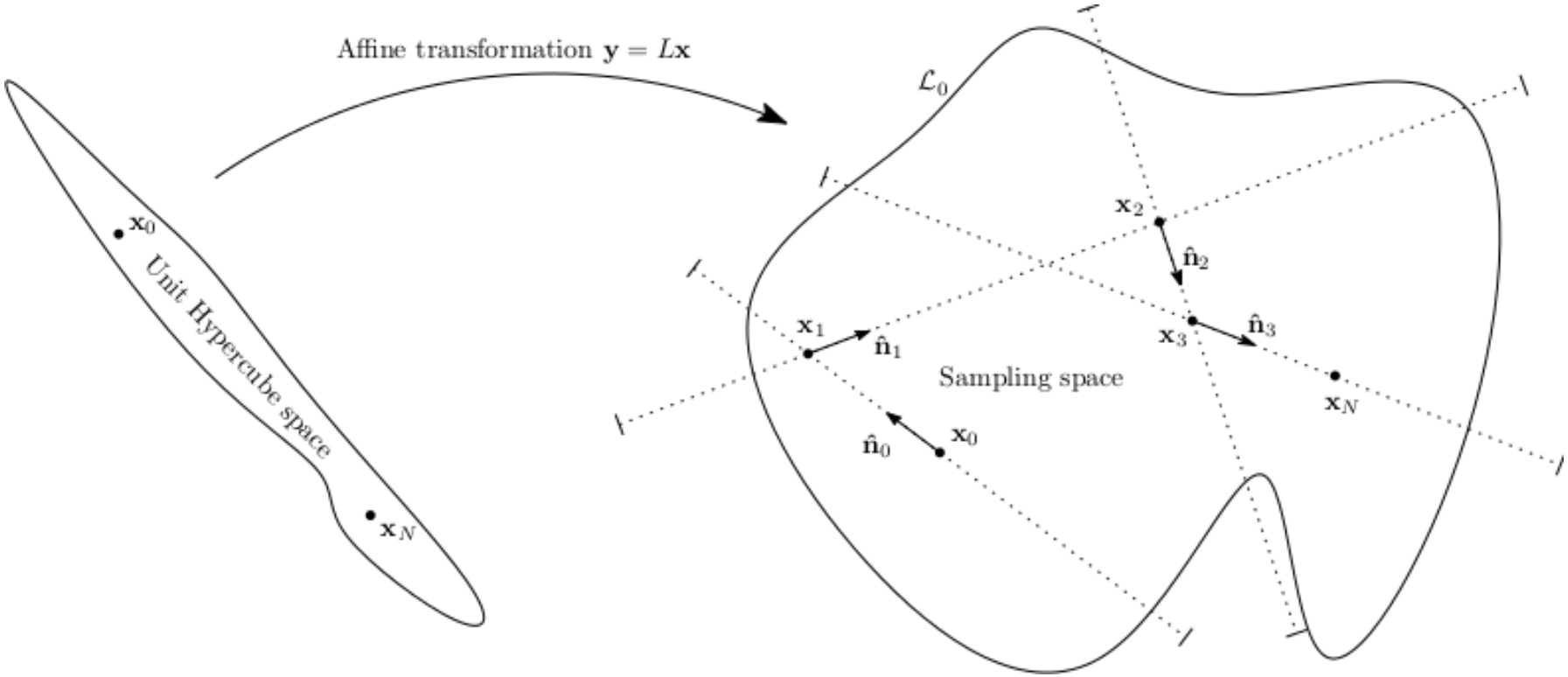
MultiNest

arXiv:0809.3437 arXiv:0704.3704 arXiv:1306.2144, Feroz, Hobson



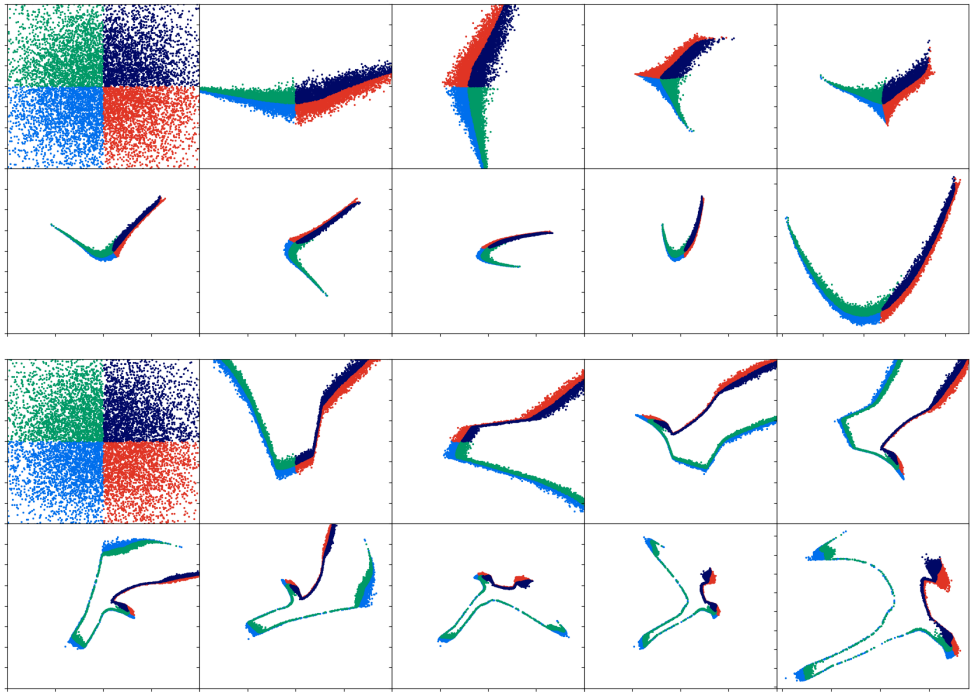
PolyChord

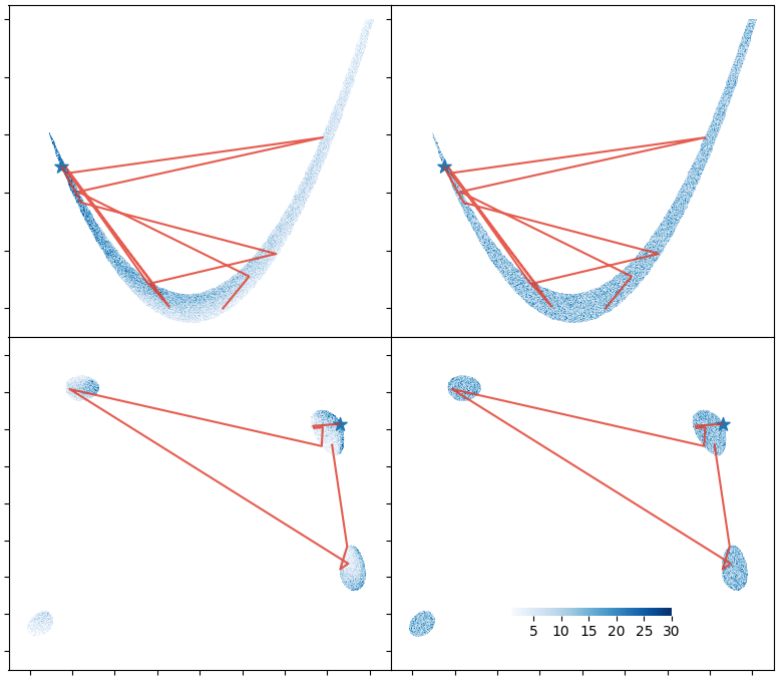
arXiv:1502.01856 arXiv:1506.00171, Handley, Hobson, Lasenby



NeuralNest

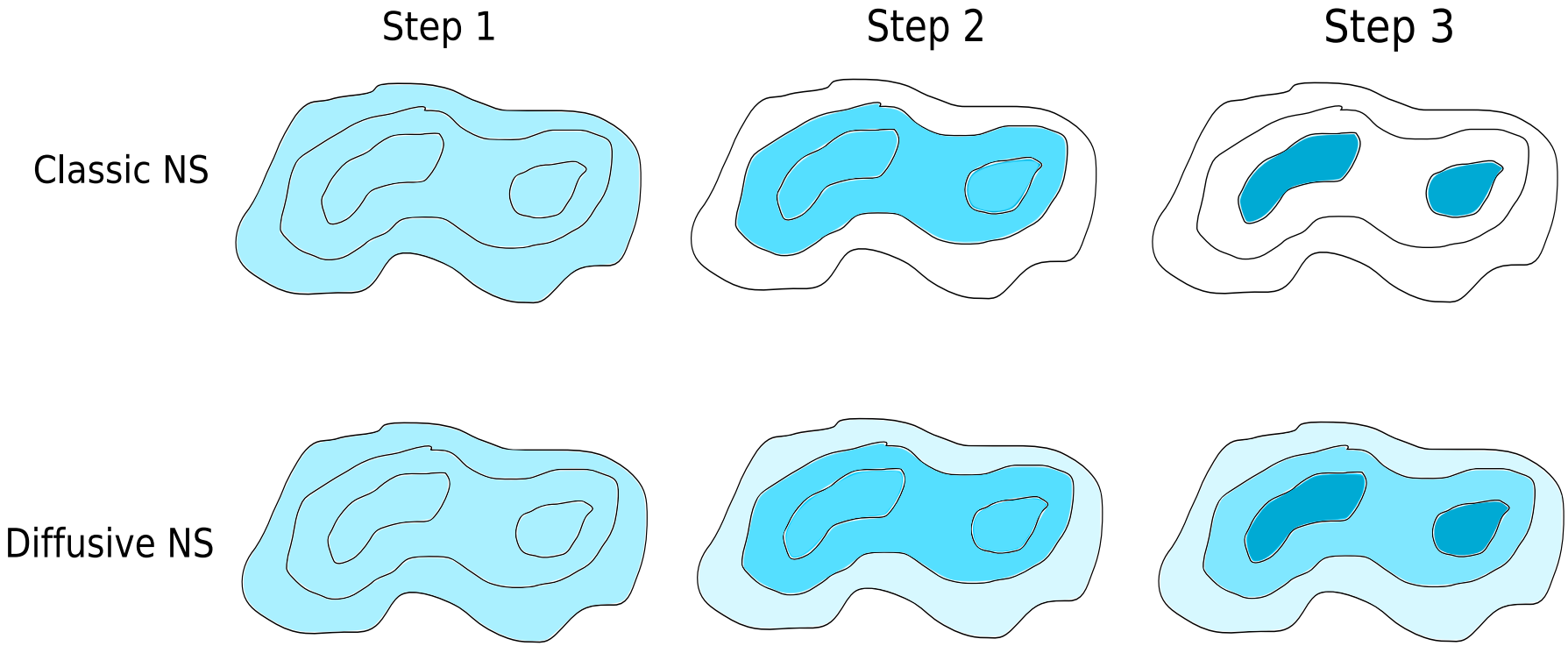
arXiv:1903.10860, Moss





Diffusive nested sampling

arXiv:0912.2380, Brewer

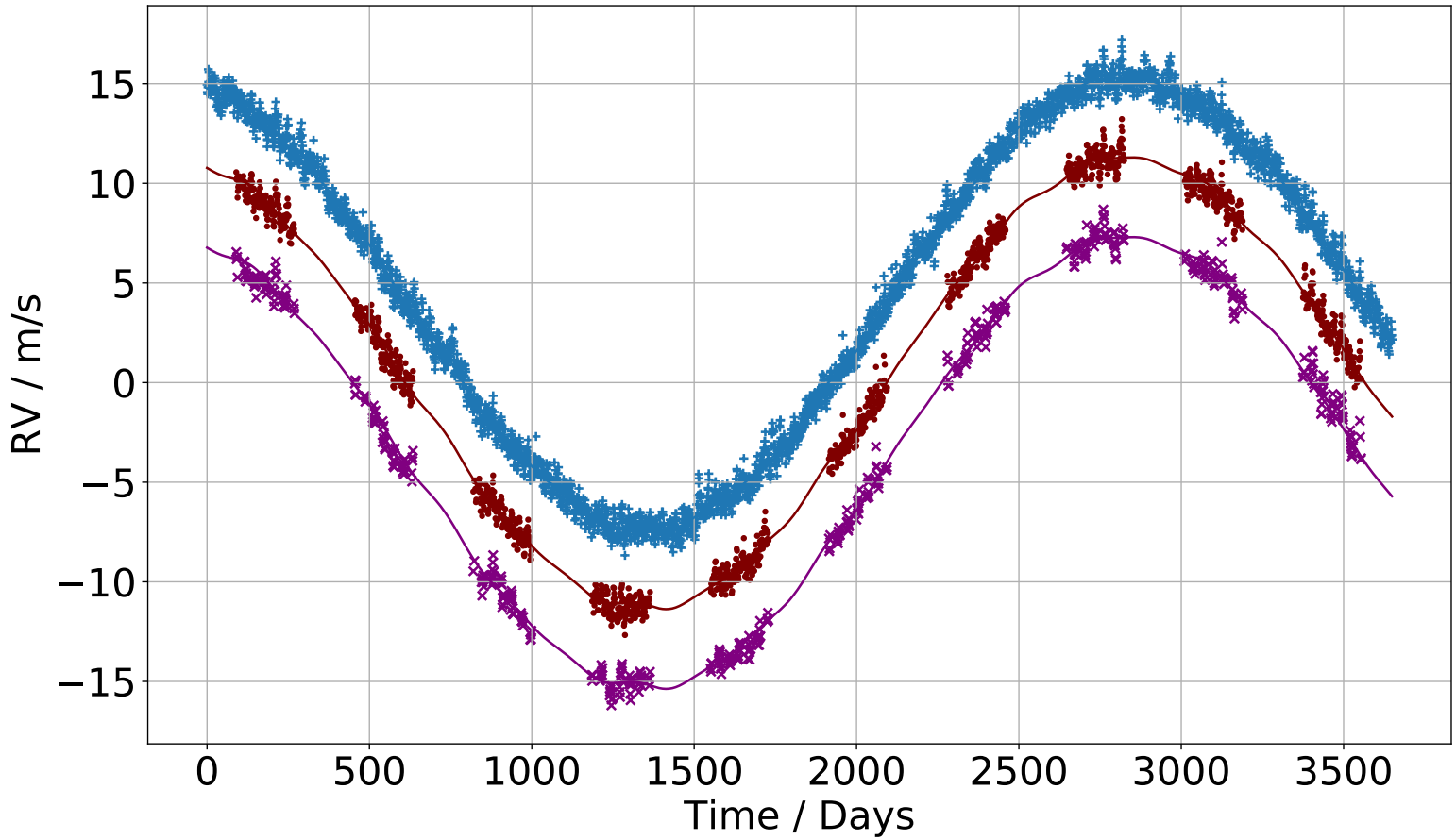


PolyChord vs MultiNest

- MultiNest excels in low dimensions $D < 10 - 20$.
- PolyChord can go up to ~ 150.
- Crossover is problem dependent
- PolyChord can also exploit fast-slow hierarchy

Exoplanets

Nested sampling in action (arXiv:1806.00518, Hall, Walker-Smith, Handley, Queloz)



- Simple radial velocity model

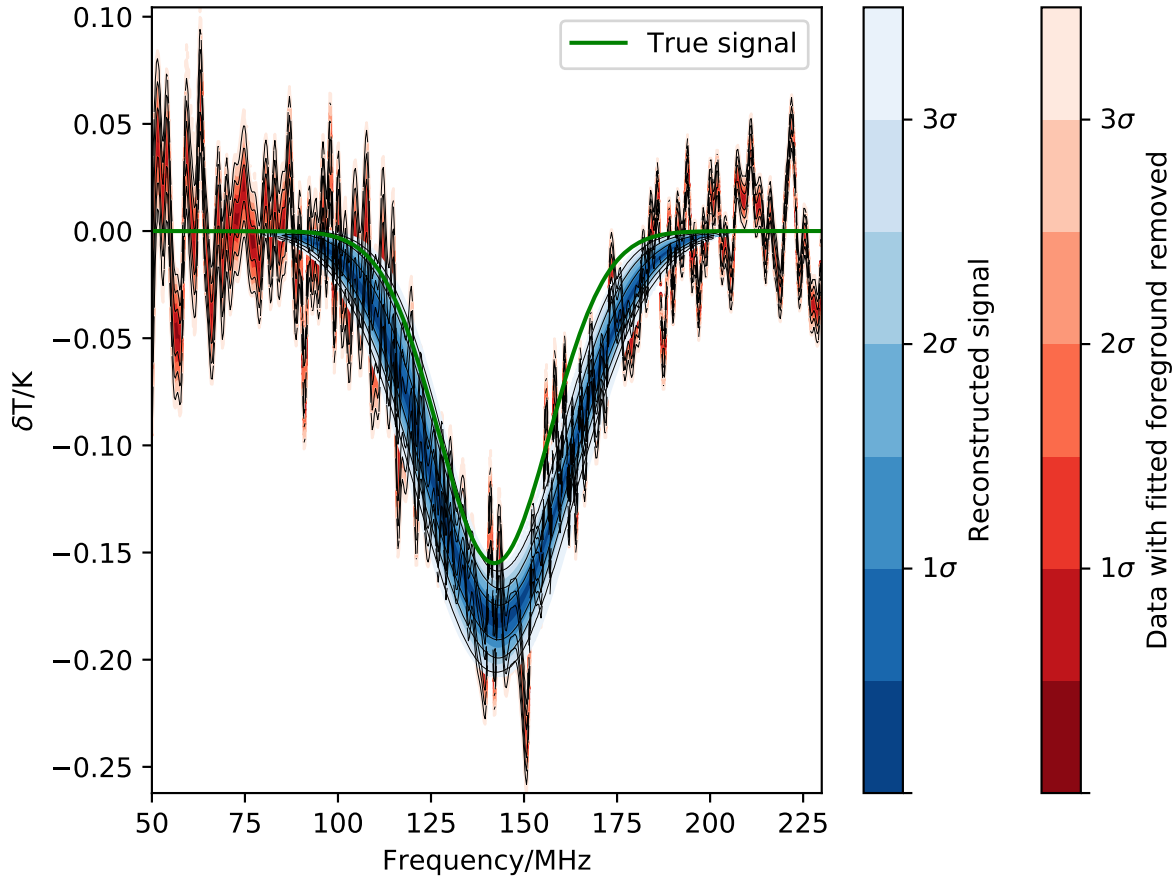
$$\nu(t;\theta) = \sum_{p=1}^{N} K_p \sin(\omega_p t + \phi_p)$$

- Fit each model to data.
- Posteriors on model parameters $[(K_p, \omega_p, \phi_p), p = 1 \cdots N]$ quantify knowledge of system characteristics.
- Evidences of models determine relative likelihood of number of planets in system
- This is an application where phase transitions matter

21cm cosmology

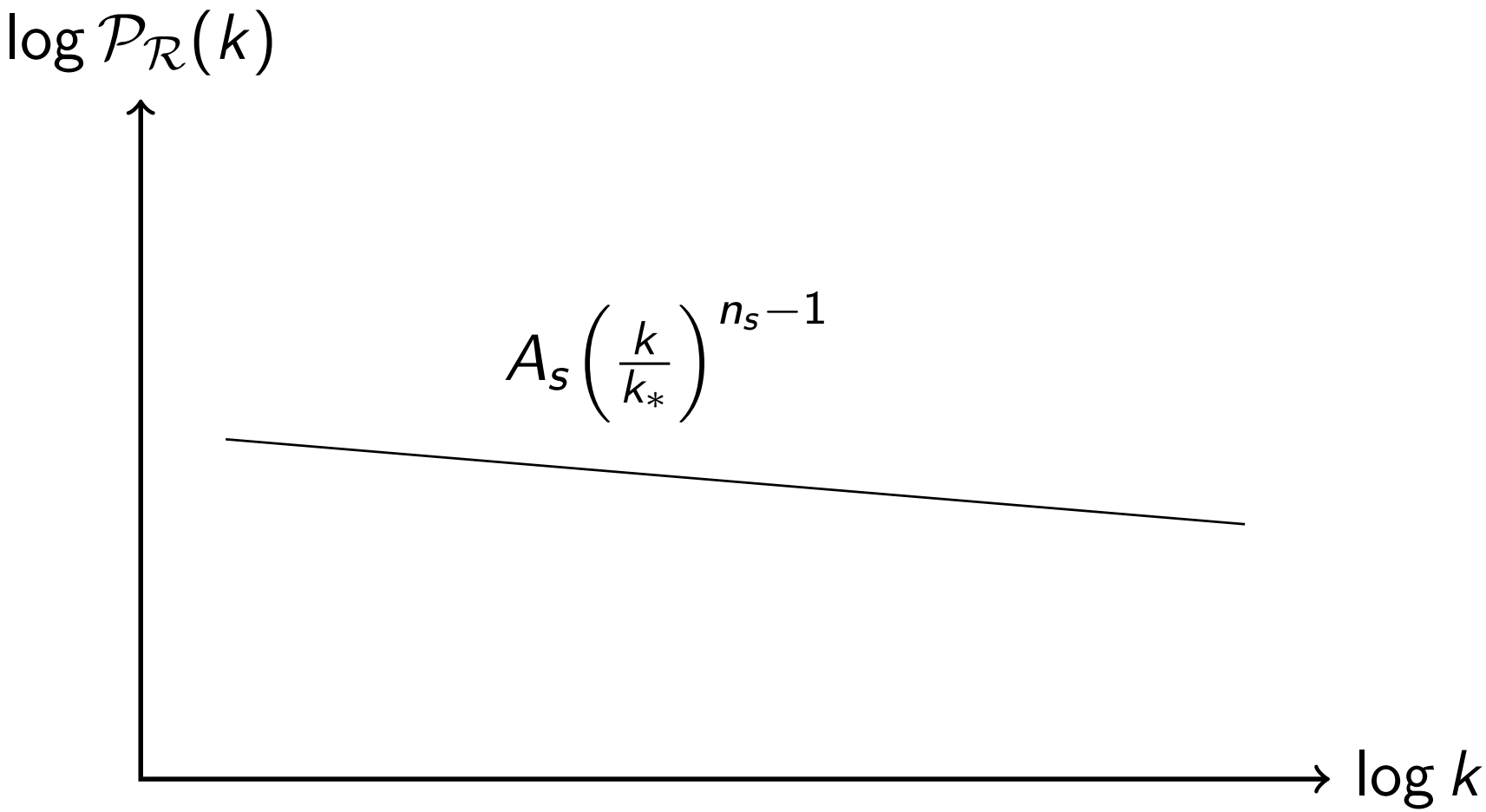
Nested sampling in action (Paper coming soon, Anstey, de Lera Acedo & Handley)

- Search for signal $T = T_{\rm fg} + T_{21\rm cm}$
- Fit parameterised models with/without $T_{21\rm cm}$
- Compare evidences for signal detection
- Use evidences to quantify complexity of beam/sky models



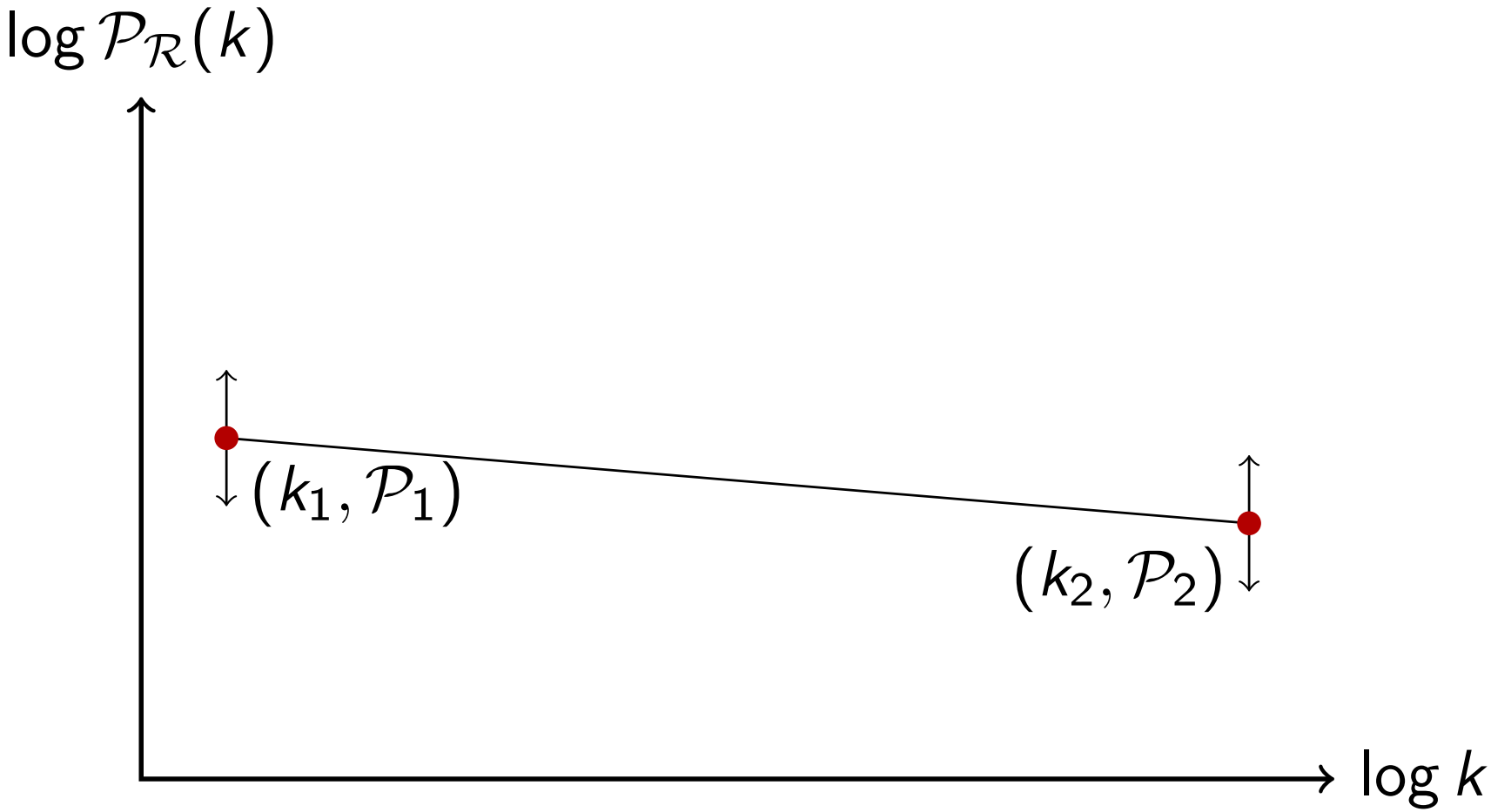
Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction

Nested Sampling in action (arXiv:1908.00906)



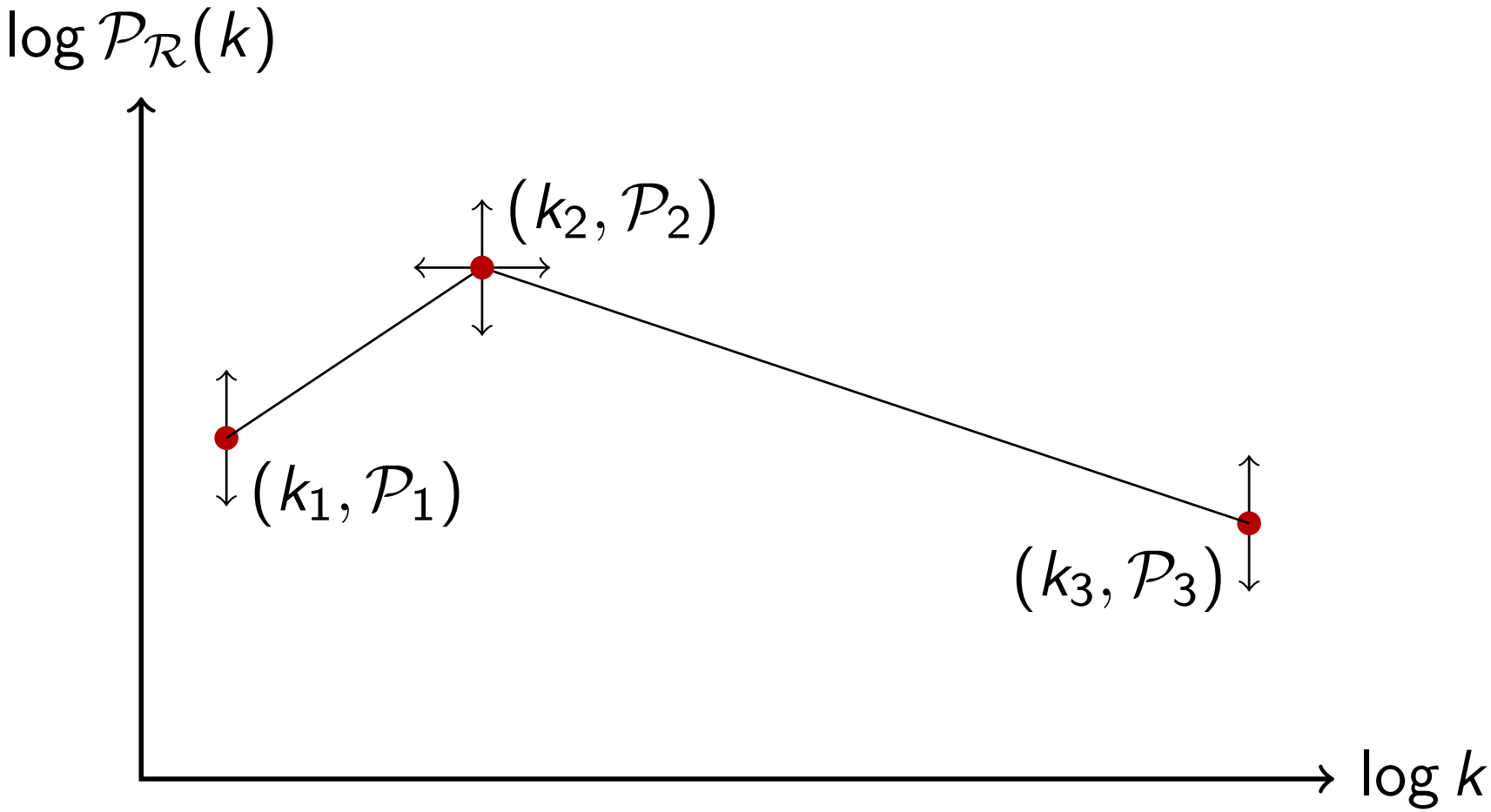
Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction

Nested Sampling in action (arXiv:1908.00906)



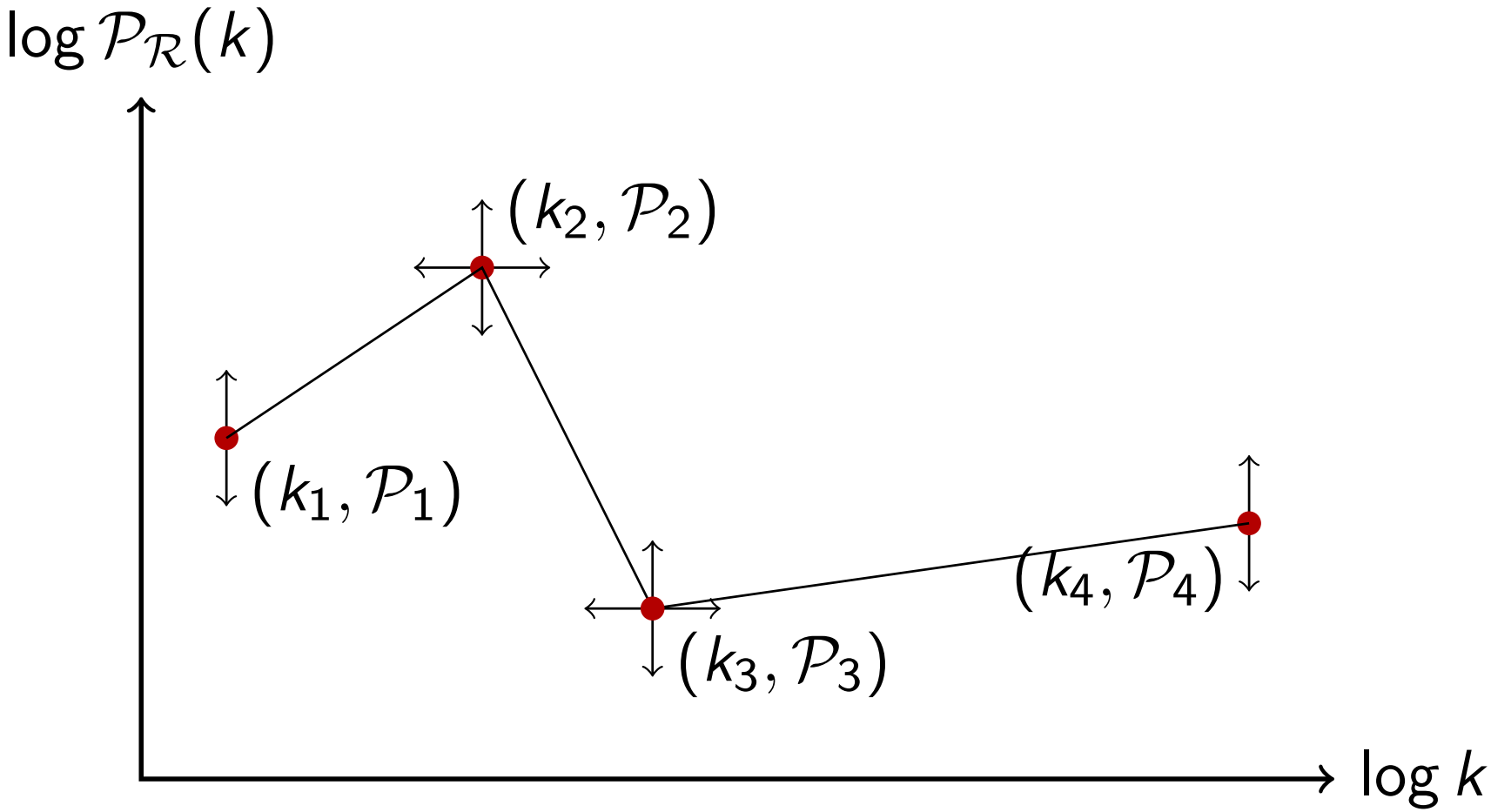
Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction

Nested Sampling in action (arXiv:1908.00906)



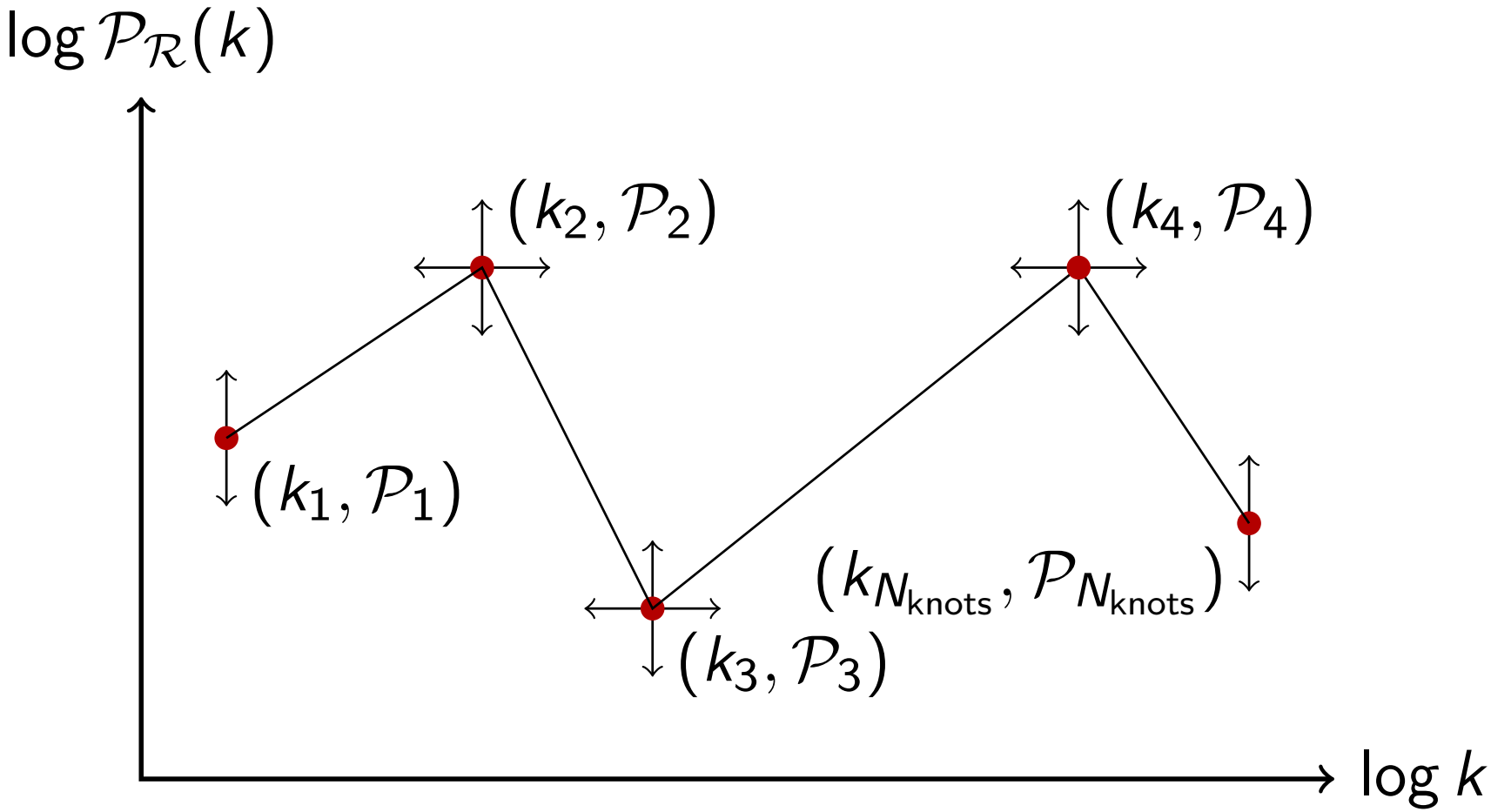
Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction

Nested Sampling in action (arXiv:1908.00906)

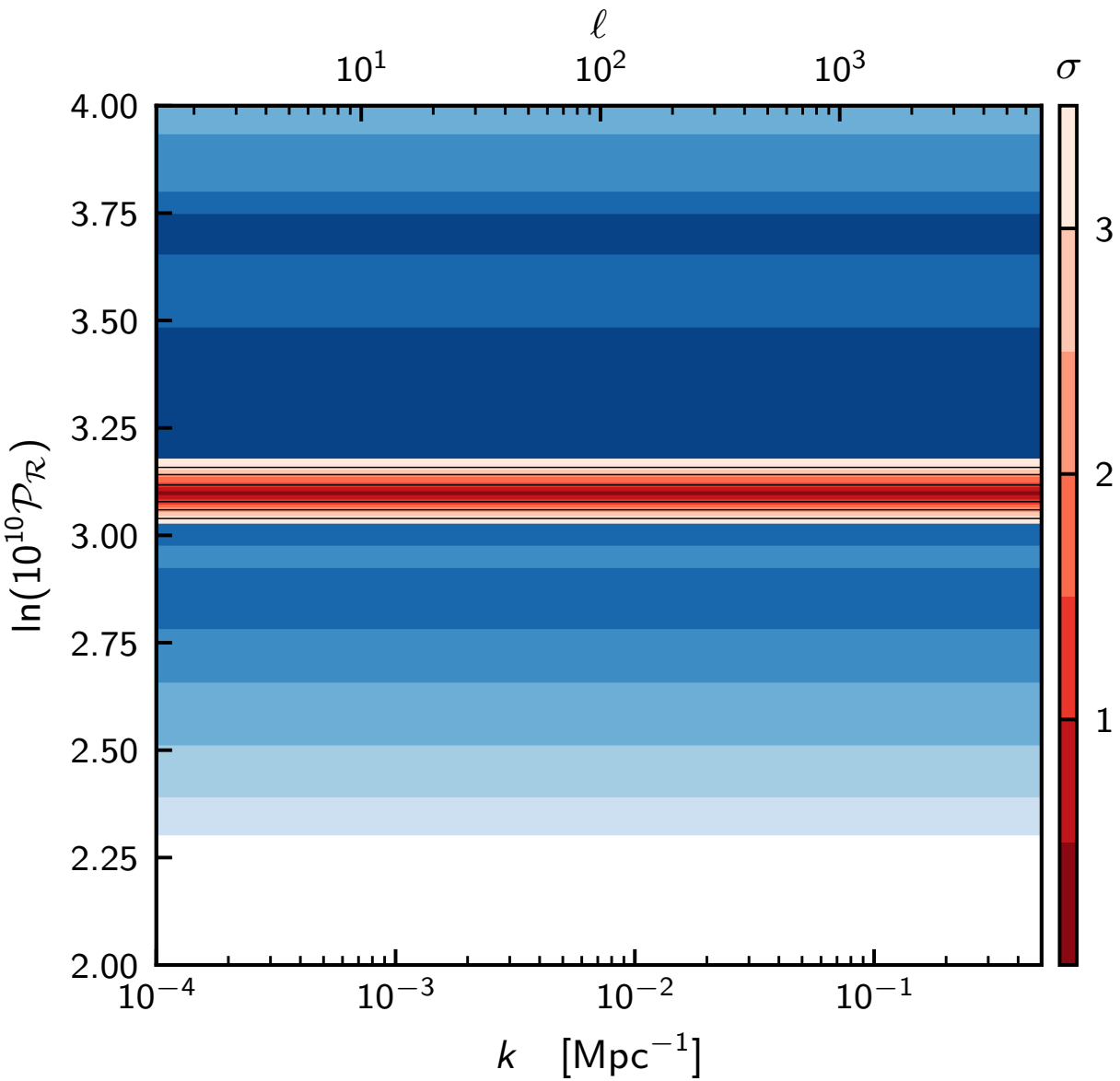


Primordial power spectrum $\mathcal{P}_{\mathcal{R}}(k)$ reconstruction

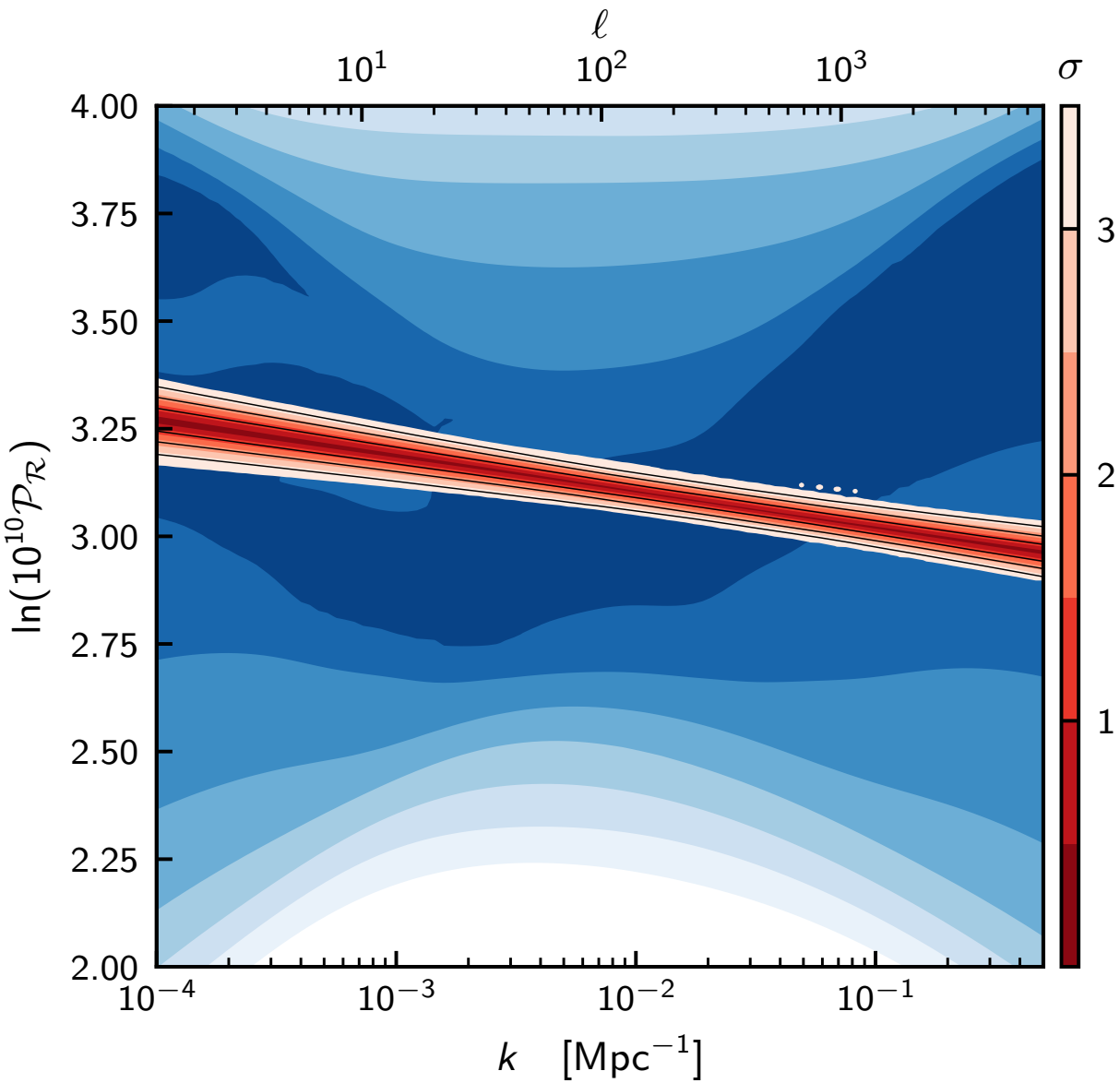
Nested Sampling in action (arXiv:1908.00906)



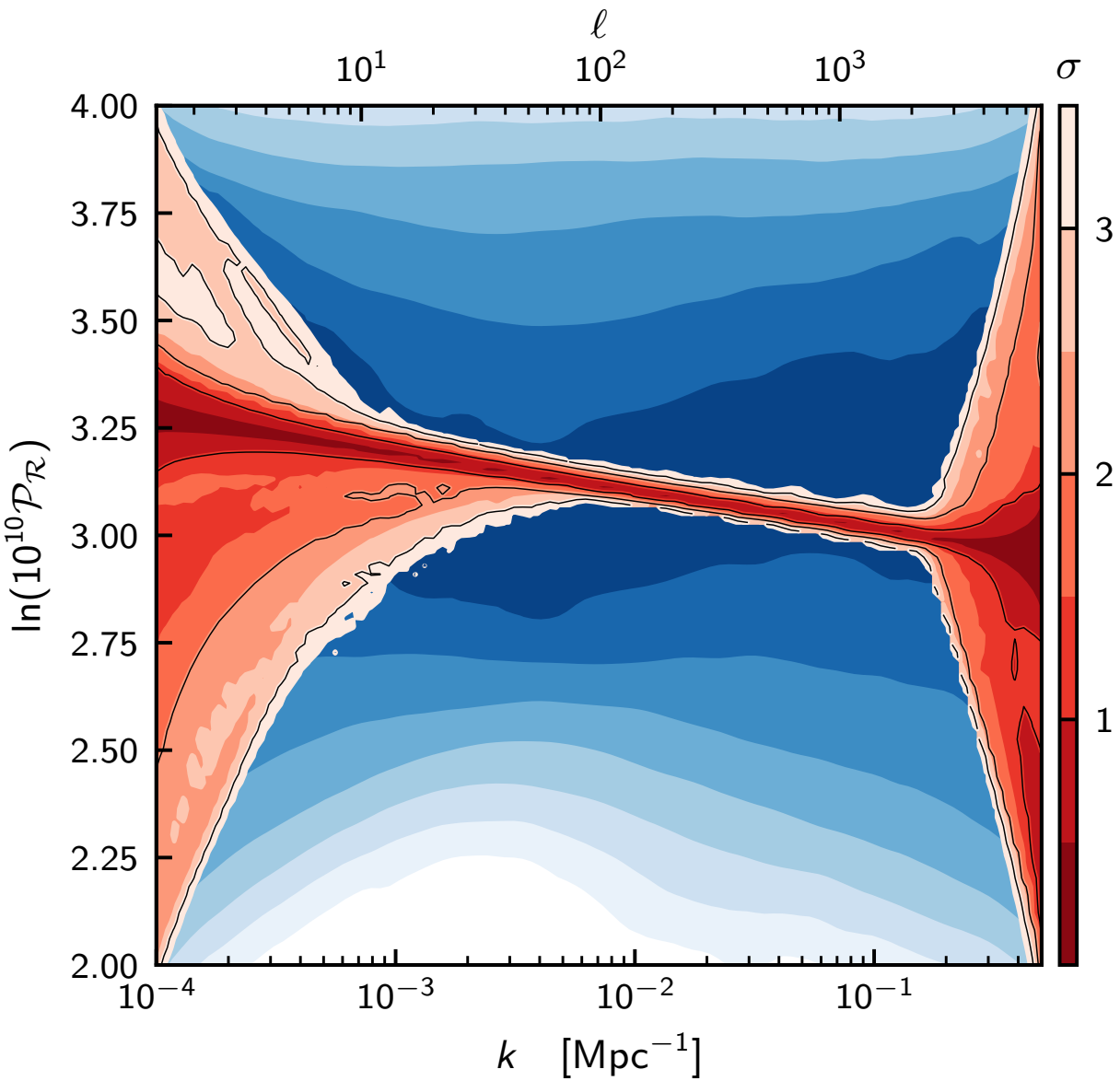
0 internal knots



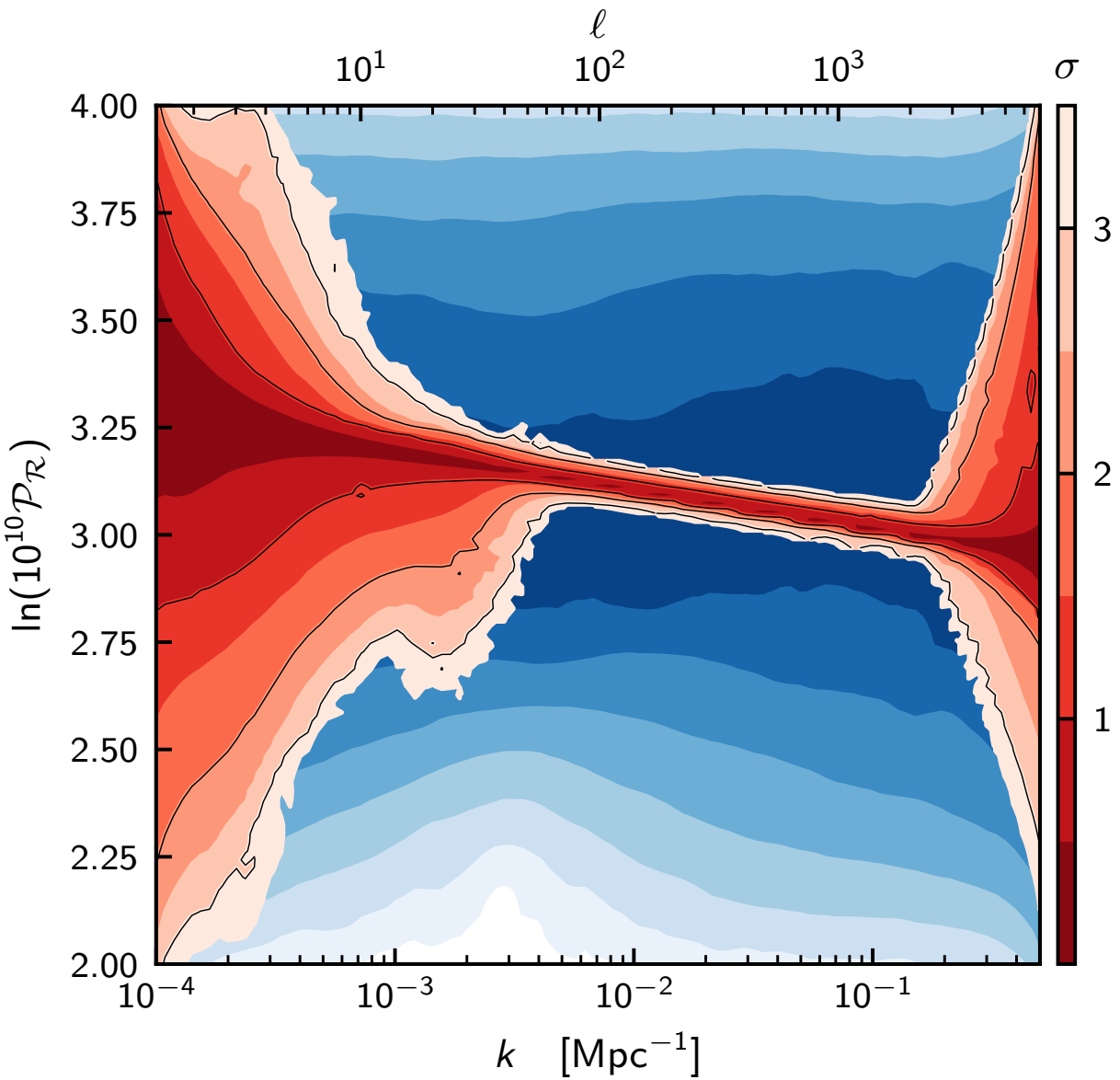
1 internal knot



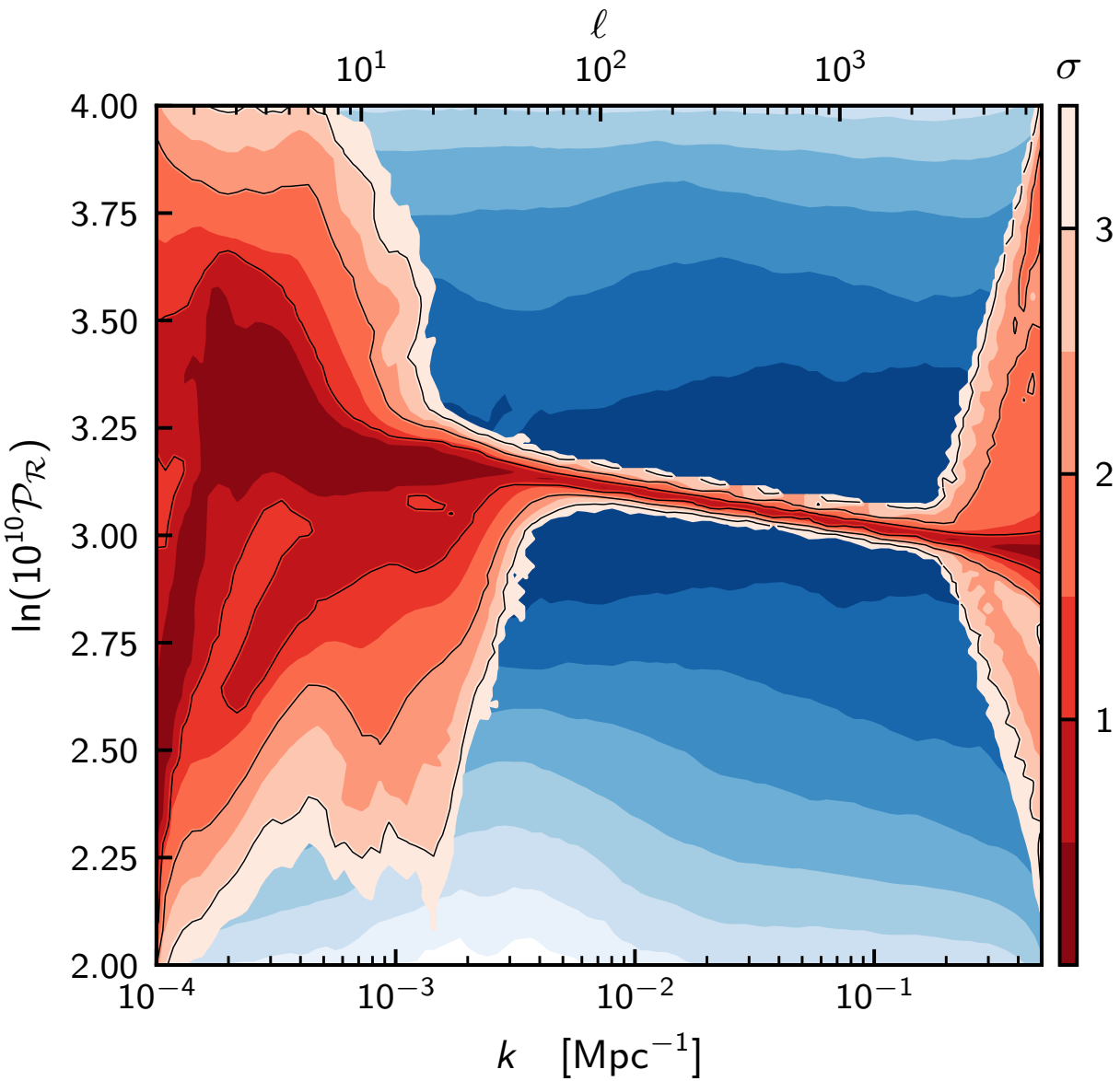
2 internal knots



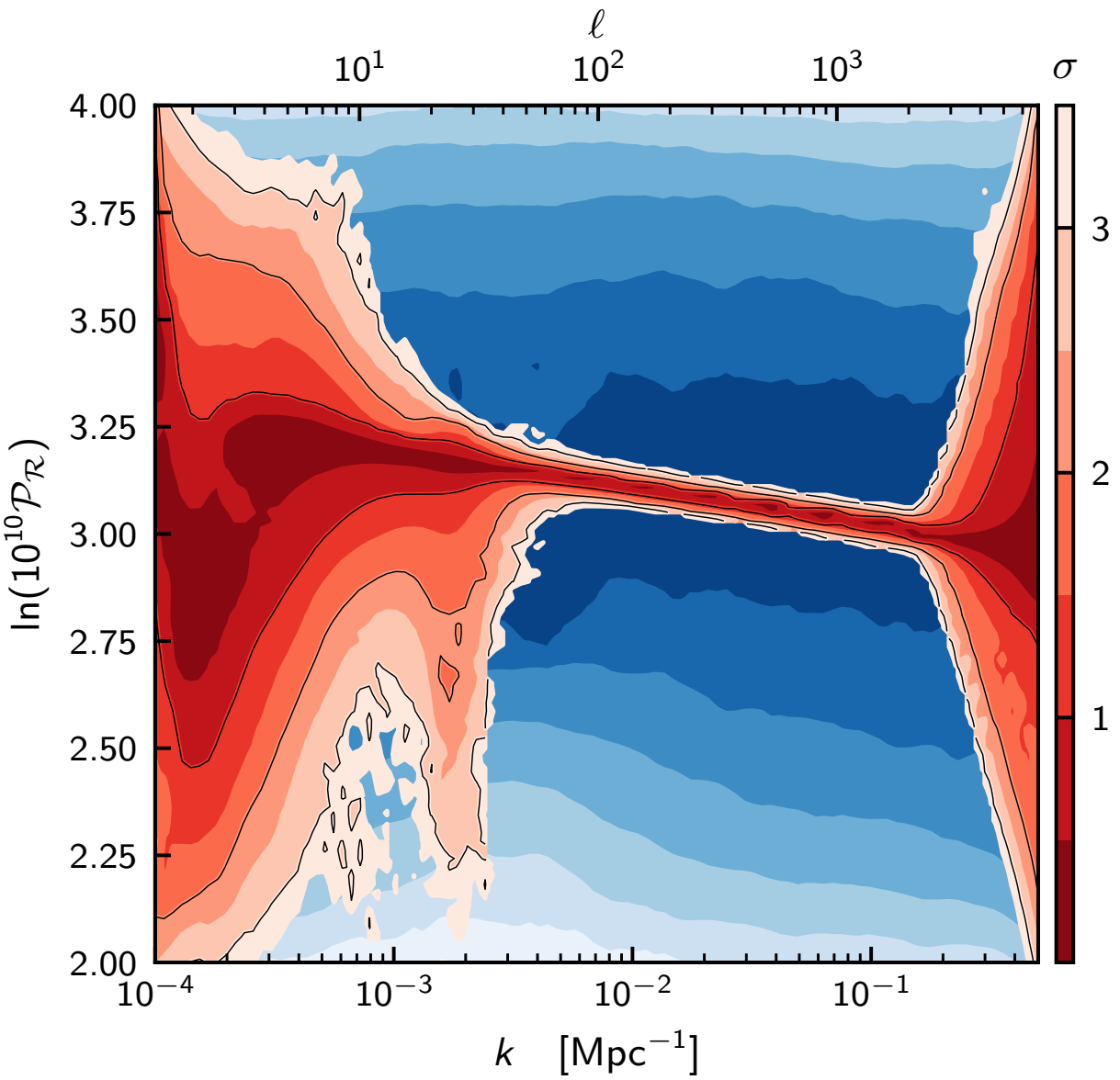
3 internal knots



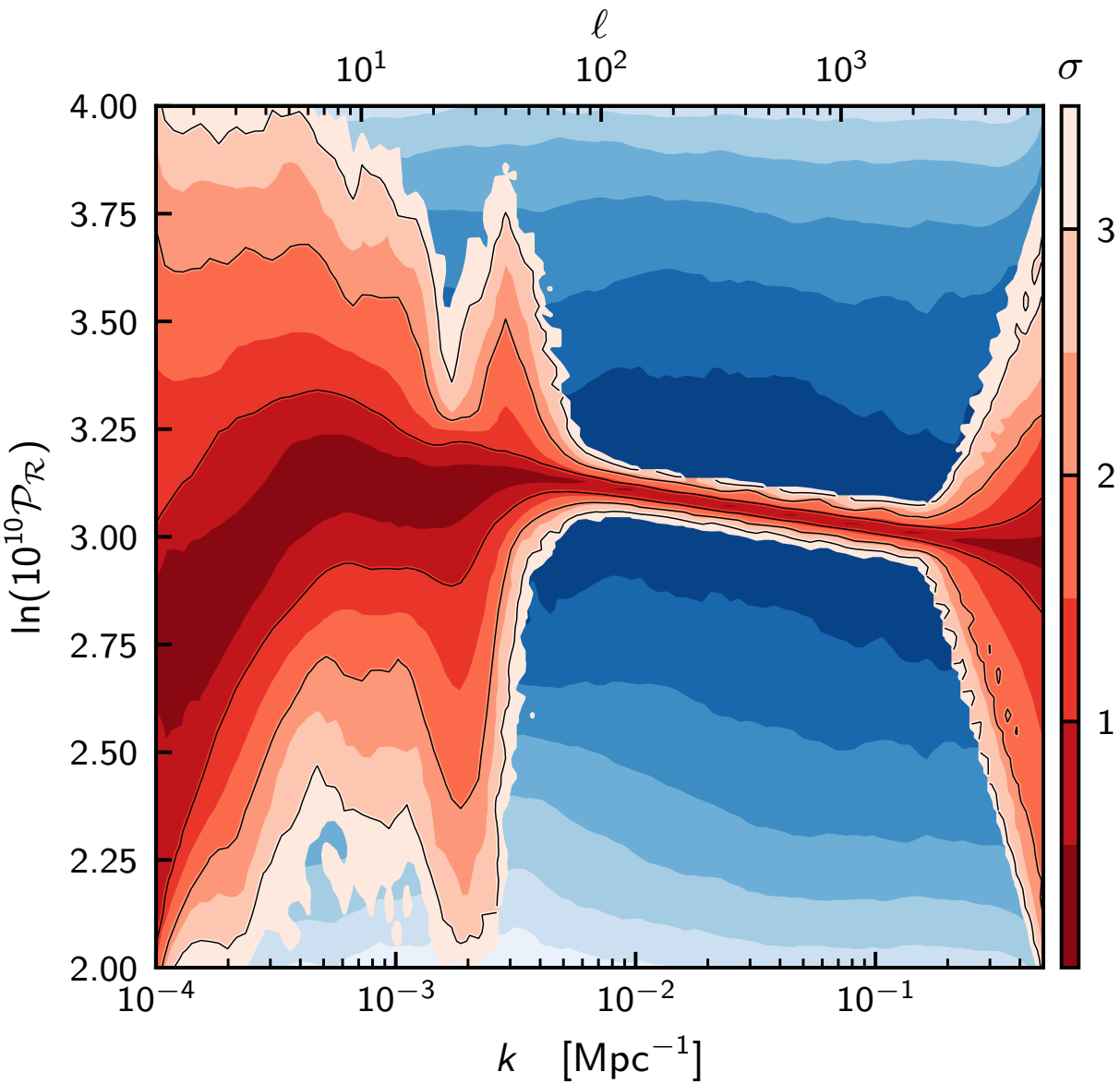
4 internal knots



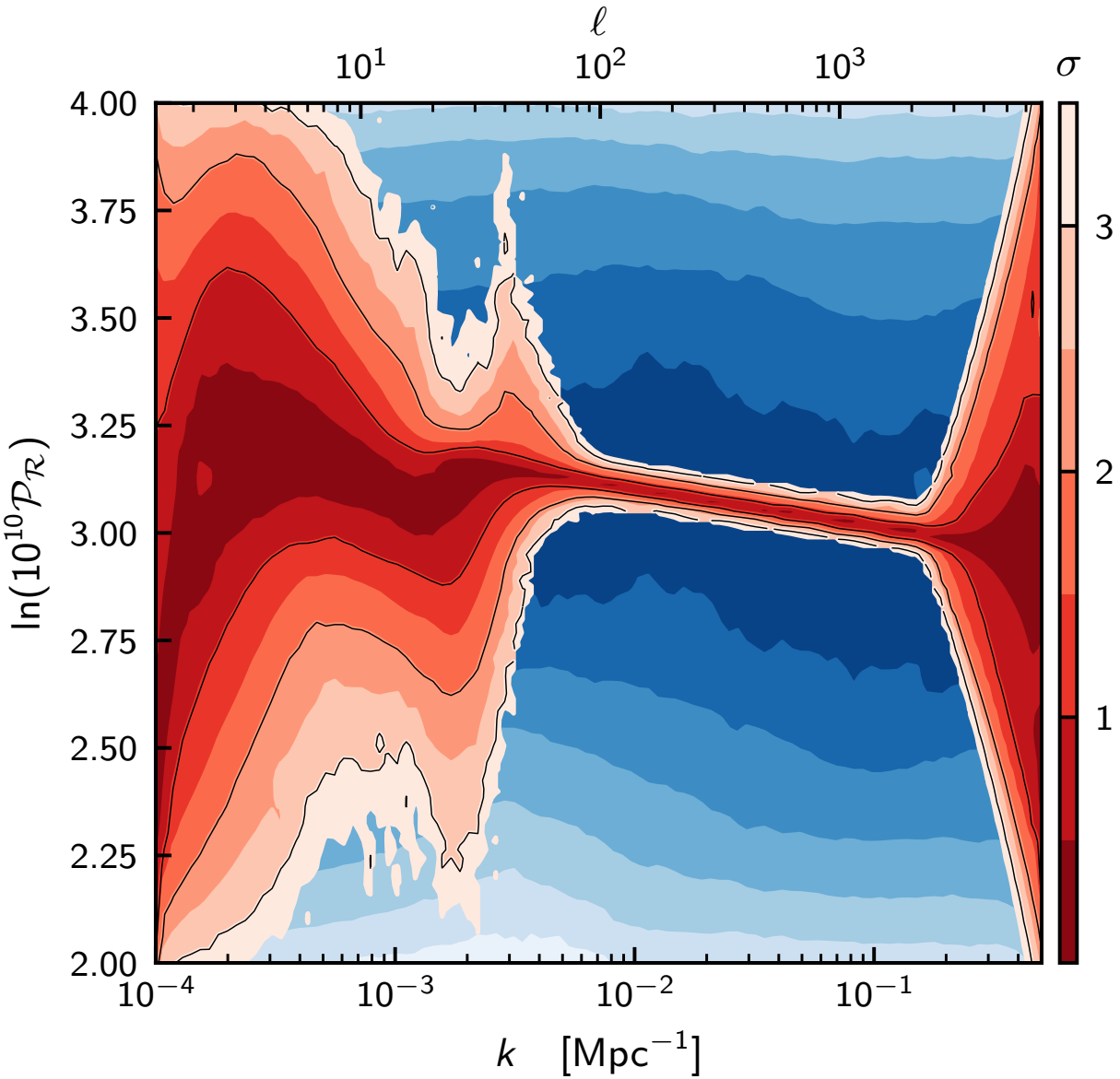
5 internal knots



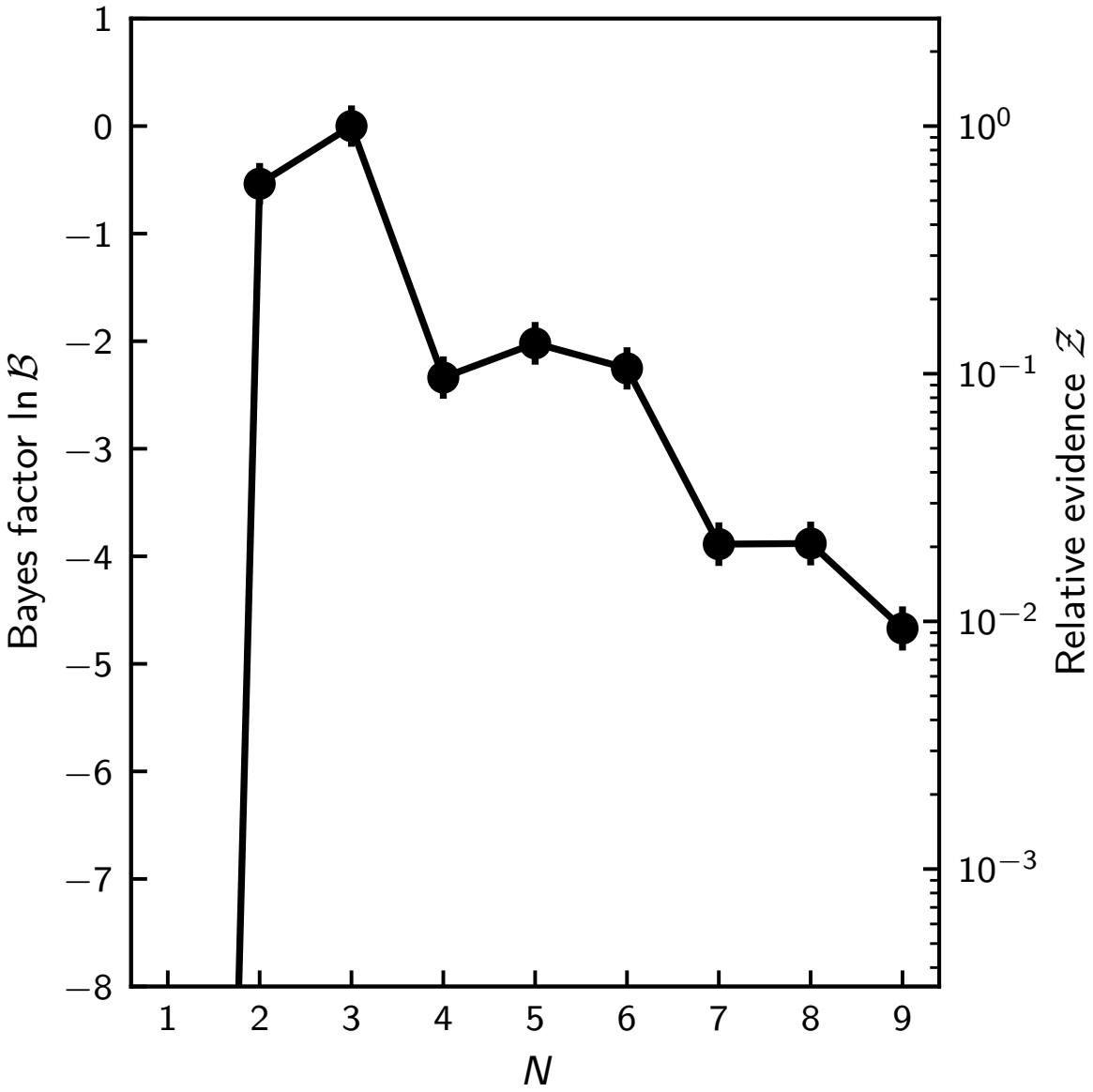
6 internal knots



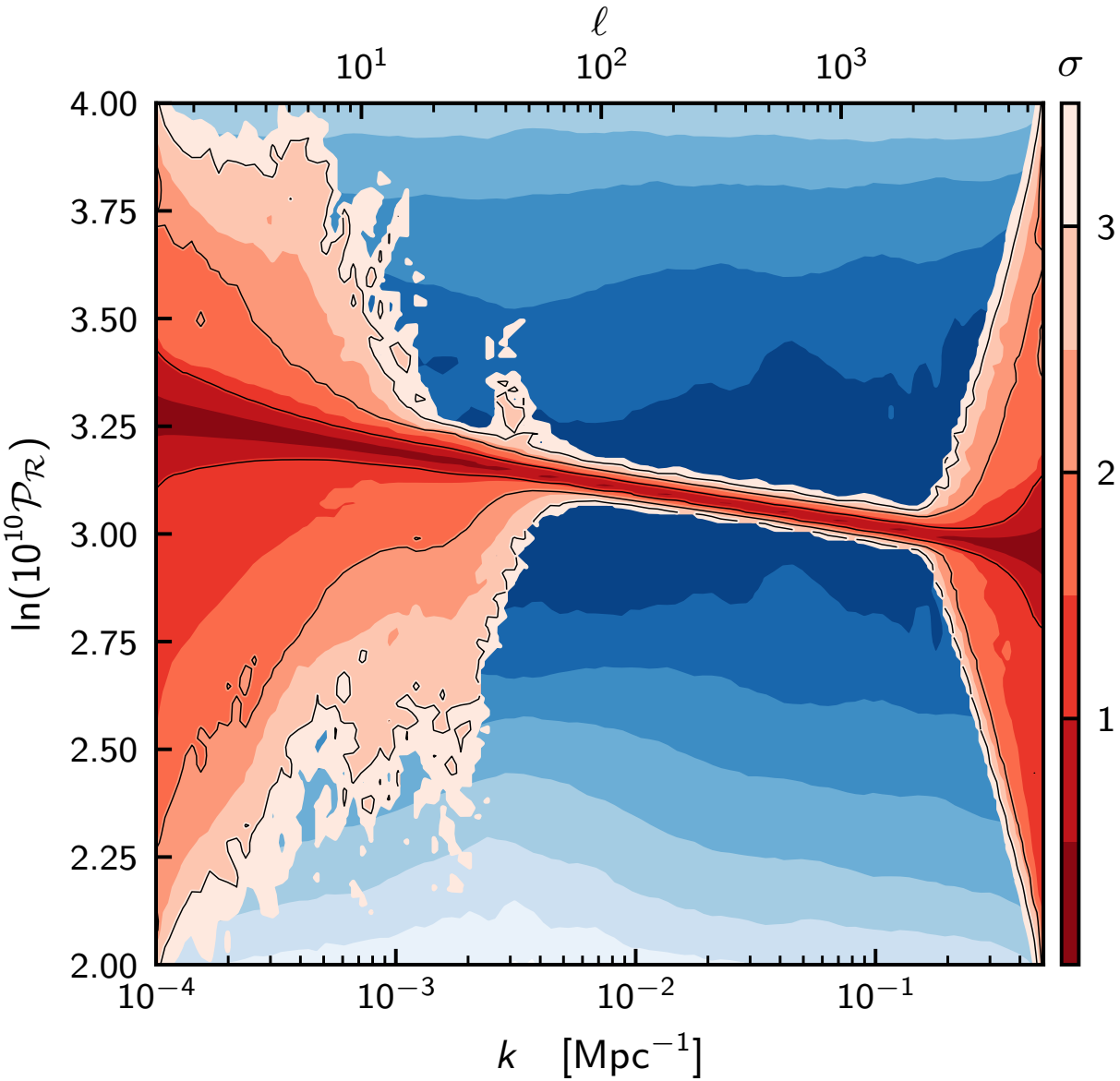
7 internal knots



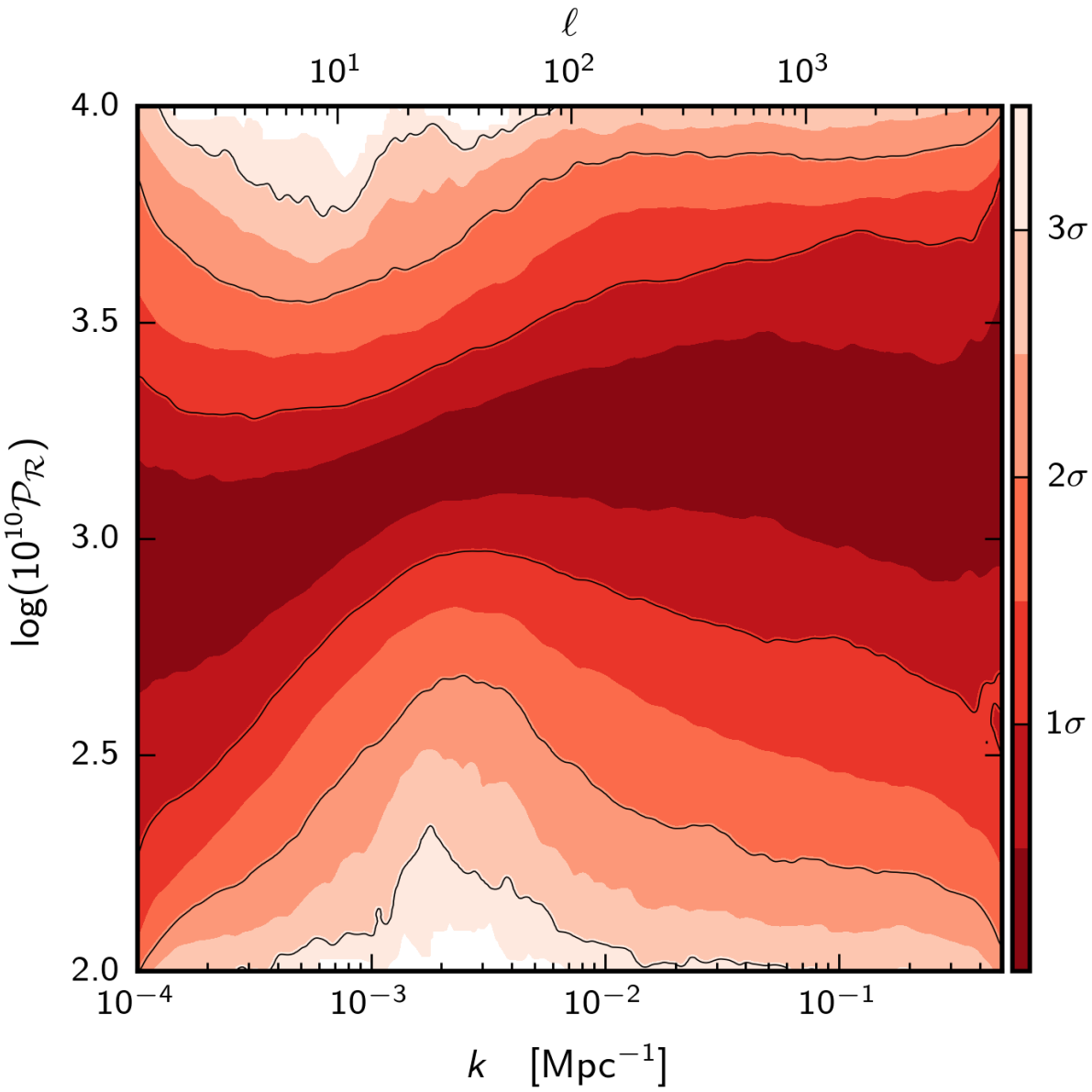
Bayes Factors



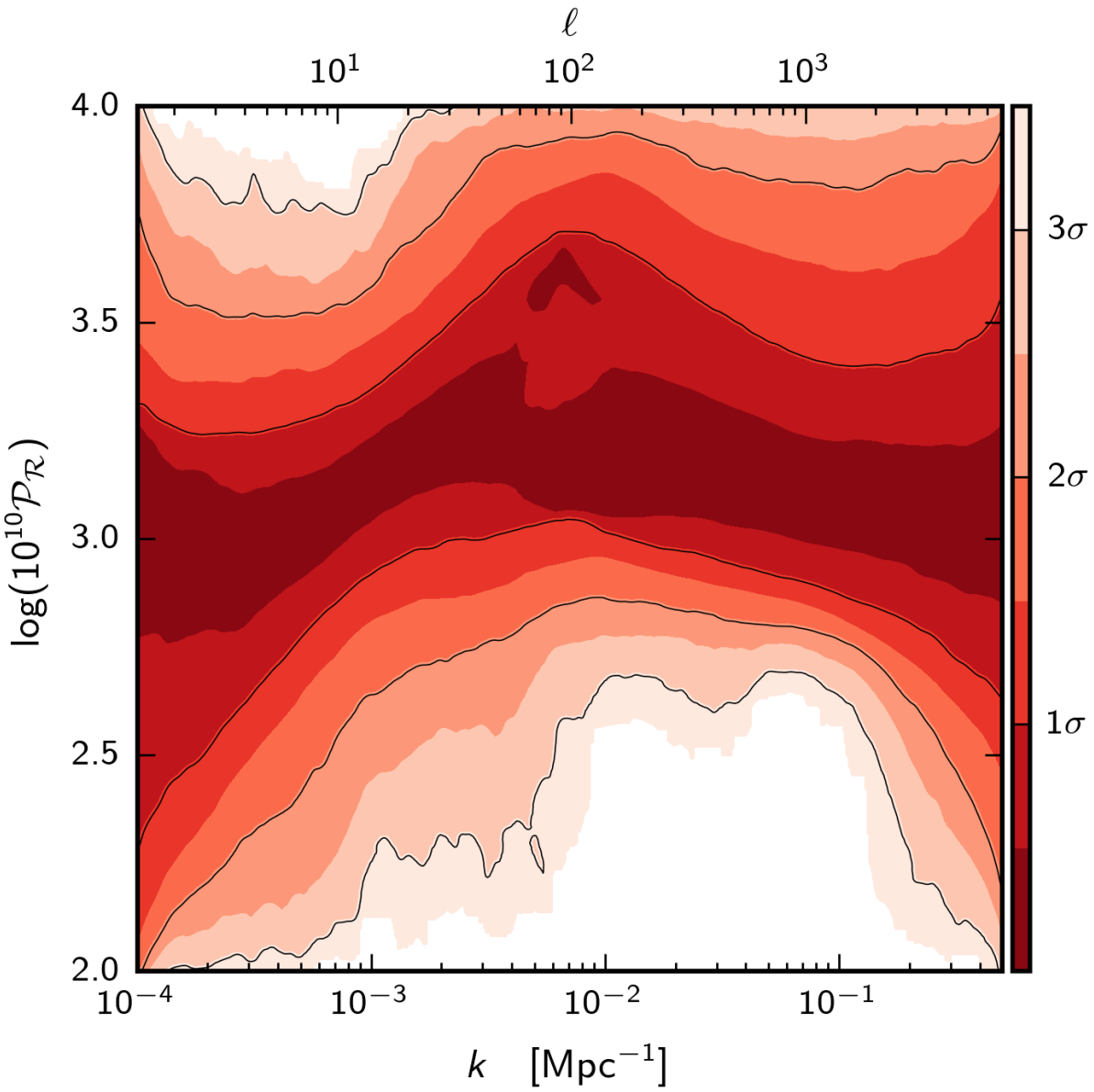
Marginalised plot



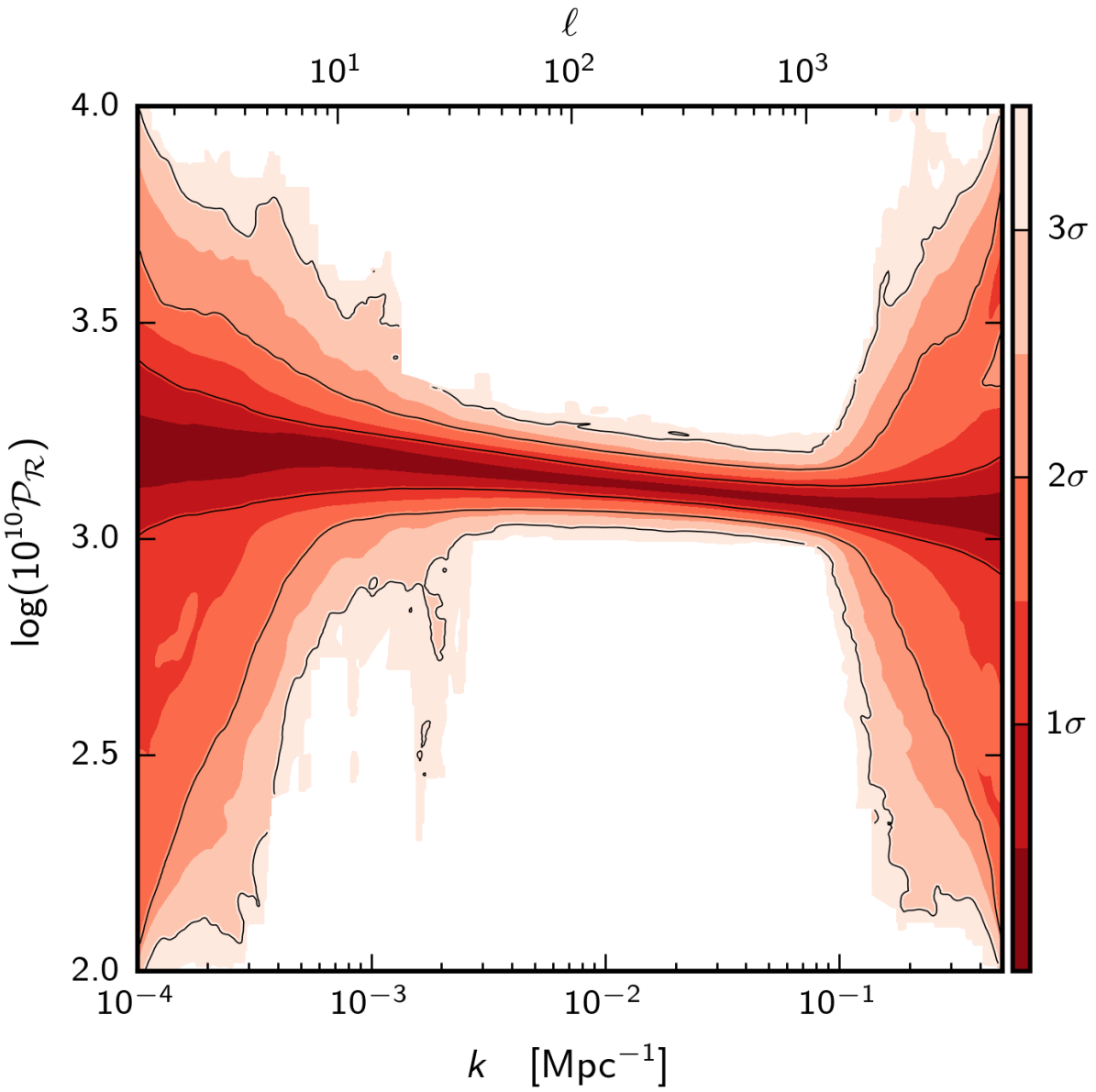
COBE (pre-2002)



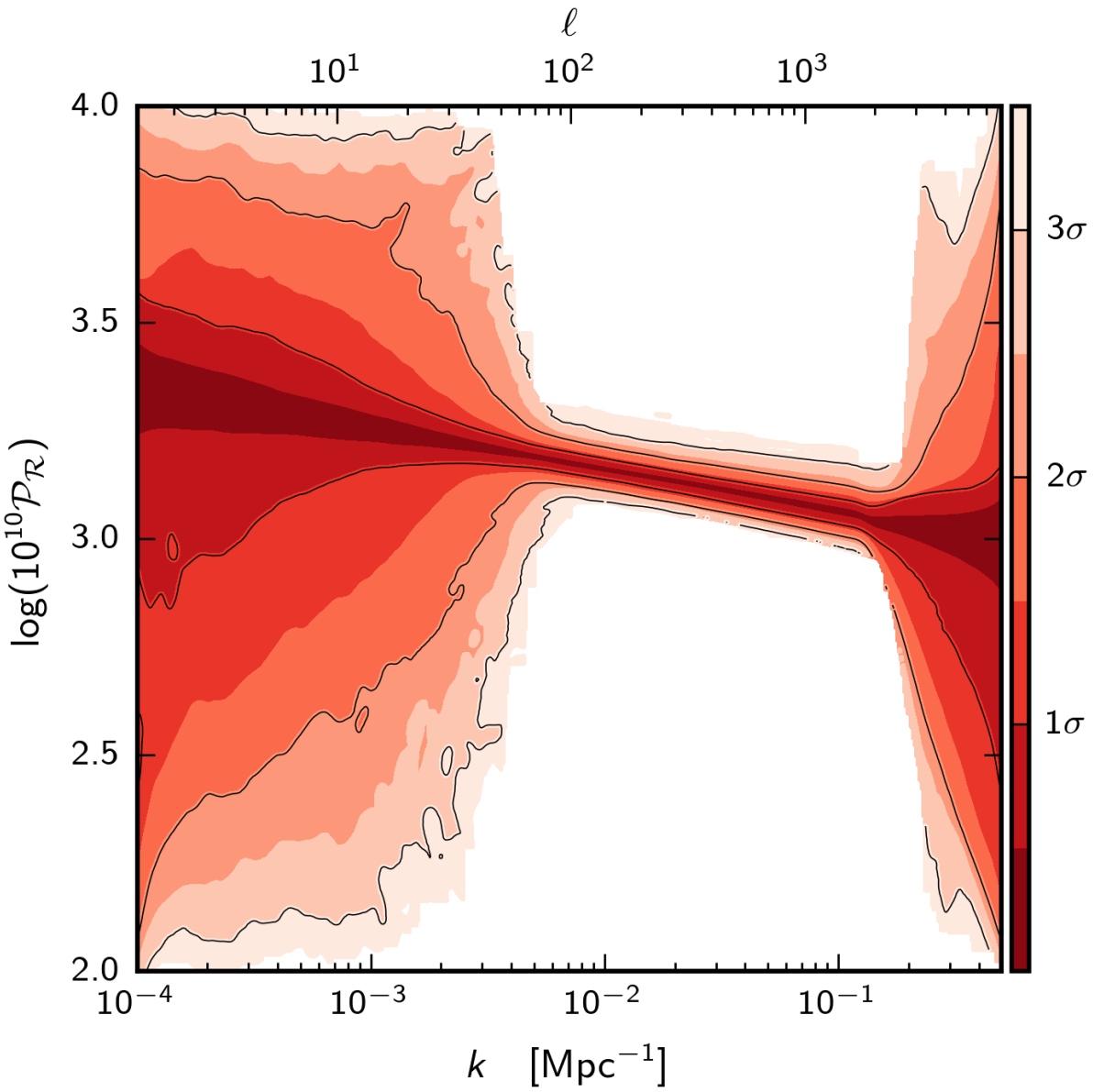
COBE et al (2002)



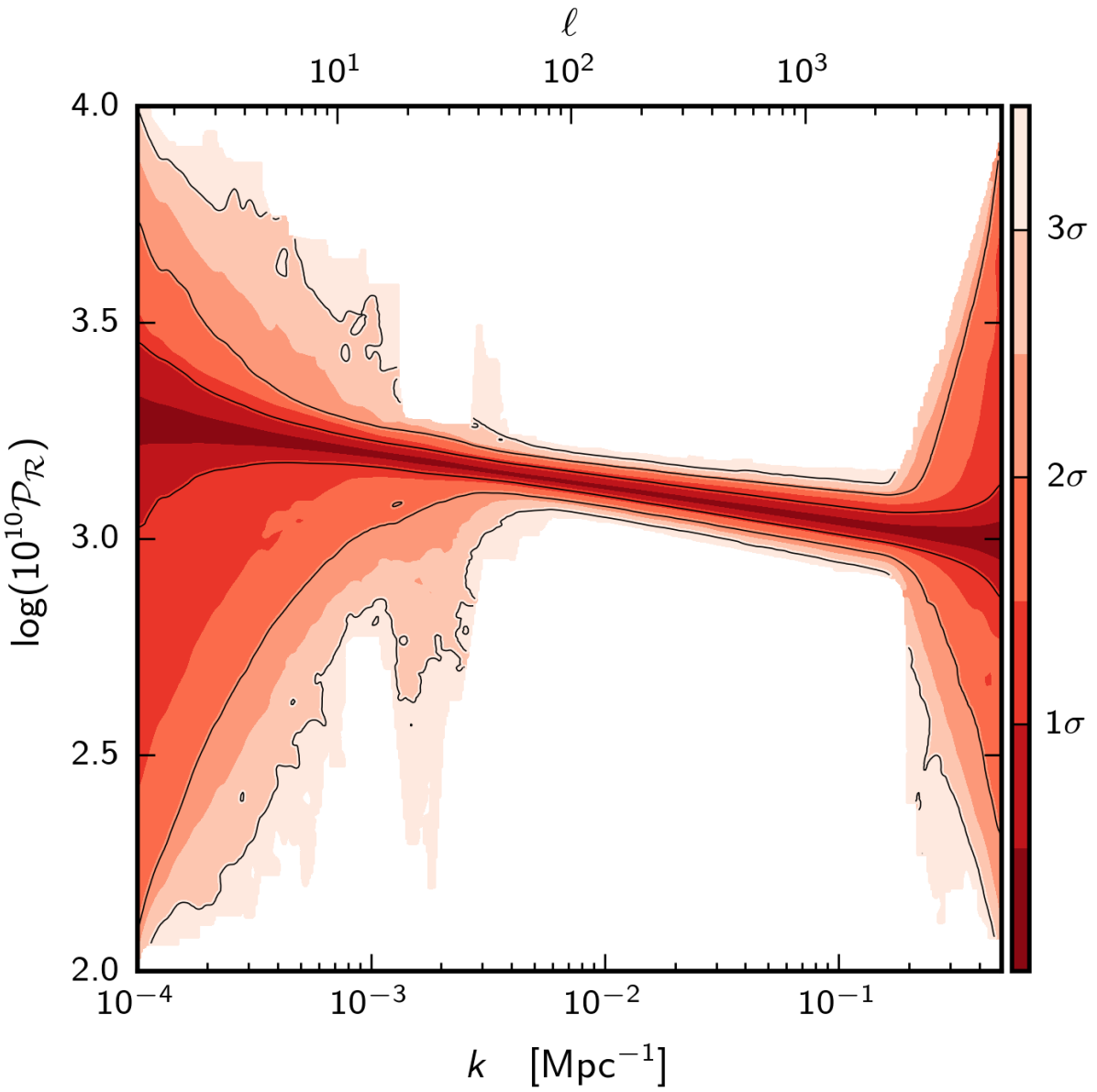
WMAP (2012)


ℓ
10^1
10^2
10^3
4.0
3.5
3.0
2.5
2.0
$\log(10^{10}\mathcal{P}_\mathcal{R})$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
k [Mpc^{-1}]
3σ
2σ
1σ

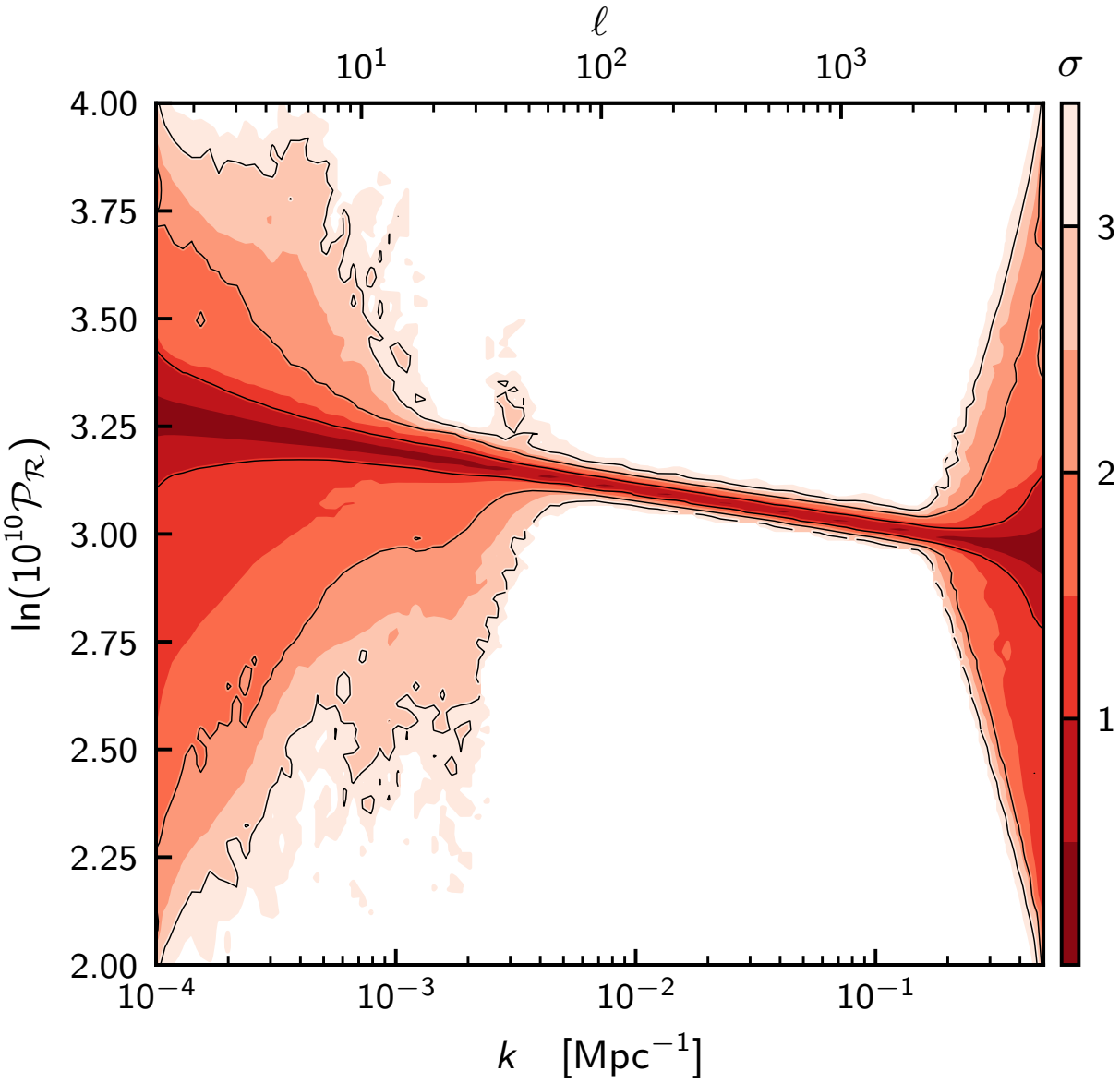
Planck (2013)


ℓ
10^1
10^2
10^3
4.0
3.5
3.0
2.5
2.0
$\log(10^{10}\mathcal{P}_\mathcal{R})$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
k [Mpc^{-1}]
3σ
2σ
1σ

Planck (2015)


ℓ
10^1
10^2
10^3
4.0
3.5
3.0
2.5
2.0
$\log(10^{10}\mathcal{P}_\mathcal{R})$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
k [Mpc^{-1}]
3σ
2σ
1σ

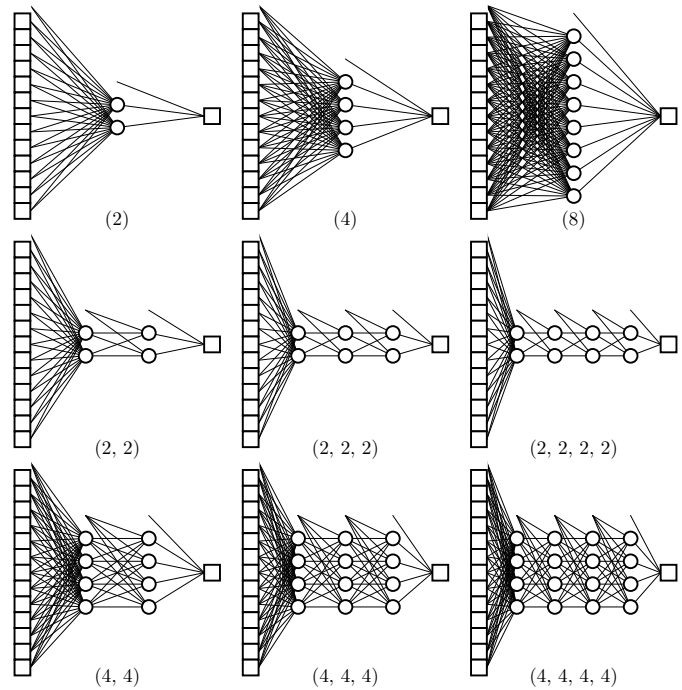
Planck (2018)

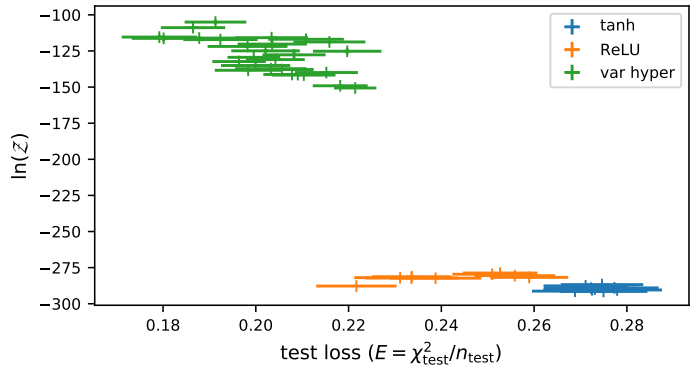

ℓ
10^1
10^2
10^3
σ
4.00
3.75
3.50
3.25
3.00
2.75
2.50
2.25
2.00
$\ln(10^{10}\mathcal{P}_\mathcal{R})$
10^{-4}
10^{-3}
10^{-2}
10^{-1}
k [Mpc^{-1}]
3
2
1

Bayesian neural networks

Sparse reconstruction (arXiv:1809.04598)

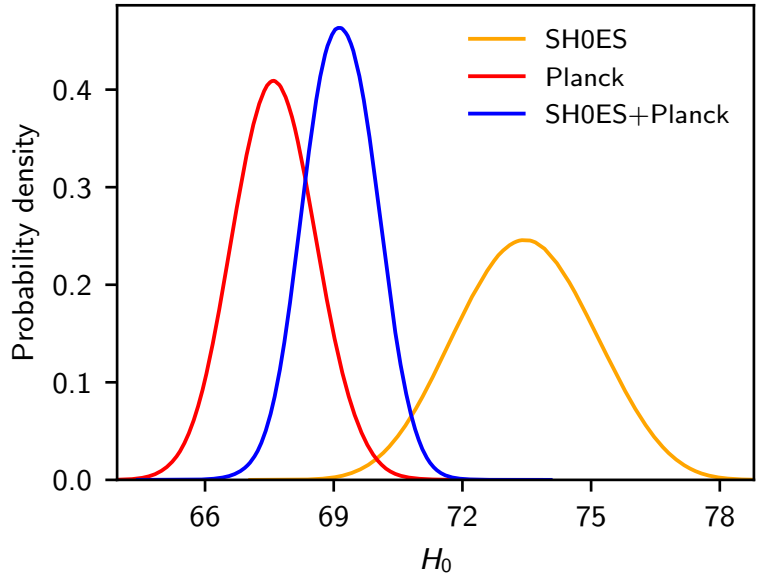
- Neural networks require:
  - Training to find weights
  - Choice of architecture/topology
- Bayesian NNs treat training as a model fitting problem
- Compute posterior of weights (parameter estimation)
- Use evidence to determine best architecture (model comparison)
- "Compromise-free Bayesian NNs" (Javid, Handley, Lasenby & Hobson)
  - Bayesian evidences correlate with out-of-sample performance
  - Can be used to determine width and number of hidden layers

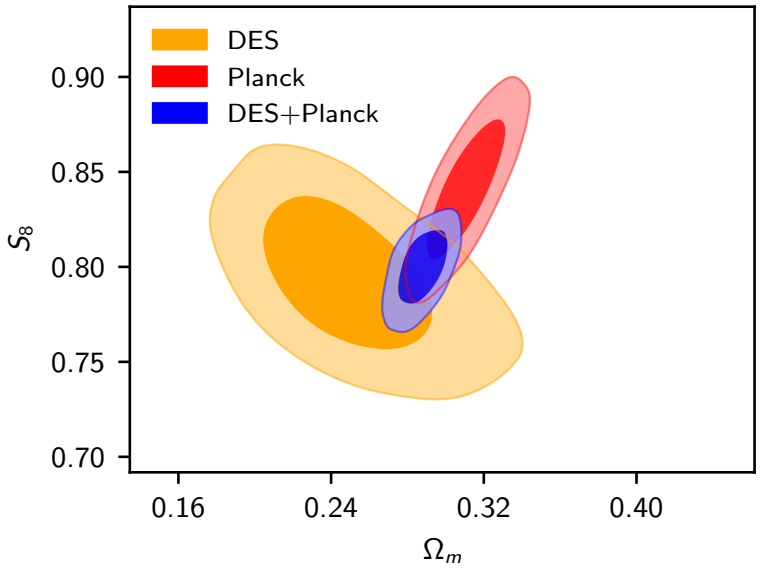




Other uses of nested sampling

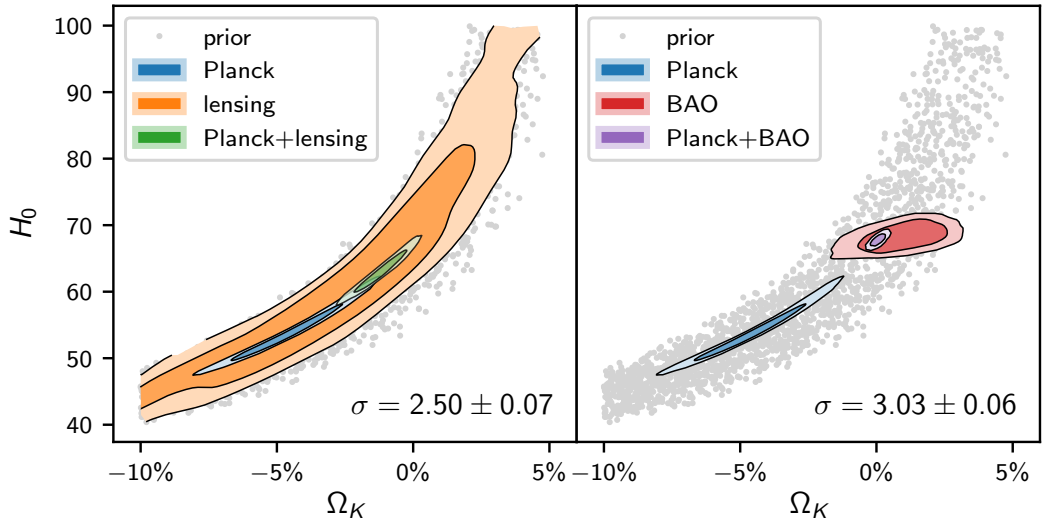
- Nested sampling estimates the density of states ΔX_i, and hence gives you access to a lot more than just posterior samples and evidences
- Kullback-Liebler divergence (arXiv:1607.00270)
- Bayesian model dimensionality (arXiv:1903.06682)
- Suspiciousness & Tension quantification (arXiv:1902.04029)
- DES tension: $\sim 2.3\sigma$

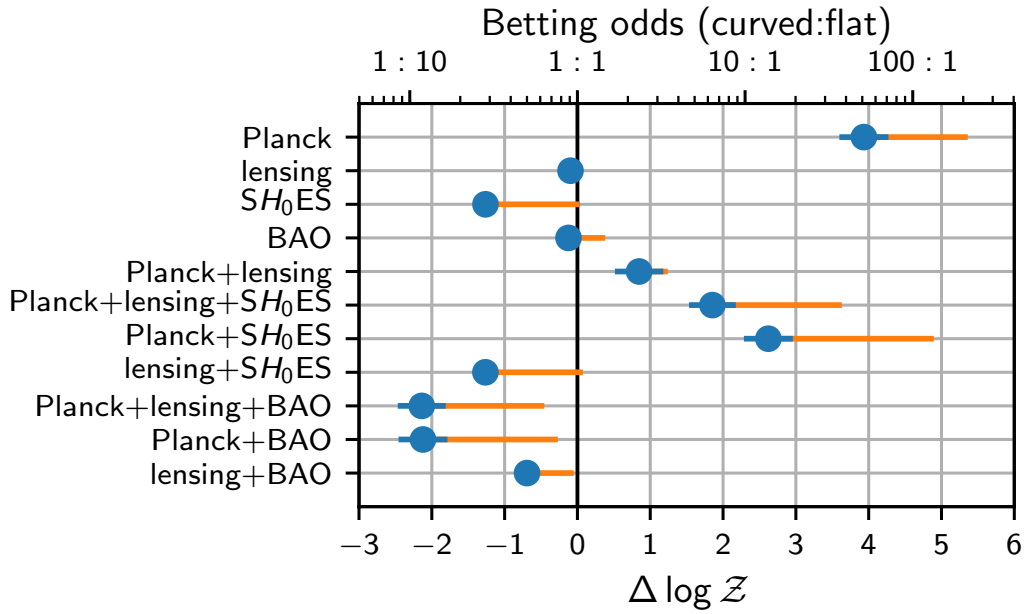


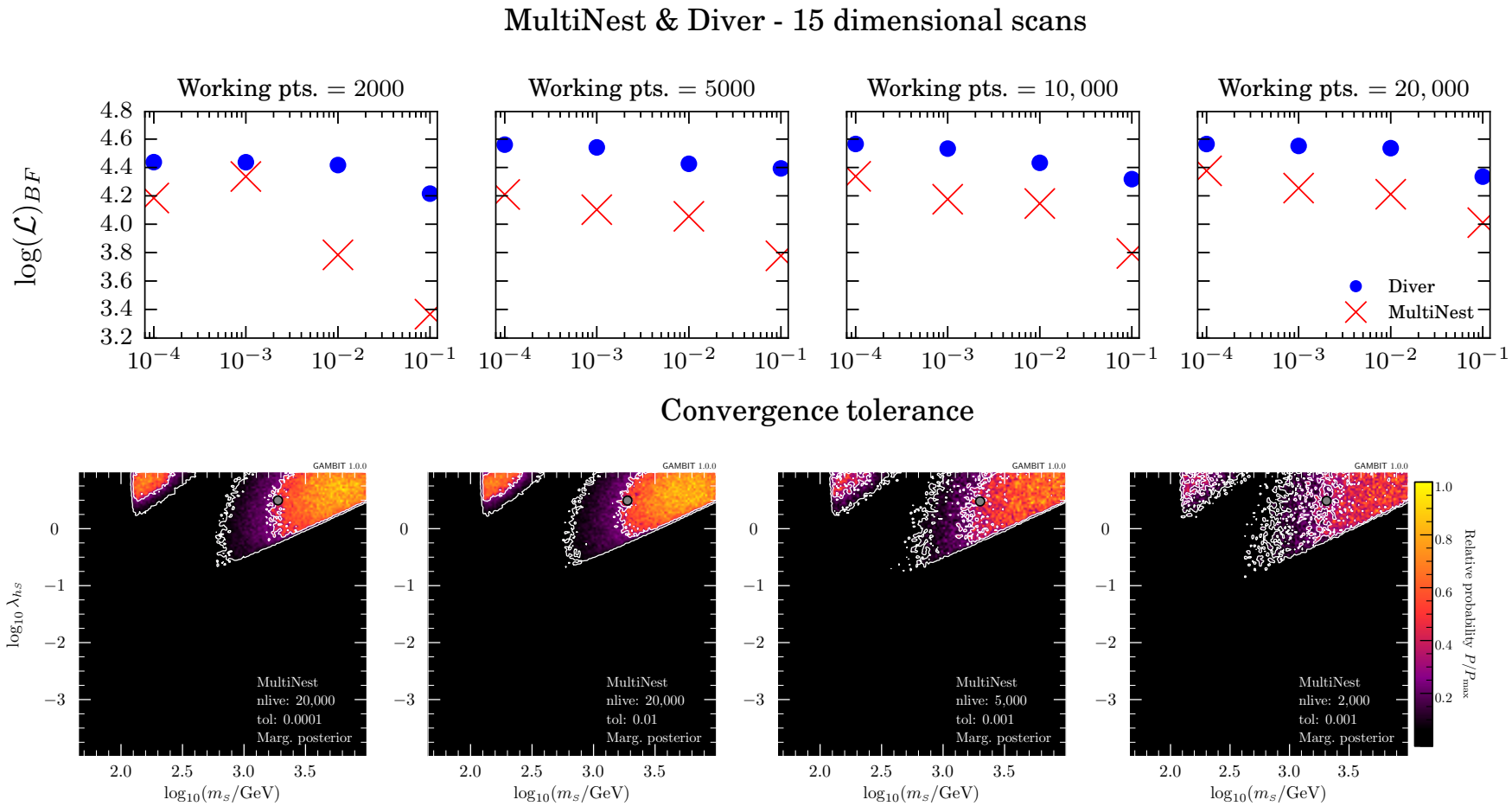


Curvature tension?

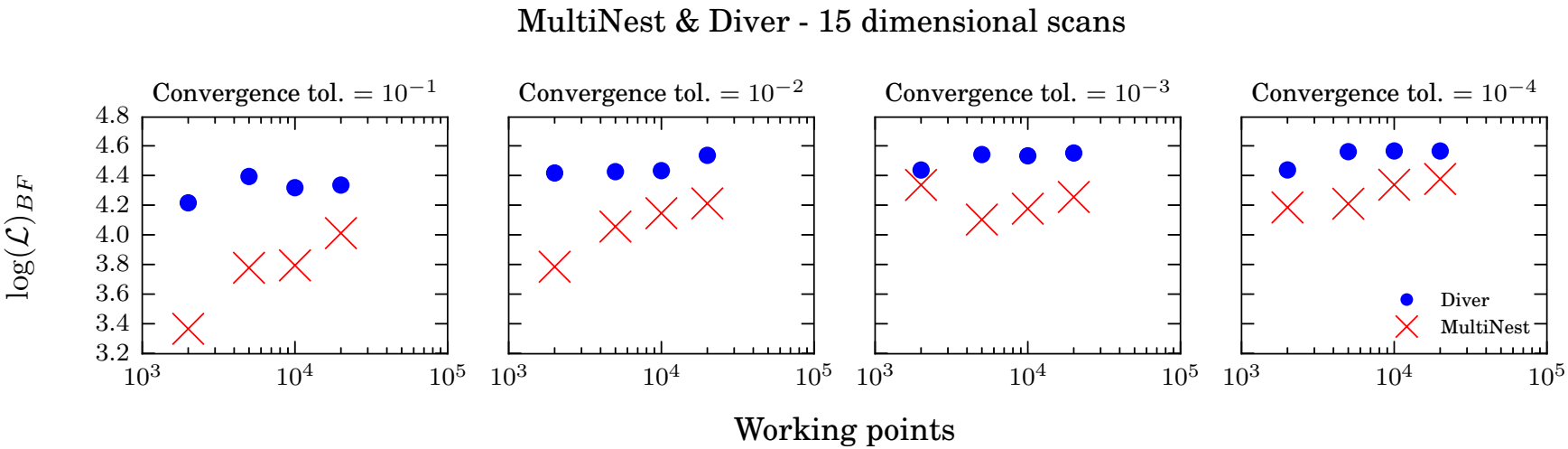
- Under the same measures of tension, CMB lensing is 2.5σ in tension with CMB TT,TE,EE
- Neglecting CMB lensing gives moderate preference for curvature
- Planck phrase these issues in terms of A_L






MultiNest & Diver - 15 dimensional scans
Working pts. = 2000
Working pts. = 5000
Working pts. = 10, 000
Working pts. = 20, 000
$\log(\mathcal{L})_{BF}$
Diver
MultiNest
Convergence tolerance
GAMBIT 1.0.0
MultiNest
nlive: 20,000
tol: 0.0001
Marg. posterior
MultiNest
nlive: 20,000
tol: 0.01
Marg. posterior
MultiNest
nlive: 5,000
tol: 0.001
Marg. posterior
MultiNest
nlive: 2,000
tol: 0.001
Marg. posterior
$\log_{10}\lambda_{hS}$
$\log_{10}(m_S/\mathrm{GeV})$
Relative probability $P/P_{\max}$

Nested sampling in particle physics (arXiv:1705.07959)



- Nested sampling is not an efficient maximiser, it is a sampler.
- Tolerance will not get you proportionally closer to the peak, or proportionally faster to the typical set.
- Better procedure would be to use it to scout out multimodal distributions, and then launch diver from its final (mode-separated) samples.
- You don't need that many live points (run time is linear in live points).

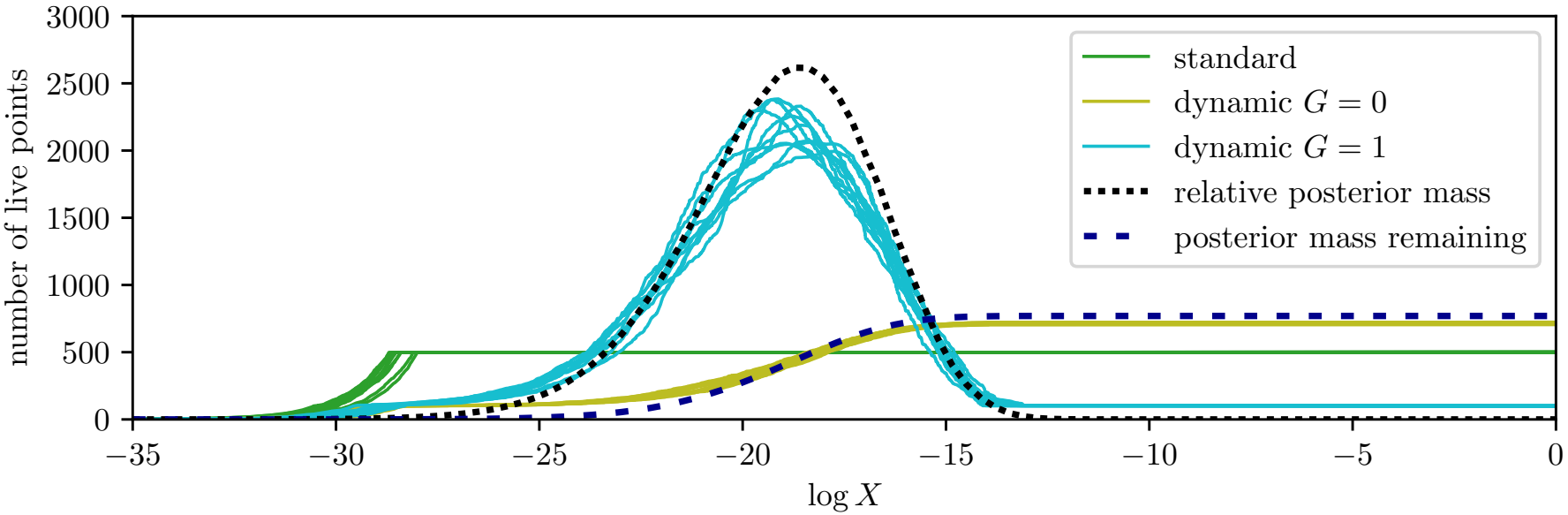
Unweaving runs

Advances in nested sampling

- John Skilling noted that two nested sampling runs can be combined in likelihood order to produce a valid run with a larger number of live points.
- The reverse is also true (arXiv:1704.03459).
- In general, a run with n live points can be "unweaved" into n runs with a single live point.
- Useful for providing convergence diagnostics and better parameter estimation (arXiv:1804.06406).

Dynamic nested sampling

Advances in nested sampling (arXiv:1704.03459, dynesty: arXiv:1904.02180)



The number of live points can be varied dynamically in order to oversample regions of interest

Multi-temperature sampling

- By compressing from prior to posterior, Nested Sampling's weighted samples are fundamentally different from traditional MCMC.
- Nested sampling tails and peaks equally.
- We can define the "temperature" of a distribution in analogy with thermodnyamics:

$$\log L \sim E \Rightarrow P \propto e^{-\beta E} = e^{-E/kT}, \quad \beta = 1$$

- Sampling at different temperatures can be useful for exploring tails.
- Nested sampling runs give you the full partition function

$$\log Z(\beta) \approx \sum_i \mathcal{L}_i^\beta \Delta X_i$$

Nested importance sampling

Future research

- Much of the time spent in a nested sampling run is spent "compressing the tails".
- Posterior-repartitioned nested sampling gives one way of speeding this up (arXiv:1908.04655)
- Sometimes we have a-priori good knowledge of the posterior bulk (analagous to an MCMC proposal distribution).

$$Z_0 = \int L(\theta)\pi_0(\theta)d\theta, \qquad Z_1 = \int L(\theta)\pi_1(\theta)d\theta$$
$$= \int L(\theta)\pi_1(\theta)\frac{\pi_0(\theta)}{\pi_1(\theta)}d\theta = \left\langle \frac{\pi_0(\theta)}{\pi_1(\theta)} \right\rangle_{P_1}$$

- This importance weighting only works if you have a lot of tail samples.

N-σ contours

Future research

- Traditional posterior samples only allow you to plot contours out to 2-3σ.
- Nested sampling fully samples the tails, so in theory one could do 20σ contours.
- Requires further thought in alternatives to kernel density estimation.

Likelihood free inference

- How can we apply Bayesian inference if we don't know the likelihood, but can simulate the system?
- Learn approximation of likelihood from simulations by fitting $f(\theta;\alpha) \approx L(\theta) = P(D|\theta)$, α are hyperparameters, D are massively compressed statistics.
- Current work in this field treats this as a "training" problem, using neural density estimators f.
- Better to fit for proxy hyperparameters α using full Bayesian approach
- Currently investigating this with mixture modelling+sparse reconstruction
- "Compromise-free Likelihood-free inference" (Handley & Alsing)

Things every nested sampling user should know

- "Burn in" can take a while, and results are not informative until then.
- Reducing the stopping criterion does not appreciably change run-time, or get you much futher from the peak, but does reduce reliability.
- Run time is linear in the number of live points, so reduce this for exploratory runs $\sim \mathcal{O}(10)$, but increase to $\sim \mathcal{O}(1000)$ for production-ready runs.
- Most nested sampling algorithms are intensely parallelisable, and work best in pure MPI mode (no openMP).

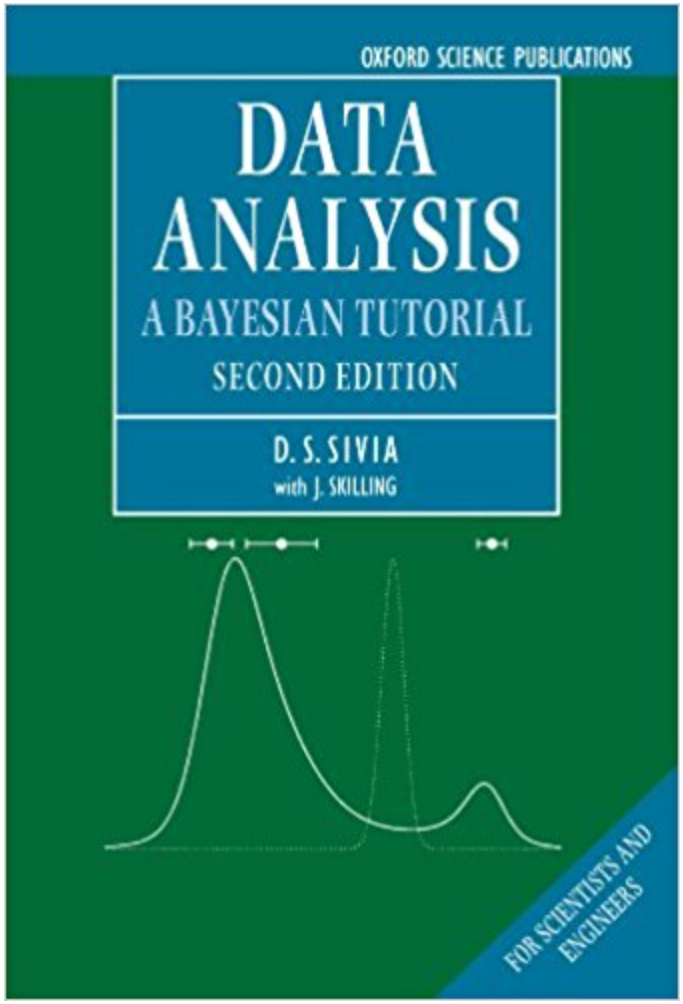
Key software

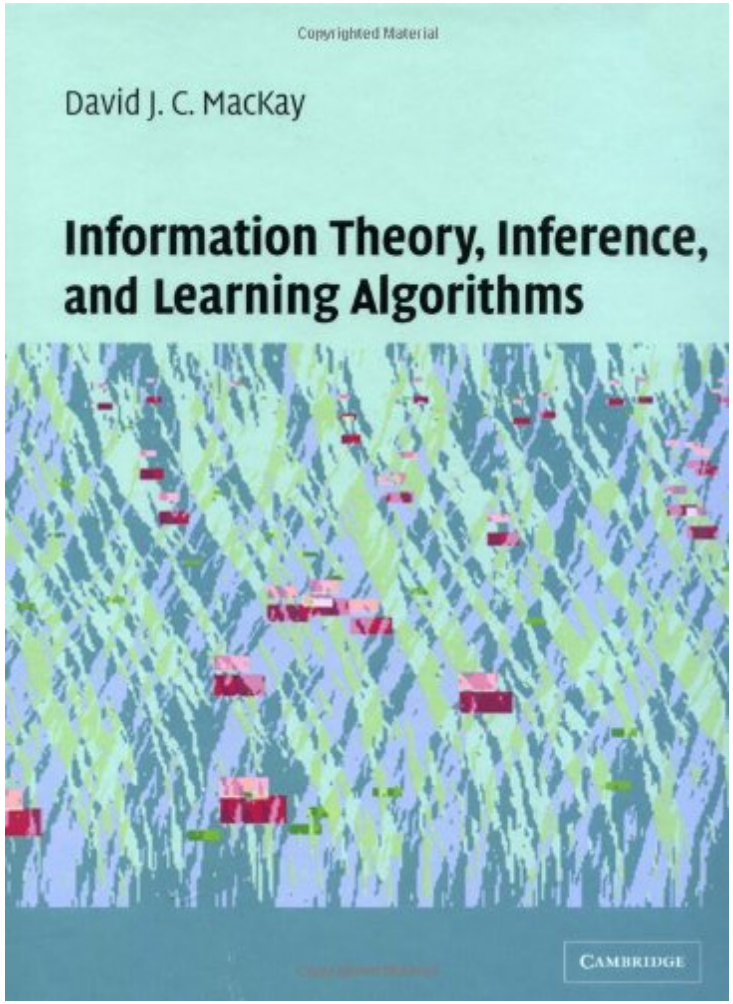
MultiNest	`github.com/farhanferoz/MultiNest`
PolyChord	`github.com/PolyChord/PolyChordLite`
DNest	`github.com/eggplantbren/DNest3`
dynesty	`github.com/joshspeagle/dynesty`
anesthetic	nested sampling visualisation `github.com/williamjameshandley/anesthetic`
fgivenx	posterior plotting of functions `github.com/williamjameshandley/fgivenx`
cosmology	Implemented as an alternative sampler in CosmoMC, MontePython, cosmosis, cobaya & GAMBIT

Summary

- Nested sampling is a rich framework for performing the full pipeline of Bayesian inference
- Plenty of further work to do on the underlying theory
- Some understanding is required in order to operate & get the most from nested sampling chains.

Further reading





- Data analysis: A Bayesian Tutorial (Sivia & Skilling)
- Information Theory, Inference and Learning Algorithms (Mackay)