Statistics

Aachen Cosmotools 2018

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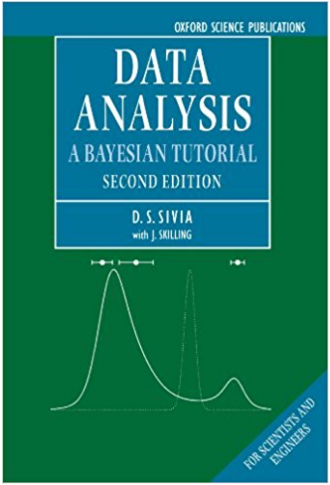
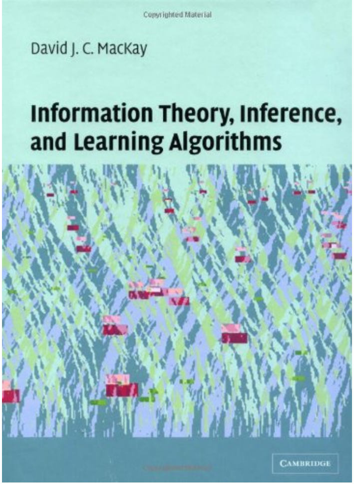
April 24, 2018

Further reading





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

Introduction

- Statistics $\equiv$ Inference $\equiv$ Machine Learning/AI.
- How to extract information about scientific models from data.
- Most cosmologists work in a *Bayesian* framework of inference, although *Frequentist* methods are also sometimes used.

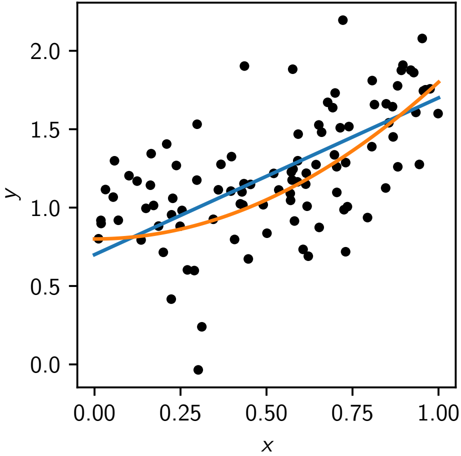
Motivating example

Fitting lines to data

- We have noisy data D
- We wish to fit a model M
- Functional form
  $y = f_M(x;\theta) = ax + b$
- e.g:

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

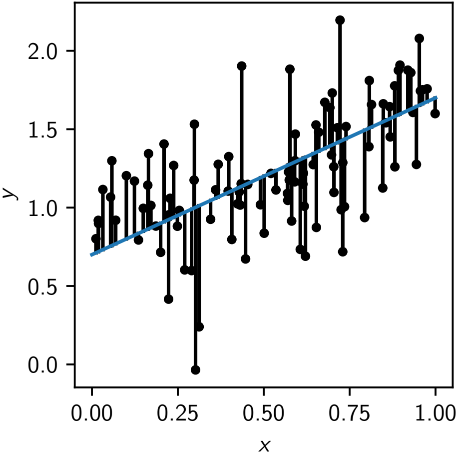
- Model parameters
  $\theta = (a, b)$



- For each parameter set θ:

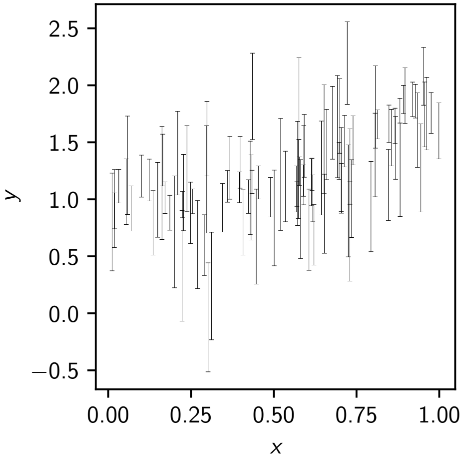
$$\chi^2(\theta) = \sum_i |y_i - f(x_i;\theta)|^2$$

- Minimise χ^2 wrt θ



- If data have non-uniform errors:

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



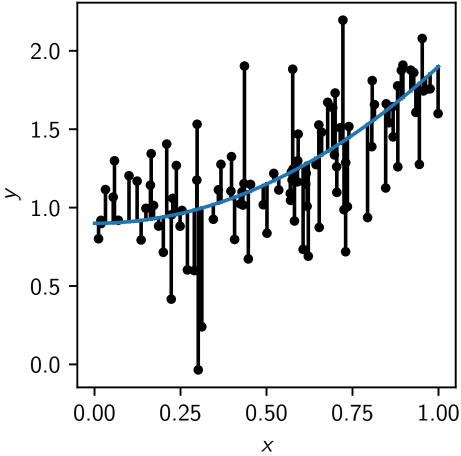
Problems with χ^2

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 even come from?



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

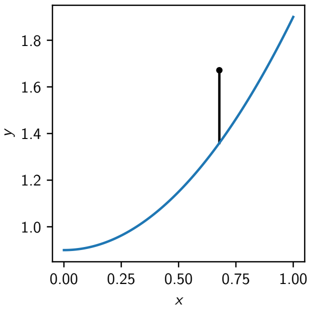
"To flip a conditional $P(x|y)$, you first de-condition on y, and then re-condition on x."

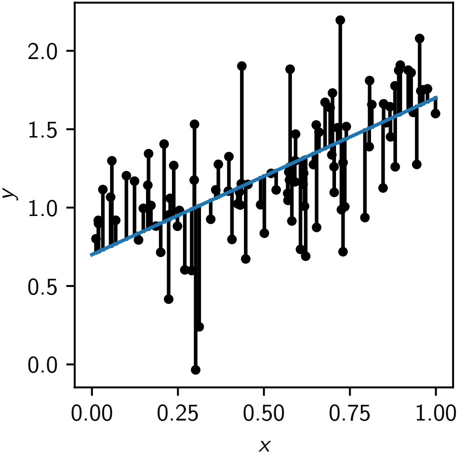
The probability of observing a datum:

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

The probability of observing the data:

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





- 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 theorem:

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

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

Terminology

Bayesian inference

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

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

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

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

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The prior
Example: Biased coins

- Need to define the **Prior** $P(\theta)$ — probability of the bias, given no data
- Represents our knowledge of parameters before the data – subjective
- Frequentists view this as a flaw in Bayesian inference.
- Bayesians view this as an advantage
- Fundamental rule of Inference:

The prior

Example: Biased coins

- Need to define the **Prior** $P(\theta)$ — probability of the bias, given no data
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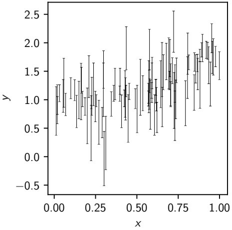
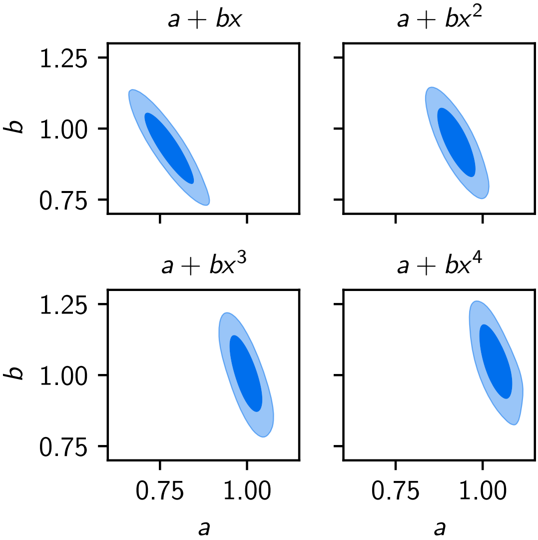
- Frequentists view this as a flaw in Bayesian inference.
- Bayesians view this as an advantage
- Fundamental rule of Inference:

You cannot extract information from data
without making assumptions

- All Bayesians do is make them explicit
- Any method that claims it is "objective" is simply hiding them

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

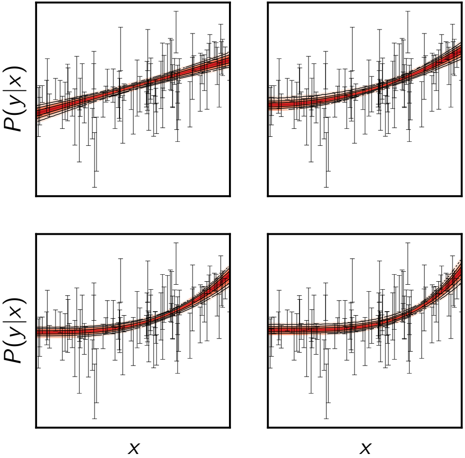




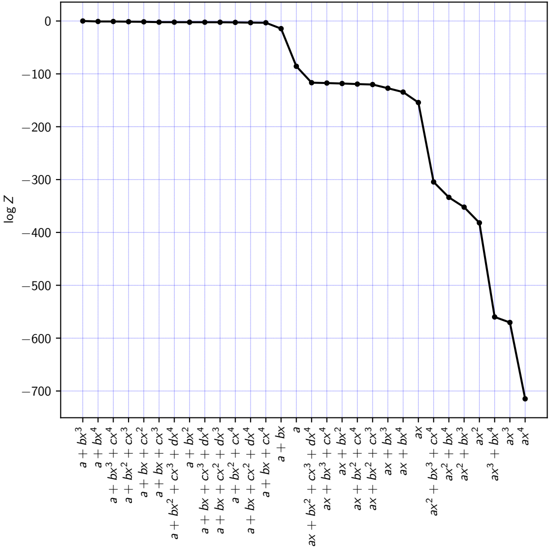
More useful to plot:

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

(all conditioned on D, M)



- We may use $Z = P(D|M)$ to determine whether a model is reasonable.



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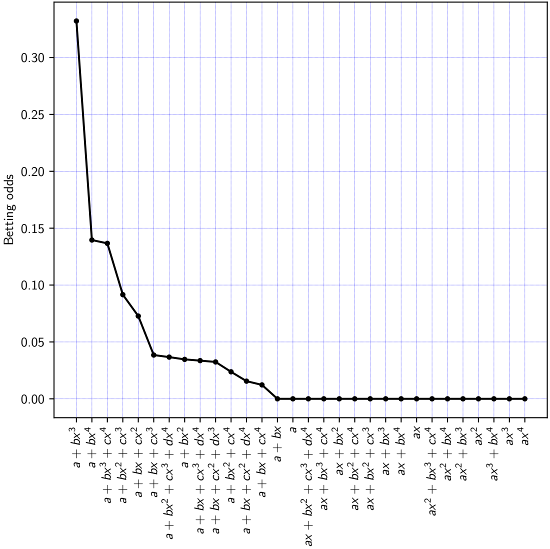
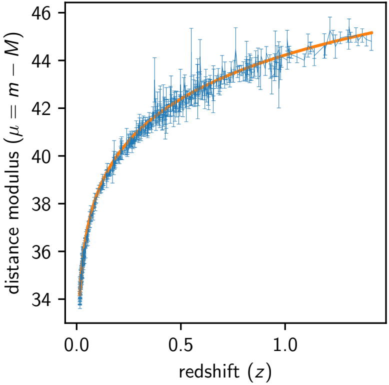


Line fitting (context)

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



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

Probability distributions

- As scientists, we are used to seeing error bars on results.
- Age of the universe (*Planck*):

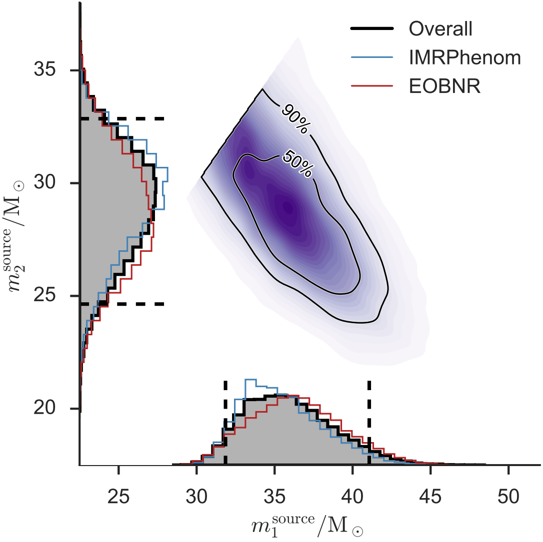
$$13.73 \pm 0.12 \,\text{billion years old.}$$

- Masses of LIGO GW150914 binary merger:

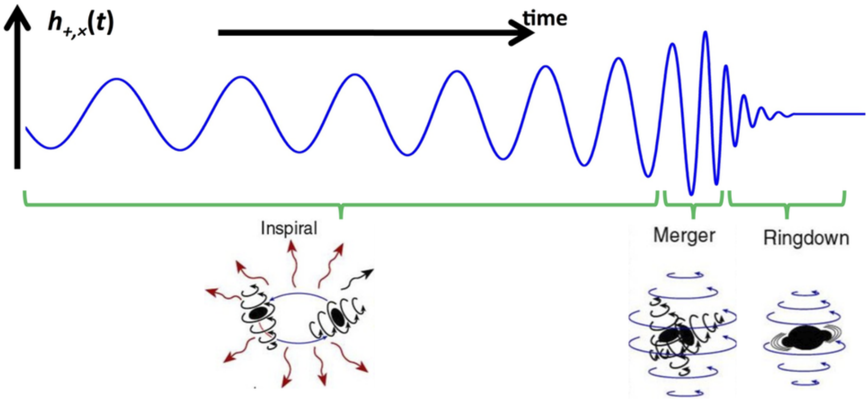
$$m_1 = 39.4^{+5.5}_{-4.9}\,M_\odot, \qquad m_2 = 30.9^{+4.8}_{-4.4}\,M_\odot$$

- These are called *credible intervals*, state that we are e.g. 90% confident of the value lying in this range.
- More importantly, these are *summary statistics*.

LIGO binary merger



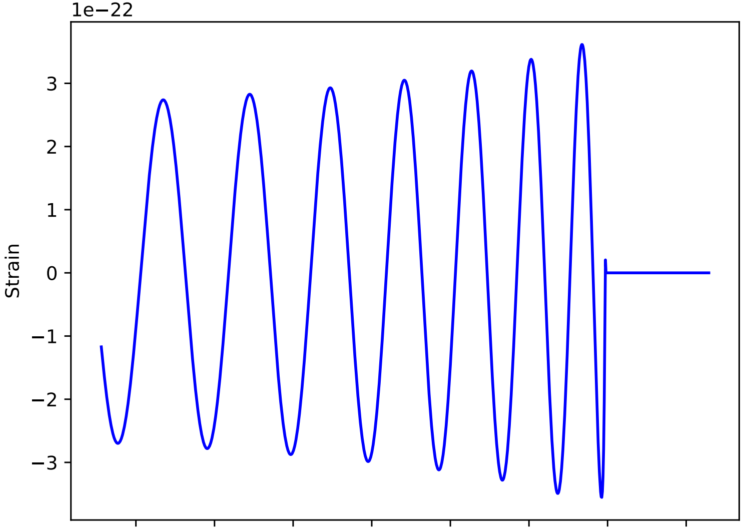
- Summary statistics summarise a full probability distribution.
- One goal of inference is to produce these probability distributions.



$h_{+,\times}(t)$
time
Inspiral
Merger
Ringdown

The model M

Extended example of inference: LIGO



The parameters Θ of the model M

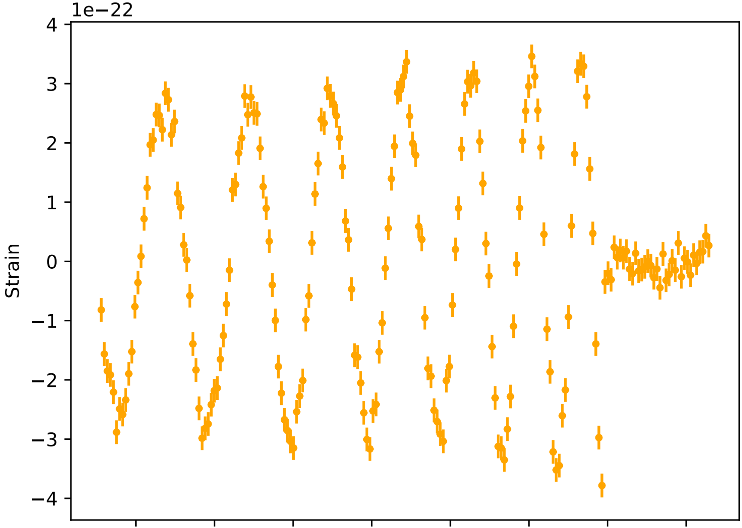
Extended example of inference: LIGO

Theoretical signal depends on:

- m_1, m_2: mass of binary
- θ, ϕ: sky location
- r: luminosity distance
- Φ_c, t_c: phase and time of coalescence
- i, θ_{sky}: inclination and angle on sky (orbital parameters)

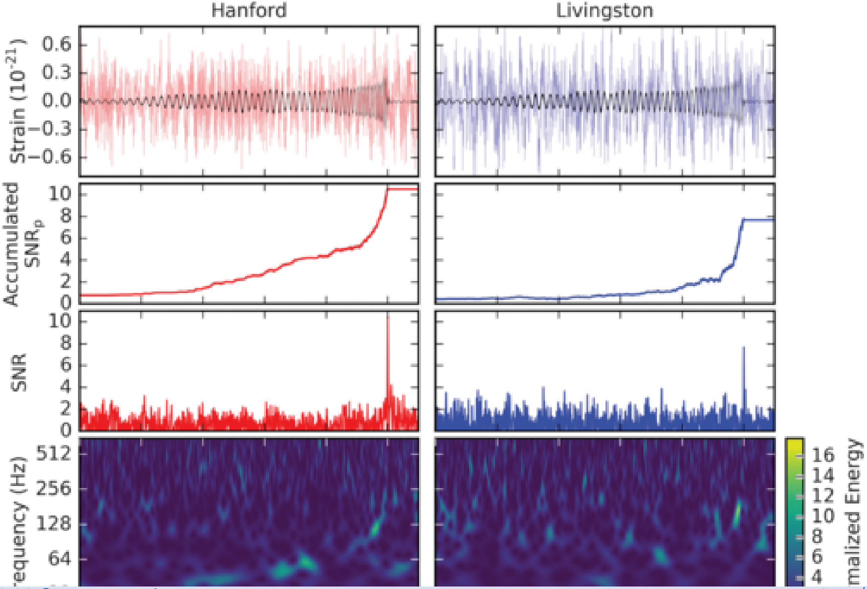
The data D

Extended example of inference: LIGO



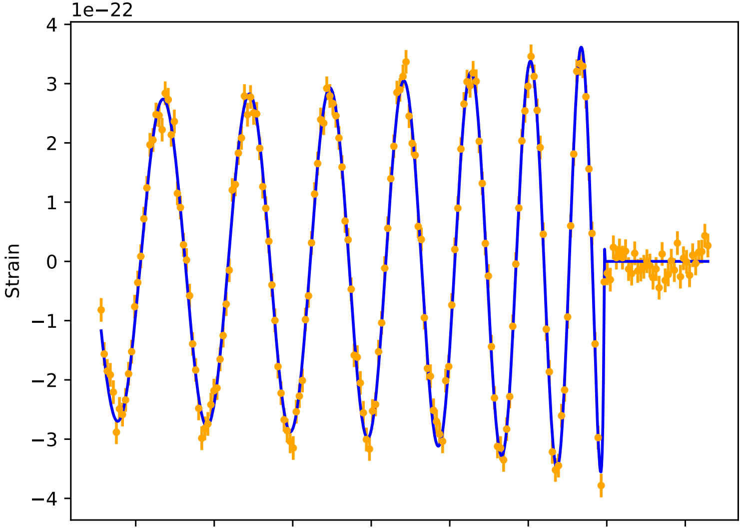
The data D

Extended example of inference: LIGO



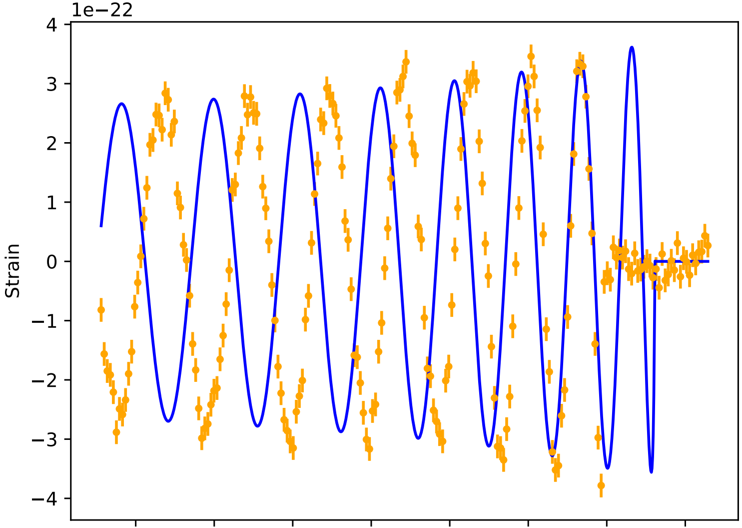
The Likelihood: well matched

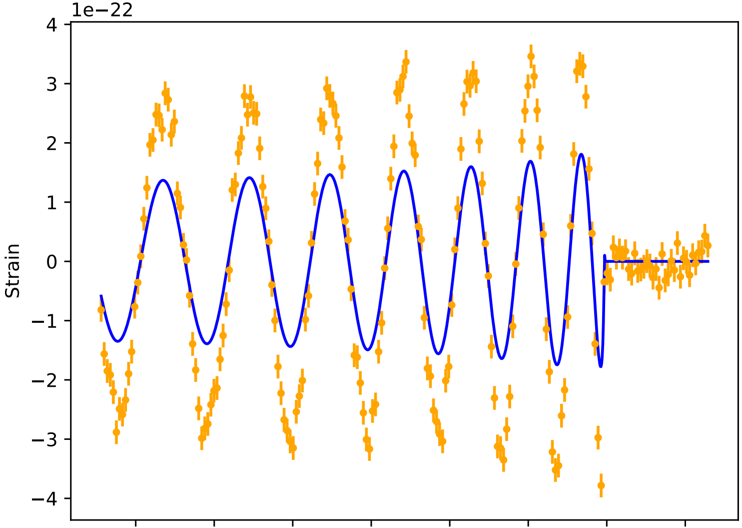
Extended example of inference: LIGO



The Likelihood: coalescence off

Extended example of inference: LIGO

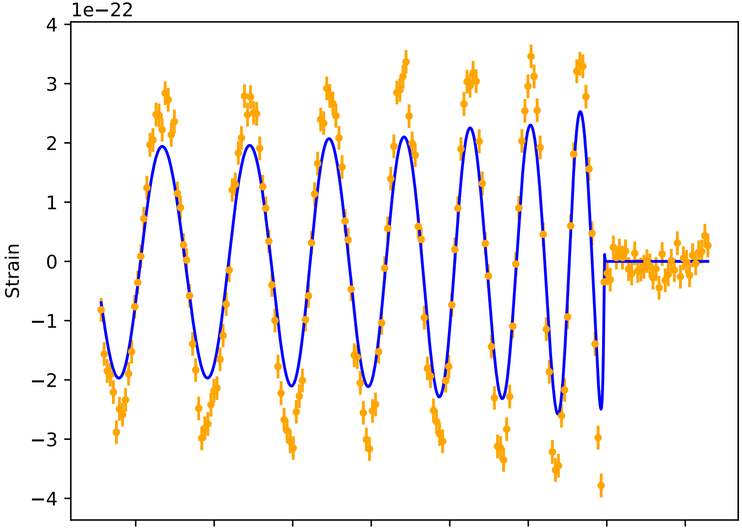




1e−22
4
3
2
1
0
−1
−2
−3
−4
Strain

The Likelihood: incorrect inclination

Extended example of inference: LIGO



- Cannot plot the full posterior distribution:

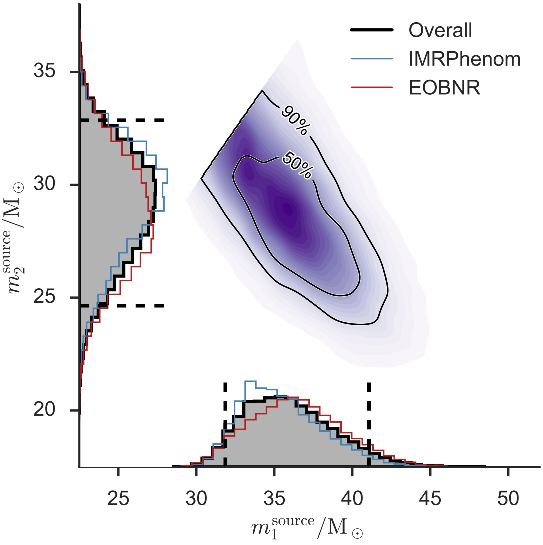
$$\mathcal{P}(\Theta) \equiv P(m_1, m_2, \theta, \phi, r, \Phi_c, t_c, i, \theta_{\mathrm{sky}}|D, M)$$

- Can plot 1D and 2D *marginalised* distributions e.g:

$$P(m_1, m_2|D, M) =$$
$$\int P(m_1, m_2, \theta, \phi, r, \Phi_c, t_c, i, \theta_{\mathrm{sky}}|D, M)\, d\theta\, d\phi\, dr\, d\Phi_c\, dt_c\, di\, d\theta_{\mathrm{sky}}$$

Posterior $\mathcal{P}$

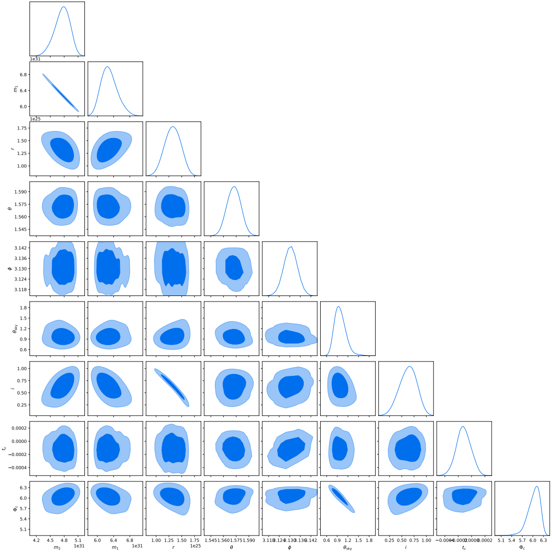
Extended example of inference: LIGO



- May do this for each pair of parameters
- Generates a *triangle plot*

Posterior $\mathcal{P}$

Extended example of inference: LIGO



- Does give insight
- Not the full picture

Evidences and model comparison

Extended example of inference: LIGO

- Up until now, we have discussed *Parameter estimation*: inferring what data tell us about parameters Θ of a model M.
- Scientifically speaking, this is only half the story.
- In general, we will have several competing models that describe the data, and we want to know which is the "best".

Parameter estimation

Another example.

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

Parameter estimation

Another example.

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

$$D = \{C_\ell\}$$

Parameter estimation

Another example.

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

$$\begin{aligned} D &= \{C_\ell\} \\ M &= \Lambda\mathrm{CDM} \end{aligned}$$

Parameter estimation

Another example.

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

$$\begin{aligned} D &= \{C_\ell\} \\ M &= \Lambda\mathrm{CDM} \\ \Theta &= \Theta_{\Lambda\mathrm{CDM}} \end{aligned}$$

Parameter estimation

Another example.

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

$$\begin{aligned} D =& \{C_\ell\} \\ M =& \Lambda\text{CDM} \\ \Theta =& \Theta_{\Lambda\text{CDM}} \\ \Theta_{\Lambda\text{CDM}} =& (\Omega_b h^2, \Omega_c h^2, 100\theta_{MC}, \tau, \ln(10^{10} A_s), n_s) \end{aligned}$$

Parameter estimation

Another example.

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

$$\begin{aligned}
D =& \{C_\ell^{(\text{Planck})}\} \\
M =& \Lambda\text{CDM} \\
\Theta =& \Theta_{\Lambda\text{CDM}} \\
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\end{aligned}$$

Parameter estimation

Another example.

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

$$\begin{aligned}
D =& \{C_\ell^{(\mathrm{Planck})}\} \\
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\end{aligned}$$

Parameter estimation

Another example.

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

$$\begin{aligned}
D =& \{C_\ell^{\text{(Planck)}}\} \\
M =& \Lambda\text{CDM} + \text{extensions} \\
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\Theta_{\text{extensions}} =& (n_{\mathrm{run}})
\end{aligned}$$

Parameter estimation

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\Theta_{\text{extensions}} =& (n_{\rm run}, n_{\rm run,run})
\end{aligned}$$

Parameter estimation

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\Theta_{\text{extensions}} =& (n_{\mathrm{run}}, n_{\mathrm{run,run}}, w)
\end{aligned}$$

Parameter estimation

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

Parameter estimation

Another example.

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

$$\begin{aligned}
D =& \{C_\ell^{(\text{Planck})}\} + \{\text{LSS}\} \\
M =& \Lambda\text{CDM} + \text{extensions} \\
\Theta =& \Theta_{\Lambda\text{CDM}} + \Theta_{\text{Planck}} + \Theta_{\text{extensions}} \\
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\end{aligned}$$

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

$$\begin{aligned}
D =& \{C_\ell^{(\text{Planck})}\} + \{\text{LSS}\} + \{\text{"Big Data"}\} \\
M =& \Lambda\text{CDM} + \text{extensions} \\
\Theta =& \Theta_{\Lambda\text{CDM}} + \Theta_{\text{Planck}} + \Theta_{\text{extensions}} \\
\Theta_{\Lambda\text{CDM}} =& (\Omega_b h^2, \Omega_c h^2, 100\theta_{MC}, \tau, \ln(10^{10} A_s), n_s) \\
\Theta_{\text{Planck}} =& (y_{\mathrm{cal}}, A_{217}^{CIB}, \xi^{tSZ-CIB}, A_{143}^{tSZ}, A_{100}^{PS}, A_{143}^{PS}, A_{143\times 217}^{PS}, A_{217}^{PS}, \\
& A^{kSZ}, A_{100}^{\mathrm{dust}\,TT}, A_{143}^{\mathrm{dust}\,TT}, A_{143\times 217}^{\mathrm{dust}\,TT}, A_{217}^{\mathrm{dust}\,TT}, c_{100}, c_{217}) \\
\Theta_{\text{extensions}} =& (n_{\mathrm{run}}, n_{\mathrm{run,run}}, w, \Sigma m_\nu, m_{\nu,\mathrm{sterile}}^{\mathrm{eff}})
\end{aligned}$$

Parameter estimation

Another example.

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

$$\begin{aligned}
D =& \{C_\ell^{(\text{Planck})}\} + \{\text{LSS}\} + \{\text{“Big Data”}\} \\
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\Theta =& \Theta_{\Lambda\text{CDM}} + \Theta_{\text{Planck}} + \Theta_{\text{extensions}} \\
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\Theta_{\text{Planck}} =& (y_{\mathrm{cal}}, A^{CIB}_{217}, \xi^{tSZ-CIB}, A^{tSZ}_{143}, A^{PS}_{100}, A^{PS}_{143}, A^{PS}_{143\times 217}, A^{PS}_{217}, \\
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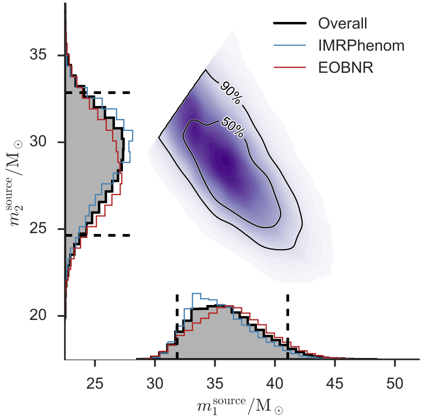
\Theta_{\text{extensions}} =& (n_{\mathrm{run}}, n_{\mathrm{run,run}}, w, \Sigma m_\nu, m^{\mathrm{eff}}_{\nu,\mathrm{sterile}})
\end{aligned}$$

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

Sampling

How to describe a high-dimensional posterior

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



Why do sampling?

Marginalisation over the posterior

- Set of N samples $S = \{\Theta^{(i)} : i = 1, \ldots N : \; \Theta^{(i)} \sim \mathcal{P}\}$
- Mean mass:

$$\bar{m}_1 \equiv \langle m_1 \rangle_{\mathcal{P}} \approx \frac{1}{N} \sum_{i=1}^{N} m_1^{(i)}$$

- Mass covariance:

$$\mathrm{Cov}(m_1, m_2) \approx \frac{1}{N} \sum_{i=1}^{N} (m_1^{(i)} - \bar{m}_1)(m_2^{(i)} - \bar{m}_2)$$

- Marginalised samples: Just ignore the other coordinates.
- N.B. Typically have *weighted* samples

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$$\bar{m}_1 \equiv \langle m_1 \rangle_{\mathcal{P}} \approx \frac{\sum_{i=1}^N w^{(i)} m_1^{(i)}}{\sum_{i=1}^N w^{(i)}}$$

- Mass covariance:

$$\mathrm{Cov}(m_1, m_2) \approx \frac{\sum_{i=1}^N (m_1^{(i)} - \bar{m}_1)(m_2^{(i)} - \bar{m}_2)}{\sum_{i=1}^N w^{(i)}}$$

- Marginalised samples: Just ignore the other coordinates.
- N.B. Typically have *weighted* samples

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.

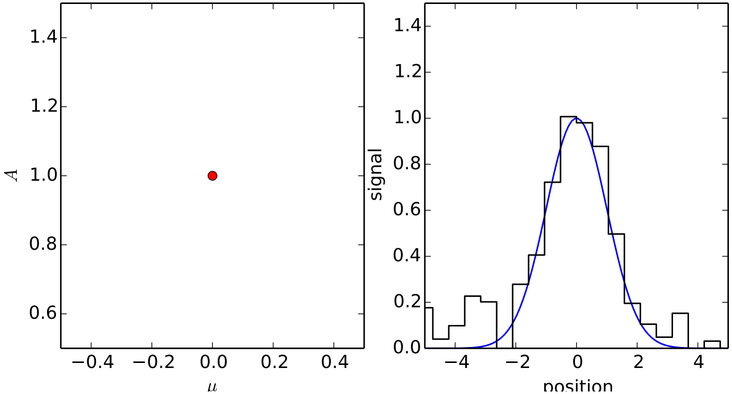
Current sampling approaches

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

Metropolis Hastings

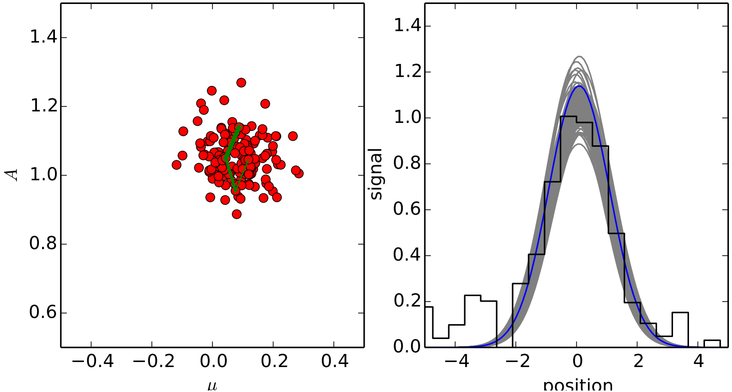
- Turn the N-dimensional problem into a one-dimensional one.
  1. Pick random direction
  2. Choose step length
  3. If uphill, make step...
  4. ...otherwise sometimes make step.

Metropolis Hastings



Metropolis Hastings

Metropolis Hastings



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.
- 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.
- Simulated annealing gives one possibility for computing evidences.
  - Inspired by thermodynamics.
  - Suffers from similar issues to MCMC.
  - Unclear how to choose correct annealing schedule

What is nested sampling?

- Nested sampling is an alternative way of sampling posteriors.
- Uses ensemble sampling to compress prior to posterior.
- In doing so, it circumvents many issues (dimensionality, topology, geometry) that beset standard approaches.

Nested Sampling

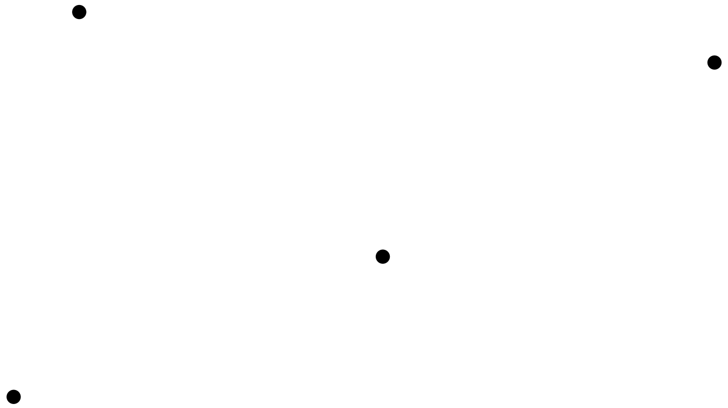
John Skilling's alternative to traditional MCMC!

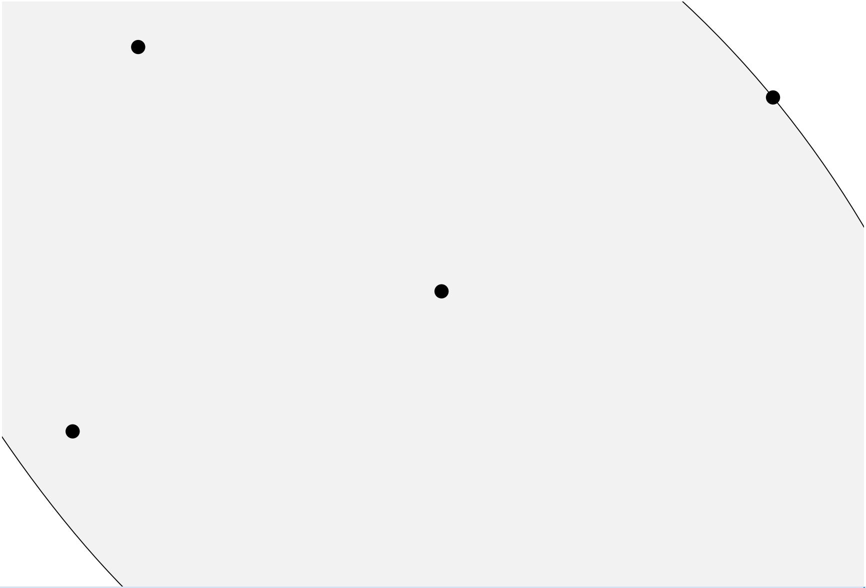
New procedure:

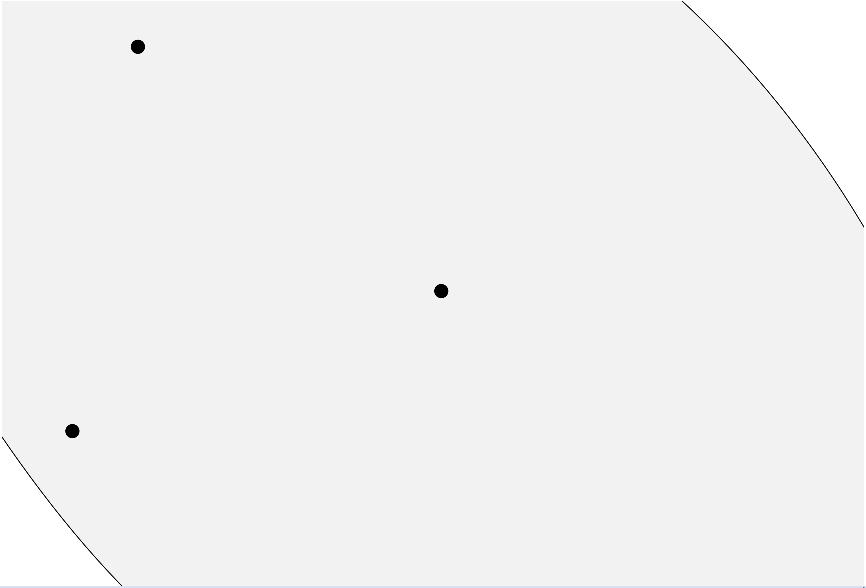
Maintain a set S of n samples, which are sequentially updated:

- 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*.

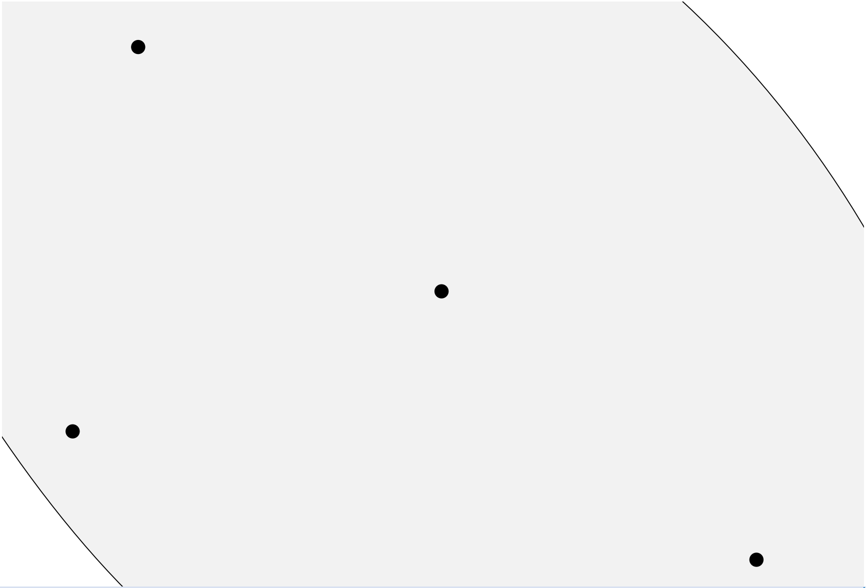


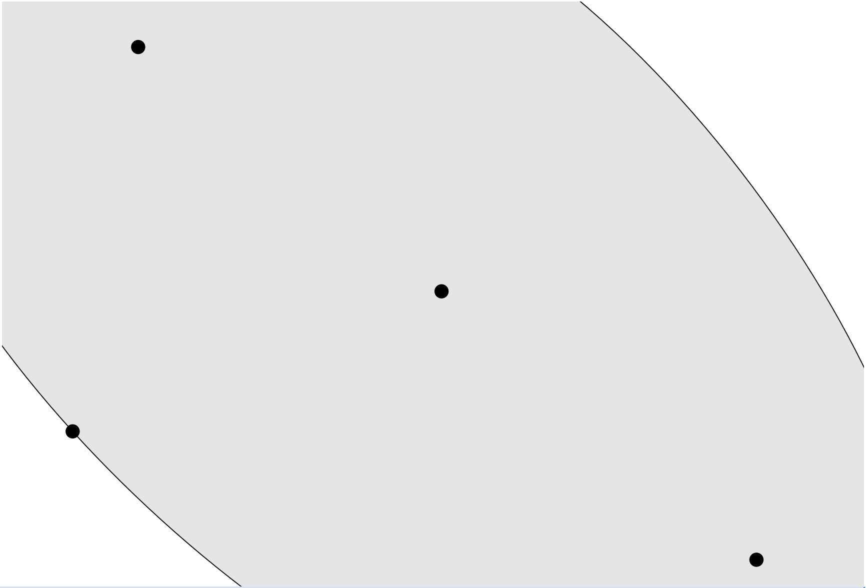




Nested Sampling

Graphical aid





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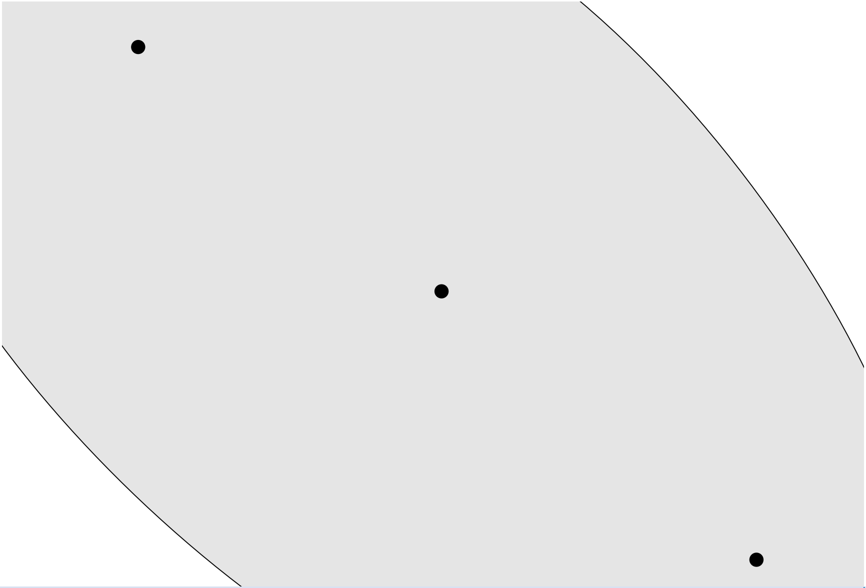

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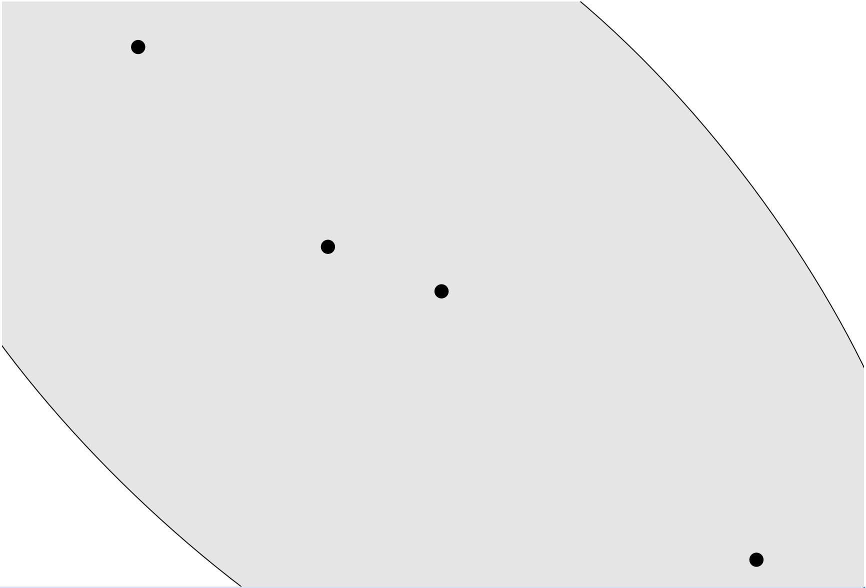
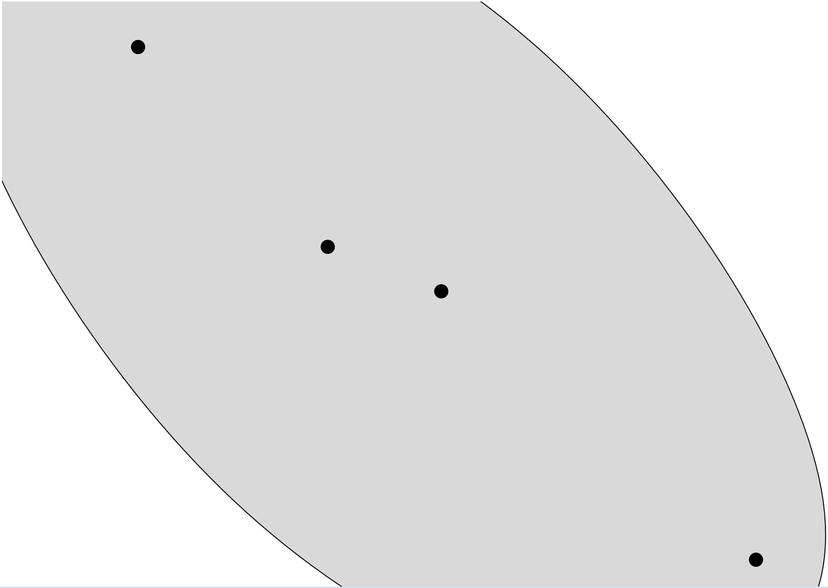
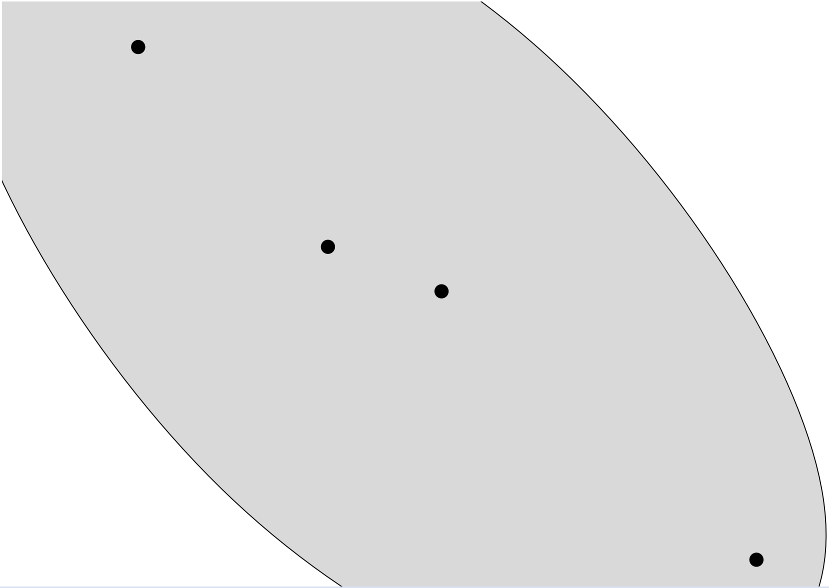
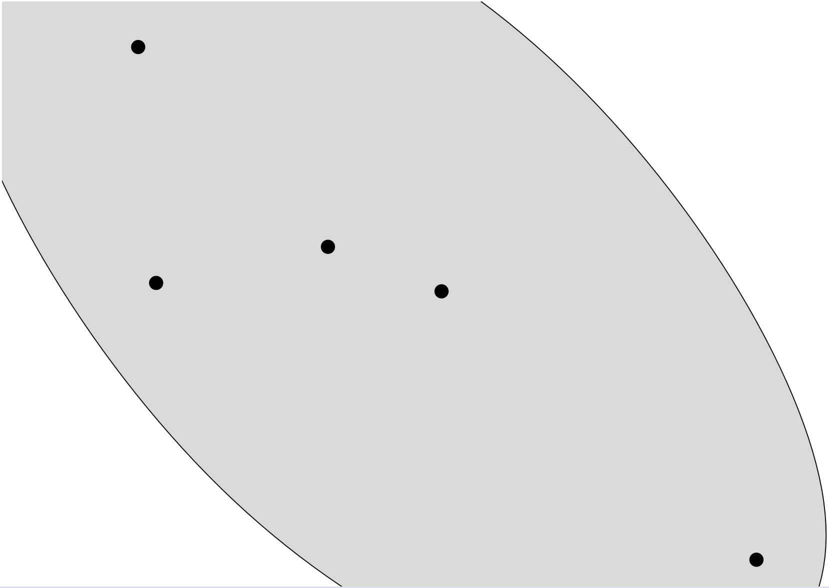
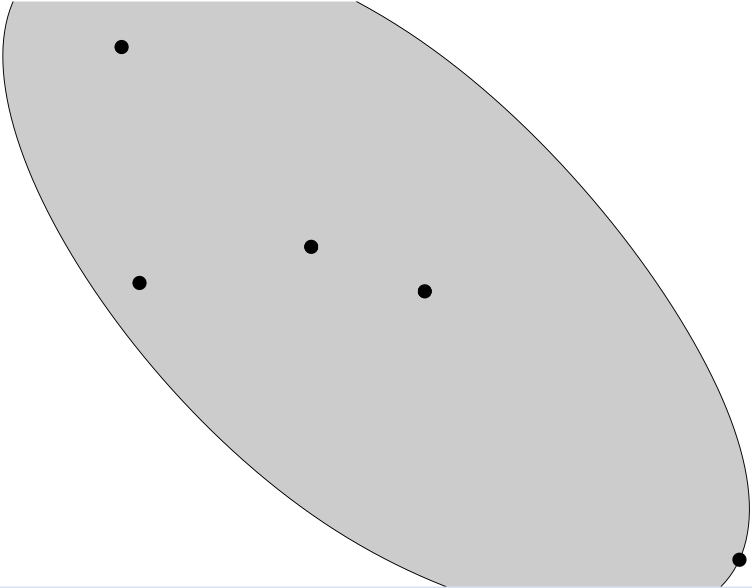






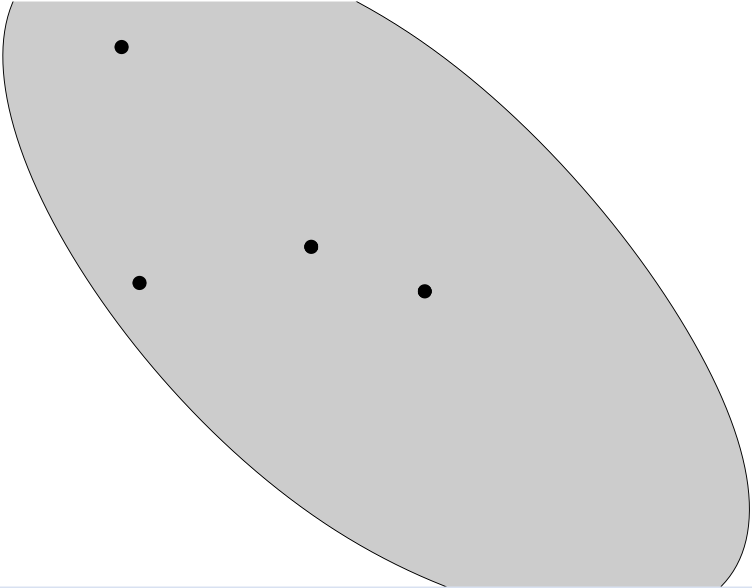


Nested Sampling
Graphical aid



Nested Sampling

Graphical aid



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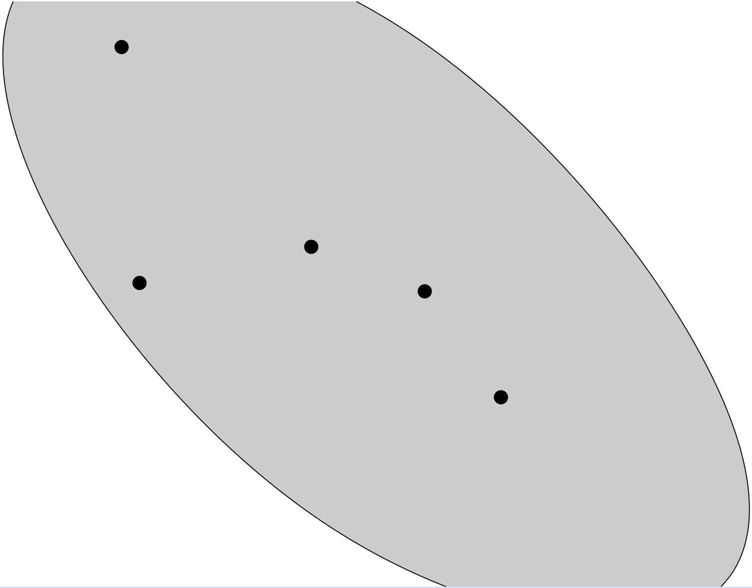

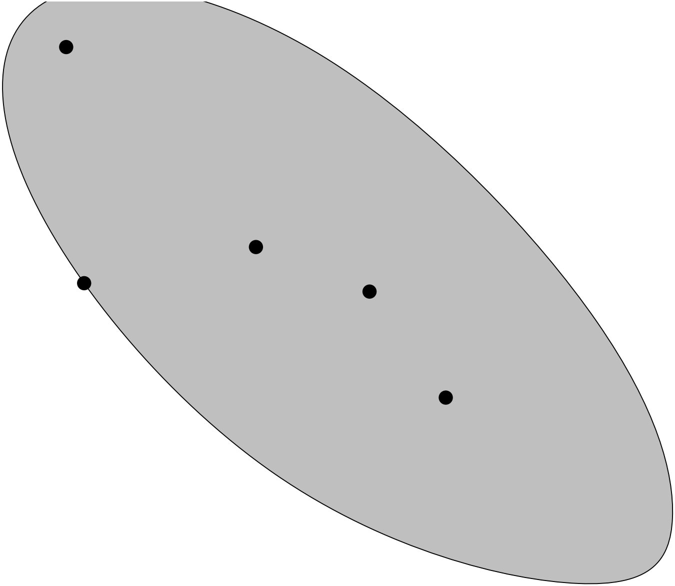

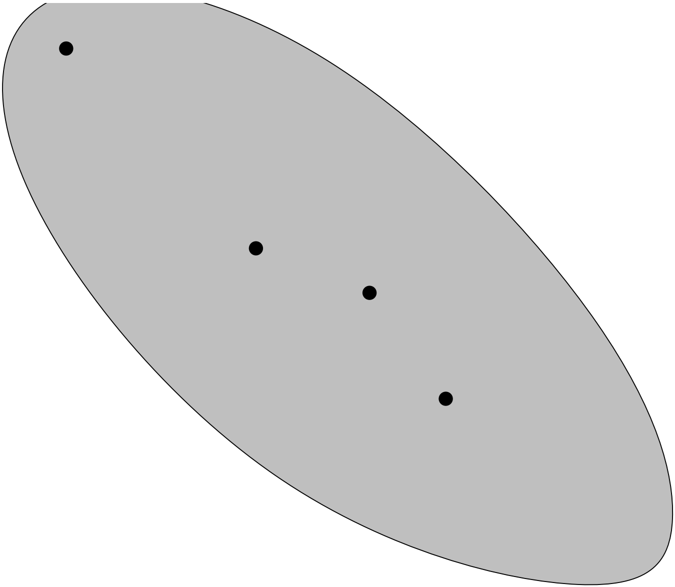

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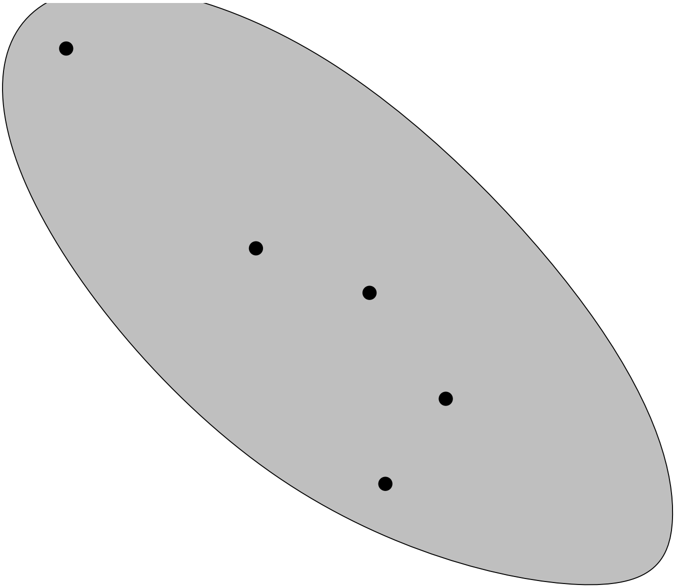

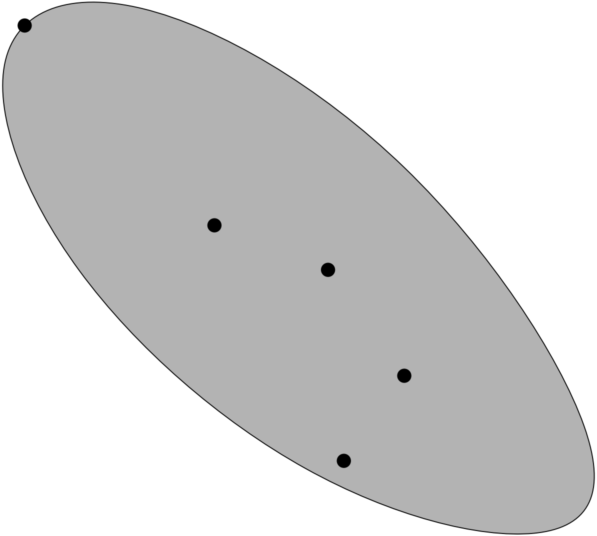

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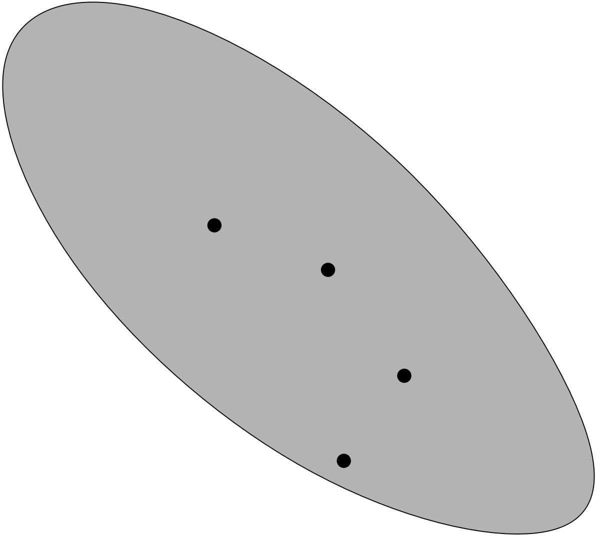

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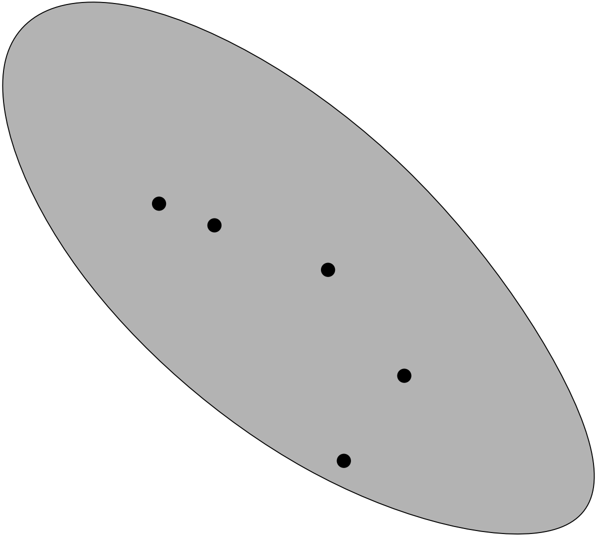

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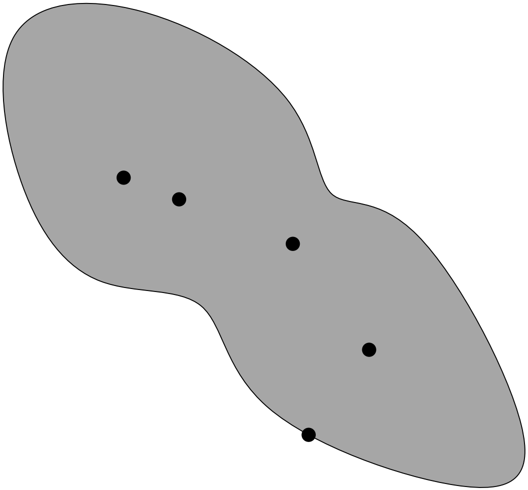

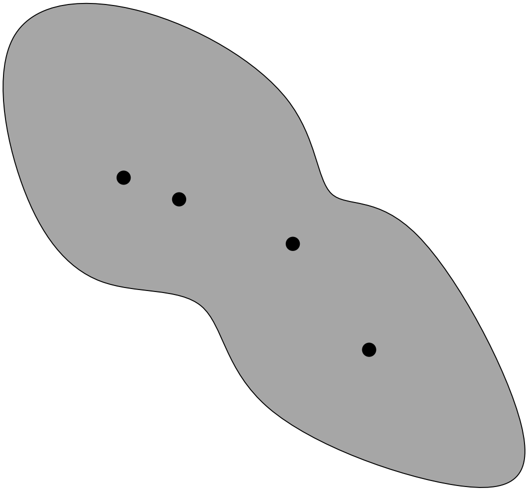

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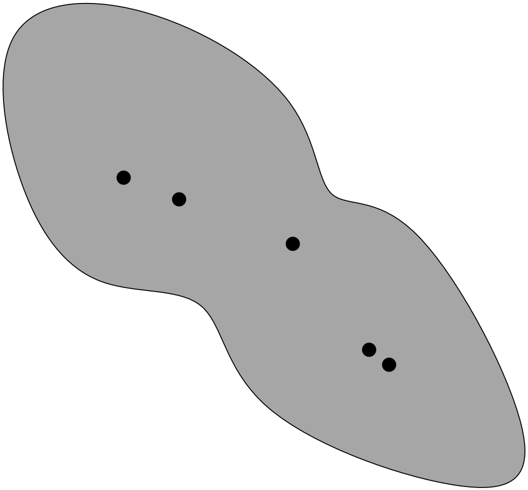

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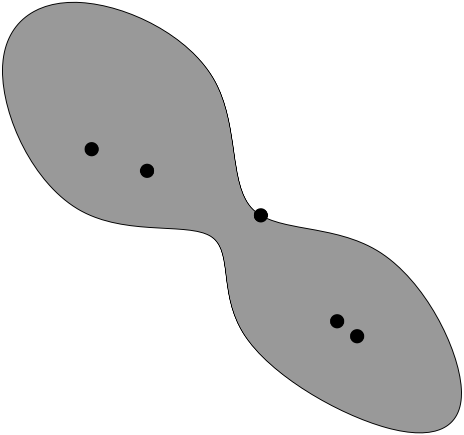

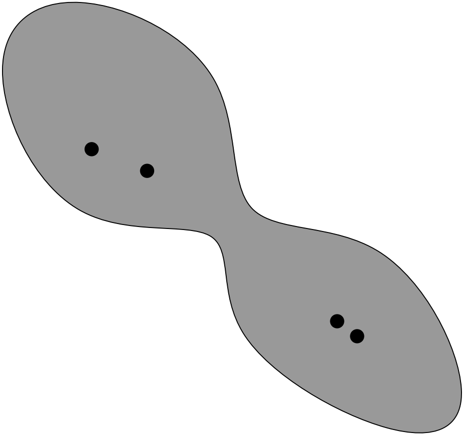

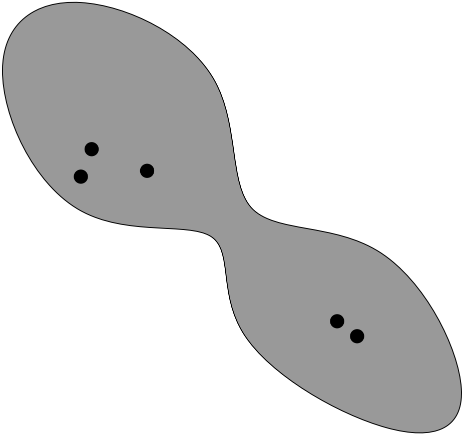

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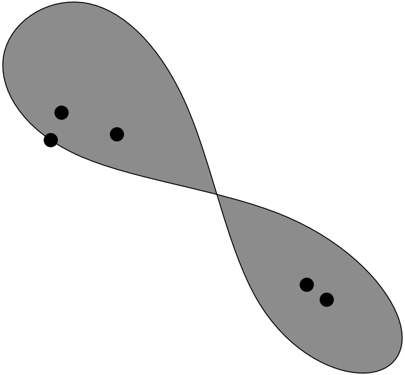

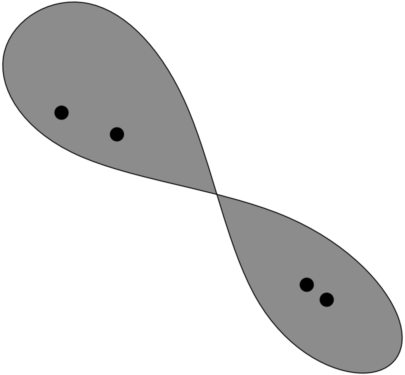

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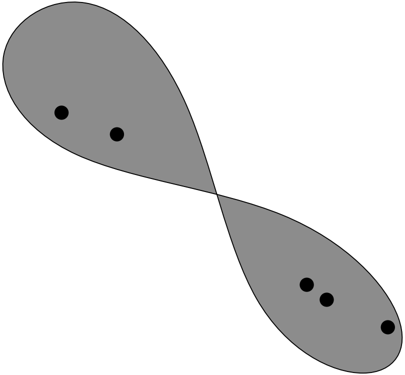

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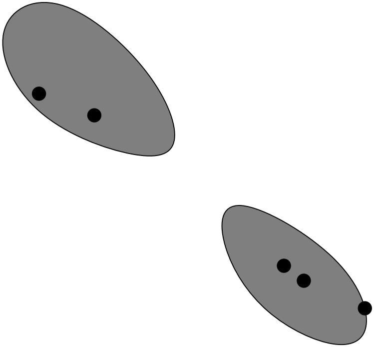

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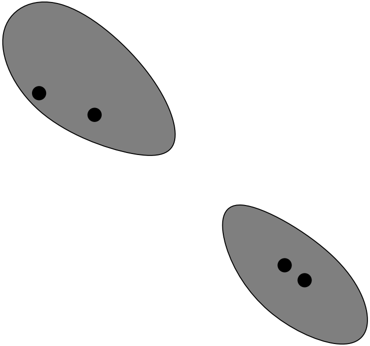

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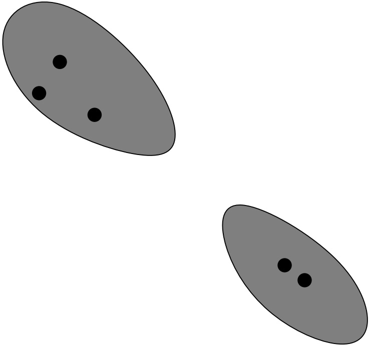

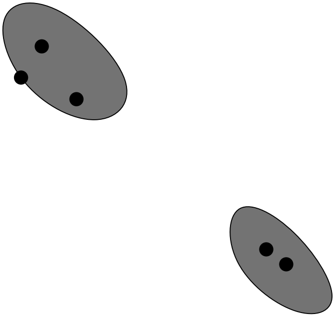

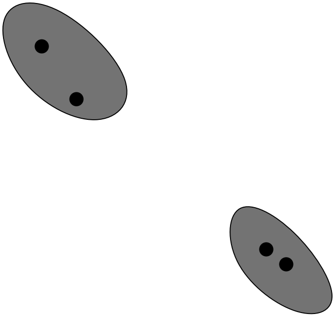

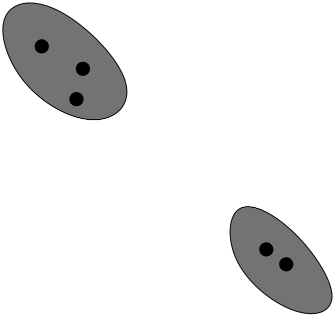

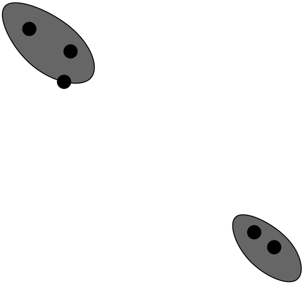

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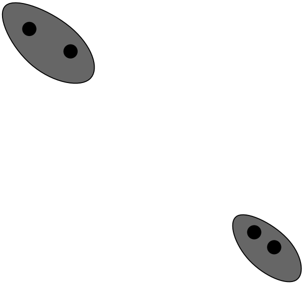

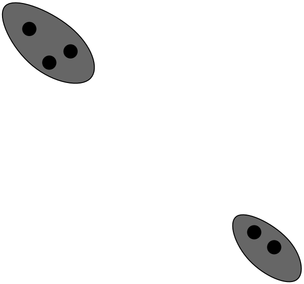

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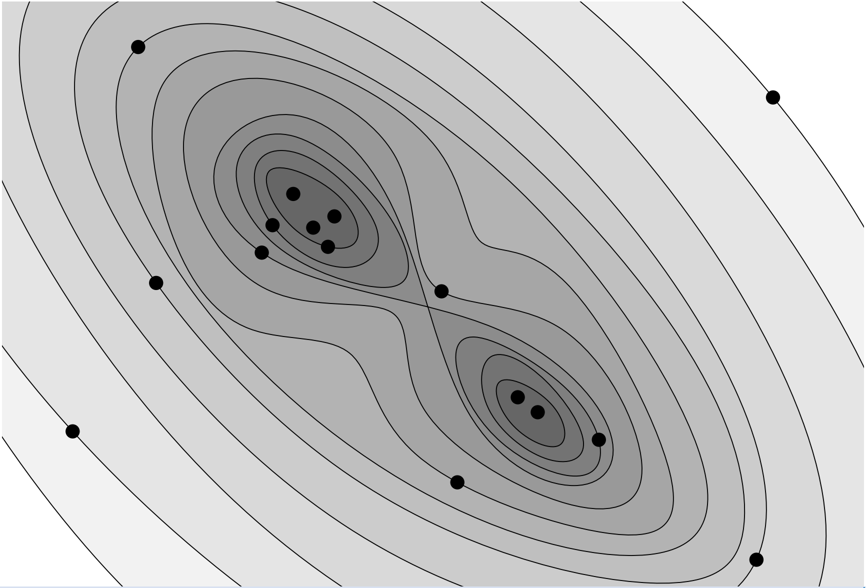


Nested sampling

- 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.

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.

Sampling within an iso-likelihood contour

Previous attempts

Rejection Sampling MultiNest; F. Feroz & M. Hobson (2009).

- Suffers in high dimensions

Hamiltonian M.J. Betancourt (2010)

Galilean F. Feroz & J. Skilling (2013)

- Requires gradients and tuning

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

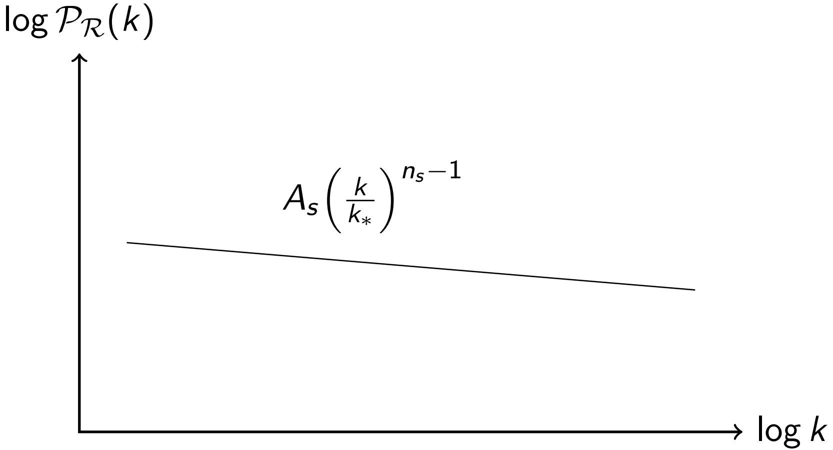
- Very promising
- Still needs tuning.

Slice Sampling PolyChord; Handley et al. (2015).

- Current "state-of-the-art".
- PolyChord 2.0 imminent.

PolyChord in action

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



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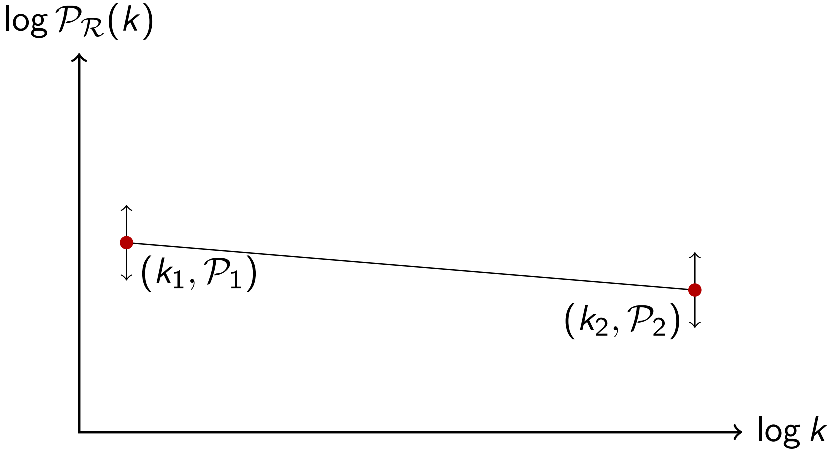

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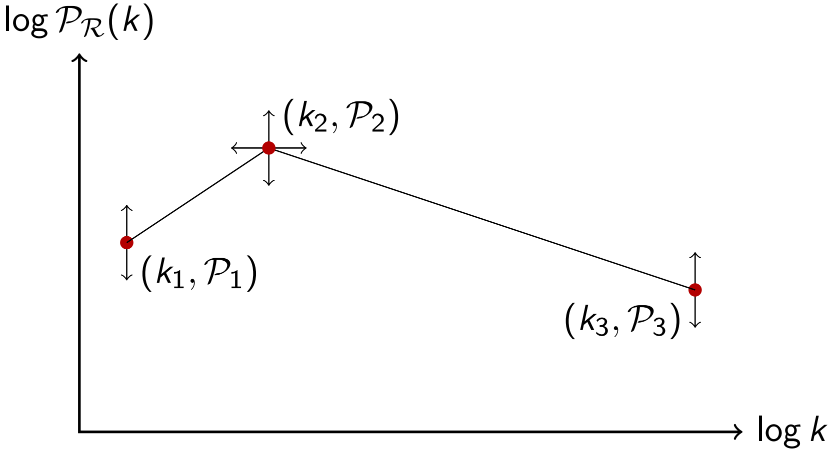

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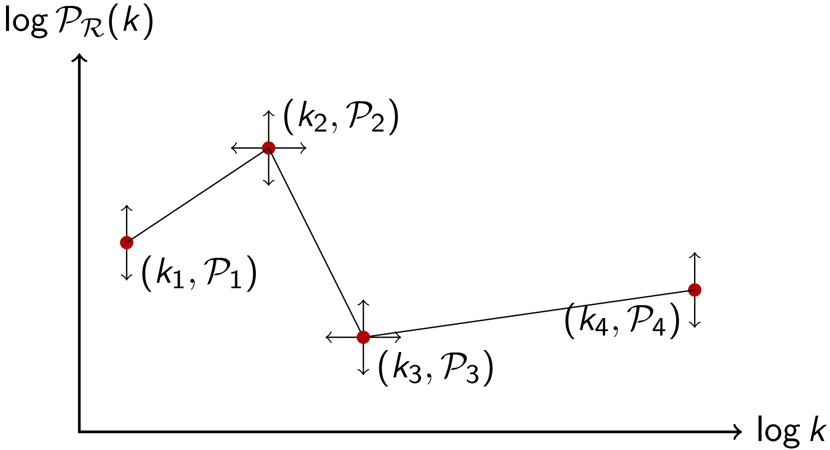
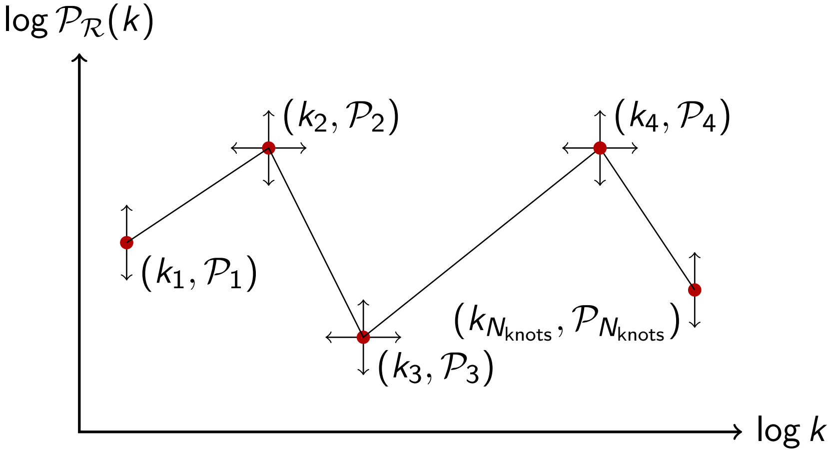
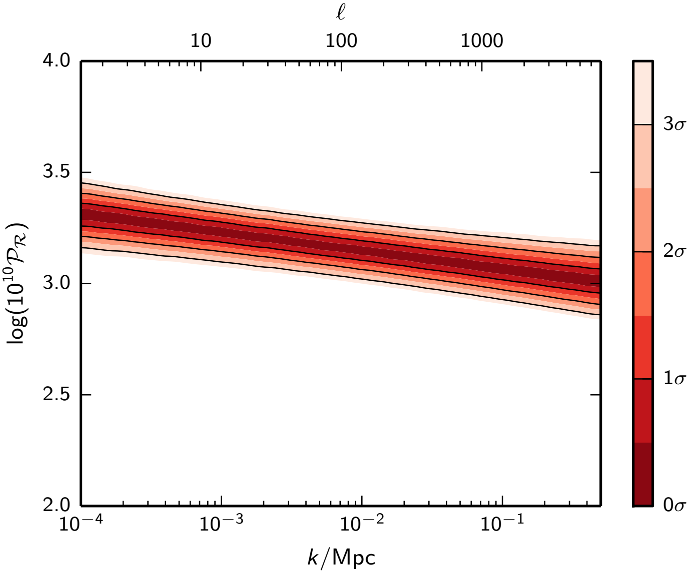




$\log \mathcal{P}_\mathcal{R}(k)$
$(k_2, \mathcal{P}_2)$
$(k_4, \mathcal{P}_4)$
$(k_1, \mathcal{P}_1)$
$(k_{N_\mathrm{knots}}, \mathcal{P}_{N_\mathrm{knots}})$
$(k_3, \mathcal{P}_3)$
$\log k$

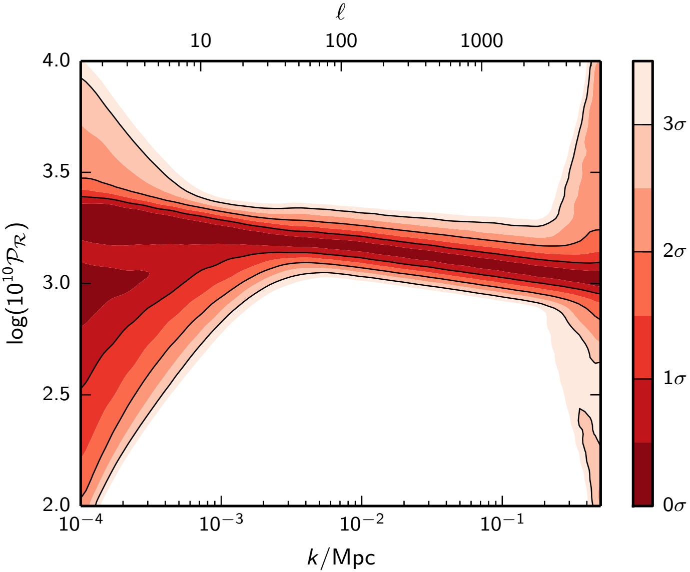
0 internal knots

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



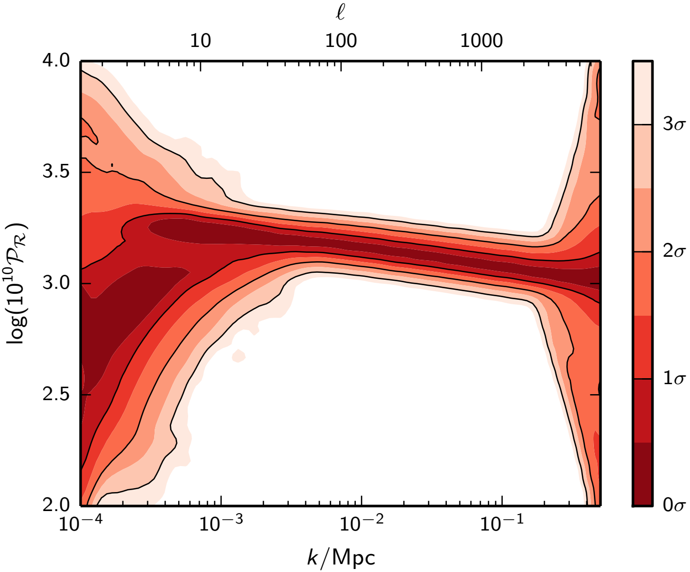
1 internal knots

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



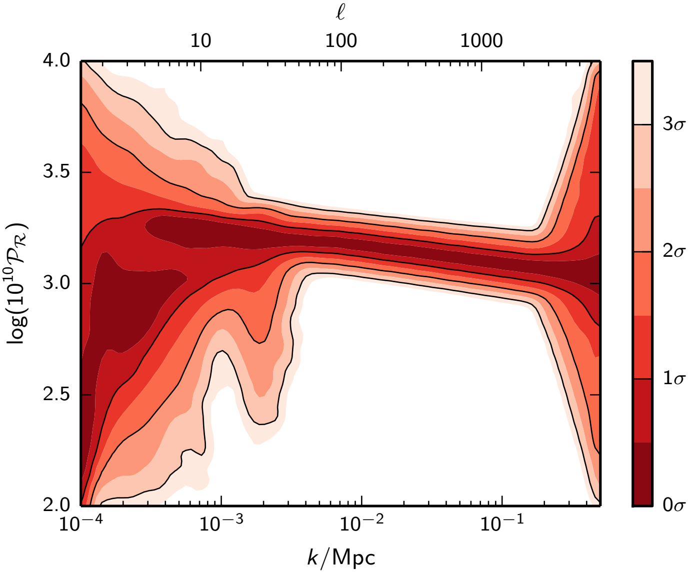
2 internal knots

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



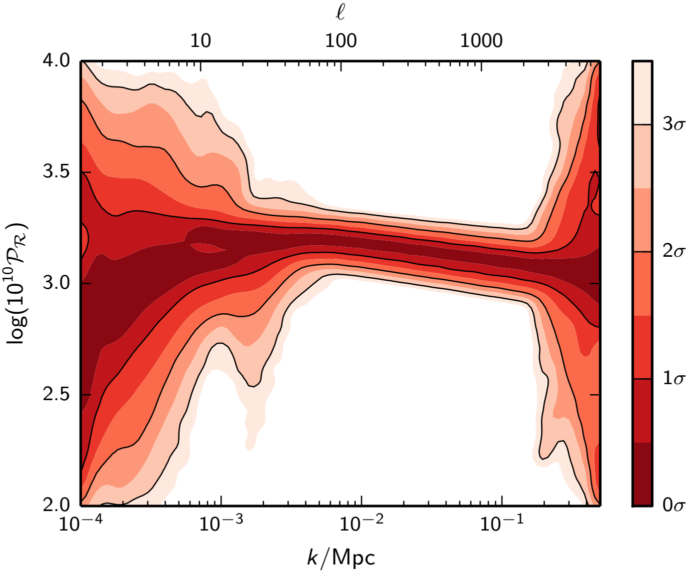
3 internal knots

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



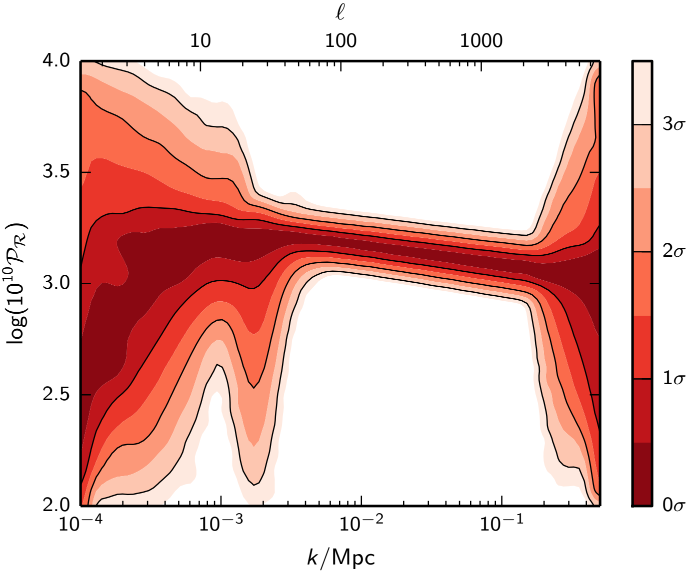
4 internal knots

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



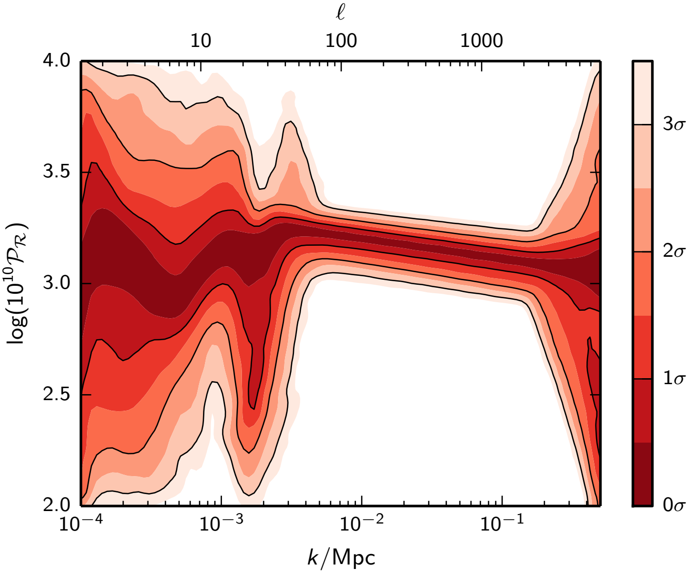
5 internal knots

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



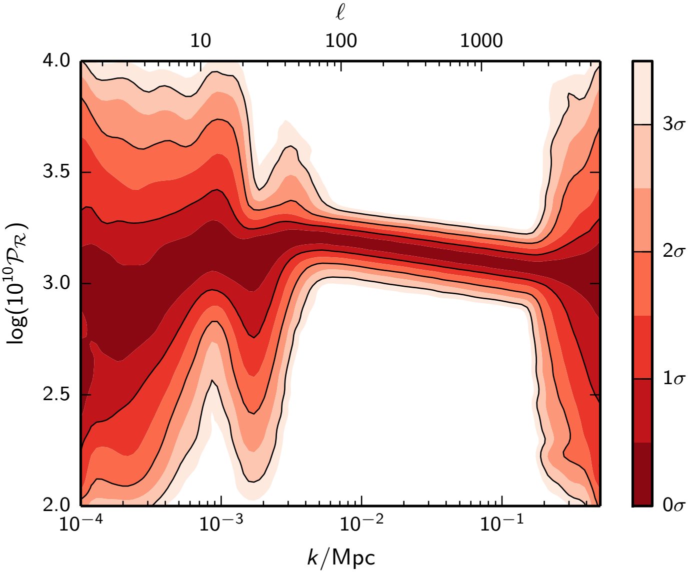
6 internal knots

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



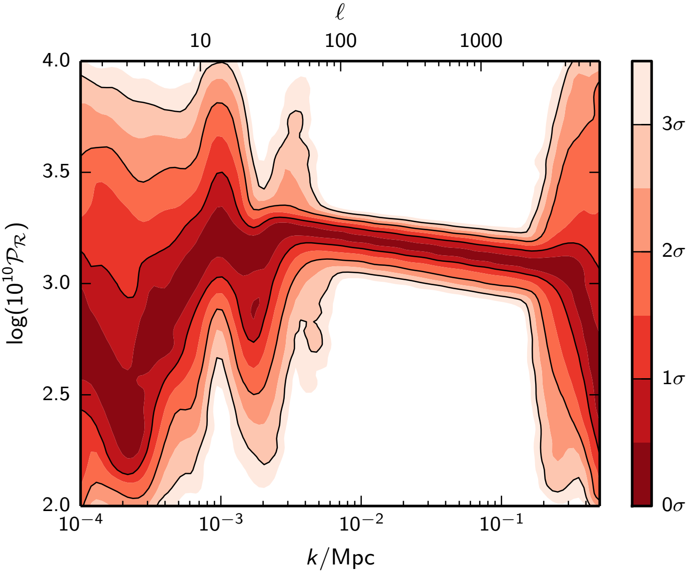
7 internal knots

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



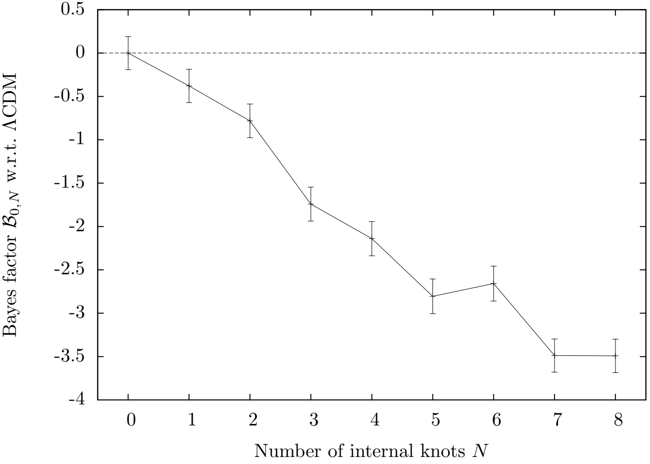
8 internal knots

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



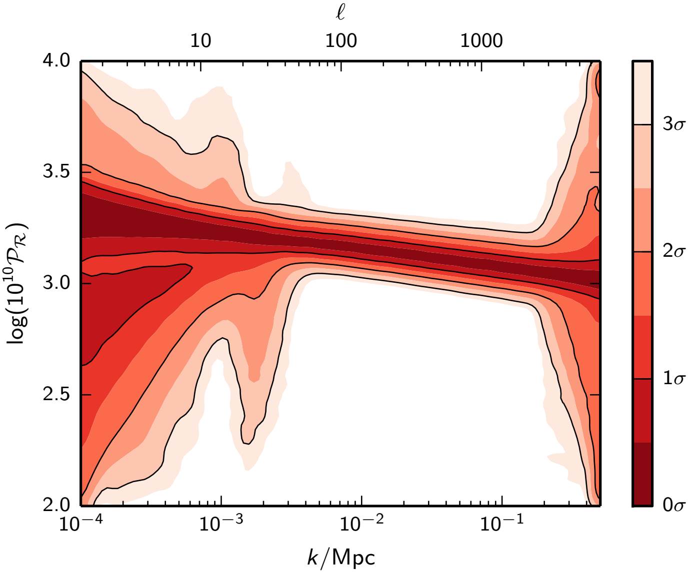
Bayes Factors

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



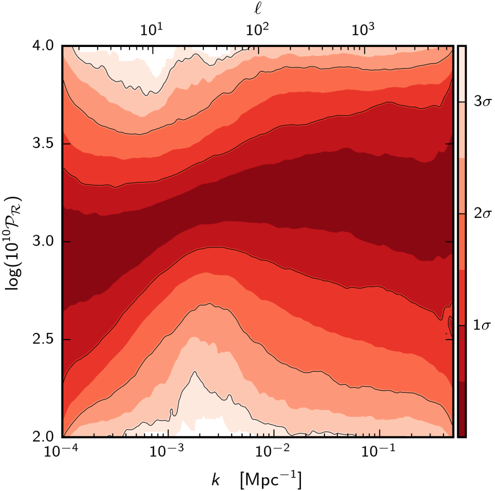
Marginalised plot

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



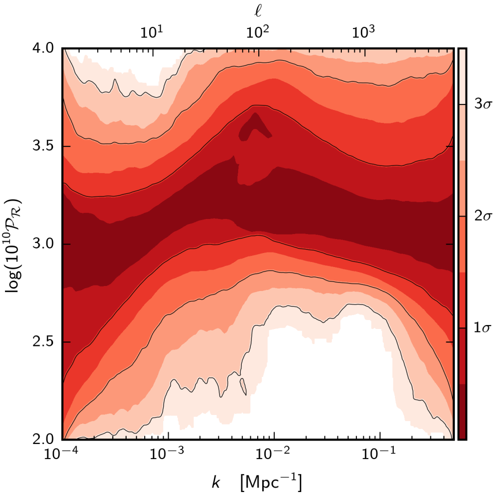
COBE (pre-2002)

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



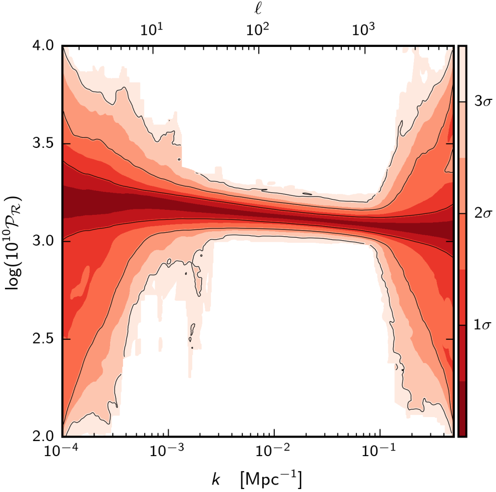
COBE et al (2002)

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



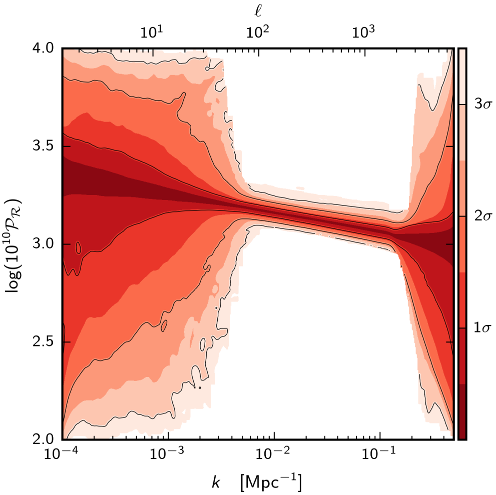
WMAP (2012)

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



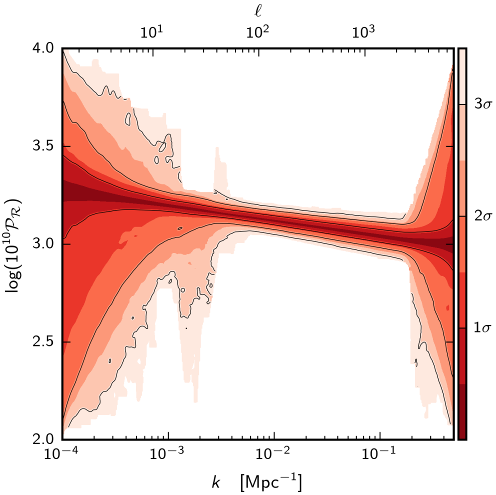
Planck (2013)

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

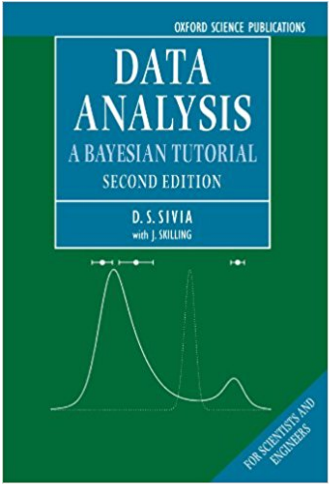


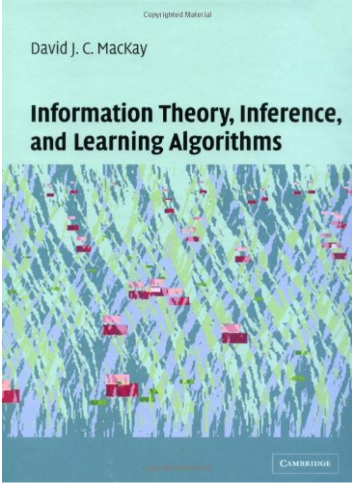
Planck (2015)

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



Further reading





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