Lecture 14: Nested Sampling for Bayesian Inference

Photo by Howard Jackman

D. Jason Koskinen
koskinen@nbi.ku.dk

Advanced Methods in Applied Statistics
Feb - Apr 2016

Comments

- No lecture this afternoon so that work can be done on the project
- I will post my solutions to problem set 2 online shortly after the assignment deadline so that students can review
- I will post some extra practice problems next week for exam preparation
- For the following nested sampling lecture, I have included intellectually accessible, i.e. clear and understandable, references at the end of the slides

Bayes' Theorem (from Lecture 5)

- One can solve the respective conditional probability equations for P(A and B) and P(B and A), setting them equal to give Bayes' theorem:

likelihood

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

prior

posterior

marginal likelihood

$$\text{posterior} \propto \text{prior} \times \text{likelihood}$$

- The theorem applies to both frequentist and Bayesian methods. Differences stem from how the theorem is applied and, in particular, whether one extends probability to include some degree of belief.

Slight Notation Shift

$$P(\Theta|D,H) = \frac{P(D|\Theta,H)\ P(\Theta|H)}{P(D|H)}$$

D are data
Θ are parameters
H is hypothesis or model

- Previously, we have focused on the posterior distribution P(Θ|D,H) which is critical for parameter estimation and we used Markov Chain Monte Carlo for calculating the marginal likelihood P(D|H)
- For model selection, versus parameter estimation, the marginal likelihood is important in it's own right. The problem is that many MCMC methods are slow (simulated annealing).

New Task

- If model selection is important then comparing models can be done via the respective posterior distributions

$$\frac{P(H_1|D)}{P(H_0|D)} = \frac{P(D|H_1)P(H_1)}{P(D|H_0)P(H_0)} = \frac{Z_1 P(H_1)}{Z_0 P(H_0)}$$

- The "marginal likelihood" is now rebranded as the "Bayesian evidence" and noted as Z
- Reversing the traditional MCMC approach, the 'evidence' is now the primary target, and the posterior is a by-product
- Note: we won't be doing model selection explicitly in this lecture, but it is the motivation for much of the following material.

Nested Sampling

- In 2004, John Skilling came up with a new Monte Carlo sampling technique, known as nested sampling, to more efficiently evaluate the bayesian evidence (Z)

$$Z = \int \mathcal{L}(\Theta)\pi(\Theta)d\Theta$$

$$\mathcal{L} \text{ is the likelihood}$$

$$\pi \text{ is the likelihood}$$

- For higher dimensions of Θ the integral for the bayesian evidence becomes challenging

Nested Sampling

- If numerical integration in higher dimensions is troublesome, then we can transform the multi-dimensional integral to a one-dimensional integral, via

$$dX = \pi(\Theta)d\Theta$$

$$X(\lambda) = \int_{\mathcal{L}(\Theta)>\lambda} \pi(\Theta)d\Theta$$

- The new prior X is defined such that

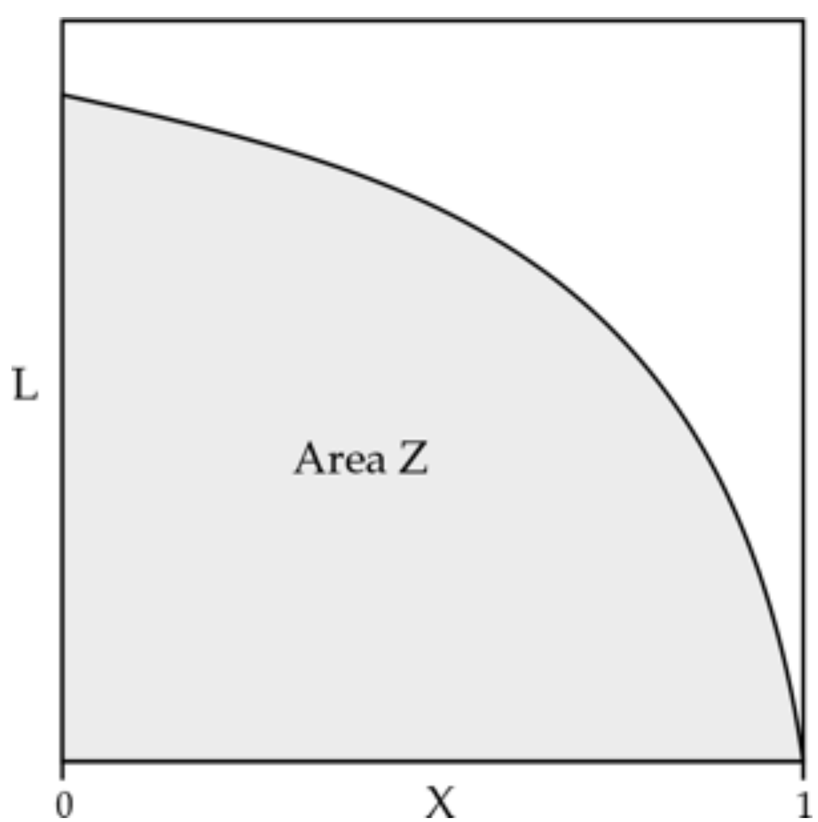
$$Z = \int_0^1 \mathcal{L}(X)dX$$

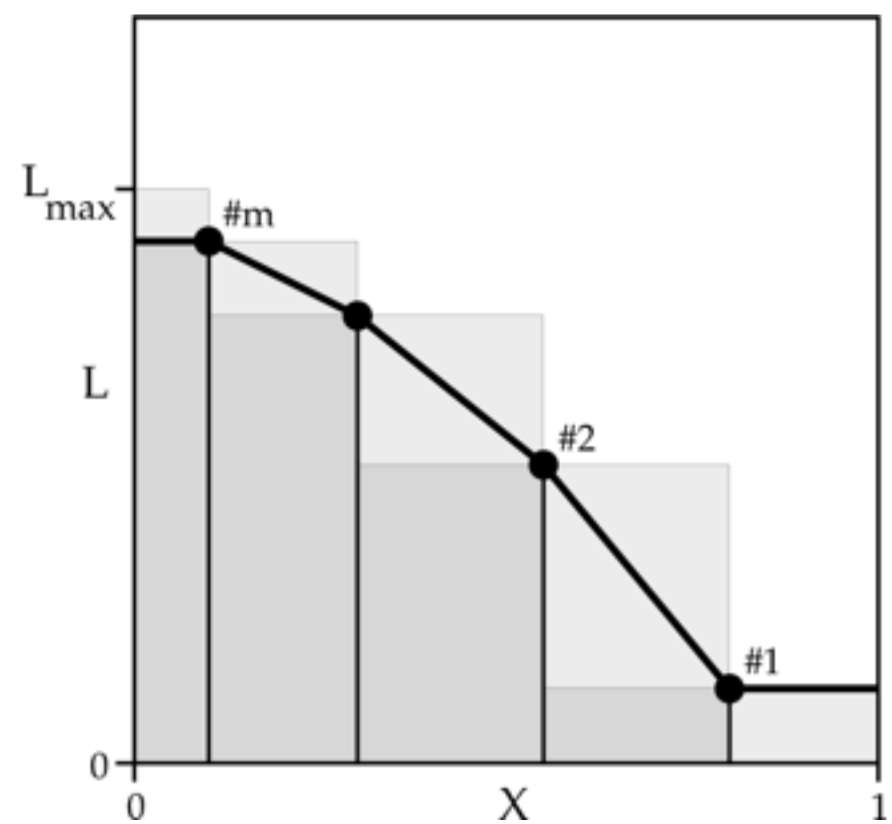
*For more justification, see the original paper by J .Skilling

- Note that X is a probability (mass) function and can only range from 0 to 1
- L(X) is also now a monotonically decreasing function
- A clever approx. to get X will be covered in a later slide

New Likelihood in 1-D

- The bayesian evidence is now the 1-D integral of the re-parameterized likelihood integrated over the re-parameterized prior
  - An analytic determination of the integral is out of the question, otherwise we would not be using numerical integration
  - Use points sampled in X to calculate the trapezoid sum
  - Diagram below (right) shows X and L for 4 sampled points

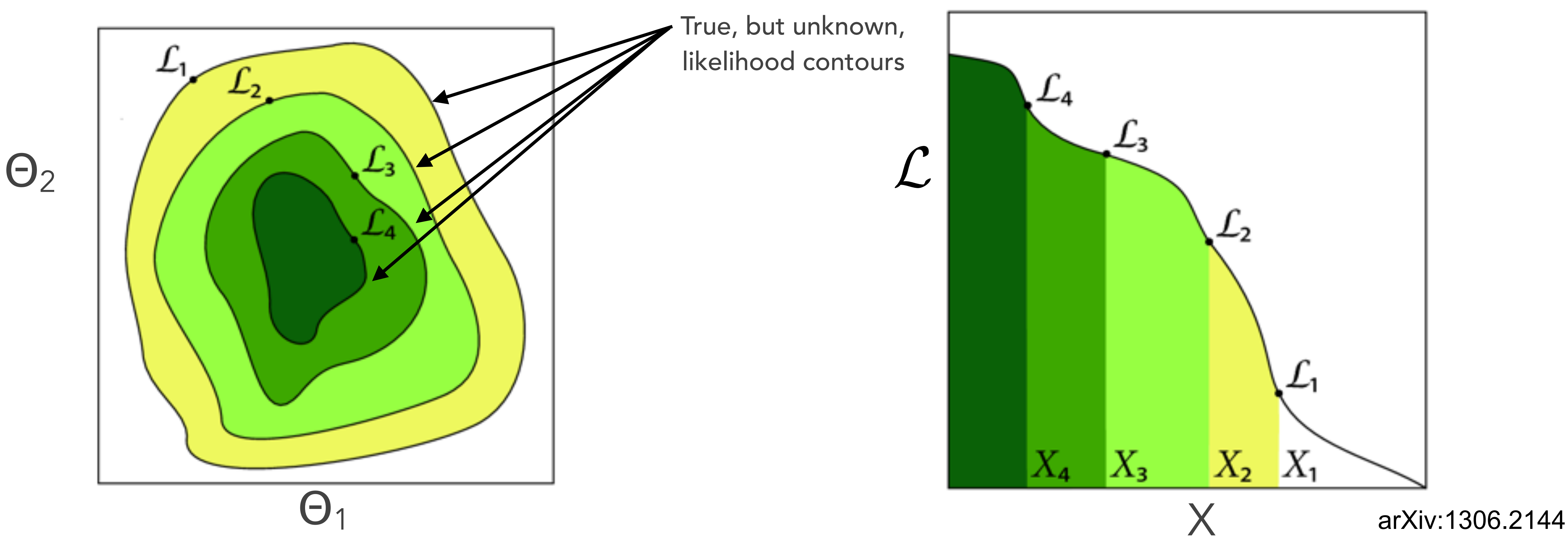




*J. Skilling

Simple Cartoon

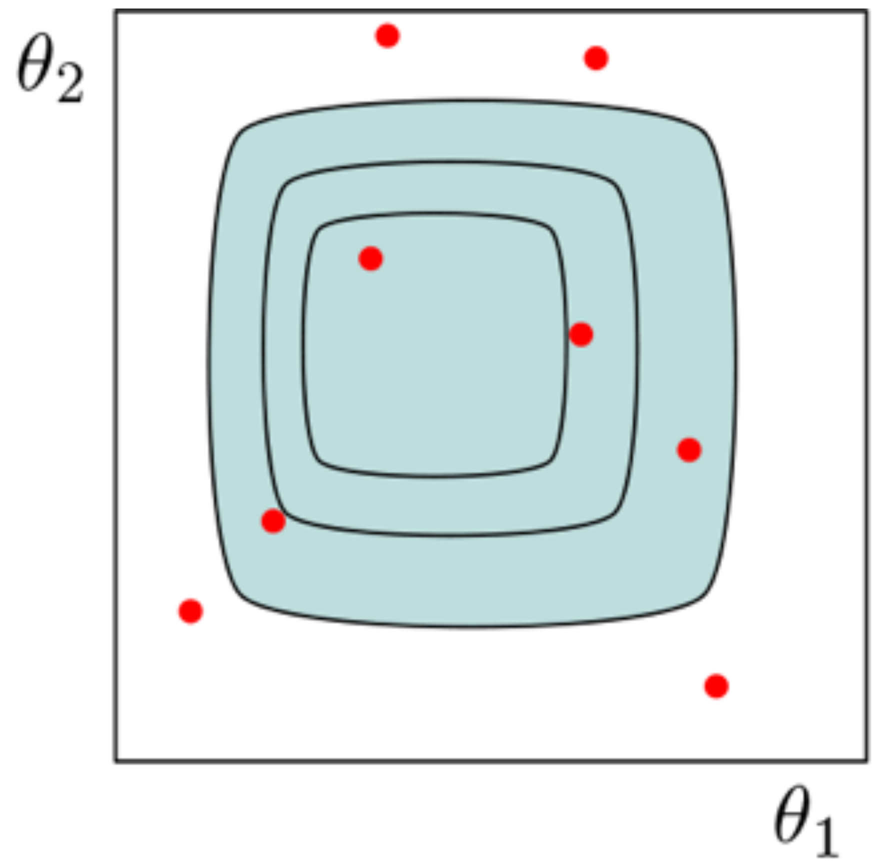
- For a simple 2-dimensional case, 4 'live' points are drawn at random. The likelihood for each point is calculated and converted to a value of X.
  - Note that multiple points of Θ_1 and Θ_2 can have the same value of X
  - This illustration nicely samples the space with only 4 points, which is uncommon and unrealistic



arXiv:1306.2144

Sampling

- Instead of relying on luck, it is better to sample the space sparsely where the new likelihood is low, and sample frequently in the space where the likelihood is high(er)



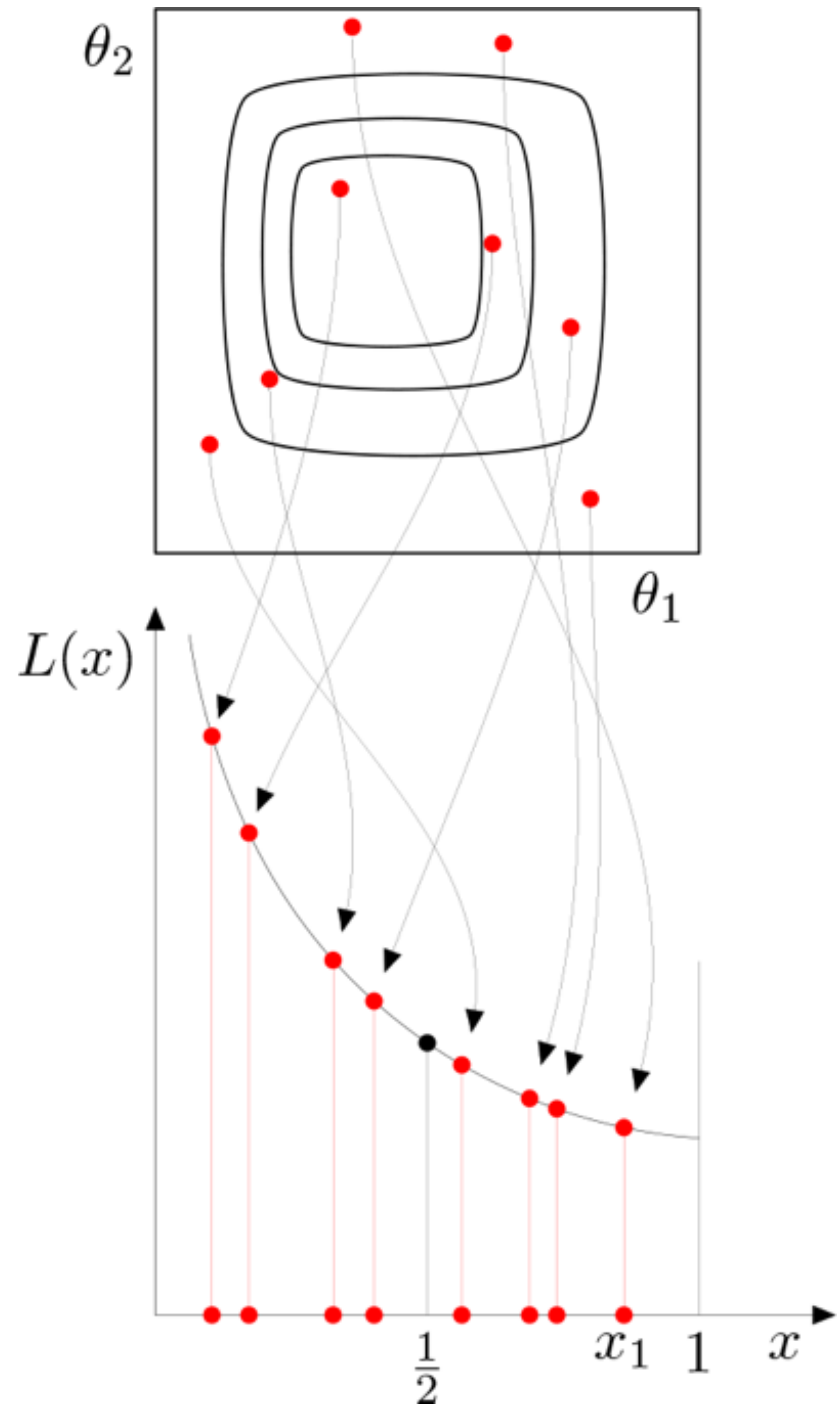
Shaded areas are the true underlying contours

Figure 51.3. $N = 8$ points drawn uniformly from the prior.

http://www.inference.phy.cam.ac.uk/bayesys/box/nested.pdf

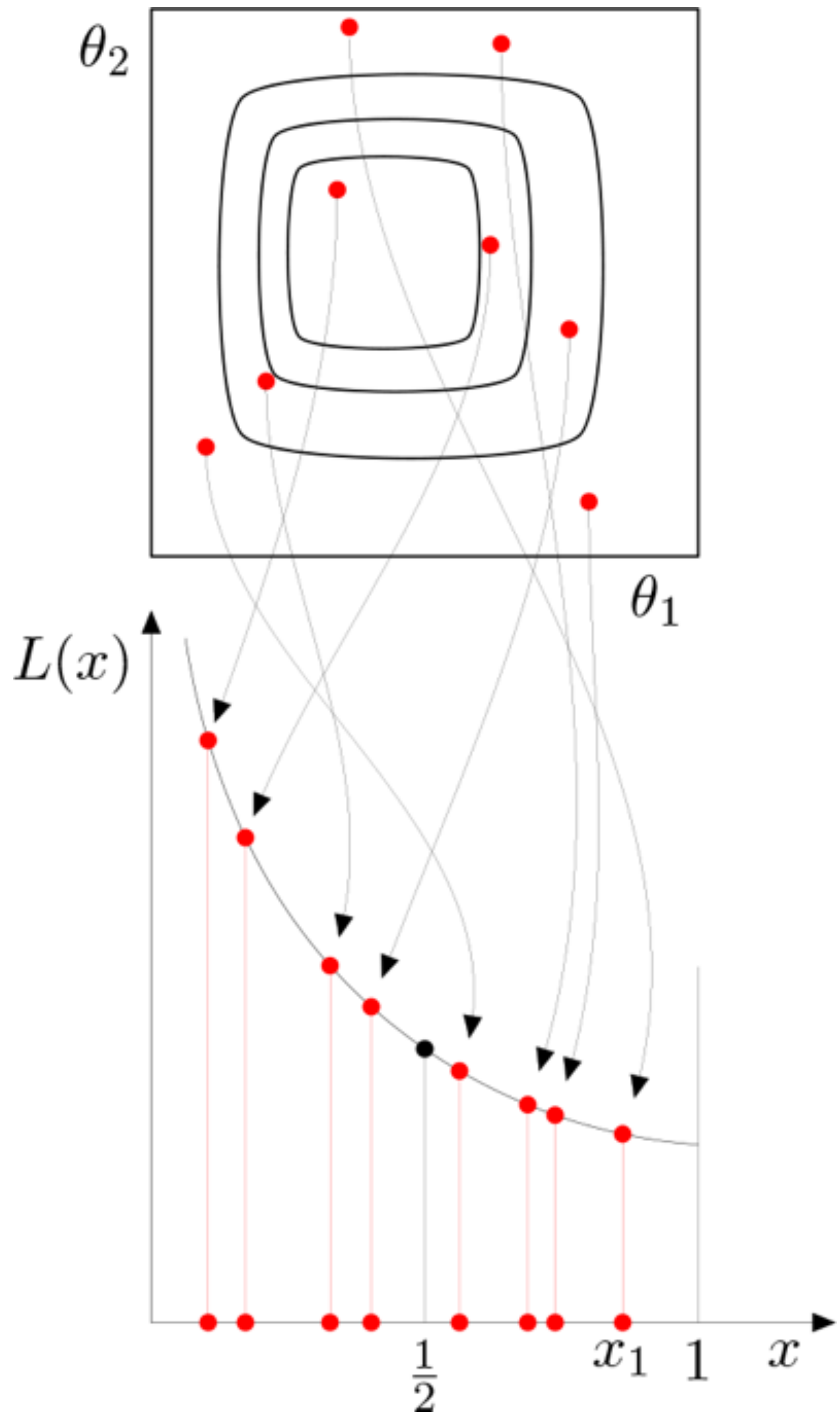
Sampling Start

- Each of the 8 initial live points has a likelihood value L(x) and a value of x
- In order to better sample where the likelihood is high, the point with the lowest L(x), i.e. x_1 in the diagram, is replaced by a new point x'
    - A new point (Θ1, Θ2), equivalently x', is drawn from the prior which produced the initial points. Normally a flat prior.
    - x' must satisfy that L(x') > L(x_{lowest})
    - Remove the point x_{lowest}, but store it's values to calculate the likelihood integral, e.g. bayesian evidence
- Next slide covers approx. for value of x



Sampling Start cont.

- The diagram at right shows the x values of each of the 8 points, but at each iteration only one value of x matters; x_{lowest} related to L_{lowest}
  - The final bayesian evidence value is the integral of all the iteratively stored x_{lowest} and L_{lowest} data
  - By construction $x_0=1$, and x_1 can be approximated as (N-1)/N, where N is the number of live points. Later banked points, x_i, are approximated as $x_i=((N-1)/N)^i$



Pseudo-Code

Generate n points from the prior
Loop for i=1,2,3,...
{
* Find the one with the lowest likelihood, L_{worst}. Remove it from the population, but store it for results. Estimate its X value as $((N-1)/N)^i$, for N live points
* Replace that point with a new one generated from the prior, but subject to the hard constraint $L>L_{worst}$.
}

The estimate of X can be
* $((N-1)/N)^i$
* $(N/(N+1))^i$
* $\exp(-i/N)$

*G. F. Lewis

Sampling more

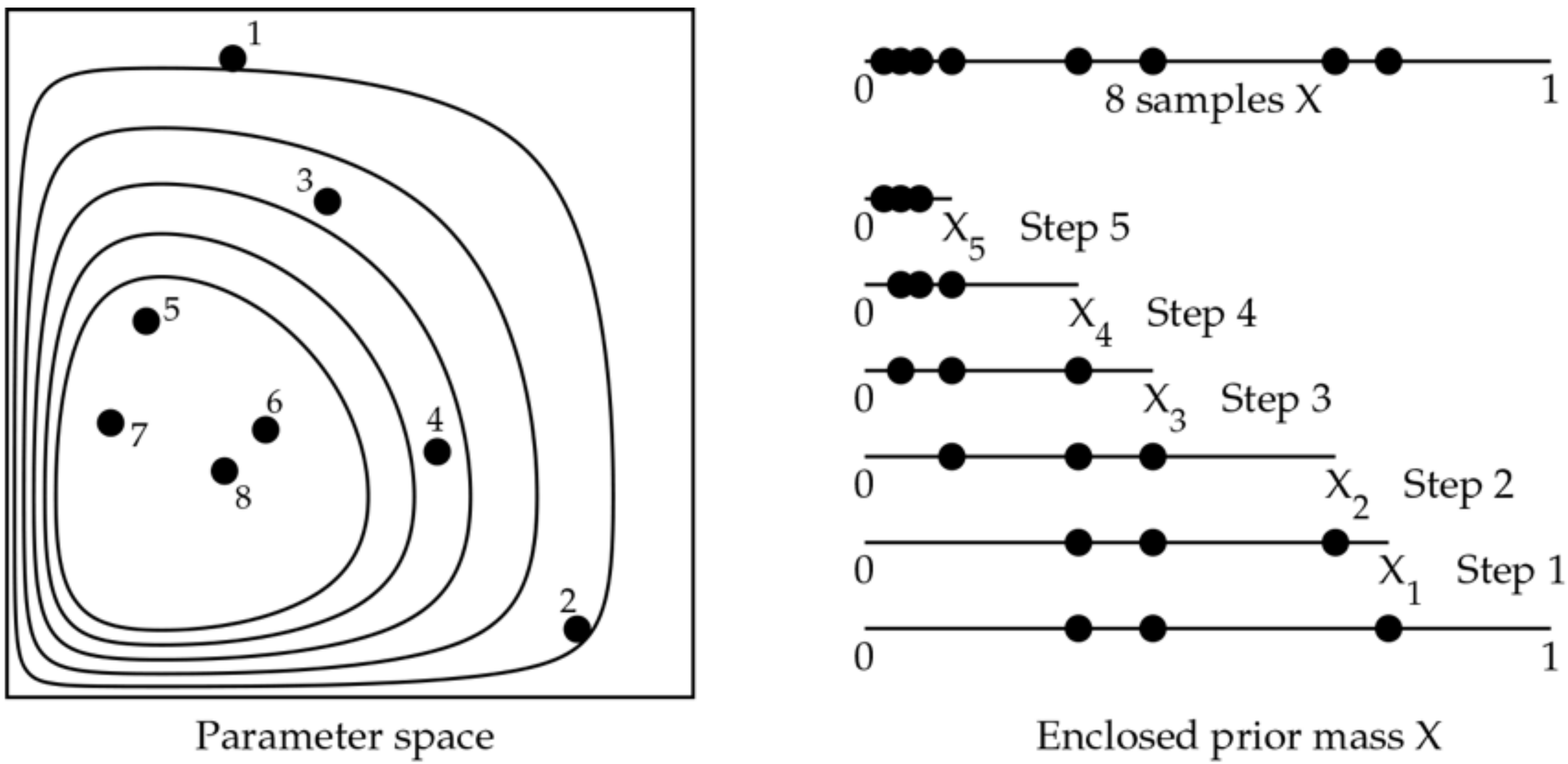
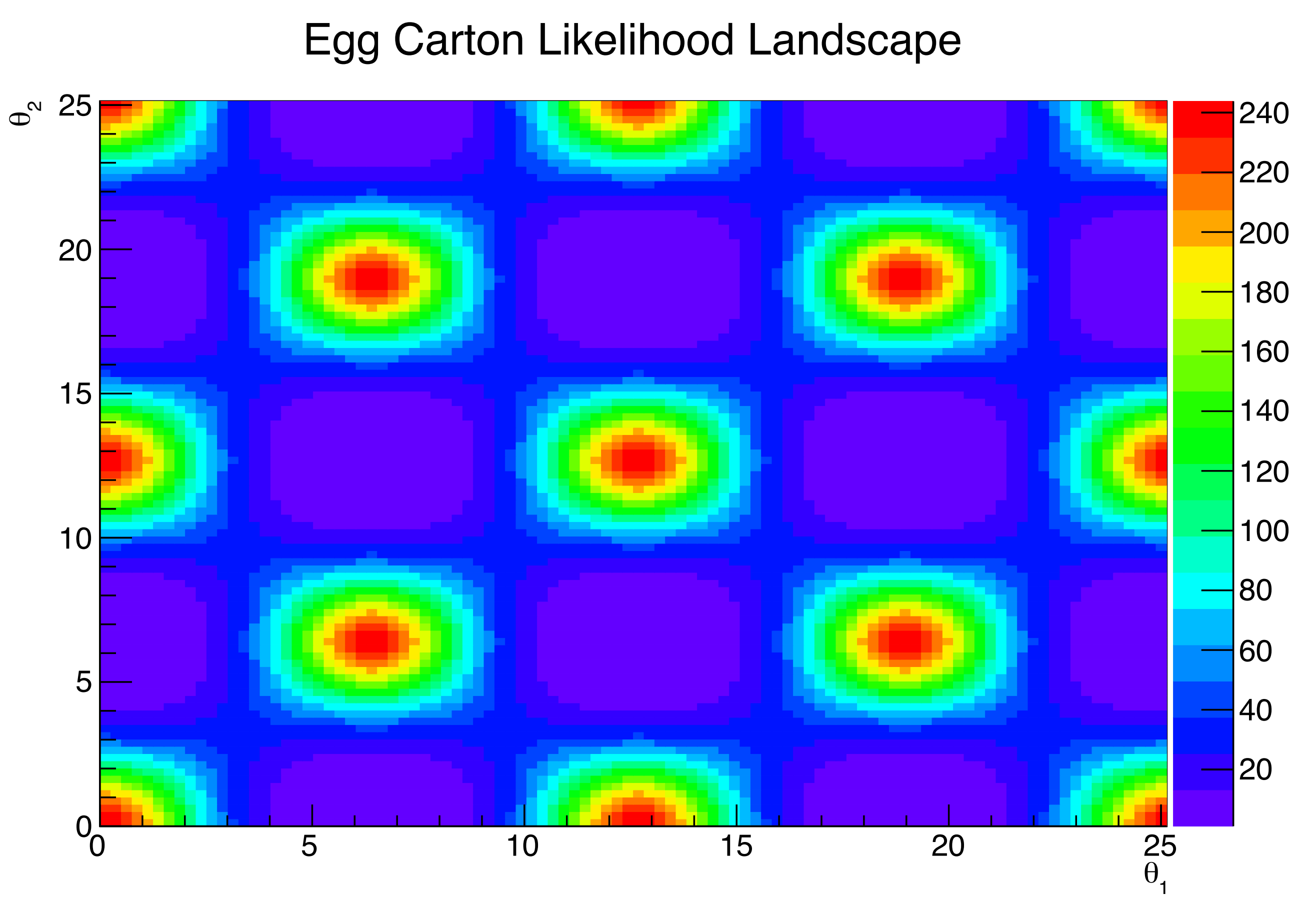


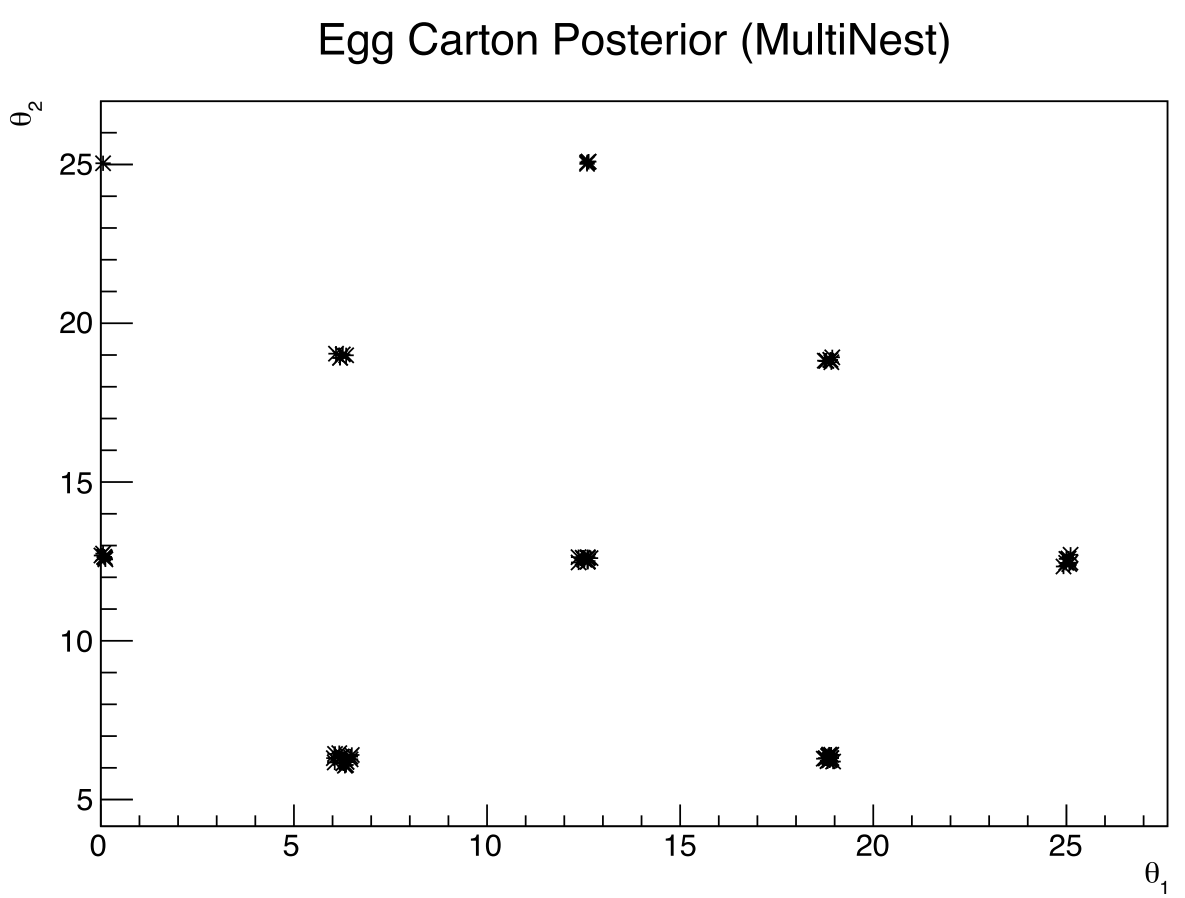
Figure 4: Nested sampling for five steps with a collection of three points. Likelihood contours shrink by factors exp(−1/3) in area and are roughly followed by successive sample points.

*J. Skilling 2006

Nested Sampling in Action

- The 'Egg Carton' likelihood landscape is a benchmark likelihood landscape for difficulty and stress testing of bayesian sampling techniques





Pros

- Samples sparsely in low likelihood regions and samples densely where the likelihood is high
- Can handle irregular likelihood landscapes
- Many applications require nothing more than setting the range over which to generate 'live points'
  - Little to no tuning
  - Most of the time the sampling prior is uniform, i.e. flat
- The true value of the maximum likelihood estimator is not essential to be known, it just needs to be within the region where the points are sampled
- Efficient when compared to MCMC methods

Cons

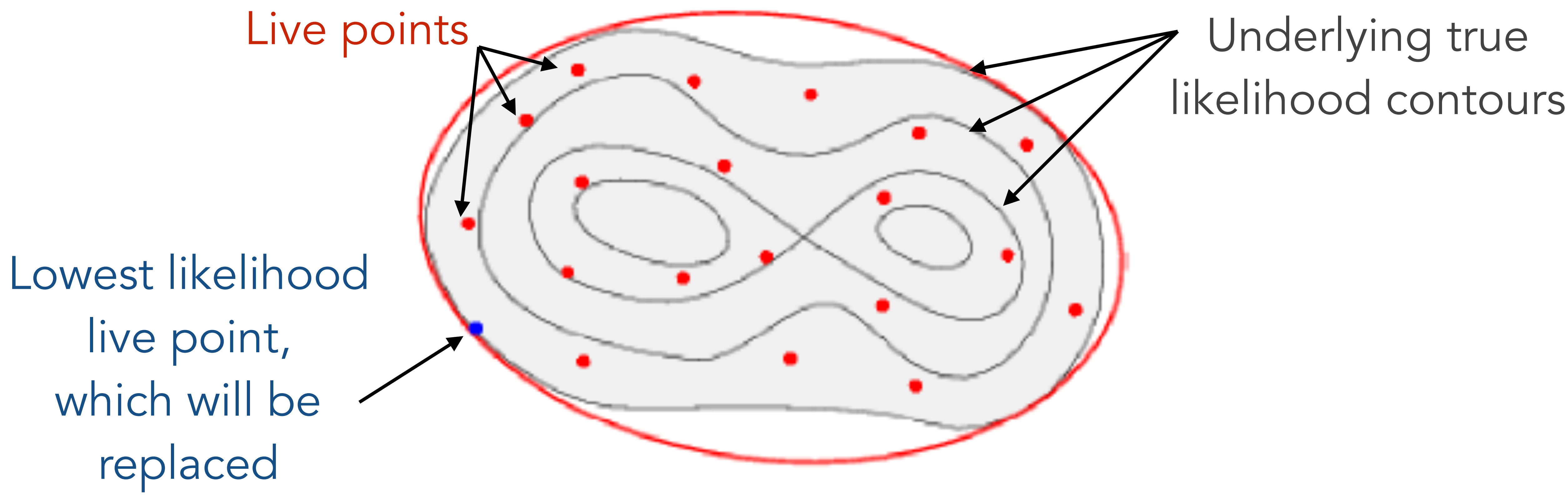
- Similar to every other fitting technique, there is no guarantee that any best-fit values are global best-fit values
- No rigorous termination criterion
  - There is always the possibility that there exist some unsampled regions in X which have very large likelihood values which will contribute to the bayesian evidence value Z
- Unlike other MCMC algorithms which sample near the current point, many nested sampling algorithms sample uniformly over the full parameter space
  - Higher dimensions can see slow-downs
- Trapezoidal summing will induce some uncertainty and possibly small bias

MultiNest Application

- Crude nested sampling was somewhat inefficient when it came to multi-modal likelihood landscapes
  - Much better than conventional maximum likelihood fitters, e.g. MIGRAD, but could still get stuck in local minima
- Instead of using a multi-dimensional uniform prior for each replacement point, use an n-dimensional ellipsoid for resampling
  - The hyper-ellipsoid is defined by the current iteration live points
  - The hyper-ellipsoid for re-sampling has a small enlargement margin as a safeguard

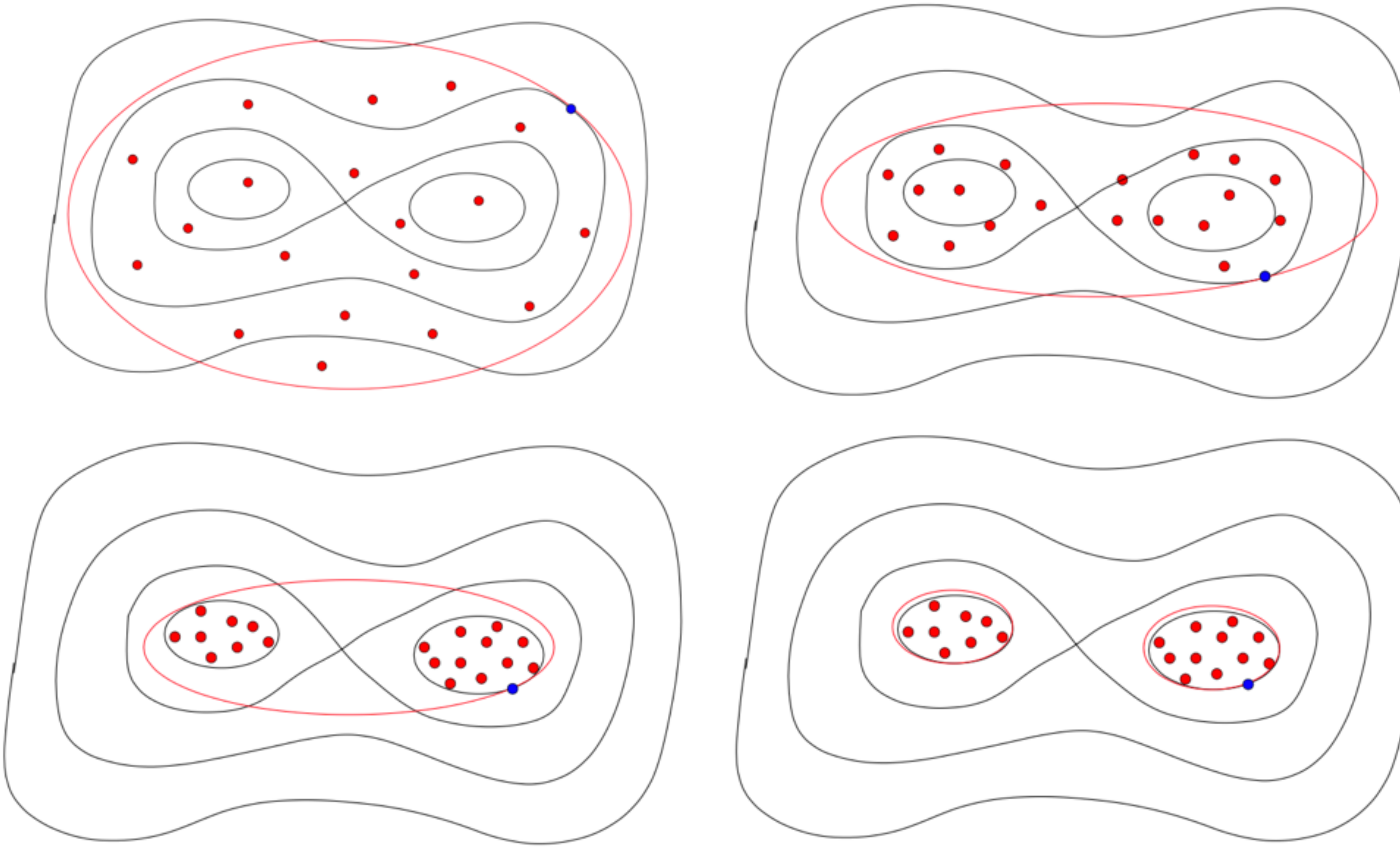
MultiNest Ellipsoid Sampling

- Start with a sample of live points using a uniform prior in n-dimensional cube
- After a few iterations resampling within an ellipsoid we have:



*F. Feroz

MultiNest Evolution



MultiNest Pictures

- Dis-joint regions, as in fig. a, as well as multi-dimensional multi-modal regions, as in figs. a and b, can be found efficiently without continual resampling of the whole space

(a) (b)

Nested Sampling

- Can be an excellent method to map out a likelihood/probability landscape that is complicated
- MultiNest is very nice, but the base package requires Fortran, even though there are nice wrapper packages in other software languages

Packages

- In Python there are a handful of nestling sampling packages
  - pymultinest (https://johannesbuchner.github.io/PyMultiNest/)
  - nestle (http://kbarbary.github.io/nestle/)
  - SuperBayeS (http://www.ft.uam.es/personal/rruiz/superbayes/?page=main.html)

Exercise Egg Carton

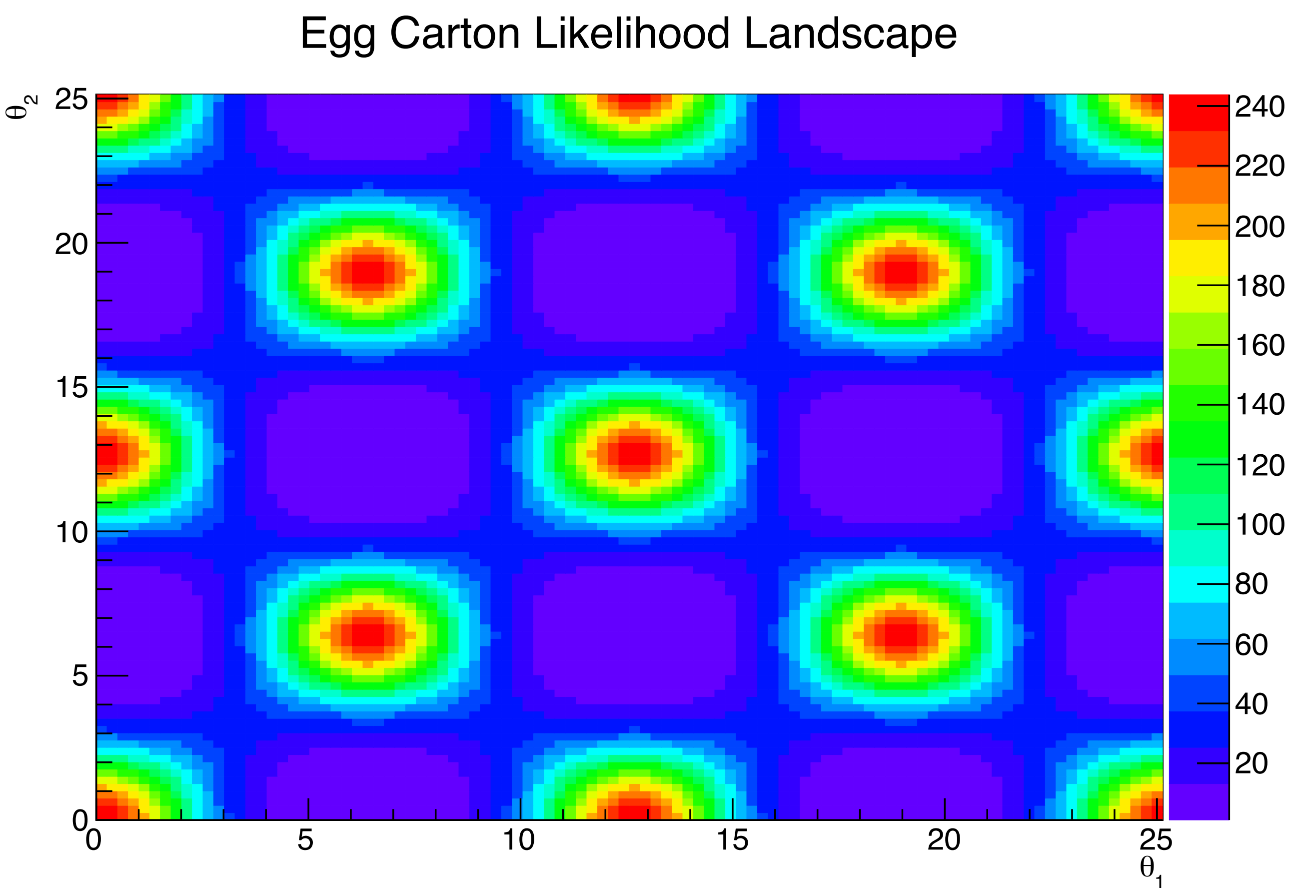
- The task is to produce a posterior distribution using a (hopefully) nested sampling algorithm for the classic 2-dimensional egg carton likelihood

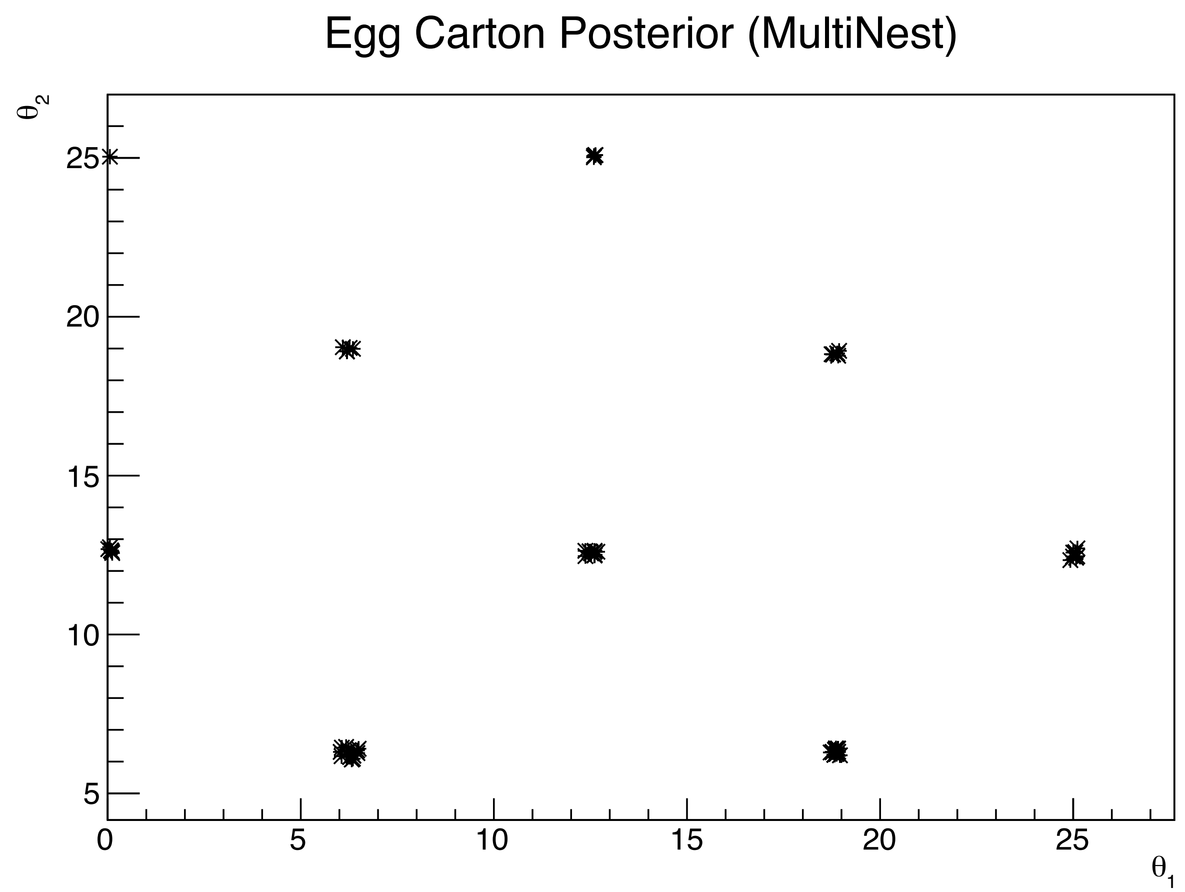
$$\mathcal{L}(\theta_1, \theta_2) \propto \cos(\theta_1)\cos(\theta_2)$$

- First, make sure you have a nested sampling algorithm package installed
- Second, make a plot of the raster scan of the the 2-D likelihood for reference
- Third, make a plot of the posterior distribution from the sampling algorithm

Exercise Egg Carton cont.

- The raster scan across θ_1 and θ_2 and the posterior distribution





Exercise Gaussian Shell/Cylinder

- Another classic example is the 2- or 3-dimensional gaussian shell
  - The probability is highest, i.e. centered, on the surface of a sphere or cylinder, and has a gaussian width
  - Looking at 3D gaussian surfaces is tough, so we will do a projection into 2D for visualization

$$\mathcal{L}(\vec{\theta}) = \mathrm{circ}(\vec{\theta}; \vec{c}, r, \sigma)$$

$$\mathrm{circ}(\vec{\theta}; \vec{c}, r, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(|\vec{\theta} - \vec{c}| - r)^2}{2\sigma^2}\right]$$

c is the center of the sphere/cylinder

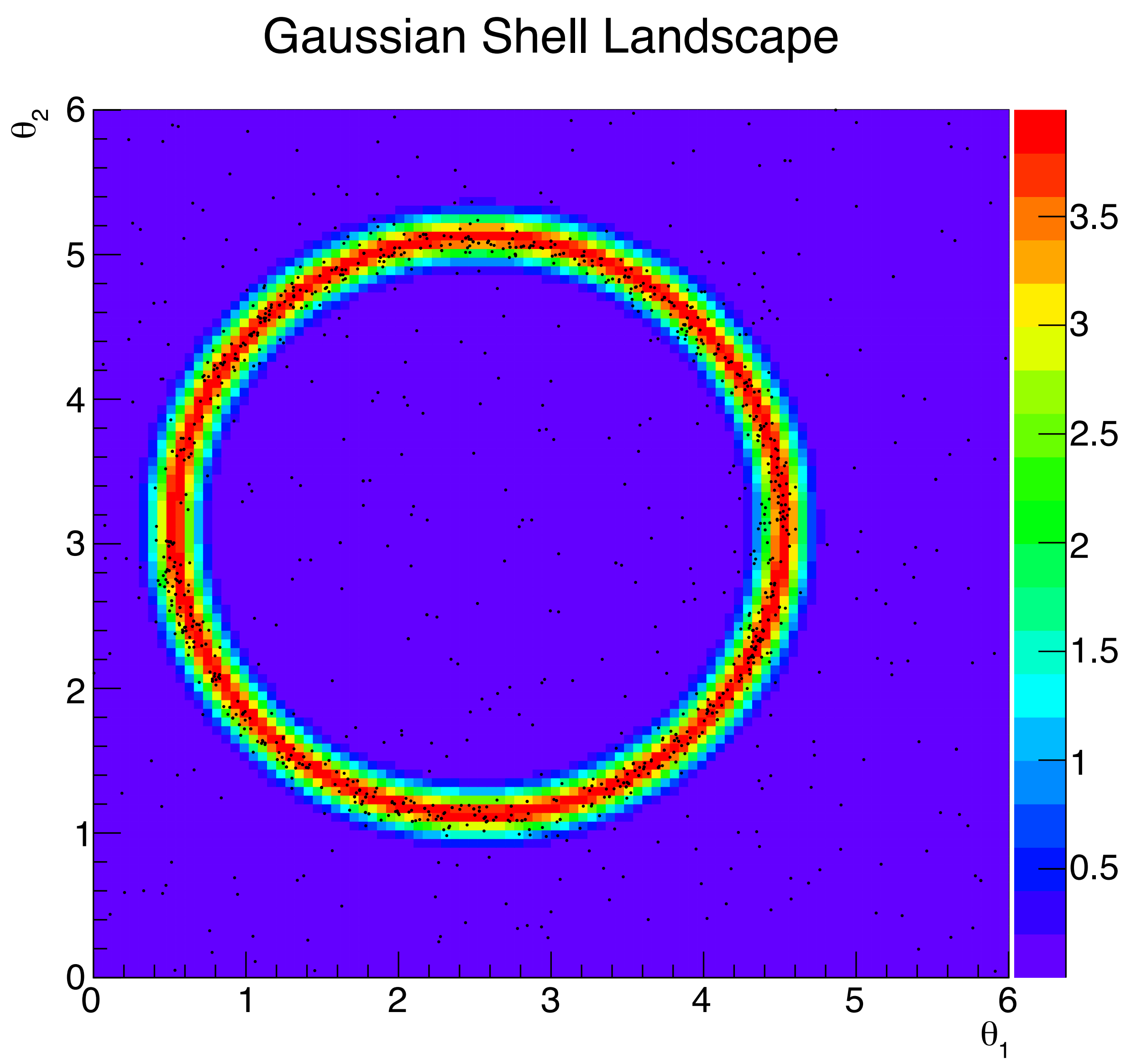
r is the radius

σ is the gaussian width

θ is a/the sample point as a vector, e.g. (x,y,z,…) in cartesian coordinates

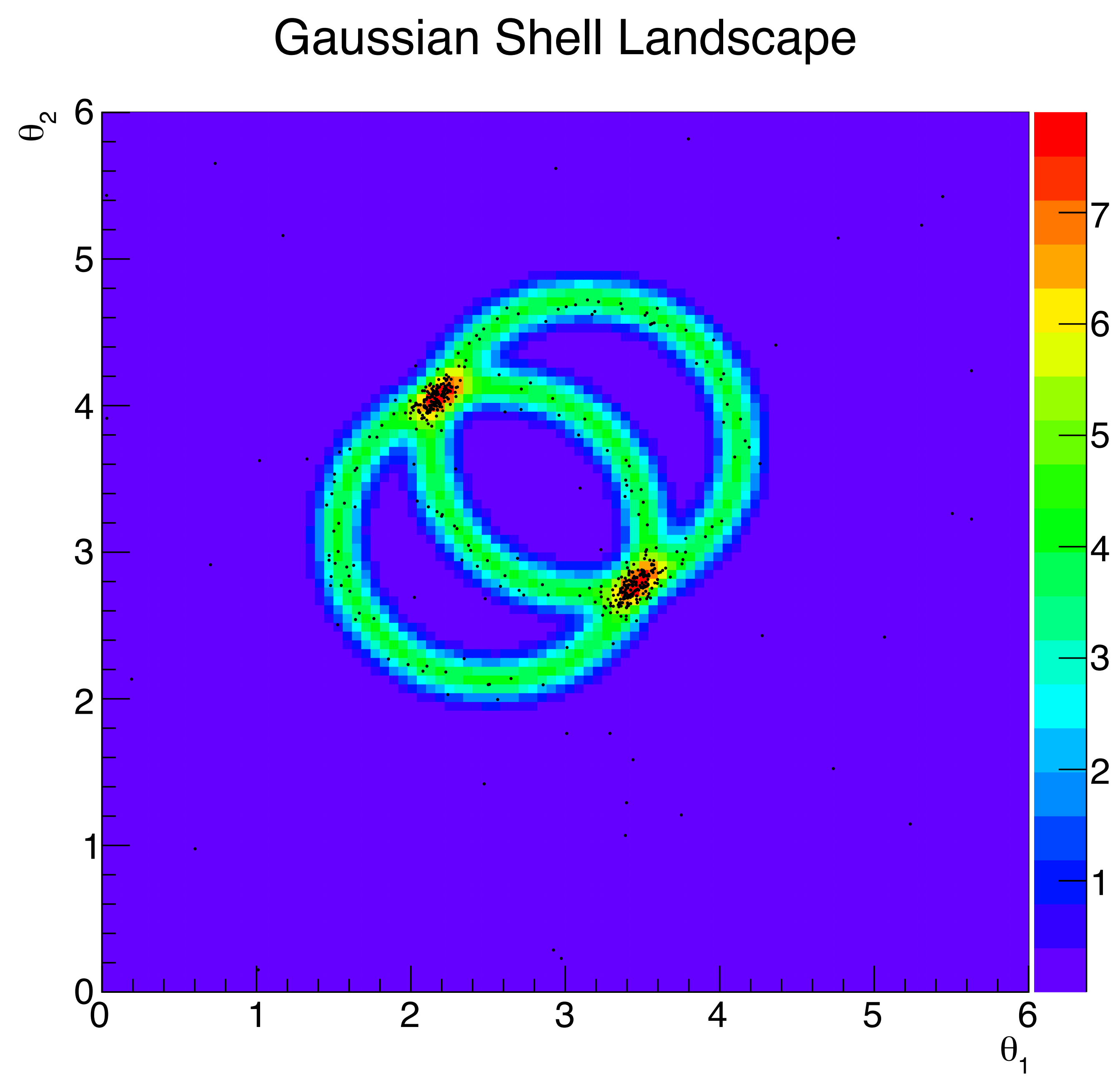
Exercise Gaussian Shell/Cylinder cont.

- Similar to the Egg Carton exercise generate the following plots:
  - For a single cylinder/sphere of r=2, σ=0.1, centered at c=(2.5, 3.1)
  - Plot the underlying probability/likelihood space
  - Plot the posterior sampling
- Note that there might be issues with the computer/machine precision when calculating exp() or ln() for negative, extremely large, or extremely small values related to the likelihood.



Exercise Gaussian Shell/Cylinder cont.

- Repeat the previous task with two overlapping spheres/ cylinders
  - For r=1, σ=0.1, with one centered at c_1=(2.5, 3.1) and the other at c_2=(3.1, 3.7)

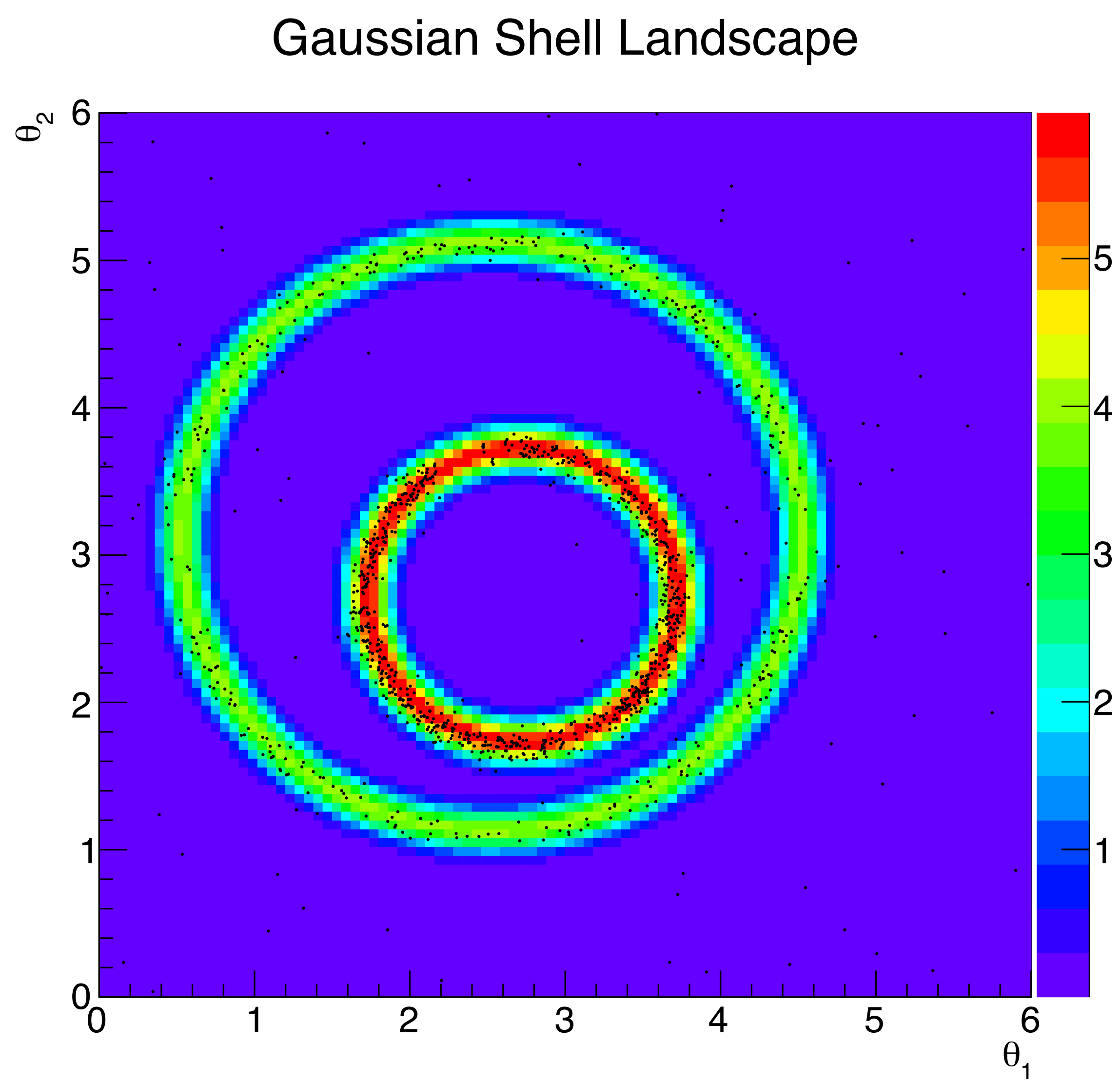


Exercise Nested Nested Cylinder

- Using the following likelihood for the two cylinders plot the underlying likelihood and posterior distribution:

$$\mathcal{L}(\vec{\theta}) = \mathrm{circ}(\vec{\theta}; \vec{c}_1, r_1, \sigma_1) + 1.5\ \mathrm{circ}(\vec{\theta}; \vec{c}_2, r_2, \sigma_2)$$

  - c_1=(2.5, 3.1) and c_2=(2.7, 2.7) and r_1=2 and r_2=1



Extra

- Try higher dimensionality landscapes, e.g. 16-dimensions, and see if the sampler starts to slow down dramatically for the gaussian shell hyper-sphere likelihood

References

- Excellent and readable paper by developed John Skilling
  - http://projecteuclid.org/euclid.ba/1340370944
- Nested sampling implementation in nice steps and detail slides (http://www2.stat.duke.edu/~fab2/nested_sampling_talk.pdf). Also a sly reference to 'going down the rabbit hole'
- MultiNest
  - Slides by F. Feroz (http://www.ics.forth.gr/ada5/pdf_files/Feroz_talk.pdf)
  - Papers (http://arxiv.org/abs/0809.3437, http://arxiv.org/abs/1306.2144)