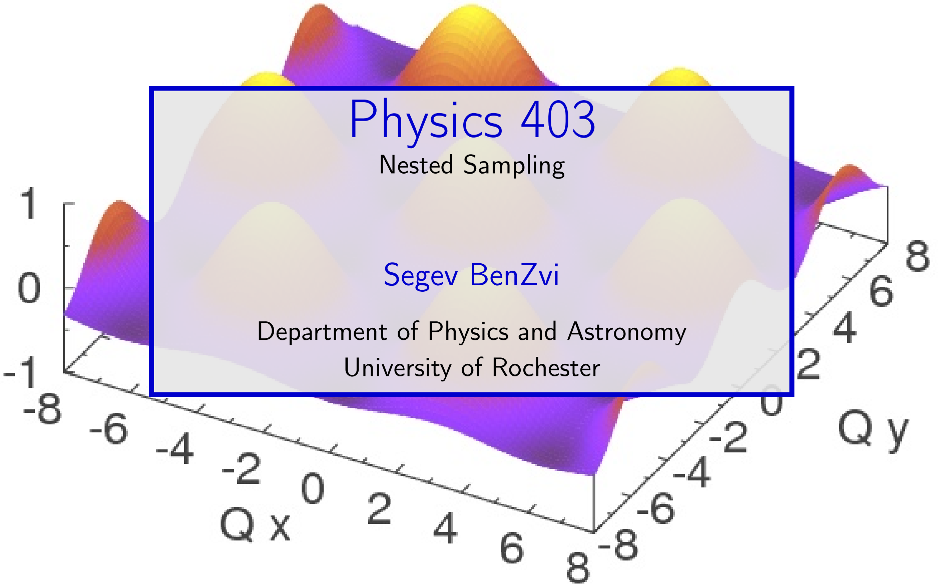
Physics 403

Nested Sampling

Segev BenZvi

Department of Physics and Astronomy
University of Rochester



Evaluating Full Posterior Distributions

Recall the types of calculations we often have to do in a Bayesian analysis (from [1]):

$$\begin{array}{ccccc} p(D|\boldsymbol{x},I)\ p(\boldsymbol{x}|I) & = & p(D,\boldsymbol{x}|I) & = & p(D|I)\ p(\boldsymbol{x}|D,I) \\ \mathcal{L}(\boldsymbol{x}) \ \times\ \pi(\boldsymbol{x}) & = & \dots & = & Z\ \times\ p(\boldsymbol{x}) \\ \text{likelihood} \times \text{prior} & = & \text{joint} & = & \text{evidence} \times \text{posterior} \\ \text{INPUT} & \Longrightarrow & \dots & \Longrightarrow & \text{OUTPUT} \end{array}$$

To fully evaluate the posterior $p(\boldsymbol{x}) = \mathcal{L}(\boldsymbol{x})\pi(\boldsymbol{x})/Z$ we have to evaluate integrals of the form

$$Z = \iint \dots \int d\boldsymbol{x}\ \ \mathcal{L}(\boldsymbol{x})\ \pi(\boldsymbol{x})$$

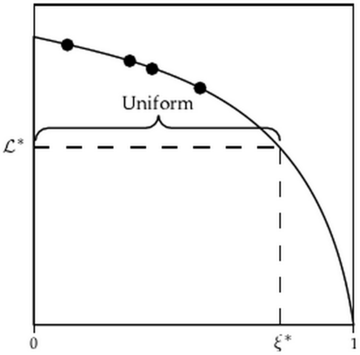
Often this can only be done numerically, so we need an efficient method of calculating high-dimensional integrals

Nested Sampling

- Nested sampling is another kind of technique useful for high-dimensional integration and posterior sampling [2, 3]
- Advantages over MCMC: can handle pathologies in parameter spaces such as strong non-linear correlations and requires fewer samples (up to a factor 100 less) for evidence calculation
- The algorithm gives results that allow for model selection as well as best parameter estimates at once
- Several packages available in Python [4, 5]
- Basic concept: use a likelihood ordering scheme to evaluate integrals like

$$Z = \iint \ldots \int d\boldsymbol{x} \;\; \mathcal{L}(\boldsymbol{x}) \, \pi(\boldsymbol{x})$$

Basics of Nested Sampling



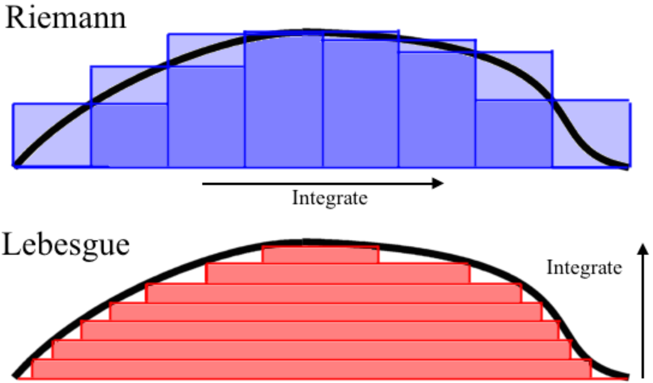
- Sample N objects $\boldsymbol{x}$ with respect to the prior such that $\mathcal{L}(\boldsymbol{x}) > \mathcal{L}^*$
- Start with $\mathcal{L}^* = 0$, so that sampling begins over the entire prior
- We uniformly sample $\xi(\mathcal{L}^*)$, the proportion of the prior with likelihood greater than $\mathcal{L}^*$:

$$\xi(\mathcal{L}^*) = \iint\limits_{\mathcal{L}(\boldsymbol{x}) > \mathcal{L}^*} \ldots \int \pi(\boldsymbol{x})\, d\boldsymbol{x}$$

- Slowly increase $\mathcal{L}^*$ so that we end up sampling in the high probability region

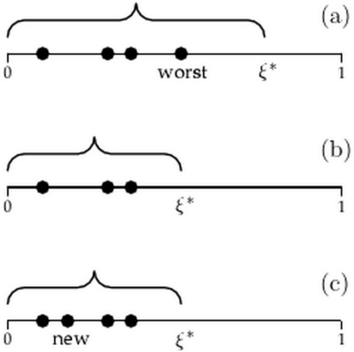
Analogy: Riemann and Lebesgue Integration

The concept is similar to Lebesgue integration



Rather than partition the domain of $\mathcal{L}$ into subintervals, we partition the range of $\mathcal{L}$ and integrate "up the hill"

Iteration Step



The algorithm in practice:

- Start with N objects restricted to $\xi < \xi^*$
- Select the object with the largest ξ (and hence smallest $\mathcal{L}$)
- Use the worst object's $(\xi, \mathcal{L})$ as the new $(\xi^*, \mathcal{L}^*)$ and then toss out the worst object
- There are now $N - 1$ objects in the new domain bounded by ξ^*, which is nested inside the old domain
- Generate a new object inside the smaller domain by uniformly sampling the prior
- Restart the loop, and proceed until $\mathcal{L}^* = \mathcal{L}_{\text{max}}$

Calculation of Marginal Evidence

- The shrinkage ratio $t = \xi/\xi^*$ at each iteration is distributed as

$$p(t) = Nt^{N-1}, \quad \text{with mean } \ln(t) = (-1 \pm 1)/N$$

- At each iteration k,

$$\mathcal{L}_k = \mathcal{L}^* \quad \text{and} \quad \xi_k = \xi^* \prod_{j=1}^{k} t_j$$

- Each shrinkage ratio is independently distributed according to $p(t)$ so

$$\ln \xi_k = (-k \pm \sqrt{k})/N$$

- If $\ln t = -1/N$ then $\xi_k = \exp(-k/n)$, and we can evaluate

$$Z = \int_0^1 \mathcal{L}(\xi)\, d\xi \approx \sum_k h_k\, \mathcal{L}_k,$$

where $h_k = \xi_{k-1} - \xi_k = \Delta\xi_k$

Generating Quantities from the Posterior Distribution

- Each sequence in the parameter space $\{\boldsymbol{x}_k\}$ has an associated weight

$$w_k = \frac{h_k \mathcal{L}_k}{Z}$$

where $h_k = \Delta\xi_k$ and $Z = \sum h_k \mathcal{L}_k$

- The weights define the posterior PDF. Any quantity $f(\boldsymbol{x})$ can be generated from the posterior in the usual way:

$$\langle f \rangle = \sum_k w_k f(\boldsymbol{x}_k)$$

$$\langle f \rangle = \sum_k w_k f^2(\boldsymbol{x}_k)$$

$$\text{var}(f) = \langle f^2 \rangle - \langle f \rangle$$

Uncertainty in Z

- Given the estimate of Z, we can calculate the information or negative entropy

$$\mathcal{H} = \int p(\xi) \ln [p(\xi)]\ d\xi \approx \sum_k \frac{h_k\, \mathcal{L}_k}{Z} \ln \left[\frac{\mathcal{L}_k}{Z}\right]$$
$$\approx (\#\ \text{active components in data}) \times \ln (\text{signal}/\text{noise})$$

- If we count until $k = N\mathcal{H}$ then the accumulated values of $\ln \xi$ are subject to an uncertainty $\sqrt{N\mathcal{H}}/N$
- This uncertainty also applies to $\ln Z$, so that

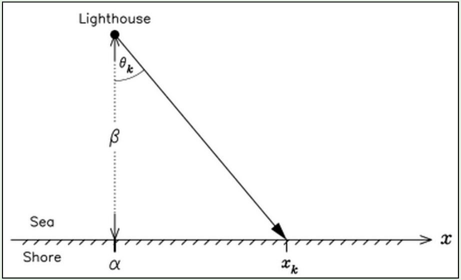
$$\ln Z \approx \ln \left(\sum_k h_k\, \mathcal{L}_k\right) \pm \sqrt{\frac{\mathcal{H}}{N}}$$

- Convergence criterion: no rigorous approach. Use your judgment. Typical: choose upper limit on the number of iterations

Lighthouse Problem

Example

A lighthouse is somewhere off the coast at position α along the shore and β out to sea. It emits a series of short collimated flashes at random intervals (and hence, random azimuths)



N flashes are detected at positions $\{x_k\}$ along the coast. Given the $\{x_k\}$, where is the lighthouse?

Parameterization of the Lighthouse Problem

- Since the lighthouse emissions are random, the azimuth angle of the k^{th} emission is uniform over $\theta = \pm 90^\circ$:

$$p(\theta_k|\alpha, \beta, I) = 1/\pi$$

- The azimuth angle is related to the position along the coast x_k by

$$\beta \tan\theta_k = x_k - \alpha$$

- Change variables to find the likelihood of the x_k:

$$p(x_k|\alpha, \beta, I) = p(\theta_k|\alpha, \beta, I)\left|\frac{\partial\theta_k}{\partial x_k}\right|$$

$$\beta \sec^2\theta \frac{\partial\theta}{\partial x} = 1$$

$$\beta[1 + \tan^2\theta]\frac{\partial\theta}{\partial x} = \beta\left[1 + \left(\frac{x-\alpha}{\beta}\right)^2\right]\frac{\partial\theta}{\partial x} = 1$$

Parameterization of the Lighthouse Problem

- Using the Jacobian we find the likelihood of the x_k:

$$p(x_k|\alpha,\beta,I) = \frac{\beta}{\pi\left[\beta^2 + (x_k-\alpha)^2\right]}$$

$$p(\boldsymbol{x}|\alpha,\beta,I) = \prod_{k=1}^{N} p(x_k|\alpha,\beta,I)$$

- What we really want is the posterior distribution of α:

$$p(\alpha,\beta|\boldsymbol{x},I) = \frac{1}{Z} p(\boldsymbol{x}|\alpha,\beta,I)\; p(\alpha,\beta|I),$$

where we expect that $p(\alpha,\beta|I) = p(\alpha|I)p(\beta|I)$ is uniform:

$$p(\alpha,\beta|I) = \begin{cases} \frac{1}{\alpha_{\text{max}}-\alpha_{\text{min}}}\frac{1}{\beta_{\text{max}}-\beta_{\text{min}}}, & \alpha\in[\alpha_{\text{min}},\alpha_{\text{max}}], \beta\in[\beta_{\text{min}},\beta_{\text{max}}] \\ 0 & \text{otherwise} \end{cases}$$

Calculating the Likelihood

The likelihood we use for nested sampling is

$$\mathcal{L}(\alpha, \beta) = \prod_{k=1}^{N} \frac{\beta}{\pi\left[\beta^2 + (x_k - \alpha)^2\right]}$$

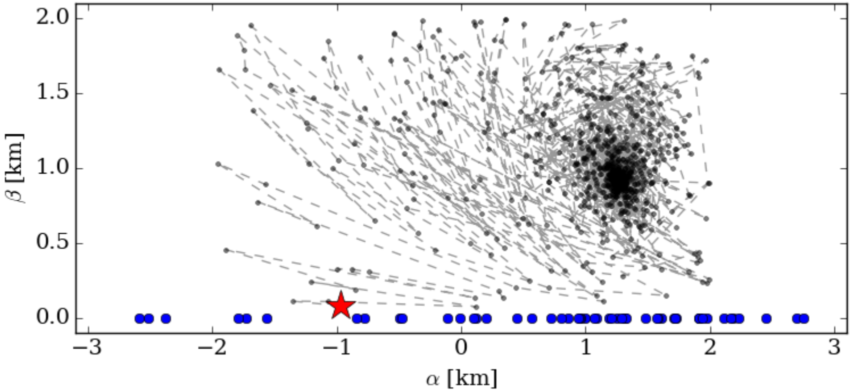
$$\ln \mathcal{L} = \ln \beta - \ln \pi - \sum_{k=1}^{N} \left(\beta^2 + (x_k - \alpha)^2\right)$$

The algorithm we apply is:

1. Generate N values of α and β from the uniform priors
2. Calculate $\mathcal{L}$ (or $\ln \mathcal{L}$) using the N points and the $\{x_k\}$
3. Pick the value with the lowest $\mathcal{L}$ and set it to $\mathcal{L}^*$
4. Use $\mathcal{L}^*$ to estimate new limits α^* and β^* and generate new values of α and β subject to these limits. Proceed until termination

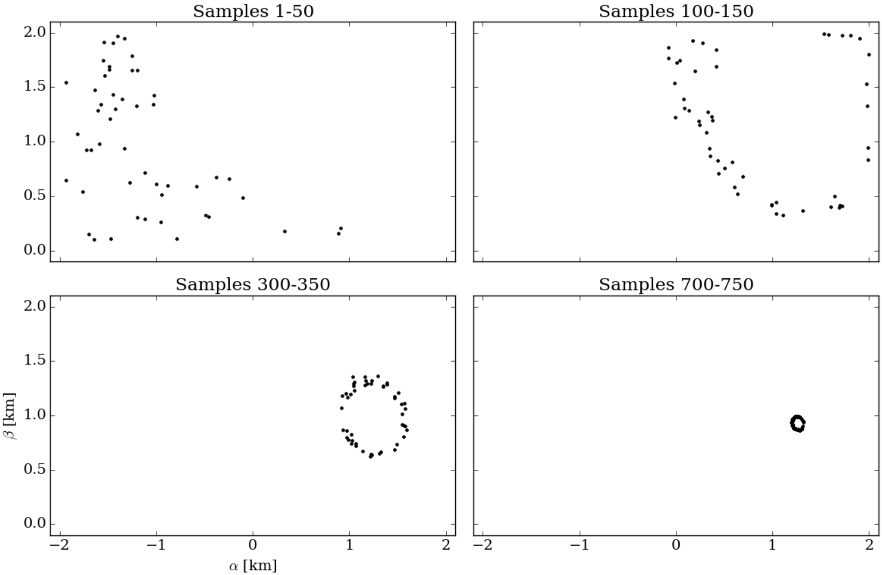
Lighthouse Problem

Chooose $\alpha \in [-2, 2]$ and $\beta \in [0, 2]$. Update α and β with uniform steps (easy to implement; could have used a Gaussian)



(α, β) moves from starting point (red star) to the region of highest probability

Sampling of the Posterior vs. Time



Best Estimate of α, β

- Using the liklihood weights from each sample

$$w_k = \frac{h_k\,\mathcal{L}_k}{Z}$$

we can get the mean α and β:

$$\langle\alpha\rangle = \sum_k w_k \alpha_k = 1.25 \pm 0.18 \text{ km}$$

$$\langle\beta\rangle = \sum_k w_k \beta_k = 1.01 \pm 0.20 \text{ km}$$

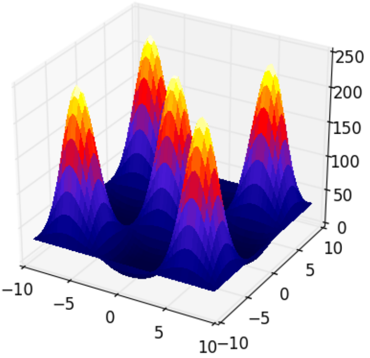
- The estimate of the evidence $\ln Z$ is

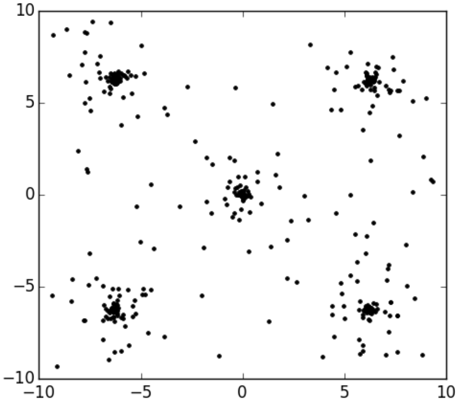
$$\ln\left(Z/\text{km}^{64}\right) = -160.53 \pm 0.17$$

- Note that Z has dimensions of km^{64} because of the 64 $\{x_k\}$

Highly Multimodal Distributions

Handles very multimodal distributions like the eggbox function





Note: the acceptance rate for points $\mathcal{L} > \mathcal{L}^*$ can be poor unless some effort is made to split up the sampling region

References I

[1] D.S. Sivia and John Skilling. *Data Analysis: A Bayesian Tutorial*. New York: Oxford University Press, 1998.

[2] J. Skilling. "Nested Sampling". In: *Proc. Bayesian Inference and Maximum Entropy Methods*. Vol. 735. Garching, Germany: AIP, July 2004, p. 395.

[3] J. Skilling. "Nested sampling for general Bayesian computation". In: *Bayesian Anal.* 1.4 (Dec. 2006), pp. 833–859.

[4] F. Feroz et al. *MultiNest: Efficient and Robust Bayesian Inference*. 2015. URL: http://ccpforge.cse.rl.ac.uk/gf/project/multinest/.

[5] K. Barbary. *Nestle Nested Sampling Package*. 2015. URL: https://github.com/kbarbary/nestle.