

An Introduction to (Dynamic) Nested Sampling

Josh Speagle

jspeagle@cfa.harvard.edu

Introduction

Background

$$\Pr(\Theta|D, M) = \frac{\Pr(D|\Theta, M) \Pr(\Theta|M)}{\Pr(D|M)}$$

Bayes' Theorem

Background

$$\Pr(\Theta|D, M) = \frac{\text{Posterior Likelihood} \Pr(D|\Theta, M) \text{ Prior } \Pr(\Theta|M)}{\text{Evidence } \Pr(D|M)}$$

Bayes' Theorem

Background

$$p(\Theta) = \frac{\text{Likelihood} \quad \text{Prior}}{\text{Evidence} \equiv \int_{\Omega_\Theta} \mathcal{L}(\Theta) \pi(\Theta) d\Theta}$$

Bayes' Theorem

The equation shows the posterior probability $p(\Theta)$ as a fraction. The numerator is the product of the likelihood $\mathcal{L}(\Theta)$ (in red) and the prior $\pi(\Theta)$ (in blue). The denominator is the evidence, represented by an integral over the parameter space Ω_Θ of the product of the likelihood and prior.

Background

$$\text{Posterior } p(\Theta) = \frac{\text{Likelihood } \mathcal{L}(\Theta) \text{ Prior } \pi(\Theta)}{\text{Evidence } \equiv \int_{\Omega_\Theta} \mathcal{L}(\Theta)\pi(\Theta)d\Theta}$$

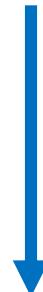
Bayes' Theorem

Posterior Estimation via Sampling

Samples $\Theta_N, \Theta_{N-1}, \dots, \Theta_2, \Theta_1 \in \Omega_\Theta$

Posterior Estimation via Sampling

Samples $\Theta_N, \Theta_{N-1}, \dots, \Theta_2, \Theta_1 \in \Omega_\Theta$



Weights $\hat{p}_N, \hat{p}_{N-1}, \dots, \hat{p}_2, \hat{p}_1 \Rightarrow \hat{p}(\Theta)$

$$= \sum_{i=1}^N \hat{p}_i \delta_D(\Theta - \Theta_i)$$

Posterior Estimation via Sampling

Samples $\Theta_N, \Theta_{N-1}, \dots, \Theta_2, \Theta_1 \in \Omega_\Theta$



Weights $\hat{p}_N, \hat{p}_{N-1}, \dots, \hat{p}_2, \hat{p}_1 \Rightarrow \hat{p}(\Theta)$

MCMC $1, 1, \dots, 1, 1 = \sum_{i=1}^N \hat{p}_i \delta_D(\Theta - \Theta_i)$

Posterior Estimation via Sampling

Samples $\Theta_N, \Theta_{N-1}, \dots, \Theta_2, \Theta_1 \in \Omega_\Theta$



Weights $\hat{p}_N, \hat{p}_{N-1}, \dots, \hat{p}_2, \hat{p}_1 \Rightarrow \hat{p}(\Theta)$

MCMC $1, 1, \dots, 1, 1$

Importance Sampling $\frac{p_N}{q_N}, \frac{p_{N-1}}{q_{N-1}}, \dots, \frac{p_2}{q_2}, \frac{p_1}{q_1}$

$$= \sum_{i=1}^N \hat{p}_i \delta_D(\Theta - \Theta_i)$$

Posterior Estimation via Sampling

Samples $\Theta_N, \Theta_{N-1}, \dots, \Theta_2, \Theta_1 \in \Omega_\Theta$



Weights $\hat{p}_N, \hat{p}_{N-1}, \dots, \hat{p}_2, \hat{p}_1 \Rightarrow \hat{p}(\Theta)$

Nested Sampling?

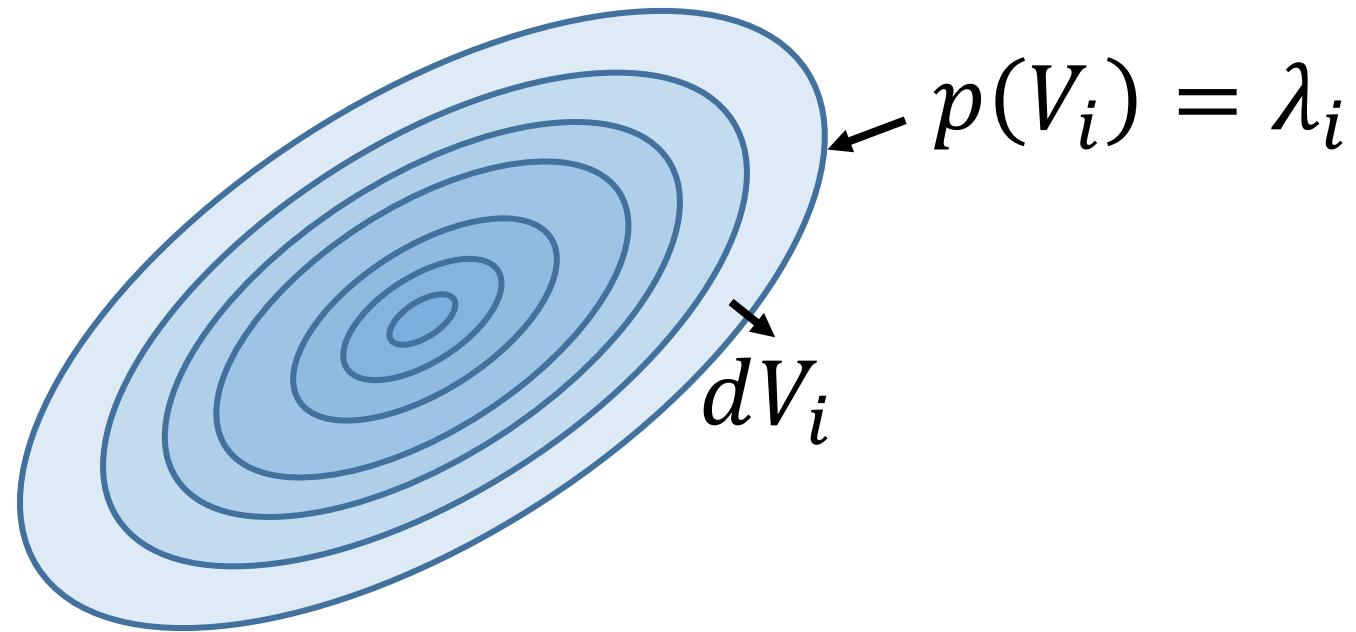
$$= \sum_{i=1}^N \hat{p}_i \delta_D(\Theta - \Theta_i)$$

Motivation: Integrating the Posterior

$$\int_{\Omega_{\Theta}} p(\Theta) d\Theta$$

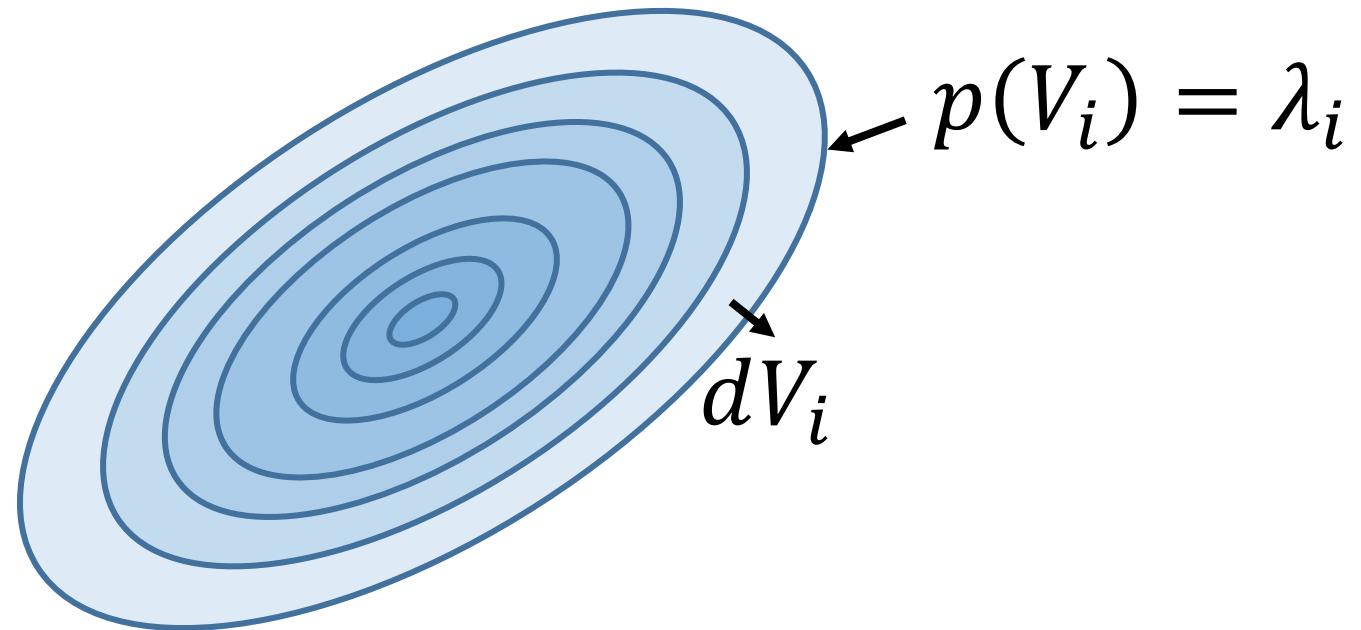
Motivation: Integrating the Posterior

$$\int_{\{\Theta: p(\Theta)=\lambda\}} \lambda dV(\lambda)$$



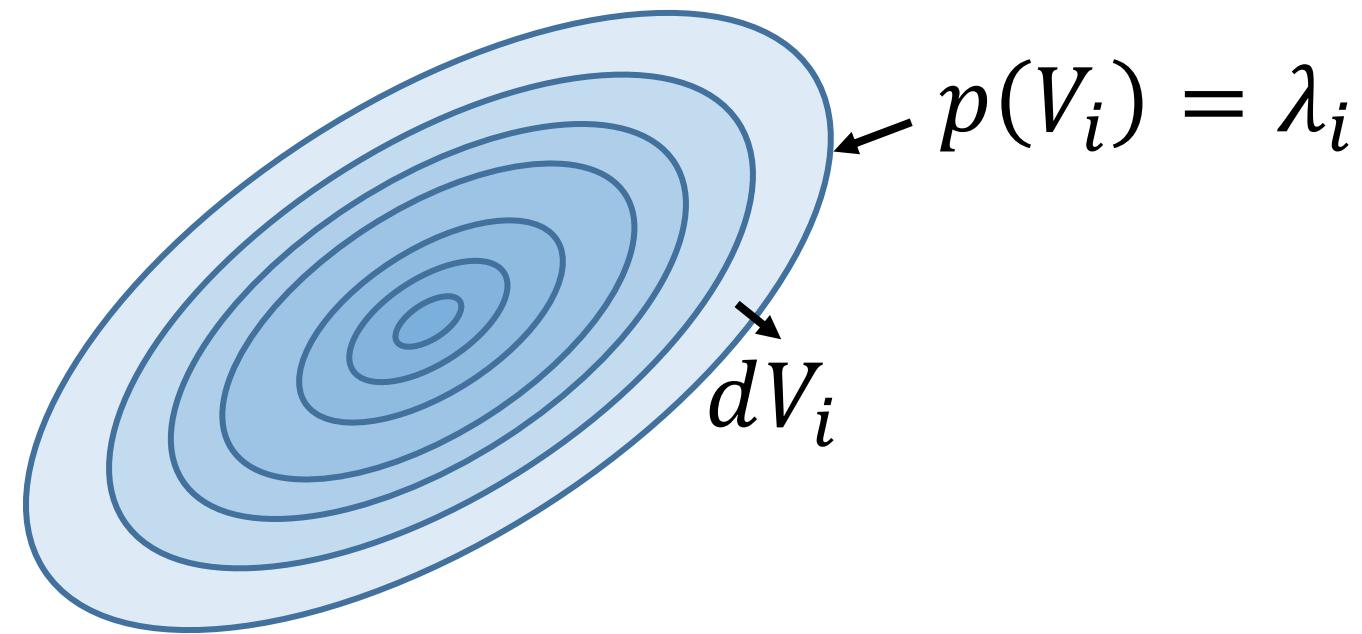
Motivation: Integrating the Posterior

$$\int_0^\infty p(V) dV(\lambda)$$



Motivation: Integrating the Posterior

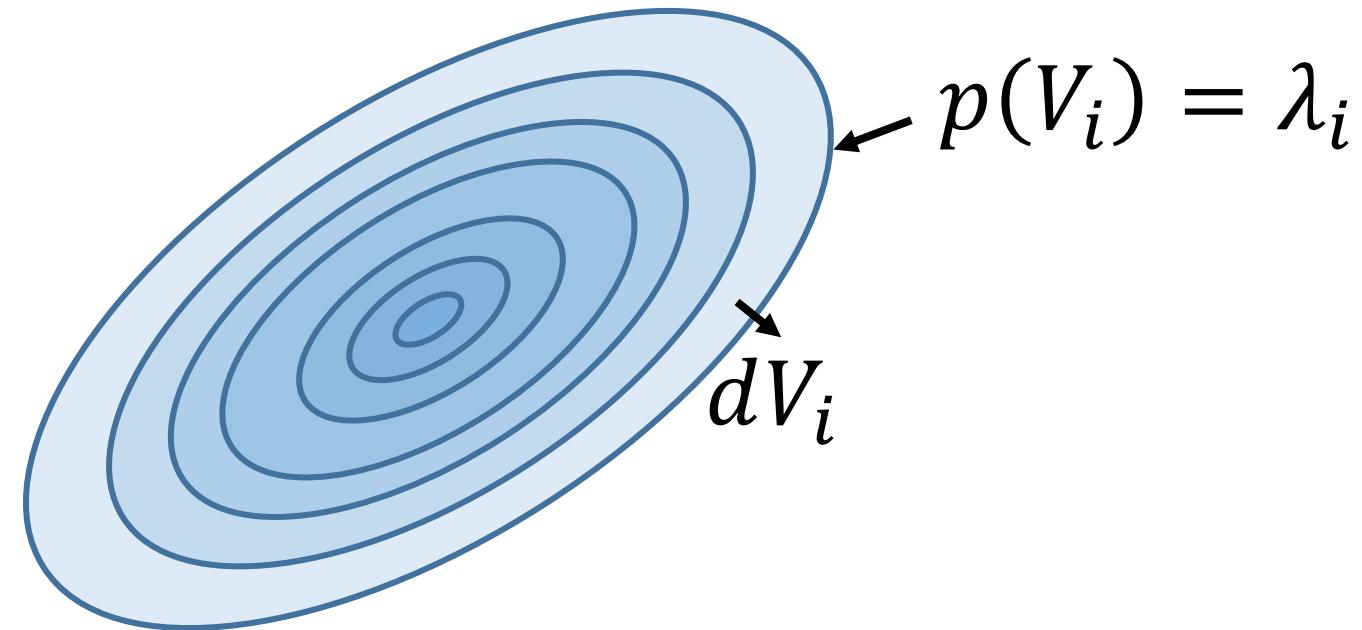
$$\int_0^\infty \text{“Amplitude”} \\ p(V) dV(\lambda) \\ \text{“Volume”}$$



Motivation: Integrating the Posterior

“Typical Set”

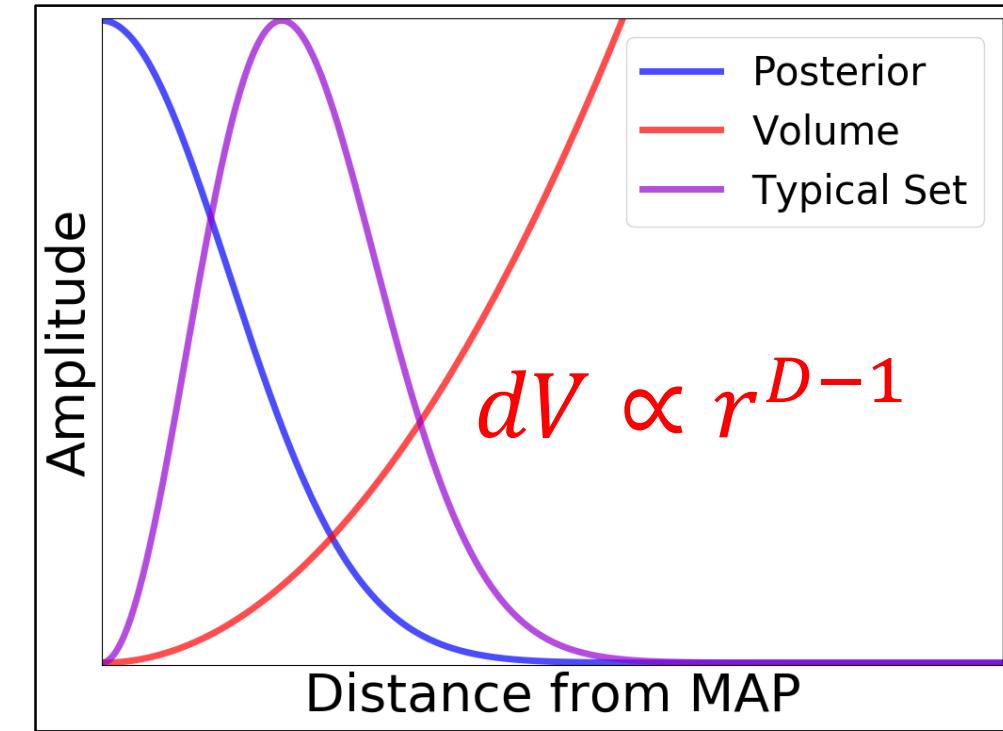
$$\int_0^\infty \overbrace{p(V)dV(\lambda)}$$



Motivation: Integrating the Posterior

“Typical Set”

$$\int_0^\infty p(V) dV(\lambda)$$



Motivation: Integrating the Posterior

$$\int_{\Omega_{\Theta}} p(\Theta) d\Theta$$

Motivation: Integrating the Posterior

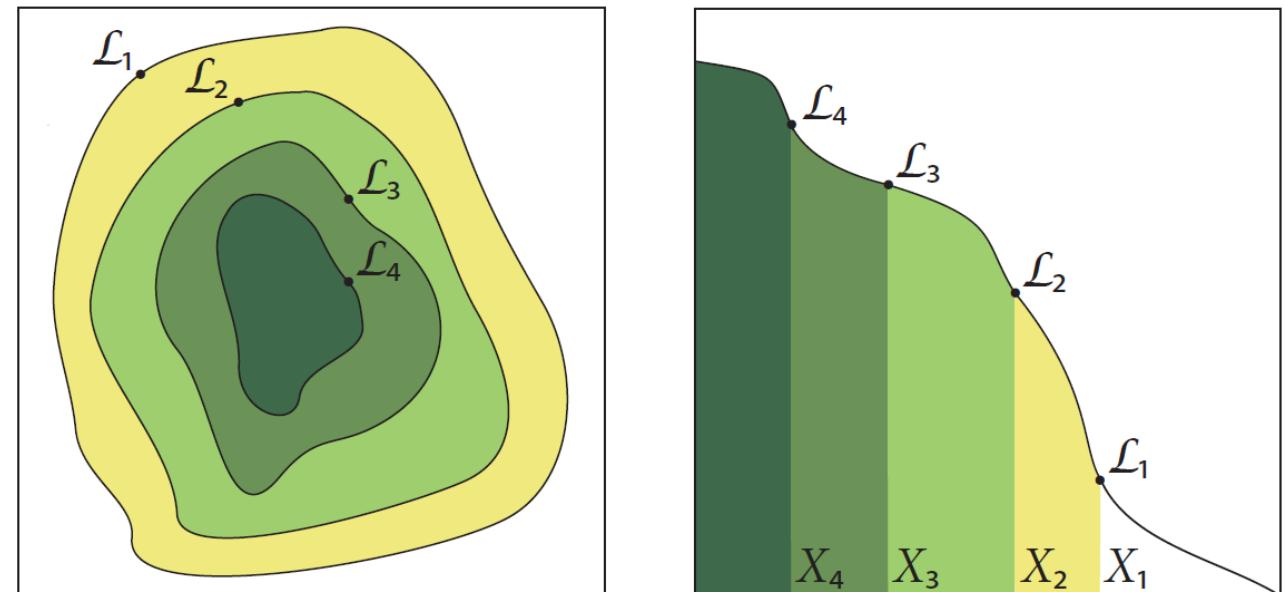
$$Z \equiv \int_{\Omega_{\Theta}} \mathcal{L}(\Theta) \pi(\Theta) d\Theta$$

Motivation: Integrating the Posterior

$$\mathcal{Z} \equiv \int_{\Omega_{\Theta}} \mathcal{L}(\Theta) \pi(\Theta) d\Theta$$

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

“Prior Volume”



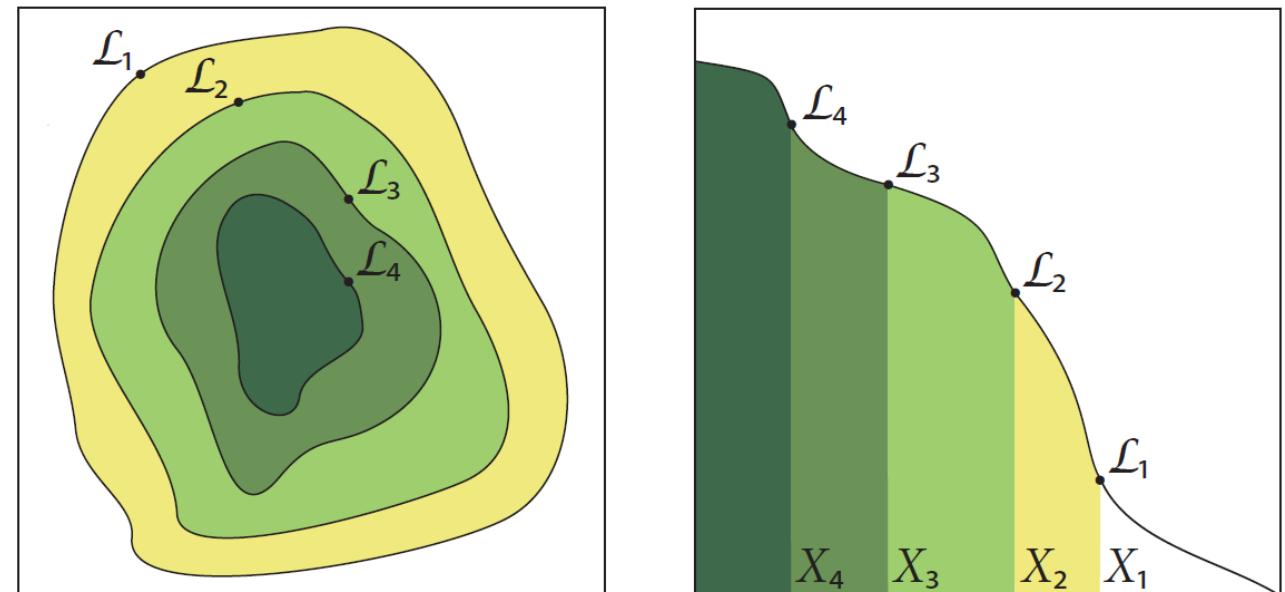
Feroz et al. (2013)

Motivation: Integrating the Posterior

$$Z = \int_0^\infty X(\lambda) d\lambda$$

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

“Prior Volume”



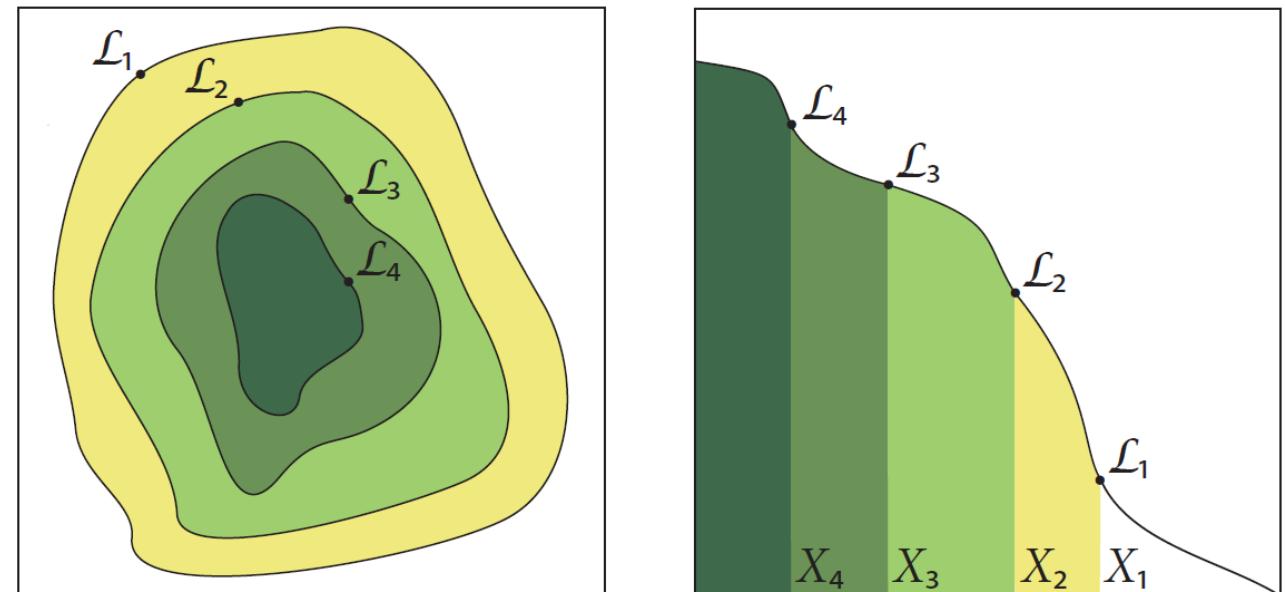
Feroz et al. (2013)

Motivation: Integrating the Posterior

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

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

“Prior Volume”



Feroz et al. (2013)

$f(\mathcal{L}_i, \dots)g(X_i, \dots)$ can be rectangles, trapezoids, etc.

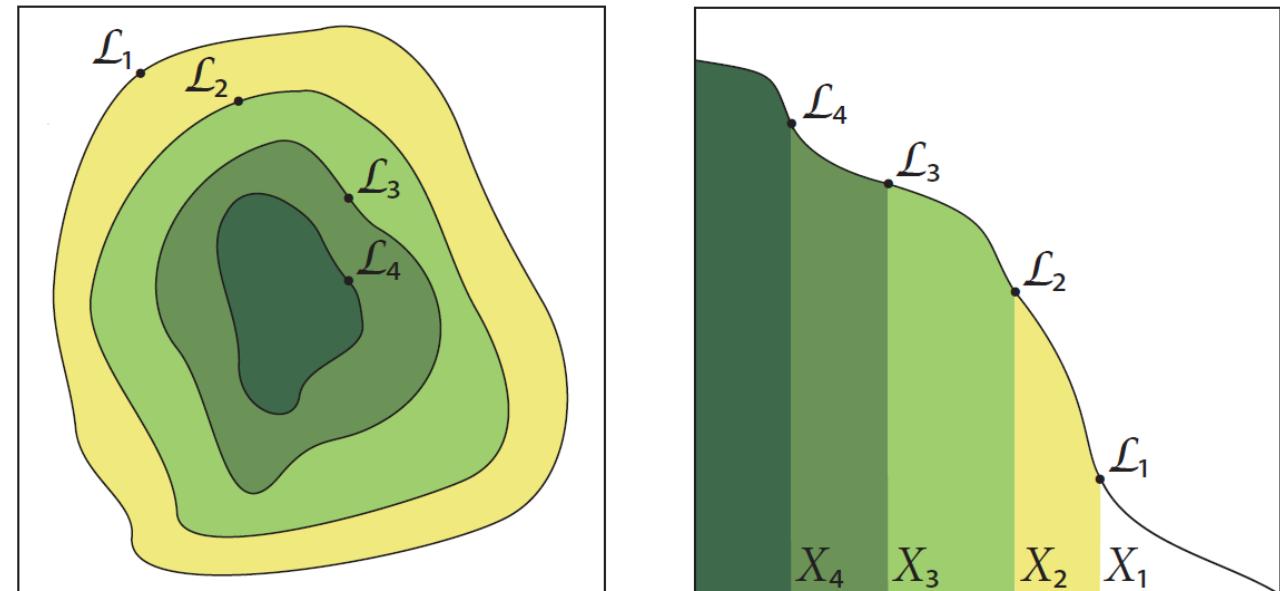
Motivation: Integrating the Posterior

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n f(\mathcal{L}_i, \dots)g(X_i, \dots)$$

Amplitude Differential Volume ΔX_i

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

“Prior Volume”



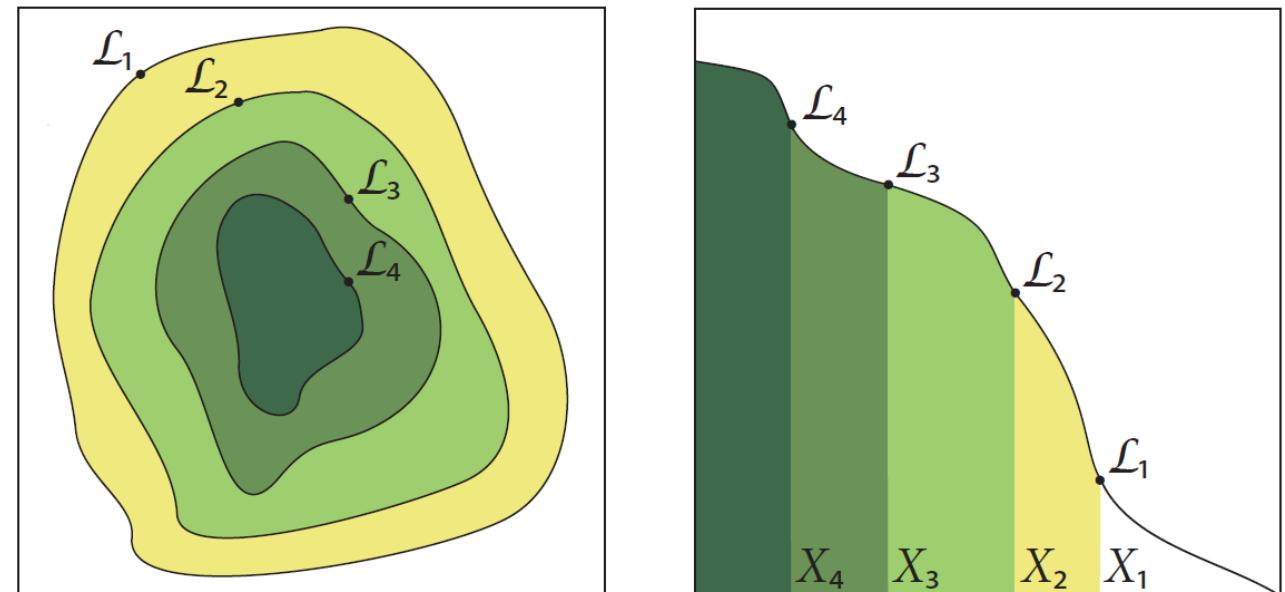
$$\hat{w}_i = f(\mathcal{L}_i, \dots)g(X_i, \dots)$$

Motivation: Integrating the Posterior

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

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

“Prior Volume”



$$\hat{w}_i = f(\mathcal{L}_i, \dots)g(X_i, \dots)$$

Motivation: Integrating the Posterior

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

We get posteriors “for free”

$$\hat{p}_i = \frac{\hat{w}_i}{\hat{\mathcal{Z}}}$$

Importance Weight

$$\begin{aligned}\widehat{w}_i &= f(\mathcal{L}_i, \dots) g(X_i, \dots) \\ &\sim f(p_i, \dots) g(V_i, \dots)\end{aligned}$$

Motivation: Integrating the Posterior

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \widehat{w}_i$$

We get posteriors “for free”

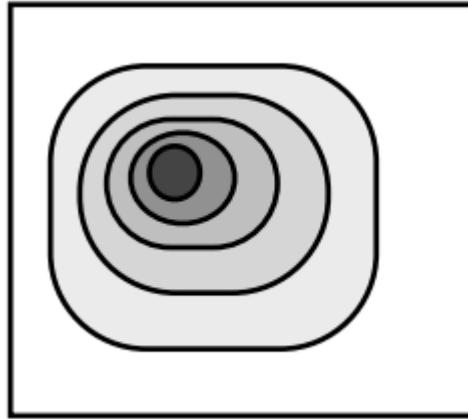
$$\hat{p}_i = \frac{\widehat{w}_i}{\hat{\mathcal{Z}}}$$

Importance Weight

Directly proportional to
typical set.

Pictures from [this 2010 talk](#) by Skilling.

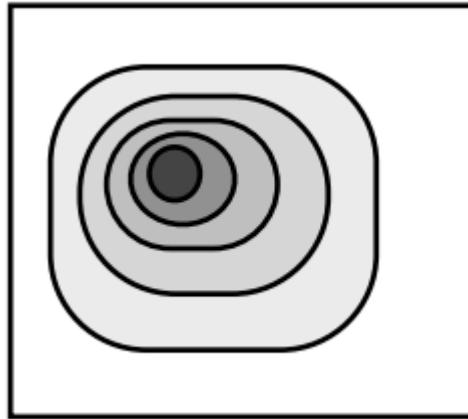
Motivation: Sampling the Posterior



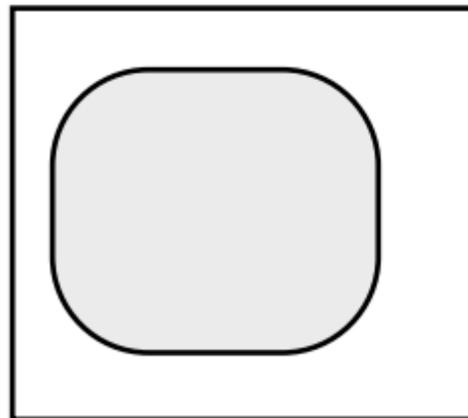
Sampling directly from the likelihood $\mathcal{L}(\Theta)$ is **hard**.

Pictures from [this 2010 talk](#) by Skilling.

Motivation: Sampling the Posterior

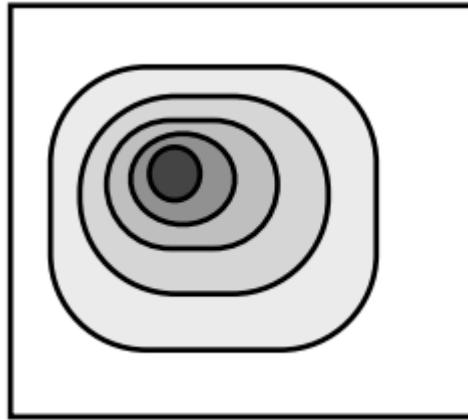


Sampling uniformly within
bound $\mathcal{L}(\Theta) > \lambda$ is **easier**.

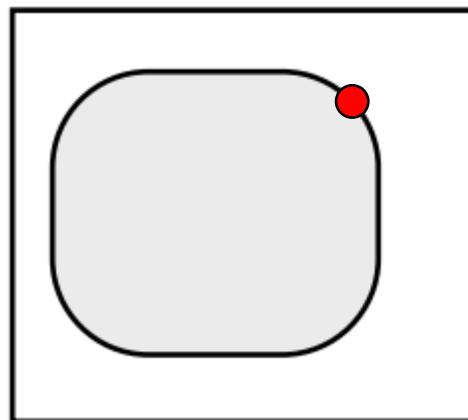


Pictures from [this 2010 talk](#) by Skilling.

Motivation: Sampling the Posterior

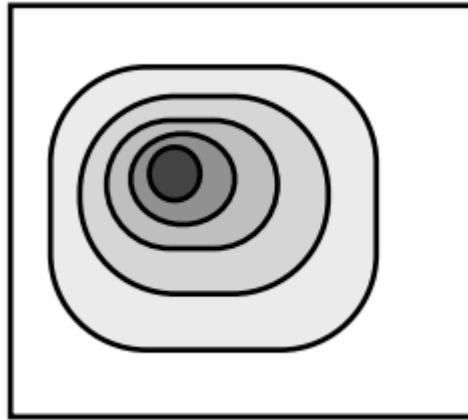


Sampling uniformly within
bound $\mathcal{L}(\Theta) > \lambda$ is **easier**.

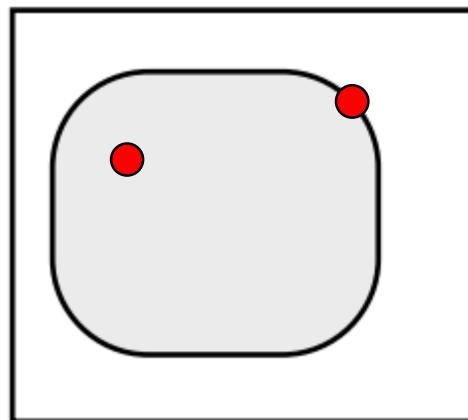


Pictures from [this 2010 talk](#) by Skilling.

Motivation: Sampling the Posterior

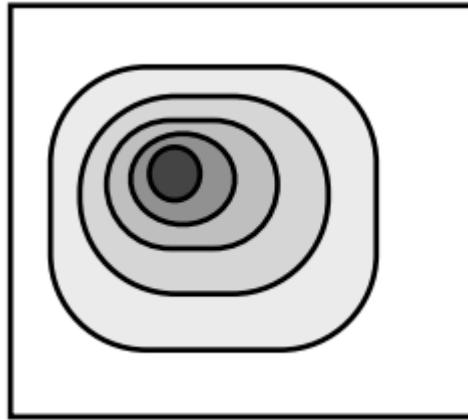


Sampling uniformly within
bound $\mathcal{L}(\Theta) > \lambda$ is **easier**.

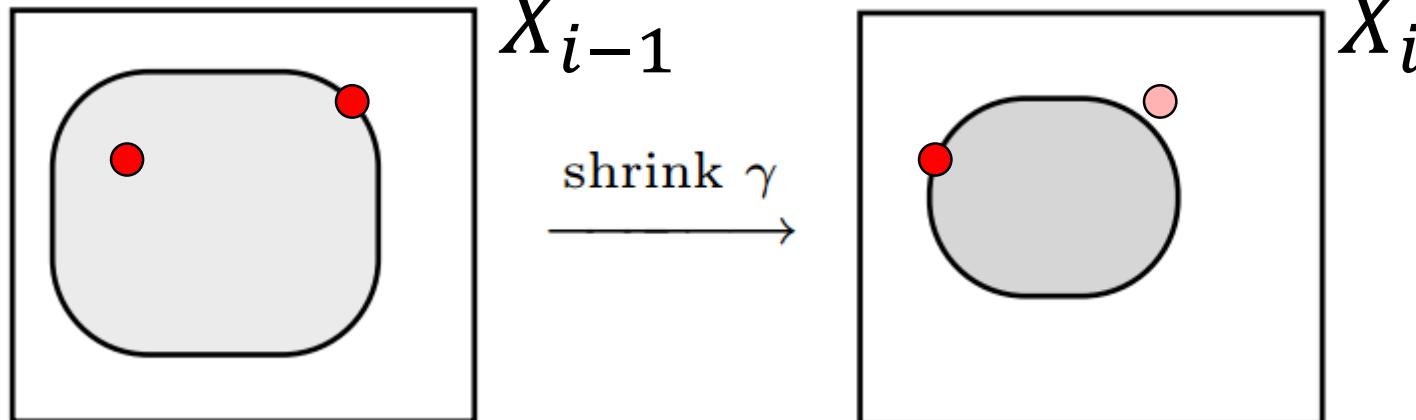


Pictures from [this 2010 talk](#) by Skilling.

Motivation: Sampling the Posterior

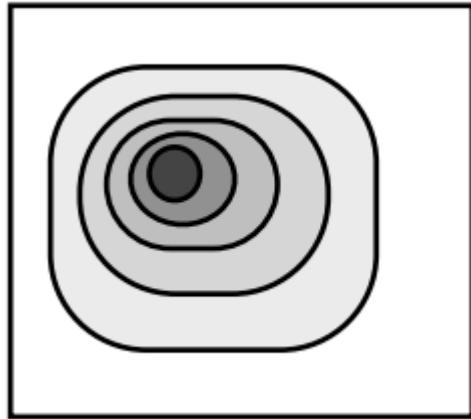


Sampling uniformly within
bound $\mathcal{L}(\Theta) > \lambda$ is **easier**.

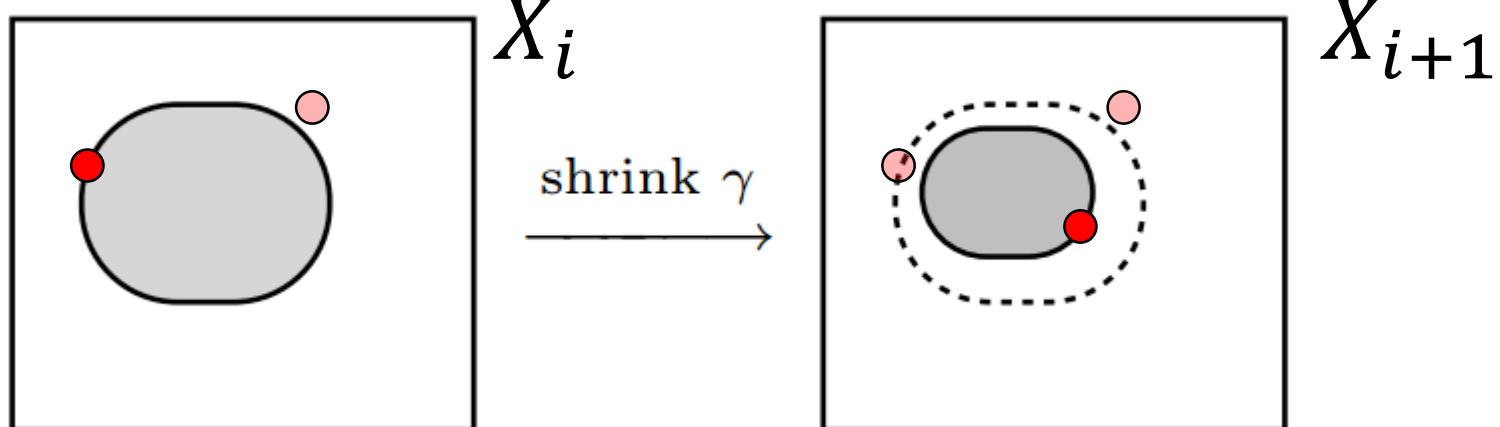


Pictures from [this 2010 talk](#) by Skilling.

Motivation: Sampling the Posterior

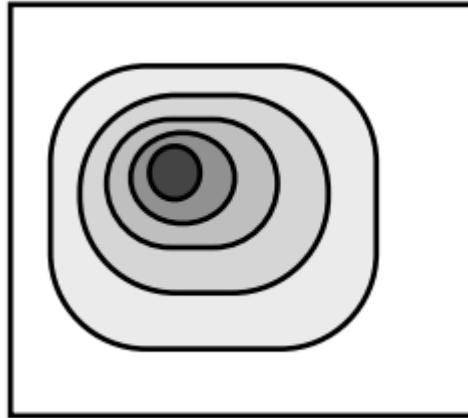


Sampling uniformly within bound $\mathcal{L}(\Theta) > \lambda$ is **easier**.



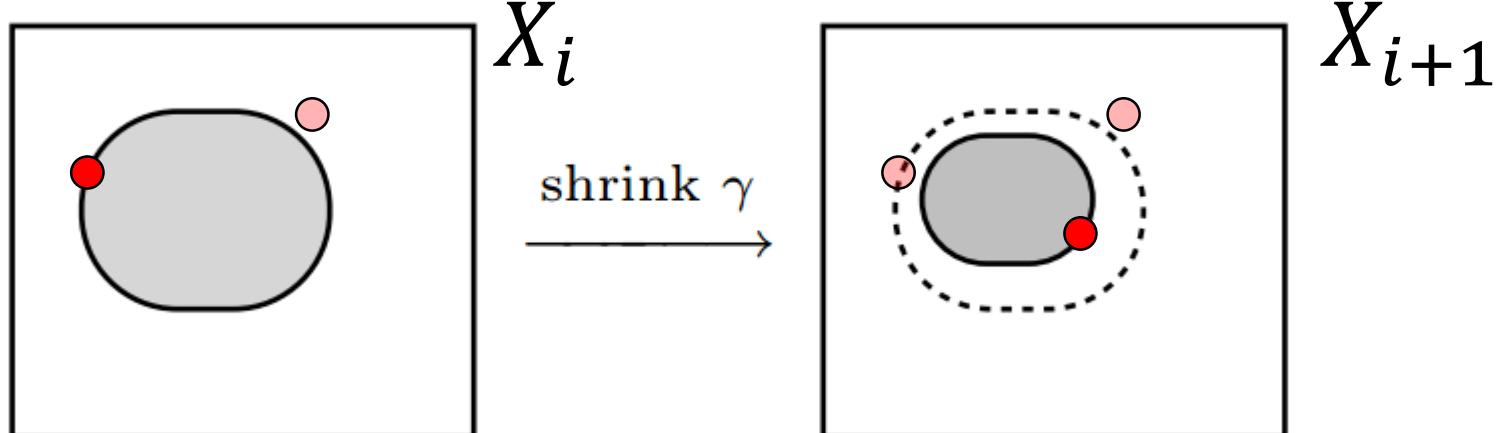
Pictures from [this 2010 talk](#) by Skilling.

Motivation: Sampling the Posterior



MCMC: Solving a Hard Problem **once**.
vs
Nested Sampling: Solving an Easier
Problem **many times**.

Sampling uniformly within
bound $\mathcal{L}(\Theta) > \lambda$ is **easier**.



How Nested Sampling Works

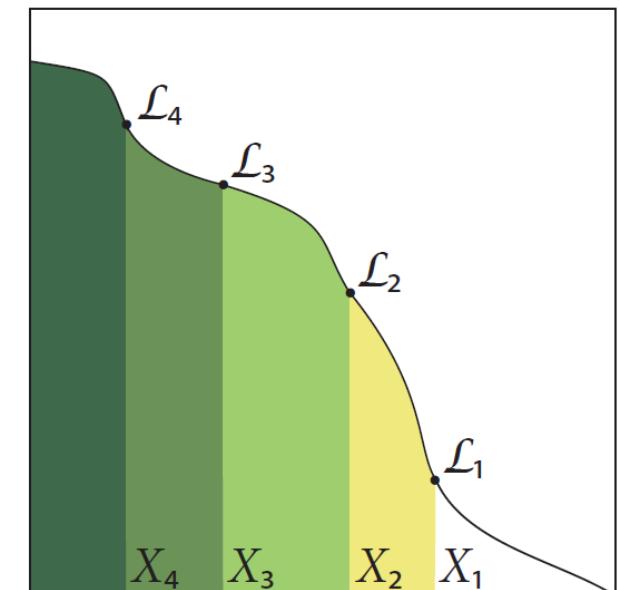
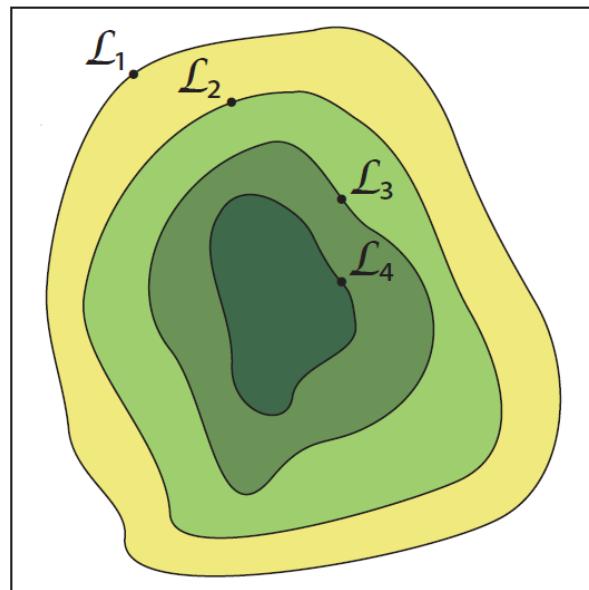
Estimating the Prior Volume

$$\hat{w}_i = f(\mathcal{L}_i, \dots)g(X_i, \dots)$$

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

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

“Prior Volume”



Estimating the Prior Volume

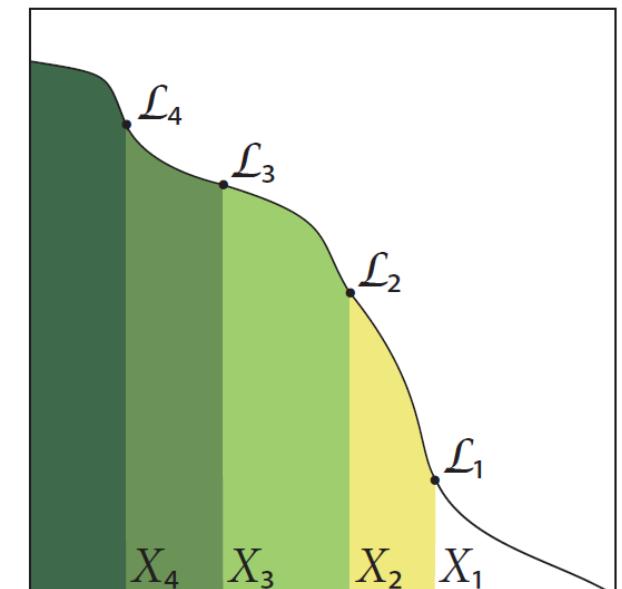
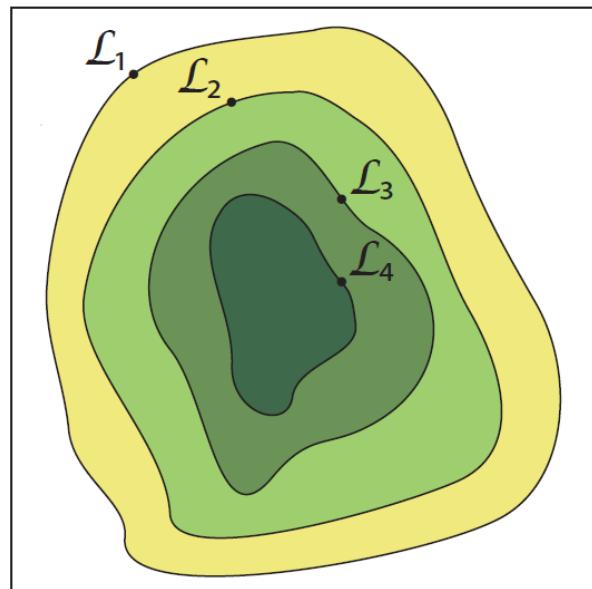
$$\hat{w}_i = \boxed{f(\mathcal{L}_i, \dots)} g(X_i, \dots)$$



$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

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

“Prior Volume”



Estimating the Prior Volume

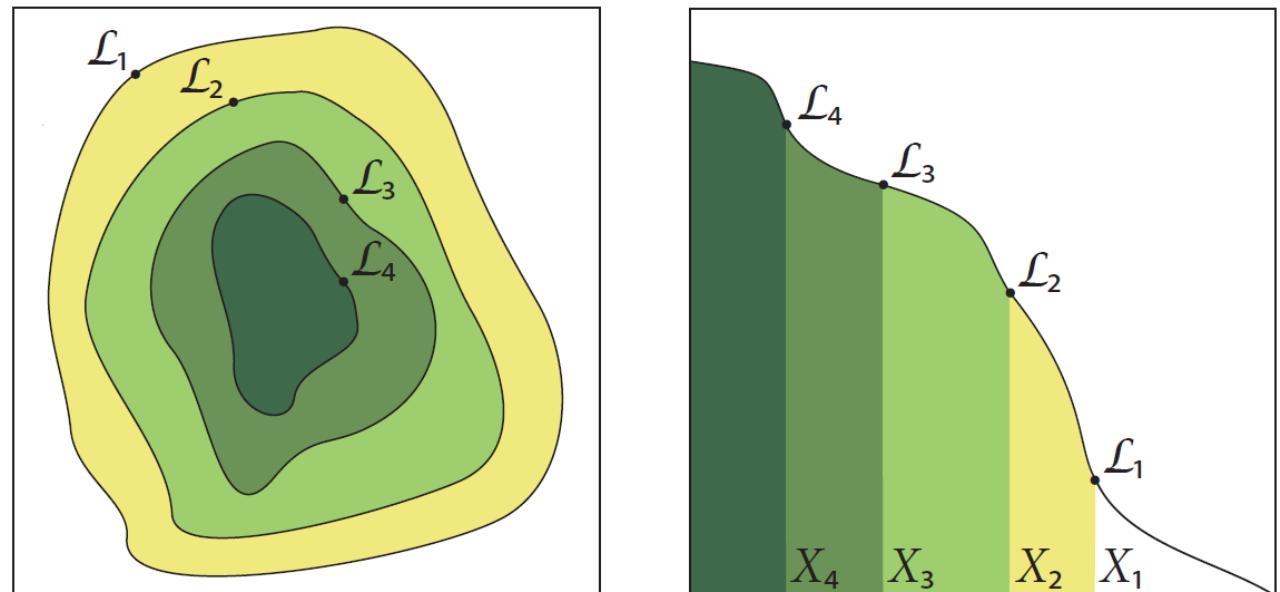
$$\hat{w}_i = f(\mathcal{L}_i, \dots) g(X_i, \dots)$$

✓ ???

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

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

“Prior Volume”



Estimating the Prior Volume

$$\hat{w}_i = f(\mathcal{L}_i, \dots) g(X_i, \dots)$$

???

✓

Probability Integral Transform

PDF

$X \sim f(x)$

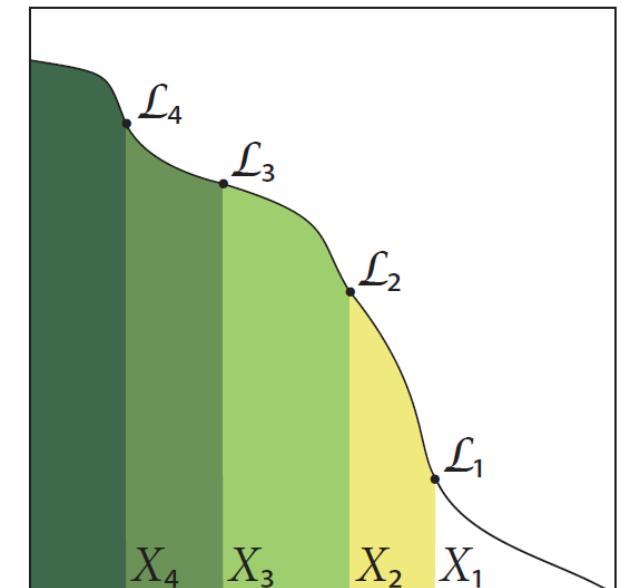
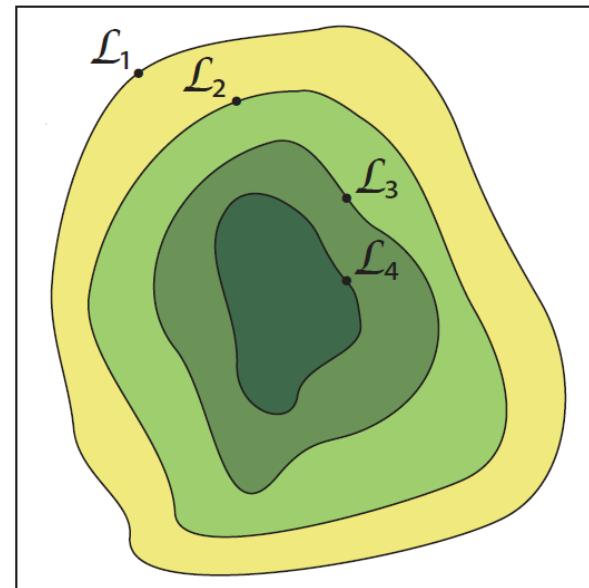
CDF

$F(X) \sim \text{Unif}$

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

$$X(\lambda) \equiv \int_{\{\boldsymbol{\Theta}: \mathcal{L}(\boldsymbol{\Theta}) > \lambda\}} \pi(\boldsymbol{\Theta}) d\boldsymbol{\Theta}$$

“Prior Volume”



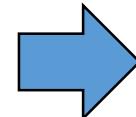
Estimating the Prior Volume

$$\hat{w}_i = f(\mathcal{L}_i, \dots) g(X_i, \dots)$$



???

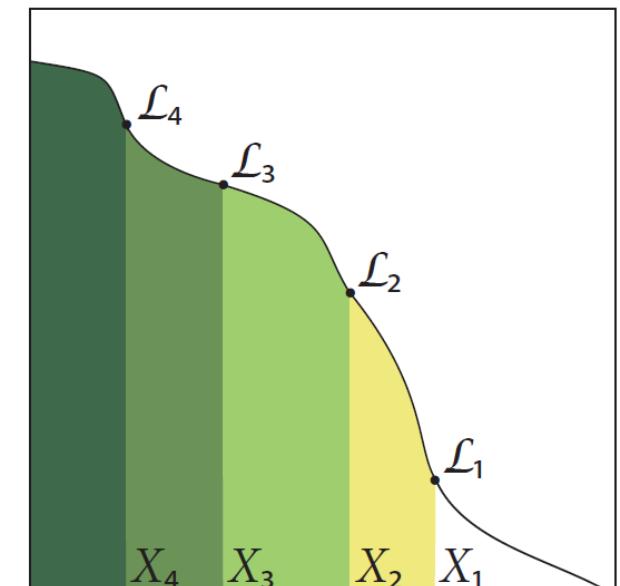
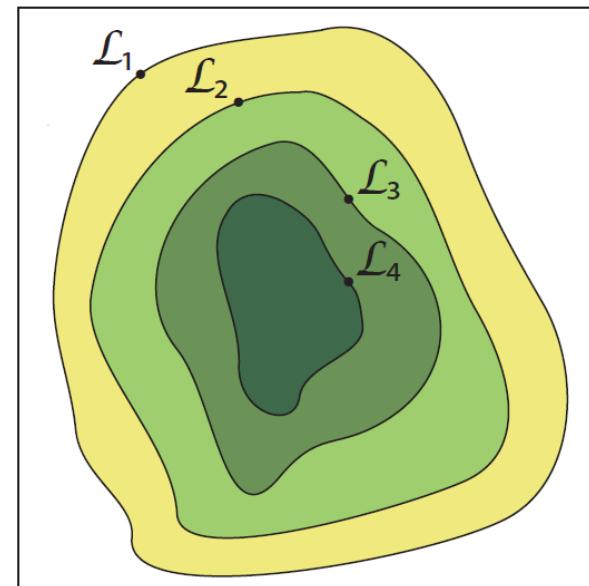
Probability Integral Transform
PDF
 $X \sim f(x)$
CDF
 $F(X) \sim \text{Unif}$



n
 $\ell - 1$
Need to sample from
the constrained prior.

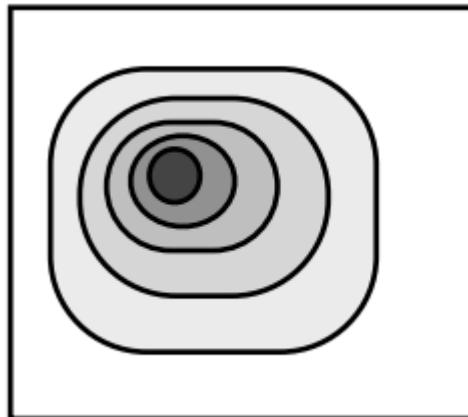
$$X(\lambda) \equiv \int_{\{\boldsymbol{\Theta} : \mathcal{L}(\boldsymbol{\Theta}) > \lambda\}} \pi(\boldsymbol{\Theta}) d\boldsymbol{\Theta}$$

“Prior Volume”

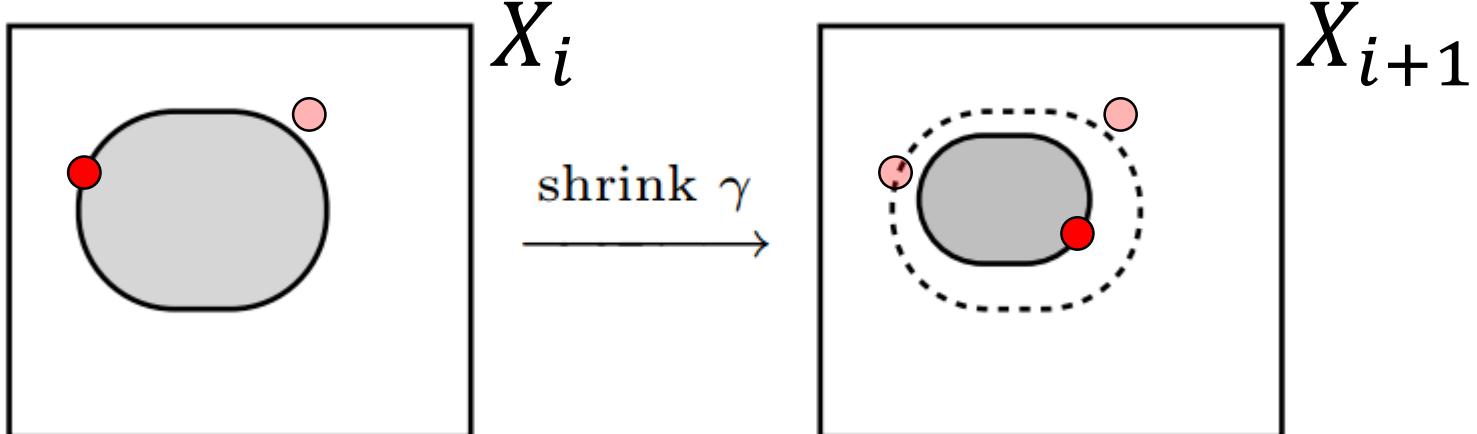


Pictures from [this 2010 talk](#) by Skilling.

Estimating the Prior Volume



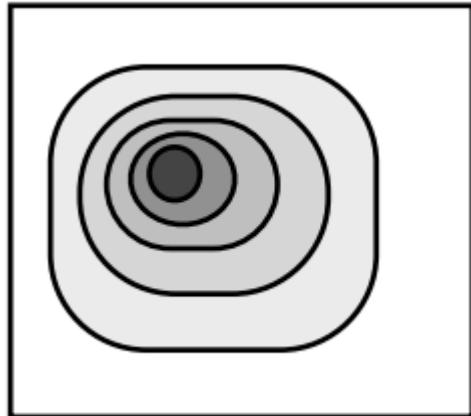
Posterior



Pictures from [this 2010 talk](#) by Skilling.

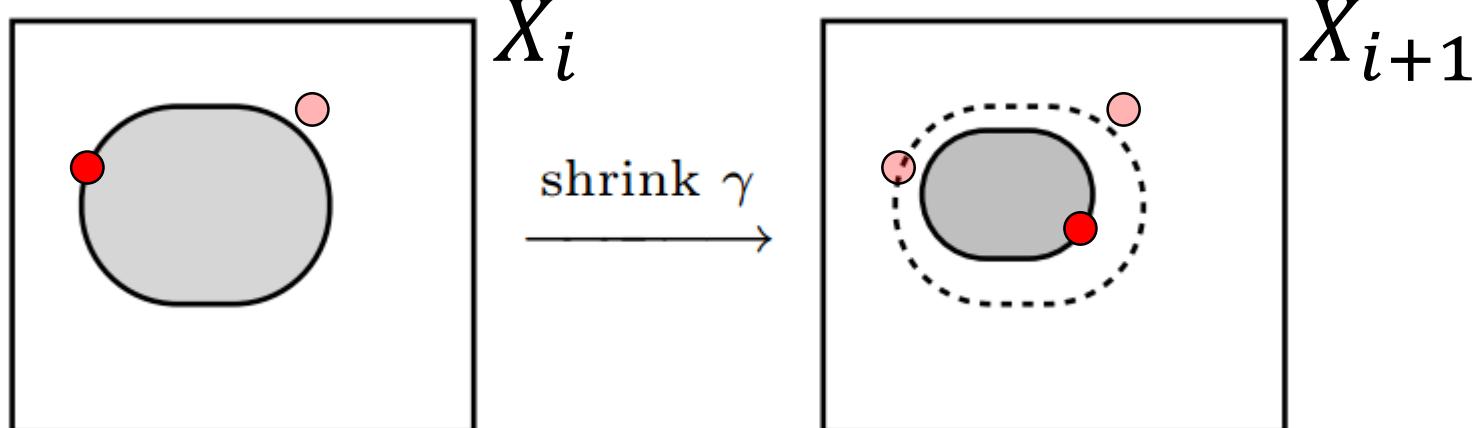
Estimating the Prior Volume

$$U_i \sim \text{Unif}$$



Posterior

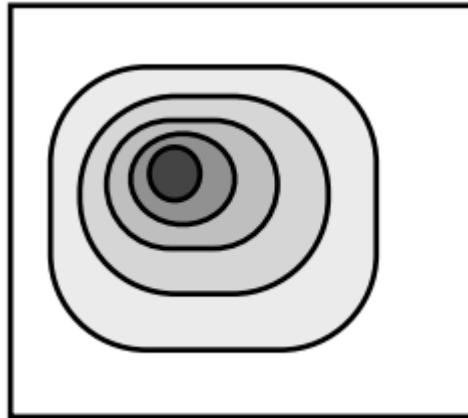
$$X_{i+1} = U_i X_i$$



Pictures from [this 2010 talk](#) by Skilling.

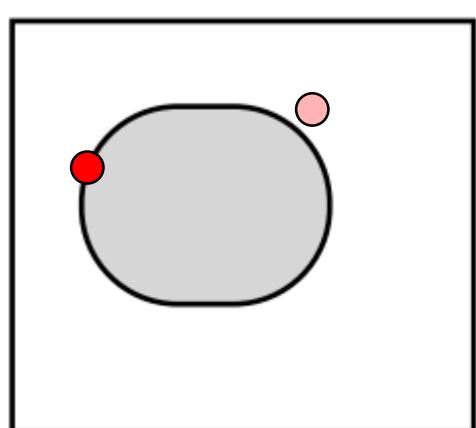
Estimating the Prior Volume

$U_0, \dots, U_i \stackrel{\text{i.i.d.}}{\sim} \text{Unif}$

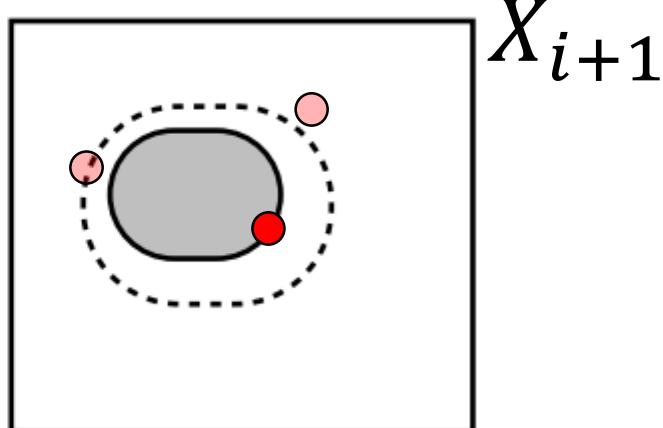


Posterior

$$X_{i+1} = \prod_{j=0}^i U_j X_0$$



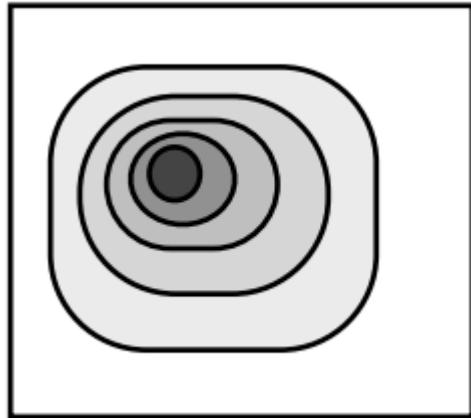
X_i
 $\xrightarrow{\text{shrink } \gamma}$



Pictures from [this 2010 talk](#) by Skilling.

Estimating the Prior Volume

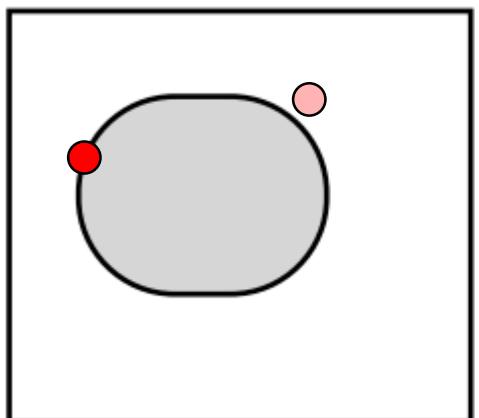
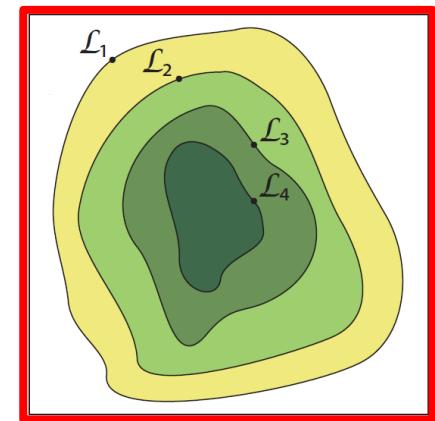
$U_0, \dots, U_i \stackrel{\text{i. i. d.}}{\sim} \text{Unif}$



Posterior

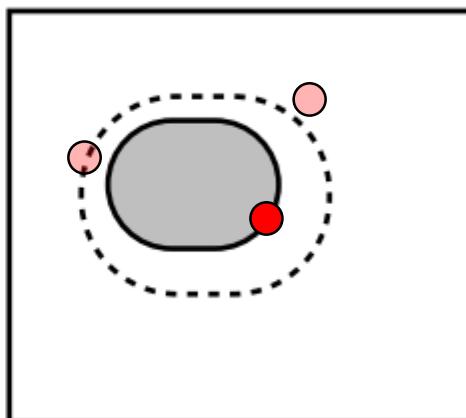
$$X_{i+1} = \prod_{j=0}^i U_j X_0$$

$$X_0 \equiv 1$$



X_i

shrink γ

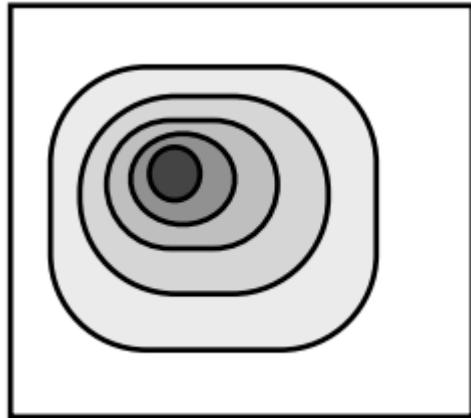


X_{i+1}

Pictures from [this 2010 talk](#) by Skilling.

Estimating the Prior Volume

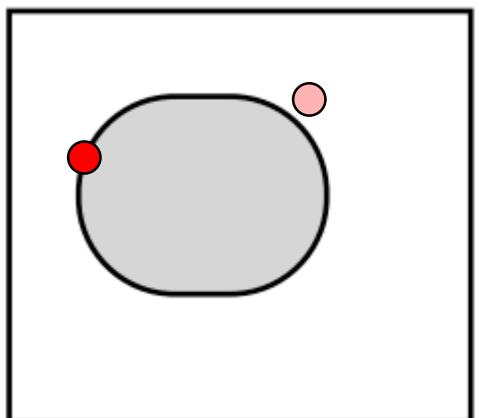
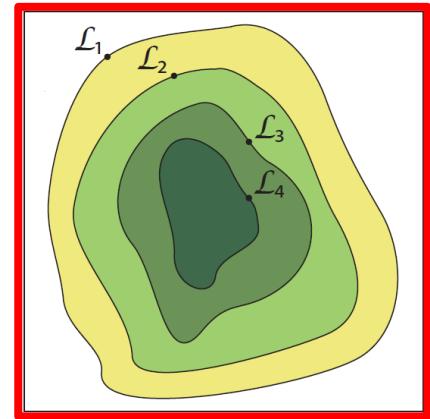
$U_0, \dots, U_i \stackrel{\text{i. i. d.}}{\sim} \text{Unif}$



Posterior

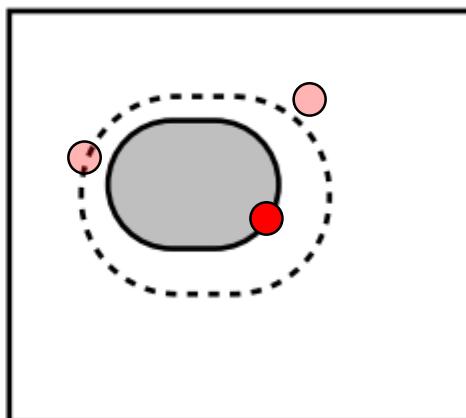
$$X_{i+1} = \prod_{j=0}^i U_j$$

$$X_0 \equiv 1$$



X_i

shrink γ



X_{i+1}

Estimating the Prior Volume

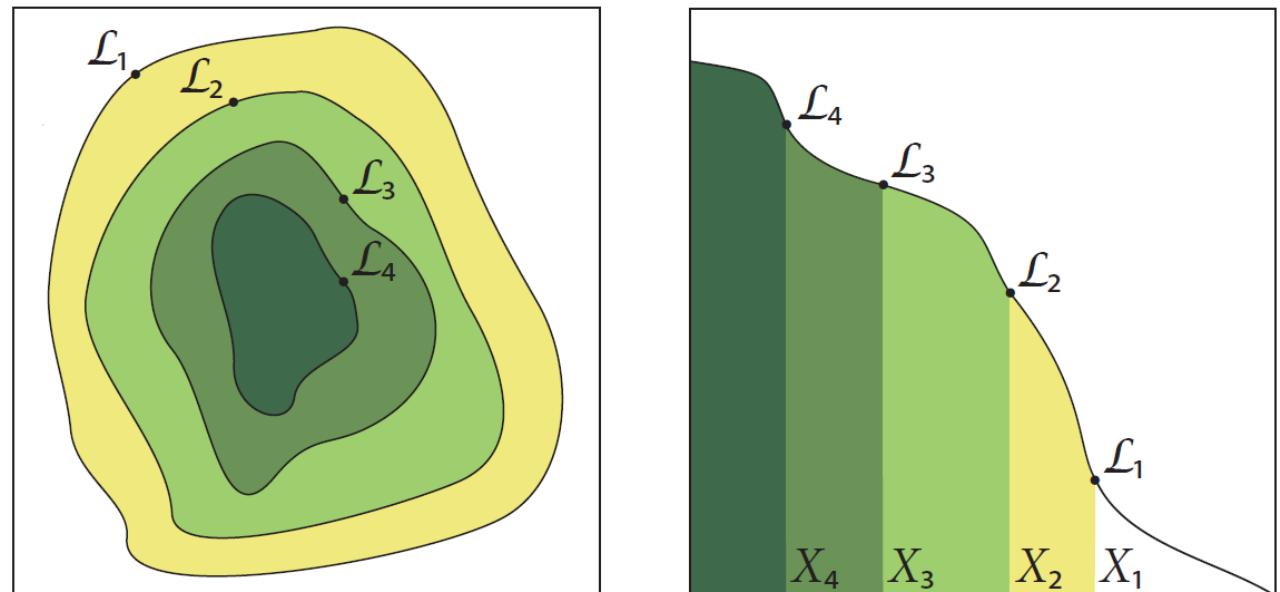
$$\hat{w}_i = f(\mathcal{L}_i, \dots) g(X_i, \dots)$$

✓ ???

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

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

“Prior Volume”



Estimating the Prior Volume

$$\hat{w}_i = f(\mathcal{L}_i, \dots) g(X_i, \dots)$$

✓

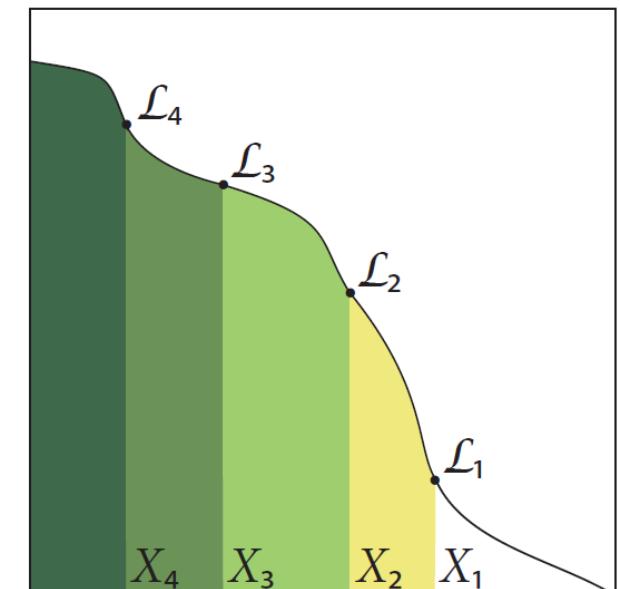
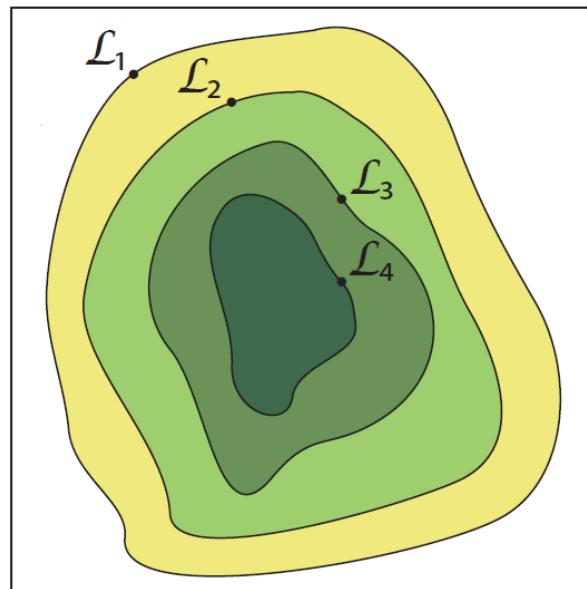
↗

$$\hat{\mathcal{Z}} \approx \sum_{i=1}^n \hat{w}_i$$

$\Pr(X_1, X_2, \dots, X_i)$
where 1st & 2nd moments
can be computed

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

“Prior Volume”



Nested Sampling Algorithm

$$\begin{array}{cccccc} \mathcal{L}_N > \mathcal{L}_{N-1} > \cdots > \mathcal{L}_2 > \mathcal{L}_1 > 0 \\ \Theta_N & \Theta_{N-1} & \cdots & \Theta_2 & \Theta_1 \end{array}$$

Nested Sampling Algorithm (Ideal)

$$\begin{array}{cccccc} \mathcal{L}_N > \mathcal{L}_{N-1} > \cdots > \mathcal{L}_2 > \mathcal{L}_1 > 0 \\ \Theta_N \quad \Theta_{N-1} \quad \cdots \quad \Theta_2 \quad \Theta_1 \end{array}$$

Samples sequentially drawn
from constrained prior $\pi_{\mathcal{L} > \mathcal{L}_i}(\Theta)$.

Nested Sampling Algorithm (**Naïve**)

$$\mathcal{L}_N > \mathcal{L}_{N-1} > \cdots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

$$\Theta_1 \sim \pi(\Theta)$$

1. Samples sequentially drawn from prior $\pi(\Theta)$.
2. New point only accepted if $\mathcal{L}_{i+1} > \mathcal{L}_i$.

Nested Sampling Algorithm (**Naïve**)

$$\mathcal{L}_N > \mathcal{L}_{N-1} > \cdots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

$$\Theta_2 \quad \Theta_1 \sim \pi(\Theta)$$

1. Samples sequentially drawn from prior $\pi(\Theta)$.
2. New point only accepted if $\mathcal{L}_{i+1} > \mathcal{L}_i$.

Nested Sampling Algorithm (Naïve)

$$\mathcal{L}_N > \mathcal{L}_{N-1} > \cdots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

$$\Theta_N \quad \Theta_{N-1} \quad \cdots \quad \Theta_2 \quad \Theta_1 \sim \pi(\Theta)$$

1. Samples sequentially drawn from prior $\pi(\Theta)$.
2. New point only accepted if $\mathcal{L}_{i+1} > \mathcal{L}_i$.

Building a Nested Sampling Algorithm

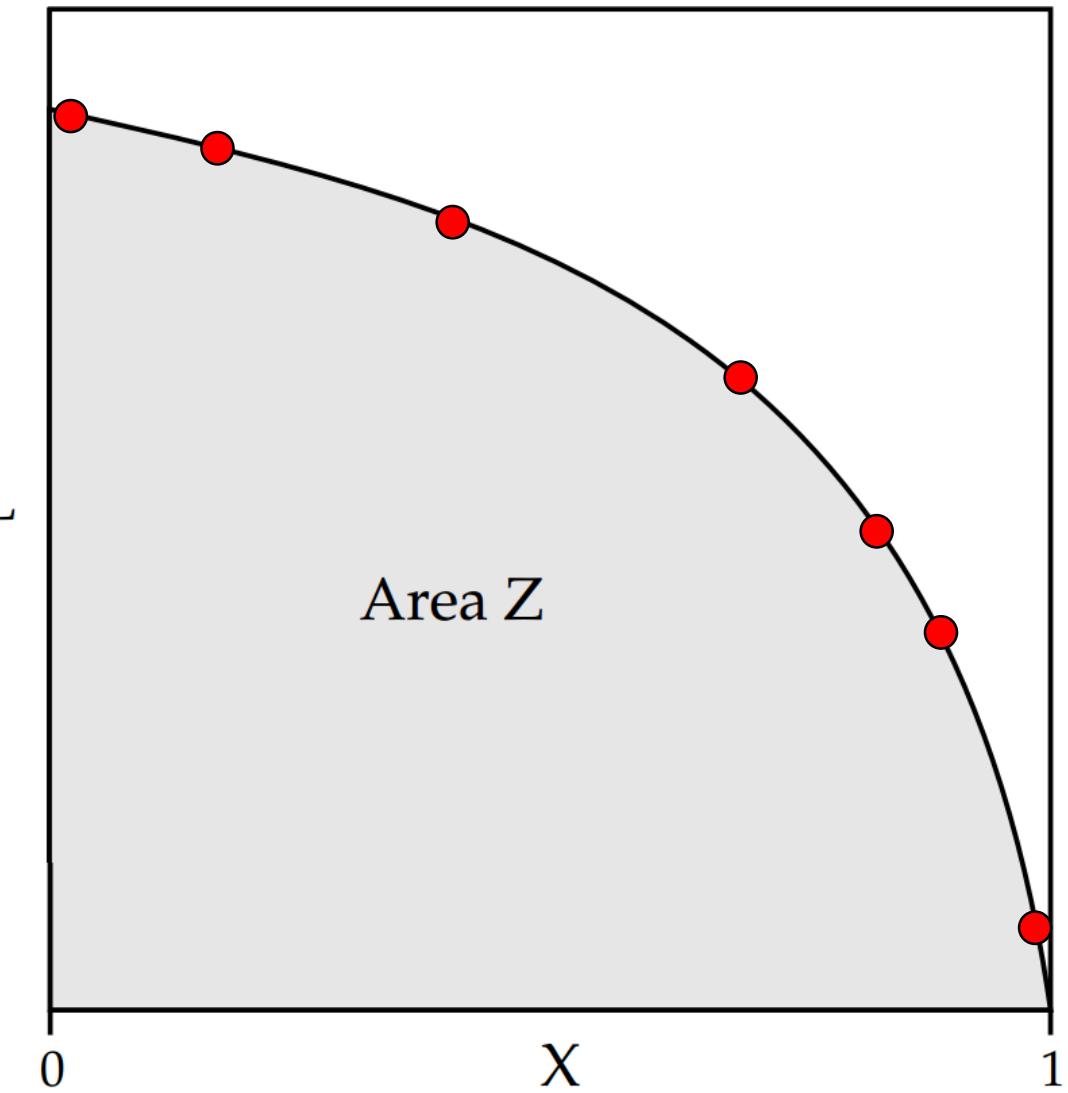
Components of the Algorithm

1. Adding more particles.
2. Knowing when to stop.
3. What to do after stopping.

Adding More Particles

$$\mathcal{L}_{N_1}^{(1)} > \dots > \mathcal{L}_2^{(1)} > \mathcal{L}_1^{(1)} > 0$$

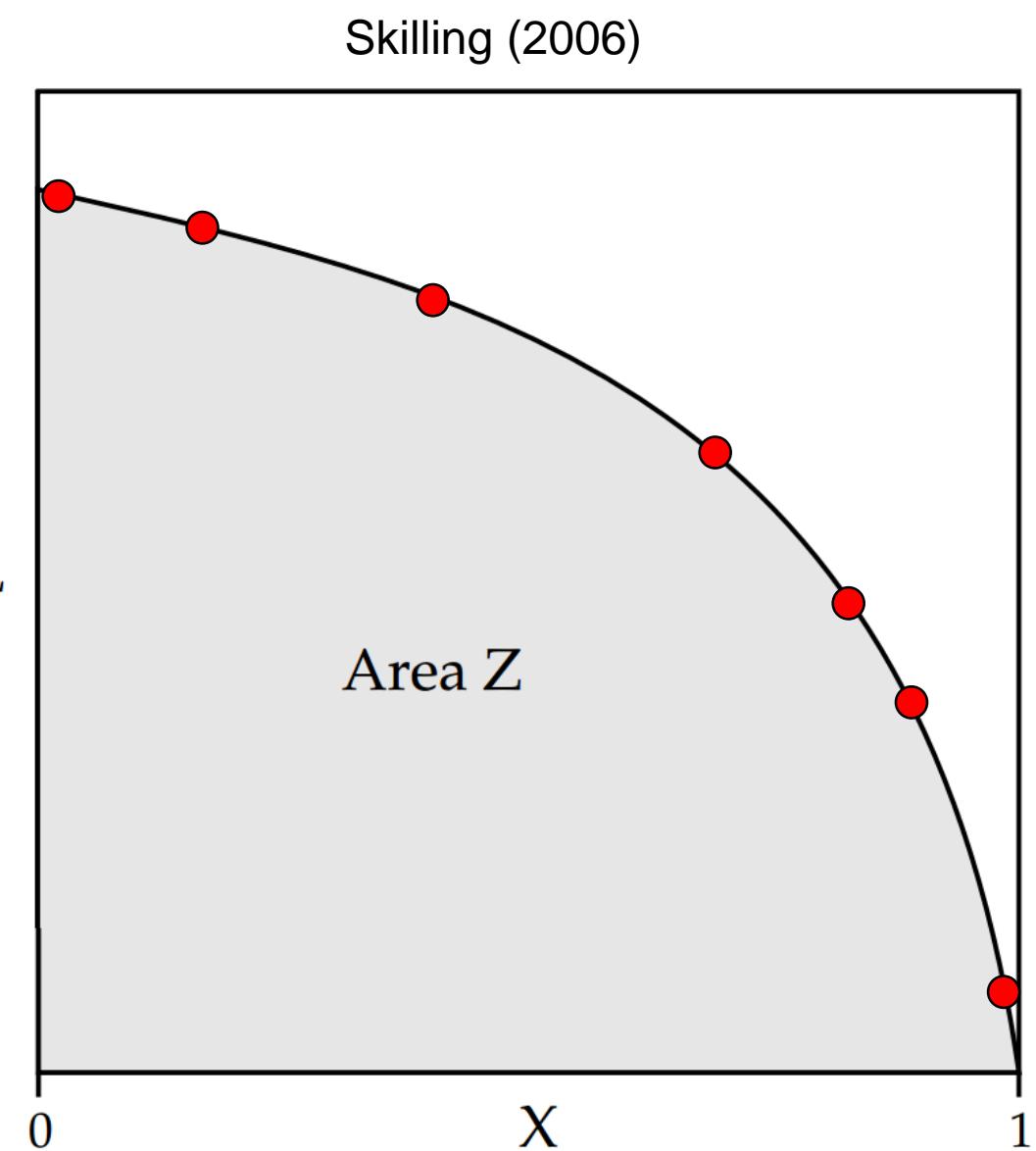
Skilling (2006)



Adding More Particles

$$\mathcal{L}_{N_1}^{(1)} > \dots > \mathcal{L}_2^{(1)} > \mathcal{L}_1^{(1)} > 0$$

$$X_{i+1}^{(1)} = \prod_{j=0}^i U_j$$

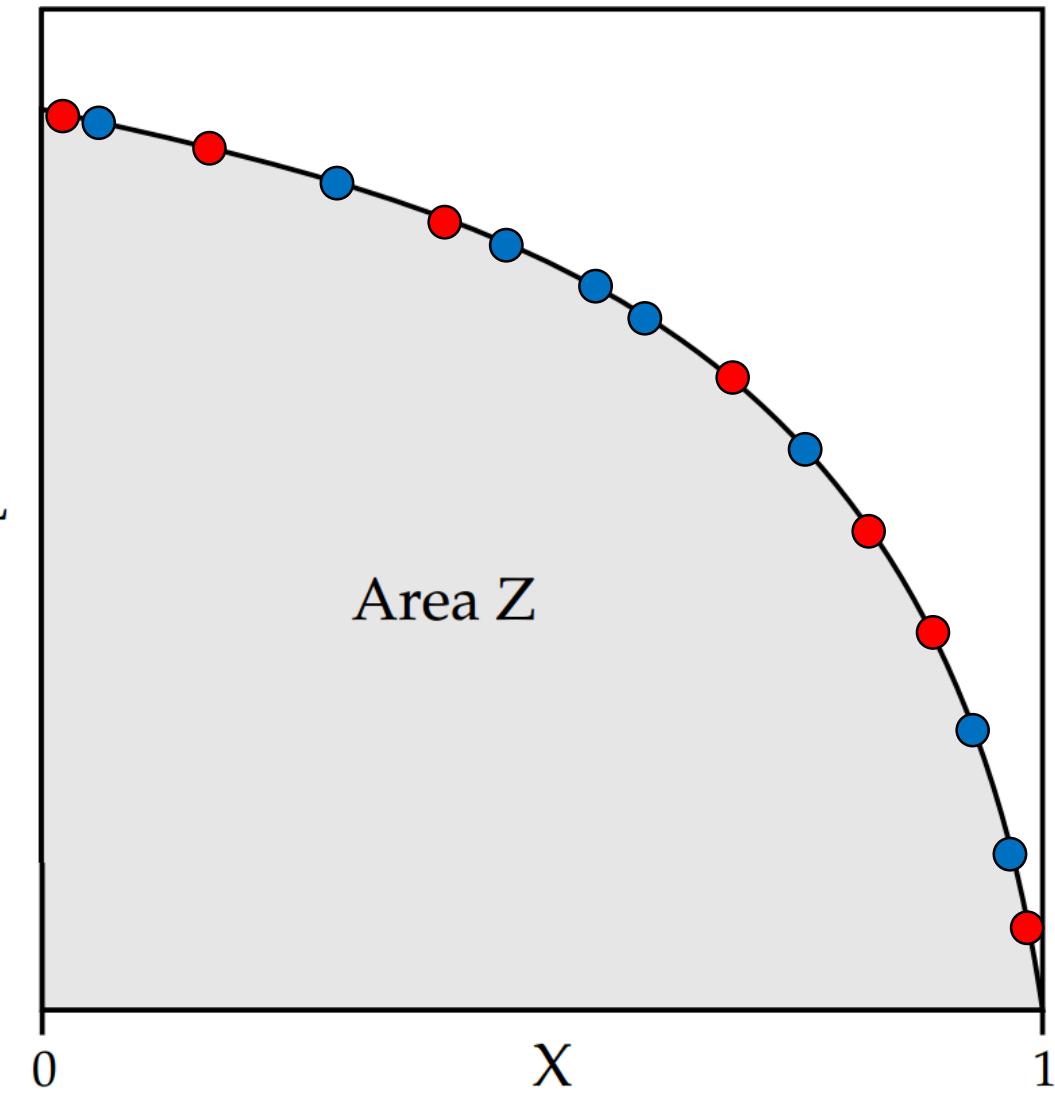


Adding More Particles

$$\mathcal{L}_{N_1}^{(1)} > \dots > \mathcal{L}_2^{(1)} > \mathcal{L}_1^{(1)} > 0$$

$$\mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > 0$$

Skilling (2006)



Adding More Particles

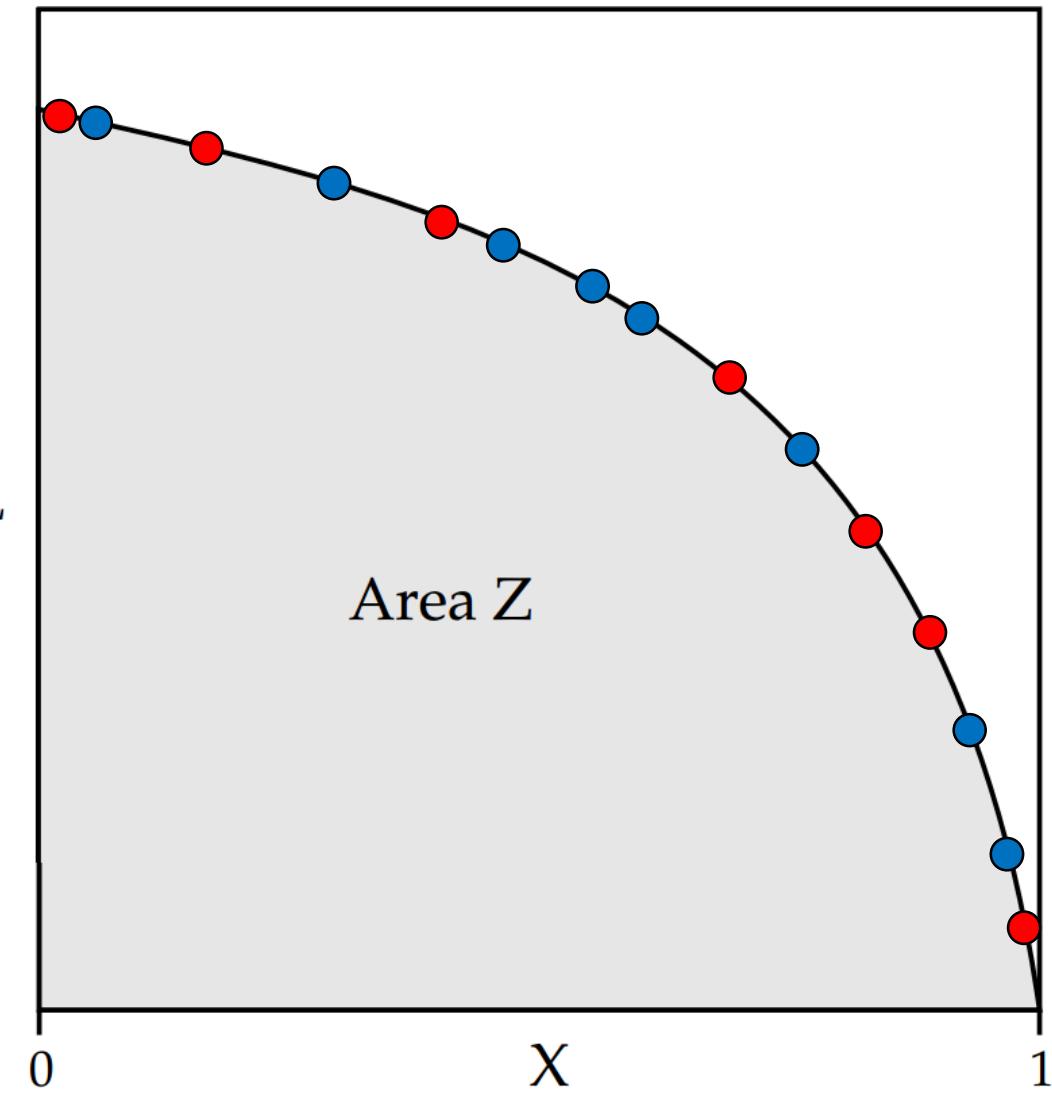
$$\mathcal{L}_{N_1}^{(1)} > \dots > \mathcal{L}_2^{(1)} > \mathcal{L}_1^{(1)} > 0$$

$$\mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > 0$$

$$X_{i+1}^{(1)} = \prod_{j=0}^i U_j$$

$$X_{j+1}^{(2)} = \prod_{k=0}^j U_k$$

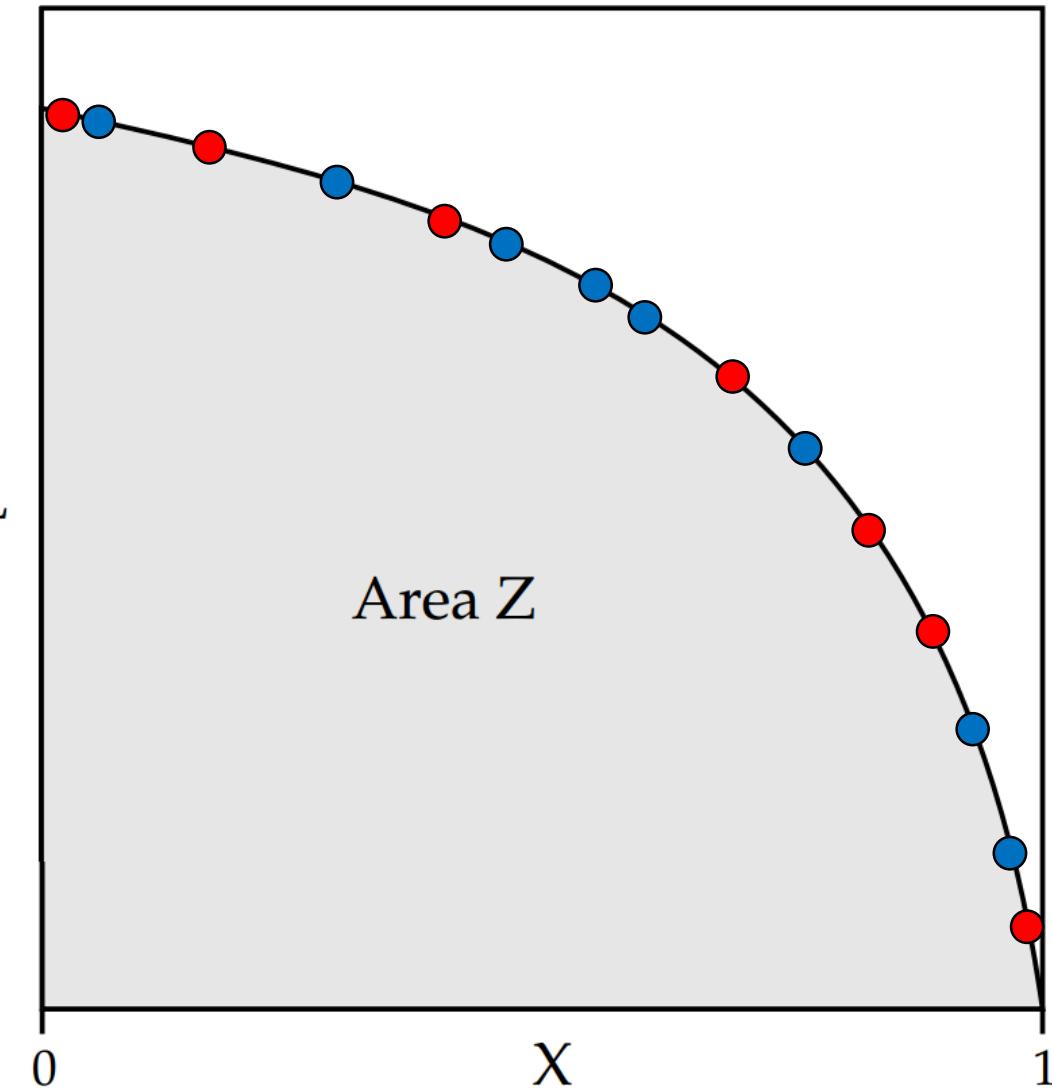
Skilling (2006)



Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

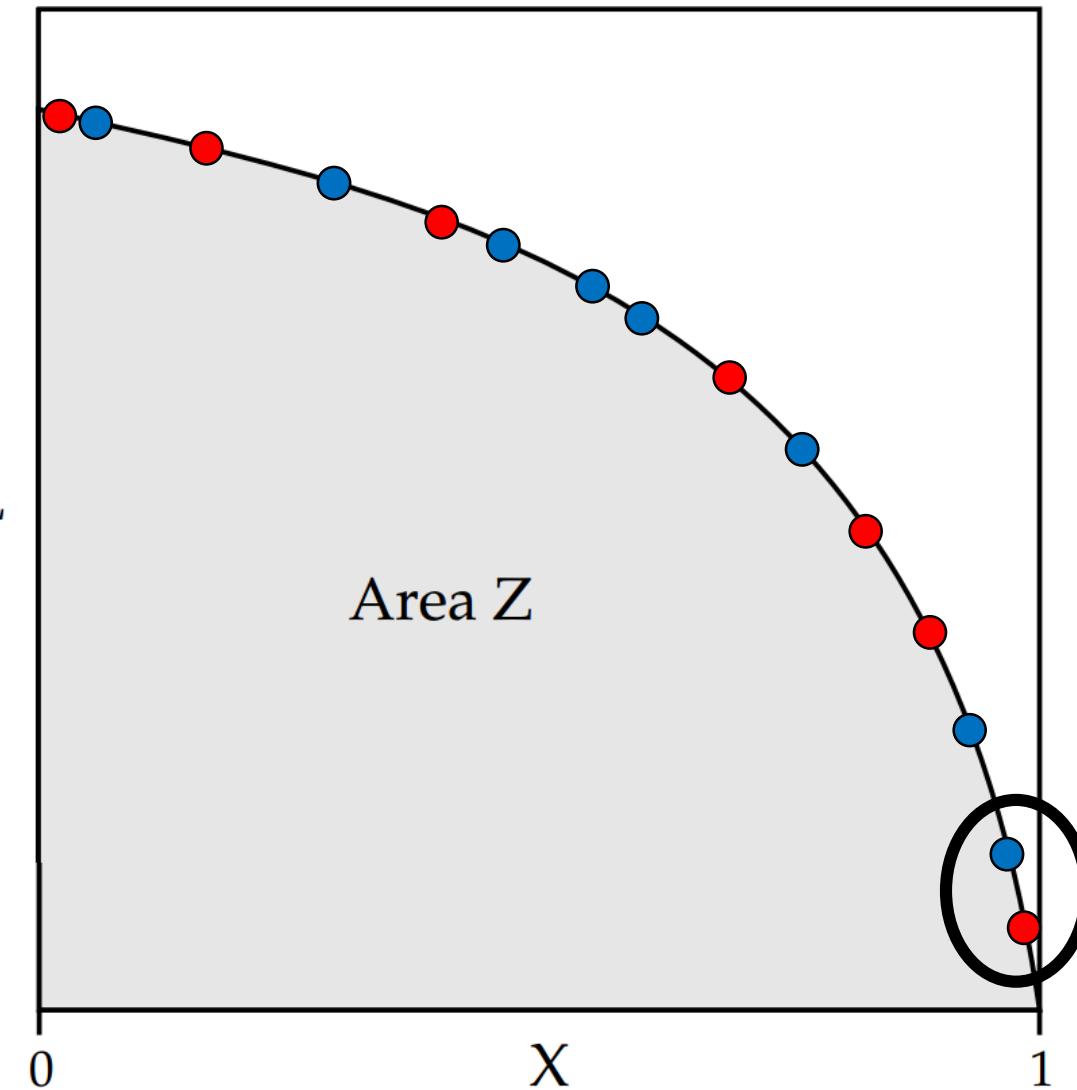
Skilling (2006)



Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

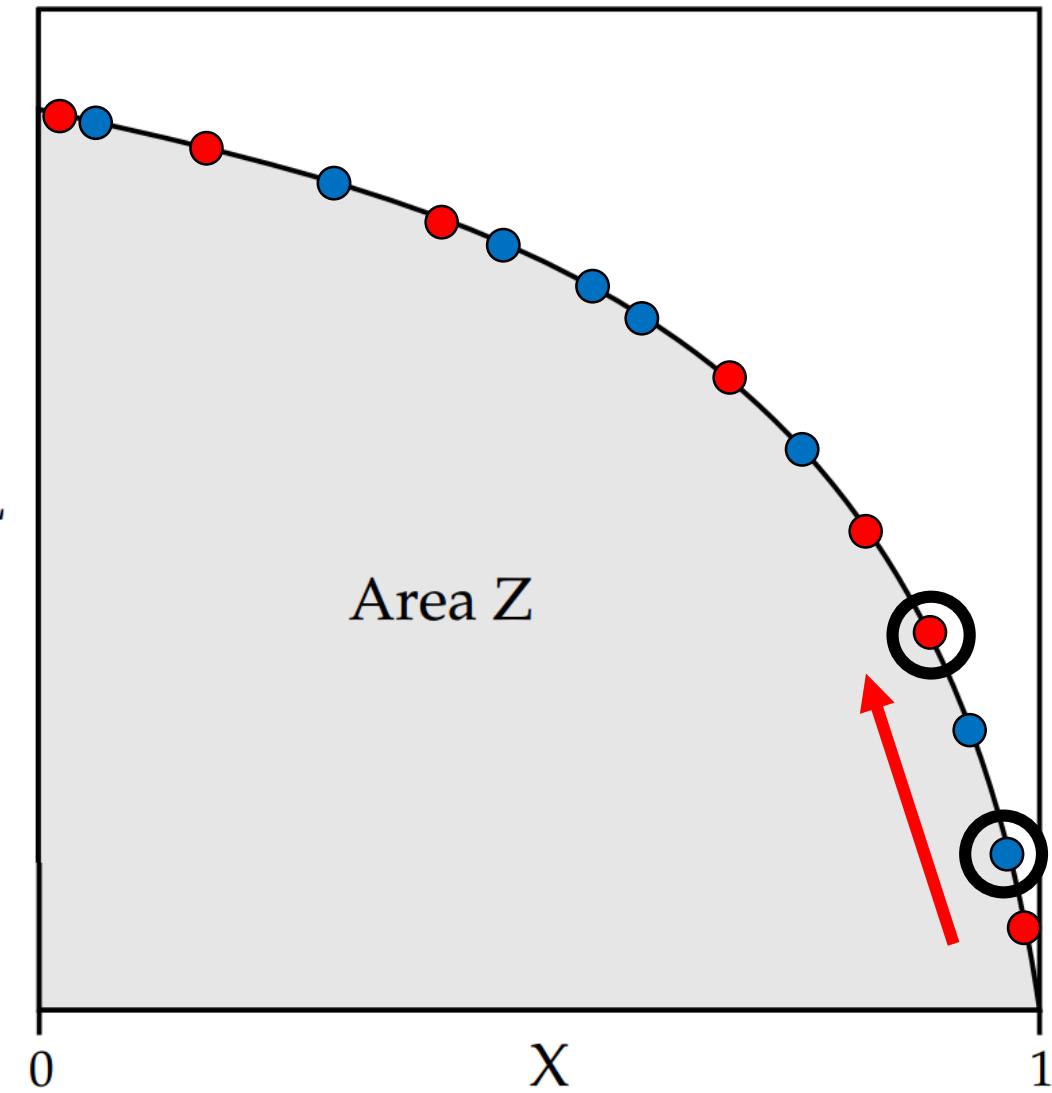
Skilling (2006)



Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

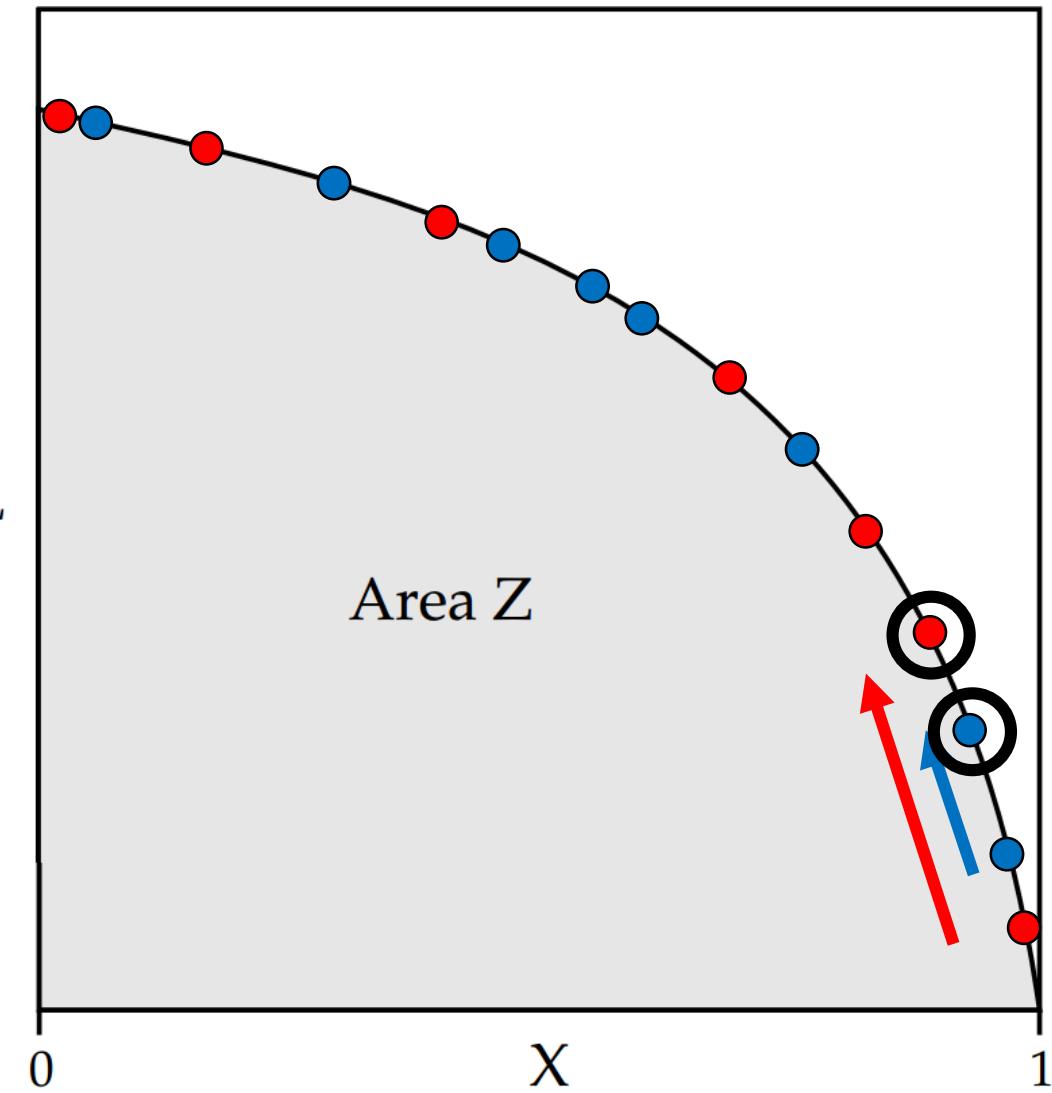
Skilling (2006)



Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

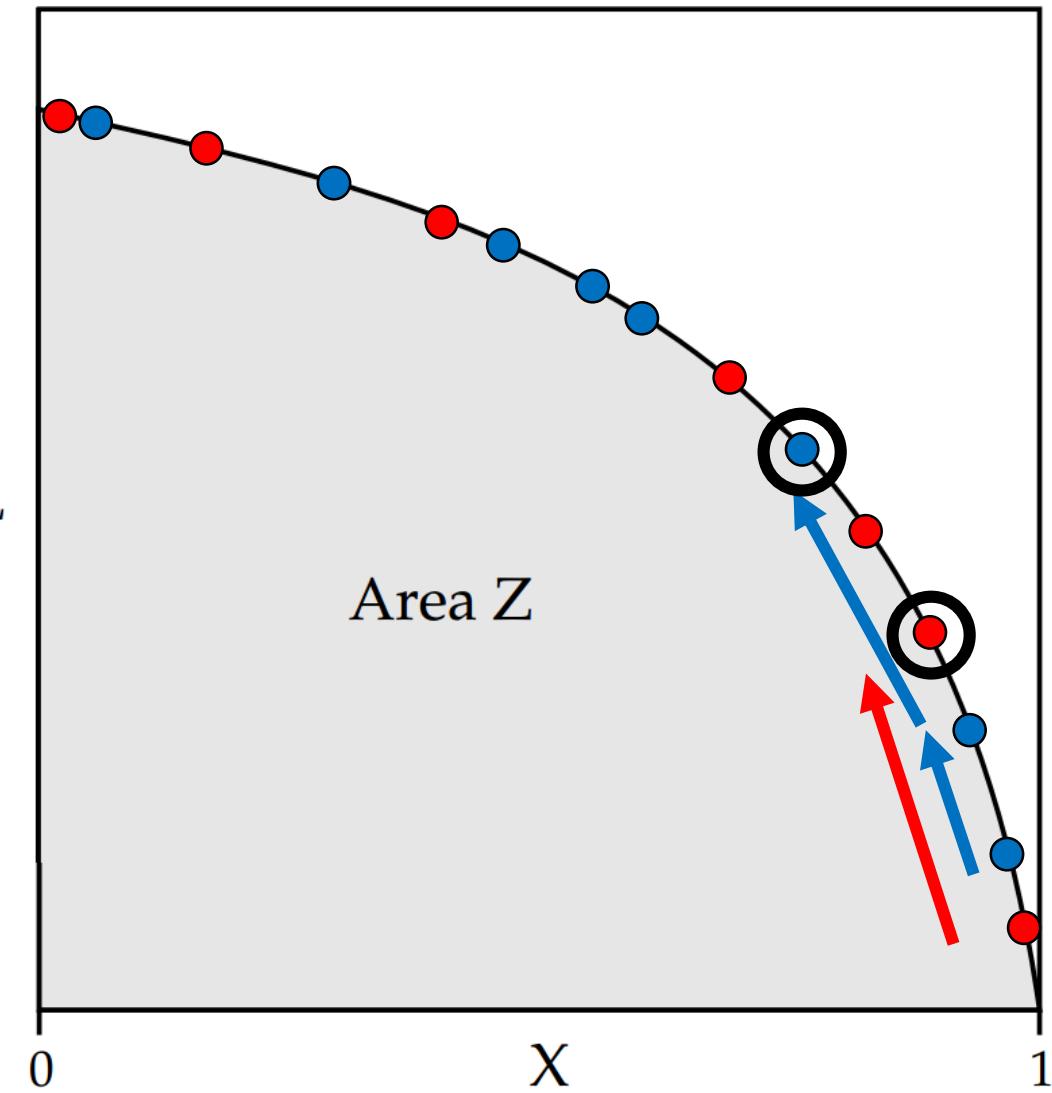
Skilling (2006)



Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

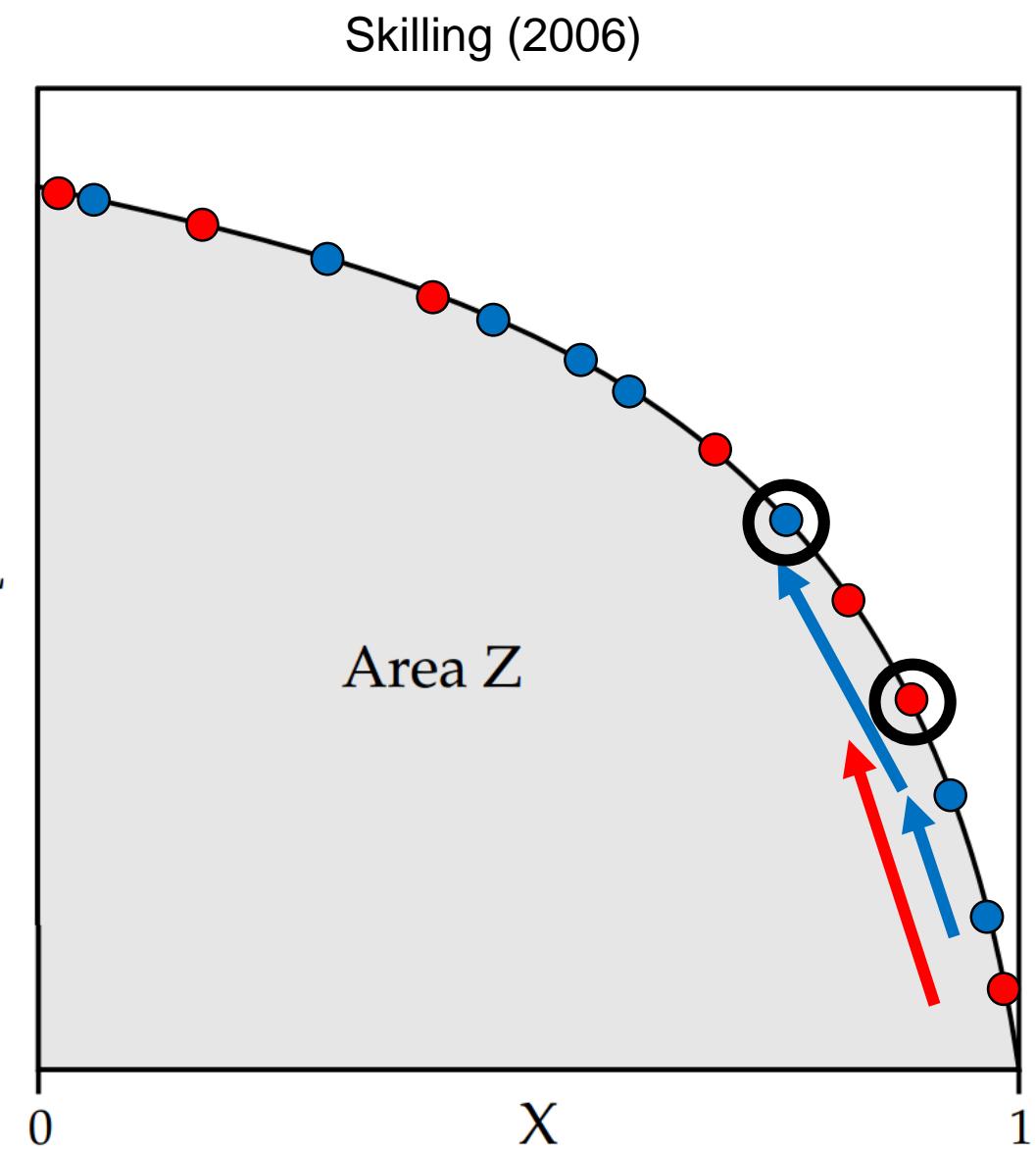
Skilling (2006)



Adding More Particles

$U_0, \dots, U_i \sim \text{Unif}$

$$\ln X_{i+1} = \sum_{j=0}^i \ln U_j$$



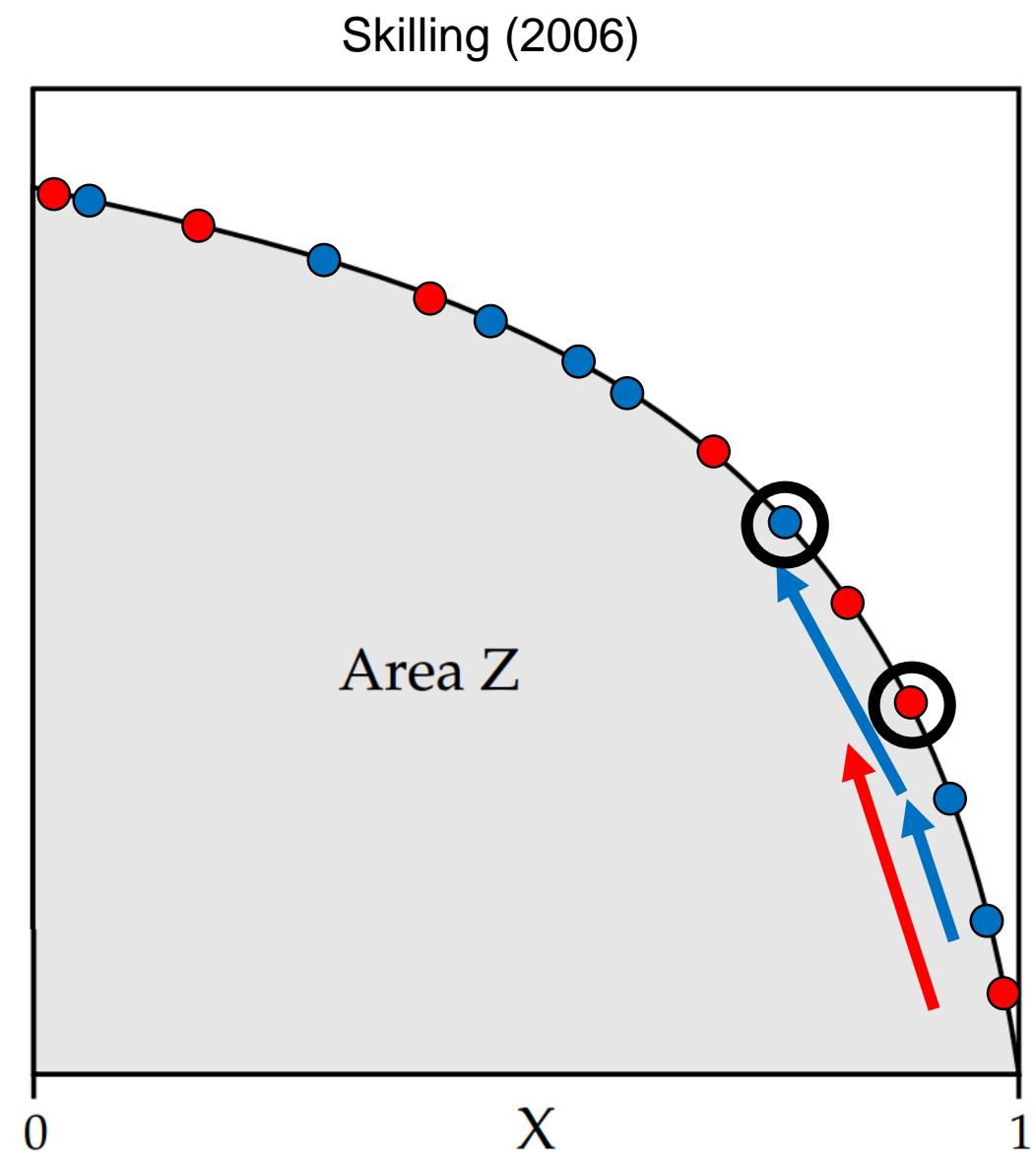
Adding More Particles

$$T_0, \dots, T_i \sim U(2)$$

Order Statistics

$$U_1, U_2 \sim \text{Unif} \Rightarrow U_{(1)}, U_{(2)}$$

$$\ln X_{i+1} = \sum_{j=0}^i \ln T_j$$



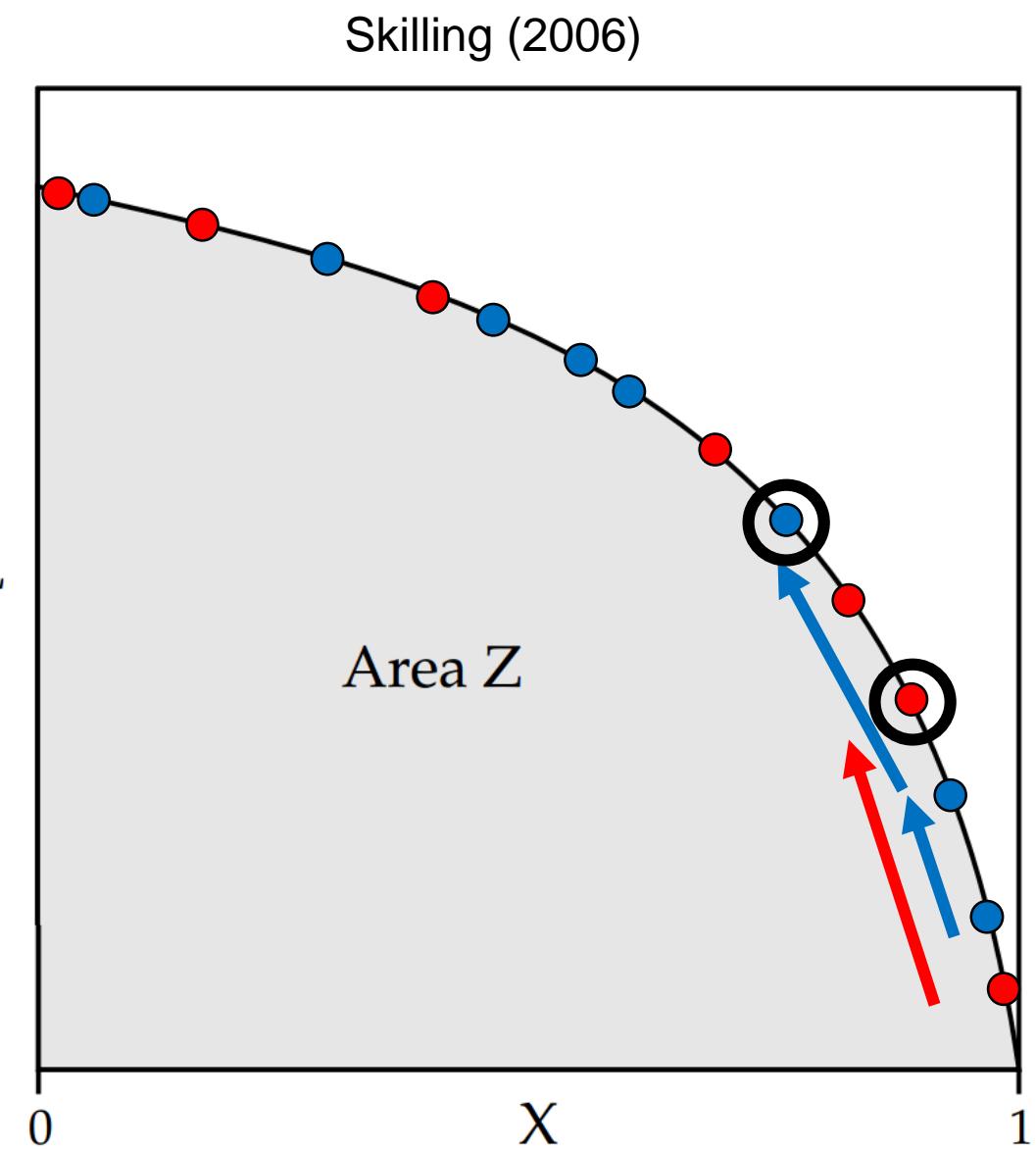
Adding More Particles

$$T_0, \dots, T_i \sim \text{Beta}(2,1)$$

Order Statistics

$$U_1, U_2 \sim \text{Unif} \Rightarrow U_{(1)}, U_{(2)}$$

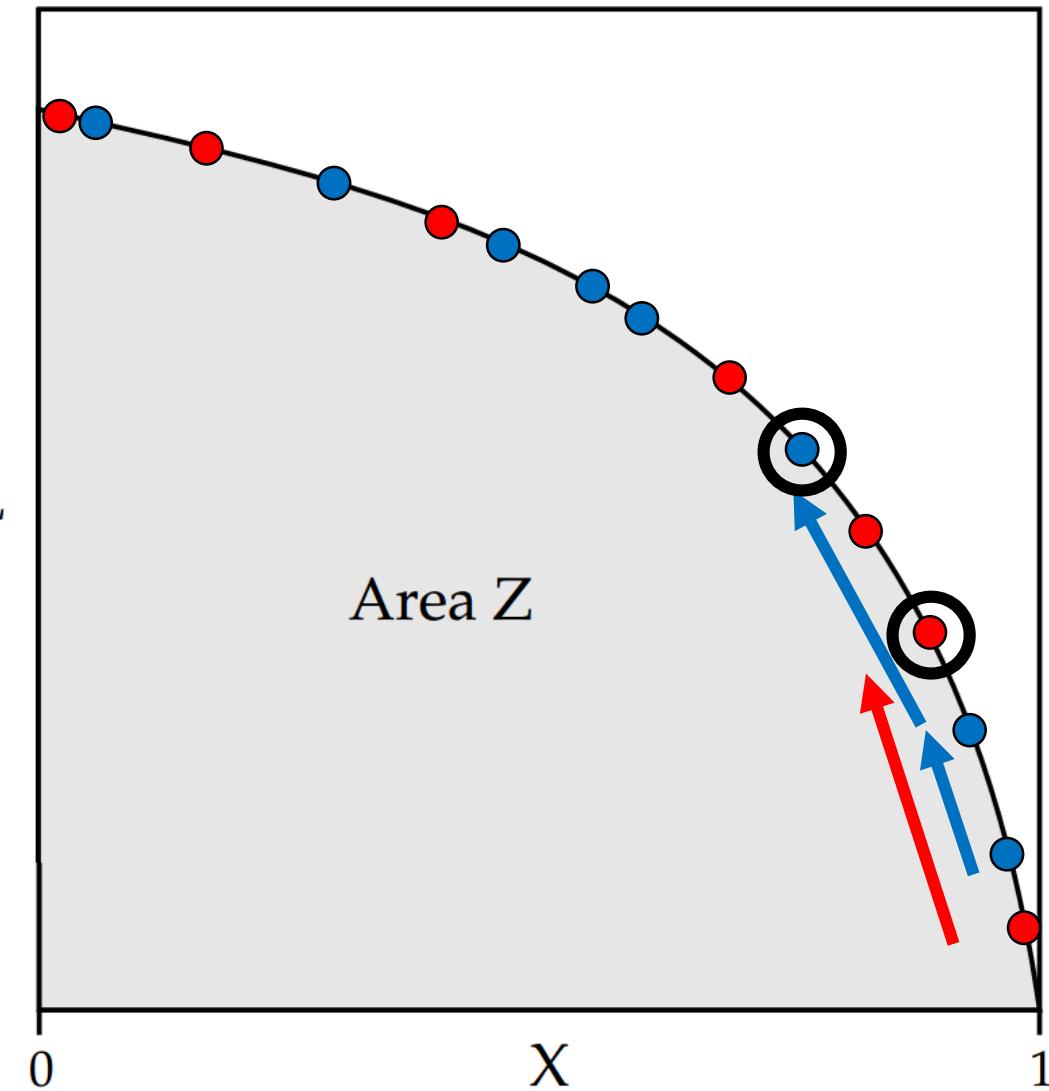
$$\ln X_{i+1} = \sum_{j=0}^i \ln T_j$$



Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

Skilling (2006)

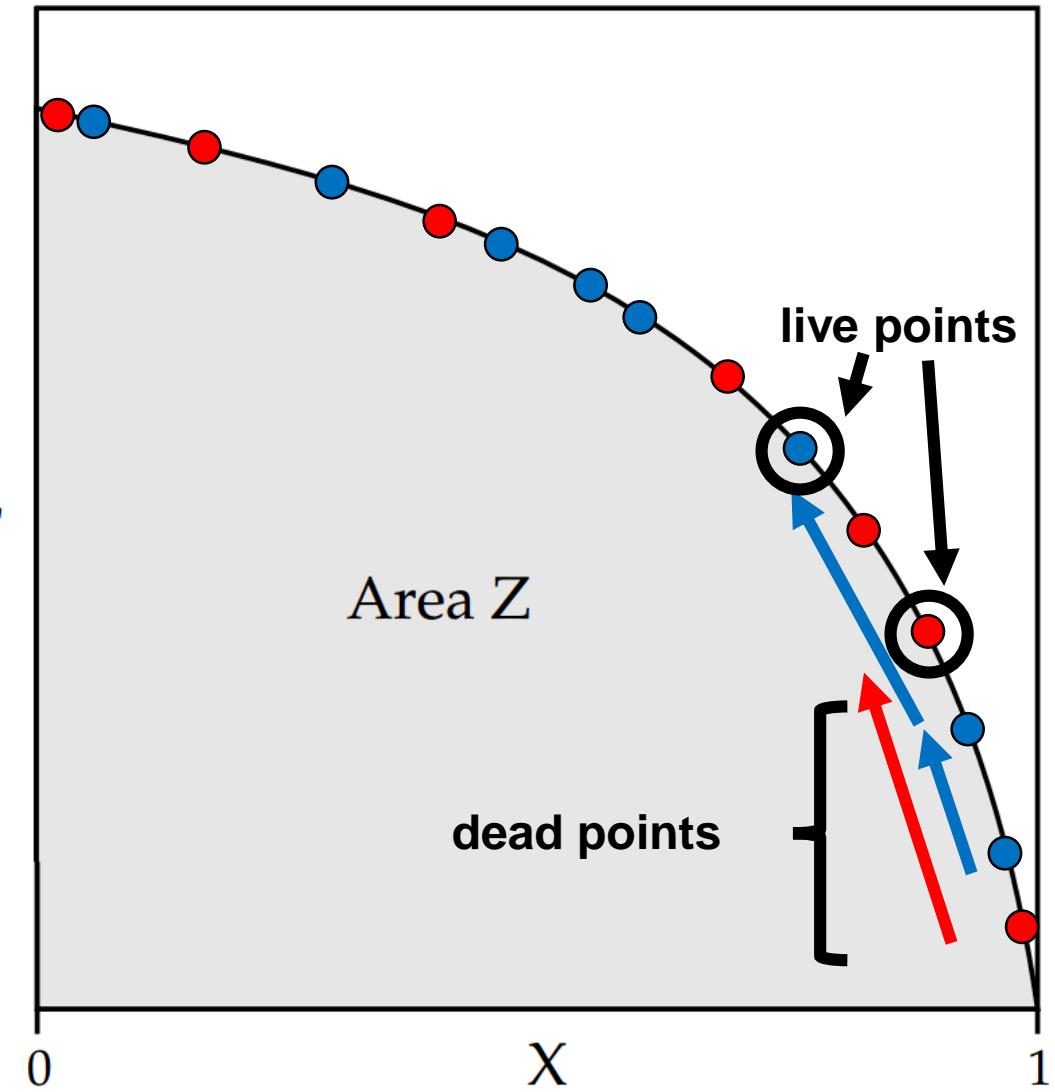


Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

One run with 2 “live points”
= 2 runs with 1 live point

Skilling (2006)

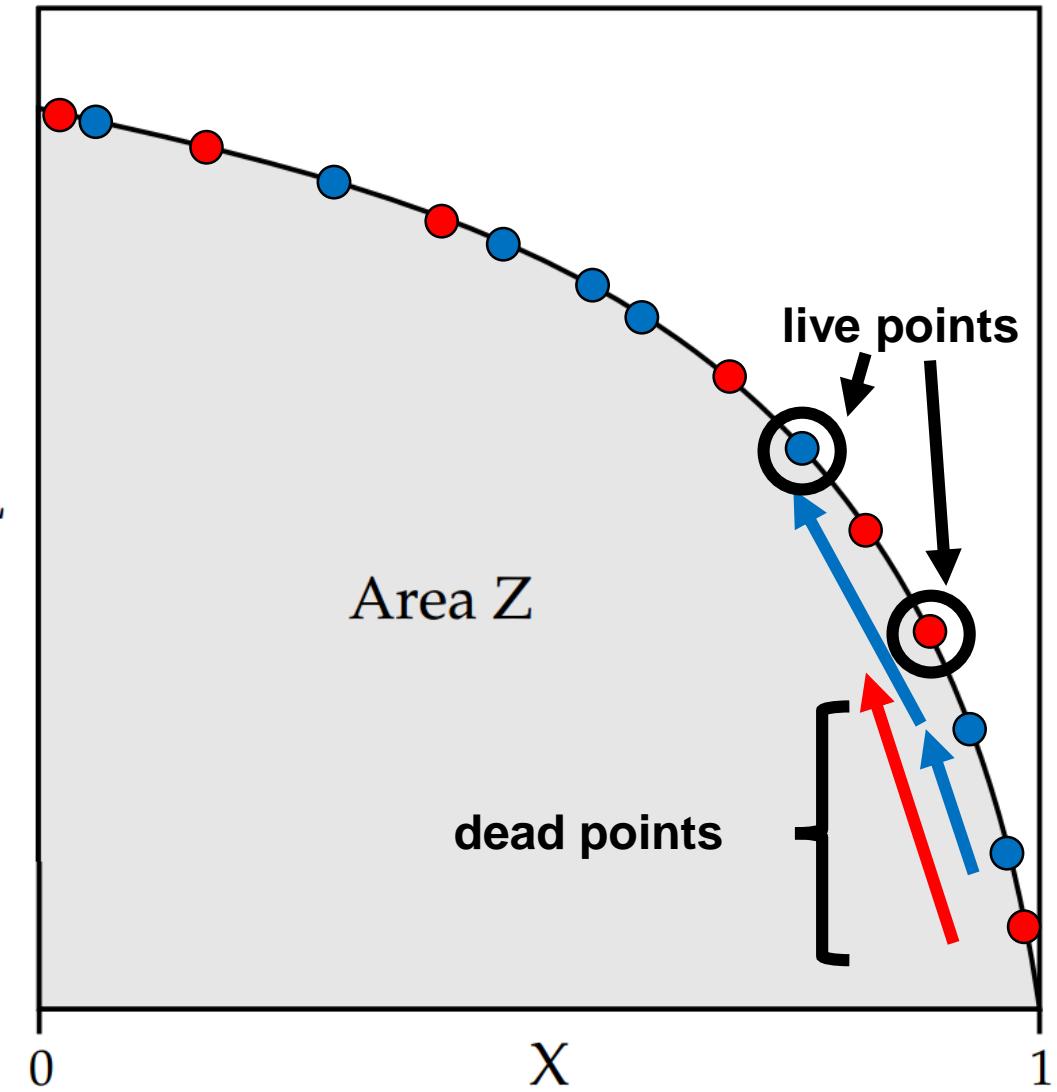


Adding More Particles

$$\begin{aligned}\mathcal{L}_{N_1}^{(1)} &> \mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(1)} \\ &> \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > \mathcal{L}_1^{(1)} > 0\end{aligned}$$

One run with K “live points”
= K runs with 1 live point

Skilling (2006)



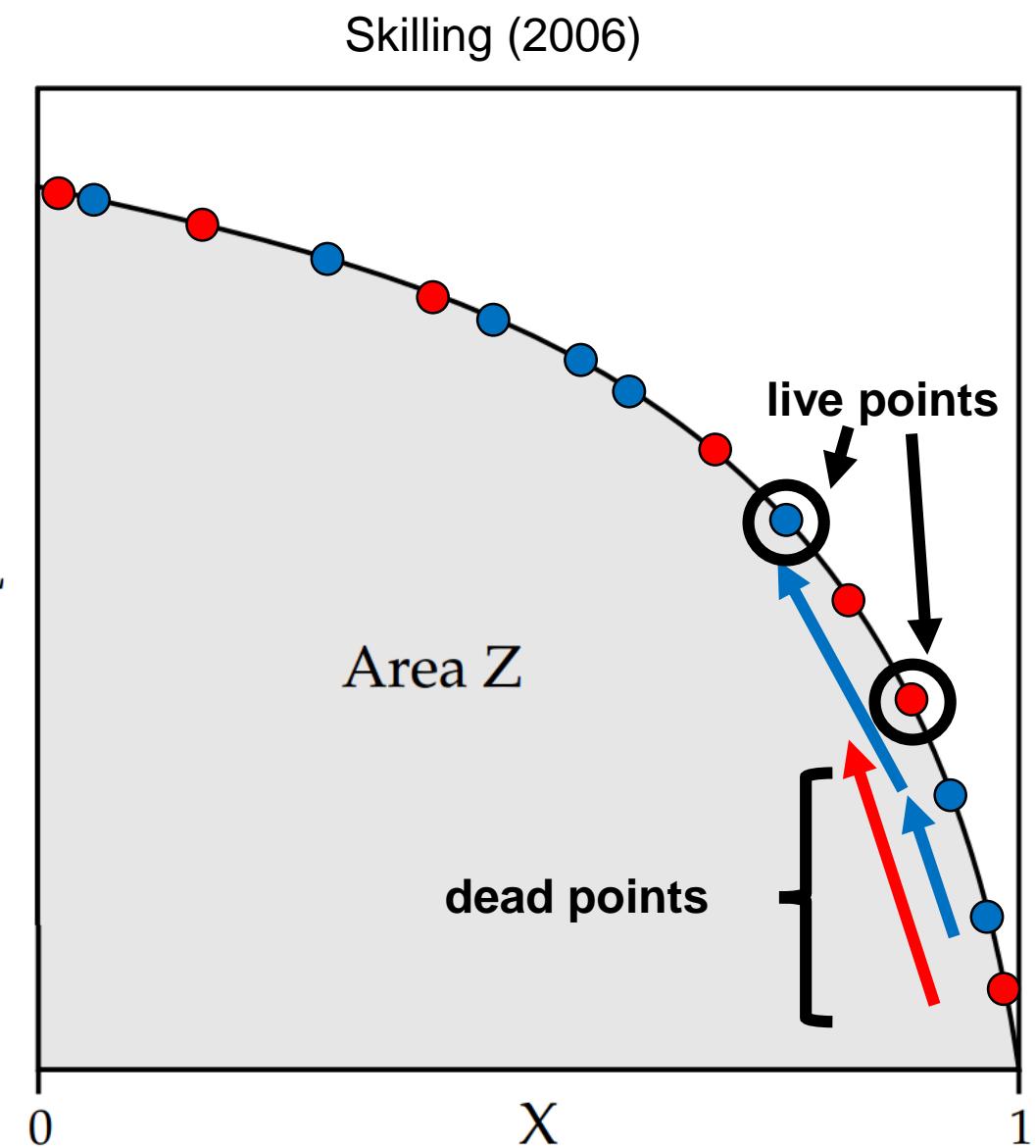
Adding More Particles

$$T_0, \dots, T_i \sim \text{Beta}(2,1)$$

Order Statistics

$$T_1, T_2 \sim \text{Unif} \Rightarrow U_{(1)}, U_{(2)}$$

$$\ln \mathbb{E}[X_{i+1}] = \sum_{j=0}^i \ln \mathbb{E}[T_j]$$



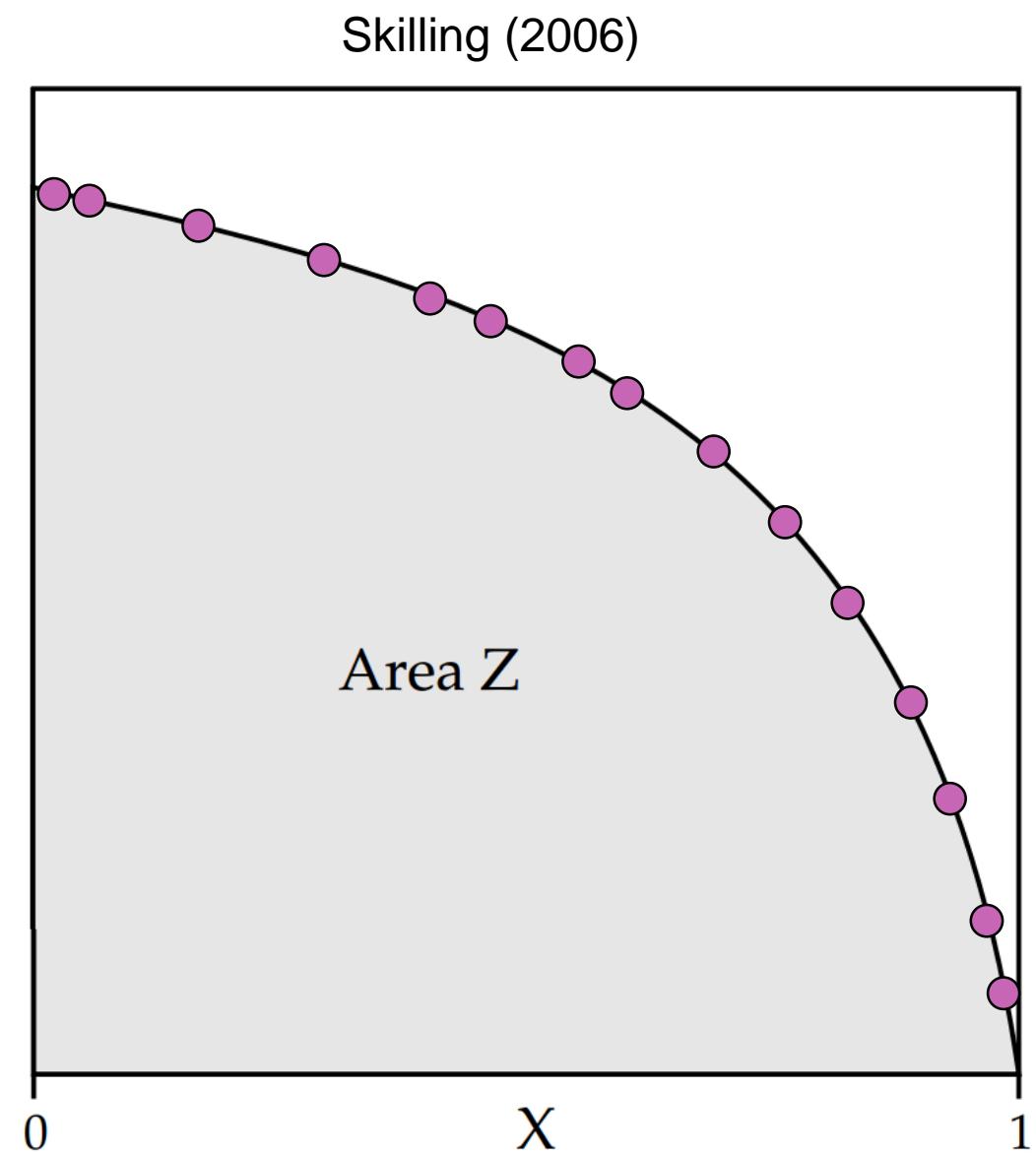
Adding More Particles

$$T_0, \dots, T_i \sim \text{Beta}(K, 1)$$

Order Statistics

$$U_1, \dots, U_K \sim \text{Unif} \Rightarrow U_{(1)}, \dots, U_{(K)}$$

$$\ln \mathbb{E}[X_{i+1}] = \sum_{j=0}^i \ln \mathbb{E}[T_j]$$



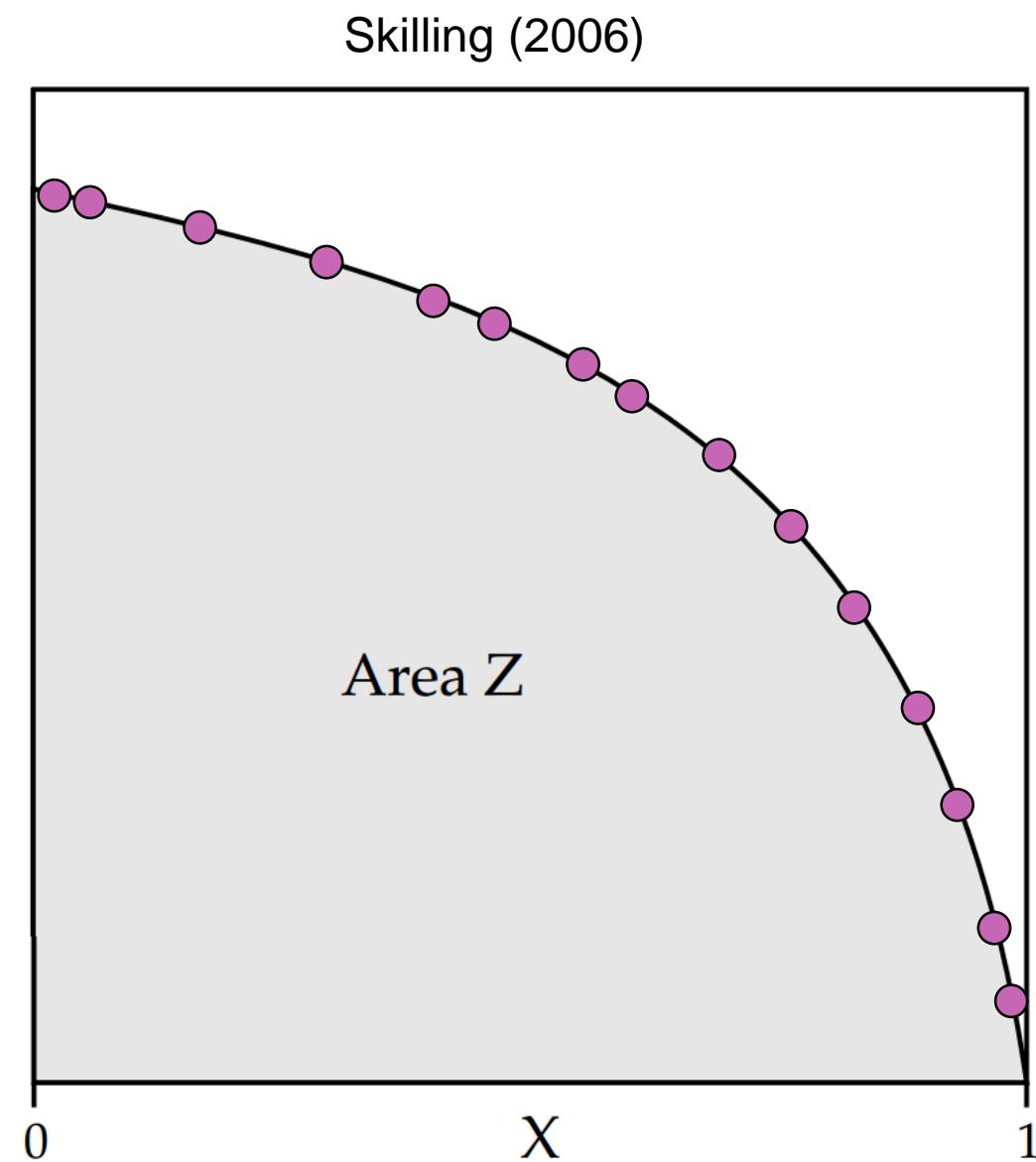
Adding More Particles

$$T_0, \dots, T_i \sim \text{Beta}(K, 1)$$

Order Statistics

$$U_1, \dots, U_K \sim \text{Unif} \Rightarrow U_{(1)}, \dots, U_{(K)}$$

$$\ln \mathbb{E}[X_{i+1}] = \sum_{j=0}^i \ln \left(\frac{K}{K+1} \right)$$



Stopping Criteria

$$\hat{Z} = \hat{Z}_i + Z_{\text{in}}$$

Stopping Criteria

$$\frac{\hat{z}_i}{\hat{z}_i + z_{in}} > f$$

Stopping Criteria

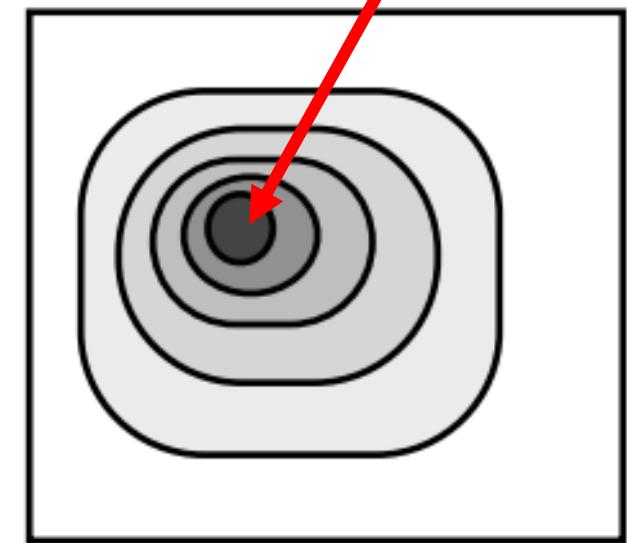
$$\hat{Z} = \sum_{j=1}^i \hat{w}_j + Z_{\text{in}}$$

Stopping Criteria

$$\hat{Z} \leq \sum_{j=1}^i \hat{w}_j + \mathcal{L}_{(K)} X_n$$

Maximum Likelihood

Uniform slab

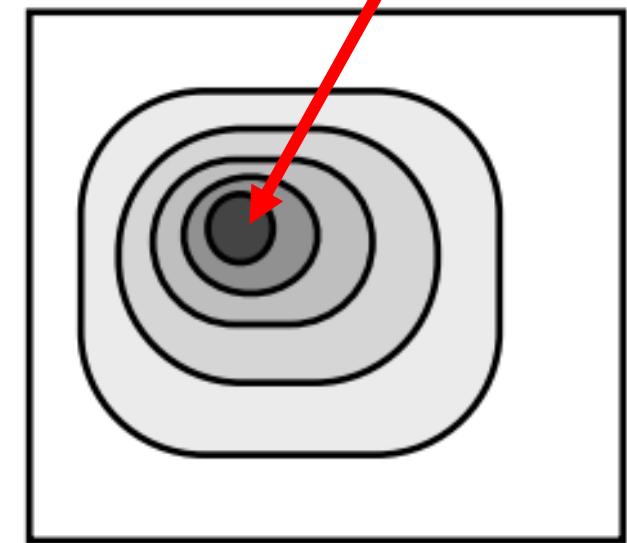


Stopping Criteria

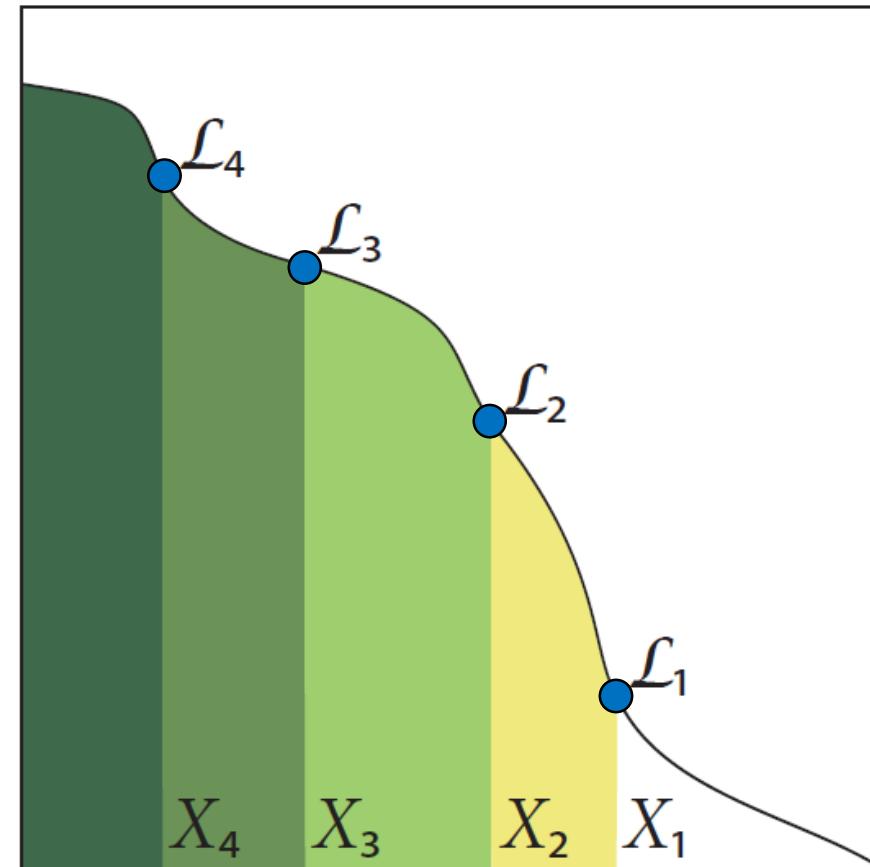
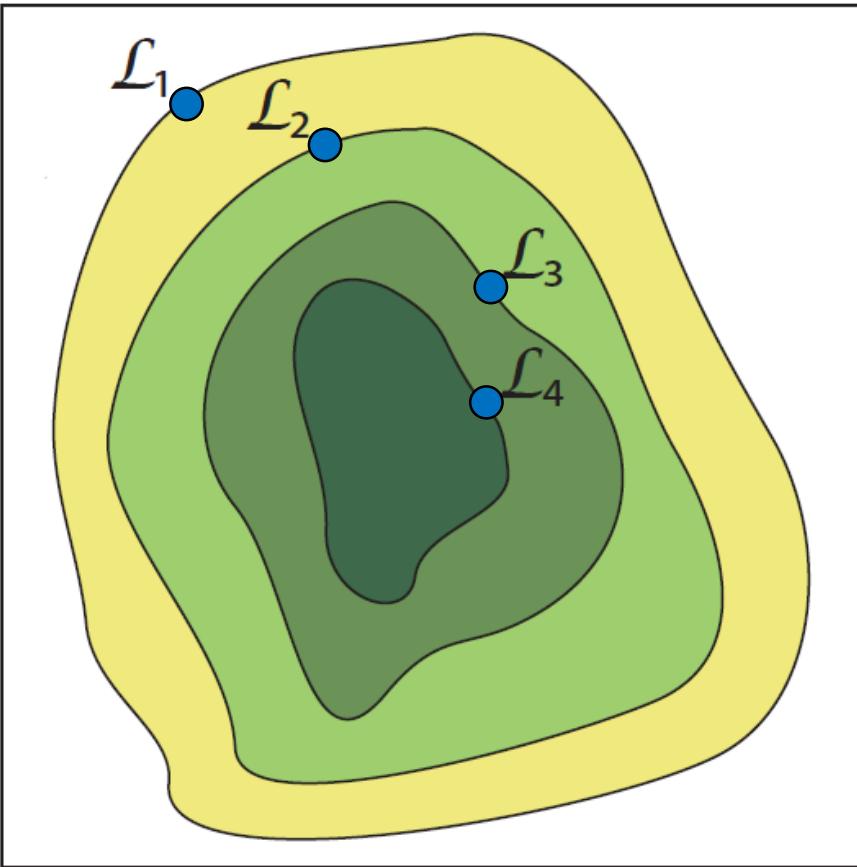
$$\hat{Z} \lesssim \sum_{j=1}^i \hat{w}_j + \mathcal{L}_{(K)} \hat{X}_n$$

Maximum Likelihood

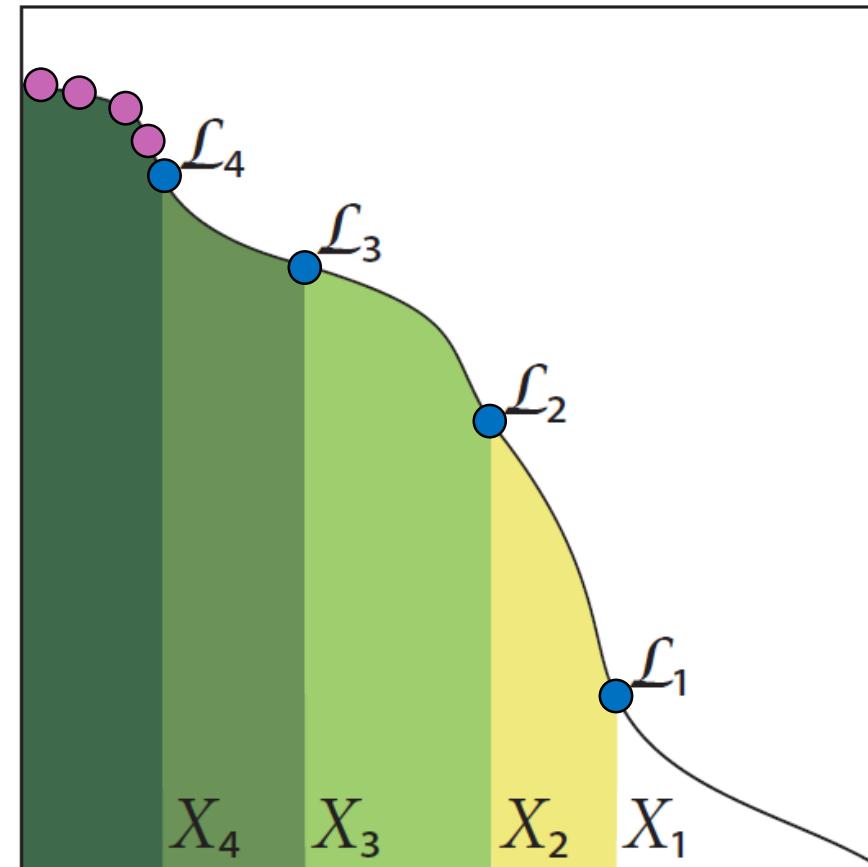
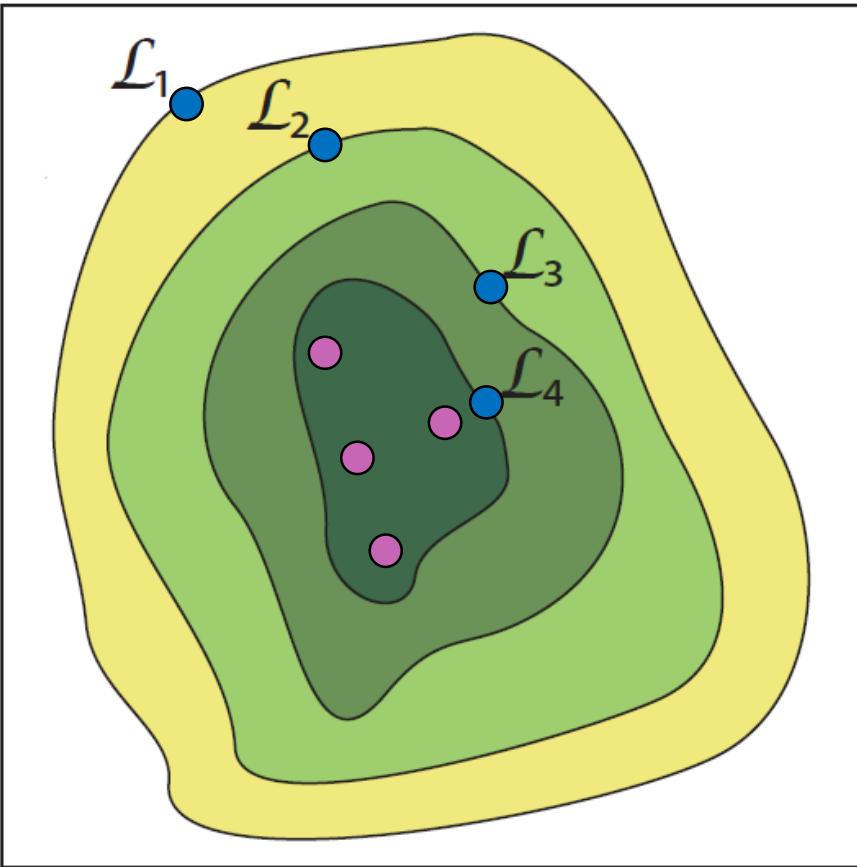
Uniform slab



“Recycling” the Final Set of Particles



“Recycling” the Final Set of Particles



“Recycling” the Final Set of Particles

$$\dots, \chi_{N+1}^{[k]}, \dots \sim U_k X_N \quad U_1, \dots, U_K \sim \text{Unif}$$

“Recycling” the Final Set of Particles

$$\dots, \chi_{N+1}^{[k]}, \dots \sim U_k X_N \quad U_1, \dots, U_K \sim \text{Unif}$$

$$\mathcal{L}_N > \mathcal{L}_{N-1} > \dots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

“Recycling” the Final Set of Particles

$$\dots, \chi_{N+1}^{[k]}, \dots \sim U_k X_N \quad U_1, \dots, U_K \sim \text{Unif}$$

$$\mathcal{L}_{N+K} > \dots > \mathcal{L}_{N+1} > \mathcal{L}_N > \mathcal{L}_{N-1} > \dots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

“Recycling” the Final Set of Particles

$$\dots, \chi_{N+1}^{[k]}, \dots \sim U_k X_N \quad U_1, \dots, U_K \sim \text{Unif}$$

$$\mathcal{L}_{N+K} > \dots > \mathcal{L}_{N+1} > \mathcal{L}_N > \mathcal{L}_{N-1} > \dots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

$$X_{N+k} = \chi_{N+1}^{(K-k+1)}$$

“Recycling” the Final Set of Particles

$$U_1, \dots, U_K \sim \text{Unif}$$
$$\dots, X_{N+k}, \dots \sim U_{(K-k+1)} X_N$$

$$\mathcal{L}_{N+K} > \dots > \mathcal{L}_{N+1} > \mathcal{L}_N > \mathcal{L}_{N-1} > \dots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

$$X_{N+k} = \chi_{N+1}^{(K-k+1)}$$

“Recycling” the Final Set of Particles

$$U_1, \dots, U_K \sim \text{Unif}$$
$$\dots, X_{N+k}, \dots \sim U_{(K-k+1)} X_N$$

$$\mathcal{L}_{N+K} > \dots > \mathcal{L}_{N+1} > \mathcal{L}_N > \mathcal{L}_{N-1} > \dots > \mathcal{L}_2 > \mathcal{L}_1 > 0$$

$$X_{N+k} = \chi_{N+1}^{(K-k+1)}$$

Rényi Representation

“Recycling” the Final Set of Particles

$$\ln \mathbb{E}[X_N] = \sum_{i=1}^N \ln\left(\frac{K}{K+1}\right)$$

“Recycling” the Final Set of Particles

$$\ln \mathbb{E}[X_{N+k}] = \sum_{i=1}^N \ln\left(\frac{K}{K+1}\right) + \ln\left(\frac{K-k+1}{K+1}\right)$$

“Recycling” the Final Set of Particles

$$\ln \mathbb{E}[X_{N+k}] = \sum_{i=1}^N \ln\left(\frac{K}{K+1}\right) + \sum_{j=1}^k \ln\left(\frac{K-j+1}{K-j+2}\right)$$

“Recycling” the Final Set of Particles

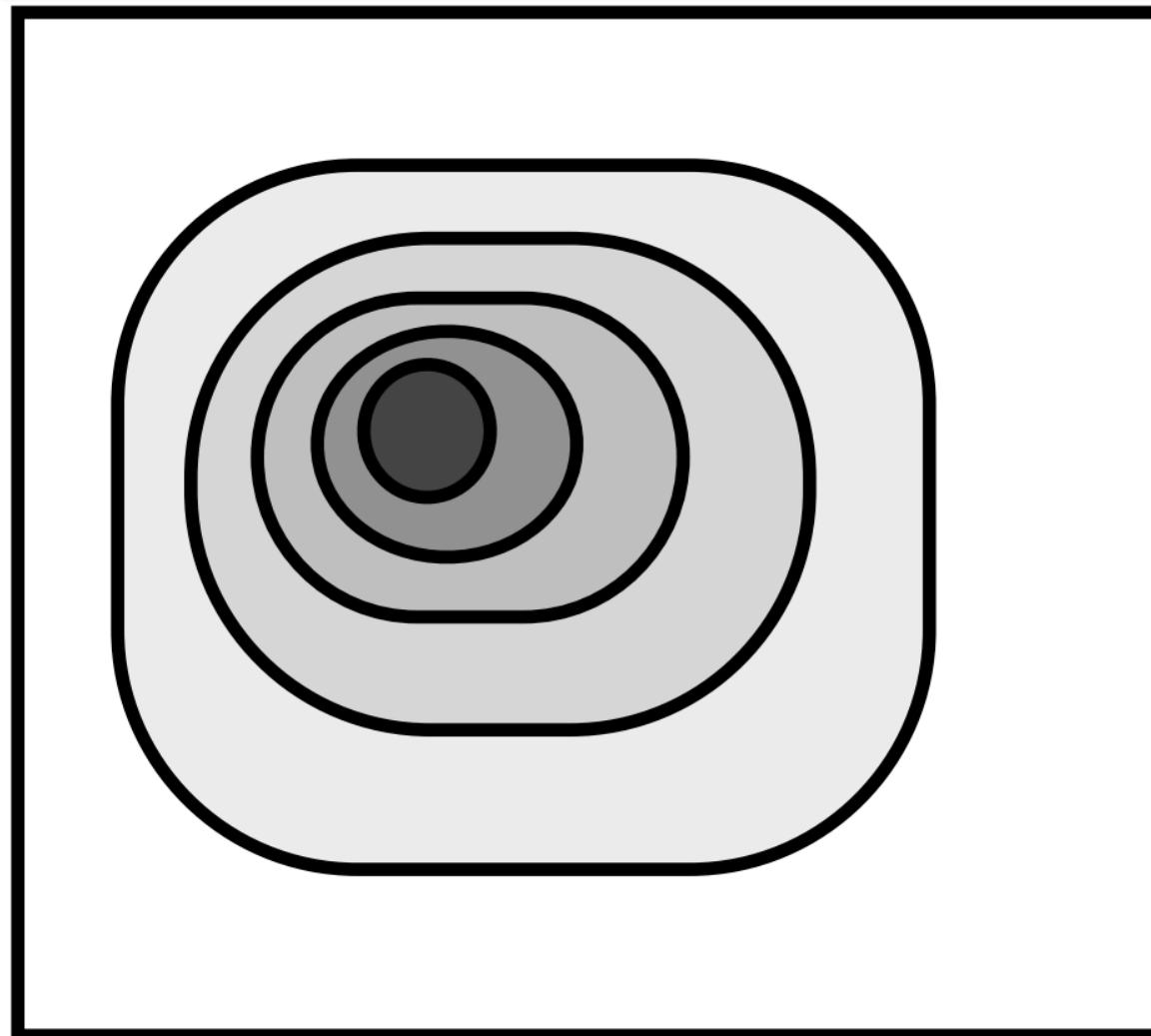
$$\ln \mathbb{E}[X_{N+k}] = \sum_{i=1}^N \ln \left(\frac{K}{K+1} \right) + \sum_{j=1}^k \ln \left(\frac{K-j+1}{K-j+2} \right)$$

Exponential Shrinkage Uniform Shrinkage

Nested Sampling Errors

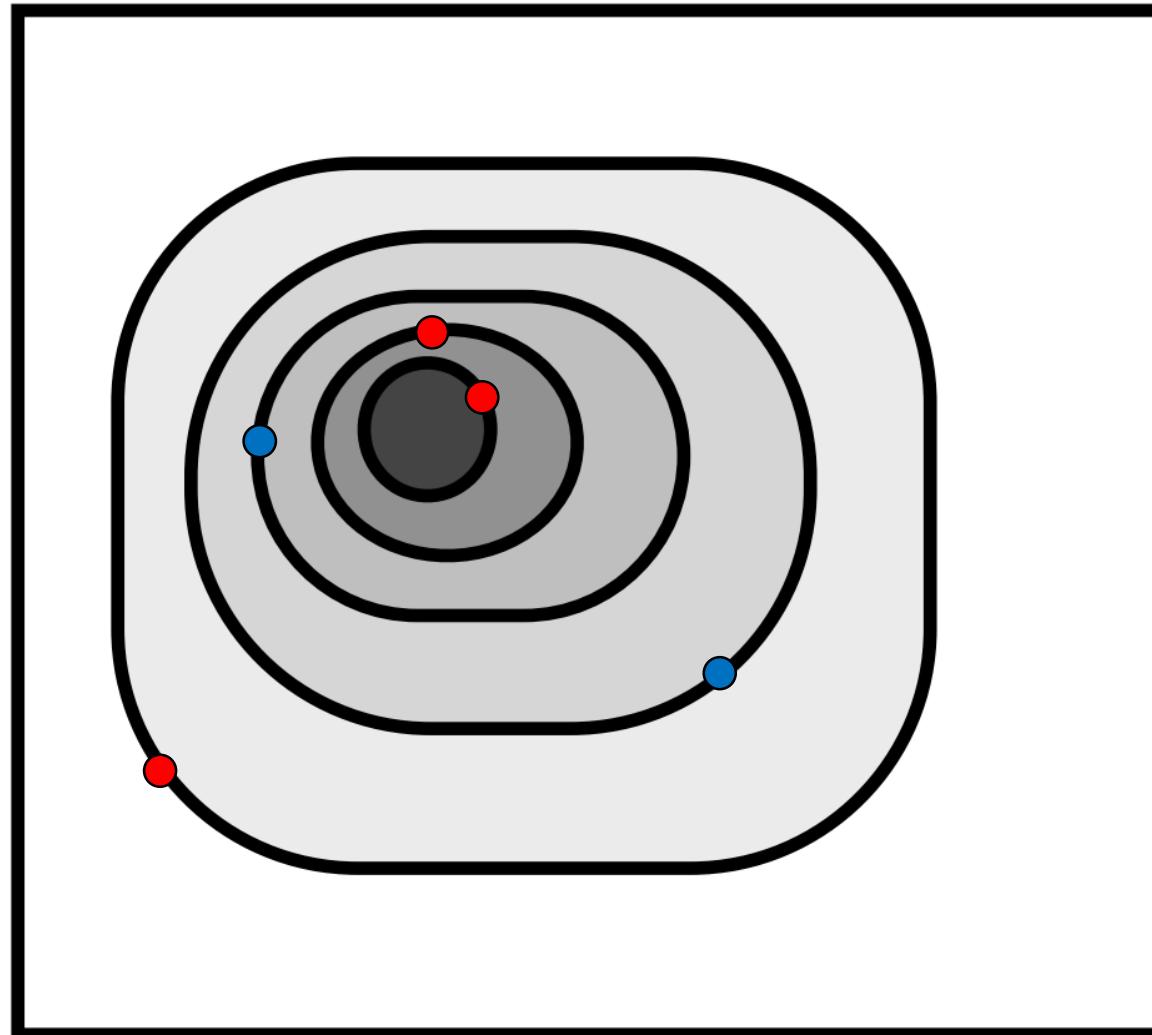
Pictures from [this 2010 talk](#) by Skilling.

Nested Sampling Uncertainties



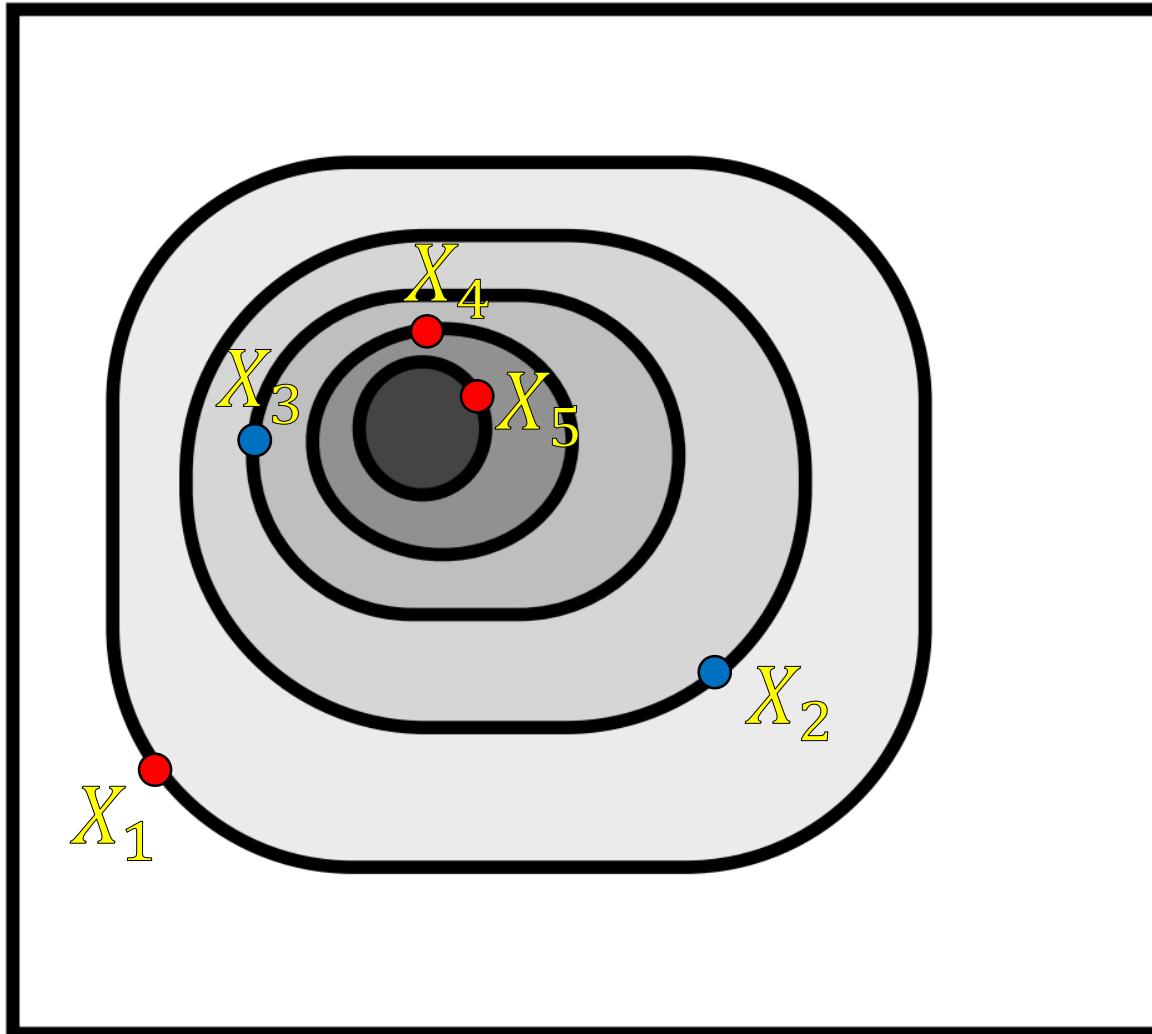
Pictures from [this 2010 talk](#) by Skilling.

Nested Sampling Uncertainties



Pictures from [this 2010 talk](#) by Skilling.

Nested Sampling Uncertainties



Statistical
uncertainties

- Unknown prior
volumes

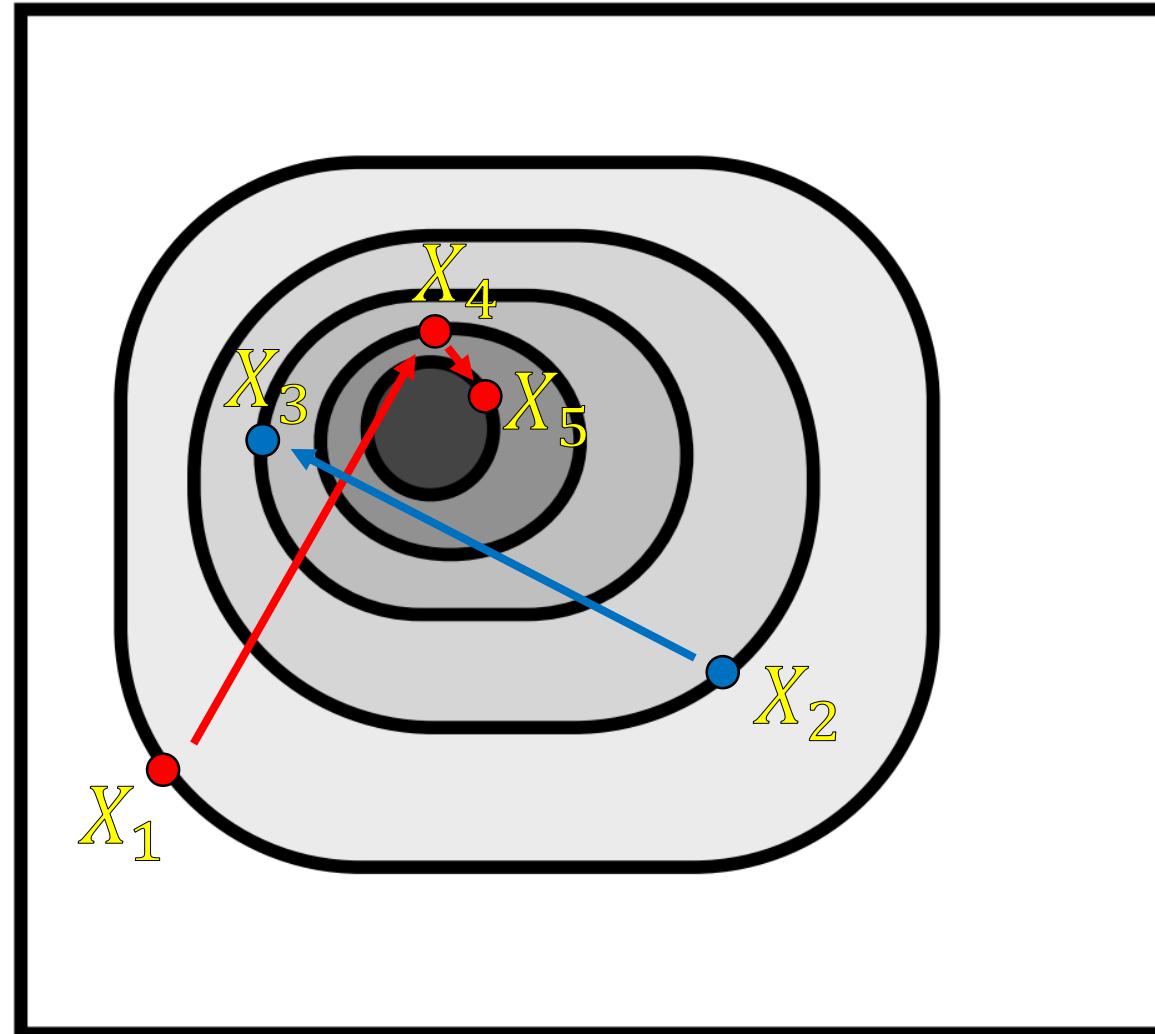
Nested Sampling Uncertainties

Sampling uncertainties

- Number of samples (counting)
- Discrete point estimates for contours
- Particle path dependencies

Statistical uncertainties

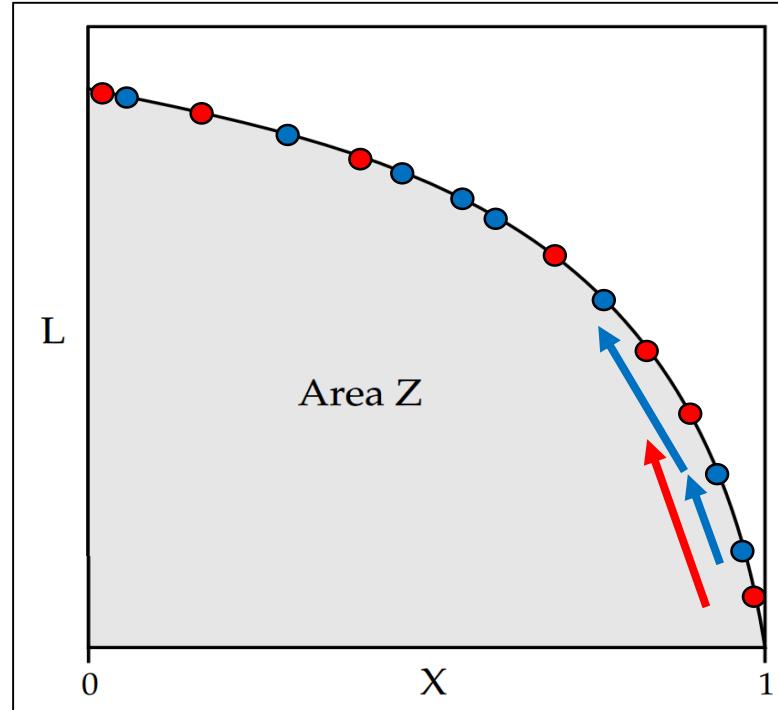
- Unknown prior volumes



Sampling Error: Poisson Uncertainties

“Distance” from prior to posterior

$$\mathbb{V}[N] = \mathbb{E}[N] \sim \frac{? ? ?}{\mathbb{E}[\Delta \ln X]}$$



Based on Skilling (2006)
and Keeton (2011)

Sampling Error: Poisson Uncertainties

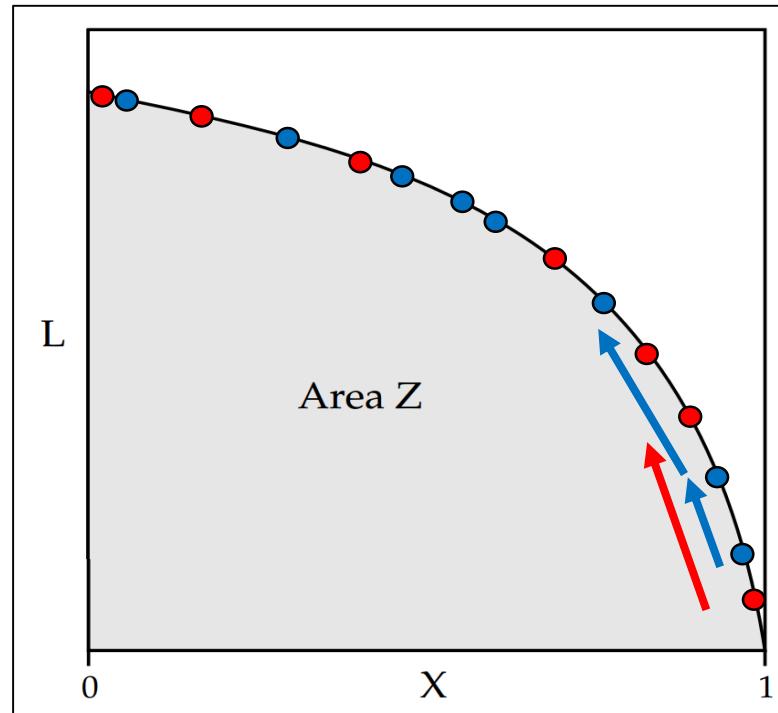
Kullback-Leibler divergence from

π to $p \rightarrow$ “information gained”.

$$H(\pi|p) \equiv \int_{\Omega_{\Theta}} p(\Theta) \ln \frac{p(\Theta)}{\pi(\Theta)} d\Theta$$

Sampling Error: Poisson Uncertainties

$$\text{V}[N] = \mathbb{E}[N] \sim \frac{H(\pi|p)}{\mathbb{E}[\Delta \ln X]}$$



Based on Skilling (2006)
and Keeton (2011)

Sampling Error: Poisson Uncertainties

$$\mathbb{V}[N] = \mathbb{E}[N] \sim \frac{H(\pi|p)}{\mathbb{E}[\Delta \ln X]}$$

$$\mathbb{V}[\ln \hat{\mathcal{Z}}]$$

Sampling Error: Poisson Uncertainties

$$\mathbb{V}[N] = \mathbb{E}[N] \sim \frac{H(\pi|p)}{\mathbb{E}[\Delta \ln X]}$$

$$\mathbb{V}[\ln \hat{\mathcal{Z}}] \sim \mathbb{V}[\ln \hat{X}_H]$$

Sampling Error: Poisson Uncertainties

$$\mathbb{V}[N] = \mathbb{E}[N] \sim \frac{H(\pi|p)}{\mathbb{E}[\Delta \ln X]}$$

$$\mathbb{V}[\ln \hat{\mathcal{Z}}] \sim \mathbb{V}[\ln \hat{X}_H] \sim (\sigma[N] \mathbb{E}[\Delta \ln X])^2$$

Sampling Error: Poisson Uncertainties

$$\mathbb{V}[N] = \mathbb{E}[N] \sim \frac{H(\pi|p)}{\mathbb{E}[\Delta \ln X]}$$

$$\begin{aligned}\mathbb{V}[\ln \hat{\mathcal{Z}}] &\sim \mathbb{V}[\ln \hat{X}_H] \sim (\sigma[N] \mathbb{E}[\Delta \ln X])^2 \\ &\sim H(\pi|p) \mathbb{E}[\Delta \ln X]\end{aligned}$$

Sampling Error: Poisson Uncertainties

$$\mathbb{V}[N] = \mathbb{E}[N] \sim \frac{H(\pi|p)}{\mathbb{E}[\Delta \ln X]}$$

$$\begin{aligned}\mathbb{V}[\ln \hat{\mathcal{Z}}] &\sim \mathbb{V}[\ln \hat{X}_H] \sim (\sigma[N] \mathbb{E}[\Delta \ln X])^2 \\ &\sim \sum_{i=1}^{N+K} \Delta H_i \mathbb{E}[\Delta \ln X_i] \\ &= 1/K\end{aligned}$$

Based on Skilling (2006)
and Keeton (2011)

Sampling Error: Monte Carlo Noise

$$\mathbb{E}_p[f(\boldsymbol{\Theta})] = \int_{\Omega_{\boldsymbol{\Theta}}} f(\boldsymbol{\Theta}) p(\boldsymbol{\Theta}) d\boldsymbol{\Theta}$$

Formalism following Higson et al.
(2017) and Chopin and Robert (2010)

Sampling Error: Monte Carlo Noise

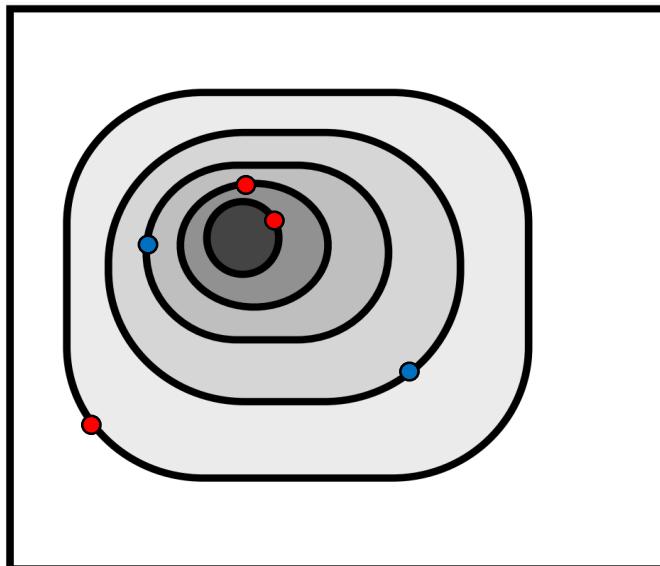
$$\mathbb{E}_p[f(\boldsymbol{\Theta})] = \int_{\Omega_{\boldsymbol{\Theta}}} f(\boldsymbol{\Theta}) p(\boldsymbol{\Theta}) d\boldsymbol{\Theta} = \frac{1}{Z} \int_0^1 \tilde{f}(X) \mathcal{L}(X) dX$$
$$\tilde{f}(X) = \mathbb{E}_{\pi}[f(\boldsymbol{\Theta}) | \mathcal{L}(\boldsymbol{\Theta}) = \mathcal{L}(X)]$$

Formalism following Higson et al.
(2017) and Chopin and Robert (2010)

Sampling Error: Monte Carlo Noise

$$\mathbb{E}_p[f(\boldsymbol{\Theta})] = \int_{\Omega_{\boldsymbol{\Theta}}} f(\boldsymbol{\Theta}) p(\boldsymbol{\Theta}) d\boldsymbol{\Theta} = \frac{1}{Z} \int_0^1 \tilde{f}(X) \mathcal{L}(X) dX$$

$$\tilde{f}(X) = \mathbb{E}_{\pi}[f(\boldsymbol{\Theta}) | \mathcal{L}(\boldsymbol{\Theta}) = \mathcal{L}(X)]$$

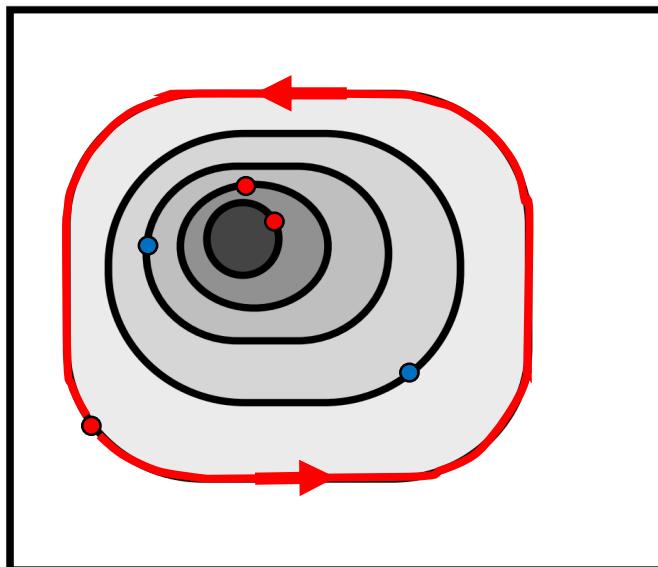


Formalism following Higson et al.
(2017) and Chopin and Robert (2010)

Sampling Error: Monte Carlo Noise

$$\mathbb{E}_p[f(\boldsymbol{\Theta})] = \int_{\Omega_{\boldsymbol{\Theta}}} f(\boldsymbol{\Theta}) p(\boldsymbol{\Theta}) d\boldsymbol{\Theta} = \frac{1}{Z} \int_0^1 \tilde{f}(X) \mathcal{L}(X) dX$$

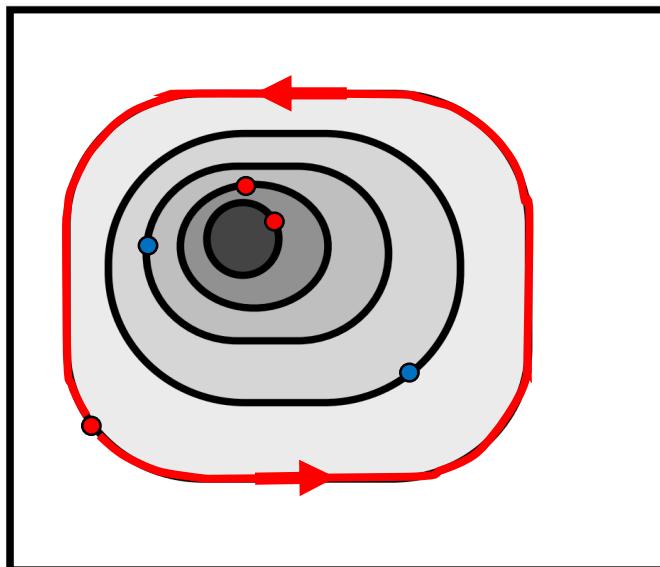
$$\tilde{f}(X) = \mathbb{E}_{\pi}[f(\boldsymbol{\Theta}) | \mathcal{L}(\boldsymbol{\Theta}) = \mathcal{L}(X)]$$



Formalism following Higson et al.
(2017) and Chopin and Robert (2010)

Sampling Error: Monte Carlo Noise

$$\mathbb{E}_p[f(\boldsymbol{\Theta})] = \int_{\Omega_{\boldsymbol{\Theta}}} f(\boldsymbol{\Theta}) p(\boldsymbol{\Theta}) d\boldsymbol{\Theta} = \frac{1}{Z} \int_0^1 \tilde{f}(X) \mathcal{L}(X) dX$$



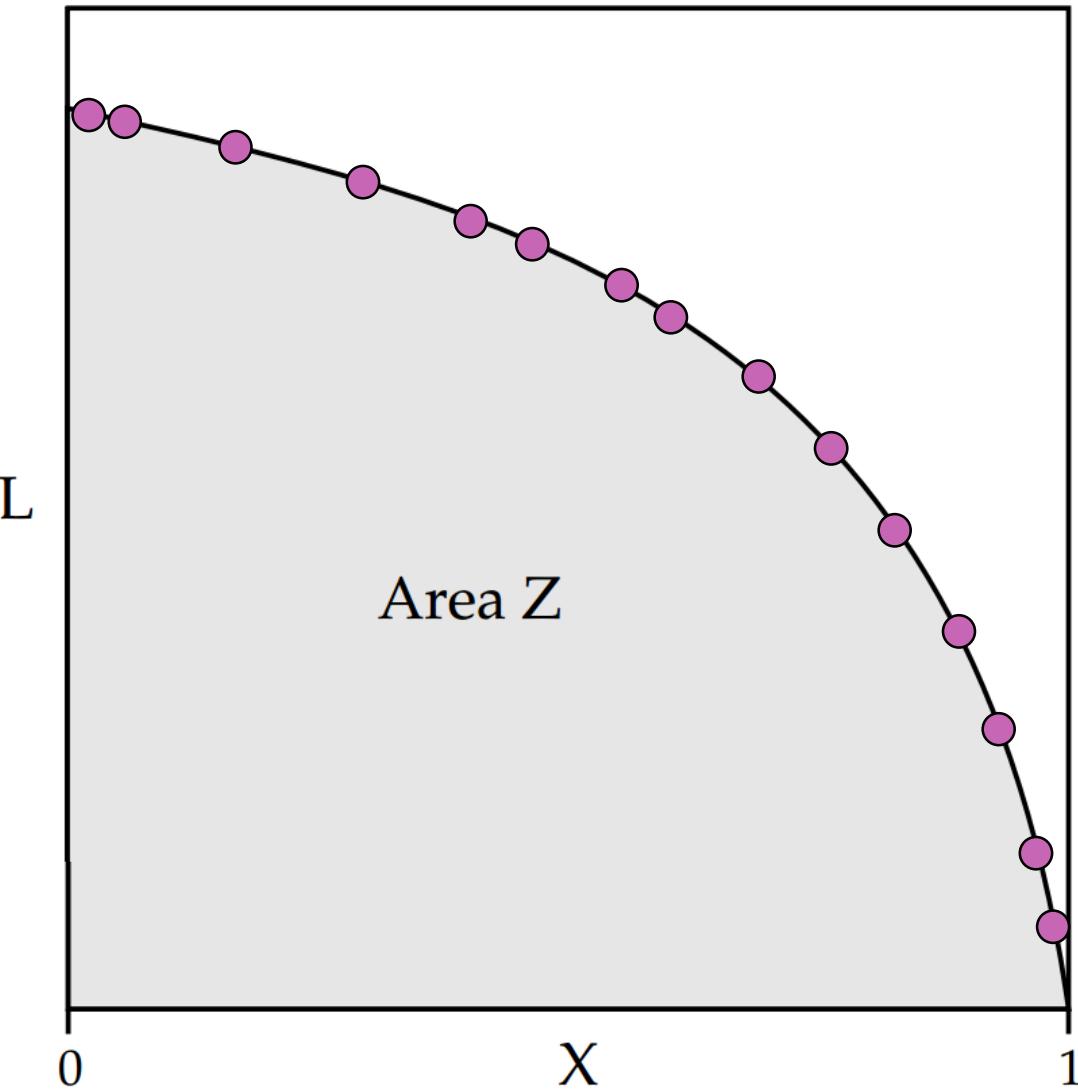
$$\approx \sum_{i=1}^{N+K} \hat{p}_i \tilde{f}(\boldsymbol{\Theta}_i)$$

Formalism following Higson et al.
(2017) and Chopin and Robert (2010)

Exploring Sampling Uncertainties

$$\begin{aligned}\mathcal{L}_N &> \mathcal{L}_{N-1} > \dots \\ &> \mathcal{L}_2 > \mathcal{L}_1 > 0\end{aligned}$$

One run with \mathbf{K} “live points”
= \mathbf{K} runs with 1 live point!

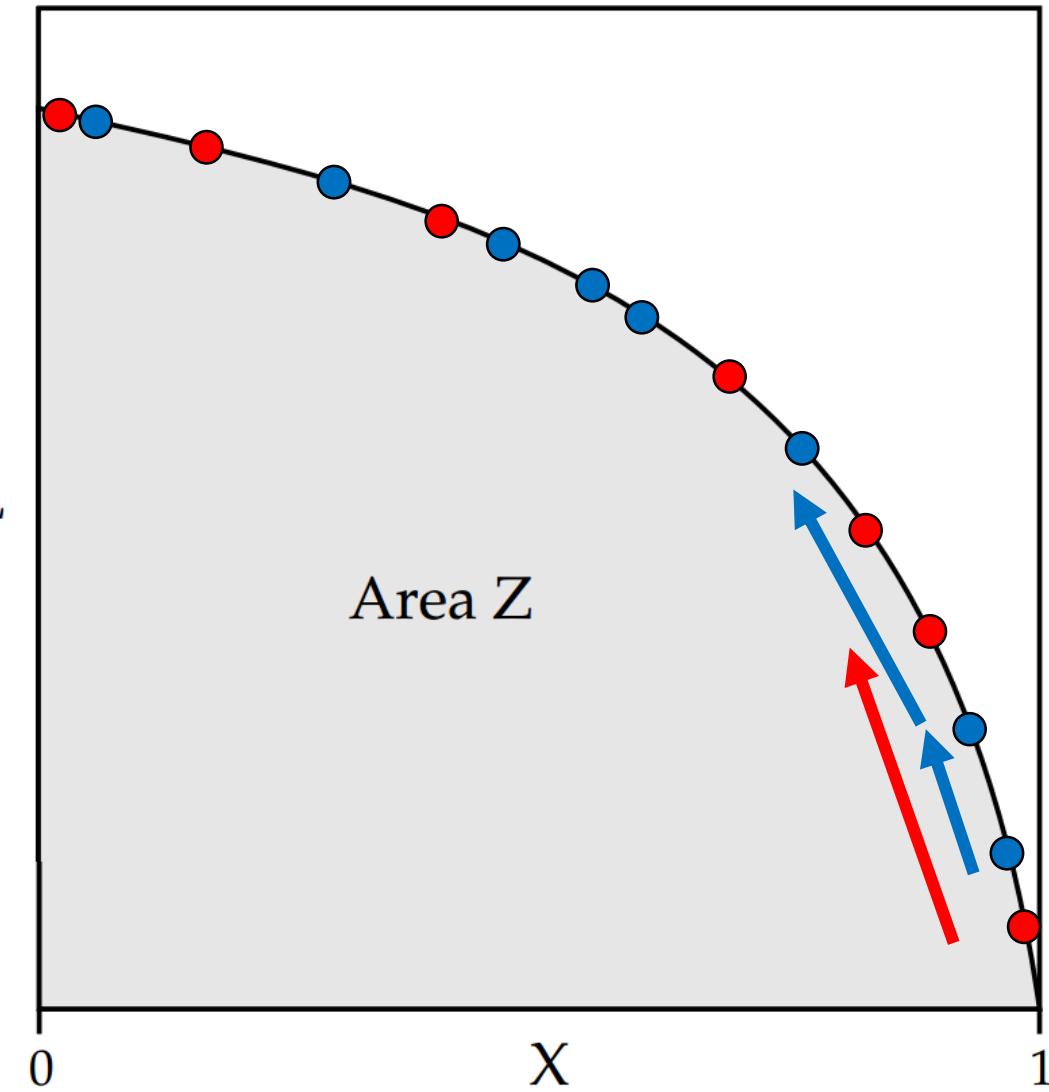


Exploring Sampling Uncertainties

$$\mathcal{L}_{N_1}^{(1)} > \dots > \mathcal{L}_2^{(1)} > \mathcal{L}_1^{(1)} > 0$$

$$\mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > 0$$

One run with **K** “live points”
= **K** runs with 1 live point!



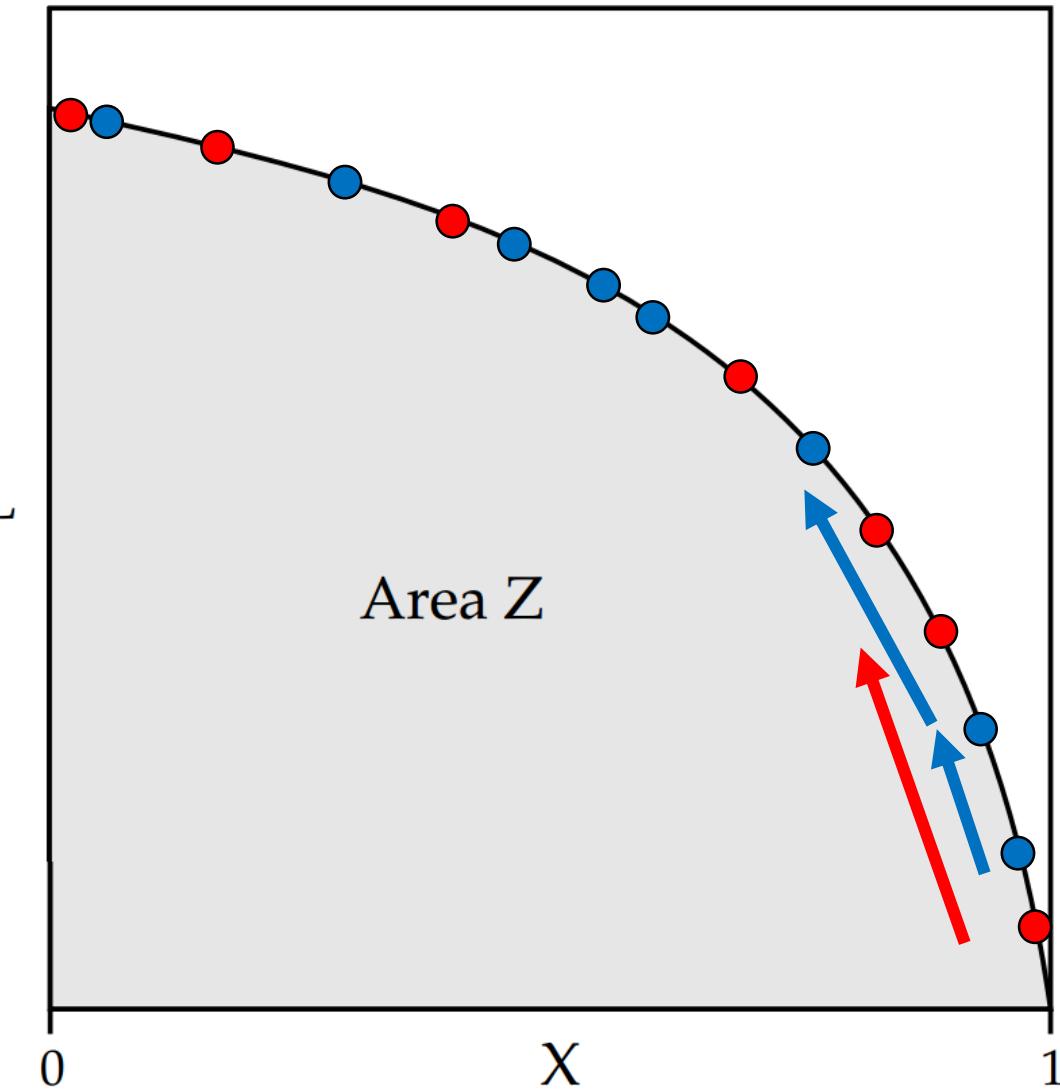
Exploring Sampling Uncertainties

Original run

$$\left\{ \mathcal{L}_{(i)}^{(\cdot)} \right\} = \left\{ \mathcal{L}_{(i)}^{(1)} \right\}, \left\{ \mathcal{L}_{(i)}^{(2)} \right\}, \dots$$

“strand”
“strand”

One run with K “live points”
= K runs with 1 live point!

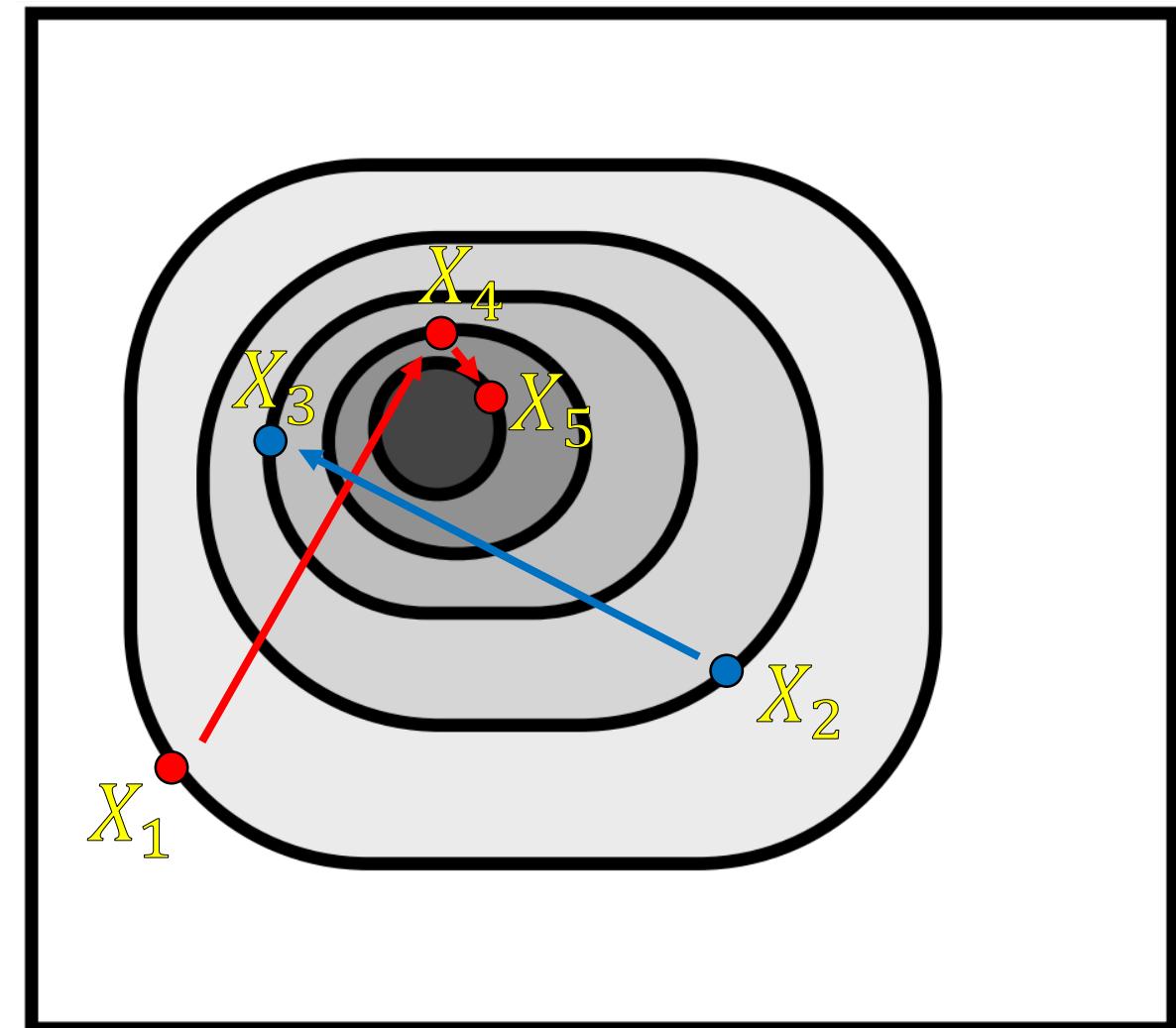


Exploring Sampling Uncertainties

Original run

$$\left\{ \mathcal{L}_{(i)}^{(\cdot)} \right\} = \left\{ \mathcal{L}_{(i)}^{(1)} \right\}, \left\{ \mathcal{L}_{(i)}^{(2)} \right\}, \dots$$

“strand”
“strand”



Exploring Sampling Uncertainties

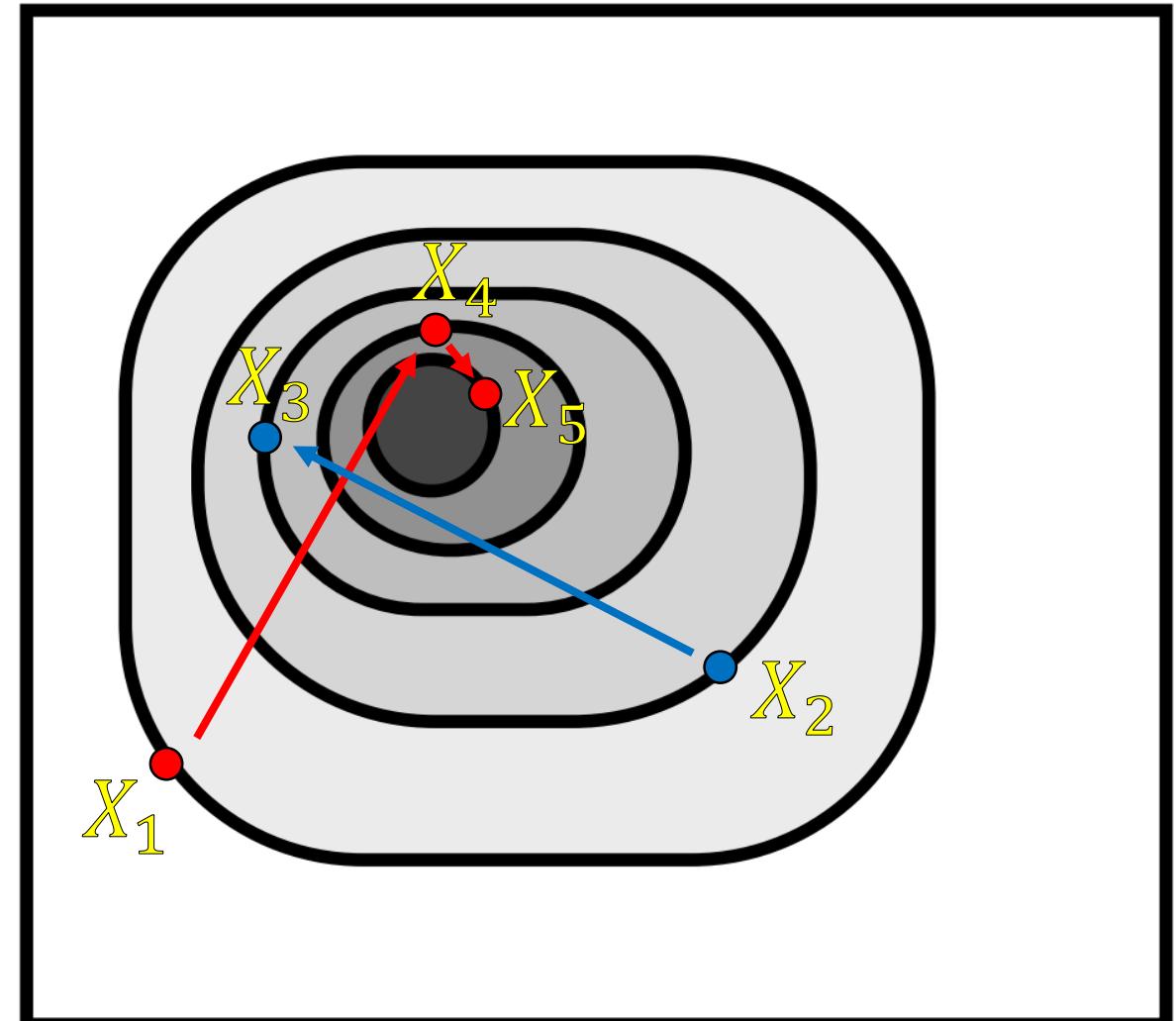
Original run

$$\{\mathcal{L}_{(i)}^{(\cdot)}\} = \{\mathcal{L}_{(i)}^{(1)}\}, \{\mathcal{L}_{(i)}^{(2)}\}, \dots$$

“strand”
“strand”

We would like to sample K paths from
the set of all possible paths $P(\{\mathcal{L}_{(i)}\}, \dots)$.
However, we don't have access to it.

$$\{\mathcal{L}_{(i)}^{(\cdot)}\}' = \{\mathcal{L}_{(i)}^{(1)}\}', \{\mathcal{L}_{(i)}^{(2)}\}', \dots$$



Exploring Sampling Uncertainties

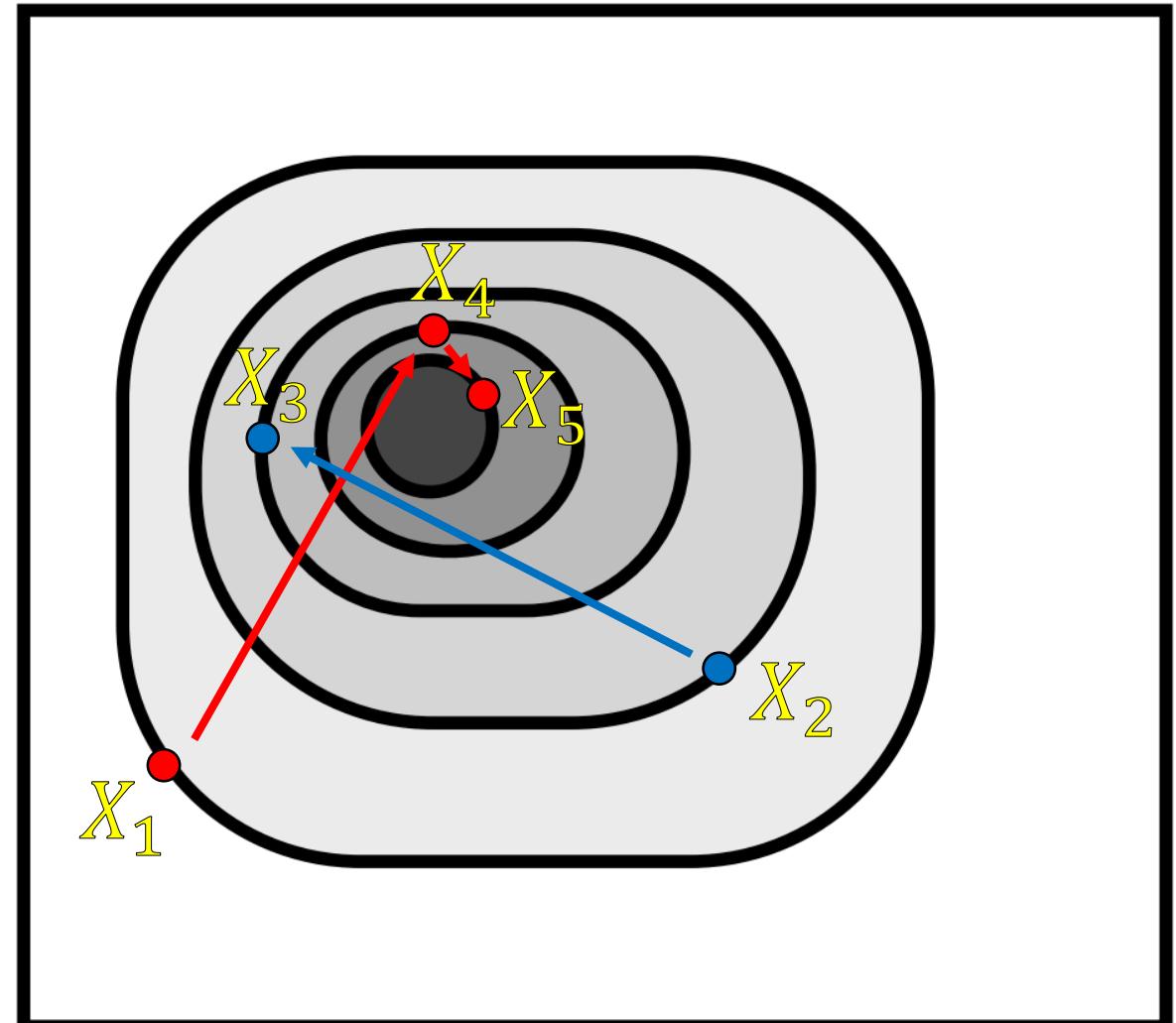
Original run

$$\{\mathcal{L}_{(i)}^{(\cdot)}\} = \{\mathcal{L}_{(i)}^{(1)}\}, \{\mathcal{L}_{(i)}^{(2)}\}, \dots$$

“strand”
“strand”

We would like to sample K paths from the set of all possible paths $P(\{\mathcal{L}_{(i)}\}, \dots)$. However, we don't have access to it.
Use bootstrap estimator.

$$\widetilde{\{\mathcal{L}_{(i)}^{(\cdot)}\}}' = \{\mathcal{L}_{(i)}^{(1)}\}, \{\mathcal{L}_{(i)}^{(1)}\}, \{\mathcal{L}_{(i)}^{(2)}\}, \dots$$



Exploring Sampling Uncertainties

Original run

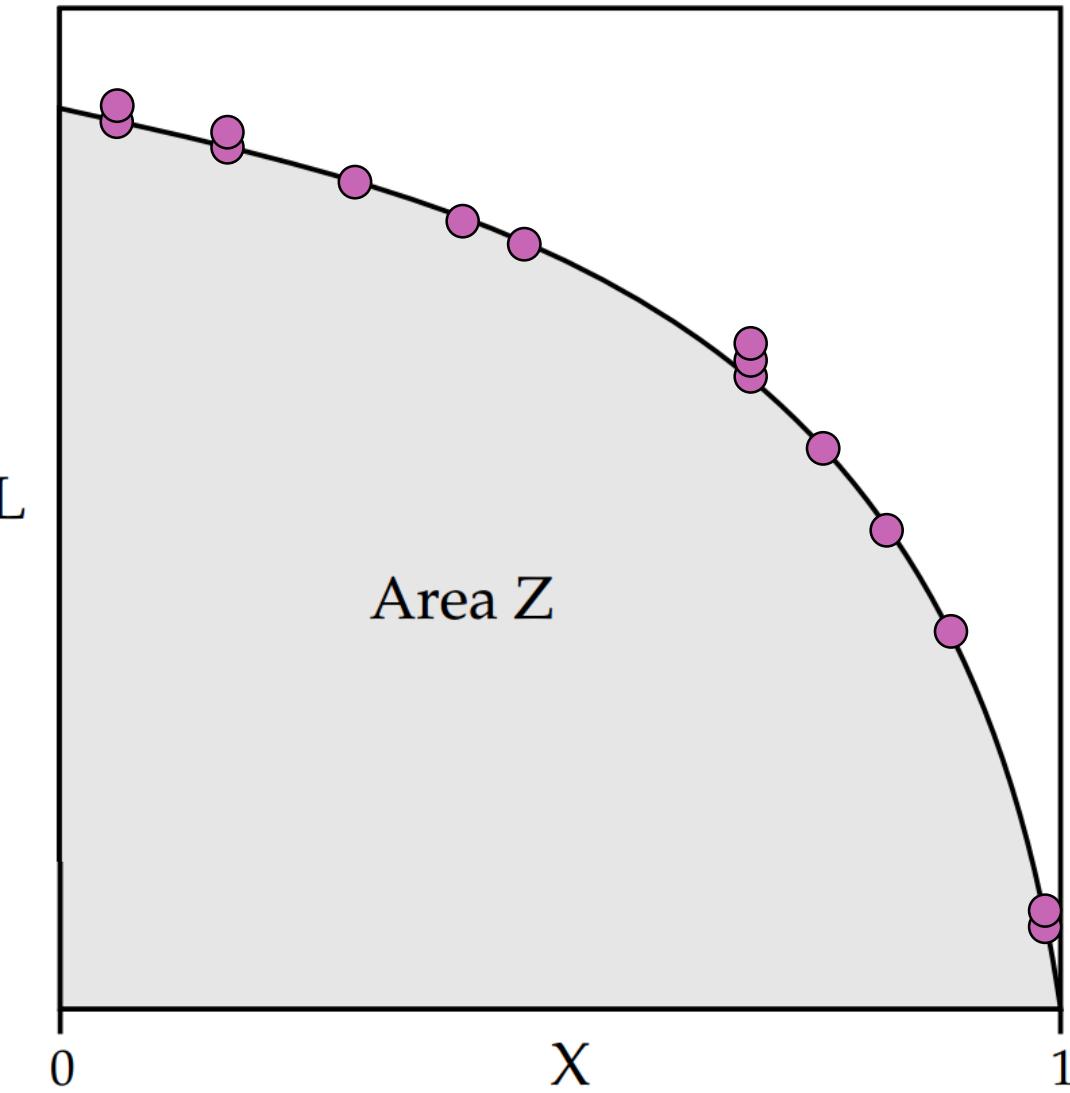
$$\left\{ \mathcal{L}_{(i)}^{(\cdot)} \right\} = \left\{ \mathcal{L}_{(i)}^{(1)} \right\}, \left\{ \mathcal{L}_{(i)}^{(2)} \right\}, \dots$$

“strand”
“strand”

We would like to sample K paths from
the set of all possible paths $P(\{\mathcal{L}_{(i)}\}, \dots)$.
However, we don't have access to it.
Use bootstrap estimator.

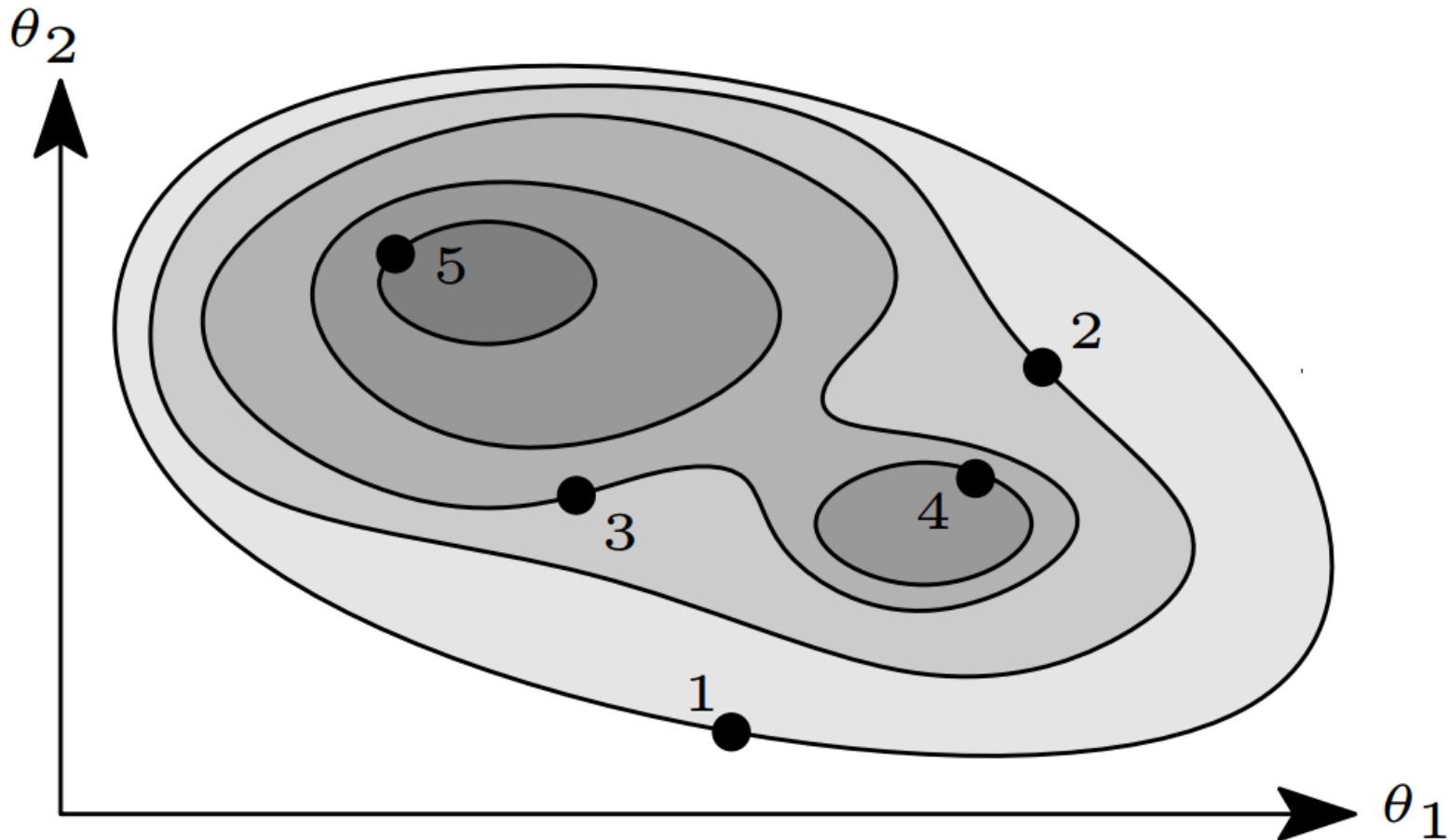
$$\tilde{p}'_i = \frac{\tilde{w}'_i}{\tilde{Z}'}$$

$$\tilde{Z}' \approx \sum_{i=1}^{N'} \tilde{w}'_i$$

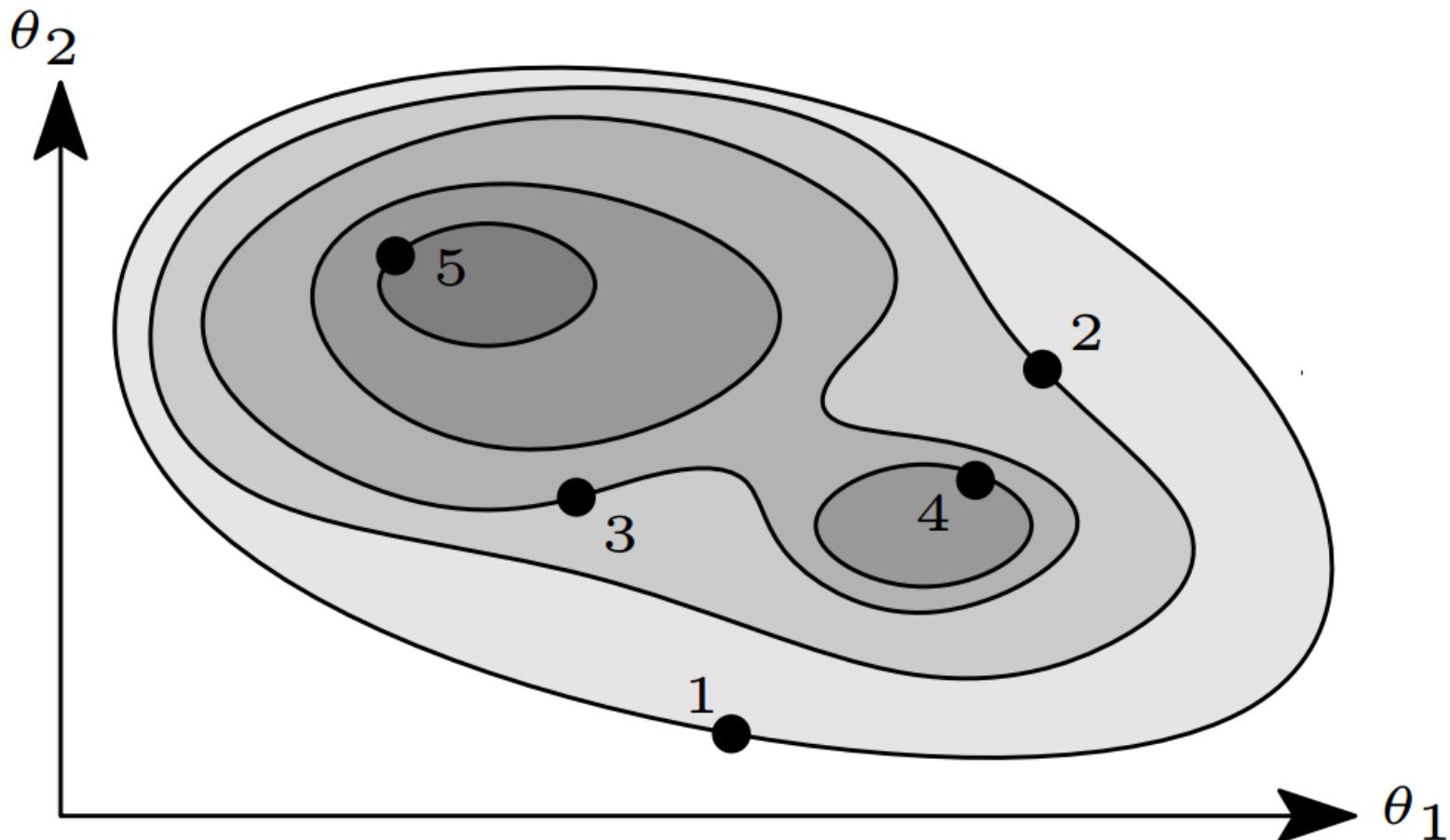


Nested Sampling In Practice

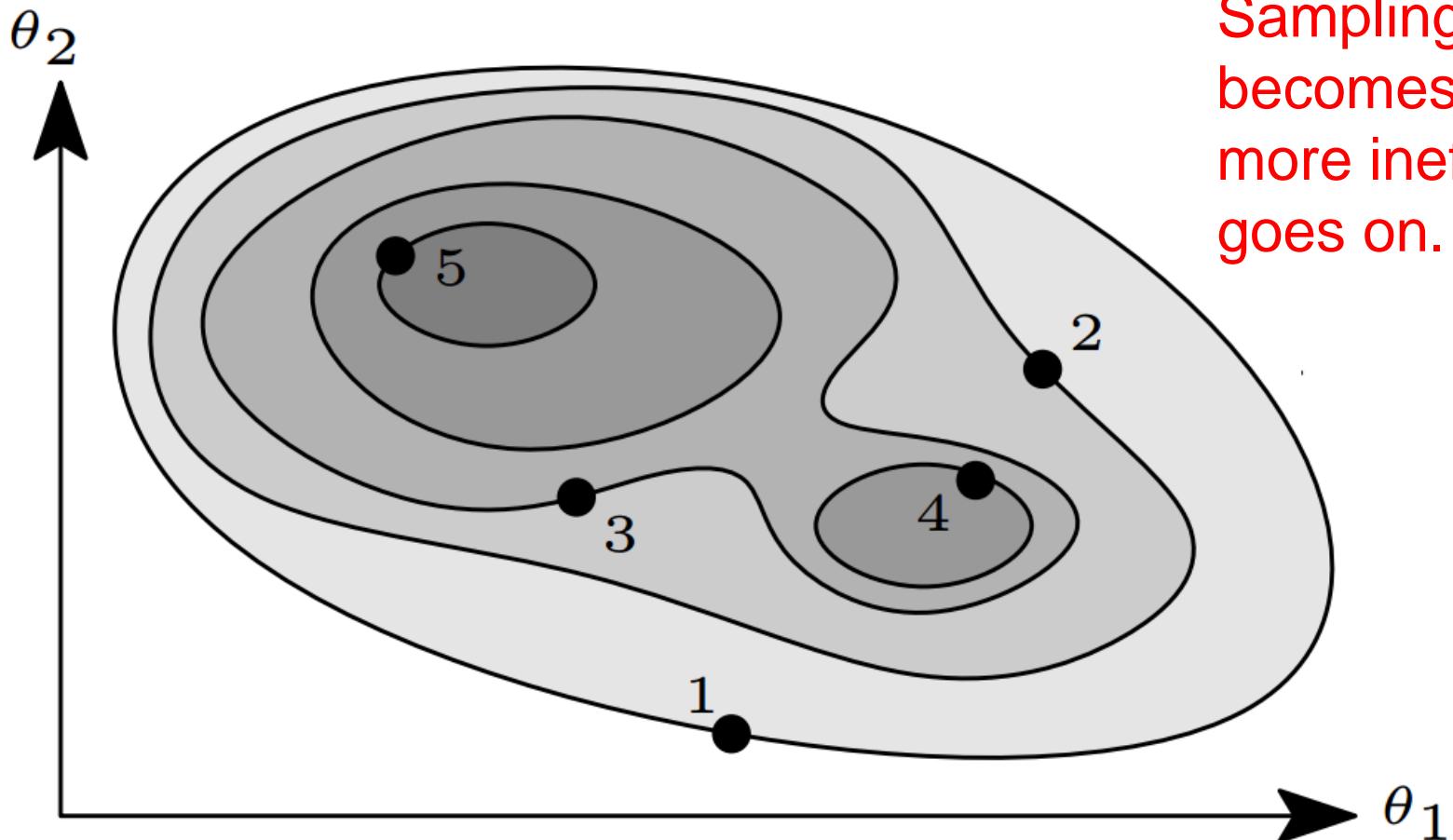
Nested Sampling In Practice



Method 0: Sampling from the Prior



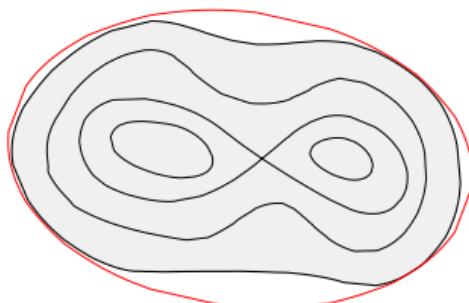
Method 0: Sampling from the Prior



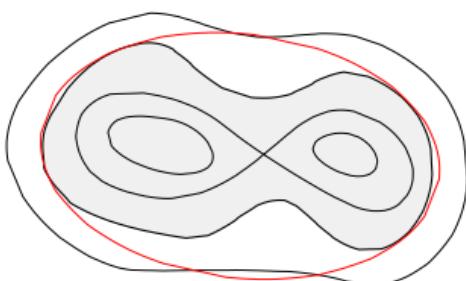
Method 1: Constrained Uniform Sampling

Proposal:

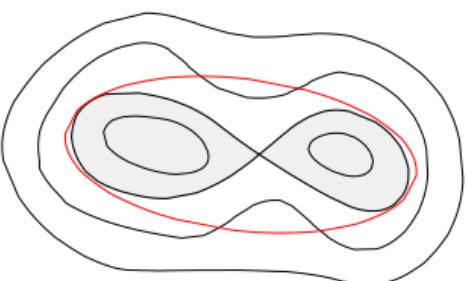
Bound the iso-likelihood contours in real time and sample from the newly **constrained prior**.



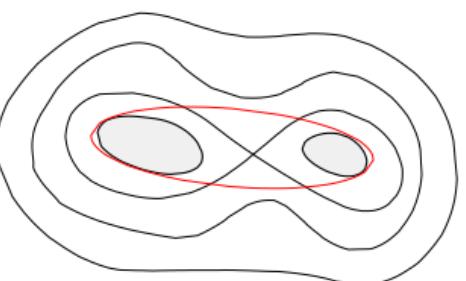
(a)



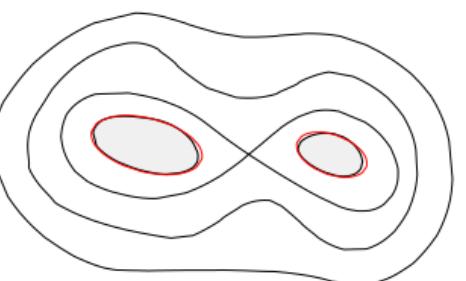
(b)



(c)



(d)

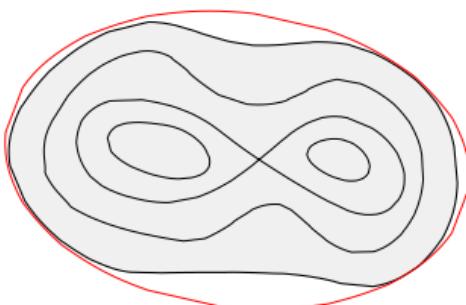


(e)

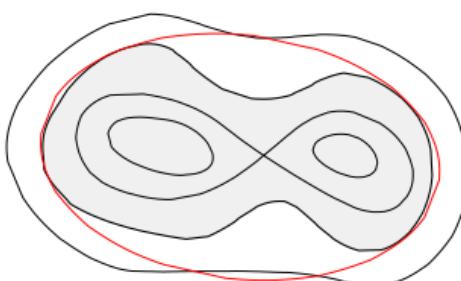
Method 1: Constrained Uniform Sampling

Issues:

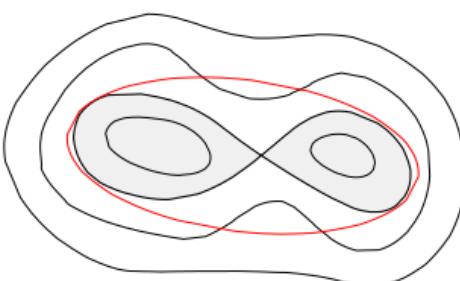
- How to ensure bounds always encompass iso-likelihood contours?
- How to generate flexible bounds?



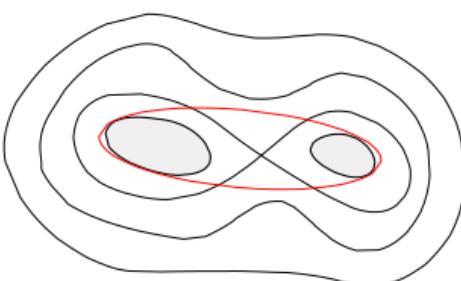
(a)



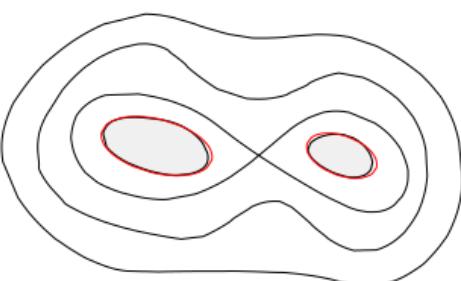
(b)



(c)



(d)

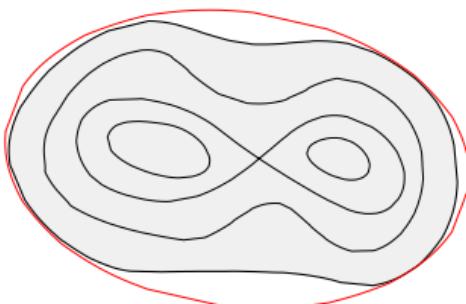


(e)

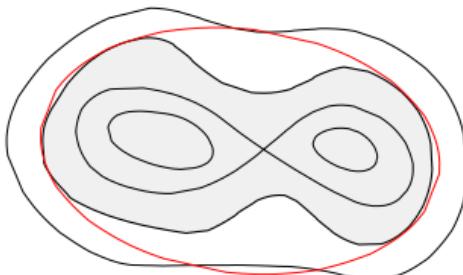
Method 1: Constrained Uniform Sampling

Issues:

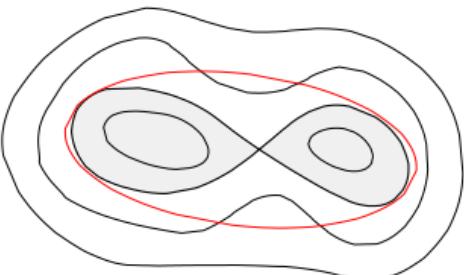
- How to ensure bounds always encompass iso-likelihood contours? Bootstrapping.
- How to generate flexible bounds? Easier with uniform (transformed) prior.



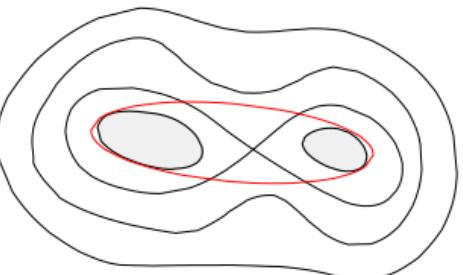
(a)



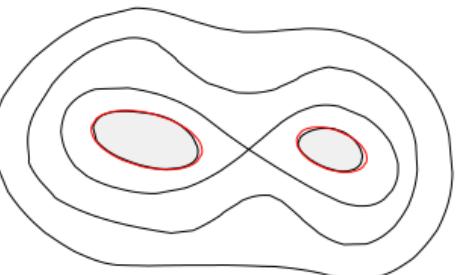
(b)



(c)



(d)

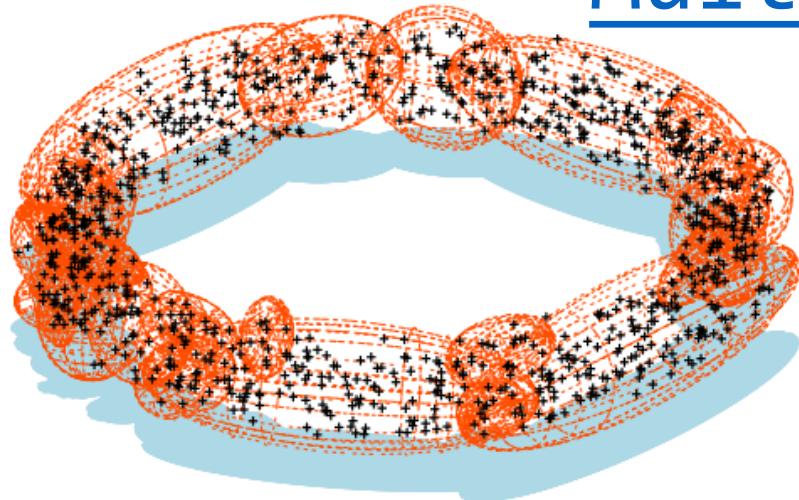


(e)

Method 1: Constrained Uniform Sampling

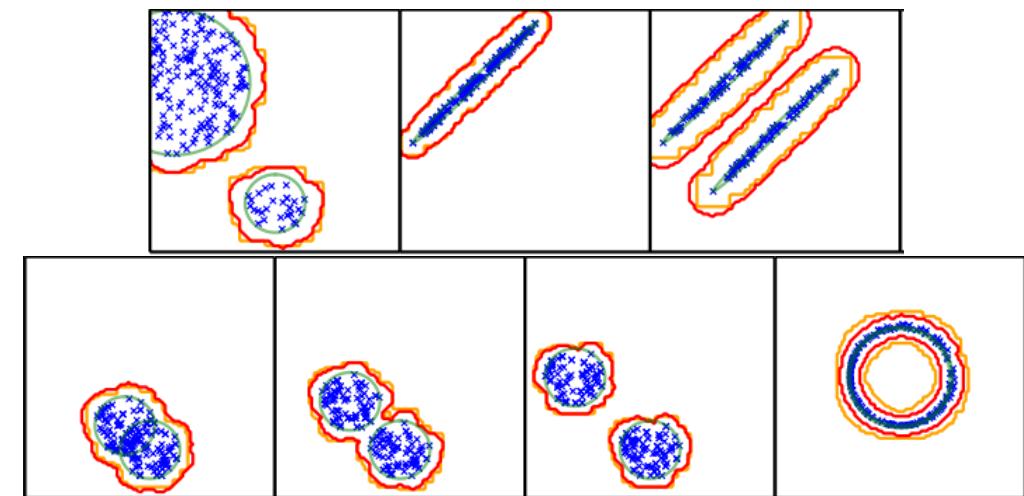
Ellipsoids

MultiNest



Feroz et al. (2009)

Balls/Cubes

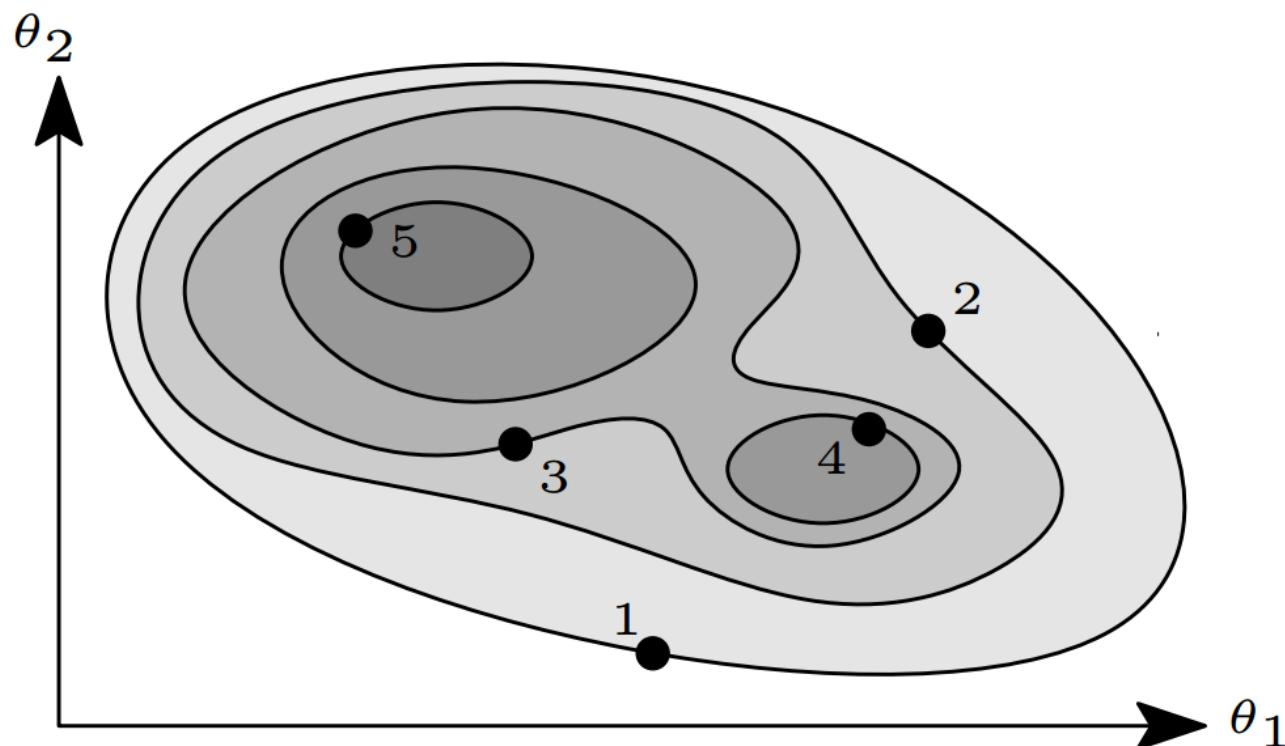


Buchner (2014)

Method 2: “Evolving” Previous Samples

Proposal:

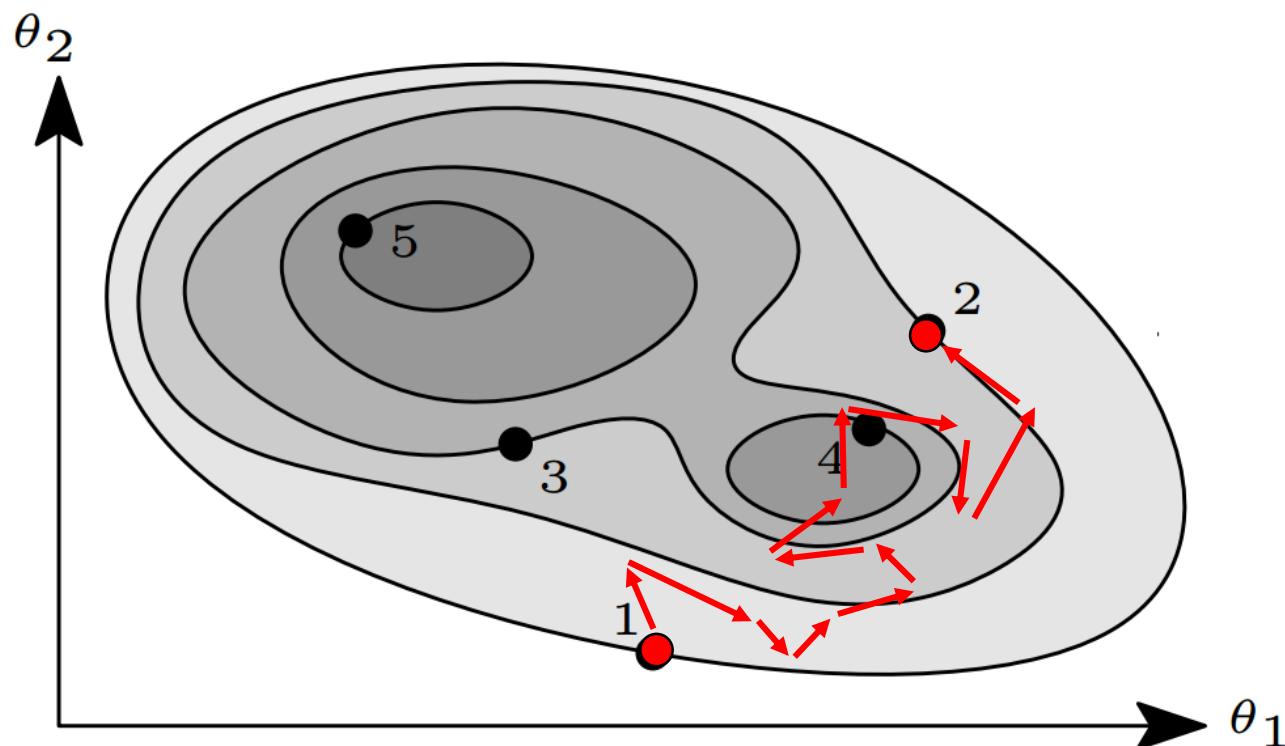
Generate independent samples subject to the likelihood constraint by “evolving” copies of current live points.



Method 2: “Evolving” Previous Samples

Proposal:

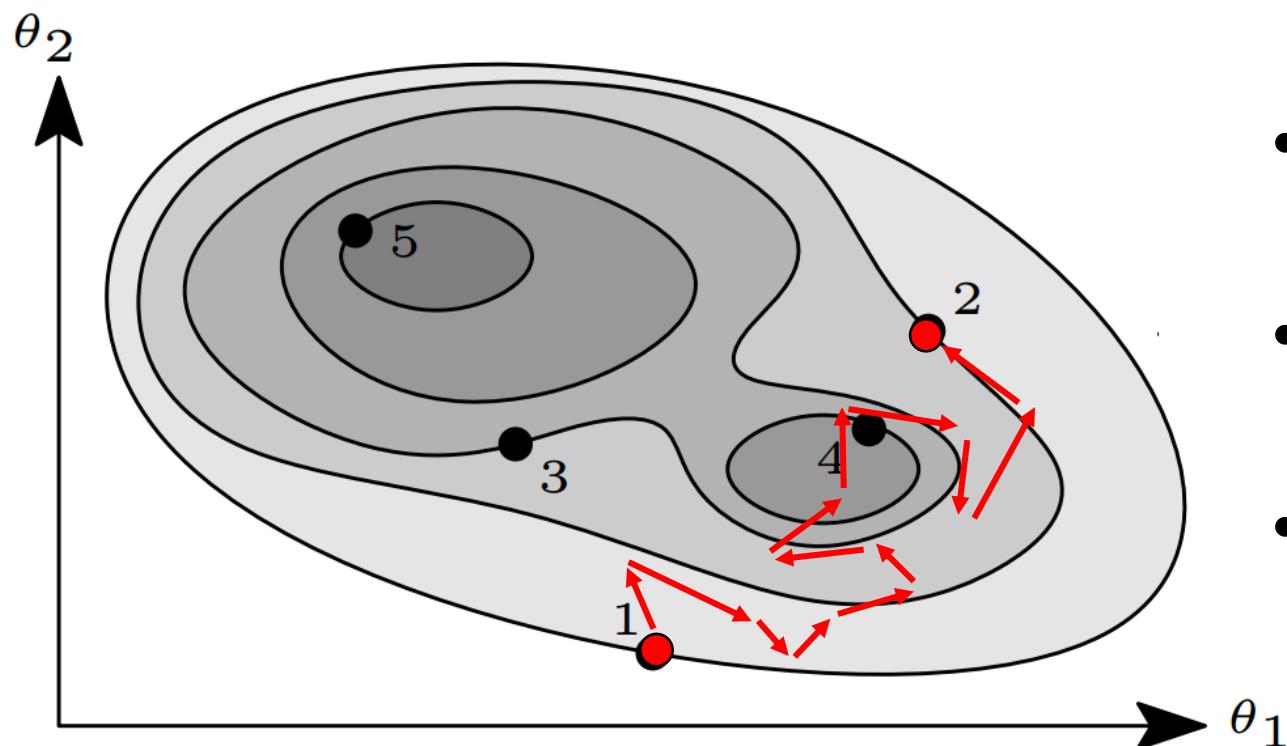
Generate independent samples subject to the likelihood constraint by “evolving” copies of current live points.



Method 2: “Evolving” Previous Samples

Proposal:

Generate independent samples subject to the likelihood constraint by “evolving” copies of current live points.

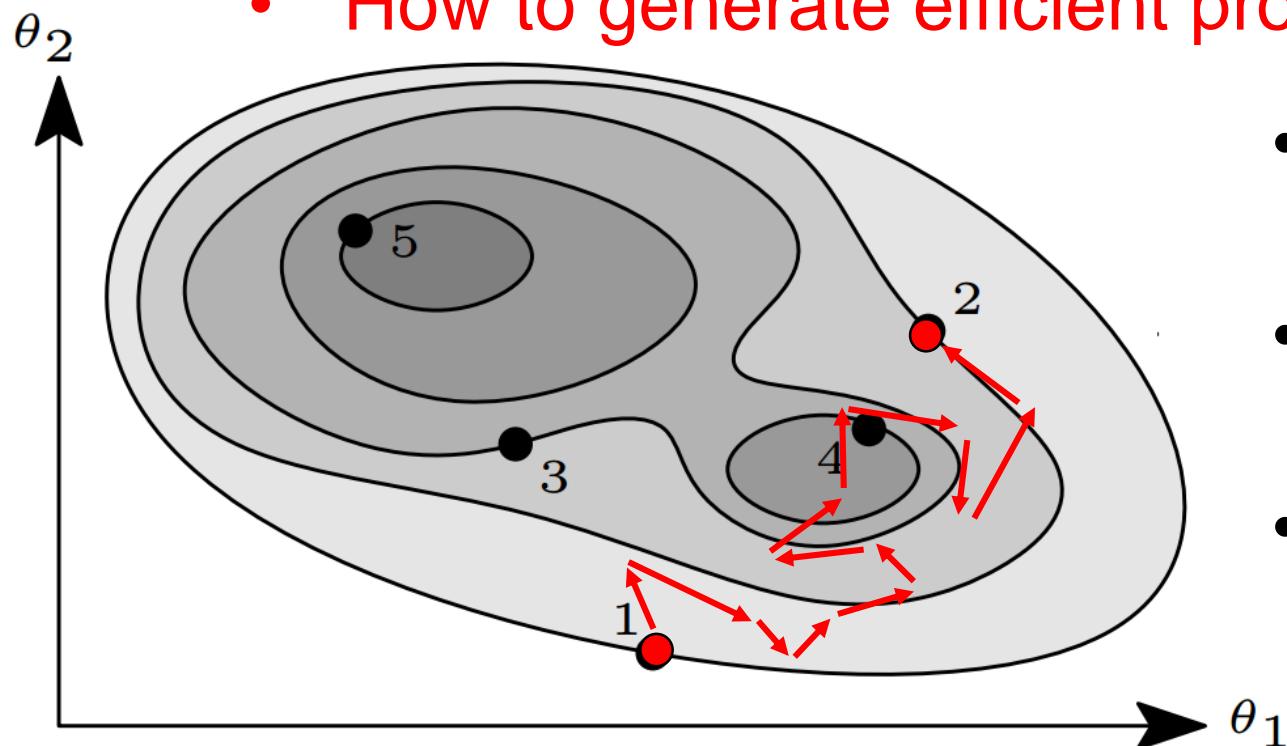


- Random walks (i.e. MCMC)
- Slice sampling [PolyChord](#)
- Random trajectories (i.e. HMC)

Method 2: “Evolving” Previous Samples

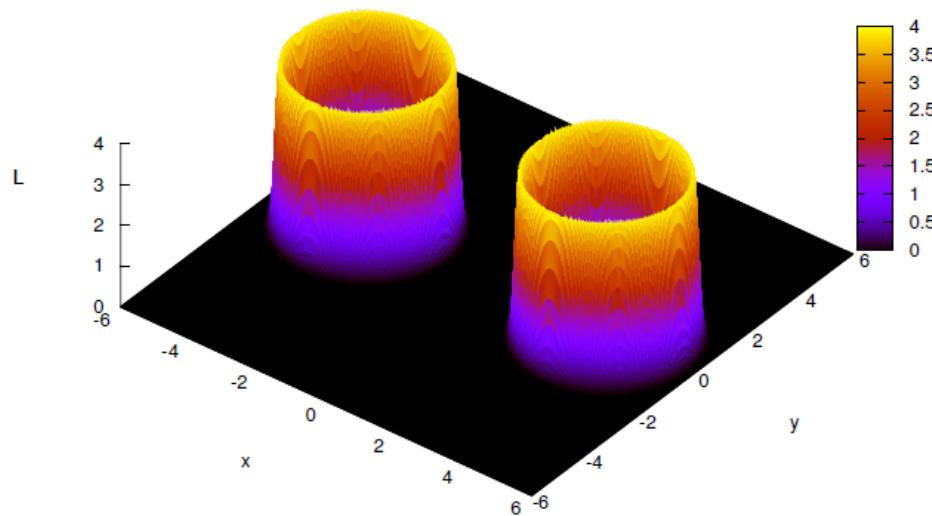
Issues:

- How to ensure samples are independent (thinning) and properly distributed within likelihood constraint?
- How to generate efficient proposals?

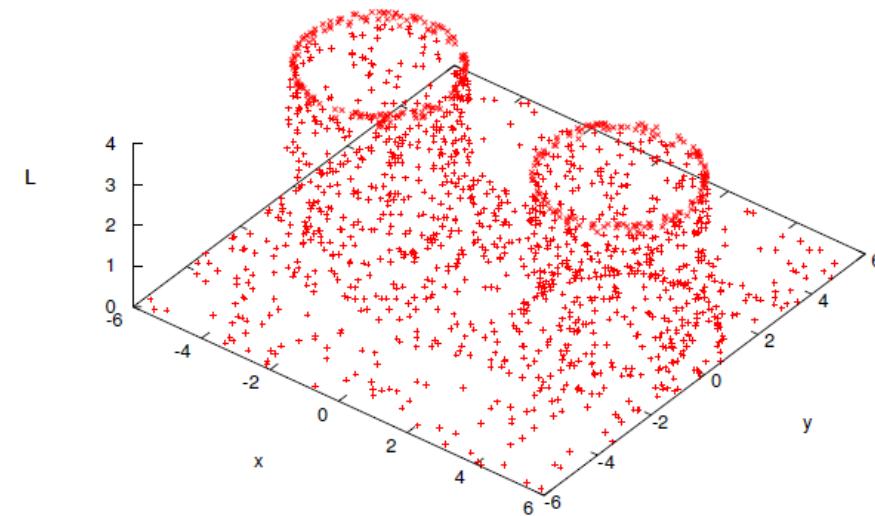


- Random walks (i.e. MCMC)
- Slice sampling [PolyChord](#)
- Random trajectories (i.e. HMC)

Example: Gaussian Shells



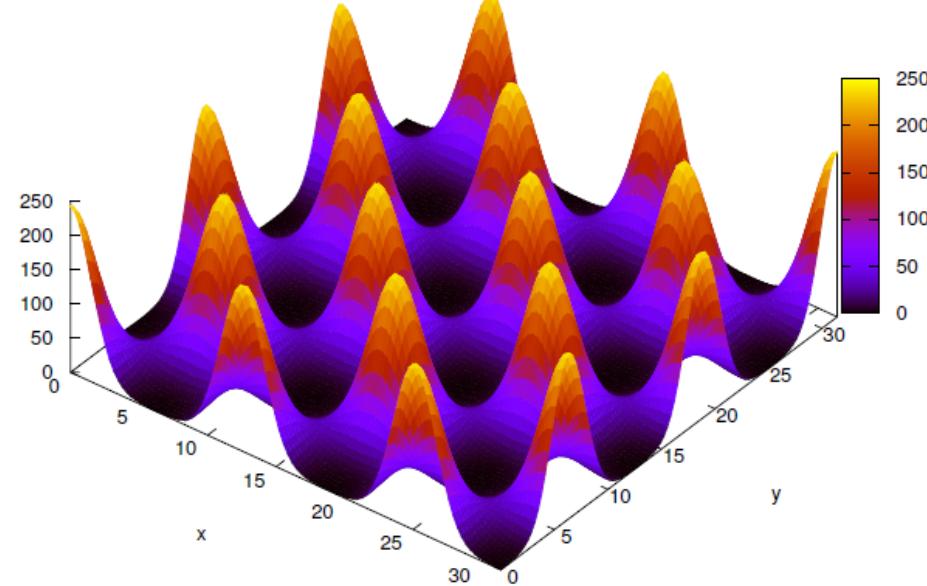
(a)



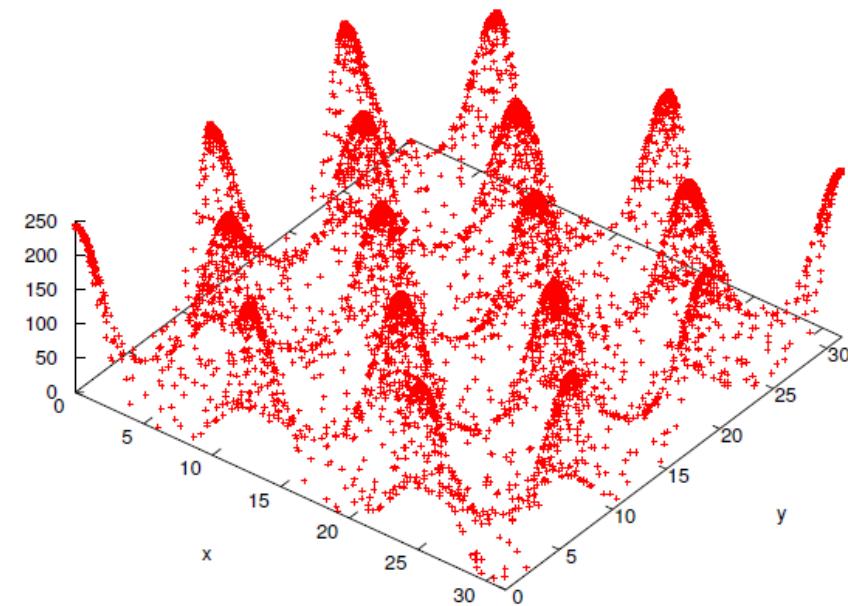
(b)

Feroz et al. (2013)

Example: Eggbox



(a)



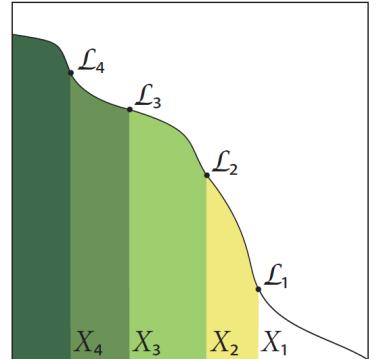
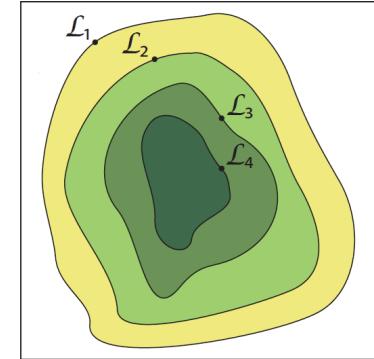
(b)

Feroz et al. (2013)

Summary: (Static) Nested Sampling

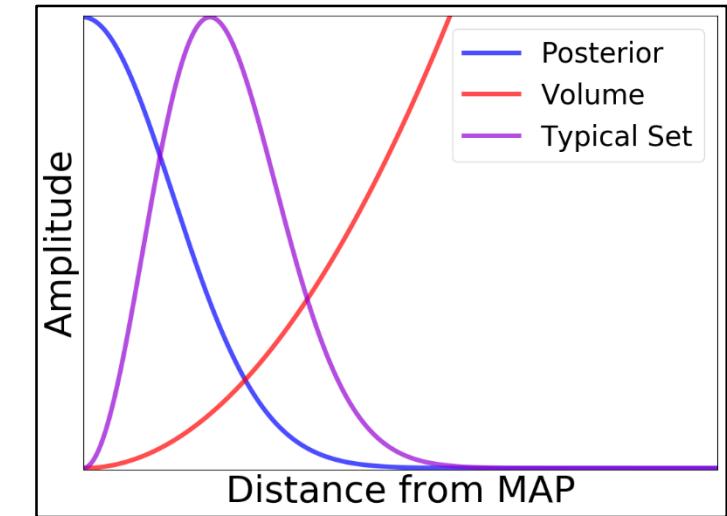
Summary: (Static) Nested Sampling

1. Estimates the evidence \hat{Z} .



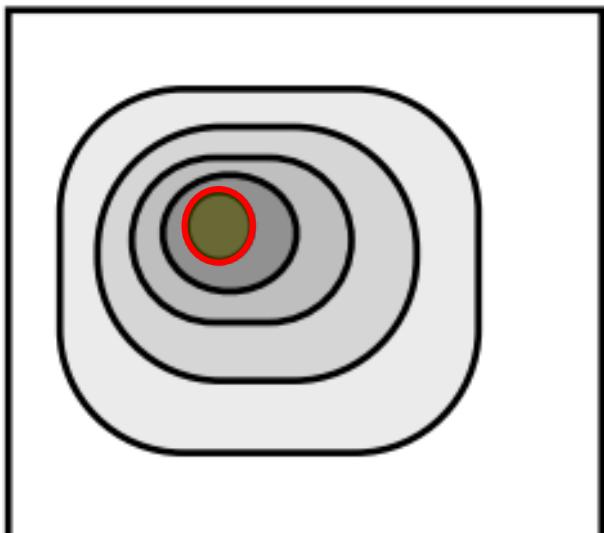
Summary: (Static) Nested Sampling

1. Estimates the evidence \tilde{Z} .
2. Estimates the posterior $\hat{p}(\Theta)$.



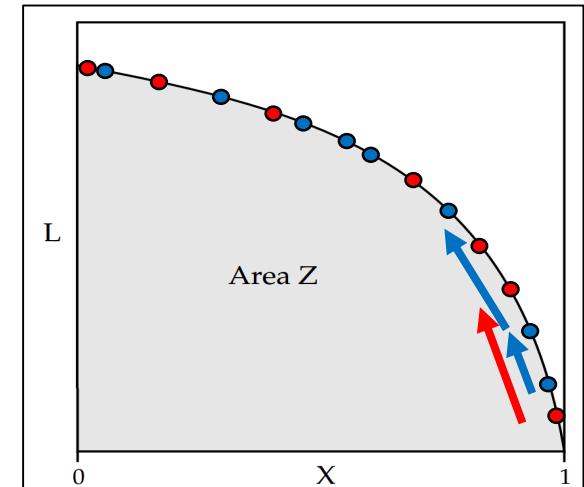
Summary: (Static) Nested Sampling

1. Estimates the evidence $\hat{\mathcal{Z}}$.
2. Estimates the posterior $\hat{p}(\boldsymbol{\Theta})$.
3. Possesses well-defined stopping criteria.



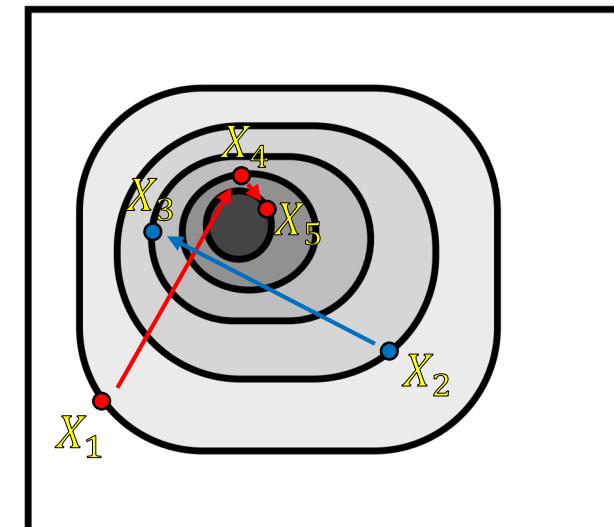
Summary: (Static) Nested Sampling

1. Estimates the evidence $\hat{\mathcal{Z}}$.
2. Estimates the posterior $\hat{p}(\boldsymbol{\Theta})$.
3. Possesses well-defined stopping criteria.
4. Combining runs improves inference.



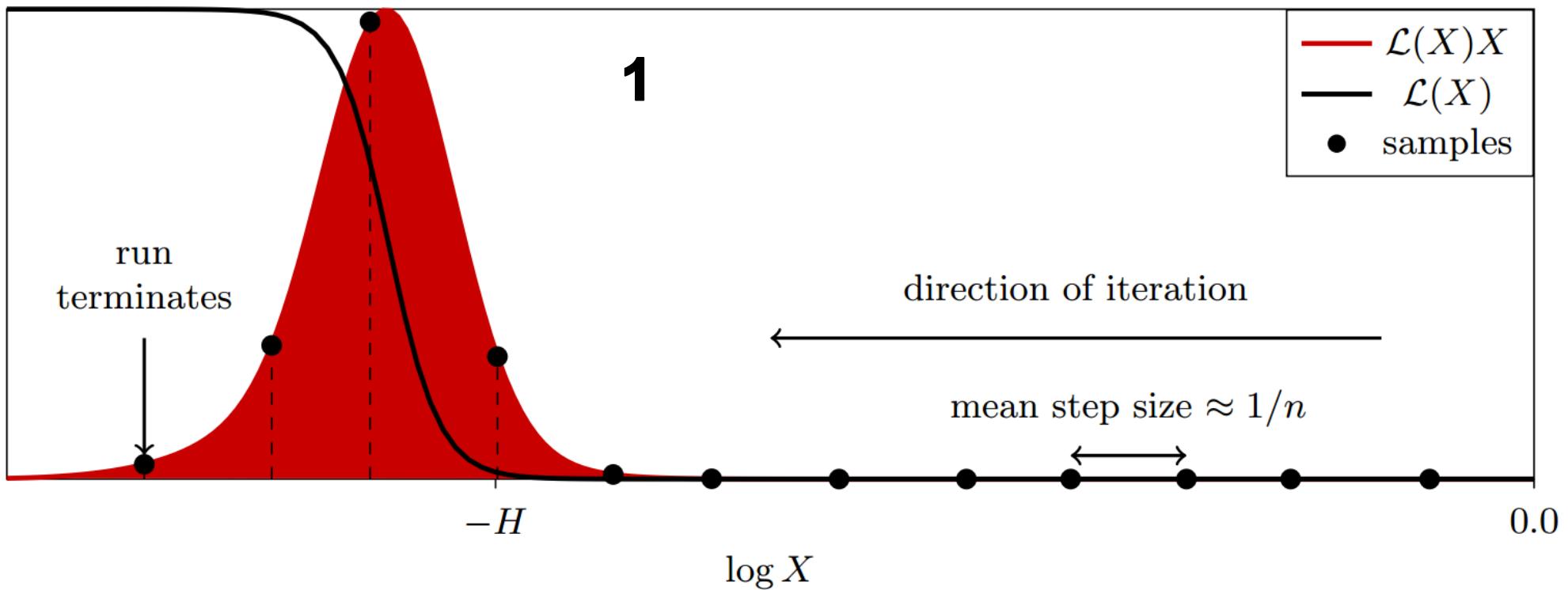
Summary: (Static) Nested Sampling

1. Estimates the evidence $\hat{\mathcal{Z}}$.
2. Estimates the posterior $\hat{p}(\boldsymbol{\Theta})$.
3. Possesses well-defined stopping criteria.
4. Combining runs improves inference.
5. Sampling and statistical uncertainties can be simulated from a single run.



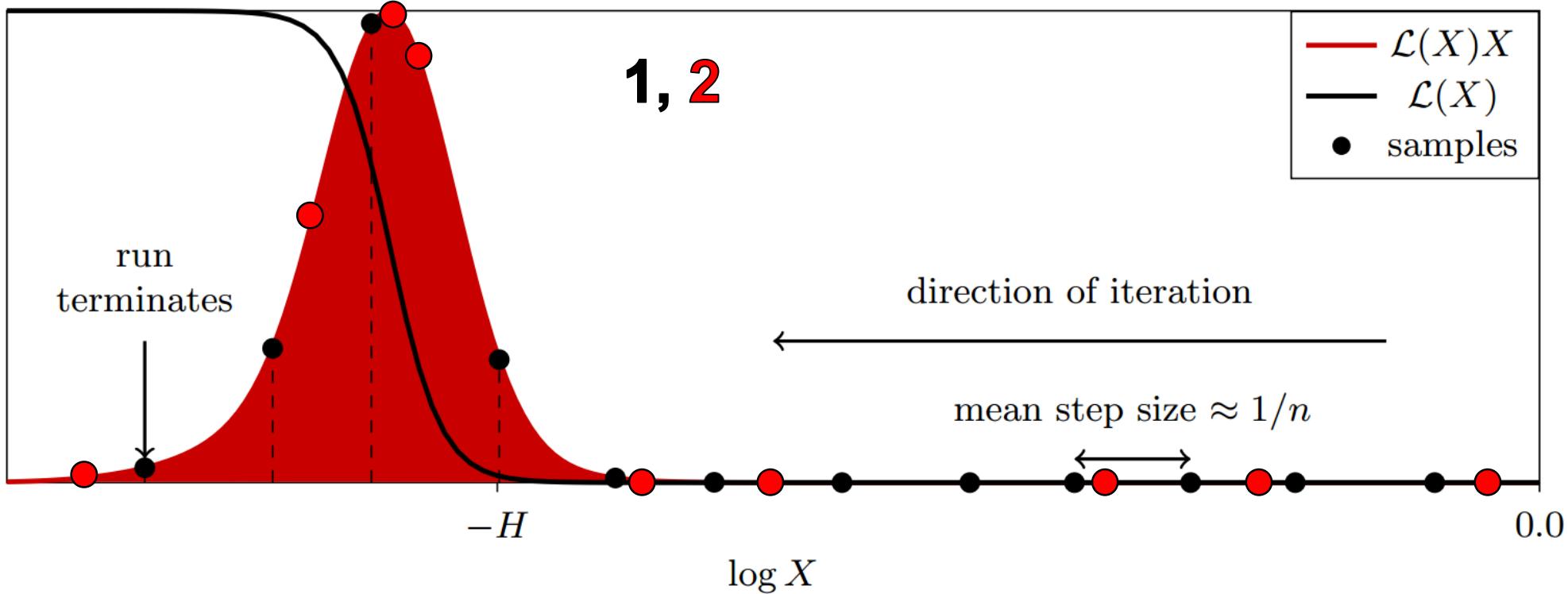
Dynamic Nested Sampling

Dynamic Nested Sampling



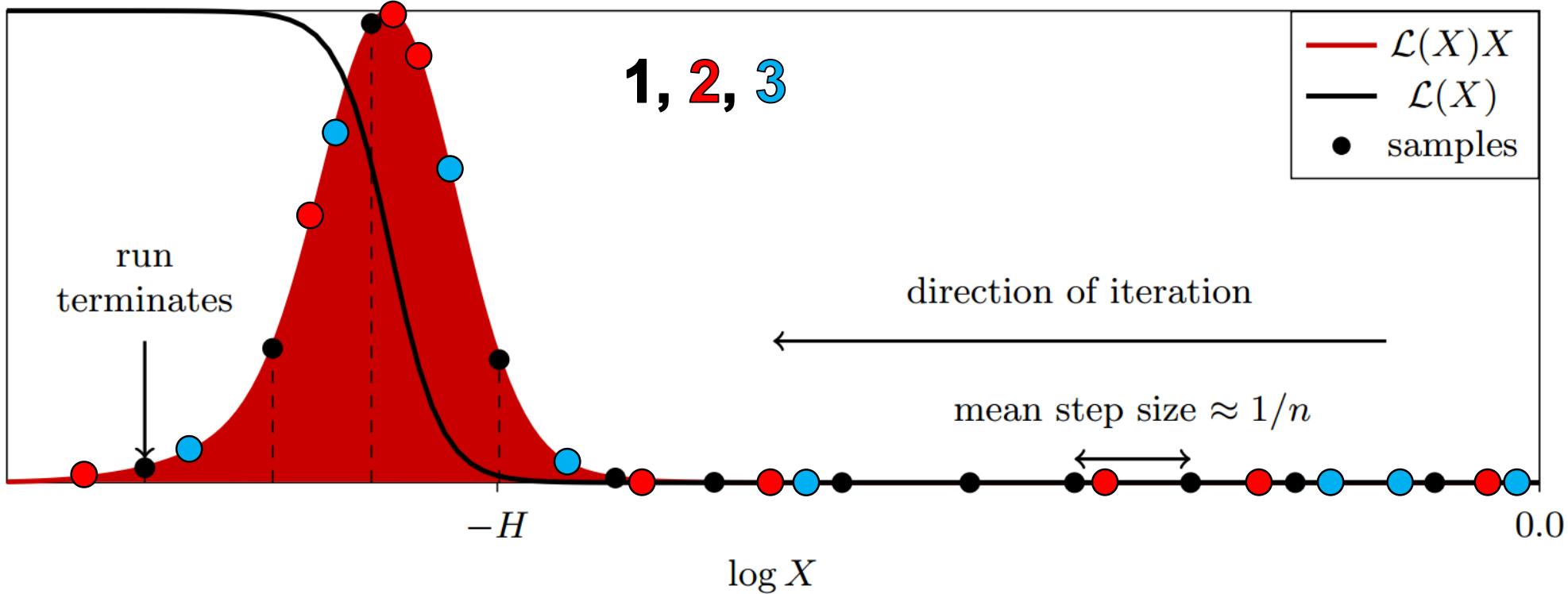
Higson et al. (2017)
[arxiv:1704.03459](https://arxiv.org/abs/1704.03459)

Dynamic Nested Sampling



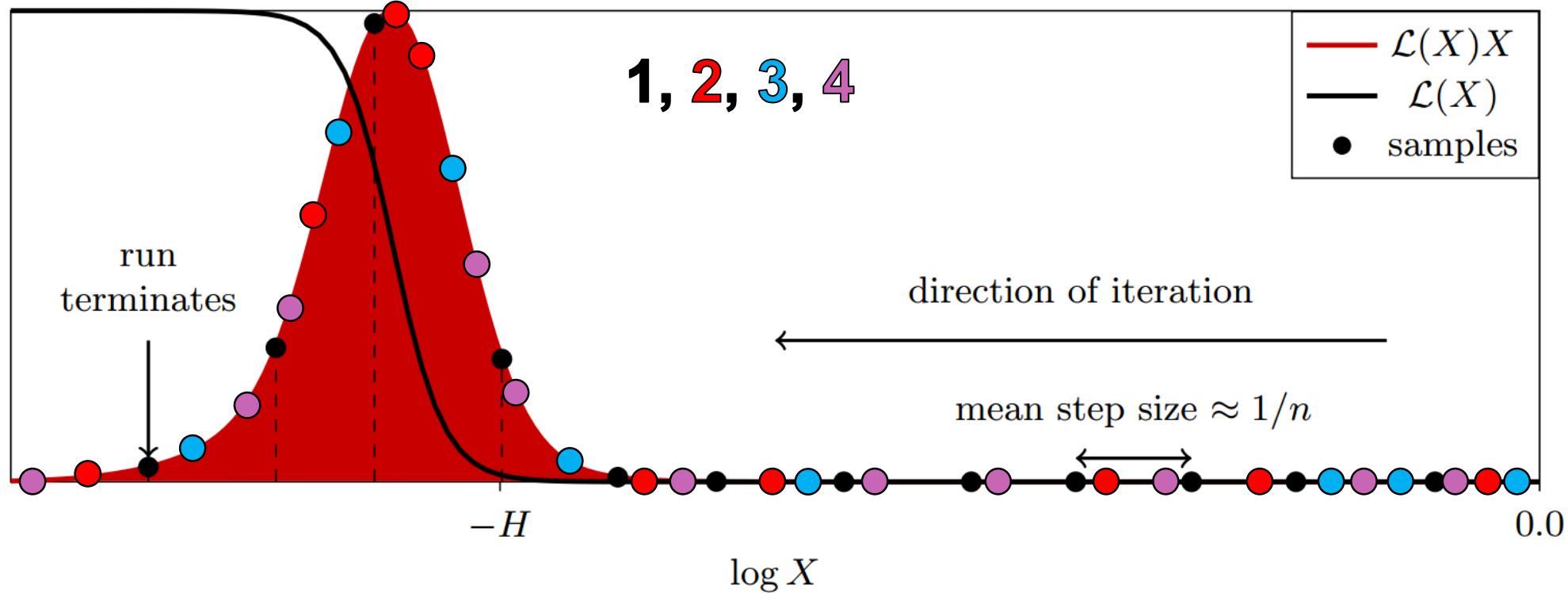
Higson et al. (2017)
[arxiv:1704.03459](https://arxiv.org/abs/1704.03459)

Dynamic Nested Sampling



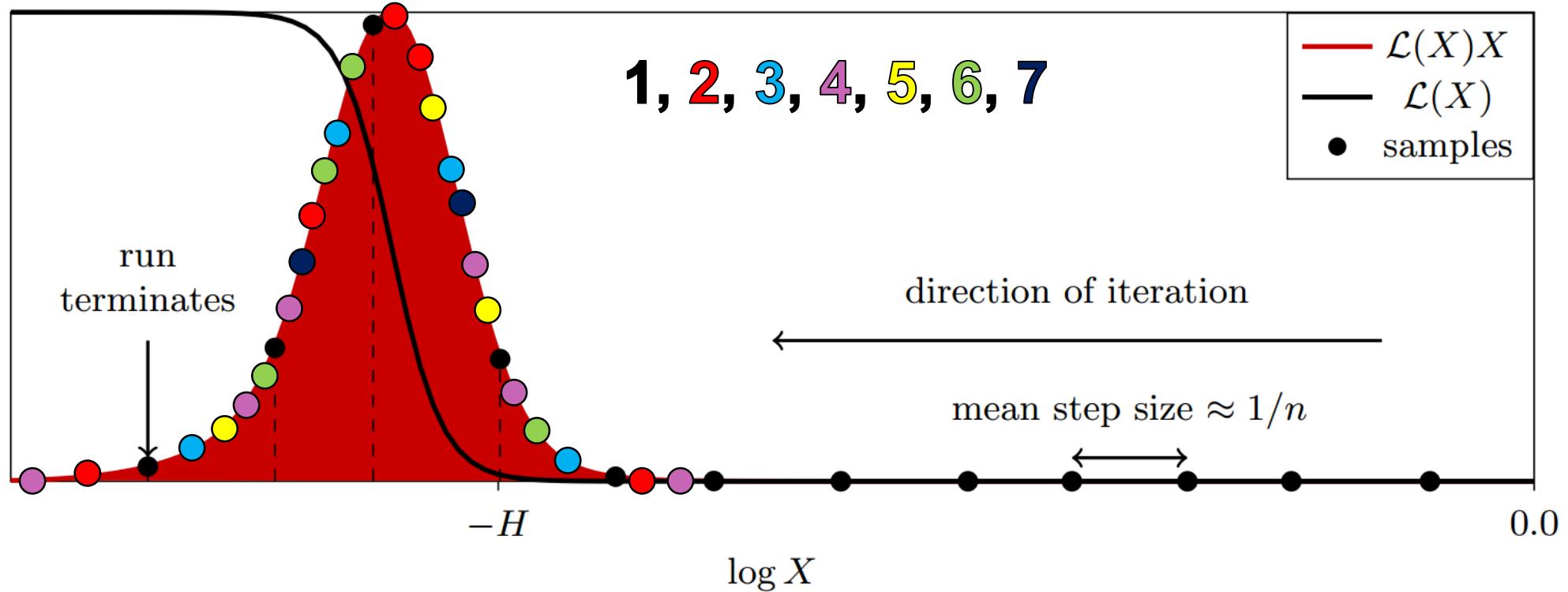
Higson et al. (2017)
[arxiv:1704.03459](https://arxiv.org/abs/1704.03459)

Dynamic Nested Sampling



Higson et al. (2017)
[arxiv:1704.03459](https://arxiv.org/abs/1704.03459)

Dynamic Nested Sampling

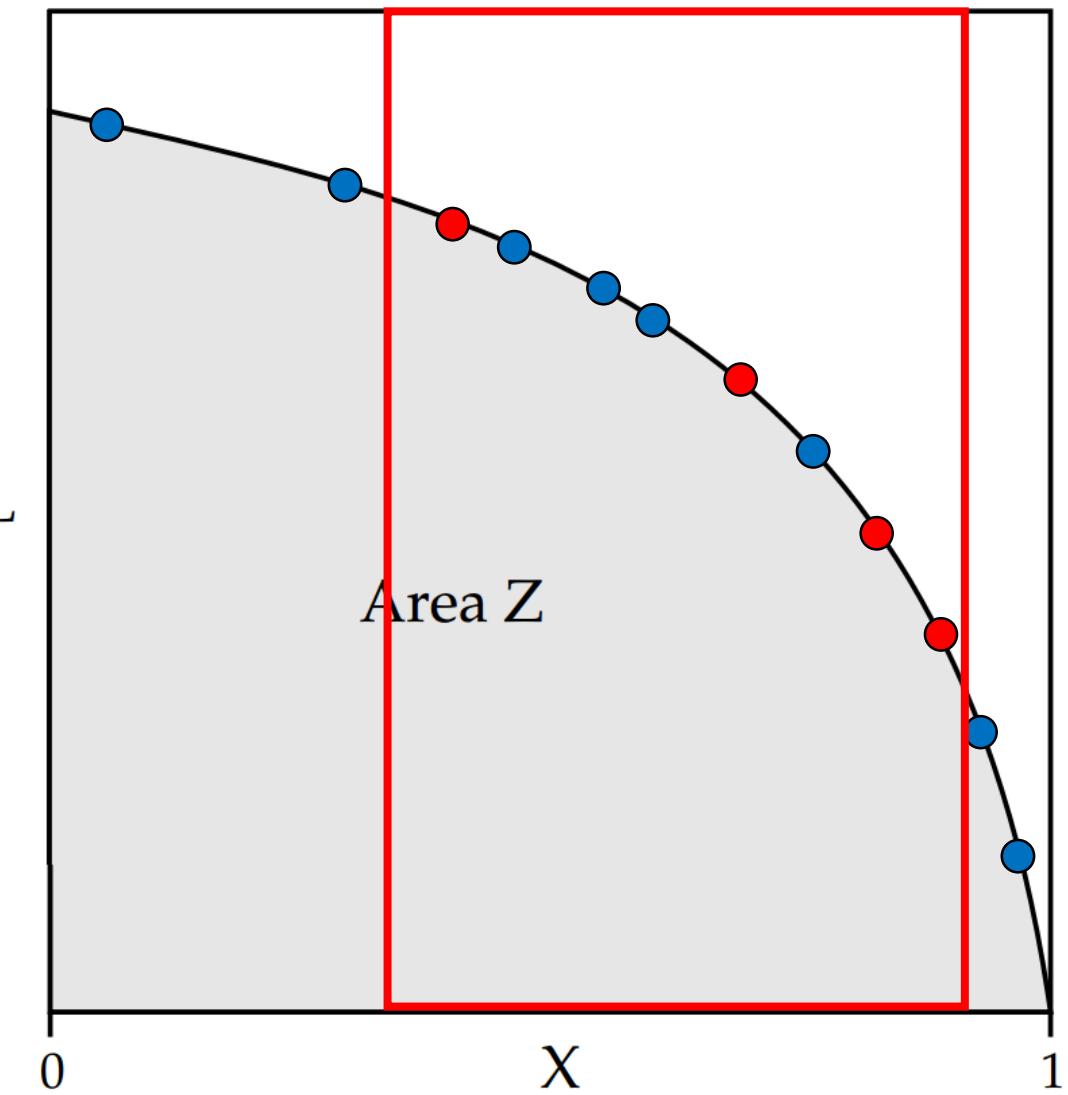


Higson et al. (2017)
[arxiv:1704.03459](https://arxiv.org/abs/1704.03459)

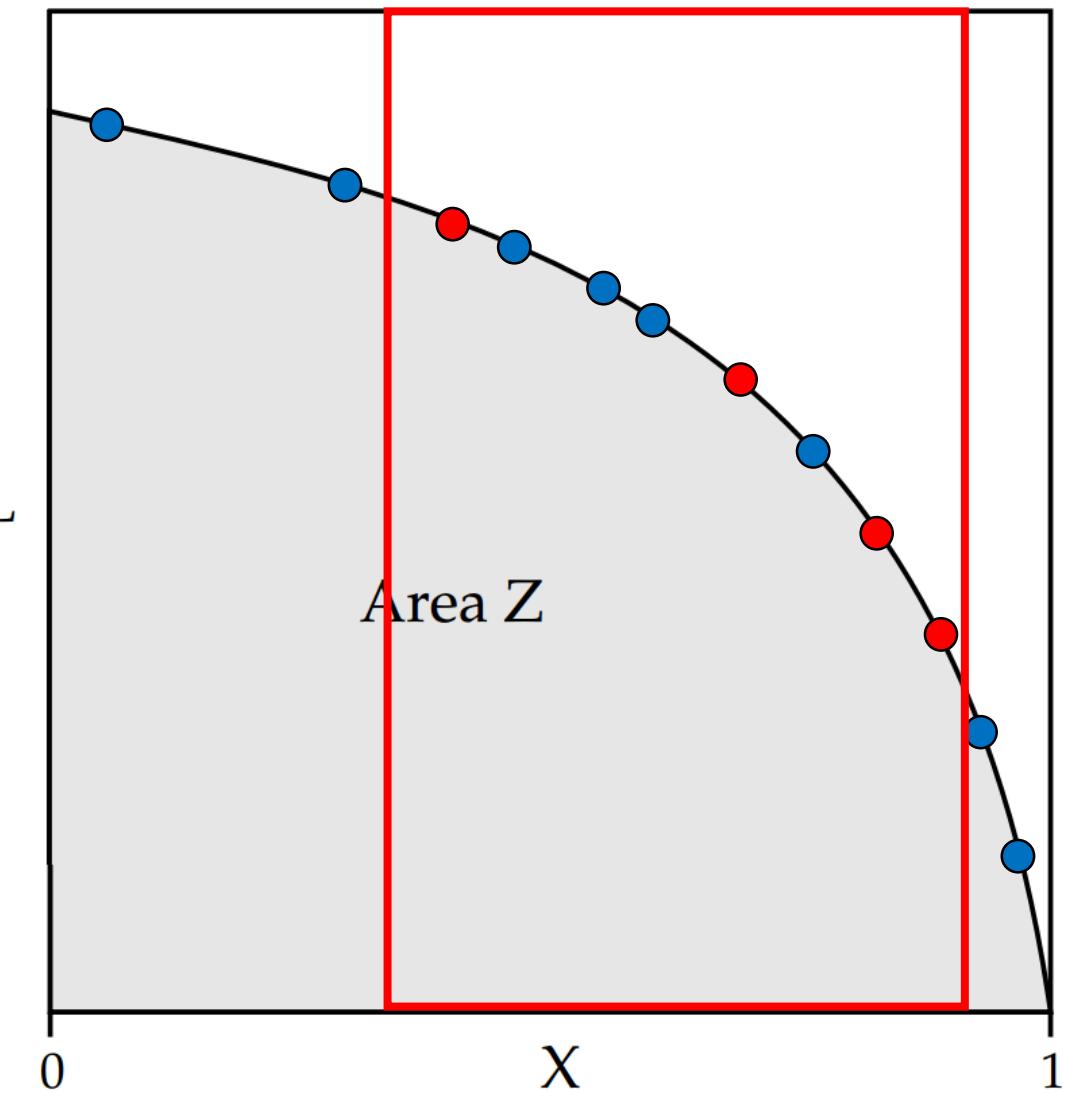
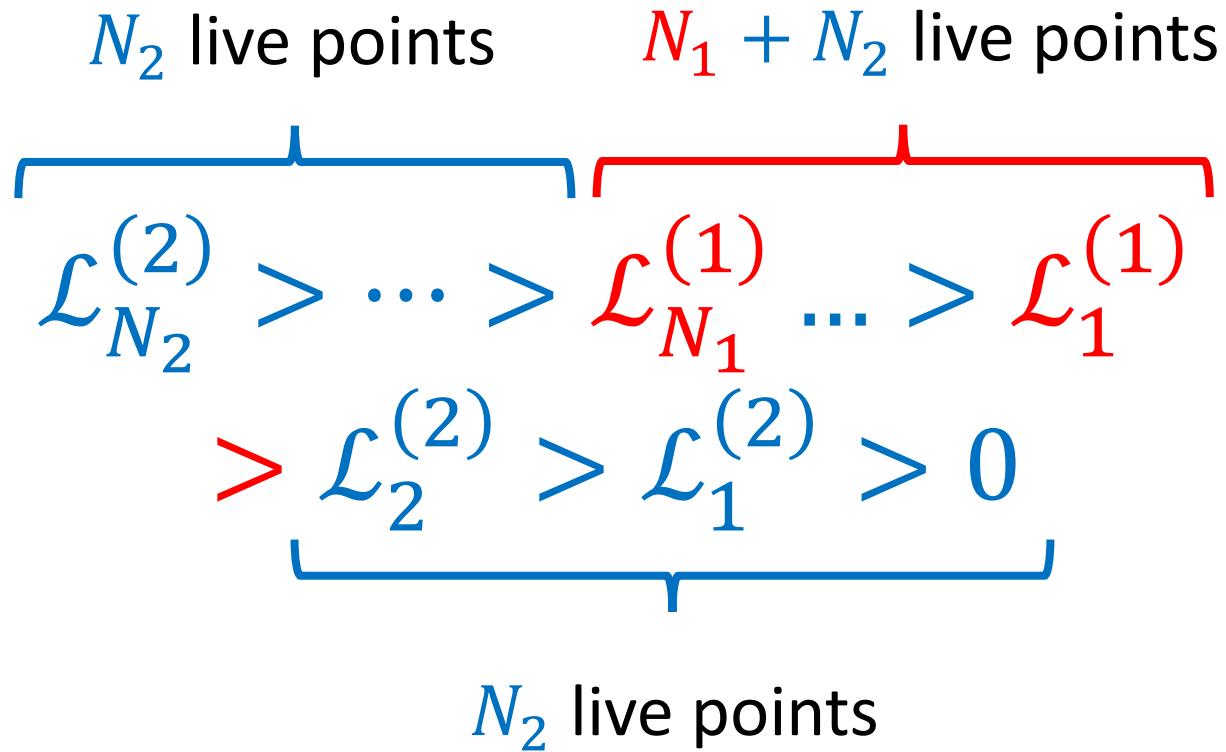
Dynamic Nested Sampling

$$\mathcal{L}_{\max}^{(1)} > \mathcal{L}_{N_1}^{(1)} > \dots > \mathcal{L}_2^{(1)} > \mathcal{L}_1^{(1)} > \mathcal{L}_{\min}^{(1)}$$

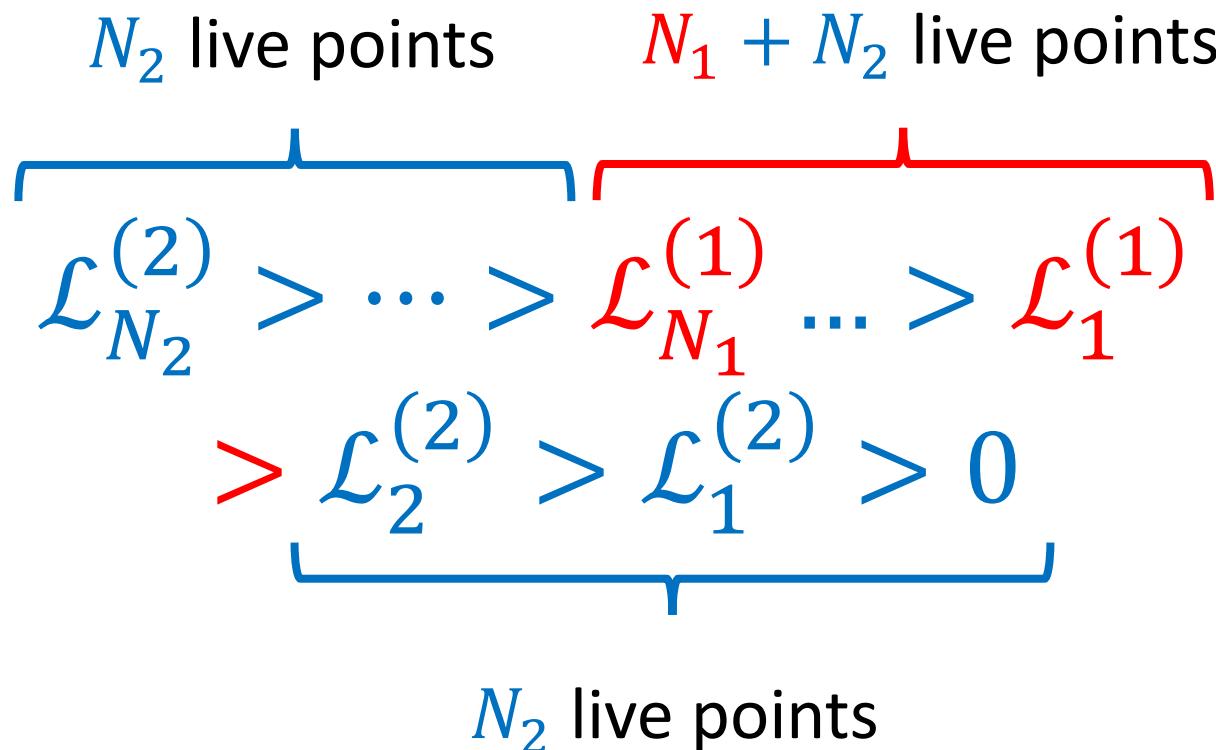
$$\mathcal{L}_{N_2}^{(2)} > \dots > \mathcal{L}_2^{(2)} > \mathcal{L}_1^{(2)} > 0$$



Dynamic Nested Sampling

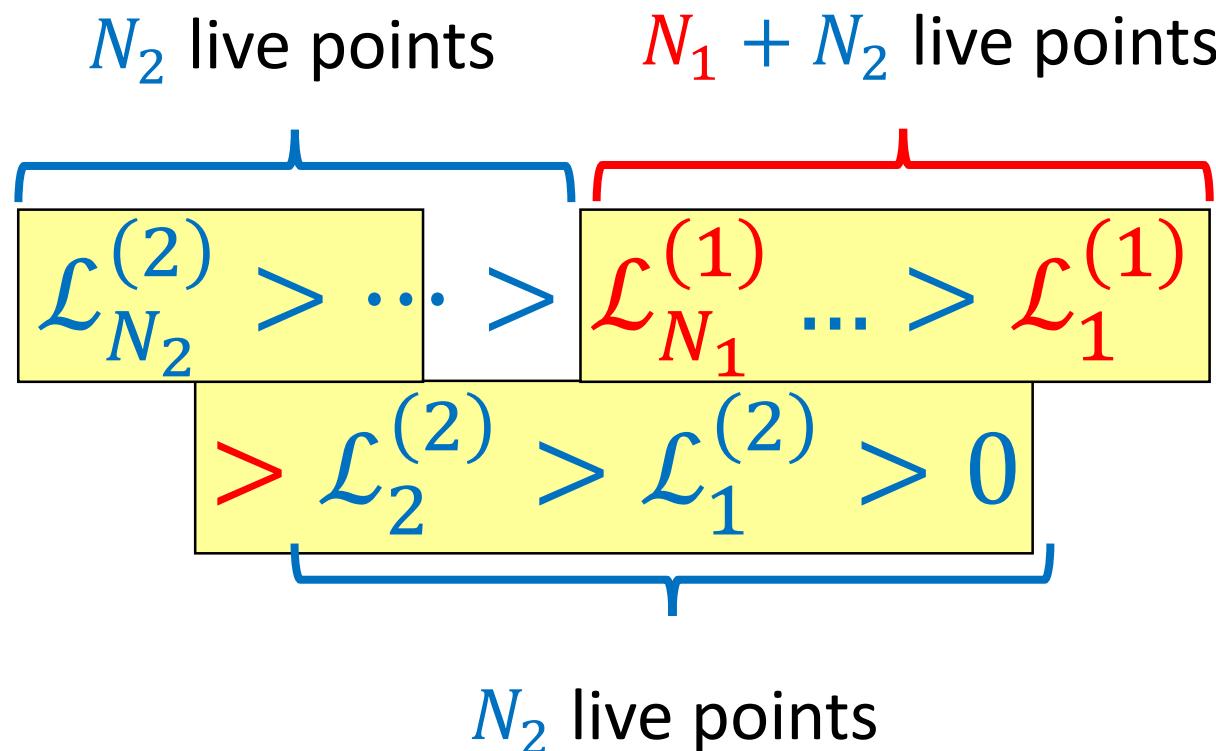


Dynamic Nested Sampling



$$\ln X_{i+1} = \sum_{j=1}^i \ln T_j$$

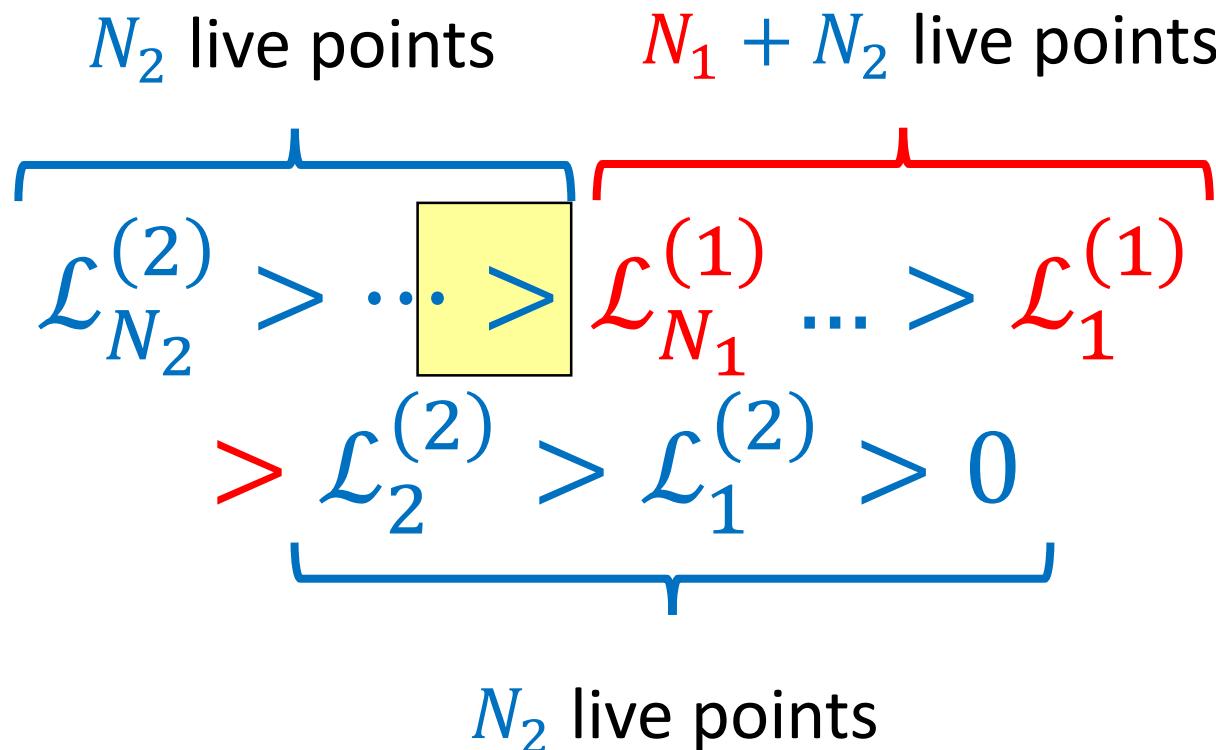
Dynamic Nested Sampling



$$\ln X_{i+1} = \sum_{j=1}^i \ln T_j$$

Constant/Increasing
 $K_{i+1} \geq K_i$:
 $T_{i+1} \sim \text{Beta}(K_{i+1}, 1)$

Dynamic Nested Sampling



$$\ln X_{i+1} = \sum_{j=1}^i \ln T_j$$

Constant/Increasing
 $K_{i+1} \geq K_i$:
 $T_{i+1} \sim \text{Beta}(K_{i+1}, 1)$

Decreasing sequence
 $K_{i+j>i} < K_i$:
 $T_{i+1}, \dots, T_{i+j} \sim U_{(K_i)}, \dots, U_{(K_i-j+1)}$

Static Nested Sampling

$$\ln \mathbb{E}[X_{N+k}] = \sum_{i=1}^N \ln \left(\frac{K}{K+1} \right) + \sum_{j=1}^k \ln \left(\frac{K-j+1}{K-j+2} \right)$$

Exponential shrinkage Uniform shrinkage

Dynamic Nested Sampling

$$\ln \mathbb{E}[X_N] = \sum_{i=1}^{n_1} \ln \left(\frac{K_i}{K_i + 1} \right) + \sum_{j=1}^{n_2} \ln \left(\frac{K_{n_1} - j + 1}{K_{n_1} - j + 2} \right)$$

Exponential shrinkage Uniform shrinkage

$$+ \dots + \sum_{j=1}^{K_{\text{final}}} \ln \left(\frac{K_{\text{final}} - j + 1}{K_{\text{final}} - j + 2} \right)$$

Benefits of Dynamic Nested Sampling

- Can accommodate new “strands” within a particular range of prior volumes without changing overall statistical framework.
- Particles can be adaptively added until stopping criteria are reached, allowing targeted estimation.

Benefits of Dynamic Nested Sampling

- Can accommodate new “strands” within a particular range of prior volumes without changing overall statistical framework.
- Particles can be adaptively added until stopping criteria are reached, allowing targeted estimation.

Allocating Samples

Posterior weight

$$I_P(i) \sim \hat{p}_i$$

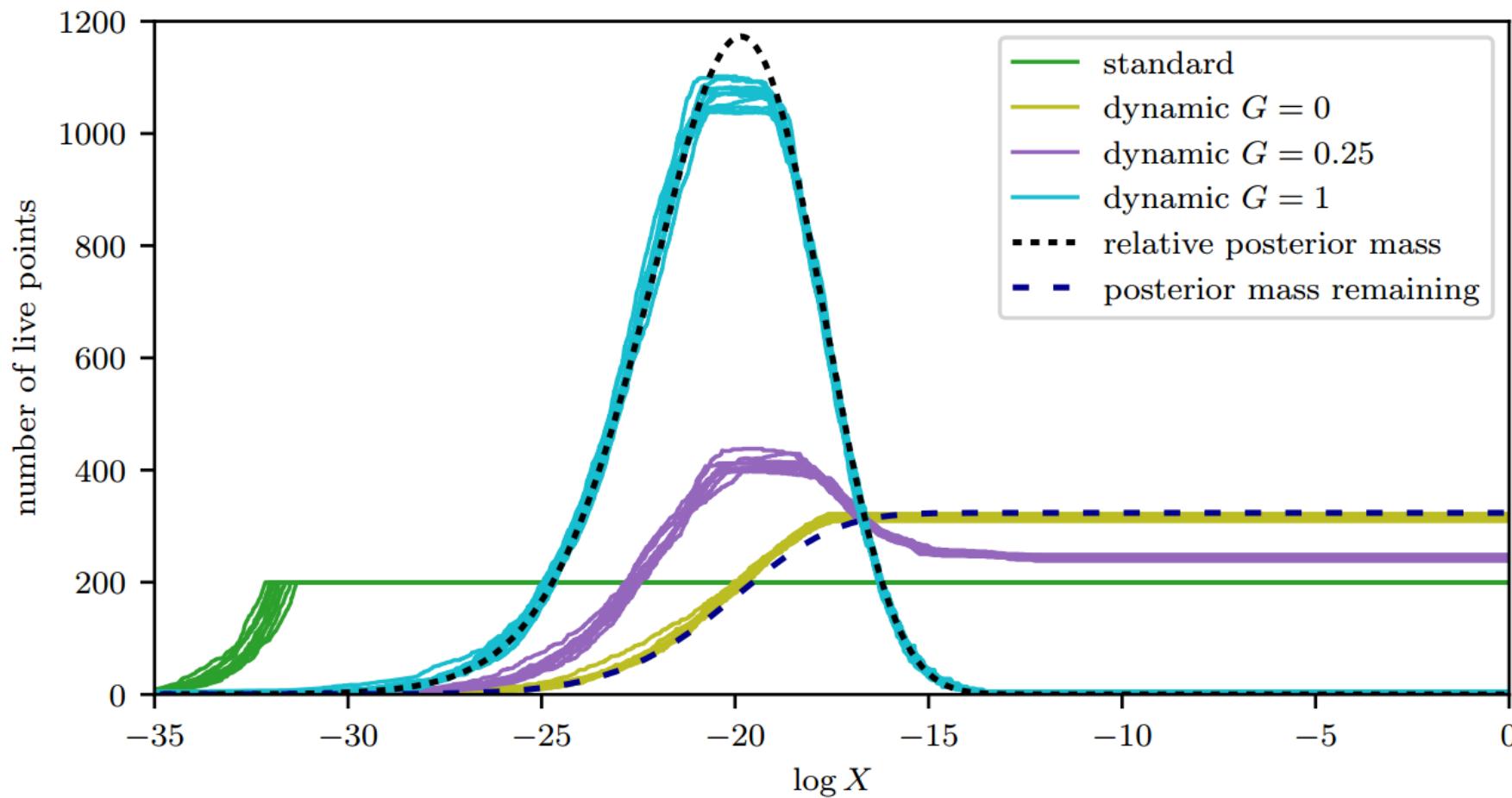
Weight Function

$$I(G, i) = G \frac{I_P(i)}{\sum_j I_P(j)} + (1 - G) \frac{I_Z(i)}{\sum_j I_Z(j)}$$

Evidence weight

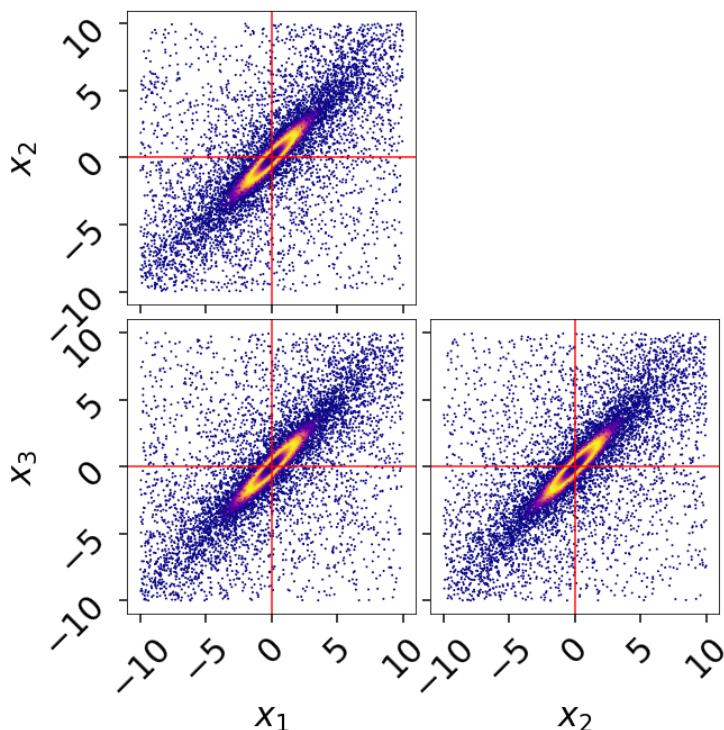
$$I_Z(i) \sim \frac{\mathbb{E}[\mathcal{Z}_{>i}]}{K_i}$$

Allocating Samples

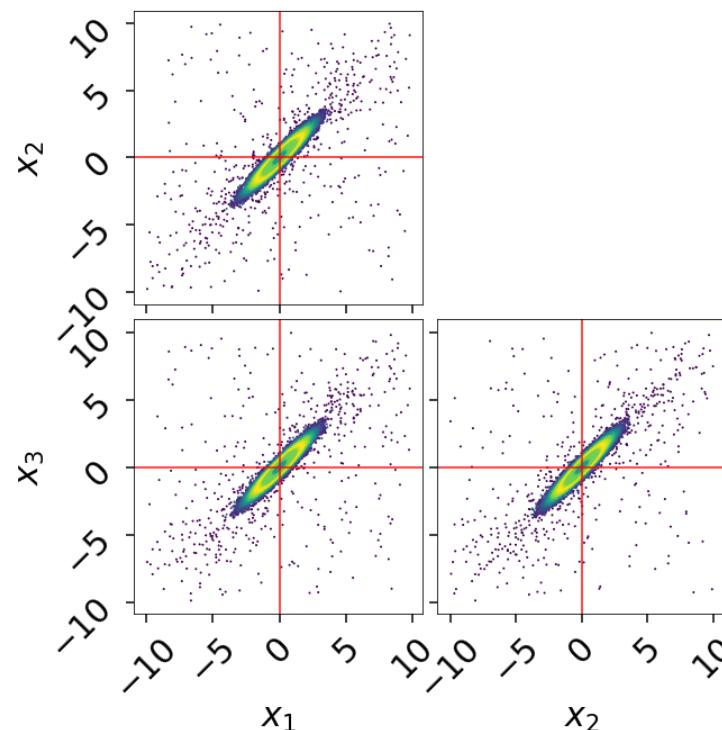


Allocating Samples

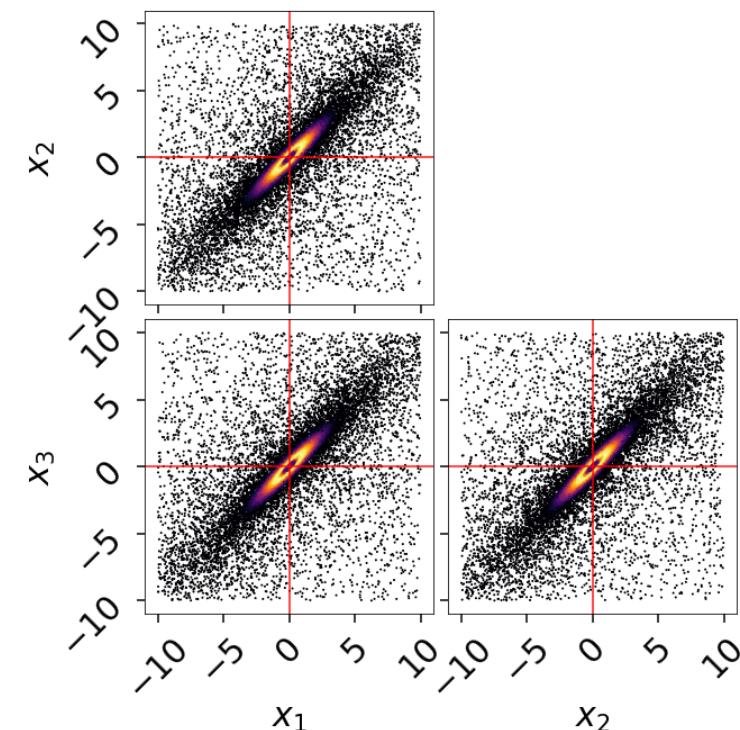
3-D correlated multivariate Normal



Static



Dynamic
(posterior)



Dynamic
(evidence)

How Many Samples is Enough?

How Many Samples is Enough?

- **III-posed question: depends on application!**

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

Assume general case: we want D-dimensional
 $\hat{p}(\{\Theta_i\})$ and $\tilde{p}(\{\Theta_i\})$ densities to be “close”.



“True” posterior
constructed over
same “domain”.

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

Assume general case: we want D-dimensional $\hat{p}(\{\Theta_i\})$ and $\tilde{p}(\{\Theta_i\})$ densities to be “close”.

$$H(\tilde{p}|\hat{p}) \equiv \int_{\Omega_\Theta} \hat{p}(\Theta) \ln \frac{\hat{p}(\Theta)}{\tilde{p}(\Theta)} d\Theta$$

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

Assume general case: we want D-dimensional $\hat{p}(\{\Theta_i\})$ and $\tilde{p}(\{\Theta_i\})$ densities to be “close”.

$$H(\tilde{p}|\hat{p}) = \sum_{i=1}^N \hat{p}_i \ln(\hat{p}_i/\tilde{p}_i)$$

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

Assume general case: we want D-dimensional $\hat{p}(\{\Theta_i\})$ and $\tilde{p}(\{\Theta_i\})$ densities to be “close”.

We want access to $P(\{\hat{p}_i\}|\tilde{p})$, but we don’t know $\tilde{p}(\Theta)$.

$$H(\tilde{p}|\hat{p}) = \sum_{i=1}^N \hat{p}_i \ln(\hat{p}_i/\tilde{p}_i)$$

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

Assume general case: we want D-dimensional $\hat{p}(\{\Theta_i\})$ and $\tilde{p}(\{\Theta_i\})$ densities to be “close”.

We want access to $\Pr(\{\hat{p}_i\}|p(\Theta))$, but we don’t know $p(\Theta)$.

Use bootstrap estimator.

$$H(\hat{p}|\tilde{p}') = \sum_{i=1}^N \tilde{p}'_i \ln(\tilde{p}'_i/\hat{p}_i)$$

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

Assume general case: we want D-dimensional $\hat{p}(\{\Theta_i\})$ and $\tilde{p}(\{\Theta_i\})$ densities to be “close”.

We want access to $\Pr(\{\hat{p}_i\}|p(\Theta))$, but we don’t know $p(\Theta)$.

Use bootstrap estimator.

$$H(\hat{p}|\tilde{p}') = \sum_{i=1}^N \tilde{p}'_i \ln(\tilde{p}'_i/\hat{p}_i)$$

Random variable

How Many Samples is Enough?

- In any sampling-based approach to estimating $p(\Theta)$ with $\hat{p}(\Theta)$, how many samples are necessary?

Assume general case: we want D-dimensional
 $\hat{p}(\{\Theta_i\})$ and $\tilde{p}(\{\Theta_i\})$ densities to be “close”.

We want access to $\Pr(\{\hat{p}_i\}|p(\Theta))$, but we don’t know $p(\Theta)$.

Use bootstrap estimator.

**Possible stopping criterion:
fractional (%) variation in H.**

Dynamic Nested Sampling Summary

1. Can sample from multi-modal distributions.
2. Can simultaneously estimate the evidence \hat{Z} and posterior $\hat{p}(\Theta)$.
3. Combining independent runs improves inference (“trivially parallelizable”).
4. Can simulate uncertainties (sampling and statistical) from a single run.
5. Enables adaptive sample allocation during runtime using arbitrary weight functions.
6. Possesses evidence/posterior-based stopping criteria.

Examples and Applications

Dynamic Nested Sampling with **dynesty**

Beta release

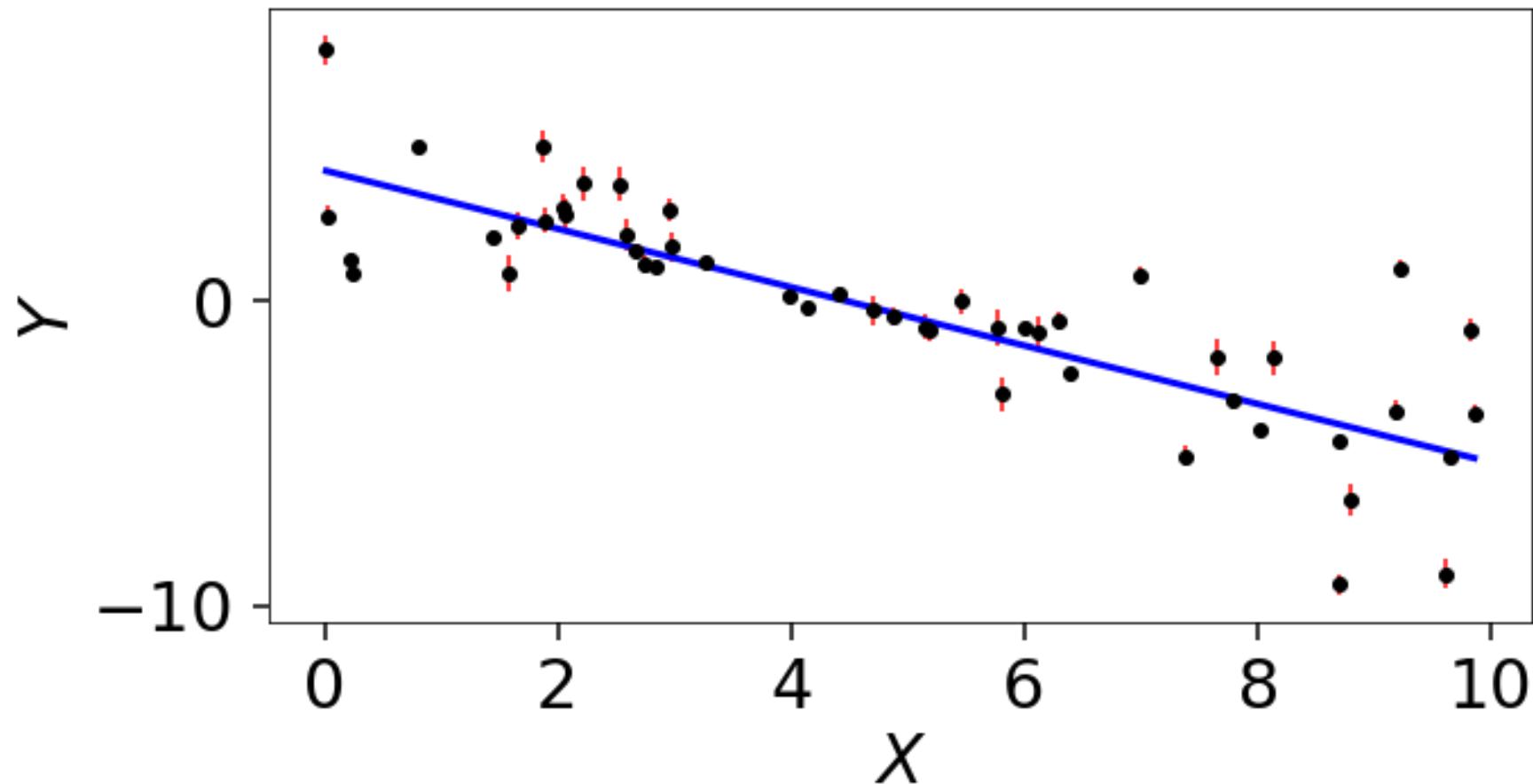
- Pure Python.
- Easy to use.
- Modular.
- Open source.
- Parallelizable.
- Flexible bounding/sampling methods.
- Thorough documentation!

dynesty.readthedocs.io

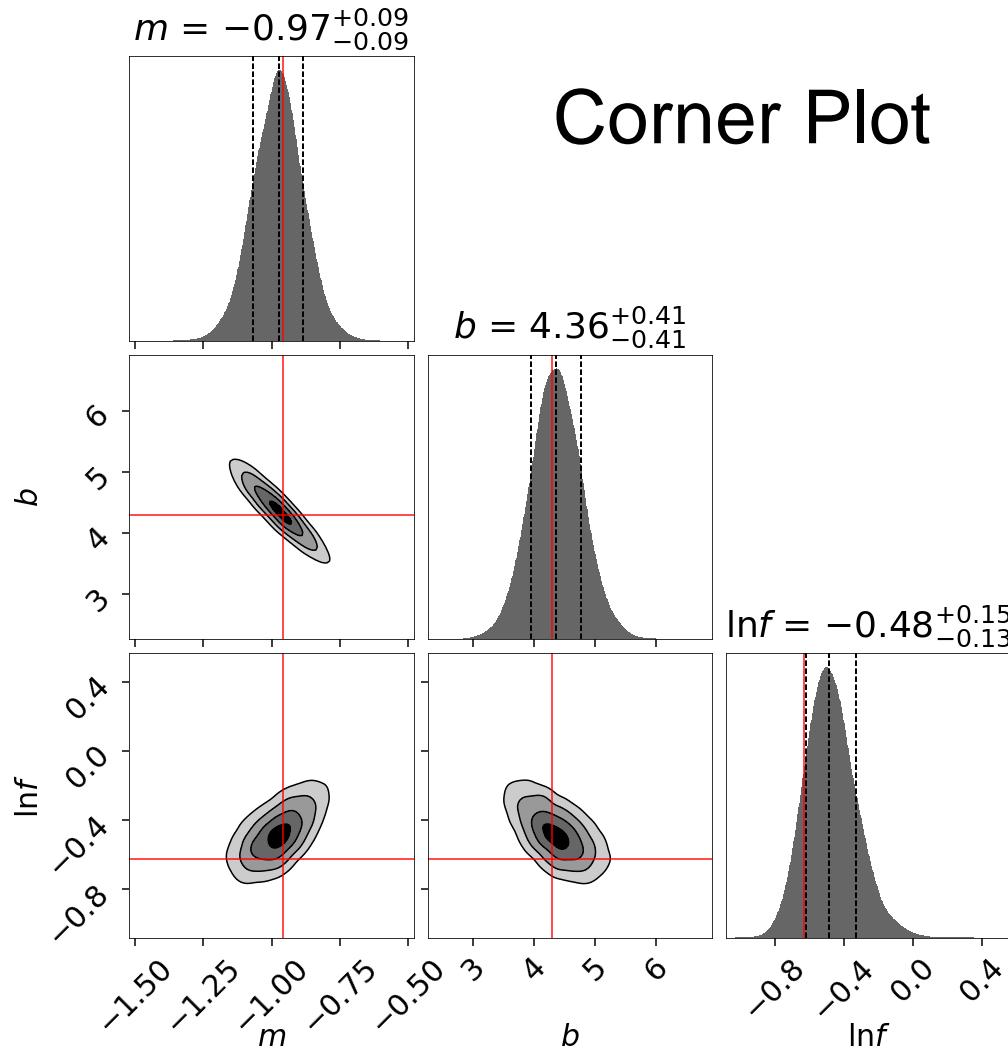
Example:

Example: Linear Regression (Posterior)

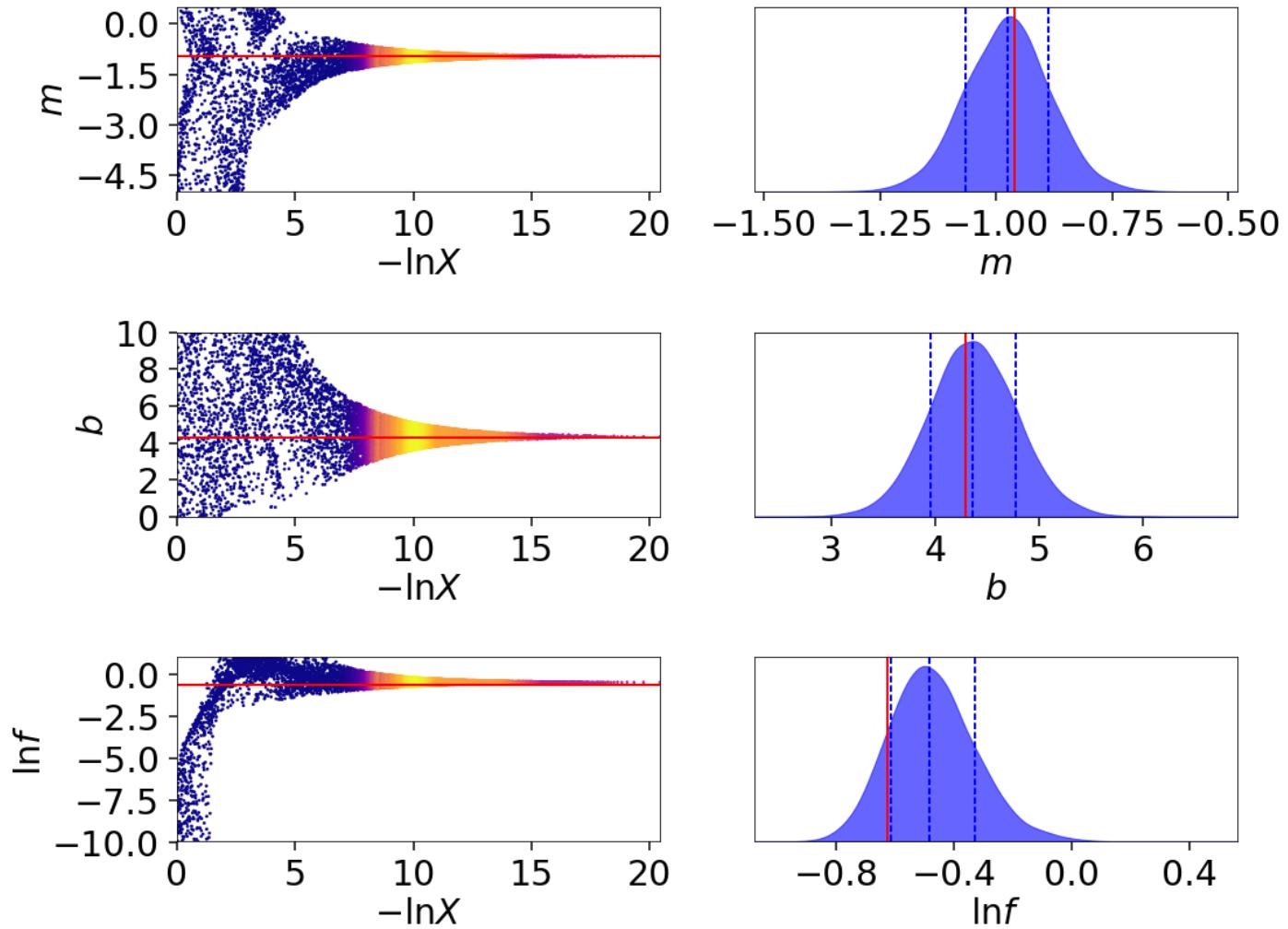
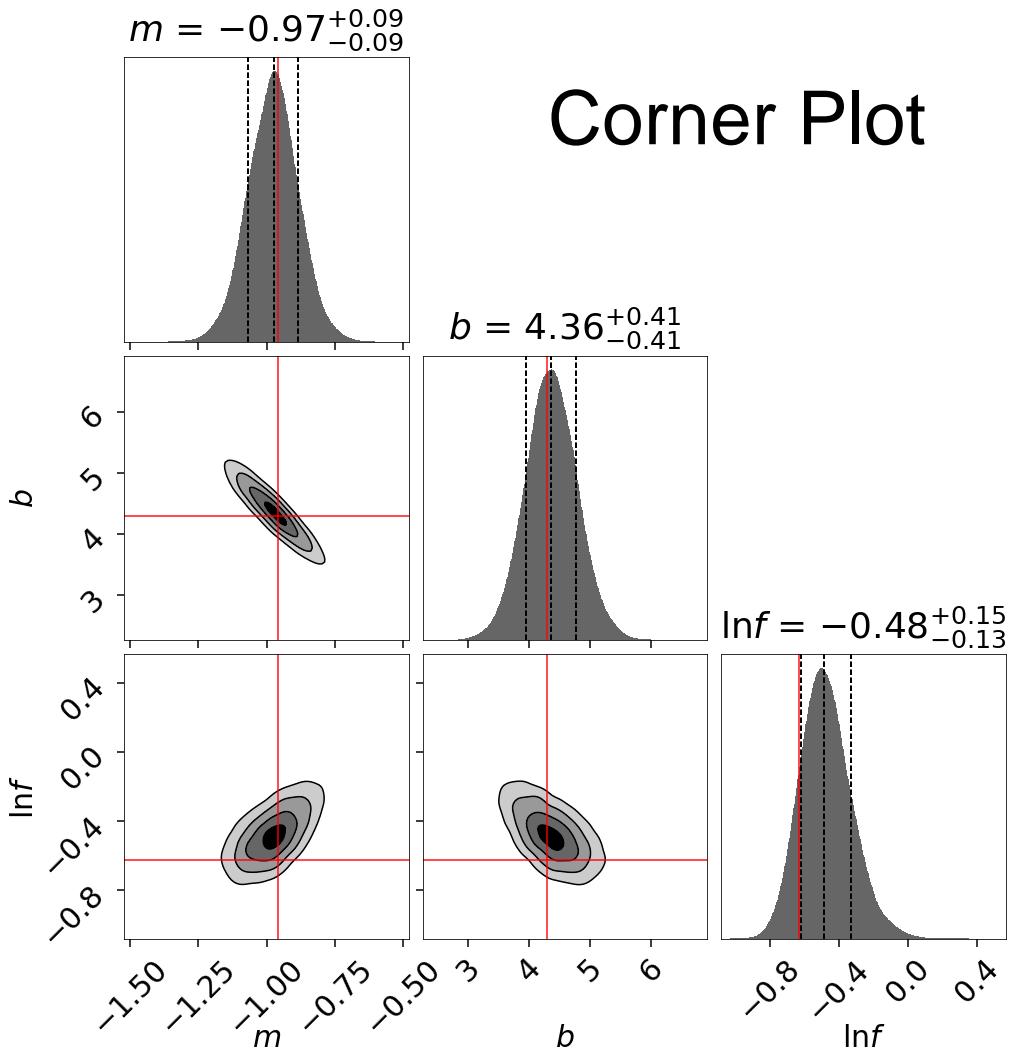
$$\Theta = \{a, b, \ln f\}$$



Example: Linear Regression (Posterior)

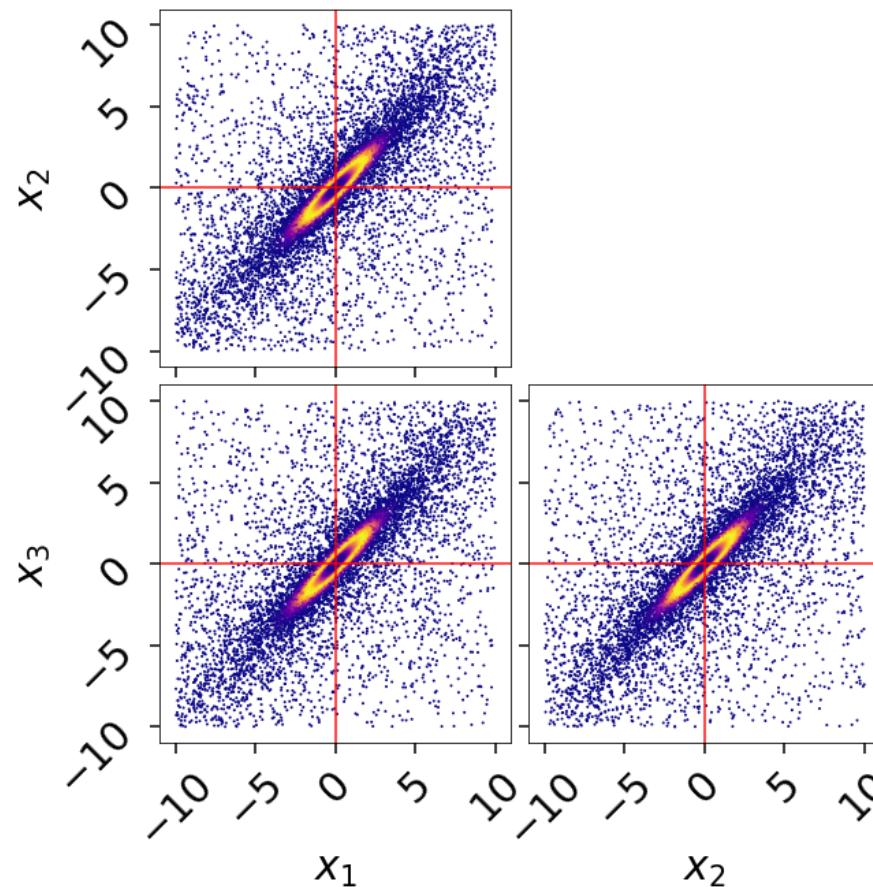


Example: Linear Regression (Posterior) Trace Plot

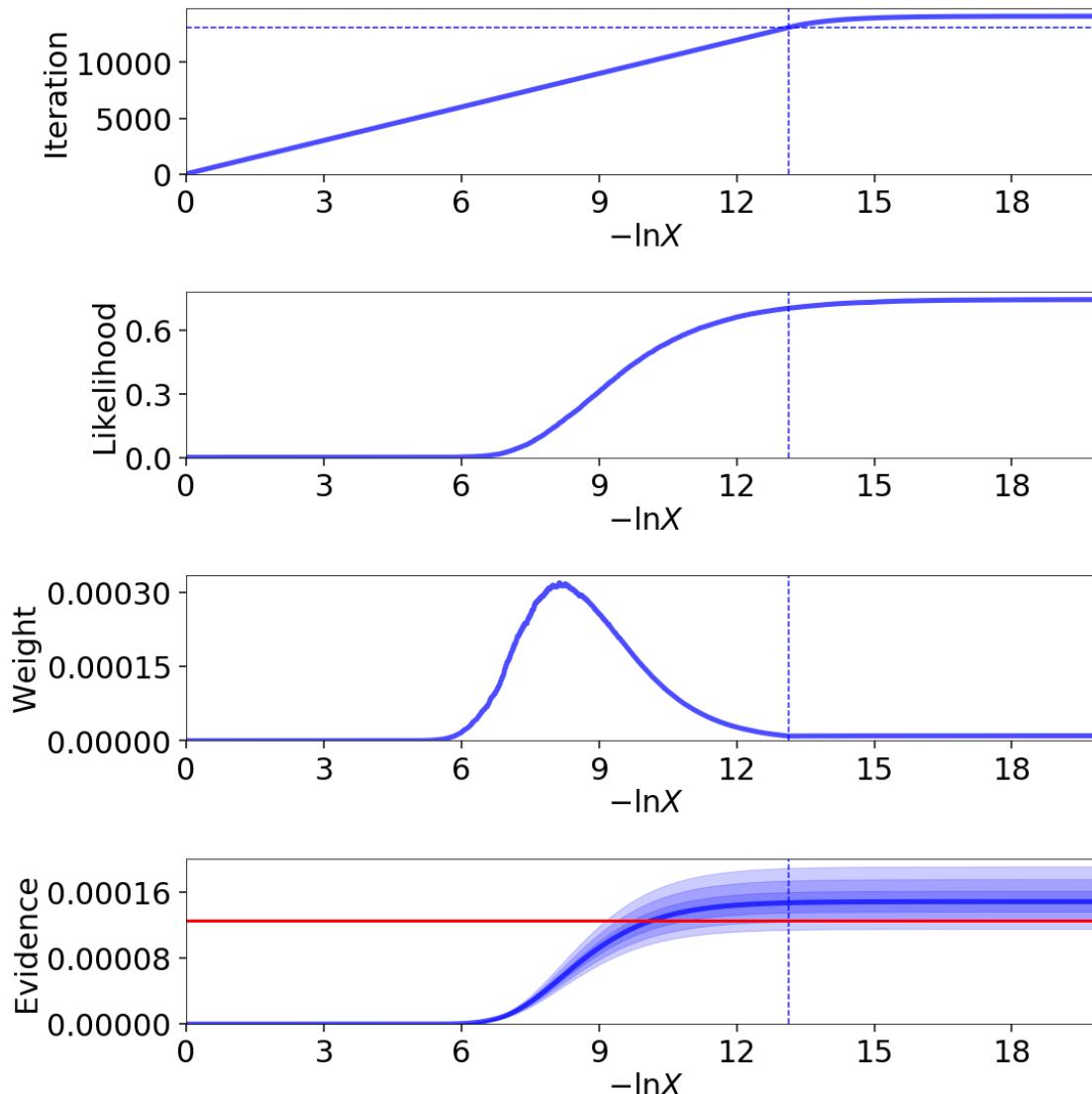


Example: Multivariate Normal (Evidence)

$$\Theta = \{x_1, x_2, x_3\}$$

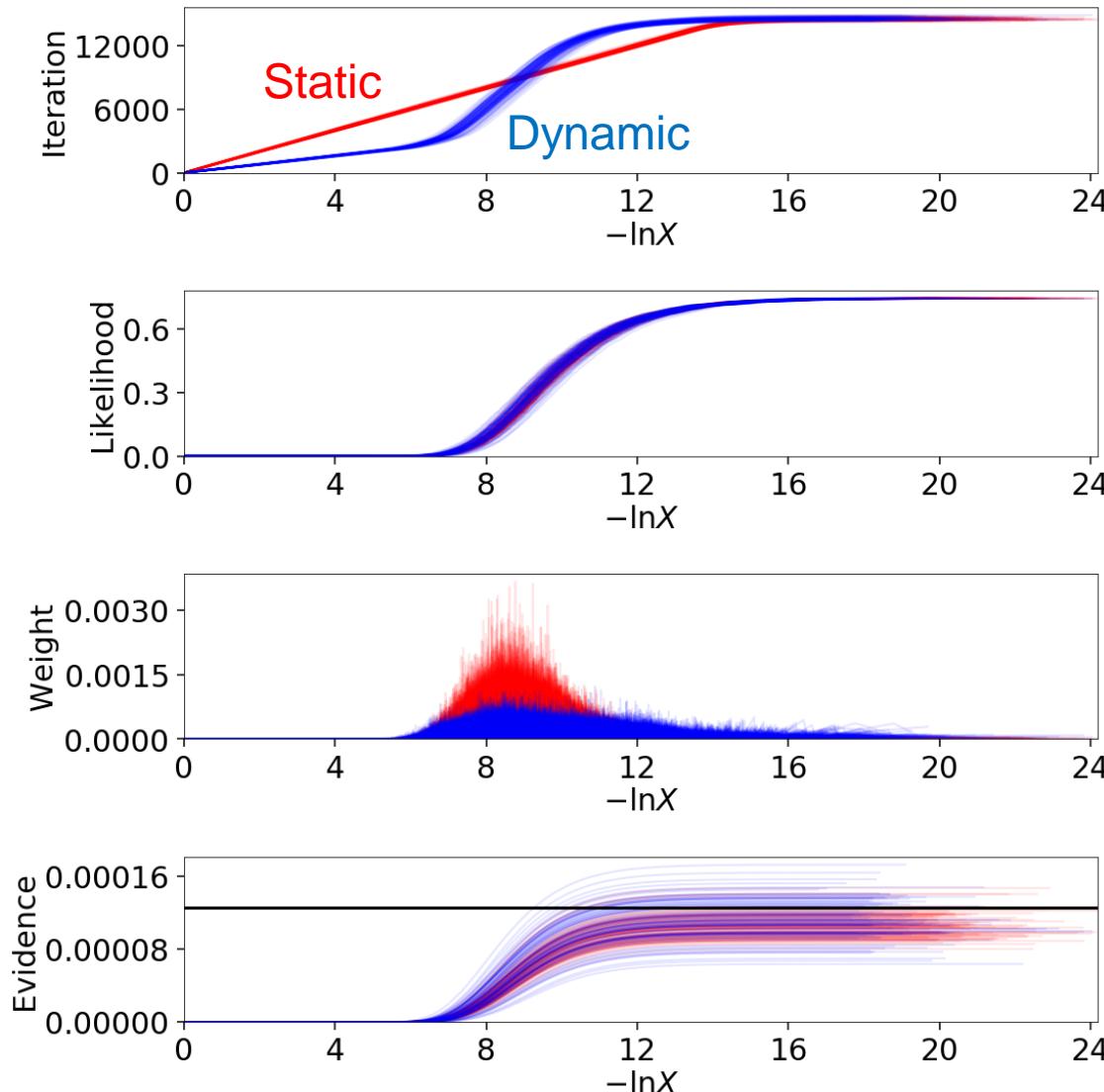


Example: Multivariate Normal (Evidence)



“Summary” Plot

Example: Multivariate Normal (Errors)



“Summary” Plot

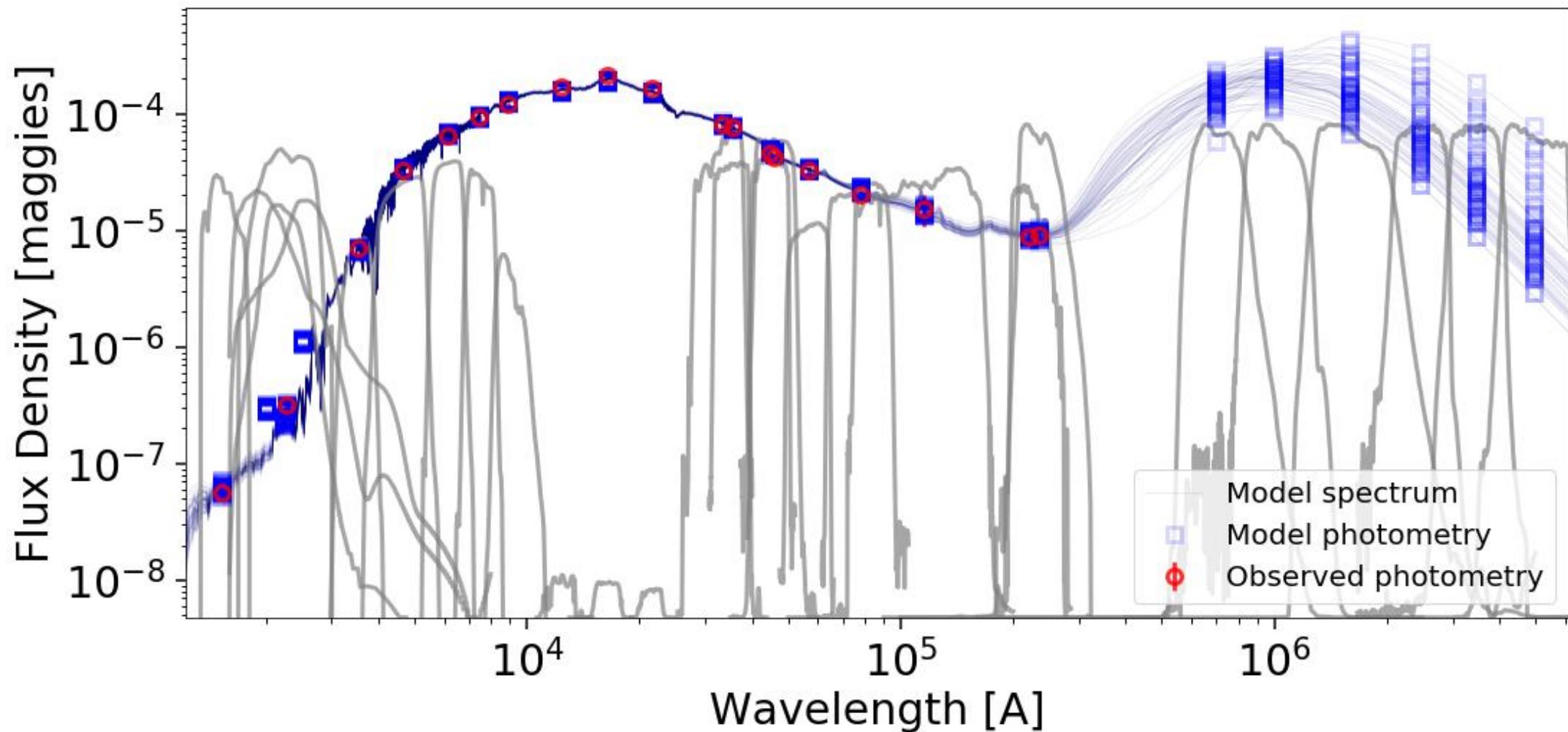
Application:

Application:

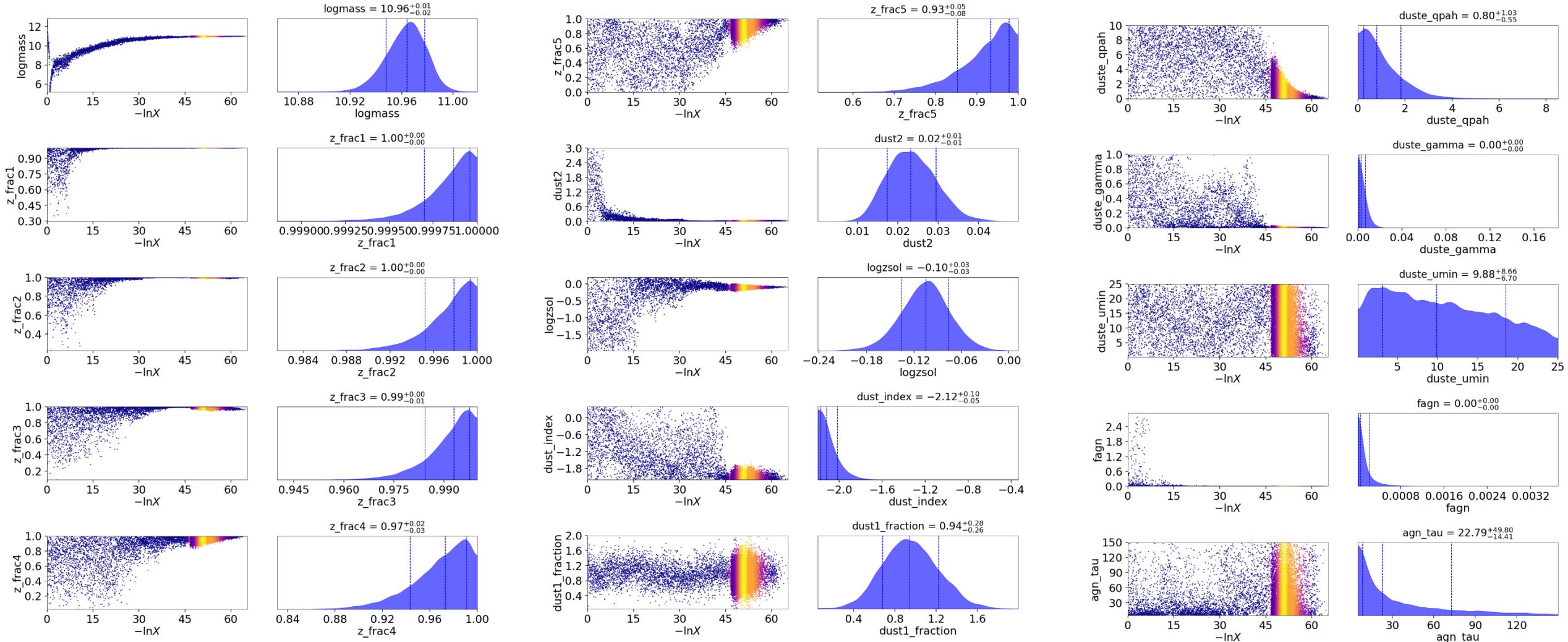
- All results are preliminary but agree with results from MCMC methods (derived using [emcee](#)).
- Samples allocated with 100% posterior weight, automated stopping criterion (2% fractional error in simulated KLD).
- `dynesty` was substantially (~3-6x) more efficient at generating good samples than `emcee`, **before thinning**.

Application: Modeling Galaxy SEDs

$$\Theta = \{\ln M_*, \ln Z, \sigma_5, \delta_6, \alpha_2\} \quad D=15$$



Application: Modeling Galaxy SEDs



Application: Modeling Galaxy SEDs

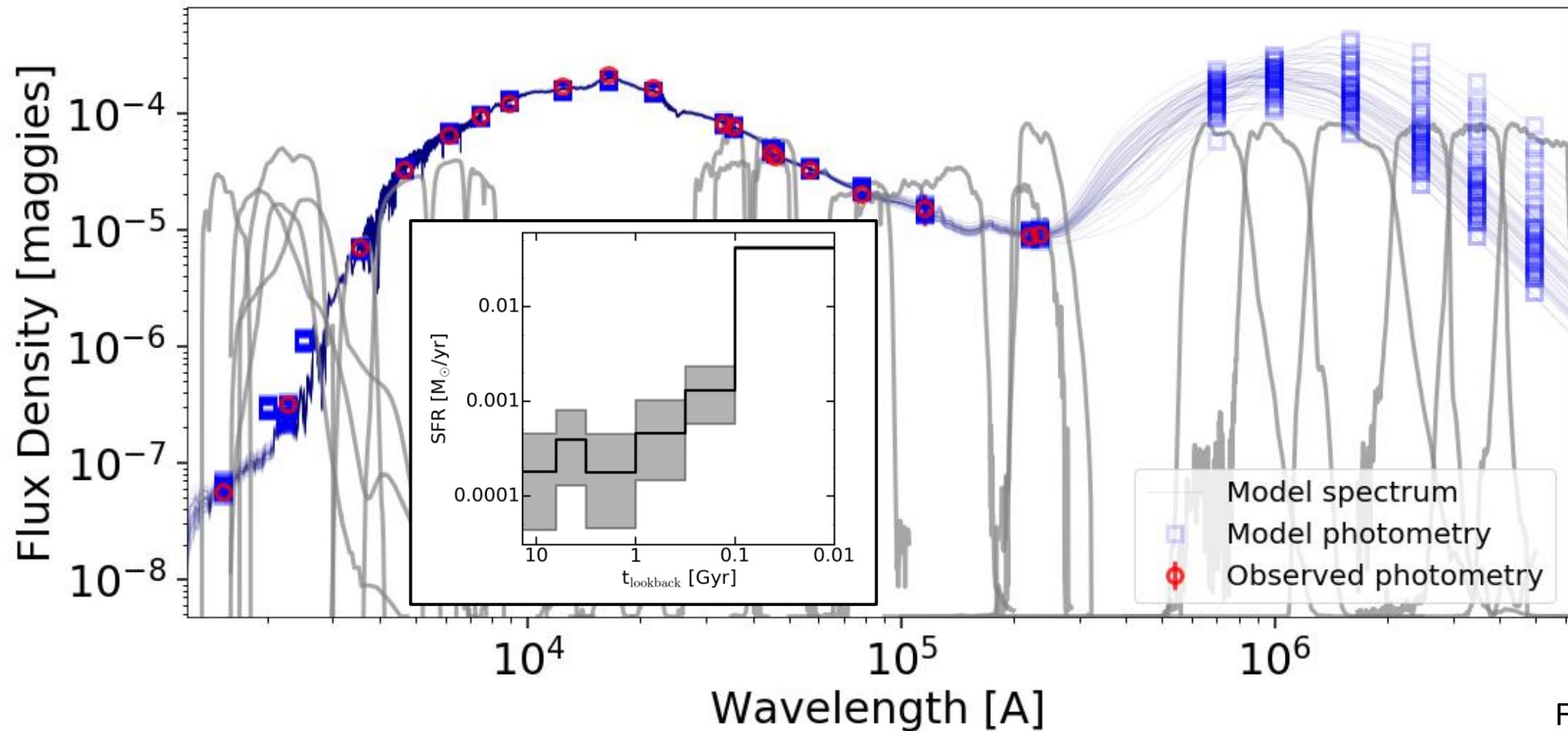


Fig: Joel Leja

Application: Supernovae Light Curves

$$\Theta = \{t_e, \rho_4, \epsilon_3, \delta_3, \sigma^2\} \quad D=12$$

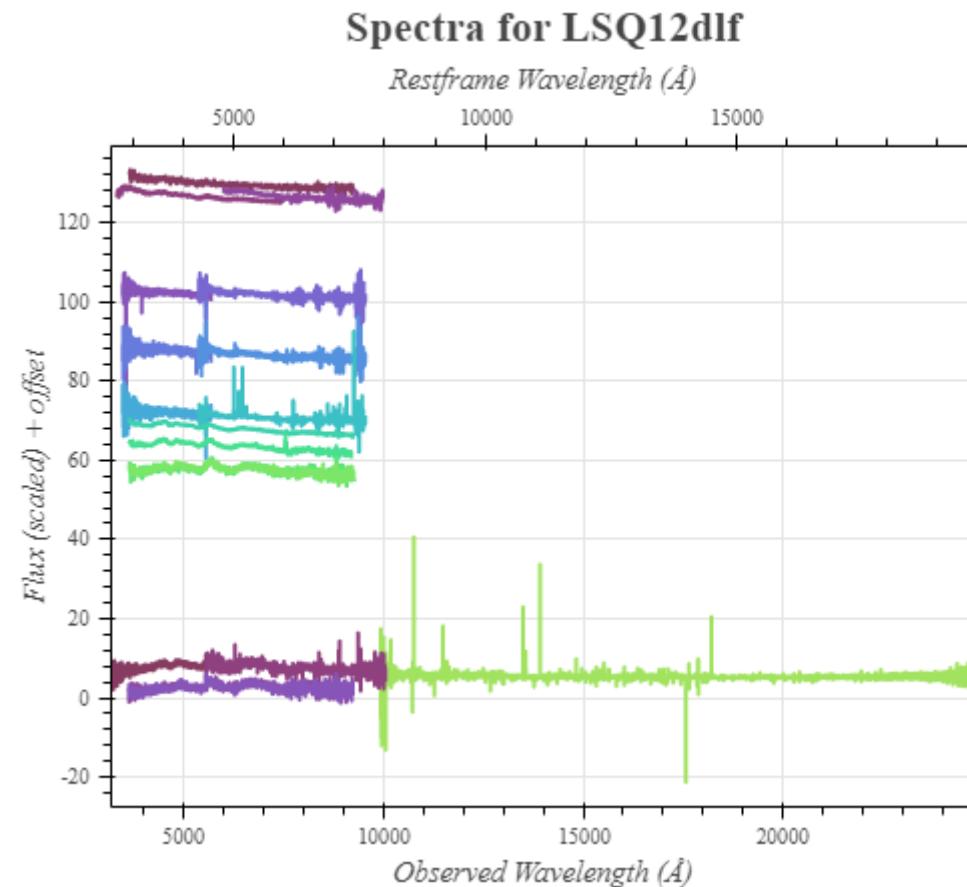
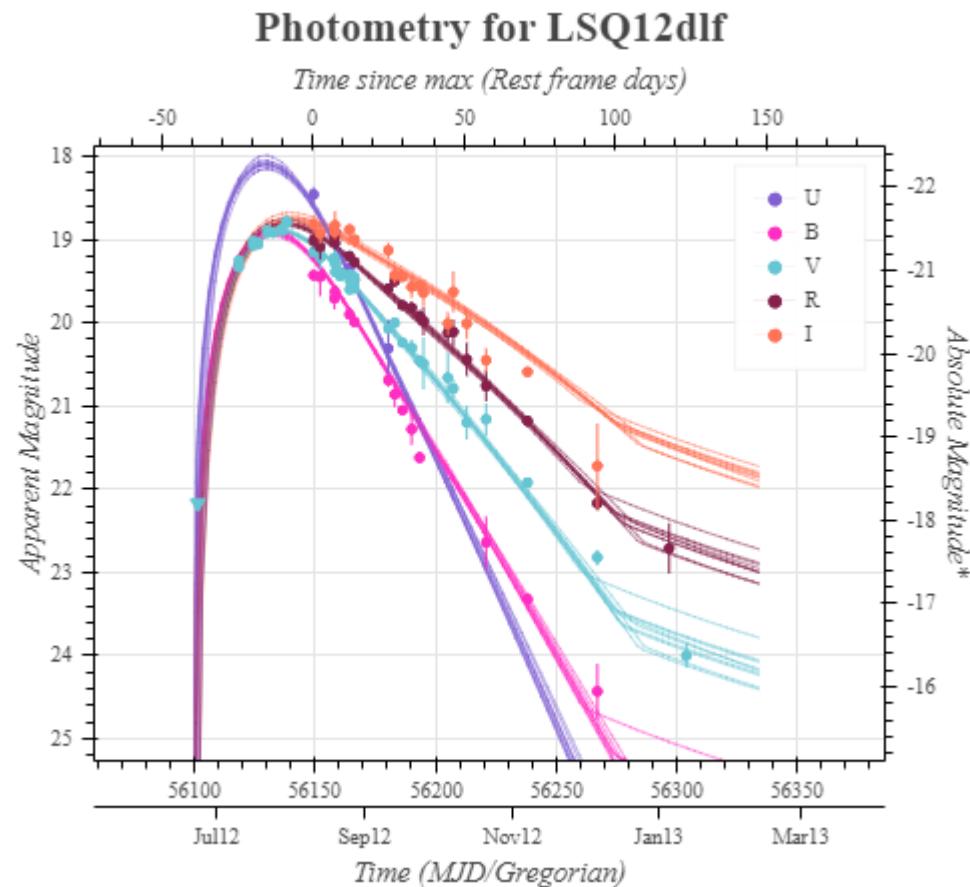
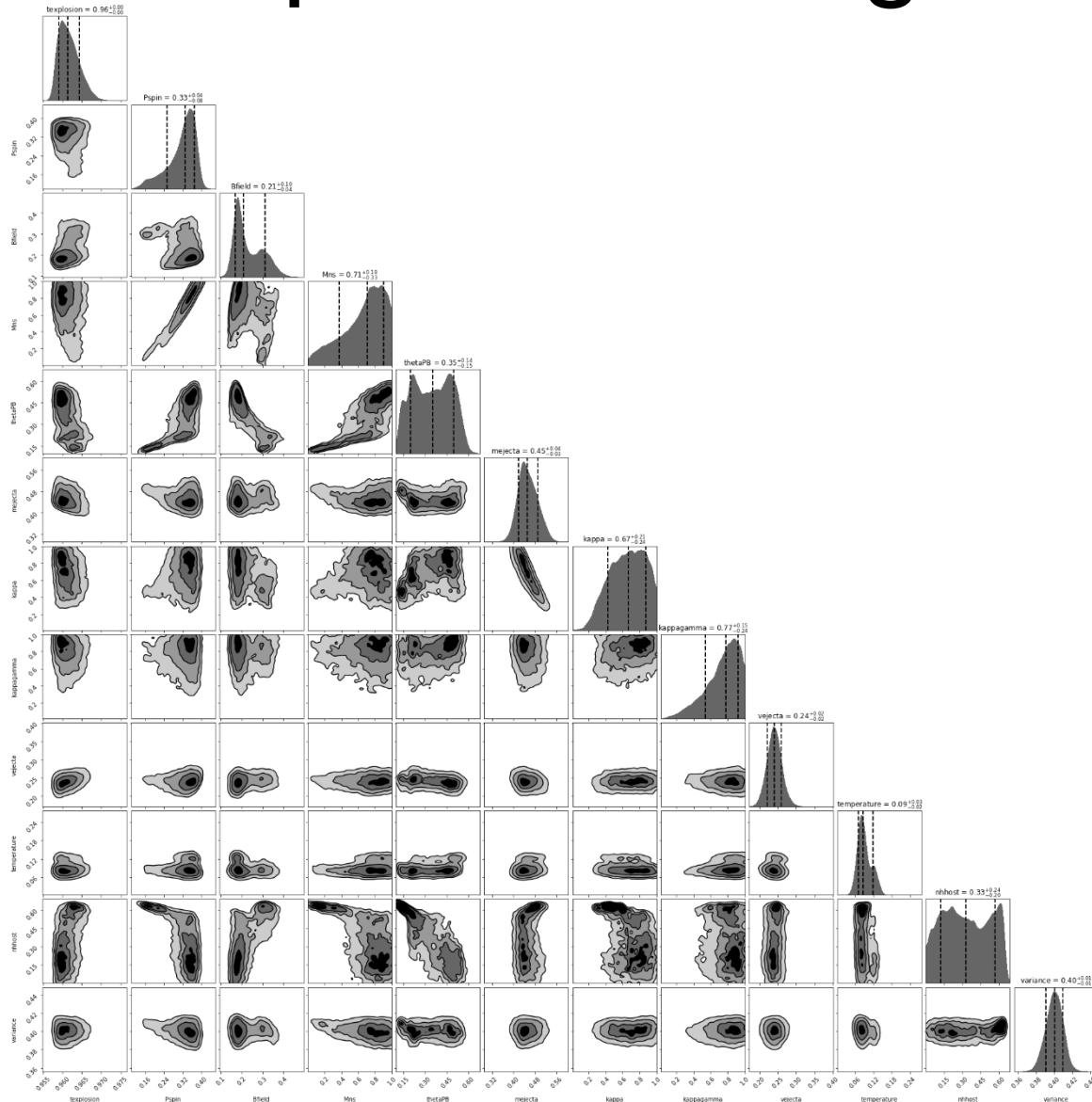


Fig: Open Supernova Catalog ([LSQ12dlf](#)), James Guillochon

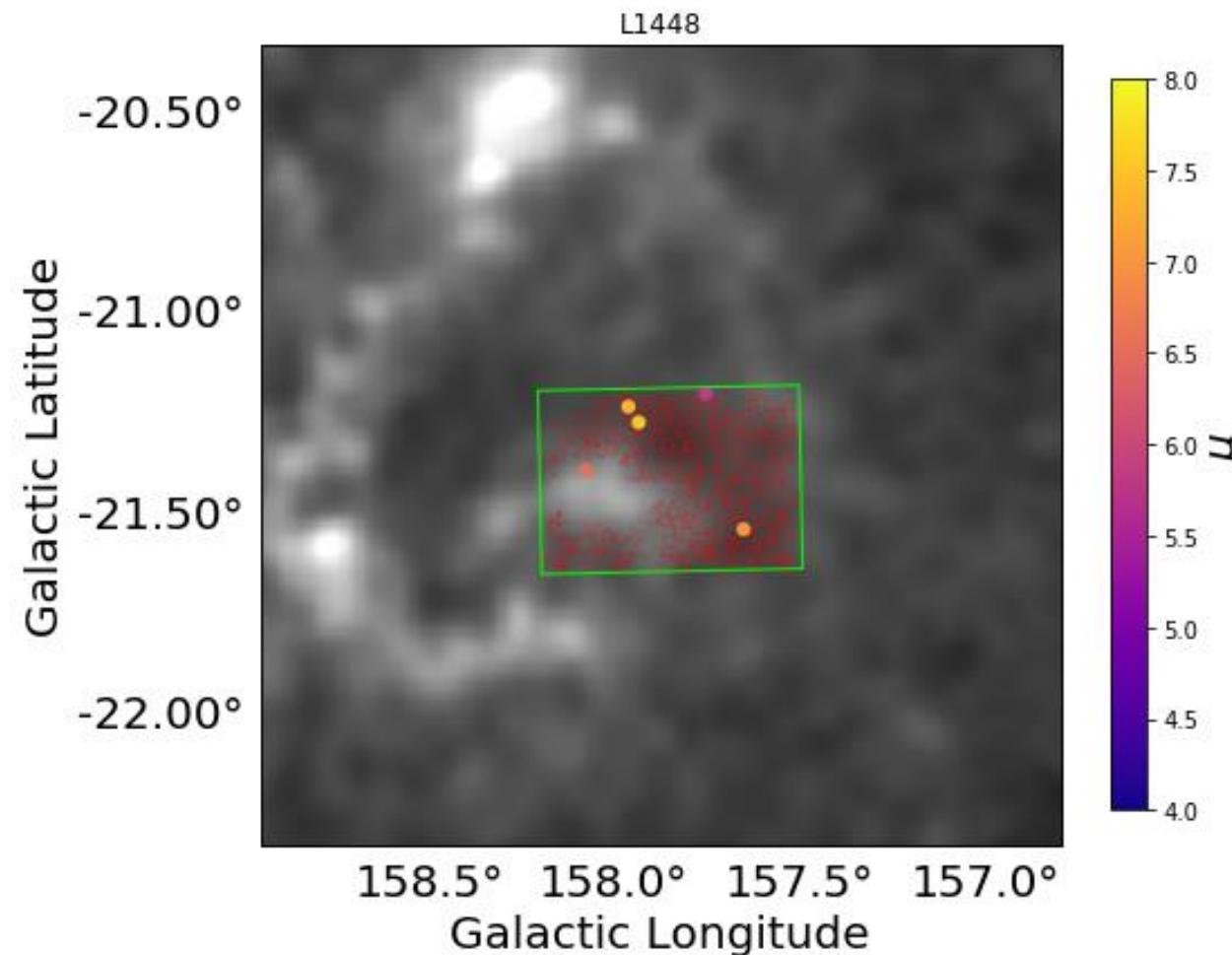
Application: Supernovae Light Curves



Application: Molecular Cloud Distances

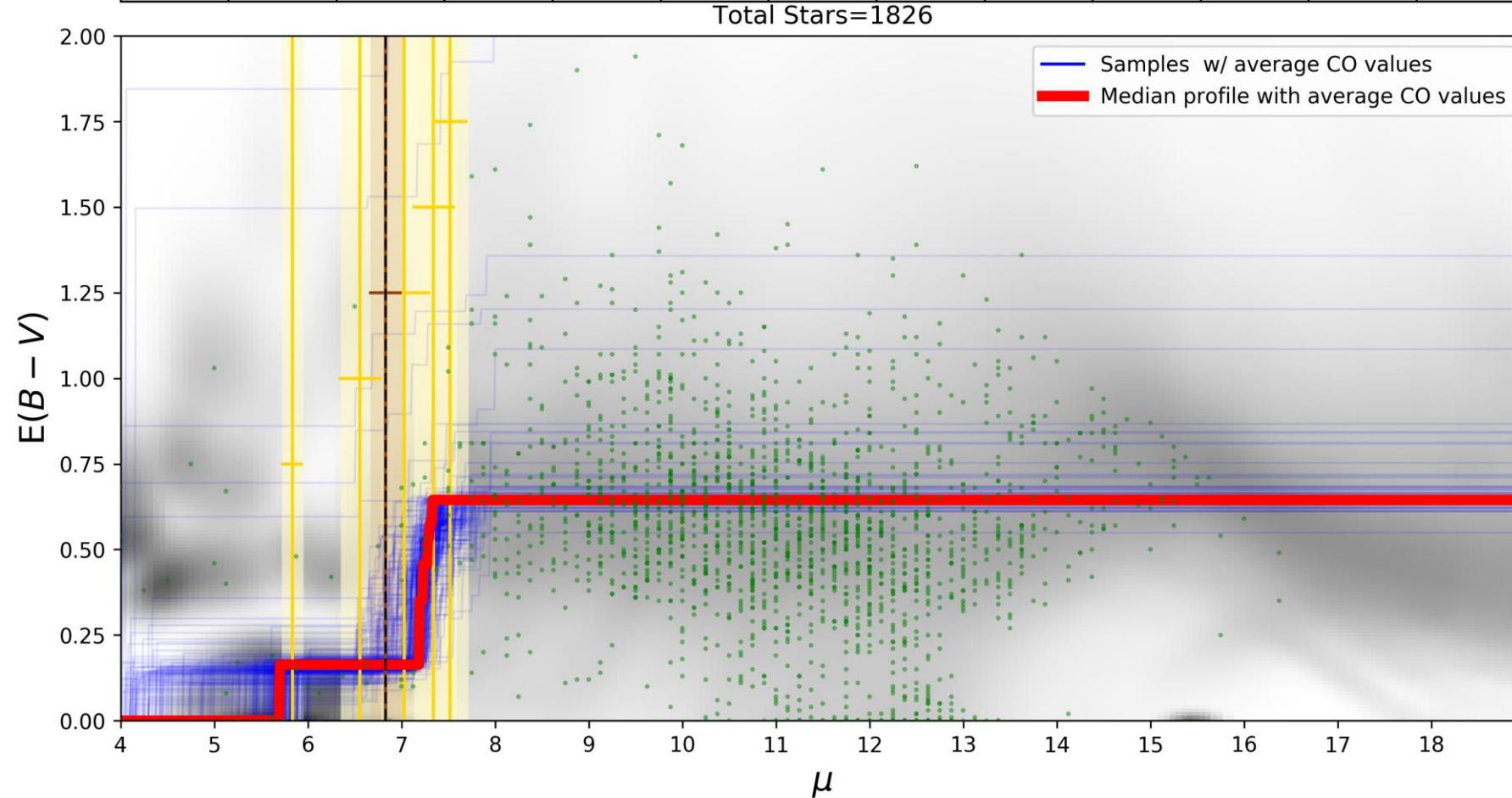
$$\Theta = \{f_2, d_5, c_5, p_o\}$$

D=13



Application: Molecular Cloud Distances

dfore	rfore	P_b	d1	d2	d3	d4	d5	c1	c2	c3	c4	c5
$5.70^{+0.15}_{-0.17}$	$0.16^{+0.01}_{-0.01}$	$0.04^{+0.00}_{-0.00}$	$7.31^{+0.10}_{-0.11}$	$7.29^{+0.13}_{-0.12}$	$7.24^{+0.10}_{-0.08}$	$7.20^{+0.06}_{-0.07}$	$7.34^{+0.13}_{-0.13}$	$0.79^{+0.07}_{-0.07}$	$0.57^{+0.04}_{-0.05}$	$0.76^{+0.05}_{-0.06}$	$1.16^{+0.09}_{-0.08}$	$1.66^{+0.11}_{-0.10}$
			-1.2 km/s	0.8 km/s	2.8 km/s	4.9 km/s	6.9 km/s					



Dynamic Nested Sampling with **dynesty**

Beta release

- Pure Python.
- Easy to use.
- Modular.
- Open source.
- Parallelizable.
- Flexible bounding/sampling methods.
- Thorough documentation!

dynesty.readthedocs.io