A Simple Approach to Parallel Nested Sampling

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Outline

Introduction

2 Bayesian inference and nested sampling

3 Combining independent chains







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Introduction

- Nested sampling's precision is limited by N.
- Increasing N requires more computation.
- Concurrently-run, independent nested sampling results can be combined to increase the effective value of *N*.
- Several examples demonstrate this technique's utility.



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4 Examples

5 Conclusion



Parameter estimation and model selection

Parameter estimation

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



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Parameter estimation and model selection

Parameter estimation

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

Abbreviations

$$Pr(\boldsymbol{\Theta}|\boldsymbol{D}, M) \equiv \mathscr{P}(\boldsymbol{\Theta}) \qquad Pr(\boldsymbol{D}|\boldsymbol{\Theta}, M) \equiv \mathscr{L}(\boldsymbol{\Theta})$$
$$Pr(\boldsymbol{\Theta}|M) \equiv \pi(\boldsymbol{\Theta}) \qquad Pr(\boldsymbol{D}|M) \equiv \mathscr{Z}$$



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Parameter estimation and model selection

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Model selection

 $\Pr(M|D) \propto \Pr(D|M)\Pr(M)$



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Model selection

Model posterior ratio

$$\frac{\Pr\left(M_{1}|\boldsymbol{D}\right)}{\Pr\left(M_{2}|\boldsymbol{D}\right)} = \frac{\Pr\left(\boldsymbol{D}|M_{1}\right)}{\Pr\left(\boldsymbol{D}|M_{2}\right)} \frac{\Pr\left(M_{1}\right)}{\Pr\left(M_{2}\right)}$$



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Model selection

Model posterior ratio

$$\frac{\Pr(M_1|D)}{\Pr(M_2|D)} = \frac{\Pr(D|M_1)}{\Pr(D|M_2)} \frac{\Pr(M_1)}{\Pr(M_2)}$$

Evidence integral

$$\Pr(\boldsymbol{D}|\boldsymbol{M}) = \int_{\boldsymbol{\Theta}} \Pr(\boldsymbol{D}|\boldsymbol{\Theta}, \boldsymbol{M}) \Pr(\boldsymbol{\Theta}|\boldsymbol{M}) \, \mathrm{d}\boldsymbol{\Theta}$$



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Nested sampling

Prior mass

$$X(L) = \int_{\{\Theta: \mathcal{L}(\boldsymbol{\Theta}) > L\}} \pi(\boldsymbol{\Theta}) \,\mathrm{d}\boldsymbol{\Theta}$$



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Nested sampling

Prior mass

$$X(L) = \int_{\{\Theta: \mathcal{L}(\Theta) > L\}} \pi(\Theta) \,\mathrm{d}\Theta$$

Alternate evidence integral

$$\mathscr{Z} = \int_0^1 L(X) \,\mathrm{d}X$$



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Estimating the prior mass

For a set of parameters Θ , the likelihood can be computed exactly. Prior mass, however, generally must be estimated.



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Shrinkage

$$t_i = \frac{X_i}{X_{i-1}}$$



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For a set of parameters Θ , the likelihood can be computed exactly. Prior mass, however, generally must be estimated.

Shrinkage

$$t_i = \frac{X_i}{X_{i-1}}$$

Shrinkage distribution

$$t_i \sim \text{Beta}(N, 1)$$



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$$X_i = \prod_{k=1}^i t_k$$



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$$X_i = \prod_{k=1}^i t_k$$

Estimating evidence with quadrature

$$Z \approx \sum_{i=1}^{m} \left(X_{i-1} - X_i \right) L_i$$



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Uncertainty in evidence estimate

$$\exp\left(\pm\sqrt{H/N}\right)$$



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Uncertainty in evidence estimate

$$\exp\left(\pm\sqrt{H/N}\right)$$

Larger N gives a smaller uncertainty in the evidence estimate. Raising N requires more computation time. Unless we can combine samples from independent runs!

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Combining independent chains – general case

General case: ${\it M}$ ordered sets of discarded samples with associated prior mass ${\it X}$

$$\begin{aligned} \boldsymbol{X}^{1} &= \left\{ X_{1}^{1}, X_{2}^{1}, \cdots, X_{Q_{1}}^{1} \right\} \\ \boldsymbol{X}^{2} &= \left\{ X_{1}^{2}, X_{2}^{2}, \cdots, X_{Q_{2}}^{2} \right\} \\ &\vdots \\ \boldsymbol{X}^{M} &= \left\{ X_{1}^{M}, X_{2}^{M}, \cdots, X_{Q_{M}}^{M} \right\} \end{aligned}$$



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Combining independent chains – simplest case

Simplest case has two sets of one discarded sample each.

$$\boldsymbol{X}^1 = \left\{ \boldsymbol{X}_1^1 \right\}$$
$$\boldsymbol{X}^2 = \left\{ \boldsymbol{X}_1^2 \right\}$$

Combined set is

$$\hat{\boldsymbol{X}}^{1,2} = \left\{ \hat{X}_1^{1,2}, \hat{X}_2^{1,2} \right\}$$

What is the distribution of the shrinkage from the larger member to the smaller member of $\hat{X}^{1,2}$?



Combining independent chains - shrinkage

The shrinkage t is defined

$$t_i = \frac{X_i}{X_{i-1}}$$

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For the first sample,

$$t_1 = \frac{X_1}{1} = X_1$$

In our example,

$$\hat{X}_{1}^{1,2} = \hat{t}_{1}^{1,2} \sim \text{Beta}(N,1)$$



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Combining independent chains – highest order statistic

For a set with n members i.i.d. as f(x) with CDFs F(x), the density of the *i*th order statistic is

$$f_{\hat{X}_{(i)}}(x) = \frac{n!}{(n-i)! (i-1)!} f(x) [F(x)]^{i-1} [1 - F(x)]^{n-i}$$

In our example,

$$f_{\hat{X}_{(2)}}(x) = 2f(x)[1 - F(x)]$$

$$f_{t_i}(x) = N x^{N-1}$$
 $F_{t_i}(x) = x^N$



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Combining independent chains – highest order statistic

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In our example,

$$f_{\hat{X}_{(2)}}(x) = 2f(x)[1 - F(x)]$$

$$f_{t_i}(x) = N x^{N-1}$$
 $F_{t_i}(x) = x^N$

$$f_{X_{(2)}}(x) = 2Nx^{2N-1}$$



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Generalization

- Show empirically that, in general, shrinkage in combined set is distributed as $\text{Beta}(N \times M, 1)$
- Procedure
 - ▶ Generate 32 sets of 10,000 shrinkage samples from *Beta*(100, 1).
 - Get prior mass values from cumulative product of shrinkage samples in each set.
 - Combine sets of prior mass samples, then sort by prior mass.
 - Compute actual shrinkage between each consecutive pair of samples.
 - Compare sample mean of log t with $\frac{1}{N}$ and $\frac{1}{N \times M}$.



Generalization results

- $\frac{1}{N} = 1/100 = 0.01$
- $\frac{1}{N \times M} = 1/3200 = 3.125 \times 10^{-4}$
- Log geometric mean of combined shrinkage samples: $3.200 \times 10^{-4} \pm 4.146 \times 10^{-5}$
- Relative error with $\frac{1}{N}$: 96.80%
- Relative error with $\frac{1}{N \times M}$: 2.393%



Many ways to implement:

- Concurrent independent nested sampling runs using multiple supercomputer nodes, processor cores, GPU cores, etc.
- Concurrent or non-concurrent independent NS runs by different users, later combined to improve precision
- If original evidence estimate is not precise enough, subsequent NS runs can be used to improve precision



Advantages

- Runs are independent (i.e., no communication is required), so the speed-up is nearly ideal.
- Posterior distributions with multiple high-probability modes can be sampled effectively.
- Precision can be improved with subsequent runs.



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Examples

- Eggcrate likelihood function
- Modified lighthouse problem
- Sum of sinusoidal signals in noise



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Nested sampling implementation details

- Evidence is estimated by sampling shrinkage distribution instead of using geometric mean
- Log-evidence error bars are the standard deviations of the log-evidence samples



Eggcrate

Prior

$$\pi(\boldsymbol{\Theta}) = \left(\frac{1}{10\pi}\right)^2 \mathbb{1}_{[0,10\pi]} \left(\boldsymbol{\Theta}_1\right) \mathbb{1}_{[0,10\pi]} \left(\boldsymbol{\Theta}_2\right)$$



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Eggcrate

Prior

$$\pi(\boldsymbol{\Theta}) = \left(\frac{1}{10\pi}\right)^2 \mathbb{1}_{[0,10\pi]} \left(\boldsymbol{\Theta}_1\right) \mathbb{1}_{[0,10\pi]} \left(\boldsymbol{\Theta}_2\right)$$

Likelihood

$$\mathscr{L}(\boldsymbol{\Theta}) = \exp\left\{\left[2 + \cos\left(\frac{\Theta_1}{2}\right)\cos\left(\frac{\Theta_2}{2}\right)\right]^5\right\}$$



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Eggcrate

Prior

$$\pi(\boldsymbol{\Theta}) = \left(\frac{1}{10\pi}\right)^2 \mathbb{1}_{[0,10\pi]} \left(\boldsymbol{\Theta}_1\right) \mathbb{1}_{[0,10\pi]} \left(\boldsymbol{\Theta}_2\right)$$

Likelihood

$$\mathscr{L}(\boldsymbol{\Theta}) = \exp\left\{\left[2 + \cos\left(\frac{\Theta_1}{2}\right)\cos\left(\frac{\Theta_2}{2}\right)\right]^5\right\}$$

Posterior

$$\mathscr{P}(\boldsymbol{\Theta}) = \frac{\left(\frac{1}{10\pi}\right)^2 \exp\left\{\left[2 + \cos\left(\frac{\Theta_1}{2}\right)\cos\left(\frac{\Theta_2}{2}\right)\right]^5\right\} \mathbb{1}_{[0,10\pi]}(\Theta_1)\mathbb{1}_{[0,10\pi]}(\Theta_2)}{235.88}$$

Eggcrate parameters

- N = 20
- *M* = 32



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Eggcrate results: log-posterior and histogram



$\log \mathcal{Z} = 235.1 \pm 1.336$

Compare the above value with the value from Feroz, et al., 2009 computed using standard quadrature: 235.88.

Lighthouse problem



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Lighthouse problem

Prior

$$\Pr\left(\alpha_{j}\right) = (1/200)\mathbb{1}_{\left[-100,100\right]}\left(\alpha_{j}\right)$$
$$\Pr\left(\beta_{j}\right) = (1/100)\mathbb{1}_{\left[0,100\right]}\left(\beta_{j}\right)$$



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Lighthouse problem

Prior

$$\Pr\left(\alpha_{j}\right) = (1/200)\mathbb{1}_{\left[-100,100\right]}\left(\alpha_{j}\right)$$
$$\Pr\left(\beta_{j}\right) = (1/100)\mathbb{1}_{\left[0,100\right]}\left(\beta_{j}\right)$$

Original likelihood

$$\mathscr{L}(\boldsymbol{\Theta}) = \Pr\left(x_k | \alpha_j, \beta_j\right) = \frac{\beta_j}{\pi\left(\beta_j^2 + \left(x_k - \alpha_j\right)^2\right)}$$



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Lighthouse problem extension

New likelihood for one observation

$$\mathscr{L}(\boldsymbol{\Theta}) = \Pr\left(x_k | \boldsymbol{\alpha}, \boldsymbol{\beta}\right) = \sum_{j=1}^J A_j \frac{\beta_j}{\pi \left(\beta_j^2 + \left(x_k - \alpha_j\right)^2\right)}$$



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Lighthouse problem extension

New likelihood for one observation

$$\mathscr{L}(\boldsymbol{\Theta}) = \Pr\left(x_k | \boldsymbol{\alpha}, \boldsymbol{\beta}\right) = \sum_{j=1}^J A_j \frac{\beta_j}{\pi \left(\beta_j^2 + \left(x_k - \alpha_j\right)^2\right)}$$

New likelihood for multiple observations

$$\mathscr{L}(\boldsymbol{\Theta}) = \Pr\left(\boldsymbol{x} | \boldsymbol{\alpha}, \boldsymbol{\beta}\right) = \prod_{k=1}^{K} \sum_{j=1}^{J} A_{j} \frac{\beta_{j}}{\pi \left(\beta_{j}^{2} + \left(x_{k} - \alpha_{j}\right)^{2}\right)}$$



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Lighthouse problem parameters

- 1000 observations of 2 lighthouses
- *N* = 40
- *M* = 4

Table: Lighthouse parameters

j	A_{j}	α_{j}	β_j
1	0.5	-10.0	1
2	0.5	10.0	1



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Lighthouse results



Lighthouse results

Table: Lighthouse problem results

J	$\langle \log \mathscr{Z} \rangle$	Stdev(log \mathcal{Z}
1	-12680	1.160
2	-9254	1.107
3	-9260	1.445
4	-9300	1.377



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Signal model: sum of sinusoidal signals corrupted by additive white Gaussian noise (AWGN) $% \left(AWGN\right) =0$

$$s(t) = \left[\sum_{j=1}^{J} A_j \cos\left(\omega_j t\right) + B_j \sin\left(\omega_j t\right)\right]$$
$$d(t) = s(t) + n(t)$$



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Sinusoidal signals in noise

Joint prior

$$\pi(\boldsymbol{\Theta}) = \left(\frac{1}{(20)(20)(512\pi)}\right)^{J} \prod_{j=1}^{J} \mathbb{1}_{[-10,10]} \left(A_{j}\right) \mathbb{1}_{[-10,10]} \left(B_{j}\right) \mathbb{1}_{[0,512\pi]} \left(\omega_{j}\right)$$



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Sinusoidal signals in noise

Joint prior

$$\pi(\boldsymbol{\Theta}) = \left(\frac{1}{(20)(20)(512\pi)}\right)^{J} \prod_{j=1}^{J} \mathbb{1}_{[-10,10]} \left(A_{j}\right) \mathbb{1}_{[-10,10]} \left(B_{j}\right) \mathbb{1}_{[0,512\pi]} \left(\omega_{j}\right)$$

For observed time series $d(t_k)$ such that $1 \le k \le K$,

Likelihood

$$\mathscr{L}(\boldsymbol{\Theta}) = \left(\frac{1}{\sqrt{2\pi\sigma}}\right)^{K} \exp\left\{-\left[\sum_{k=1}^{K} \left(s\left(t_{k}\right) - d\left(t_{k}\right)\right)^{2}\right] / \left(2\sigma^{2}\right)\right\}$$



Sinusoidal signals in noise

Test signal parameters:

- *J* = 2
- $f_s = 512$ samples/s
- K = 1000
- $\sigma^2 = 0.01$
- *N* = 25
- *M* = 4

Table: Sinusoidal signal parameters

j	A_{j}	B_{j}	ω_{j}
1	1.0	0.0	68π
2	0.0	1.0	160 <i>π</i>



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Sinusoidal signals in noise - truncated signal plot



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Sinusoidal signals in noise - results

Table: Signal problem results

J	$\langle \log \mathcal{Z} \rangle$	Stdev(log \mathcal{Z})
1	-2546	1.174
2	-553.7	1.349
3	-583.5	1.568



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Conclusion

- Combining the results of independent nested sampling runs decreases the shrinkage between consecutive samples.
- This is demonstrated using an analytical example for the simplest case and a numerical test for a more general case.
- This technique is effective for determining the evidence in several example problems, including for distributions with several prominent modes.
- Simple, effective, extensible.

