Lecture 4: Parameter Estimation

Outline:

- Review of GW likelihood, Bayes' theorem
- Why do we want to sample from the posterior?
  - "typical set"
  - Expectation values and Monte-Carlo integration
- How can we get posterior samples?
  examples:
  - inverse transform
  - rejection sampling
  - Markov-Chain Monte Carlo
  - parallel tempering
- Examples of GW parameter estimation: corner plots, correlations, weird likelihood surfaces

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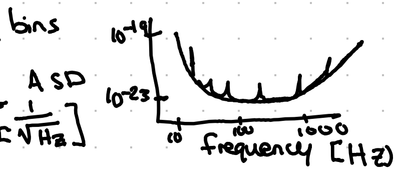
1) From last time:

data = signal + noise

$d(t) = h(t) + n(t)$ timeseries

$\vec{d} = \vec{h} + \vec{n}$ take discrete time samples

noise is approximately stationary and Gaussian
→ noise at each frequency follows a Gaussian described by PSD, noise is uncorrelated between frequency bins



Define an inner product

$$(A|B) \equiv 4\,\mathrm{Re} \int_0^\infty df \, \frac{\tilde{A}^*(f)\,\tilde{B}(f)}{S_n(f)}$$

$$p(n) \propto \exp\left[-\tfrac{1}{2}(n|n)\right]$$

GW likelihood: signal (strain) depends on parameters $\vec{\theta}$ (masses, spins, distance, etc.)

so, $\vec{n} = \vec{d} - \vec{h}(\vec{\theta})$

$$p(\vec{d}\,|\,\vec{\theta}, \underset{\text{model assumptions}}{H}) \propto \exp\left[-\tfrac{1}{2}(d - h(\vec{\theta})\,|\,d - h(\vec{\theta}))\right]$$

We want to infer $\vec{\theta}$. Posterior:

$$p(\vec{\theta}\,|\,\vec{d}, H) = \frac{p(\vec{d}\,|\,\vec{\theta}, H)\, p(\vec{\theta}\,|\,H)}{p(\vec{d}\,|\,H)}$$

$$= \frac{\text{likelihood} \times \text{prior}}{\text{evidence}}$$

We will talk more about the evidence next week!

For now, just ignore (treat as normalization factor), so

$$p(\vec{\theta}\,|\,\vec{d}, H) \propto p(\vec{d}\,|\,\vec{\theta}, H)\, p(\vec{\theta}\,|\,H)$$

Why samples?

Maximum likelihood is not enough for many applications or maximum a posteriori

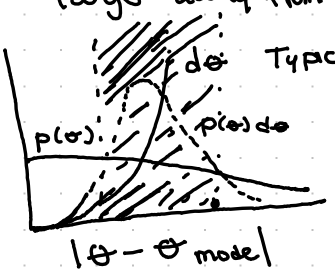
Especially in high dimensions

The probability contained in a given region of param. space V is

$$\int_V p(\theta)\, d\theta$$

prob. density × volume

$p(\theta)$ peaks at the mode, but $d\theta$ is much larger away from the mode in high-dimensions



samples allow us to compute expectation values

consider $X = f(\theta)$

$$\mathbb{E}[X] = \int_V f(\theta)\, p(\theta)\, d\theta$$

$$\sigma^2[X] = \mathbb{E}[(X - \mathbb{E}[X])^2] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$$

If we have samples $\theta \sim p(\theta)$, then we can estimate

$$\int_V f(\theta)\, p(\theta)\, d\theta \approx \langle f(\theta) \rangle_{\theta \sim p(\theta)} = \frac{1}{N} \sum_{i=1}^{N} f(\theta_i)$$

This Monte Carlo estimate of the integral is unbiased:

$$\mathbb{E}[\langle f \rangle] = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}[f(\theta_i)] = \frac{1}{N} \sum_{i=1}^{N} \int_V f(\theta)\, p(\theta)\, d\theta$$

$$= \int_V f(\theta)\, p(\theta)\, d\theta \quad \checkmark$$

and converges with $\sqrt{N}$:

$$\sigma^2[\langle f \rangle] = \sigma^2\left[\frac{1}{N} \sum_{i=1}^{N} f(\theta_i)\right]$$

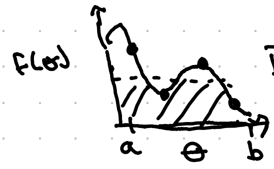
$$= \frac{1}{N^2} \sum_{i=1}^{N} \sigma^2[f(\theta_i)]$$

if samples are independent, variance of sum is sum of variance

$$= \frac{1}{N} \sigma^2[f(\theta)]$$

if samples are not independent, replace N with "effective sample size"

Ex: if $p(\theta)$ is uniform,



$$\frac{1}{b-a} \int_a^b f(\theta)\, d\theta \approx \langle f(\theta) \rangle \cdot \frac{(b-a)}{b-a}$$

How can we get $\{\vec{\theta}_i\}$ samples from $p(\vec{\theta})$?

- inverse transform sampling from target with pdf $p(x)$

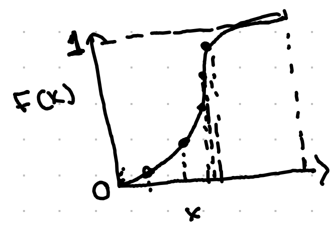
In 1-d, CDF $F(x) = \int_0^x \underbrace{p(x')}_{\text{pdf}}\, dx'$

$0 < F(x) < 1$

draw $y_i = F(x_i)$ from uniform distribution

$y \sim U(0,1)$

$F^{-1}(y_i) = x_i$



- rejection sampling from target with pdf $p(x)$

draw samples from some easy-to-sample distribution

$x_i \sim g(x)$

Keep x_i with probability $\dfrac{p(x)}{K g(x)}$ where K is a constant s.t. $p(x) \leq K g(x) \;\forall x$

$\underbrace{\text{Markov Chain}}$ $\underbrace{\text{Monte Carlo}}_{\text{random sampling}}$

sequence of random variables where next step in the sequence depends only on the previous

Efficient, multi-dim. sampling that preferentially samples the "typical set."

<u>Target distribution</u> $\pi(\theta) = p(d|\theta, H)\, p(\theta|H)$

(switching notation a bit, π is not a pdf because it's not normalized)

<u>proposal distribution</u> $q(\theta^{(n+1)}|\theta^{(n)})$

<u>acceptance prob</u> $\alpha(\theta^{(n+1)}|\theta^{(n)})$

<u>Transition prob.</u> $P(\theta^{(n+1)}|\theta^{(n)})$ given by q and α

We want our chain to respect <u>detailed balance</u>

$$\pi(\theta^{(n+1)})\, P(\theta^{(n)}|\theta^{(n+1)}) = \pi(\theta^{(n)})\, P(\theta^{(n+1)}|\theta^{(n)})$$

i.e. probability of being in state $(n+1)$ and transitioning to (n) is the same as the reverse.

This yields a <u>stationary distribution</u>, i.e. if

$\theta^{(n)}$ drawn from π, $\theta^{(n+1)}$ also drawn from π

and we will "eventually" converge to the target distribution

Metropolis Hastings algorithm

$$\alpha(\theta^{(n+1)}|\theta^{(n)}) = \min\left[1, \frac{\pi(\theta^{(n+1)})\, q(\theta^{(n)}|\theta^{(n+1)})}{\pi(\theta^{(n)})\, q(\theta^{(n+1)}|\theta^{(n)})}\right]$$

In this case, transition prob is

$$p(\theta^{(n+1)}|\theta^{(n)}) = q(\theta^{(n+1)}|\theta^{(n)})\alpha(\theta^{(n+1)}|\theta^{(n)}) + (1-b)\delta(\theta^{(n)}-\theta^{(n+1)})$$

$$b = \int d\theta^{(n+1)}\, q(\theta^{(n+1)}|\theta^{(n)})\alpha(\theta^{(n+1)}|\theta^{(n)})$$

This choice satisfies detailed balance.

Proof: If $\theta^{(n+1)} = \theta^{(n)}$, trivial

If $\theta^{(n+1)} \neq \theta^{(n)}$,

$$\alpha(\theta^{n+1}|\theta^n) = \min\{1, r\}$$

If $r>1$,

LHS: $\pi(\theta^n)\, q(\theta^{n+1}|\theta^n)\cdot 1$

RHS: $\pi(\cancel{\theta^{n+1}})\, q(\cancel{\theta^n|\theta^{n+1}})\cdot \frac{1}{r}$

$$= \text{''} \quad \text{''} \cdot \frac{\pi(\theta^n)\, q(\theta^{n+1}|\theta^n)}{\cancel{\pi(\theta^{n+1})}\, q(\cancel{\theta^n|\theta^{n+1}})} \quad ✓$$

If $r<1$,

LHS: $\pi(\theta^n)\, q(\theta^{n+1}|\theta^n)\cdot r$ similar cancellations

RHS: $\pi(\theta^{n+1})\, q(\theta^n|\theta^{n+1})\cdot 1$

Note that often proposal q is taken to be a Gaussian, so that

$$q(\theta^{n+1}|\theta^n) = q(\theta^n|\theta^{n+1})$$

and $r = \dfrac{\pi(\theta^{n+1})}{\pi(\theta^n)}$

Challenges:

- correlations

good jump in one direction isn't necessarily a good jump in another direction

- multimodal

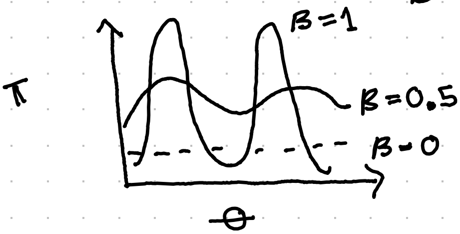
how do you discover second modes?

One technique is Parallel Tempering MCMC

Run multiple chains with different target distributions

$$\pi_\beta(\theta) = [p(d|\theta, H)]^\beta \, p(\theta|H)$$

$\beta = \frac{1}{T} \leftarrow$ temperature



$\beta = 1$ (cold chain) is our posterior

$\beta \to 0$ (hot chain) is our prior

hot chain can hop around much more easily.

Progress the chains together
every N iterations, propose a swap between
neighboring chains i and j

accept the swap with probability

$$A_{ij} = \min\left[1, \frac{\pi_{\beta_i}(\theta_j)}{\pi_{\beta_j}(\theta_i)}\right]$$

$$= \min\left[1, \frac{p(d|\theta_j)}{p(d|\theta_i)}\right]^{\beta_i - \beta_j}$$

helps explore parameter space (find new modes)

also used to calculate evidences
("thermodynamic integration")

Define an evidence for each temperature chain

$$Z_\beta \equiv \int d\theta\, \pi_\beta(\theta) \quad \text{so that } p_\beta(\theta) = \frac{\pi_\beta(\theta)}{Z_\beta}$$

[The evidence we want is $\beta = 1$]

consider

$$\frac{\partial}{\partial\beta}\ln(Z_\beta) = \frac{1}{Z_\beta}\frac{\partial}{\partial\beta}Z_\beta$$

$$= \frac{1}{Z_\beta}\int d\theta \frac{\partial}{\partial\beta}\pi_\beta(\theta)$$

$$= \int d\theta \frac{1}{Z_\beta}\frac{\partial \pi_\beta(\theta)}{\partial\beta}\cdot\frac{\pi_\beta(\theta)}{\pi_\beta(\theta)}$$

$$= \int d\theta\, p_\beta(\theta)\frac{\partial \ln \pi_\beta(\theta)}{\partial\beta}$$

$$\frac{\partial \ln \pi_\beta(\theta)}{\partial\beta} = \frac{\partial}{\partial\beta}\left[\ln\left[(p(d|\theta,H))^\beta\right] + \ln p(\theta|H)\right]$$

$$= \frac{\partial}{\partial\beta}\left[\beta \ln p(d|\theta,H)\right.$$

$$= \ln p(d|\theta,H)$$ which is just the log-likelihood

so

$$\frac{\partial}{\partial\beta}\ln(Z_\beta) = \int d\theta\, p_\beta(\theta)\ln p(d|\theta,H)$$

$$= \mathbb{E}_\beta\left[\ln p(d|\theta,H)\right]$$

Easy to estimate for each chain β by
taking average over points in the chain

Once we have $\mathbb{E}_\beta[\ln p(d|\theta,H)]$ computed for
each chain, we can numerically integrate

$$\int_0^1 \frac{\partial}{\partial\beta}\ln(Z_\beta)\, d\beta = \ln Z_1 - \ln \underbrace{Z_0}_{1 \text{ if prior is normalized}}$$

$$= Z_1$$