

From Gaussians to Periodograms

(*Lecture 2*)

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Summary of Lecture 1

Overview of Bayesian inference

- What to do: Calculate $p(H_i|D, \dots)$
- What's different about it:
 - ▶ Problem solving vs. solution characterization
 - ▶ Parameter space vs. sample space integrals
- How to do it:
 - ▶ Large N : Laplace Approximation
 - ▶ Exact: Analytic, Adaptive/randomized quadrature, posterior sampling

Today's Lecture

- Simple example: Coin flipping
- Inference with Gaussians
 - ▶ Estimating the mean (σ known & unknown)

$$d_i = \mu + \epsilon_i$$

- ▶ Superposed nonlinear models (Bretthorst algorithm)

$$d_i = \sum_{\alpha=1}^M A_\alpha g_\alpha(x_i; \theta) + \epsilon_i$$

Example: Coin Flipping!

Parameter Estimation

M = Assumed independence of flips

H_i = Statements about a , the probability for heads on the next flip → seek $p(a|D, M)$

D = Sequence of results from N previous flips:

THTHHHTHHHHT ($n = 8$ heads in $N = 12$ flips)

Likelihood:

$$\begin{aligned} p(D|a, M) &= p(\text{tails}|a, M) \times p(\text{heads}|a, M) \times \dots \\ &= a^n(1-a)^{N-n} \\ &= \mathcal{L}(a) \end{aligned}$$

Prior:

Starting with no information about a beyond its definition, use as an “uninformative” prior $p(a|M) = 1$. Justifications:

- Intuition: Don’t prefer any a interval to any other of same size
- Bayes’s justification: “Ignorance” means that before doing the N flips, we have no preference for how many will be heads:

$$P(n \text{ heads}|M) = 1/N \rightarrow p(a|M) = 1$$

Consider this a *convention*—an assumption added to M to make the problem well posed.

Prior Predictive:

$$\begin{aligned} p(D|M) &= \int da \ a^n (1-a)^{N-n} \\ &= B(n+1, N-n+1) = \frac{n!(N-n)!}{(N+1)!} \end{aligned}$$

A *Beta integral*, $B(a, b) \equiv \int dx \ x^{a-1} (1-x)^{b-1} = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$.

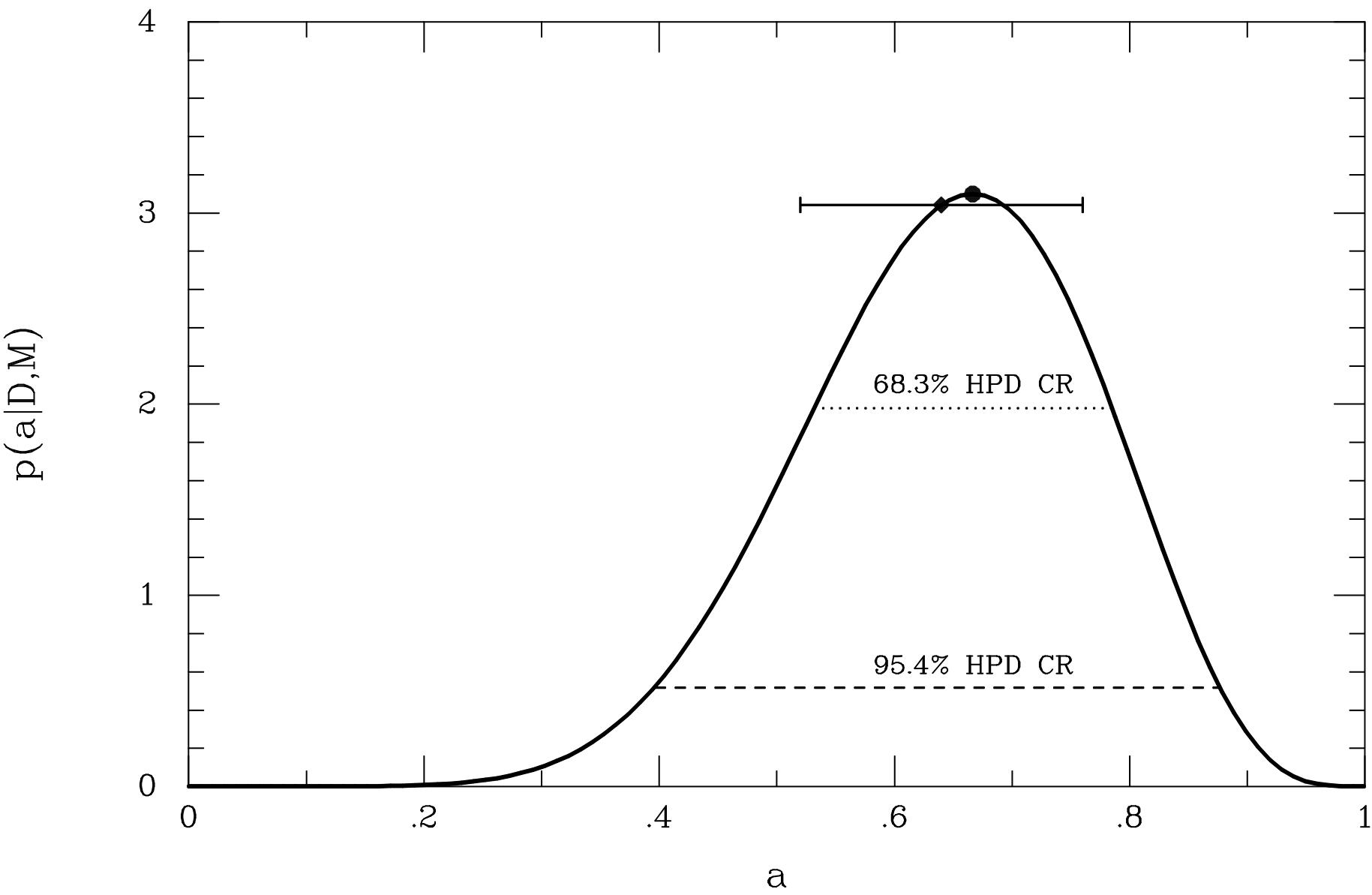
Posterior:

$$p(a|D, M) = \frac{(N+1)!}{n!(N-n)!} a^n (1-a)^{N-n}$$

A *Beta distribution*. Summaries:

- Best-fit: $\hat{a} = \frac{n}{N} = 2/3$; $\langle a \rangle = \frac{n+1}{N+2} \approx 0.64$
- Uncertainty: $\sigma_a = \sqrt{\frac{(n+1)(N-n+1)}{(N+2)^2(N+3)}} \approx 0.12$
Find credible regions numerically, or with incomplete beta function

Note that the posterior depends on the data only through n , not the N binary numbers describing the sequence. n is a (minimal) *Sufficient Statistic*.



Model Comparison: Fair Flips?

M_1 : $a = 1/2$

M_2 : $a \in [0, 1]$ with flat prior.

Maximum Likelihoods:

$$M_1 : \quad p(D|M_1) = \frac{1}{2^N} = 2.44 \times 10^{-4}$$

$$M_2 : \quad \mathcal{L}(2/3) = \left(\frac{2}{3}\right)^n \left(\frac{1}{3}\right)^{N-n} = 4.82 \times 10^{-4}$$

$$\frac{p(D|M_1)}{\mathcal{L}(2/3)} = 0.51$$

Maximum likelihoods favor M_2 (biased flips).

Bayes Factor (ratio of model likelihoods):

$$p(D|M_1) = \frac{1}{2^N}; \quad \text{and} \quad p(D|M_2) = \frac{n!(N-n)!}{(N+1)!}$$

$$\begin{aligned} \rightarrow B_{12} \equiv \frac{p(D|M_1)}{p(D|M_2)} &= \frac{(N+1)!}{n!(N-n)!2^N} \\ &= 1.57 \end{aligned}$$

Bayes factor (odds) favors M_1 (fair flips).

Note that for $n = 6$, $B_{12} = 2.93$; for this small amount of data, we can never be very sure the coin is fair.

If $n = 0$, $B_{12} \approx 1/315$; if $n = 3$, $B_{12} \approx 1/4.8$; for extreme data, 12 flips can be enough to lead us to strongly suspect the coin flipping is not fair.

Coin Flipping: Binomial Distribution

Suppose $D = n$ (number of heads in N flips), rather than the actual sequence. What is $p(a|n, M)$?

Likelihood:

Let S = a sequence of flips with n heads.

$$\begin{aligned} p(n|a, M) &= \sum_S p(S|a, M)p(n|S, a, M) \\ &= a^n (1 - a)^{N-n} C_{n,N} \end{aligned}$$

$C_{n,N}$ = # of sequences of length N with n heads.

$$\rightarrow p(n|a, M) = \frac{N!}{n!(N-n)!} a^n (1 - a)^{N-n}$$

The *Binomial Distribution* for n given a, N .

Posterior:

$$p(a|n, M) = \frac{\frac{N!}{n!(N-n)!} a^n (1-a)^{N-n}}{p(n|M)}$$

$$\begin{aligned} p(n|M) &= \frac{N!}{n!(N-n)!} \int da \ a^n (1-a)^{N-n} \\ &= \frac{1}{N+1} \end{aligned}$$

$$\rightarrow p(a|n, M) = \frac{(N+1)!}{n!(N-n)!} a^n (1-a)^{N-n}$$

Same result as when data specified the actual sequence.

Lessons from Coin Flip Analyses

- Sufficiency: Calculation of the likelihood identified a sufficient statistic
- Only dependence of likelihood on *parameters* matters
- Demonstration of “Occam factors”:
 - ▶ Simpler model can be favored
 - ▶ Experiments can have limited strength

Inference With Gaussians

Gaussian PDF:

$$p(x|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \text{ over } [-\infty, \infty]$$

Common abbreviated notation: $x \sim N(\mu, \sigma^2)$

Parameters:

$$\mu = \langle x \rangle \equiv \int dx \ x \ p(x|\mu, \sigma)$$

$$\sigma^2 = \langle (x - \mu)^2 \rangle \equiv \int dx \ (x - \mu)^2 \ p(x|\mu, \sigma)$$

Gauss's Observation: Sufficiency

Suppose our data consist of N measurements, $d_i = \mu + \epsilon_i$. Suppose the noise contributions are independent, and $\epsilon_i \sim N(0, \sigma^2)$.

$$\begin{aligned} p(D|\mu, \sigma, M) &= \prod_i p(d_i|\mu, \sigma, M) \\ &= \prod_i p(\epsilon_i = d_i - \mu|\mu, \sigma, M) \\ &= \prod_i \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(d_i - \mu)^2}{2\sigma^2}\right] \\ &= \frac{1}{\sigma^N (2\pi)^{N/2}} e^{-Q/2\sigma^2} \end{aligned}$$

Find dependence of Q on μ by completing the square:

$$\begin{aligned} Q &= \sum_i (d_i - \mu)^2 \\ &= \sum_i d_i^2 + N\mu^2 - 2N\mu\bar{d} \quad \text{where } \bar{d} \equiv \frac{1}{N} \sum_i d_i \\ &= N(\mu - \bar{d})^2 + Nr^2 \quad \text{where } r^2 \equiv \frac{1}{N} \sum_i (d_i - \bar{d})^2 \end{aligned}$$

Likelihood depends on $\{d_i\}$ only through \bar{d} and r :

$$\mathcal{L}(\mu, \sigma) = \frac{1}{\sigma^N (2\pi)^{N/2}} \exp\left(-\frac{Nr^2}{2\sigma^2}\right) \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right)$$

The sample mean and variance are *sufficient statistics*.

Estimating a Normal Mean

Model: $d_i = \mu + \epsilon_i$, $\epsilon_i \sim N(0, \sigma^2)$, σ is known $\rightarrow I = (\sigma, M)$.

Parameter space: μ ; seek $p(\mu|D, \sigma, M)$

Likelihood:

$$\begin{aligned} p(D|\mu, \sigma, M) &= \frac{1}{\sigma^N (2\pi)^{N/2}} \exp\left(-\frac{Nr^2}{2\sigma^2}\right) \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right) \\ &\propto \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right) \end{aligned}$$

“Uninformative” prior:

Translation invariance $\Rightarrow p(\mu) \propto C$, a constant.

This prior is *improper* unless bounded.

Prior predictive:

$$\begin{aligned} p(D|\sigma, M) &= \int d\mu C \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right) \\ &= C(\sigma/\sqrt{N})\sqrt{2\pi} \end{aligned}$$

... minus a tiny bit from tails, using a proper prior.

Posterior:

$$p(\mu|D, \sigma, M) = \frac{1}{(\sigma/\sqrt{N})\sqrt{2\pi}} \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right)$$

Posterior is Gaussian at \bar{d} with standard deviation $w = \sigma/\sqrt{N}$.

68.3% HPD credible region for μ is $\bar{d} \pm \sigma/\sqrt{N}$.

Note that C drops out \rightarrow limit of infinite prior range is well behaved.

Informative Conjugate Prior:

Use a Gaussian prior, $\mu \sim N(\mu_0, w_0^2)$

Posterior:

Remains Gaussian with

$$\begin{aligned}\hat{\mu} &= \frac{\bar{d}}{1 + \frac{w^2}{w_0^2}} + \frac{\mu_0}{1 + \frac{w_0^2}{w^2}} \\ w' &= w \frac{1}{\sqrt{1 + w^2/w_0^2}}\end{aligned}$$

“Principle of stable estimation:” The prior affects inferences only when data are not informative.

Estimating a Normal Mean: Unknown σ

Model: $d_i = \mu + \epsilon_i$, $\epsilon_i \sim N(0, \sigma^2)$, σ is *unknown*

Parameter space: (μ, σ) ; seek $p(\mu|D, \sigma, M)$

Likelihood:

$$\begin{aligned} p(D|\mu, \sigma, M) &= \frac{1}{\sigma^N (2\pi)^{N/2}} \exp\left(-\frac{Nr^2}{2\sigma^2}\right) \exp\left(-\frac{N(\mu - \bar{d})^2}{2\sigma^2}\right) \\ &\propto \frac{1}{\sigma^N} e^{-Q/2\sigma^2} \end{aligned}$$

where $Q = N [r^2 + (\mu - \bar{d})^2]$

Uninformative Priors:

Assume priors for μ and σ are independent.

Translation invariance $\Rightarrow p(\mu) \propto C$, a constant.

Scale invariance $\Rightarrow p(\sigma) \propto 1/\sigma$.

Joint Posterior for μ, σ :

$$p(\mu, \sigma | D, M) \propto \frac{1}{\sigma^{N+1}} e^{-Q/2\sigma^2}$$

Marginal Posterior:

$$p(\mu|D, M) \propto \int d\sigma \frac{1}{\sigma^{N+1}} e^{-Q/2\sigma^2}$$

Let $\tau = \frac{Q}{2\sigma^2}$ so $\sigma = \sqrt{\frac{Q}{2\tau}}$ and $|d\sigma| = \tau^{-3/2} \sqrt{\frac{Q}{2}} d\tau$

$$\begin{aligned} \Rightarrow p(\mu|D, M) &\propto 2^{N/2} Q^{-N/2} \int d\tau \tau^{\frac{N}{2}-1} e^{-\tau} \\ &\propto Q^{-N/2} \end{aligned}$$

Write $Q = Nr^2 \left[1 + \left(\frac{\mu - \bar{d}}{r} \right)^2 \right]$ and normalize:

$$p(\mu|D, M) = \frac{\left(\frac{N}{2} - 1\right)!}{\left(\frac{N}{2} - \frac{3}{2}\right)! \sqrt{\pi}} \frac{1}{r} \left[1 + \frac{1}{N} \left(\frac{\mu - \bar{d}}{r/\sqrt{N}} \right)^2 \right]^{-N/2}$$

“Student’s t distribution,” with $t = \frac{(\mu - \bar{d})}{r/\sqrt{N}}$

A “bell curve,” but with power-law tails

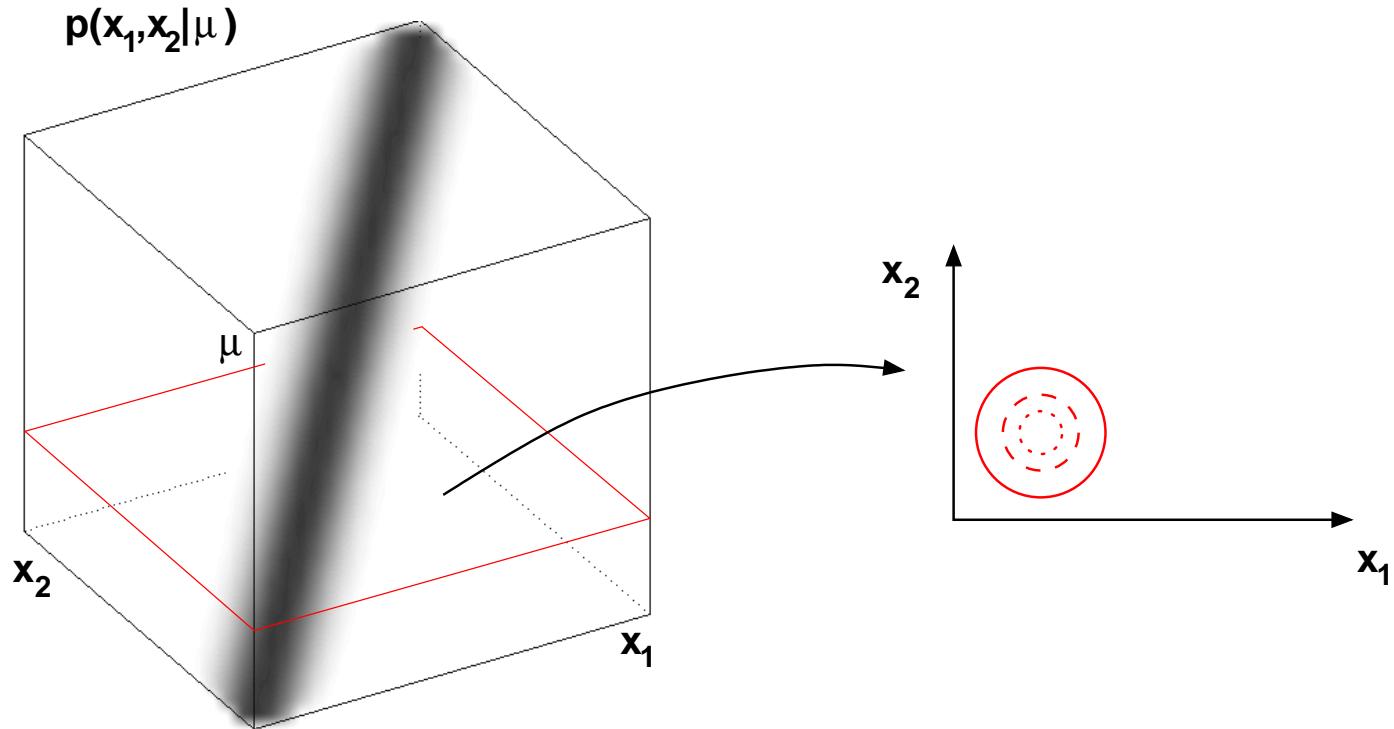
Large N :

$$p(\mu|D, M) \sim e^{-N(\mu - \bar{d})^2/2r^2}$$

A Frequentist Confidence Region

Infer μ : $x_i = \mu + \epsilon_i;$

$$p(x_i|\mu, M) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x_i - \mu)^2}{2\sigma^2}\right]$$



68% confidence region: $\bar{x} \pm \sigma/\sqrt{N}$

Monte Carlo Algorithm:

1. Pick a null hypothesis, $\mu = \mu_0$
2. Draw $x_i \sim N(\mu_0, \sigma^2)$ for $i = 1$ to N
3. Find \bar{x} ; check if $\mu_0 \in \bar{x} \pm \sigma/\sqrt{N}$
4. Repeat $M >> 1$ times; report fraction (≈ 0.683)
5. *Hope result is independent of μ_0 !*

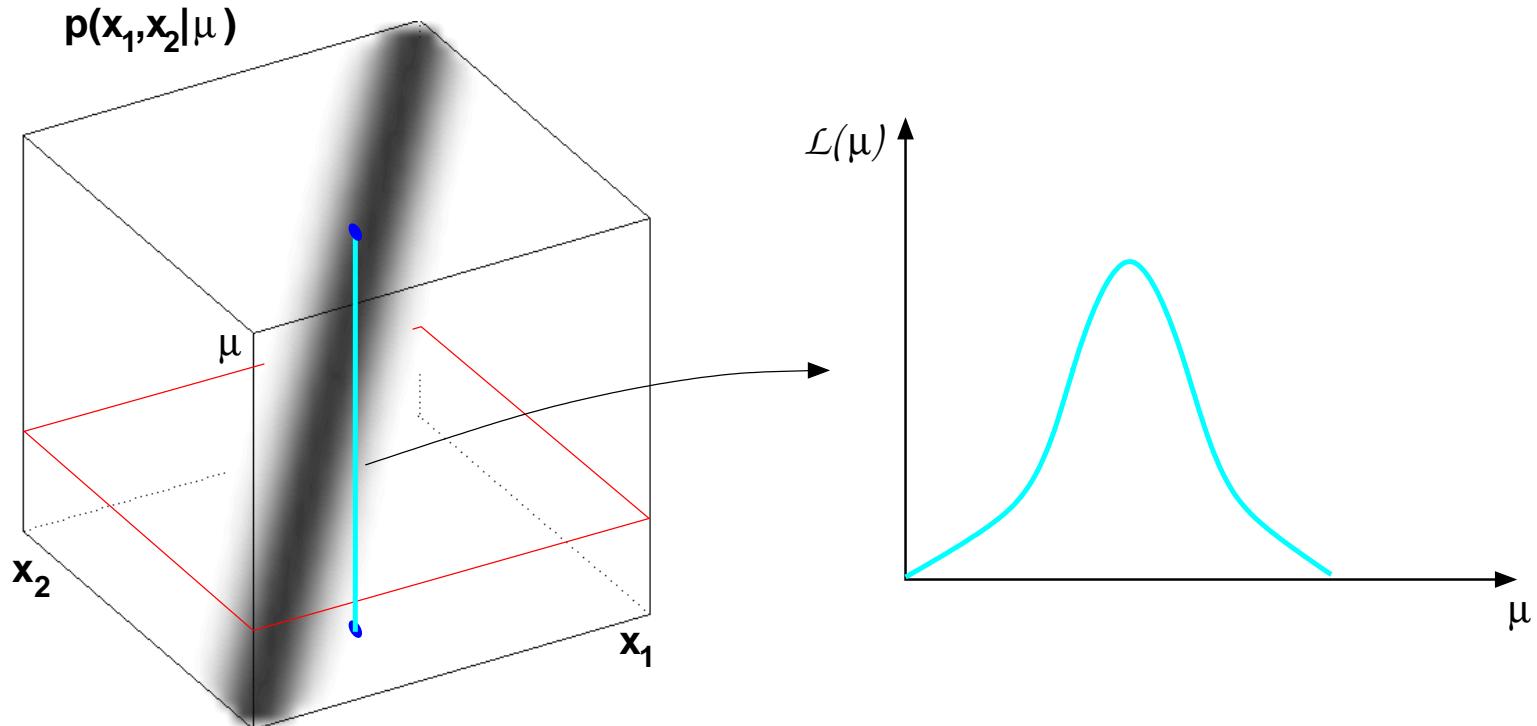
A Monte Carlo calculation of the N -dimensional integral:

$$\int dx_1 \frac{e^{-\frac{(x_1 - \mu)^2}{2\sigma^2}}}{\sigma\sqrt{2\pi}} \cdots \int dx_N \frac{e^{-\frac{(x_N - \mu)^2}{2\sigma^2}}}{\sigma\sqrt{2\pi}} \times [\mu_0 \in \bar{x} \pm \sigma/\sqrt{N}] \\ = \int d(\text{angles}) \int_{\bar{x} - \sigma/\sqrt{N}}^{\bar{x} + \sigma/\sqrt{N}} d\bar{x} \exp \left[-\frac{(\bar{x} - \mu)^2}{2(\sigma/\sqrt{N})^2} \right] \cdots \approx 0.683$$

A Bayesian Credible Region

Infer μ : Flat prior;

$$\mathcal{L}(\mu) \propto \exp \left[-\frac{(\bar{x} - \mu)^2}{2(\sigma/\sqrt{N})^2} \right]$$



68% credible region: $\bar{x} \pm \sigma/\sqrt{N}$

68% credible region: $\bar{x} \pm \sigma/\sqrt{N}$

$$\frac{\int_{\bar{x}-\sigma/\sqrt{N}}^{\bar{x}+\sigma/\sqrt{N}} d\mu \exp\left[-\frac{(\bar{x}-\mu)^2}{2(\sigma/\sqrt{N})^2}\right]}{\int_{-\infty}^{\infty} d\mu \exp\left[-\frac{(\bar{x}-\mu)^2}{2(\sigma/\sqrt{N})^2}\right]} \approx 0.683$$

Equivalent to a Monte Carlo calculation of a 1-d integral:

1. Draw μ from $N(\bar{x}, \sigma^2/N)$ (i.e., prior $\times \mathcal{L}$)
2. Repeat $M >> 1$ times; histogram
3. Report most probable 68.3% region

This simulation uses hypothetical *hypotheses* rather than hypothetical *data*.

When Will Results Differ?

When models are linear in the parameters and have additive Gaussian noise, frequentist results are identical to Bayesian results with flat priors.

This mathematical coincidence will *not* occur if:

- The choice of statistic is not obvious (no sufficient statistics)
- There is no identity between parameter space and sample space integrals (due to nonlinearity or the form of the sampling distribution)
- There is important prior information

Also, some problems can be quantitatively addressed only from the Bayesian viewpoint; e.g., systematic error.

The Bretthorst Algorithm

Superposed Nonlinear Models

N samples of a superpos'n of nonlinear functions plus Gaussian errors,

$$d_i = \sum_{\alpha=1}^M A_\alpha g_\alpha(x_i; \theta) + \epsilon_i$$

or $\vec{d} = \sum_{\alpha} A_\alpha \vec{g}_\alpha(\theta) + \vec{\epsilon}.$

E.g., sinusoidal signal:

$$\begin{aligned} f(x) &= A \cos(\omega x + \phi) \\ &= A_1 \cos \omega x + A_2 \sin \omega x \\ &= A_1 g_1(x, \omega) + A_2 g_2(x, \omega) \end{aligned}$$

The log-likelihood is a quadratic form in A_α ,

$$\mathcal{L}(A, \theta) \propto \frac{1}{\sigma^N} \exp \left[-\frac{Q(A, \theta)}{2\sigma^2} \right]$$

with
$$Q = \left[\vec{d} - \sum_{\alpha} A_{\alpha} \vec{g}_{\alpha} \right]^2$$
$$= d^2 - 2 \sum_{\alpha} A_{\alpha} \vec{d} \cdot \vec{g}_{\alpha} + \sum_{\alpha, \beta} A_{\alpha} A_{\beta} \eta_{\alpha \beta}$$

where $\eta_{\alpha \beta} = \vec{g}_{\alpha} \cdot \vec{g}_{\beta}$

Goals:

- Estimate θ given a prior, $\pi(\theta)$.
- Estimate amplitudes.
- Compare rival models.

The algorithm:

- Switch to orthonormal set of models, $\vec{h}_\mu(\theta)$ by diagonalizing $\eta_{\alpha\beta}$; new amplitudes $B = \{B_\mu\}$.

$$Q = \sum_{\mu} \left[B_{\mu} - \vec{d} \cdot \vec{h}_{\mu}(\theta) \right]^2 + r^2(\theta, B)$$

residual $\vec{r}(\theta, B) = \vec{d} - \sum_{\mu} B_{\mu} \vec{h}_{\mu}$

$$p(B, \theta | D, I) \propto \frac{\pi(\theta) J(\theta)}{\sigma^N} \exp \left[-\frac{r^2}{2\sigma^2} \right] \exp \left[\frac{-1}{2\sigma^2} \sum_{\mu} (B_{\mu} - \hat{B}_{\mu})^2 \right]$$

where $J(\theta) = \prod_{\mu} \lambda_{\mu}(\theta)^{-1/2}$

- Marginalize B 's analytically.

$$p(\theta|D, I) \propto \frac{\pi(\theta)J(\theta)}{\sigma^{N-M}} \exp\left[-\frac{r^2(\theta)}{2\sigma^2}\right]$$

$r^2(\theta) =$ residual sum of squares
from least squares

- If σ unknown, marginalize using $p(\sigma|I) \propto \frac{1}{\sigma}$.

$$p(\theta|D, I) \propto \pi(\theta)J(\theta) [r^2(\theta)]^{\frac{M-N}{2}}$$

Detecting Periodic Signals

Conventional approach:

FT of signal \approx DFT of data

$$\rightarrow \text{use } S(\omega) = \frac{2}{N} \left[\left(\sum_i d_i \cos \omega t_i \right)^2 + \left(\sum_i d_i \sin \omega t_i \right)^2 \right]$$

Schuster periodogram (evenly spaced data)

Lomb-Scargle periodogram (unevenly spaced data)

Interpret data power spectrum as signal power spectrum corrupted by noise and sampling “window”

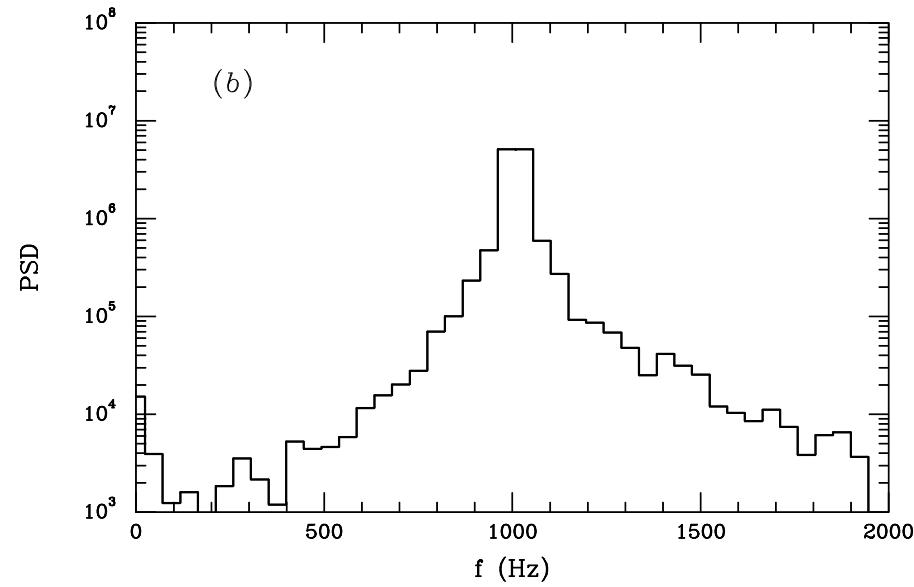
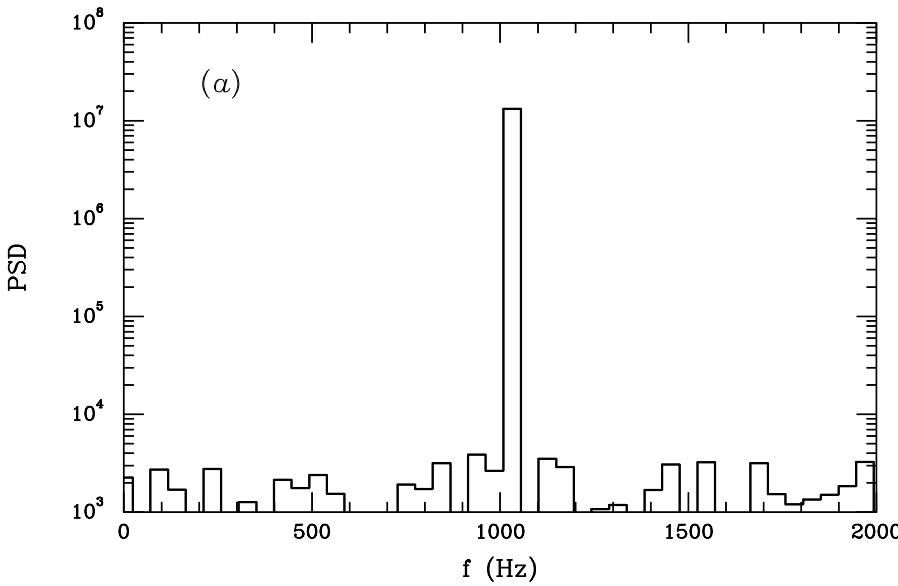
Under simple null hypotheses, $N/2$ values given by DFT are *statistically independent* \Rightarrow focus on those

Problem: Leakage in the Power Spectrum

1024 samples at 48 kHz sampling rate

$S/N = 5$, white noise

$f = 1031.25$ Hz (Fourier frequency) and $f = 1008$ Hz



⇒ Attempt to reduce leakage by tapering/smoothing data

Bayesian approach (Jaynes & Bretthorst):

Explicit periodic signal model:

$$\begin{aligned} f(t) &= A \cos(\omega t - \phi) && \text{parameters } \omega, A, \phi \\ &= A_1 \cos \omega t + A_2 \sin \omega t && \text{parameters } \omega, A_1, A_2 \end{aligned}$$

$$d_i = f(t_i) + e_i \quad \text{Gaussian error pdfs; rms} = \sigma$$

Estimate ω assuming signal present.

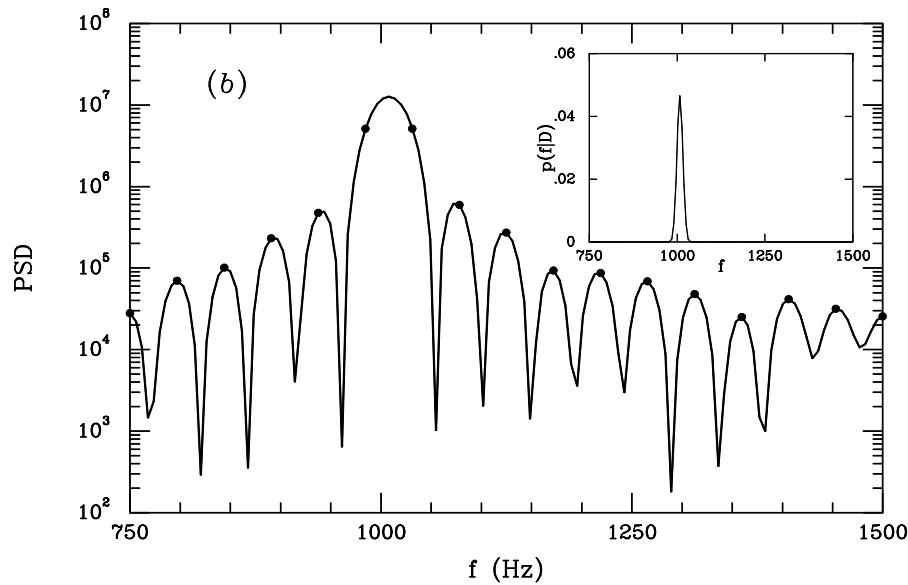
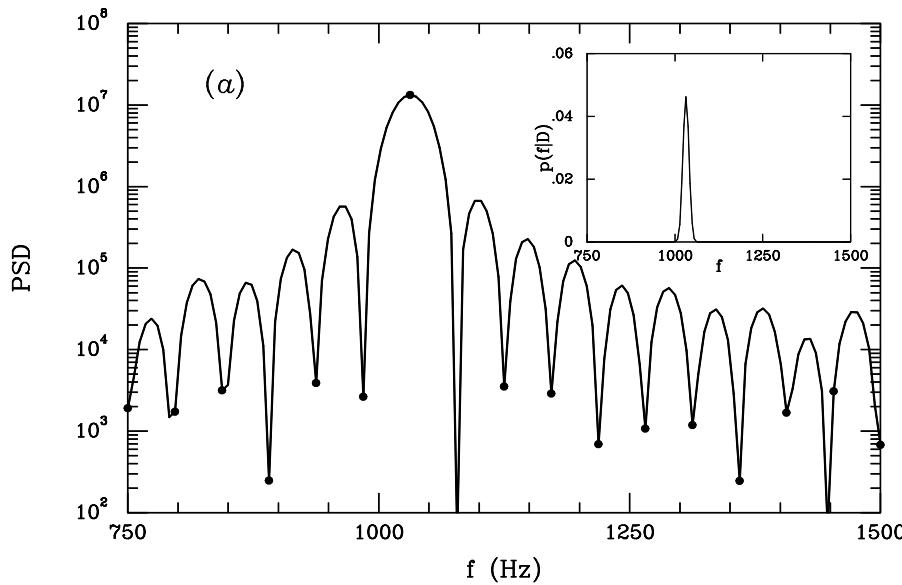
$$\begin{aligned} p(\omega|D) &\propto \int dA_1 \int dA_2 p(\omega, A_1, A_2) \mathcal{L}(\omega, A_1, A_2) \\ &\propto p(\omega) J(\omega) \exp \left[\frac{S(\omega)}{\sigma^2} \right] \end{aligned}$$

Continuous Periodogram and Posterior Distribution for ω

1024 samples at 48 kHz sampling rate

$S/N = 5$

$f = 1031.25$ Hz (Fourier frequency) and $f = 1008$ Hz



New aspects:

- Periodogram is not a power spectrum, but the logarithm of the marginal *pdf* for ω
- No special role for Fourier frequencies
- No “leakage;” log *pdf* has similar structure for *all* signal frequencies, but sidelobes get *exponentiated* away.
- Detect signal using signal model likelihood:

$$\mathcal{L}(\text{signal}) \approx \exp\left[\frac{S_{\max}}{\sigma^2}\right] \times \frac{\text{peak width}}{\text{prior search range}}$$

- Conventional periodograms optimal only for *single sinusoids*
- Noise estimated using *peak amplitude* (rms residual)

Astrophysical Applications

Bayes + Gaussians + linear & nonlinear parameters

- Periodic signals:
 - ▶ Cepheid/RR Lyrae variables — Bretthorst, Jefferys & Berger
 - ▶ X-ray flare stars — Gregory
 - ▶ Planet detection — TJL, Scargle, Bretthorst
- Gravitational radiation from binary inspiral (LIGO) — Finn, Flanagan, Cutler...
- Cosmic background radiation (signal=variance) — Readhead, Lasenby, Bond, Jaffe...

Key Ideas

- Sufficiency—For some problems, inferences depend on only a few features of the data. The Bayesian algorithm identifies these automatically.
- For simple Gaussian problems, Bayesian and frequentist results are similar; but this is a mathematical coincidence.
- A powerful modeling framework: Superposed nonlinear models + Gaussian noise
- A new interpretation of the Fourier power spectrum with significant practical consequences