STSCI 4780
Information, decision, design

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Agenda

1. **BDA research community**
2. Information theory & reference priors
3. Decision theory
4. Experimental design
5. Recap

Bayesian data analysis research community

- Valencia International Meetings on Bayesian Statistics
  - Organized by José Bernardo (Dennis Lindley's student) and several prominent Bayesian statisticians
  - Every 4 years from 1979 to 2010
  - 9 highly-cited proceedings volumes
  - Bayesian Cabarets; The Bayesian Songbook
- The International Society for Bayesian Analysis (ISBA): Bayesian.org
  - Sections: OBayes, BayesComp...
  - Biannual ISBA World Meeting; sectional meetings
  - Journal: *Bayesian Analysis*
  - Bayesian work is prominent in many statistics & machine learning journals; see esp.: JASA, JRSS B, Biometrika, JMLR, Statistical Science
  - Bayesian work is prominent in machine learning: NeurIPS, ICML

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Limitations of the Jeffreys prior

- Only considered sound for a single parameter (or considering a single parameter at a time in some multiparameter problems)
- Only applicable to continuous spaces

$\rightarrow$ Seek more general notions of "objective" or "uninformative" that reproduce good things about the Jeffreys prior

Reference priors seek to minimize the influence of the prior on the *expected information content* of the posterior

Uncertainty, information, and entropy

Other rules for assigning "non-informative" priors rely on a more formal measure of the *information content* (or its complement, amount of *uncertainty*) in a probability distribution

Intuitively appealing metric-based measures, like standard deviation or interval size, are not general enough; e.g., they don't apply to categorical distributions

Desiderata for an *uncertainty functional* $\mathcal{S}_N[\vec{p}]$—a map from a PMF $\vec{p} = (p_1, p_2, \ldots, p_N)$ to a single scalar quantifying the amount of uncertainty it expresses (treat PDFs later):

- $\mathcal{S}_N[\vec{p}]$ should be continuous w.r.t. the p_is
- *Uncertainty grows with multiplicity*: When the p_i are all equal, $s(N) = \mathcal{S}_N[\vec{p}]$ should grow monotonically with N
- *Invariance w.r.t. decomposition into subgroups*

$\Rightarrow$ functional equations for $\mathcal{S}_N[\vec{p}]$ $\Rightarrow$ *Shannon entropy*

Information Gain as Entropy Change

Entropy and uncertainty

Shannon entropy = a scalar measure of the degree of uncertainty expressed by a probability distribution

$$\begin{aligned} \mathcal{S} &= \sum_i p_i \log \frac{1}{p_i} \qquad \text{“Average surprisal”} \\ &= -\sum_i p_i \log p_i \end{aligned}$$

Information gain

Information gain upon learning D = decrease in uncertainty:

$$\begin{aligned} \mathcal{I}(D) &= \mathcal{S}[\{p(H_i)\}] - \mathcal{S}[\{p(H_i|D)\}] \\ &= \sum_i p(H_i|D) \log p(H_i|D) - \sum_i p(H_i) \log p(H_i) \end{aligned}$$

A 'Bit' About Entropy

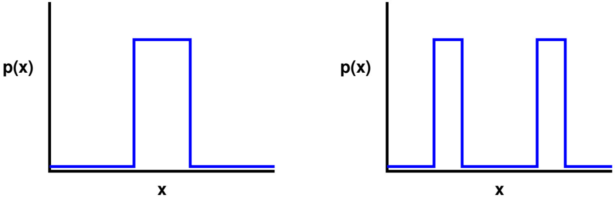
Entropy of a Gaussian

$$p(x) \propto e^{-(x-\mu)^2/2\sigma^2} \quad \rightarrow \quad \mathcal{S} \propto \log(\sigma)$$

$$p(\vec{x}) \propto \exp\left[-\frac{1}{2}\vec{x}\cdot \mathsf{V}^{-1}\cdot\vec{x}\right] \quad \rightarrow \quad \mathcal{S} \propto \log(\det \mathsf{V})$$

$\rightarrow$ Asymptotically like log Fisher matrix

A log-measure of "volume" or "spread," not range



These distributions have the same entropy/amount of information.

Expected information gain

When the data are yet to be considered, the *expected* information gain averages over D; straightforward use of the product rule/Bayes's theorem gives:

$$\begin{aligned}\mathbb{E}\mathcal{I} &= \int dD\, p(D)\, \mathcal{I}(D) \\ &= \int dD\, p(D)\, \sum_i p(H_i|D) \log\left[\frac{p(H_i|D)}{p(H_i)}\right]\end{aligned}$$

For a continuous hypothesis space labeled by parameter(s) θ,

$$\mathbb{E}\mathcal{I} = \int dD\, p(D)\, \int d\theta p(\theta|D) \log\left[\frac{p(\theta|D)}{p(\theta)}\right]$$

This is the expectation value of the *Kullback-Leibler divergence* between the prior and posterior:

$$\mathcal{D} \equiv \int d\theta\, p(\theta|D) \log\left[\frac{p(\theta|D)}{p(\theta)}\right]$$

Reference priors

Bernardo (later joined by Berger & Sun) advocates *reference priors*, priors chosen to maximize the KLD between prior and posterior, as an "objective" expression of the idea of a "non-informative" prior: reference priors let the data most strongly dominate the prior (on average)

- Rigorous definition invokes asymptotics and delicate handling of non-compact parameter spaces to make sure posteriors are proper
- For 1-D problems, the reference prior is the Jeffreys prior
- In higher dimensions, the reference prior is *not* the Jeffreys prior; it behaves better
- The construction in higher dimensions is complicated and depends on separating interesting vs. nuisance parameters (but see Berger, Bernardo & Sun 2015, "Overall objective priors")
- Reference priors are typically improper on non-compact spaces
- They give Bayesian inferences good frequentist properties
- A constructive numerical algorithm exists

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Naive Decision Making

A Bayesian analysis results in probabilities for two hypotheses:

$$p(H_1|I) = 5/6; \qquad\qquad p(H_2|I) = 1/6$$

Equivalently, the odds favoring H_1 over H_2 are

$$O_{12} = 5$$

We must base future actions on either H_1 or H_2.

Which should we choose?

Naive decision maker: *Choose the most probable,* H_1

Naive Decision Making—Deadly!

Russian Roulette

$H_1 =$ Chamber is empty; $\qquad H_2 =$ Bullet in chamber

What is your choice now?

Decisions should depend on consequences!

Unattributed JavaScript at `http://www.javascriptkit.com/script/script2/roulette.shtml`

Bayesian Decision Theory

Decisions depend on consequences

Might bet on an improbable outcome provided the payoff is large if it occurs and/or the loss is small if it doesn't

Utility and loss functions

Compare consequences via *utility* quantifying the benefits of a decision, or via *loss* quantifying costs

$$\text{Utility} = U(a, o) \qquad \begin{aligned} a &= \text{Choice of action (decide b/t these)} \\ o &= \text{Outcome (what we are uncertain of)} \end{aligned}$$

Loss $L(a, o) = U_{\max} - U(a, o)$

Russian Roulette Utility

Suppose you're offered \$6,000 to play

	Outcomes	
Actions	Empty (*click*)	Bullet (*BANG!*)
Play	\$6,000	−\$Life
Pass	0	0

Uncertainty & expected utility

We are uncertain of what the outcome will be
$\rightarrow$ Expected utility *averages over outcomes*:

$$\mathbb{E}U(a) = \sum_{\text{outcomes}} P(o|\ldots)\, U(a, o)$$

The best action *maximizes the expected utility*:

$$\hat{a} = \arg\max_a \mathbb{E}U(a)$$

I.e., minimize expected loss.

Axiomatized: von Neumann & Morgenstern; Ramsey, de Finetti, Savage

Russian Roulette Expected Utility

	Outcomes		
Actions	Empty (*click*)	Bullet (*BANG!*)	$\mathbb{E}U$
Play	\$6,000	$-$\$Life	\$5000$-$\$Life/6
Pass	0	0	0

As long as \$Life $>$ \$30,000, *don't play!*

Decision theory and parametric models

Decision theory can motivate specific posterior summaries:

- Point estimates for parameters ("Bayes estimators"):
  - Posterior median: best for absolute error loss
  - Posterior mean: best for squared error loss
  - Posterior mode: best for 0/1 loss ("all or nothing" prize)
- HPD regions best if penalize regions for increasing size

For model choice, *explanatory* vs. *predictive* criteria can lead to different choices

- They trade off bias vs. variance differently
- E.g., AIC comes from a *predictive* criterion, and BIC/Bayes factors from an *explanatory* criterion

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Experimental design as decision making

When we perform an experiment we have choices of actions:

- What sample size to use
- What times or locations to probe/query
- Whether to do one sensitive, expensive experiment or several less sensitive, less expensive experiments
- Whether to stop or continue a sequence of trials
- ...

We must choose amidst uncertainty about the data we may obtain and the resulting consequences for our experimental results

$\Rightarrow$ Seek a principled approach for optimizing experiments, accounting for all relevant uncertainties

Bayesian experimental design

Actions $= \{e\}$, possible experiments (sample sizes, sample times/locations, stopping criteria . . .).

Outcomes $= \{d_e\}$, values of future data from experiment e.

Utility measures value of d_e for achieving experiment goals, possibly accounting for the cost of the experiment.

Choose the experiment that maximizes

$$\mathbb{E}U(e) = \sum_{d_e} p(d_e|\ldots)\, U(e, d_e)$$

To predict d_e we must consider various hypotheses, H_i, for the data-producing process $\rightarrow$ Average over H_i uncertainty:

$$\mathbb{E}U(e) = \sum_{d_e} \left[\sum_{H_i} p(H_i|\ldots) p(d_e|H_i,\ldots) \right] U(e, d_e)$$

Information-based utility

Many scientific studies do not have a single, clear-cut goal.

Broad goal: Learn/explore, with resulting information made available for a variety of future uses.

Example: Astronomical measurement of orbits of minor planets or exoplanets

- Use to infer physical properties of a body (mass, habitability)
- Use to infer distributions of properties among the population (constrains formation theories)
- Use to predict future location (collision hazard; plan future observations)

Motivates using a "general purpose" utility that measures *what is learned* about the H_i describing the phenomenon

Lindley (1956, 1972) and Bernardo (1979) advocated using $\mathcal{I}(D)$ as such a general-purpose utility

MaxEnt sampling for parameter estimation

Setting:

- We have specified a model, M, with uncertain parameters θ
- We have data $D \to$ current posterior $p(\theta|D, M)$
- The entropy of the noise distribution doesn't depend on θ

$$\to \mathbb{E}\mathcal{I}(e) \quad = \quad \text{Const} - \sum_{d_e} p(d_e|D, I) \log p(d_e|D, I)$$

Maximum entropy sampling.
(Sebastiani & Wynn 1997, 2000)
To learn the most, sample where you know the least.

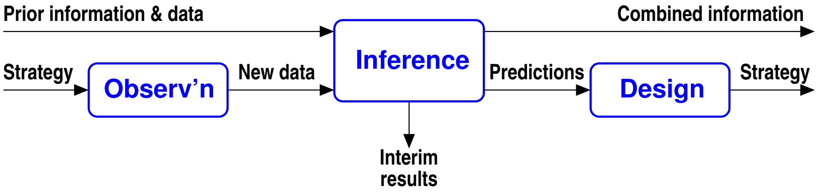
Scientific method

Science is more than a body of knowledge; it is a way of thinking.
The method of science, as stodgy and grumpy as it may seem,
is far more important than the findings of science.
—Carl Sagan

Classic hypothetico-deductive approach

- Form hypothesis (based on past observation/experiment)
- Devise experiment to test predictions of hypothesis
- Perform experiment
- Analysis $\rightarrow$
  - Devise new hypothesis if hypothesis fails
  - Devise new experiment if hypothesis corroborated

Bayesian Adaptive Exploration



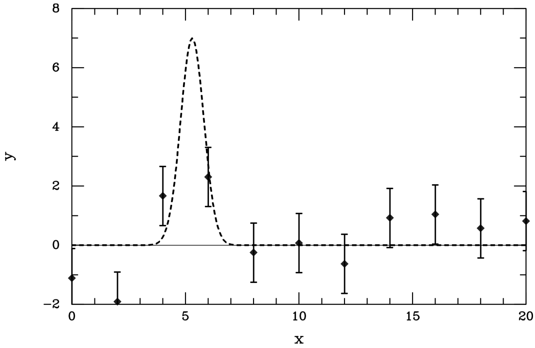
- Observation — Gather new data based on observing plan
- Inference — Interim results via posterior sampling
- Design — Predict future data; explore where expected information from new data is greatest

Locating a bump

Object is 1-d Gaussian of unknown loc'n, amplitude, and width.
True values:

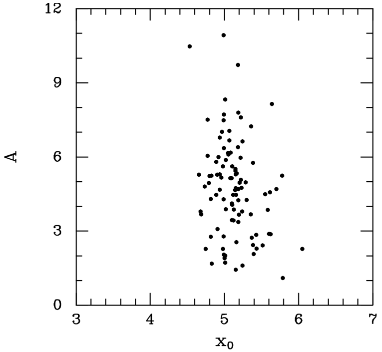
$$x_0 = 5.2, \qquad \text{FWHM} = 0.6, \qquad A = 7$$

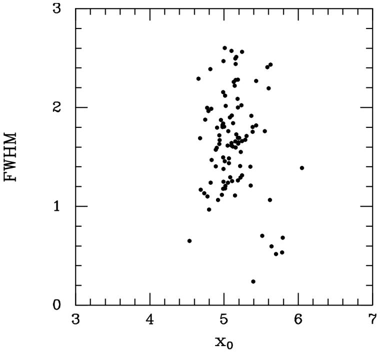
Initial scan with crude ($\sigma = 1$) instrument provides 11 equispaced observations over $[0, 20]$. Subsequent observations will use a better ($\sigma = 1/3$) instrument.



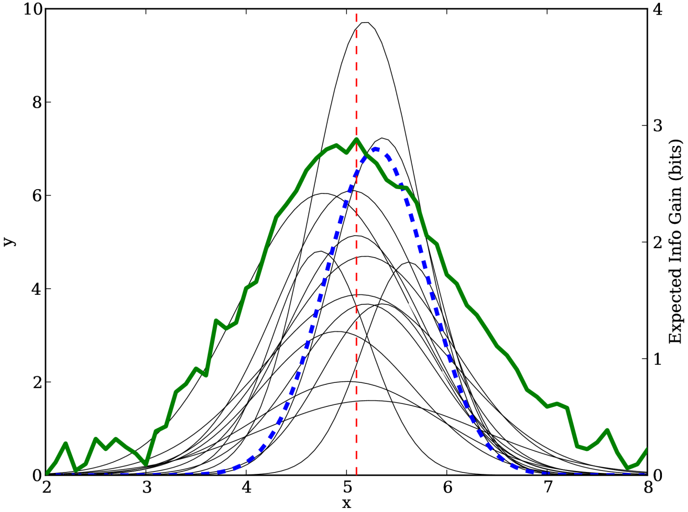
Cycle 1 Interim Inferences

Generate $\{x_0, FWHM, A\}$ via posterior sampling.

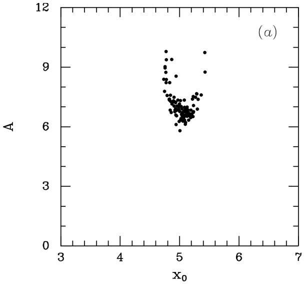


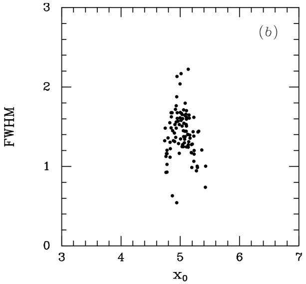


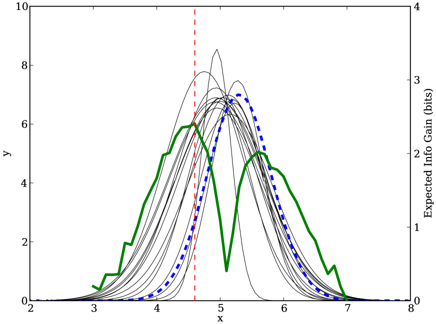
Cycle 1 Design: Predictions, Entropy



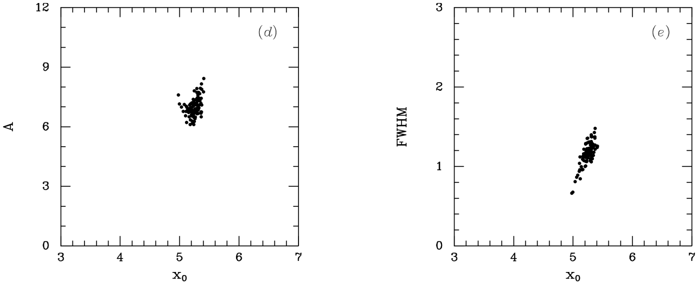
Cycle 2: Inference, Design

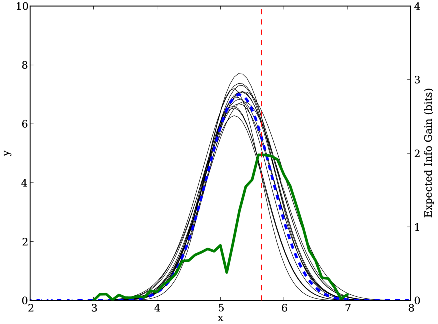




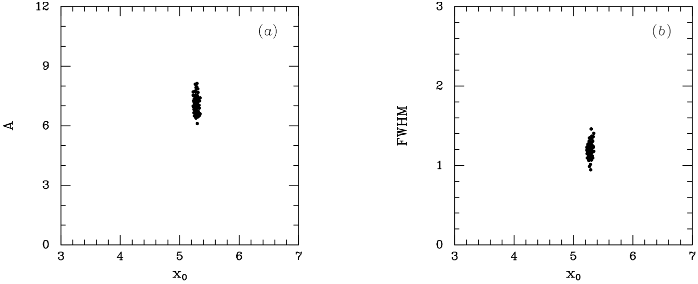


Cycle 3: Inference, Design

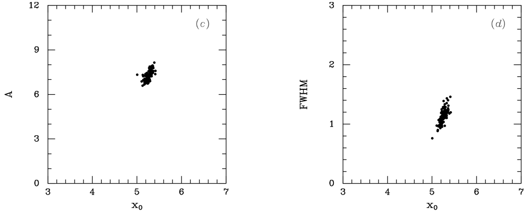




Cycle 4: Inferences



Inferences from *non-optimal* datum



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Recap: Bayesian inference in one slide

Probability as generalized logic

Probability quantifies the *strength of arguments*

To appraise hypotheses, calculate probabilities for arguments from data and modeling assumptions to each hypothesis

Use *all* of probability theory for this

Bayes's theorem

$$p(\text{Hypothesis} \mid \text{Data}) \quad \propto \quad p(\text{Hypothesis}) \times p(\text{Data} \mid \text{Hypothesis})$$

Data *change* the support for a hypothesis $\propto$ ability of hypothesis to *predict* the data

Law of total probability

$$p(\text{Hypothes}\underline{\textbf{es}} \mid \text{Data}) \quad = \quad \sum p(\text{Hypothes}\underline{\textbf{is}} \mid \text{Data})$$

The support for a *composite/compound* hypothesis must account for all the ways it could be true