Optimal Scheduling of Exoplanet Observations via Bayesian Adaptive Exploration

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GISS Workshop — 25 Feb 2011
First, a word from our sponsor (NASA!)

ASTROPHYSICS RESEARCH PROGRAM REVIEW

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Linda Sparke  
Astrophysics Research Program Manager, NASA HQ

Jon Morse  
Director, Astrophysics Division, NASA HQ
Locations of Kepler Planet Candidates

- **Earth-size**
- **Super-Earth size**
  - 1.25 - 2.0 Earth-size
- **Neptune-size**
  - 2.0 - 6.0 Earth-size
- **Giant-planet size**
  - 6.0 - 22 Earth-size
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 →
  - 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
Agenda

1. Motivation: Exoplanets via Doppler RV observations
2. Bayesian adaptive exploration
3. Toy problem: Bump hunting
4. BAE for HD 222582
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Finding Exoplanets via Stellar Reflex Motion

All bodies in a planetary system orbit wrt the system’s center of mass, including the host star:

**Astrometric Method**
Sun’s Astrometric Wobble from 10 pc

**Doppler Radial Velocity (RV) Method**
Doppler Shift Along Line-of-Sight

≈ 490 of ≈ 530 currently confirmed exoplanets found using RV method
RV method is used to confirm & measure transiting exoplanet candidates
RV Data Via Precision Spectroscopy

Millipixel spectroscopy

Meter-per-second velocities

RMS = 11.4 m s\(^{-1}\)
\(\mu\text{rms} = 3.39 \text{ m s}^{-1}\)
A Variety of Related Statistical Tasks

- **Planet detection** — Is there a planet present? Are multiple planets present?
- **Orbit estimation** — What are the orbital parameters? Are planets in multiple systems interacting?
- **Orbit prediction** — What planets will be best positioned for follow-up observations?
- **Population analysis** — What types of stars harbor planets? With what frequency? What is the distribution of planetary system properties?
- **Optimal scheduling** — How may astronomers best use limited, expensive observing resources to address these goals?

*Bayesian approach tightly integrates these tasks*
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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.

⇒ Seek a principled approach for optimizing experiments, accounting for all relevant uncertainties.
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.

\[ U(a, o) \]
\[ L(a, o) = U_{\max} - U(a, o) \]

\[ a = \text{Choice of action (decide b/t these)} \]
\[ o = \text{Outcome (what we are uncertain of)} \]
Bayesian Decision Theory

**Uncertainty & expected utility**

We are uncertain of what the outcome will be
→ *average 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
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 → Average over $H_i$ uncertainty:

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

Multiple sums/integrals

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

Average over both hypothesis and data spaces

Plus an optimization

\[ \hat{e} = \arg \max_{e} E U(e) \]

Aside: The dual averaging—over hypothesis and data spaces—hints (correctly!) of connections between Bayesian and frequentist approaches.
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
Information Gain as Entropy Change

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

\[ S = \sum_i p_i \log \frac{1}{p_i} \]

“Average surprisal”

= \(- \sum_i p_i \log p_i\)

Information gain

Existing data \(D\) \(\rightarrow\) interim posterior \(p(H_i|D)\)
Information gain upon learning \(d\) = decrease in uncertainty:

\[ \mathcal{I}(d) = S[p(H_i|D)] - S[p(H_i|d, D)] \]

= \(\sum_i p(H_i|d, D) \log p(H_i|d, D) - \text{Const (wrt } d)\)

Lindley (1956, 1972) and Bernardo (1979) advocated using
\(\mathcal{I}(d)\) as utility
A ‘Bit’ About Entropy

Entropy of a Gaussian

\[ p(x) \propto e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad \rightarrow \quad I \propto -\log(\sigma) \]

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

\[ \rightarrow \text{Asymptotically like Fisher matrix criteria} \]

Entropy is a log-measure of “volume,” not range

These distributions have the same entropy/amount of information.
**Prediction & expected information**

Information gain from datum $d_t$ at time $t$:

$$\mathcal{I}(d_t) = \sum_i p(H_i|d_t, D) \log p(H_i|d_t, D)$$

We don’t know what value $d_t$ will take → average over prediction uncertainty

*Expected information* at time $t$:

$$\mathbb{E}\mathcal{I}(t) = \int dd_t \ p(d_t|D) \mathcal{I}(d_t)$$

*Predictive distribution* for value of future datum:

$$p(d_t|D) = \sum_i p(d_t, H_i|D) = \sum_i p(H_i|D) \ p(d_t|H_i)$$

$$= \sum_i \text{Interim posterior} \times \text{Single-datum likelihood}$$

*There is a heck of a lot of averaging going on!*
MaxEnt sampling for parameter estimation cases

Setting:

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

$$\rightarrow E\mathcal{I}(t) = \text{Const} - \int dd_t \ p(d_t|D, I) \log p(d_t|D, I)$$

*Maximum entropy sampling.*

(Sebastiani & Wynn 1997, 2000)

>To learn the most, sample where you know the least.
Nested Monte Carlo integration for \( \mathbb{E} \mathcal{I} \)

Entropy of predictive dist’n:

\[
S[d_t|D, M] = -\int dd_t \ p(d_t|D, M_1) \log p(d_t|D, M)
\]

- Sample predictive via \( \theta \sim \text{posterior} \), \( d_t \sim \text{sampling dist’n given } \theta \)
- Evaluate predictive as \( \theta \)-mixture of sampling dist’ns

Posterior sampling in parameter space

- Many models are (linearly) separable \( \rightarrow \) handle linear “fast” parameters analytically
- When priors prevent analytical marginalization, use interim priors & importance sampling
- Treat nonlinear “slow” parameters via adaptive or population-based MCMC; e.g., diff’l evolution MCMC
Motivation: Exoplanets via Doppler RV observations

Bayesian adaptive exploration

Toy problem: Bump hunting

BAE for HD 222582
Locating a bump

Object is 1-d Gaussian of unknown loc’n, amplitude, and width.

True values:

\[ x_0 = 5.2, \quad \text{FWHM} = 0.6, \quad A = 7 \]

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 $\{x_0, \text{FWHM}, A\}$ via posterior sampling.
Cycle 1 Design: Predictions, Entropy
Cycle 2: Inference, Design
Cycle 4: Inferences

Inferences from *non-optimal* datum
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HD 222582: G5V at 42 pc in Aquarius, $V = 7.7$

Vogt$^+$ (2000) reported planet discovery based on 24 RV measurements
Keplerian Radial Velocity Model

Parameters for single planet

- $\tau =$ orbital period (days)
- $e =$ orbital eccentricity
- $K =$ velocity amplitude (m/s)
- Argument of pericenter $\omega$
- Mean anomaly at $t = 0$, $M_0$
- Systemic velocity $v_0$

Requires solving Kepler’s equation for every $(\tau, e, M_0)$—A strongly nonlinear model!
Cycle 1 Interim inferences
The next period
The distant future
New Data

Red points = 13 subsequent observations, Butler$^+$ (2006)

- Use 37-point best fit to simulate three new optimal observations
- Compare 24 + 3 & all-data inferences
Cycle 2 Interim inferences (25 pts)

\[ \prod \sigma_i \text{ is reduced } 2.4x \]
Cycle 3 Interim inferences (26 pts)

\[ \prod \sigma_i \text{ is reduced further } 1.5x \]
Cycle 4 Interim inferences (27 pts)

\[ \prod \sigma_i \text{ is reduced further } 30x \]
All-data inferences (37 pts)

\[ \prod \sigma_i \text{ is } 7x \text{ larger than } 24 + 3 \text{ BAE pts} \]
Outlook

- Explore more cases, e.g., multiple planets, marginal detections
- Explore other adaptive MCMC algorithms
- Extend to include planet *detection*:
  - Total entropy criterion smoothly moves between detection & estimation
  - MaxEnt sampling no longer valid
  - Marginal likelihood computation needed
  - Non-greedy designs likely needed
Thanks to my collaborators!

*Cornell Astronomy*
  David Chernoff

*Duke Statistical Sciences*
  Merlise Clyde, Jim Berger, Bin Liu, Jim Crooks
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Final Provocation

Much data analysis is *sequential*:

- Sequential experimentation/exploration
- Chains of discovery (individual objects/events → population)

Herman Chernoff on sequential analysis (1996):

*I became interested in the notion of experimental design in a much broader context, namely: what’s the nature of scientific inference and how do people do science? The thought was not all that unique that it is a sequential procedure...*

*Although I regard myself as non-Bayesian, I feel in sequential problems it is rather dangerous to play around with non-Bayesian procedures.... Optimality is, of course, implicit in the Bayesian approach.*
Jetsam

jetsam: material that has been thrown overboard from a ship, esp. material discarded to lighten the vessel
Conventional RV Orbit Fitting

Analysis method: Identify best candidate period via periodogram; fit parameters with nonlinear least squares/min $\chi^2$

System: HD 3651

$P = 62.23$ d
$e = 0.63$
$m \sin i = 0.20$ M$_J$
$a = 0.28$ AU

Fischer et al. 2003
Challenges for Conventional Approaches

- Multimodality, nonlinearity, nonregularity, sparse data → Asymptotic uncertainties not valid
- Reporting uncertainties in derived parameters ($m \sin i$, $a$) and predictions
- Lomb-Scargle periodogram not optimal for eccentric orbits or multiple planets
- Accounting for marginal detections
- Combining info from many systems for pop’n studies
- Scheduling future observations
Periodogram-Based Bayesian Pipeline
Differential Evolution MCMC

Ter Braak 2006 — Combine evolutionary computing & MCMC

Follow a population of states, where a randomly selected state is considered for updating via the (scaled) vector difference between two other states.

Behaves roughly like RWM, but with a proposal distribution that automatically adjusts to shape & scale of posterior

Step scale: Optimal $\gamma \approx 2.38/\sqrt{2d}$, but occasionally switch to $\gamma = 1$ for mode-swapping
Expected Information via Nested Monte Carlo

Assume we have posterior samples $\theta_i \sim p(\theta|D, M)$

**Evaluating** predictive dist’n:

$$p(d_e|D, M) = \int d\theta \ p(\theta|D, M) \ p(d_e|\theta, M)$$

$$\rightarrow \hat{p}(d_e) = \frac{1}{N_\theta} \sum_{i=1}^{N_\theta} p(d_e|\theta_i, M)$$

**Sampling** predictive dist’n:

$$\theta_i \sim p(\theta|D, M)$$

$$d_{e,j} \sim p(d_e|\theta, M)$$

**Entropy** of predictive dist’n:

$$S[d_e|D, M] = - \int dd_e \ p(d_e|D, M_1) \log p(d_e|D, M)$$

$$\approx - \frac{1}{N_d} \sum_{j=1}^{N_d} \log \hat{p}(d_{e,j})$$