Bayes-Optimal Methods for Optimization via Simulation: The Probabilistic Bisection Algorithm

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I am interested in Bayesian sequential experimental design

Many of the problems I’m interested in have this form:

- There is some unknown function \( f : \mathbb{X} \mapsto \mathbb{Y} \).
- We have a Bayesian prior distribution on \( f \).
- We want to learn something about \( f \), such as:
  - Optimization: Find a point \( x \) such that \( f(x) \) is large.
  - Level-set estimation: Find \( \{ x : f(x) > a \} \), for some constant \( a \).
  - Sensitivity analysis: Find \( i \) such that \( |\partial f(x)/\partial x_i| \) is large.
- We have the ability to evaluate \( f(x) \), for some \( x \)’s that we may choose in a sequential fashion.
- Evaluating \( f \) is really expensive, so we can’t do it too many times.
- How should we choose our \( x \)’s?
Example: Website optimization at Yelp
Example: Detecting edges in computer vision
Example: Learning user preferences at arxiv.org
Example: Root-finding experiments in biology
These problems are all partially observable Markov decision processes

In these problems:

- The value function gives the value-to-go of the optimal policy, as a function of the current posterior.
- If we knew the value function, we could figure out the optimal measurement to take next.
- In principal, the value function can be computed via dynamic programming.
- In practice, the curse of dimensionality usually prevents us from solving the dynamic program.

In this talk, we will consider one problem in which we can circumvent the curse of dimensionality, and efficiently compute the optimal policy.
We consider the stochastic root-finding problem

Consider a function \( g : [0, 1] \rightarrow \mathbb{R} \).
Suppose there is a unique \( X^* \in [0, 1] \) such that
- \( g(x) > 0 \) for \( x < X^* \),
- \( g(x) < 0 \) for \( x > X^* \).
Our **goal** is to find \( X^* \in [0, 1] \).
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We can only observe \( Y_n(X_n) = g(X_n) + \varepsilon_n(X_n) \), where \( \varepsilon_n(X_n) \) is conditionally independent noise with zero mean (median).
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We must decide:

- Where to place samples \( X_n \) for \( n = 0, 1, 2, \ldots \)
  to best support estimation of \( X^* \) after \( n \) iterations.
This problem, or a multivariate version of it, arises in many applications

- Optimization via simulation
  - Maximizing a concave function via noisy observations of its gradient.
- Medicine, Biology, Chemistry:
  - Estimating the median effective dose (ED50), the median lethal dose (LD50), the half maximal inhibitory concentration (IC50), . . .
- Machine Learning:
  - Regression with big datasets
  - Other kinds of parameter estimation problems with big datasets
- Computer vision:
  - Edge detection
  - Object detection and tracking
  - Scanning electron microscopy
Stochastic approximation is a standard method for solving this problem, due to [Robbins and Monro, 1951]

1. Choose an initial estimate \( X_0 \in [0, 1] \);

2. Select a tuning sequence \((a_n)_n \geq 0, \sum_{n=0}^{\infty} a_n^2 < \infty, \) and \( \sum_{n=0}^{\infty} a_n = \infty. \) (Example: \( a_n = d/n \) for \( d > 0. \))

3. \( X_{n+1} = \Pi_{[0,1]}(X_n + a_n Y_n(X_n)) \), where \( \Pi_{[0,1]} \) is the projection to \([0, 1]\).
Stochastic approximation works well when the tuning sequence is well-chosen.

$$a_n = 1/n, \ varepsilon_n \sim N(0,0.5)$$

This shows stochastic approximation when the tuning sequence is well-chosen.
Stochastic approximation works poorly when the tuning sequence is poorly chosen.

\[ a_n = \frac{10}{n}, \varepsilon_n \sim N(0,0.5) \]

This shows stochastic approximation when the tuning sequence is too large.
Stochastic approximation works poorly when the tuning sequence is poorly chosen

\[ a_n = 0.5/n, \varepsilon_n \sim N(0,0.5) \]

This shows stochastic approximation when the tuning sequence is too small.
Stochastic approximation can work poorly when the noisy has heavy tails

\[ a_n = \frac{1}{n}, \; \varepsilon_n \sim t_3 \]
We consider a different approach

What about a bisection algorithm?

- Noise will cause the deterministic bisection algorithm to fail.
- We develop a noise-tolerant version of the bisection algorithm, using a dynamic programming analysis of a stylized version of the problem.
- This new method will be better than stochastic approximation in some situations, and worse in others.
To do bisection, we will use “left/right” observations

By observing one or more samples $Y_n(x)$, at a fixed $x$, we can obtain (noisy) information about:

- the sign of $g(x)$; and
- whether $X^*$ is to the left or right of $x$. 
We can get noisy “left/right” observations

Let $Z_n(X_n)$ be such a noisy left/right observation, with the following properties:

$$Z_n(X_n) = \begin{cases} 
\text{sign}(g(X_n)) & \text{with probability } p(X_n), \\
-\text{sign}(g(X_n)) & \text{with probability } 1 - p(X_n),
\end{cases}$$

for some function $p(\cdot)$, which may, or may not, be known.
Here is the simplest way to construct a noisy left/right observation

- We could take $Z_n(X_n) = \text{sign}(Y_n(X_n))$.
- This construction requires only a single observation to construct $Z_n$.
- Under this construction, with homoscedastic normal noise and $g(\cdot)$ as given below left, $p(\cdot)$ is given below right:

![Graph showing $g(x)$ and $p(x)$]

- When constructed in this way, $p(\cdot)$ is generally unknown, and $p(x)$ may be arbitrarily close to $1/2$. 
There are other ways to construct a noisy left/right observation

- We can also construct $Z_n(X_n)$ by sampling repeatedly at a single point $X_n$.
- In particular, we can sample sequentially using an $\alpha$-level test of power 1 [Siegmund, 1985] for the mean of $Y_n(x)$.

Under a parametric assumption (additive normal noise, or Bernoulli observations), this ensures $p(x) \geq p_c$ for all $x \neq X^*$. Here, $p_c > 1/2$ is a known constant that we choose when we design the $\alpha$-level test.
Here is the program for the rest of the talk

First, we consider a stylized setting where \( p(\cdot) \) is constant and known.

- We perform a Bayesian analysis, and find the optimal policy using dynamic programming.
- This Bayes-optimal policy was first proposed in 1964 by Horstein, though it was not known to be Bayes-optimal.

Second, we create an algorithm that can be used in practice.

- This algorithm allows \( p(\cdot) \) to be unknown, but requires it to be bounded below by a known constant, \( p_c > 1/2 \).
- This assumption is met using sequential sampling, as previously noted.
- We show consistency, how to construct a confidence interval, and find frequentist rates of convergence.
Stylized Setting: $p(\cdot)$ is known and constant

Practical Setting: $p(\cdot)$ is unknown, and bounded below by $p_c > 1/2$. 
We first consider a stylized setting

- Recall that $p(X_n)$ is the probability that our noisy left/right observation $Z_n(X_n)$ is correct.
- For the moment, assume that $p(·)$ is constant, known, and strictly greater than $1/2$.
- This assumption is not generally met in practice.
We perform a Bayesian analysis

\[ n = 0, X_n = 0.5, Z_n(X_n) = 1 \]

We place a Bayesian prior density \( f_0 \) on the root \( X^* \), e.g., Uniform([0, 1]).
We perform a Bayesian analysis

We place a Bayesian prior density $f_0$ on the root $X^*$, e.g., Uniform([0,1]).

Then each observation $Z_n(X_n)$ produces a new posterior density $f_n$ on $x_*$, 
$$f_n(x) = \mathbb{P}\{X^* \in dx \mid X_{1:n}, Z_{1:n}\}$$
Here is an animation of the sequence of posterior densities

\[ f_n(x) \]

where \( n = 0, X_n = 0.5, Z_n(X_n) = 1 \)
Here is an animation of the sequence of posterior densities.

For $n = 0$, $X_n = 0.5$, $Z_n(X_n) = 1$.

For $n = 1$, $X_n = 0.61538$, $Z_n(X_n) = 1$.
Here is an animation of the sequence of posterior densities

\[ f_n(x) \]

\( n = 0, X_n = 0.5, Z_n(X_n) = 1 \)

\( n = 1, X_n = 0.61538, Z_n(X_n) = 1 \)

\( n = 2, X_n = 0.70414, Z_n(X_n) = -1 \)
Here is an animation of the sequence of posterior densities

$n = 0, X_n = 0.5, Z_n(X_n) = 1$

$n = 1, X_n = 0.61538, Z_n(X_n) = 1$

$n = 2, X_n = 0.70414, Z_n(X_n) = -1$

$n = 3, X_n = 0.63587, Z_n(X_n) = -1$
We measure performance by the entropy of the posterior

- We have a finite budget of $N$ measurements.
- After this budget is exhausted, we measure our remaining uncertainty by the entropy of the posterior distribution on the root’s location,

$$H(f_N) = - \int f_N(x) \log f_N(x) \, dx.$$ 

- We wish to find an adaptive method for choosing $X_n$ so as to minimize the expected entropy of the posterior.
Our problem is a dynamic programming problem

- We wish to find an adaptive method for choosing $x_n$ so as to minimize the expected entropy of the posterior.

\[
\inf_{\pi} \mathbb{E}^{\pi}[H(f_N)],
\]

- This can be formulated as a dynamic programming problem.

- The value function is

\[
V_n(f_n) = \inf_{x_n} \mathbb{E}[H(f_N) | f_n].
\]

- The value function satisfies the dynamic programming recursion:

\[
V_n(f_n) = \inf_{x_n \in [0,1]} \mathbb{E}[V_{n+1}(f_{n+1}) | f_n].
\]
In principle we could solve the dynamic program via brute force.

- We can parameterize the posterior $f_n$ in terms of the points previously measured, $X_1, \ldots, X_n$, and the responses $Z_1, \ldots, Z_n$. (holding $f_0$ fixed).
- Thus, we can identify $f_n$ with a point in $S_n = [0, 1]^n \times \{0, 1\}^n$.
- If we had enough memory on our computer to store $V(f_n)$ for a dense grid of points in $S_n$, we could solve the problem using dynamic programming:
  - Compute $V_n(f_n)$ (with some small error) using the dynamic programming (DP) recursion:
    \[ V_n(f_n) = \inf_{x_n \in [0,1]} \mathbb{E}[V_{n+1}(f_{n+1}) \mid f_n]. \]
  - Then compute a near-optimal $x_n$ for any given $f_n$ by finding the value attaining the infimum in the DP recursion.
In practice we do not have the computing power to solve the dynamic program via brute force.

- Our state space at time $n$ is $S_n = [0, 1]^n \times \{0, 1\}^n$.
- If we discretize each dimension of $[0, 1]^n$ into 100 pieces, our dense grid in $S_n$ has $100^n \times 2^n$ points.
- If we store each $V_n(f_n)$ in double-precision floating point (64 bits), this would require:
  - 2.4 TB of storage for $n = 5$.
  - 465 TB for $n = 6$.
  - \ldots
  - $7.5 \times 10^{11}$ TB for $n = 10$.
- This exponential scaling in the storage requirement is called the curse of dimensionality.
Instead, we solve the dynamic program via trickery.

**Theorem**

Suppose $p(\cdot) = p$ is constant, known, and bounded away from $1/2$, and we use the entropy loss function. Then, the value function can be written explicitly as

$$V(f_n) = H(f_n) - (N - n)[-p \log_2(p) - (1 - p) \log_2(1 - p)],$$

and the policy that chooses $X_n$ at the median of $f_n$ is optimal.

This result appears in [Jedynak, Frazier, Sznitman 2011], and is also shown in a more elementary way in [Waeber, Frazier, Henderson 2013].
Animation showing the posterior under the optimal policy

\[ n = 0, X_n = 0.5, Z_n(X_n) = 1 \]
Animation showing the posterior under the optimal policy

\[ n = 1, \ X_n = 0.61538, \ Z_n(X_n) = 1 \]
Animation showing the posterior under the optimal policy

\[ n = 2, X_n = 0.70414, Z_n(X_n) = -1 \]
Animation showing the posterior under the optimal policy

\[ n = 3, \ X_n = 0.63587, \ Z_n(X_n) = -1 \]
Animation showing the posterior under the optimal policy

\[ n = 4, \quad X_n = 0.55589, \quad Z_n(X_n) = -1 \]
Animation showing the posterior under the optimal policy

$n = 5, X_n = 0.46446, Z_n(X_n) = -1$
Animation showing the posterior under the optimal policy

\[ n = 10, X_n = 0.39721, Z_n(X_n) = -1 \]
Animation showing the posterior under the optimal policy

\[ n = 20, X_n = 0.20046, Z_n(X_n) = 1 \]
Animation showing the posterior under the optimal policy

\[ n = 30, X_n = 0.36118, Z_n(X_n) = 1 \]
Animation showing the posterior under the optimal policy

\[ n = 40, \ X_n = 0.39722, \ Z_n(X_n) = 1 \]
Animation showing the posterior under the optimal policy

\[ n = 50, X_n = 0.36904, Z_n(X_n) = 1 \]
Animation showing the posterior under the optimal policy

\[ n = 100, X_n = 0.3752, Z_n(X_n) = 1 \]
Animation showing the posterior under the optimal policy

\[ n = 150, X_n = 0.37261, Z_n(X_n) = 1 \]
This algorithm converges exponentially fast

- We used entropy as our measure of residual uncertainty because it makes the dynamic program tractable.
- In practice, we are interested in other measures, such as expected absolute loss.

**Theorem**

*Under the policy that chooses $X_n$ at the median of $f_n$, when $p(\cdot)$ is constant, known, and bounded away from $1/2$,*

$$E|X_n - X^*| = O(e^{-rn}) \text{ for some } r > 0$$

[Waeber, Frazier, Henderson 2013].

The value of $r$ depends on $p(\cdot)$.

In contrast, under stochastic approximation, $E|X_n - X^*| = O(n^{-1/2})$ (assuming a well-chosen tuning sequence, and that certain technical conditions are met).
This algorithm outperforms stochastic approximation when $p(\cdot)$ is constant and known.
This algorithm is not new

- This algorithm was introduced in [Horstein, 1963], and is called the **Probabilistic Bisection Algorithm**, though it was not known to be Bayes-optimal.

- A discretized version was introduced in [Burnashev and Zigangirov, 1974].

- Analyses of the discretized version, or other related problems: [Feige et al., 1994], [Karp and Kleinberg, 2007], [Ben-Or and Hassidim, 2008], [Nowak, 2008], [Nowak, 2009], ...

- Survey paper: [Castro and Nowak, 2008]
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Survey paper: [Castro and Nowak, 2008]

“The [probabilistic bisection] algorithm seems to work extremely well in practice, but it is hard to analyze and there are few theoretical guarantees for it, especially pertaining error rates of convergence.”
Outline

1. Stylized Setting: $p(\cdot)$ is known and constant

2. Practical Setting: $p(\cdot)$ is unknown, and bounded below by $p_c > 1/2$. 
Although our analysis was idealized, we can use probabilistic bisection in practice

- The previous analysis assumed $p(\cdot)$ was known and constant.
  - This assumption is not met in practice.
- We now use the sequential sampling method to construct our left/right observations $Z_n(X_n)$. These satisfy $p(\cdot) \geq p_c$.
- We still use the probabilistic bisection algorithm, but update $f_n$ using $p_c$ instead of the unknown $p(X_n)$.
  - $f_n$ is no longer a true Bayesian posterior density.
We will analyze probabilistic bisection in this practical setting

We will give theorems related to consistency, confidence intervals, and rates of convergence for probabilistic bisection in this practical setting.

These theorems will assume:

- $X^* \in [0, 1]$ fixed and unknown.
- $X_n \neq X^*$ for any finite $n \in \mathbb{N}$.
- $p(X_n) \geq p_c$ for all $n \in \mathbb{N}$.

We use the notation $q_c = 1 - p_c$. 
Probalistic bisection is consistent

Theorem

\[ X_n \rightarrow X^* \text{ almost surely as } n \rightarrow \infty. \]
We can create a confidence interval for $X^*$

- Notation: $q_c = 1 - p_c; \mu = p_c \ln 2p_c + q_c \ln 2q_c$.
- For $\alpha \in (0, 1)$, define $b_n = n\mu - n^{1/2}(-0.5\ln \alpha)^{1/2}(\ln 2p_c - \ln 2q_c)$.
- Our confidence interval will be:
  \[ J_n = \text{conv}(x \in [0, 1] : f_n(x) \geq e^{b_n}). \]

**Theorem**

For $\alpha \in (0, 1)$,

\[ \mathbb{P}(X^* \in J_n) \geq 1 - \alpha, \]

for all $n \in \mathbb{N}$.

In contrast, we unaware of a method for a creating a true confidence interval using stochastic approximation.
This confidence interval shrinks at an exponential rate

**Theorem**

Choose $p_c \geq 0.85$, $\alpha \in (0, 1)$. For $0 < r < \mu - q_c \ln 2 p_c$ there exists a $N(p_c, r, \alpha) \in \mathbb{N}$, such that

$$
P(|J_n| \leq e^{-rn}, X^* \in J_n) \geq 1 - \alpha,
$$

for all $n \geq N(p_c, r, \alpha)$. 
Our estimates of the root converge at an exponential rate

**Theorem**

Define $\hat{X}_n$ to be any point in $J_n$, then there exists $r > 0$ such that

$$\mathbb{E}[|X^* - \hat{X}_n|] = O(e^{-rn}).$$

- This is extremely fast compared to stochastic approximation:
  $$O(e^{-rn}) \text{ vs. } O(n^{-1/2}).$$

- And we have true confidence intervals for $X^*$.

- But $n$ is the number of measurement points, what about total wall-clock time?
We have considered iteration count, but wall-clock time is more important.

At each iteration of this bisection algorithm we:

- Sample sequentially at $X_n$, observing $S_m(X_n) = \sum_{i=1}^{m} Y_{n,i}(X_n)$, until

  \[
  N_n = \inf \left\{ m : |S_m| \geq \left[ (m+1)(\log(m+1) + 2\log(1/\alpha)) \right]^{1/2} \right\},
  \]

- We should measure performance by wall-clock time: $T_n = \sum_{i=1}^{n} N_n$. 

![Graph showing the relationship between $m$ and $S_m(X_n)$.](attachment:graph.png)
Considering wall-clock time is especially important if \( g(x) \to 0 \) as \( x \to X^* \)

Suppose we have iid normal noise.

- If \( g(\cdot) \) jumps across 0 at \( X^* \), then the expected number of samples required per iteration of the bisection algorithm remains bounded as \( x \) approaches \( X^* \).

- If \( g(x) \to 0 \) as \( x \to X^* \), then the expected number of samples per iteration grows to infinity.

Under stochastic approximation, one iteration always requires one sample.
Stochastic approximation and probabilistic bisection have very different sample paths

\[ X^* - X_n \]

Robbin–Monro, \( a_n = \frac{1}{n} \), \( \varepsilon_n \sim N(0,1) \)

Bisection, \( p = 0.75 \), \( \varepsilon_n \sim N(0,1) \)
Numerical comparisons show stochastic approximation is faster than probabilistic bisection in wall-clock time.
Theory shows stochastic approximation is faster than probabilistic bisection in wall-clock time

- We use this result from [Farrell, 1964]:
  \[ \mathbb{E}_{g(x)}[N] \sim \left( \frac{1}{g(x)} \right)^2 \log \log \left( \frac{1}{|g(x)|} \right) \text{ as } g(x) \to 0, \]

and for all tests of power one, if \( P_0(N = \infty) > 0 \), then

\[ \lim_{g(x) \to 0} g(x)^2 \mathbb{E}_{g(x)}[N] = \infty. \]

**Theorem**

*If \( g(x) \to 0 \) as \( x \to X^* \), and we have homoscedastic normal noise, then \(|X^* - X_n|(T_n)^{1/2})_n \) is not tight.*

- If
  \[ g(x) \to 0 \text{ as } x \to X^*, \]

and if we use \( X_n \) as the best estimate of \( X^* \) then the Probabilistic Bisection Algorithm with power one tests is *asymptotically slower* than Stochastic Approximation.
We conjecture that probabilistic bisection is almost as fast as stochastic approximation in wall-clock time

- $X_n$ might not be the best estimate for $X^*$ when we use power one tests.
- Intuitively, observations where we spend more time should also be closer to $X^*$, hence an estimator of the form

$$\tilde{X}_n = \frac{1}{T_n} \sum_{i=1}^{n} N_i X_i$$

should perform better.

**Conjecture:** For any $\varepsilon > 0$ it holds that

$$\mathbb{E}[|\tilde{X}_n - X^*|] = O(T_n^{-\frac{1}{2} + \varepsilon}),$$

(if $g$ satisfies some growth conditions).
Numerical Comparison Cont.

\[ E[|X^* - X_n|] \]

Robbins–Monro \((a_n = 1/n)\)

Bisection, Siegmund \((p_c = 0.85)\)

Polyak–Ruppert

Bisection Averaging
Conclusions

**Advantages:**
- Provides true confidence interval of the root $X^*$.
- Works extremely well if there is a jump at $g(X^*)$ (geometric rate of convergence).
- Only one tuning parameter.
- Better use of prior information.
- Better ability to track progress.
- Robust finite-time performance

**Drawbacks:**
- Asymptotically slower than stochastic approximation (but not by much).
- Higher computational cost per iteration.

**Future Research:**
- Use parallel computing (very little switching of $(X_n)_n$).
- Extension to higher dimensions.
Thank You

Any questions?
The Bayesian learner is optimal for noisy binary search (and pretty good for quantum as well).

An interval estimation problem for controlled observations.

Active learning and sampling.

Asymptotic behavior of expected sample size in certain one sided tests.

Computing with noisy information.


