AI for Adaptive Experiment Design

Yisong Yue
Goal-Oriented Experiment Design

- Iterative & adaptive
- Utility maximizing (find best outcome)
Many Applications (Goal-Oriented)

Robotics & Control
image credit @ mwarmandfield

Protein Engineering
image credit @ creativebiomart

Drug Discovery
from Slideshare

Material Science
image credit @ phys.org
AI for Goal-Oriented Experiment Design

Hypothesis Space

Nature Paper

$100M

Useful Result
Batch Supervised Learning

Data: X

Target Signal: Y

$$f(x) \approx y$$

Data Collected Up Front!
Experiment Design as Interactive Learning

- Collect data on the fly
  - Not available a priori

- Limited budget on data collection

- How to choose?
Three Modes of Interactive Learning

**Active Learning**
- **Goal:** Discover truth
- E.g., model of world
- Maximize accuracy

**(Bayesian) Optimization**
- **Goal:** Best single prediction
- E.g., best protein
- Maximize final utility

**Multi-Armed Bandits**
- **Goal:** Utility over time
- E.g., recommender systems
- Maximize utility over time

Focus of Talk
Learning Setup (Bayesian)

Given: input space $X$
Unknown: fitness $F(x) = y$
Maintain: posterior $P(F|D)$  ($D=$measurements)

---

**Experiment Designer**

Add $(x_t, y_t)$ to $D$
Update posterior $P(F|D)$

**Experiment Platform**

Choose $x_t$
Measure $y_t$

$t = t + 1$

Upper Confidence Bound: $\text{argmax}_x \mu(x) + \beta \sigma(x)$
Posterior Sampling: $\text{argmax}_x f(x), \ f \sim P(F|D)$
Active Learning Simple Example

• 1 feature
• Learn threshold function
Active Learning Simple Example

• 1 feature
• Learn threshold function
Comparison with Passive/Batch Learning

• # samples to be within $\varepsilon$ of true model

• Passive Learning: $O\left(\frac{1}{\varepsilon}\right)$

• Active Learning: $O\left(\log \frac{1}{\varepsilon}\right)$
(Bayesian) Optimization Example

$X = \text{space of proteins}$

$F(x) = \text{fitness landscape}$

Image Credit: Frances Arnold

Frances Arnold
Bandits Example

• How to split trials to collect information
• **Static Experimental Design**
  • Standard practice
  • (pre-planned)

Bandits Example

• Adapt experiments based on outcomes
Each Experiment Matters ("Cumulative Regret")

Two Cousins, Two Paths Thomas McLaughlin, left, was given a promising experimental drug to treat his lethal skin cancer in a medical trial; Brandon Ryan had to go without it.

Comparison
(Active Learning, Bayesian Optimization, Bandits)

• Similarities:
  • Same interaction protocol
  • Query $F(x)$
  • “Sequential experimental design”

• Active Learning: learn $F(x)$ as accurately as possible

• (Bayesian) Optimization: find maximizer $F(x^*)$

• Bandits: maximize $\sum_i F(x_i)$

Discovering “truth”
Best result only
Each experiment matters “Regret Minimization”
Algorithmic & Theoretical Questions
(see papers for details)

• Analyze convergence to $F(x^*)$?

• Guarantee side constraints (e.g., safety)?

• Corrupted or indirect measurements?

• Efficiently search combinatorial design spaces?

• Incorporate domain knowledge such as physics?
Real-World Bayesian Optimization

Safety, Preference

Multi-Fidelity

Combinatorial, Physics, ...

Photo credit: Yury Tokpanov
Treating Lower Spine Injuries

Medtronic human array

10 mm

49 mm

Each patient is unique
$10^9$ possible configurations!

Image source: williamcapicottomd.com

Yanan Sui
Joel Burdick

SCI Patient
Learning Setup

Update posterior $P(F|D)$

Electrode Array

$y_t$ Receive Response

$t = t + 1$

$x_t$ Apply Stimulus

SCI Patient

Yanan Sui
Joel Burdick
Challenges

• Many actions
  • $10^6$ to $10^9$

• Measuring utility difficult

• Safety
Modeling Correlations: Gaussian Processes

- Defined by $GP(\mu, k)$
  - Sample a function: $f \sim GP(\mu, k)$
    - Expected value: $E[f(x)] = \mu(x)$
    - Correlation of $f(x_1)$ & $f(x_2)$: $k(x_1, x_2)$
- Finite input domain: (e.g., 10 choices of $x$)
  - Reduces to multivariate Gaussian distribution
Benefits of Gaussian Processes

• Reason about uncertainty
  • What is the spread of outcomes for f(x)?

• Correlations over input space
  • Measuring f(x₁) gives information on f(x₂)

• Work with domain experts to build correlations
  • *Ongoing work: automatically learn correlation structure!*
Challenges

• Many actions
  • $10^6$ to $10^9$

• Measuring utility difficult

• Safety

Gaussian Processes w/ Low Dimensional Kernels
Measurements via Preference Feedback

Multi-dueling Bandits with Dependent Arms, Sui, Zhuang, Burdick & Yue, UAI 2017
Correlational Dueling Bandits with Application to Clinical Treatment in Large Decision Spaces, Sui, Yue & Burdick, IJCAI 2017
Aside: Preference Elicitation in Search (Interleaving)

<table>
<thead>
<tr>
<th>Ranking A</th>
<th>Ranking B</th>
</tr>
</thead>
<tbody>
<tr>
<td><a href="http://www.napavalley.com">www.napavalley.com</a></td>
<td>en.wikipedia.org/wiki/Napa_Valley</td>
</tr>
<tr>
<td>2. Napa Valley Wineries - Plan your wine...</td>
<td>2. Napa Valley – The authority for lodging...</td>
</tr>
<tr>
<td><a href="http://www.napavalley.com/wineries">www.napavalley.com/wineries</a></td>
<td><a href="http://www.napavalley.com">www.napavalley.com</a></td>
</tr>
<tr>
<td><a href="http://www.napavalley.edu/homex.asp">www.napavalley.edu/homex.asp</a></td>
<td>books.google.co.uk/books?isbn=...</td>
</tr>
<tr>
<td>4. Been There</td>
<td>Tips</td>
</tr>
<tr>
<td><a href="http://www.ivebeenthere.co.uk">www.ivebeenthere.co.uk</a></td>
<td><a href="http://www.napalinks.com">www.napalinks.com</a></td>
</tr>
<tr>
<td>5. Napa Valley Wineries and Chambers</td>
<td>5. Napa Valley College</td>
</tr>
<tr>
<td><a href="http://www.napavintners.com">www.napavintners.com</a></td>
<td><a href="http://www.napavalley.edu/homex.asp">www.napavalley.edu/homex.asp</a></td>
</tr>
<tr>
<td><a href="http://www.napavalley.com">www.napavalley.com</a></td>
<td><a href="http://www.napavalley.com/wineries">www.napavalley.com/wineries</a></td>
</tr>
<tr>
<td>7. Napa Valley College</td>
<td>7. Napa Valley Hotels – Bed and Breakfast...</td>
</tr>
<tr>
<td><a href="http://www.napavalley.edu/homex.asp">www.napavalley.edu/homex.asp</a></td>
<td><a href="http://www.napalinks.com">www.napalinks.com</a></td>
</tr>
</tbody>
</table>

Presented Ranking

| www.napavalley.com                             | en.wikipedia.org/wiki/Napa_Valley             |
| en.wikipedia.org/wiki/Napa_Valley             | www.napavalley.com                            |
| 3. Napa: The Story of an American Eden...      | 3. Napa Valley Wineries – Plan your wine...   |
| books.google.co.uk/books?isbn=...              | www.napavalley.com/wineries                  |
| 4. Napa Valley Wineries – Plan your wine...   | 4. Napa Valley Hotels – Bed and Breakfast...  |
| www.napavalley.com/wineries                   | www.napalinks.com                             |
| 5. Napa Valley Hotels – Bed and Breakfast...  | 5. Napa Valley College                        |
| www.napalinks.com                              | www.napavalley.edu/homex.asp                  |
| 6. Napa Valley College                         | 6. Napa Valley Wineries – Plan your wine...   |
| www.napavalley.edu/homex.asp                   | www.napavalley.com/wineries                  |
| 7. NapaValley.org                              | 7. Napa Valley Hotels – Bed and Breakfast...  |
| www.napavalley.org                             | www.napalinks.com                             |

B wins!

“Large Scale Validation and Analysis of Interleaved Search Evaluation” Chapelle et al., 2012.
Aside: Deployment on Yahoo! Search Engine

Comparing Two Ranking Functions

Interleaving is more sensitive and more reliable

"Large Scale Validation and Analysis of Interleaved Search Evaluation," Chapelle et al., TOIS 2012.
Challenges

• Many actions
  • $10^6$ to $10^9$

• Measuring utility difficult

• Safety

Gaussian Processes w/
Low Dimensional Kernels

Preference Feedback
Gaussian Process Safety Model

Safety Threshold

Unsafe!  Almost  Unsafe!  Safe!

Stagewise Safe Bayesian Optimization with Gaussian Processes, Sui, Zhuang, Burdick & Yue, ICML 2018
Challenges

• Many actions
  • $10^6$ to $10^9$

• Measuring utility difficult

• Safety

Gaussian Processes w/ Low Dimensional Kernels

Preference Feedback

Uncertainty Quantification Using Gaussian Processes
Multi-dueling Bandits with Dependent Arms, Sui, Zhuang, Burdick & Yue, UAI 2017
Correlational Dueling Bandits with Application to Clinical Treatment in Large Decision Spaces, Sui, Yue & Burdick, IJCAI 2017
Stagewise Safe Bayesian Optimization with Gaussian Processes, Sui, Zhuang, Burdick & Yue, ICML 2018
Algorithmic Insights

Stagewise Safe Bayesian Optimization with Gaussian Processes, Sui, Zhuang, Burdick & Yue, ICML 2018
Algorithmic Insights

Stagewise Safe Bayesian Optimization with Gaussian Processes, Sui, Zhuang, Burdick & Yue, ICML 2018
First Maximize Safety Region
• Optimistic in the face of uncertainty
• Identify reachable safety region
• Approximately maximal w/ convergence guarantees

Meta-Framework
• Leverage any Bayesian Optimization alg.
• Inherit guarantees

Stagewise Safe Bayesian Optimization with Gaussian Processes, Sui, Zhuang, Burdick & Yue, ICML 2018

Algorithmic Insights

Standard Bayesian Optimization
Clinical Experiments
Clinical Experiments

Utility of Spinal Cord Injury Therapies

Stagewise Safe Bayesian Optimization with Gaussian Processes, Sui, Zhuang, Burdick & Yue, ICML 2018
Real-World Bayesian Optimization

Safety, Preference

Multi-Fidelity

Combinatorial, Physics, ...

Photo credit: Yury Tokpanov
Nano-photonics Structure Design

Fleischman et al.: https://doi.org/10.1021/acsphotonics.8b01634
Hyperspectral Imaging
Fitness Function (Figure of Merit)

Fitness Function: \[ FOM = \frac{\Delta \text{wav}}{c \cdot \text{wav}} + \frac{c \cdot \text{peak}}{\text{peak}} + \frac{\text{noise}}{c \cdot \text{noise}} + \frac{\text{FWHM}}{c \cdot \text{FWHM}} \]
Multi-Fidelity Simulations

• Solve Maxwell’s equations
• Fidelity depends on temporal and spatial resolution
• Do we need to accurately simulate bad structures?

Electric field profiles at 550nm for different mesh sizes

Image Credit: Yury Tokpanov
A General Framework for Multi-fidelity Bayesian Optimization with Gaussian Processes, Jialin Song et al., AISTATS 2019
Algorithmic Insights

A General Framework for Multi-fidelity Bayesian Optimization with Gaussian Processes, Jialin Song et al., AISTATS 2019
**Algorithmic Insights**

**Meta-Framework**
- Use coarse level as much as possible
- Periodically check fine level to calibrate
- Switch to fine level only at end
  - Can use any Bayesian Opt. algorithm
- **Cost-Weighted Value of Information**

---

**A General Framework for Multi-fidelity Bayesian Optimization with Gaussian Processes**, Jialin Song et al., AISTATS 2019
Results

• 3 fidelities

• Balances different costs

• State-of-the-art performance

Optimizing Photonic Nanostructures via Multi-fidelity Gaussian Processes
Song, Tokpanov, Chen, Fleischman, Fountaine, Atwater, Yue, 2018

Mirrored Plasmonic Filter Design via Active Learning of Multi-Fidelity Physical Models
Song, Tokpanov, Chen, Fleischman, Fountaine, Atwater, Yue, 2020
Real-World Bayesian Optimization

Safety, Preference  Multi-Fidelity  Combinatorial, Physics, ...

Photo credit: Yury Tokpanov
Incorporate Constraints in Real Workflows

- Combinatorial Library Design
- Directed Evolution
- Prior knowledge (e.g., ΔΔ\textit{G})
- Etc...

Bruce Wittmann
Kevin Yang

Batched Stochastic Bayesian Optimization, Yang, Chen, Lee, Yue, AISTATS 2019
Preference Learning

- **Dueling Posterior Sampling for Preference-Based Reinforcement Learning**, Ellen Novoseller et al., UAI 2020
- **Preference-Based Learning for Exoskeleton Gait Optimization**, Maegan Tucker, Ellen Novoseller et al., ICRA 2020
- **Human Preference-Based Learning for High-dimensional Optimization of Exoskeleton Walking Gaits**, Maegan Tucker et al., IROS 2020
- **ROIAL: Region of Interest Active Learning for Characterizing Exoskeleton Gait Preference Landscapes**, Amy Kejun Li et al., ICRA 2021
Incorporating Physics

Interactive Controller Calibration

Landing time comparison

- Robust Regression
- GP-1
- GP-2
- GP-3
- GP-4
- GP-5

Figure 5: Comparison with GPs

Robust Regression for Safe Exploration in Control, Angie Liu, Guanya Shi, et al., L4DC 2020
Ongoing Direction:
Decision-Aware Representation Learning for Experiment Design

- Hard to hand-craft representations
- Recent trend towards learning them!
- Many interesting new questions!
  - How to propagate gradients?
  - Directly learn value of information?
Preliminary Result: Deep Kernel Bayesian Optimization
AI for Adaptive Experiment Design

• Experimental Platforms Increasingly Automated
  • Motivates using Active Learning / Bayesian Optimization / Bandits

• Real-World Considerations
  • Indirect measurements
    • Preference feedback
    • Multi-fidelity
  • Constraints
    • Safety
    • Physical constraints
  • Domain Knowledge
    • Dynamics
    • Human factors

• Cool Applications!
Multi-dueling Bandits with Dependent Arms, Yanan Sui et al., UAI 2017
Correlational Dueling Bandits with Application to Clinical Treatment in Large Decision Spaces, Yanan Sui et al., IJCAI 2017
Large Scale Validation and Analysis of Interleaved Search Evaluation, Olivier Chapelle, Thorsten Joachims, et al., TOIS 2012
Dueling Posterior Sampling for Preference-Based Reinforcement Learning, Ellen Novoseller et al., UAI 2020
Preference-Based Learning for Exoskeleton Gait Optimization, Maegan Tucker, Ellen Novoseller et al., ICRA 2020 (Best Paper Award)
Human Preference-Based Learning for High-dimensional Optimization of Exoskeleton Walking Gaits, Maegan Tucker et al., IROS 2020
ROIAL: Region of Interest Active Learning for Characterizing Exoskeleton Gait Preference Landscapes, Amy Kejun Li et al., ICRA 2021
Stagewise Safe Bayesian Optimization with Gaussian Processes, Yanan Sui et al., ICML 2018
A General Framework for Multi-fidelity Bayesian Optimization with Gaussian Processes, Jialin Song et al., AISTATS 2019
Optimizing Photonic Nanostructures via Multi-fidelity Gaussian Processes, Jialin Song et al., NeurIPS Workshop on Machine Learning for Molecules and Materials, 2018
Mirrored Plasmonic Filter Design via Active Learning of Multi-Fidelity Physical Models, Jialin Song et al., IEEE Conference on Lasers and Electro-Optics (CLEO), 2020
Batched Stochastic Bayesian Optimization, Kevin Yang et al., AISTATS 2019
Robust Regression for Safe Exploration in Control, Angie Liu, Guanya Shi, et al., L4DC 2020
Teaching Multiple Concepts to Forgetful Learners, Anette Hunziker, Yuxin Chen, et al., NeurIPS 2019
Learning to Make Decisions via Submodular Regularization, Ayya Aliева, et al., ICLR 2021
Deep Kernel Bayesian Optimization, James Bowden et al., (in preparation)
Learning Regions of Interest for Bayesian Optimization with Adaptive Level-Set Estimation, Fengxue Zhang et al., (in preparation)