AI for Adaptive Experiment Design

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Goal-Oriented Experiment Design

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

Robotics & Control
image credit @ mfarmandfield

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 $P(F|D)$  \( (D=\text{measurements}) \)

Experiment Designer

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

Experiment Platform

Measure $y_t$  \( \rightarrow \)
Choose $x_t$  \( \rightarrow \)

$t = t + 1$

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

Passive Learning
Sample from distribution

True Model

Learned Model
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

\[ X = \text{space of proteins} \]
\[ F(x) = \text{fitness landscape} \]
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”)

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 $\sum_i F(x_i)$
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

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

Medtronic human array

Image source: williamcapicottomd.com

Yanan Sui  Joel Burdick

SCI Patient
Learning Setup

Update posterior $P(F|D)$

Receive Response $y_t$

Apply Stimulus $x_t$

$t=t+1$

Electrode Array

SCI Patient

Yanan Sui
Joel Burdick
Challenges

• Many actions
  • $10^6$ to $10^9$

• Measuring utility difficult

• Safety
Modeling Correlations: Gaussian Processes

• Defined by $GP(\mu, k)$
  
  Mean function

  Covariance “kernel”

• Sample a function: $f \sim GP(\mu, k)$
  
  • Expected value of $f(x)$ is $\mu(x)$
  
  • Correlation of $f(x_1)$ & $f(x_2)$ is $k(x_1, x_2)$

• 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
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)

### Ranking A
1. Napa Valley – The authority for lodging...
   www.napavalley.com
2. Napa Valley Wineries - Plan your wine...
   www.napavalley.com/wineries
3. Napa Valley College
   www.napavalley.edu/homex.asp
4. Been There | Tips | Napa Valley
   www.ivebeenthere.co.uk
5. Napa Valley Wineries and Wine
   www.napavintners.com
6. Napa Country, California
   en.wikipedia.org/wiki/Napa_Valley

### Ranking B
   en.wikipedia.org/wiki/Napa_Valley
2. Napa Valley – The authority for lodging...
   www.napavalley.com
3. Napa: The Story of an American Eden...
   books.google.co.uk/books?isbn=...
4. Napa Valley Hotels – Bed and Breakfast...
   www.napalinks.com
5. NapaValley.org
   www.napavalley.org
6. Napa Valley College
   www.napavalley.edu/homex.asp
7. NapaValley.org
   www.napavalley.org

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

“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

Absolute Metrics
E.g., #Clicks@1, Total #Clicks, etc.

Each ranking function receives 50% traffic

"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

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
Full Learning Setup

Multiple Stimuli $x_t$

Preference Response $y_t$

$t = t + 1$

Electrode Array

Update posterior $P(F|D)$

SCI Patient

**While guaranteeing safety**

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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

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Algorithmic Insights

Safe Region

Initial Safe Action

Very Safe!

Almost Unsafe!

Hypothesis Space

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

Yanan Sui

Vincent Zhuang
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
Algorithmic Insights

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
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)

Maxwell’s equations
FDTD solver

Fitness Function: \[ FOM = \frac{\Delta \text{wav}}{\text{c.wav}} + \frac{c.\text{peak}}{\text{peak}} + \frac{\text{noise}}{c.\text{noise}} + \frac{\text{FWHM}}{c.\text{FWHM}} \]
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
A General Framework for Multi-fidelity Bayesian Optimization with Gaussian Processes, Jialin Song et al., AISTATS 2019
Algorithmic Insights

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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
Real-World Bayesian Optimization

Safety, Preference

Multi-Fidelity

Combinatorial, Physics, ...

Photo credit: Yury Tokpanov
Batched Stochastic Bayesian Optimization

• Start with initial amino acid sequence
• Choose with sites to mutate
• Mutations are probabilistic
• Combinatorial structure in experiment design

Batched Stochastic Bayesian Optimization, Yang, Chen, Lee, Yue, AISTATS 2019
Interactive Controller Calibration

\[ \tau_i(x) = f(t_i; x, t_{a}(x)) + \epsilon_i \]

Robust Regression for Safe Exploration in Control, Angie Liu, Guanya Shi, et al., arxiv
We compare against five GP models with a wide range of kernel widths. A widespread practical issue is that real test distributions rarely match the training distribution. Our work shares some similarity with existing approaches.

As discussed above, GP-based approaches can be sensitive to model selection. One could blend different kernel functions to lead to more flexible inductive bias and better fitting of the data.

There are many avenues for future work. For instance, our safety criterion was relatively simple, and there is work to be done in tuning. Finally, our deep robust regression approach is of independent interest beyond model-based control, and can be incorporated in other applications as well.

These bounds explicitly translate the error in dynamics learning to the tracking error in control. They can be incorporated with deep kernel learning and incorporating more sophisticated density estimation techniques. Another interesting direction is to incorporate with deep kernel learning and to prove that the proposed safe exploration algorithm converges to the optimal dynamics estimator in its function class, as well as the optimal controller for tracking optimal desired trajectories.

Directions to explore include incorporating other regularization techniques, relaxing from Gaussian observation noise, and developing methods that can prove tighter safety guarantees. This can lead to dramatically improved performance. One can consider employing more sophisticated criteria that require more sophisticated certification.

We explore a robust regression approach for dynamics estimation. Using robust regression, we explicitly deal with data shifts during episodic learning, and in particular can quantify uncertainty over entire trajectories. We prove the generalization and perturbation bounds for robust regression, we explicitly deal with data shifts during episodic learning, and in particular can quantify uncertainty, we develop a robust deep regression method for dynamics estimation.

In this paper, we propose an algorithmic framework for safe exploration in model-based control. To employ spectral normalization in conjunction with robust estimation.

The study of data shift has seen increasing interest in recent years, owing to the fact that many methods for safe exploration are designed under the assumption of covariate shift, although ours is the first to extend to deep neural networks with rigorous guarantees.

More broadly, dealing with domain shift is a fundamental challenge in deep learning, as highlighted in the RBF kernel. Figure 5 shows that our approach outperforms other methods.

Robust Regression for Safe Exploration in Control, Angie Liu, Guanya Shi, et al., arxiv
Any Many More…
(subjective & dynamical)

Dueling Posterior Sampling for Preference-Based Reinforcement Learning, Ellen Novoseller et al., arxiv
Preference-Based Learning for Exoskeleton Gait Optimization, Maegan Tucker, Ellen Novoseller et al., arxiv
Any Many More…
(human cognitive factors)

Connecticut Warbler

MacGillivray's Warbler

Interpretable Teaching

Teaching Forgetful Learners

Near-Optimal Machine Teaching via Explanatory Teaching Sets, Yuxin Chen, Oisin Mac Aodha, et al., AISTATS 2018
Teaching Categories to Human Learners with Visual Explanations, Oisin Mac Aodha, et al., CVPR 2018
Teaching Multiple Concepts to Forgetful Learners, Anette Hunziker, Yuxin Chen, et al., NeurIPS 2019
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., arxiv
Preference-Based Learning for Exoskeleton Gait Optimization, Maegan Tucker, Ellen Novoseller et al., arxiv
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
Batched Stochastic Bayesian Optimization, Kevin Yang et al., AISTATS 2019
Robust Regression for Safe Exploration in Control, Angie Liu, Guanya Shi, et al., arxiv
Near-Optimal Machine Teaching via Explanatory Teaching Sets, Yuxin Chen, Oisin Mac Aodha, et al., AISTATS 2018
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