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Decision Theory For Optimization

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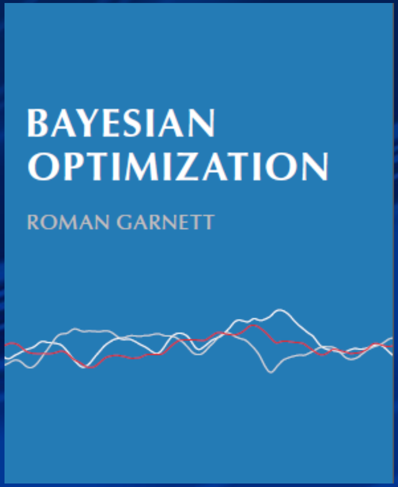


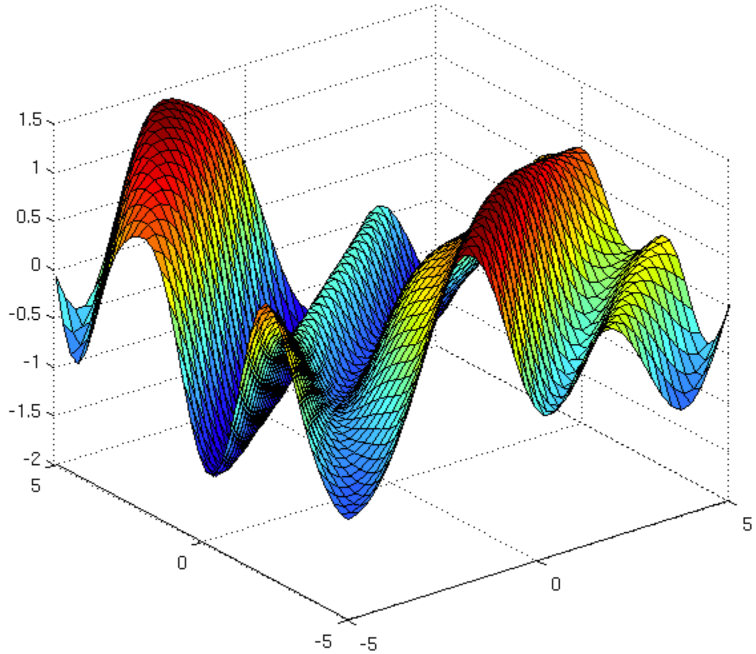
Agenda

1. Recap
2. Bayesian Decision Theory
3. Isolated Decision
4. Sequential Decisions
5. Cost & Approximation of the Optimal Policy
6. Cost-Aware Optimization
7. Summary
8. References

Black-box Function

What is Black-box Function?

- Internal working is hidden
- Evaluation is Expensive
- Gradient doesn't exists



https://python.plainenglish.io/descent-carefully-on-your-gradient-c0f030ddef81

Example – Hyperparameter Tuning

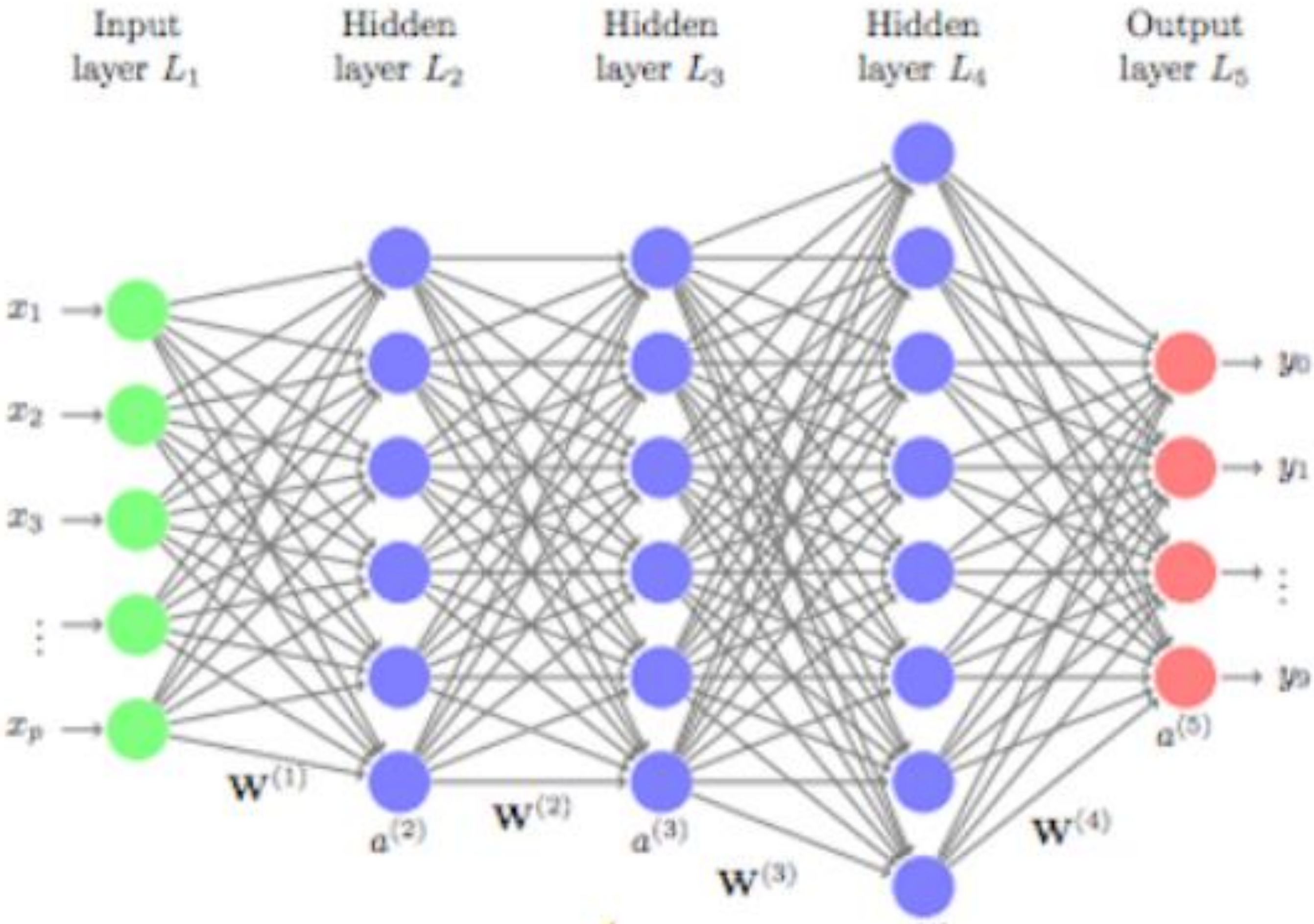


Fig: Architecture of Neural Network

Hyperparameters

- Learning Rate
- Batch size
- No. of hidden layers

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Bayesian Decision Theory

Bayesian Optimization

What is Bayesian Optimization?

- Formalization of the objective function

$$f : X \to \mathbb{R}$$

- Goal:

$$x^* \in \underset{x \in X}{\operatorname{argmax}} f(x)$$

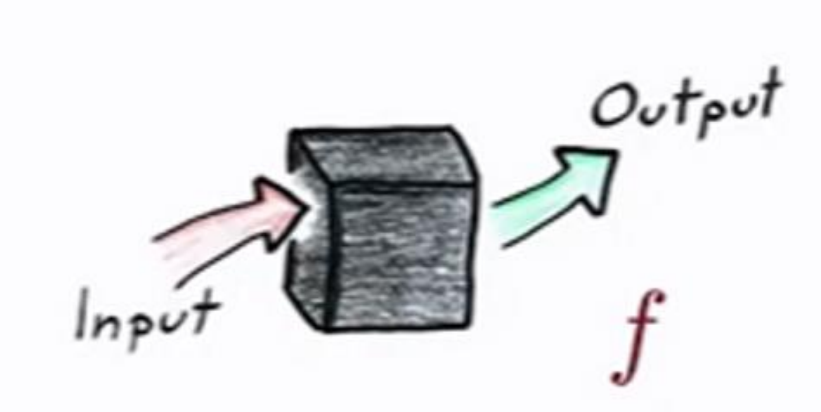


Fig. Black box Function

Sequential Algorithm

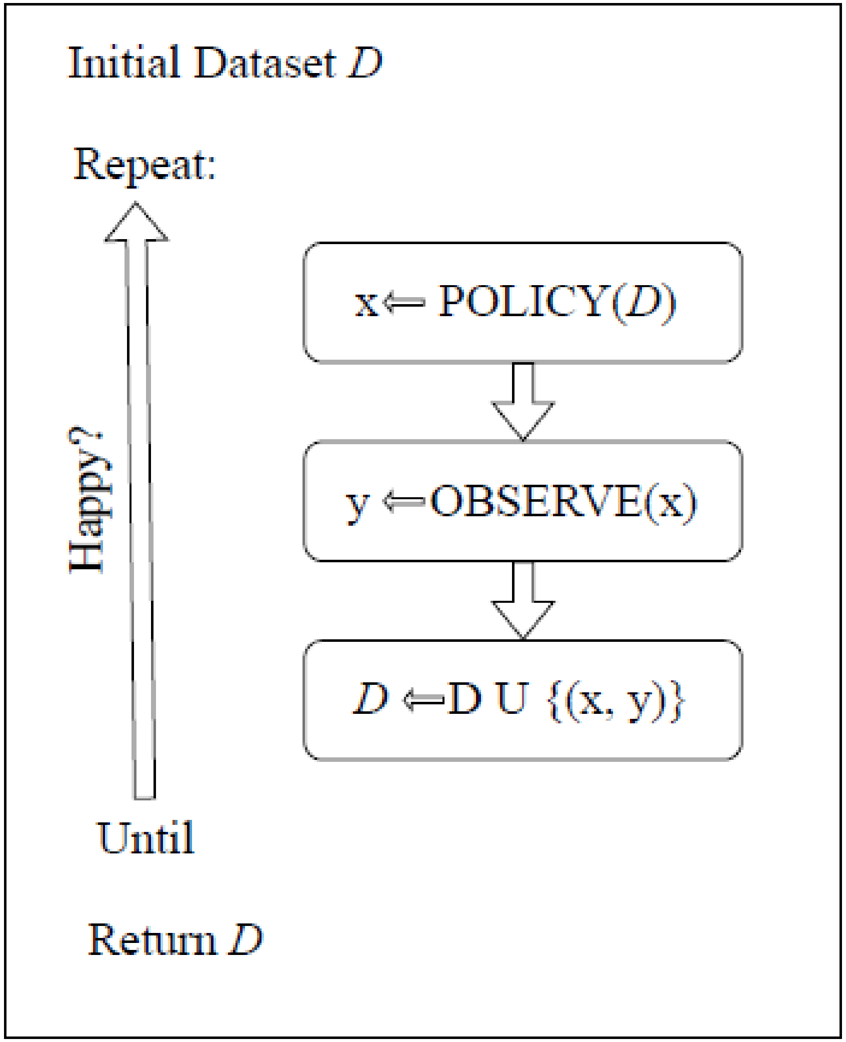
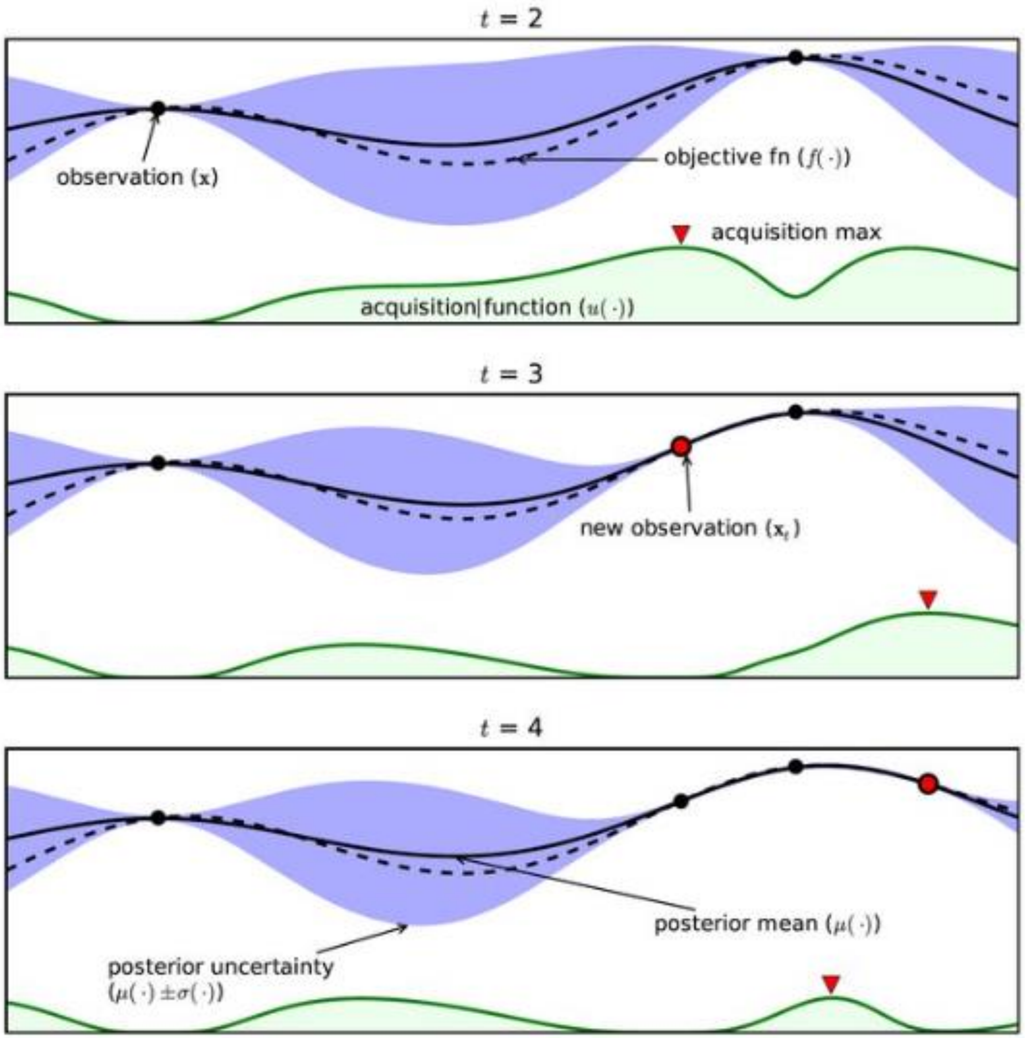


Fig Sequential Optimization Algorithm

Illustration



https://haikufactory.com/files/bayopt.pdf

Acquisition Function

- Inexpensive function that provides a score to each potential observation location
- Often used Interchangeable with Policy

Formulation of Acquisition Function

$$\alpha : X \rightarrow \mathbb{R}$$

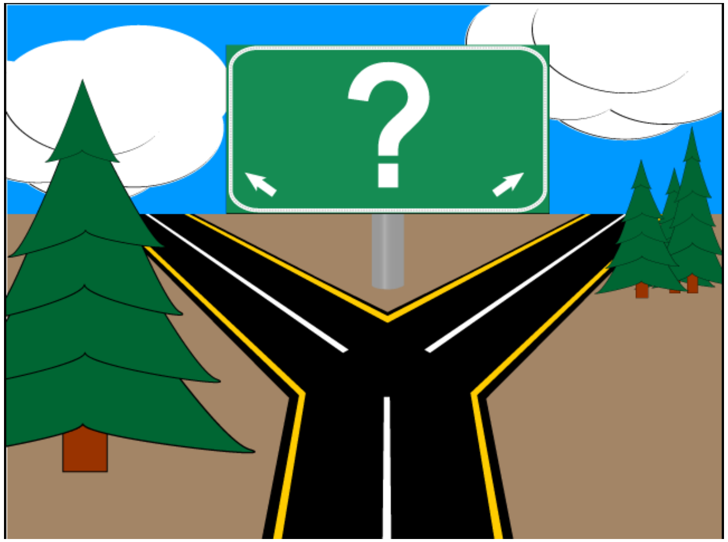
Maximizing the Acquisition Function

$$x \in \underset{x' \in X}{\operatorname{argmax}} \, \alpha\,(x'; D)$$

https://www.centernotes.com/improve-your-quality-scores-80387.html

Bayesian Decision Theory

- Bayesian Decision theory for Decision making under uncertainty
- Stopping Rule – tells about when to terminate the optimization process



https://en.wikipedia.org/wiki/Uncertainty

Isolated Decisions

Elements of Decision Problem

- Any decision problem under uncertainty has two characteristics

  1. Action Space

  $$\mathbf{A} = \boldsymbol{X} = \{\boldsymbol{x_1}, \boldsymbol{x_2}, \boldsymbol{x_3}\,.....\}$$

  2. Uncertain Element (ψ)

- Real-valued Utility Function $u(a,\psi,\mathrm{D})$
- Expected Utility

$$\mathbb{E}[\boldsymbol{u}(\boldsymbol{a},\boldsymbol{\psi},\mathbf{D})\,|\boldsymbol{a},\boldsymbol{D}] = \int \boldsymbol{u}(\boldsymbol{a},\boldsymbol{\psi},\mathbf{D})\,\mathbf{p}(\boldsymbol{\psi}|\mathbf{D})\,\mathbf{d}\boldsymbol{\psi}$$

Utility Function

- Maximizing the expected utility

$$\mathbf{a} \in \underset{a' \in A}{\mathbf{argmax}}\ \mathbb{E}\left[\boldsymbol{u}(\boldsymbol{'a},\boldsymbol{\psi},\mathbf{D}) \,\middle|\, \boldsymbol{a'}, \boldsymbol{D}\right]$$

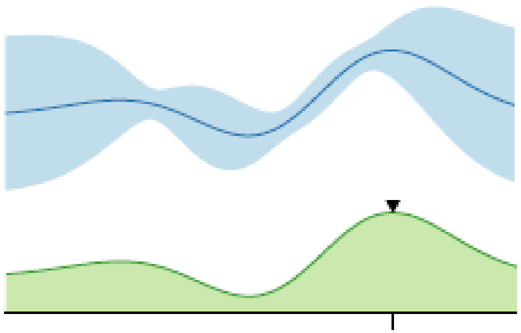
- Decision is optimal if no other action results in greater utility

- General Procedure for acting optimally under uncertainty
  1. Computing Expected Utility w.r.t the unknown variable
  2. Maximizing the Expected utility to select an action

Example for recommending an optimal action

- Utility Function

$$u(x, f) = f(x) = \phi$$



- Expected Utility for recommending a point x is

$$\mathbb{E}[u(x, f) \mid x, \mathrm{D}] = \mathbb{E}[\phi \mid x, \mathrm{D}] = \mu_D(x)$$

- Optimal Action

$$\mathbf{x} \in \underset{\mathbf{x}' \in \mathbf{X}}{\mathbf{argmax}}\ \mu_D(x')$$

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Sequential Decisions

Sequential Decision

- How it is different from Isolated Decision
- Sequential decision with a fixed budget

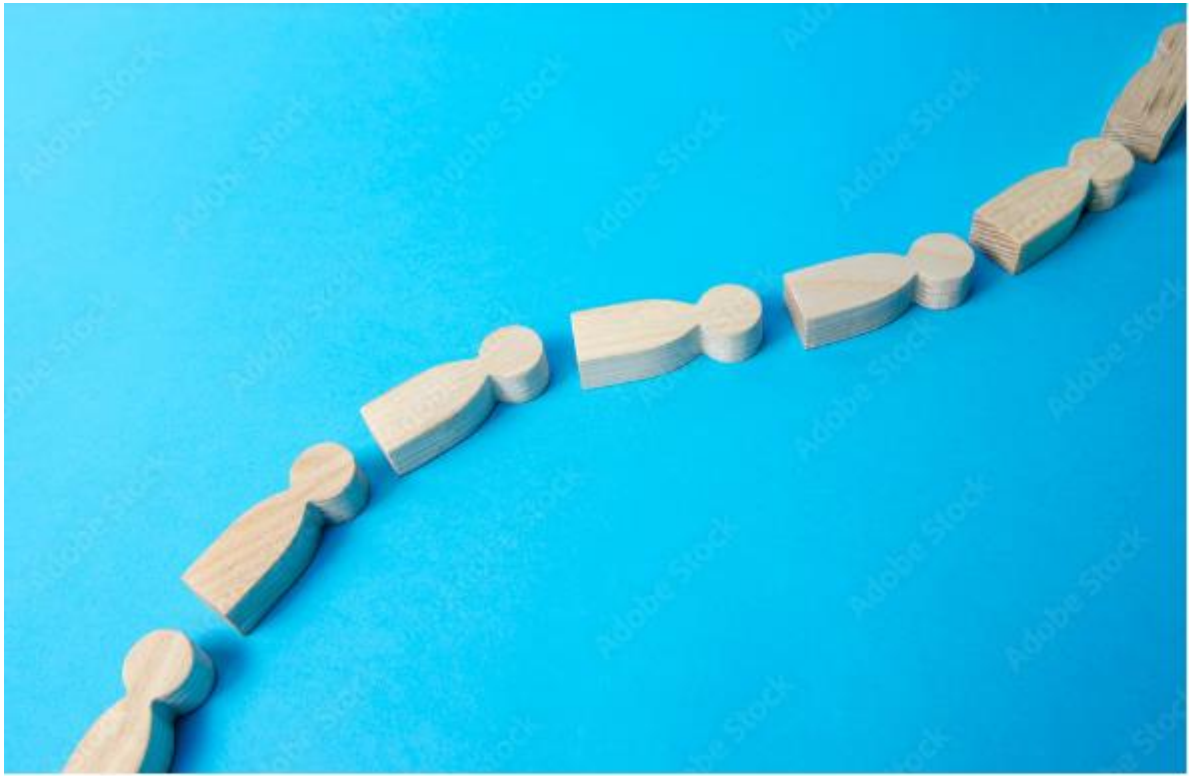


Fig: Sequential Decision

Sequential decision with a fixed budget

- Problem Formulation

An arbitrary set of data D, how should we design our next evaluation location when exactly τ observations remain before termination?

- Backward Induction

- Assumptions

  1. Each decision will have same cost

  2. Fixed budget will tell us the number of observations remaining until termination

Sequential decision with a fixed budget

- Dataset at Final stage of optimization

$$\boldsymbol{D_\tau} = \boldsymbol{D_{\tau-1}} \cup \{(\boldsymbol{x_{\tau-1}}, \boldsymbol{y_{\tau-1}})\} \longrightarrow \boldsymbol{u(D_\tau)}$$

- Expected Terminal Utility to evaluate the potential observation location x:

$$\mathbb{E}[u(D_\tau) \mid x, \mathrm{D}]$$

- Optimal Action via Maximization:

$$\mathbf{x} \in \underset{\mathrm{x}' \in \mathrm{X}}{\mathbf{argmax}}\, \mathbb{E}[u(D_\tau) \mid \boldsymbol{x}', \boldsymbol{D}]$$

- Expected Increase in the utility:

$$\alpha_\tau(x,\ D) = \mathbb{E}[u(D_\tau) \mid x, \mathrm{D}] - u(D)$$

One Observation Remaining

- Decision Horizon (τ) – How far we can look ahead in future when reasoning about the present
- When one observation remaining $\tau = 1$
- Expected increase in the utility from a final evaluation at x is

$$\alpha_1(\boldsymbol{x};\ \boldsymbol{D}) = \int u(D_1)\, \mathrm{p}(\mathrm{y} \mid \mathrm{x}, \mathrm{D})\, \mathrm{dy} - u(D)$$

- Optimal Observation:

$$\mathbf{x} \in \underset{\mathrm{x}' \in \mathrm{X}}{\operatorname{argmax}}\ \alpha_1(\boldsymbol{x}';\ \boldsymbol{D})$$

One Observation Remaining

- Final Utility:

$$u(D) + \alpha_1^*(D)$$

- Illustration :

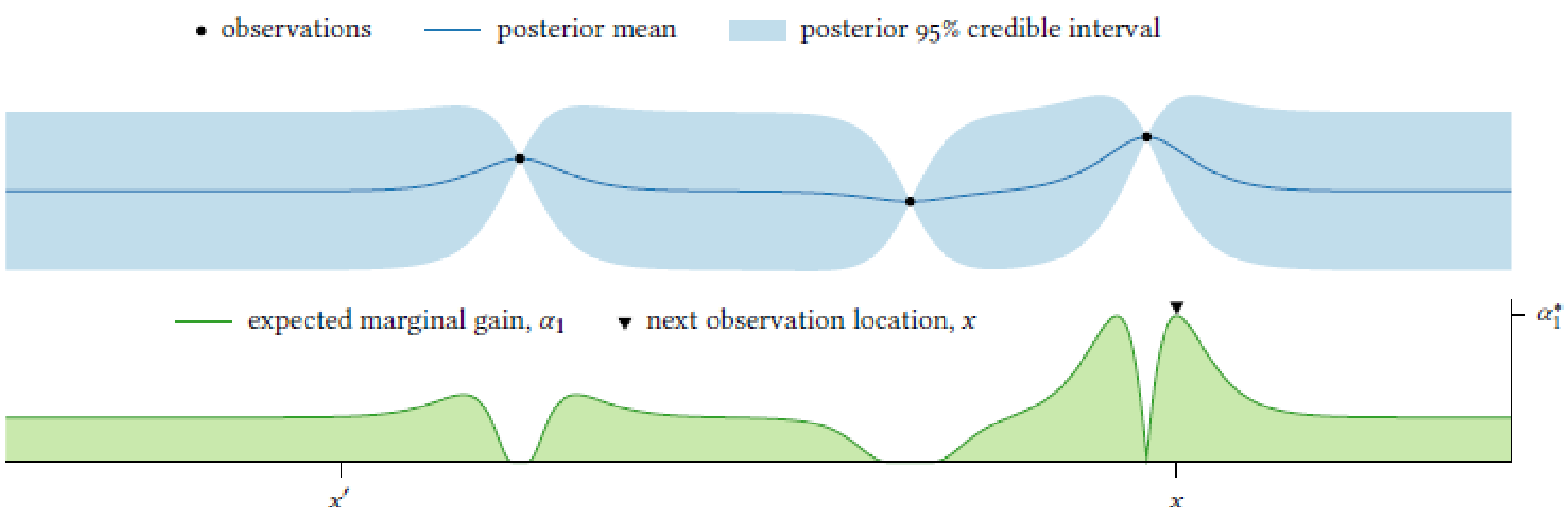


Fig: Illustration of the optimal optimization policy with a horizon of one

Two Observation Remaining

- When two observations remaining $\tau = 2$
- Expected increase in the utility at x by termination (after two observations) is:

$$\alpha_2(x;\ D) = \mathbb{E}[u(D_2) \mid x, \mathrm{D}] - u(D)$$

- Decomposing the Expected marginal gain:

$$\alpha_2(x;\ D) = \alpha_1(x;\ D) + \mathbb{E}[\alpha_1(x_2; D_1) \mid x, \mathrm{D}]$$

- Assuming Optimal Future Behaviour:

$$\alpha_2(x;\ D) = \alpha_1(x;\ D) + \mathbb{E}[\alpha_1^*(D_1) \mid x, \mathrm{D}]$$

Two Observations Remaining

- Optimal Location is where the Expected increase in the utility is maximum:

$$\mathbf{x} \in \underset{\mathbf{x'} \in \mathbf{X}}{\mathbf{argmax}}\, \alpha_2(x';\ D)$$

- Final Expected terminal Utility

$$u(D) + \alpha_2^*(D)$$

Inductive Case : Fixed Budget

- Let τ be an arbitrary decision horizon
- Assuming we can compute the value of any dataset with a horizon of $\tau - 1$.
- τ-step expected marginal gain from observing at some point x:

$$\alpha_{\tau}(x;\ D) = \mathbb{E}[u(D_{\tau}) \mid x, \mathrm{D}] - u(D)$$

- Decomposing the Expected marginal gain:

$$\alpha_{\tau}(x;\ D) = \alpha_{1}(x;\ D) + \mathbb{E}[\alpha_{\tau-1}(x_2; D_1) \mid x, \mathrm{D}]$$

- Optimal Behaviour for all remaining decisions:

$$\alpha_{\tau}(x;\ D) = \alpha_{1}(x;\ D) + \mathbb{E}[\alpha^{*}_{\tau-1}(D_1) \mid x, \mathrm{D}]$$

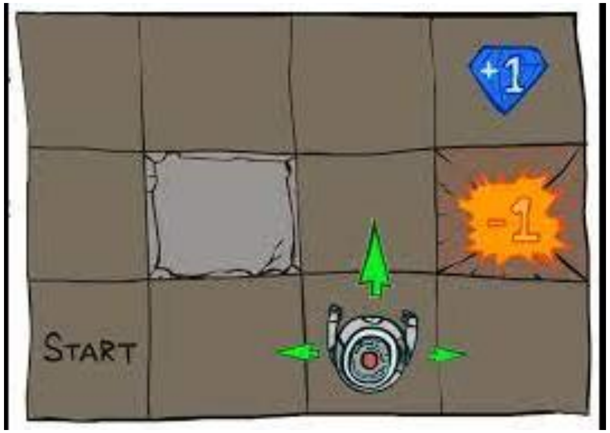
- Optimal Decision

Bellman Optimality & Bellman Equation

- Bellman Equation:

$$\alpha^*_\tau(D) = \max_{x' \in X} \{ \alpha_1(x'; D) + \mathbb{E}[\alpha^*_{\tau-1}(D_1) \mid x', D] \}$$

- Property:- "An optimal policy has the property that whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision."



https://cs.gmu.edu/~kosecka/cs747/17_reinforcement_learning_part2.pdf

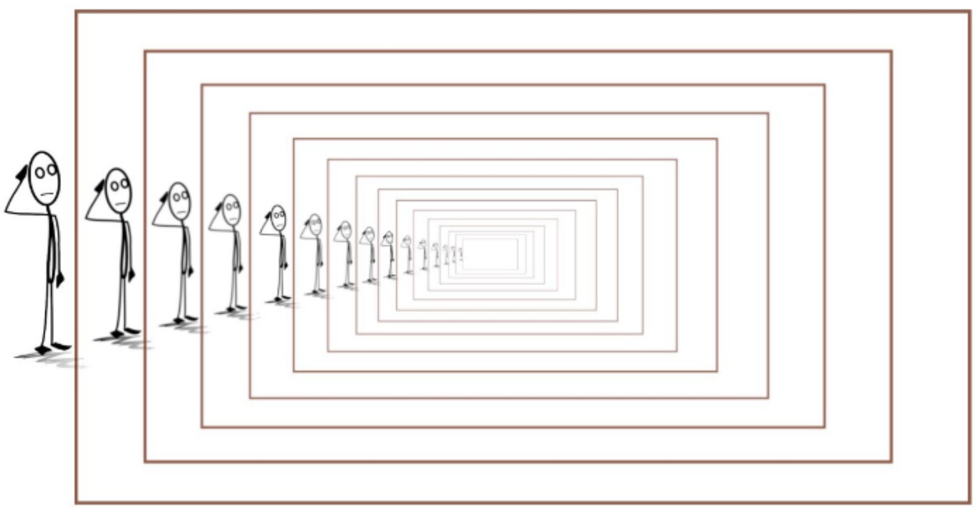
Cost & Approximation of the Optimal Policy

Cost of the optimal Policy

- Short coming of the inductive case – We can compute optimal policy for very short decision horizon

- Consider The expected two-step marginal gain to be maximized:

$$\alpha_2(x;\ D) = \alpha_1(x;\ D) + \mathbb{E}[\alpha_1^*(D_1) \mid x, \mathrm{D}]$$



https://www.linkedin.com/pulse/recursion-explained-understand-you-must-first-ignacio-chitnisky

Unrolling the optimal Policy

$x \in \operatorname{argmax} \alpha_{\tau}$:

$$\begin{aligned}
\alpha_{\tau} &= \alpha_1 + \mathbb{E}[\alpha^{*}_{\tau-1}] \\
&= \alpha_1 + \mathbb{E}[\max(\alpha_{\tau-1})] \\
&= \alpha_1 + \mathbb{E}[\max\{\alpha_1 + \mathbb{E}[\alpha^{*}_{\tau-2}]\}] \\
&= \alpha_1 + \mathbb{E}[\max\{\alpha_1 + \mathbb{E}[\max\{\alpha_1 + \mathbb{E}[\dots.]\}]
\end{aligned}$$

Cost of the optimal Policy

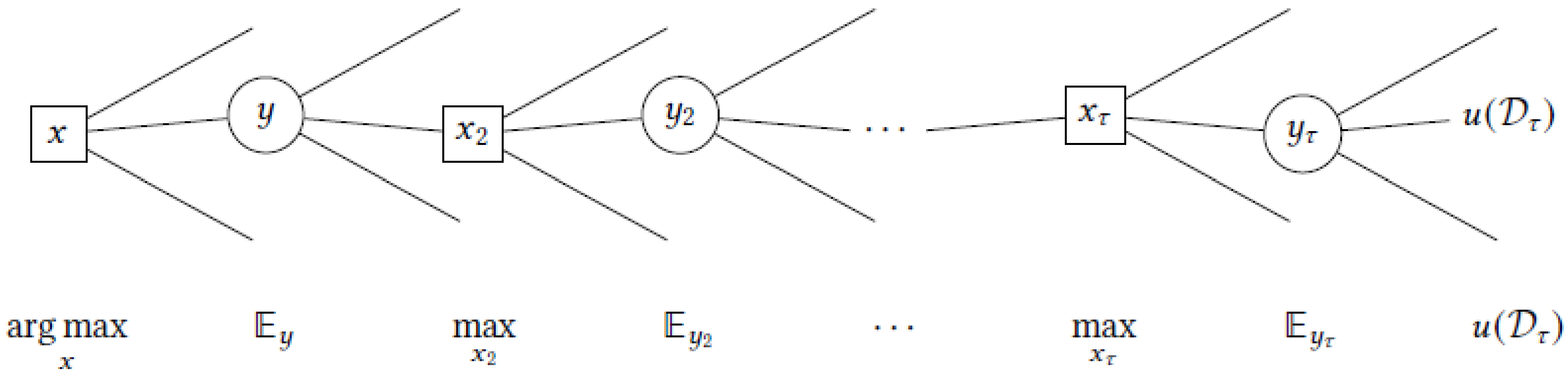


Fig: The Optimal Optimization policy as the decision tree

- Each decision costs :

$$O(nq)$$

- For Decision Horizon of τ:

$$O(n^\tau q^\tau)$$

n : evaluation budget for optimization
q : evaluation budget for quadrature

Approximating the Optimal Policy

- Limited Lookahead – Limit the number of future observations to consider in each decision.
- Let ℓ be the limited horizon to take into consideration

$$\alpha_{\tau}(x, D) \approx \alpha_{\ell}(x, D)$$

- Computational Effort required for ℓ-step lookahead policy is:

$$O(n^{\ell} q^{\ell})$$

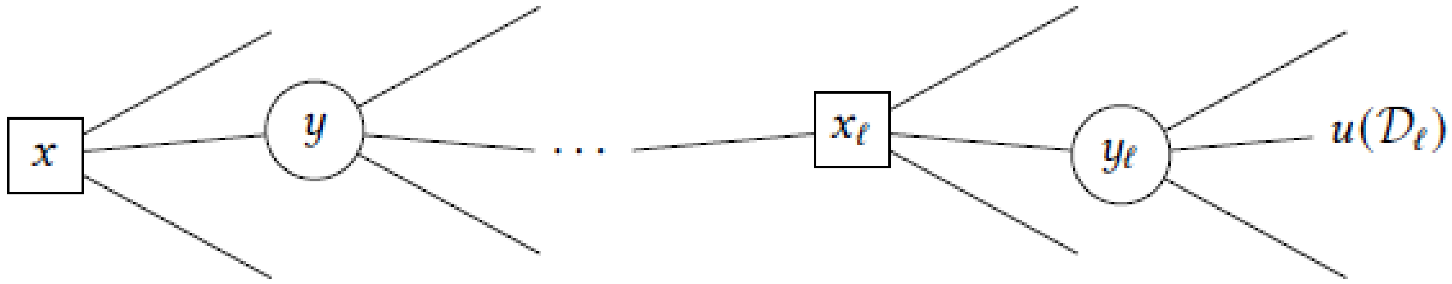


Fig: A lookahead approximation of the Optimal Policy

Approximating the optimal Policy

- Rollout – Approach to approximate policy design that emulates the structure of the optimal policy by using a tractable sub-optimal policy

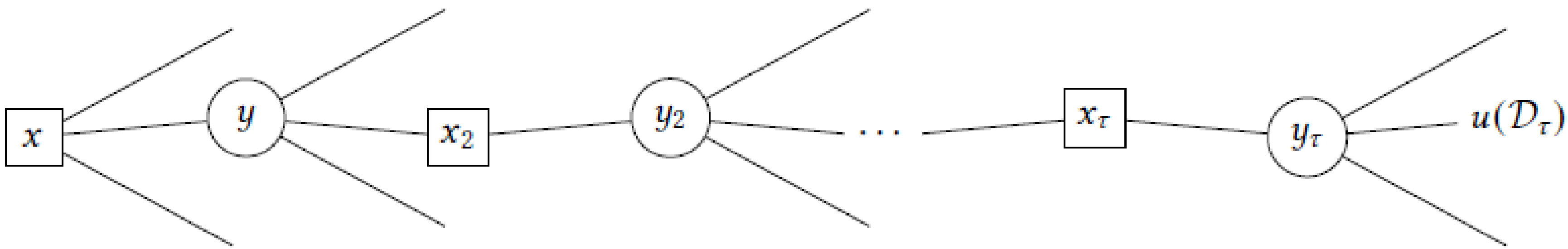


Fig: Rollout Approximation of the Optimal Policy

- Uses Base or Heuristic Policy to guide the decision
- Computational Effort required for rollout policy is:

$$O(n^2 q^\tau)$$

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Cost-Aware Optimization

Cost Aware Optimization

- When the budget is unknown and cost is associated with data acquisition, we need to dynamically decide when to terminate.

- Decision Problem under uncertainty with input domain X and Φ representing immediate termination :

$$A = X \cup \{\emptyset\}$$

- One approach to account the cost of evaluation is to do it in the utility function.

References

- Cost of gathering the Dataset D:

$$c(D) = \sum_{x \in D} c(x)$$

- Cost-adjusted utility:

$$u(D) = u'(D) - c(D)$$

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Summary

Summary

- Bayesian Optimization for optimizing the Black-box Function.

$$\boldsymbol{x}^* \in \underset{\boldsymbol{x} \in \boldsymbol{X}}{\boldsymbol{argmax}} \; \boldsymbol{f}(\mathbf{x})$$

- Sequential Algorithm and Acquisition Function
- Elements of the Decision Problem
- Optimal Policy for Isolated decision with Fixed Budget
- Sequential decisions
  - One Observation Remaining
  - Two Observation Remaining
  - Inductive case

Summary

- Computational cost for Optimal Policy
- Exponential growth with respect to the Decision Horizon
- Approximation of Optimal Policy
  - Limited Lookahead
  - Rollout
- Cost Aware Optimization

https://www.dreamstime.com/stock-illustration-optimization-cartoon-red-image78915760

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- https://www.youtube.com/watch?v=C5nqEHpdyoE

Thank You