Topics in Reinforcement Learning: AlphaZero, ChatGPT, Neuro-Dynamic Programming, Model Predictive Control, Discrete Optimization Arizona State University Course CSE 691, Spring 2024

Links to Class Notes, Videolectures, and Slides at http://web.mit.edu/dimitrib/www/RLbook.html

Dimitri P. Bertsekas dbertsek@asu.edu

Lecture 9

Combined Estimation/Control: Sequential Estimation, Bayesian Optimization, and Adaptive Control with a POMDP Approach

Application to the Wordle Puzzle

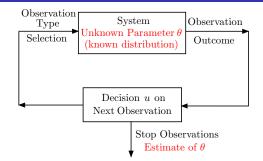
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Outline



- Bayesian Optimization of Functions with Hard-to-Compute Values
- Combined Estimation and Control Adaptive Control
- On-Line Solution of the Wordle Puzzle by Rollout

Sequential Estimation of a Parameter Vector θ



Use of costly observations to estimate a parameter vector θ

- The number and type of observations are subject to choice
- Instead, the outcomes of the observations obtained are evaluated on-line with a view towards stopping or modifying the observation process
- This involves sequential decision making, thus bringing DP to bear

Example: Select one of two hypotheses using costly sequential observations

Given a new observation, we can accept one of the hypotheses or obtain a new observation at cost C (cf. quality control, the sequential probability ratio test, 1940s).

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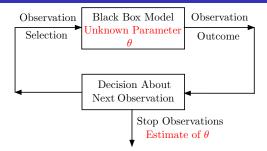
Applications of Sequential Estimation

- Classical sequential experiment design problems or sequential sampling strategies in statistics.
 - Select one of multiple hypotheses.
 - Design of clinical trials or tests for medical diagnosis.
- Classical sequential search problems (e.g., search and rescue).
- Route planning through a sensor network for sequential information collection.
- Sequential decoding problems (e.g., the Mastermind and Wordle puzzles, to be discussed later).
- Surrogate and Bayesian optimization for minimizing "black box" functions (to be discussed first).

An important distinction: Does the current choice of observation affect the availability, the quality, or the cost of future observations?

- If no, we call this a simple sequential estimation problem (we will discuss it first in the context of Bayesian optimization).
- If yes, this can be viewed as a combined estimation and control problem, and can be viewed within the context of adaptive control.

Surrogate Optimization of "Black Box" Functions

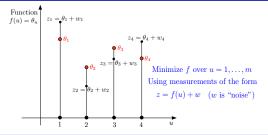


Minimize approximately a function whose values at given points are obtained only through time-consuming calculation, simulation, or experimentation

- Introduce a parametric model of the cost function with parameter θ .
- Observe sequentially the true cost function at a few observation points.
- Construct a model of the cost function (the surrogate) by estimating θ .
- Minimize the surrogate to obtain a suboptimal solution.
- How to select observation points based on results of previous observations?
- Exploration-exploitation tradeoff: Observing at points likely to have near-optimal value vs observing at points in relatively unexplored areas of the search space.

- Geostatistical interpolation ("kriging" pioneered by the South African engineers Matheron and Krige in a goldmining context): Identify locations of high gold distribution based on samples from a few boreholes.
- Design optimization, e.g., aerodynamic design using hardware prototypes, materials design, drug development, etc.
- Hyperparameter selection of machine-learning models, including the architectural parameters of the deep neural network of AlphaZero.

Bayesian Optimization of a Black Box Function f



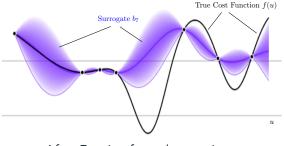
• Introduce a parameter vector $\theta = (\theta_1, \dots, \theta_m) \in \Re^m$ where $\theta_u = f(u)$, i.e., θ is f

- Observations are of the form z = f(u) + w (important special case is w = 0)
- Estimate θ with N << m noisy measurements at chosen points u₁,..., u_N
- We assume that θ has a given a priori distribution $b_0 = (b_{0,1}, \dots, b_{0,m})$ over \Re^m (values of *f* at "neighboring" points should be correlated)
- After observations at points u_1, \ldots, u_k of the form $z_{u_i} = \theta_{u_i} + w_{u_i}$, we choose the next point u_{k+1} at which to observe the value of *f*.
- Update the posterior distribution b_k with an estimator $b_{k+1} = B_k(b_k, u_{k+1}, z_{u_{k+1}})$ (b_k is essentially the surrogate cost function after the *k*th observation)
- Gaussian case: If *b*₀ and the noises *w_u* are Gaussian, *b_k* can be updated using closed form Gaussian process regression formulas.

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Illustration of the True Cost Function *f* and its Surrogate

Black is the true cost function Purple is the surrogate cost function



After 7 noise-free observations

The surrogate is specified by the posterior distribution b_k (mean and standard deviation at the different points are shown in the figure)

Key Question: How to select sequentially the observation point u_{k+1} given the observation results z_{u_1}, \ldots, z_{u_k} from previously selected points u_1, \ldots, u_k

A DP view

- Introduce a POMDP model: The posterior b_k (given the observations up to time k) is the belief state, u_k is the control, the belief estimator $b_{k+1} = B_k(b_k, u_{k+1}, z_{u_{k+1}})$ is the system. The cost function is based on the cost of the observations, and the "quality" of the surrogate obtained at the end.
- The dominant method in practice: Use a greedy/myopic policy, based on an acquisition function.
- The acquisition function $A_k(b_k, u_{k+1})$ is a heuristic measure of "benefit" for selecting point u_{k+1} for observation when the belief state is b_k .
- Myopic policy: Selects the next point at which to observe, \hat{u}_{k+1} , as

$$\hat{u}_{k+1} \in \arg \max_{u_{k+1} \in \{1,...,m\}} A_k(b_k, u_{k+1})$$

• An alternative method: Use rollout with a myopic base policy; it has been advocated in several research works since 2016, with promising results.

Examples of Acquisition Functions for Myopic Bayesian Optimization

The myopic policy maximizes over u_{k+1} the acquisition function $A_k(b_k, u_{k+1})$:

 $\hat{u}_{k+1} \in \arg \max_{u_{k+1} \in \{1,...,m\}} A_k(b_k, u_{k+1})$

A common example of acquisition function: Upper confidence bound

 $A_k(b_k, u) = T_k(b_k, u) + \beta R_k(b_k, u), \qquad \beta > 0$ is a tunable parameter

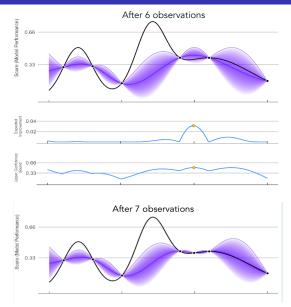
- Here $T_k(b_k, u) = -$ Mean of f(u), and $R_k(b_k, u) =$ Standard deviation of f(u) (under the posterior distribution b_k).
- $T_k(b_k, u)$ can be viewed as an exploitation index (encoding our desire to search within parts of the space where *f* takes low value), while $R_k(b_k, u)$ can be viewed as an exploration index (encoding our desire to search within parts of the space that are relatively unexplored).

Another example of acquisition function: Expected improvement

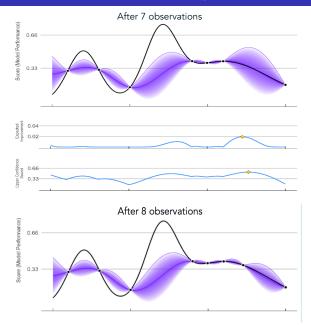
 $A_k(b_k, u)$ is the expected value of the reduction of f(u) relative to the minimal value of f obtained up to time k (under the posterior distribution b_k).

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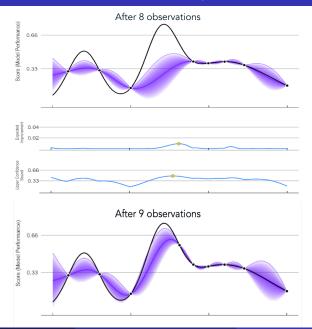
Maximization Example (From Wikipedia Article on BO): True Function is Black, Surrogate Function is Purple; Observations are Noise-Free



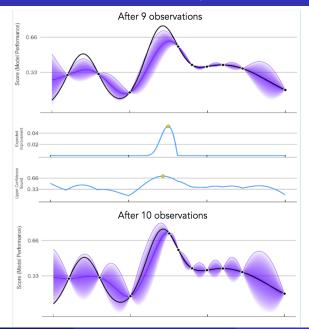
Maximization Example II



Maximization Example III



Maximization Example IV



DP Algorithm for POMDP Formulation of Bayesian Optimization

$$J_{k}^{*}(b_{k}) = \min_{u_{k+1} \in \{1,...,m\}} \left| c(u_{k+1}) + E_{z_{u_{k+1}}} \left\{ J_{k+1}^{*} \left(B_{k}(b_{k}, u_{k+1}, z_{u_{k+1}}) \right) \mid b_{k}, u_{k+1} \right\} \right|$$

where c(u) is the cost of observation at u. Proceeds backwards from a terminal cost

 $J_N^*(b_N) = G(b_N)$ (measures the quality of the surrogate obtained at the end)

Approximation in value space (replace J_{k+1}^* with \tilde{J}_{k+1})

$$\tilde{u}_{k+1} \in \arg\min_{u_{k+1} \in \{1,...,m\}} Q_k(b_k, u_{k+1})$$

where $Q_k(b_k, u_{k+1})$ is the (approximate) Q-factor corresponding to the pair (b_k, u_{k+1}) :

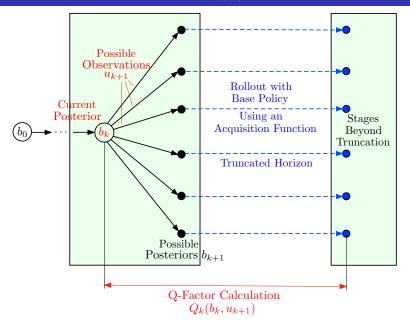
$$Q_k(b_k, u_{k+1}) = c(u_{k+1}) + E_{z_{u_{k+1}}} \Big\{ \tilde{J}_{k+1} \big(B_k(b_k, u_{k+1}, z_{u_{k+1}}) \big) \mid b_k, u_{k+1} \Big\}$$

Rollout

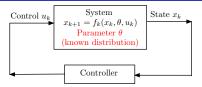
Use as \tilde{J}_{k+1} the cost function of a myopic base heuristic based on an acquisition function (or approximation thereof); first proposed by Lam, Wilcox, and Wolpert (2016), and followed up by others (promising, but relatively untested at present).

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Truncated Rollout with a Myopic Base Heuristic



Adaptive Control with a POMDP Formulation and Rollout



Deterministic system $x_{k+1} = f(x_k, \theta, u_k), \theta \in \{\theta^1, \dots, \theta^m\}$: unknown parameter

- θ has known initial distribution b_0 and stays constant. It is observed indirectly through perfect observation of x_k
- View θ as part of an augmented state (x_k, θ) that is partially observed
- Bellman equation for optimal cost function J_k^* :

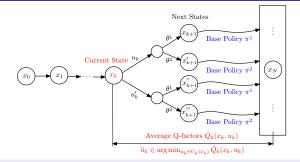
$$J_{k}^{*}(I_{k}) = \min_{u_{k}} \sum_{i=1}^{m} b_{k,i} (g(x_{k}, \theta^{i}, u_{k}) + J_{k+1}^{*}(I_{k}, u_{k}, f(x_{k}, \theta^{i}, u_{k})))$$

where $I_k = (x_0, ..., x_k, u_0, ..., u_{k-1})$ is the information state at time k, and $b_{k,i} = P\{\theta = \theta^i \mid I_k\}, i = 1, ..., m$, is the belief state (estimated on-line)

- Approximation in value space: Use approximation $\tilde{J}^i(f(x_k, \theta^i, u_k))$ in place of $J_{k+1}^*(I_k, u_k, f(x_k, \theta^i, u_k))$. Minimize over u_k to obtain a one-step lookahead policy
- Example 1: \tilde{J}^i is the cost function of the optimal policy corresponding to θ^i
- Example 2: \tilde{J}^i is the cost function of a known policy assuming $\theta = \theta^i$ (this is rollout)

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Rollout for Adaptive Control with a POMDP Formulation



At x_k , we minimize $\hat{Q}_k(x_k, u_k)$, the average Q-factor of u_k , defined by

$$\hat{Q}_k(\boldsymbol{x}_k,\boldsymbol{u}_k) = \sum_{i=1}^m \boldsymbol{b}_{k,i} \boldsymbol{Q}_k(\boldsymbol{x}_k,\boldsymbol{u}_k,\boldsymbol{\theta}^i),$$

where $Q_k(x_k, u_k, \theta^i)$ is the Q-factor computed assuming that $\theta = \theta^i$

$$Q_k(x_k, u_k, \theta^i) = g_k(x_k, \theta^i, u_k) + J_{k+1, \pi^i}(f_k(x_k, \theta^i, u_k))$$

If $\pi^i \equiv \pi$, cost improvement over π can be proved

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Reinforcement Learning

A Rollout Approach for Solving On-Line the Wordle Puzzle (Joint Work with Siddhant Bhambri and Amrita Bhattacharjee)

Overview

- There is a hidden mystery word/code word θ drawn from an initial mystery list according to a known distribution. In the standard version of the puzzle this distribution is uniform.
- The mystery list shrinks as a result of guesses/observations.
- The guesses are chosen based on feedback about the mystery word provided by the preceding guesses.
- The puzzle is solved when the mystery list shrinks to a single element.
- We want to minimize the expected number of guesses to solve the puzzle.
- Important fact: The belief distribution over the current mystery list remains uniform through the solution process.
- This makes possible the solution by exact DP, with days of computation (Selby 2022).
- Without the uniform initial belief distribution assumption (and/or small variations in the problem structure), the exact solution would be impossible.
- Rollout can solve near optimally the puzzle (and its variations) on-line much faster.

Playing Wordle Using an Online Rollout Algorithm for Deterministic POMDPs





Siddhant Bhambri

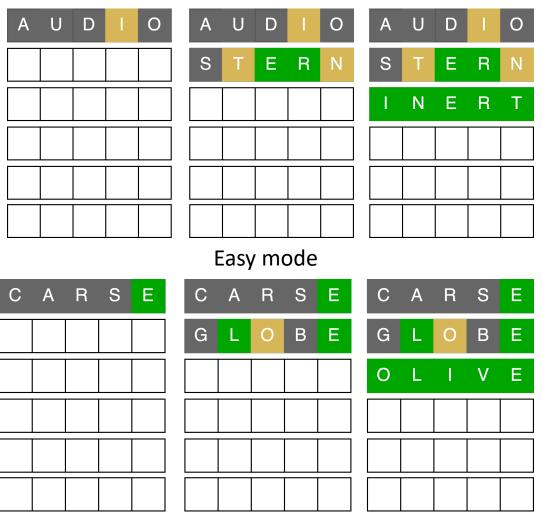


Amrita Bhattacharjee



Dimitri Bertsekas

The Wordle Puzzle

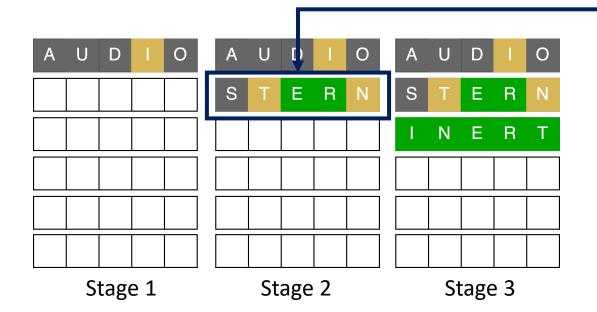


× **How To Play** Guess the Wordle in 6 tries. • Each guess must be a valid 5-letter word. • The color of the tiles will change to show how close your guess was to the word. Examples WEARY **W** is in the word and in the correct spot. I is in the word but in the wrong spot. VAGUE **U** is not in the word in any spot. Log in or create a free NYT account to link your stats. A new puzzle is released daily at midnight. If you haven't already, you can sign up for our daily reminder email. Have feedback? Email us at nytgames@nytimes.com.

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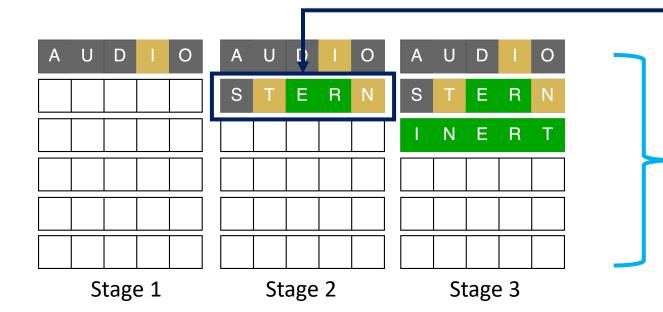
Wordle as a POMDP



States (S): Subset of the initial mystery list of 2,315 words

Actions (A): Set of 12,972 guess words

Wordle as a POMDP

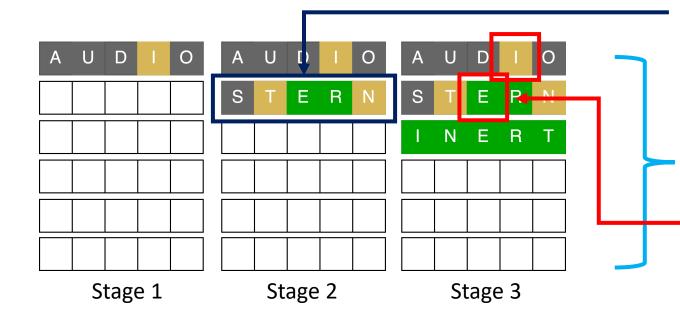


States (S): Subset of the initial mystery list of 2,315 words

Actions (A): Set of 12,972 guess words

Transitions (T): probability of going from one mystery word list to the next.

Wordle as a POMDP



States (S): Subset of the initial mystery list of 2,315 words

Actions (A): Set of 12,972 guess words

Transitions (T): probability of going from one mystery word list to the next.

Cost (C): cost of utilizing a guess word (=1)

Observations from the game: colored observations for each letter

Optimal Solution using Dynamic Programming

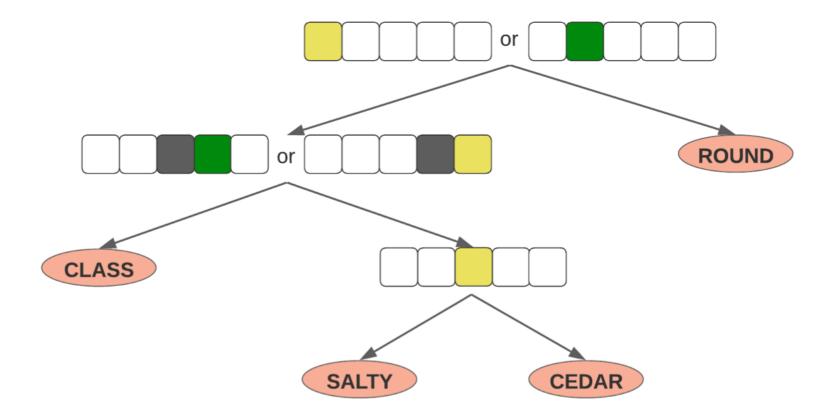


Figure adapted from *Bertsimas, D. and Paskov, A., 2022.* An Exact and Interpretable Solution to Wordle. Selby A., 2022. ``The best strategies for Wordle'.

Optimal Solution using Dynamic Programming

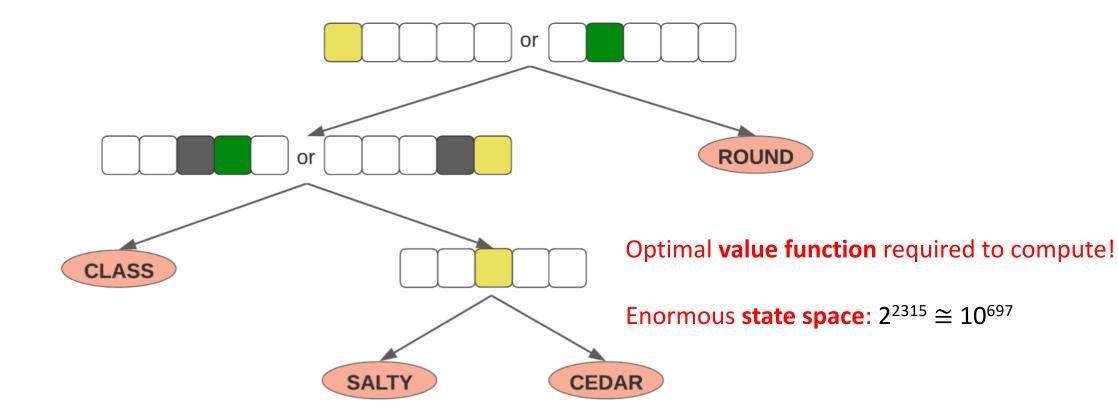
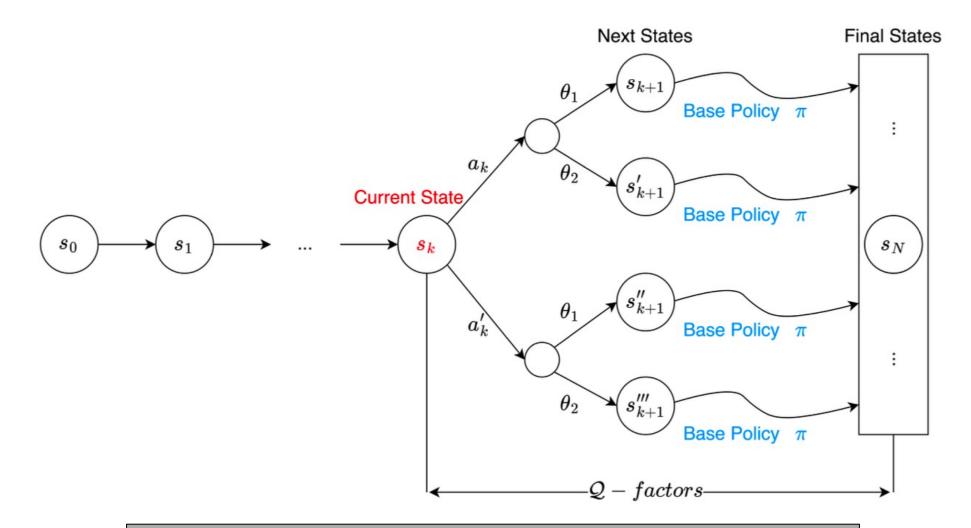


Figure adapted from *Bertsimas, D. and Paskov, A., 2022.* An Exact and Interpretable Solution to Wordle. Selby A., 2022. ``The best strategies for Wordle''.

Solution? - Approximate the Value Function!



Value Function --> Rollout Cost function: A Newton Step to solve the Bellman Eq.

A Reinforcement Learning Approach Towards POMDP and Adaptive Control

Let us denote by x_k and u_k the state and control of the system at time k, respectively.

Let us also denote by θ the unknown system parameter. We assume that θ stays fixed over time, at one of m known values $\theta_1, \dots, \theta_m$: $\theta \in \{\theta^1, \dots, \theta^m\}.$

The state x_k is assumed to be perfectly observed by the controller at each time k, and evolves according to a system equation

$$x_{k+1} = f(x_k, \theta, u_k),$$

Finally, we assume that the following information vector,

$$I_k = \{x_0, \ldots, x_k, u_0, \ldots, u_{k-1}\},\$$

is available at time k, and is used to compute the conditional probabilities

$$b_{k,i} = P\{\theta = \theta^i \mid I_k\}, \qquad i = 1, \dots, m.$$

A Reinforcement Learning Approach Towards POMDP and Adaptive Control

These probabilities form a vector

$$b_k = (b_{k,1}, \ldots, b_{k,m}),$$

Following the choice of u_k , a cost $g(x_k, \theta, u_k)$ is incurred, and we wish to choose controls to minimize the sum of the incurred costs over a given number of stages N.

Note, b_k can be updated according to an equation of the form

$$b_{k+1} = B_k(x_k, b_k, u_k, x_{k+1}),$$

where B_k is an appropriate function, which can be viewed as a recursive estimator of θ .

A Reinforcement Learning Approach Towards Wordle

- We view the mystery word θ as the unknown system parameter,
- and we view the list of the mystery words as the set $\{\theta i \mid i = 1,...,m\}$ of possible values for θ .
- The initial distribution of θ is uniform over the list of the mystery words, as is the case in the New York Times version of the puzzle. It can then be shown that the belief distribution b_k at stage k continues to be uniform over the list of eligible mystery words (those that have not been excluded by the preceding word guesses). This is an important simplification, which obviates the need for the estimator.
- An important consequence is that we may use as state x_k the list of eligible mystery words at stage k, which evolves according to a deterministic system equation $x_{k+1} = f(x_k, u_k)$, with u_k being the guess word at stage k.

The algorithm operates in the space of information vectors I_k . In particular, we denote by $J_k(I_k)$ the optimal cost starting at information vector I_k at time k. This vector evolves over a finite number of stages N according to the equation

$$I_{k+1} = (I_k, x_{k+1}, u_k) = (I_k, f(x_k, \theta, u_k), u_k), \qquad k = 0, \dots, N-1.$$

It admits a DP algorithm that takes the form

$$J_{k}^{*}(I_{k}) = \min_{u_{k} \in U(x_{k})} E_{\theta} \Big\{ g(x_{k}, \theta, u_{k}) + J_{k+1}^{*}(I_{k}, f(x_{k}, \theta, u_{k}), u_{k}) \mid I_{k}, u_{k} \Big\},$$

for k = 0, ..., N - 1, with

$$J_N^*(I_N) = g_N(x_N),$$

where we use E_{θ} {· | I_k, u_k } to denote expected value over θ , conditioned on I_k and u_k .

The Exact DP Algorithm, Approximation in Value Space & Rollout

We can rewrite this DP algorithm in terms of the conditional belief probabilities $b_{k,i}$ as

$$J_k^*(I_k) = \min_{u_k \in U(x_k)} \sum_{i=1}^m b_{k,i} \Big\{ g(x_k, \theta^i, u_k) + J_{k+1}^*(I_k, f(x_k, \theta^i, u_k), u_k) \Big\}.$$

The control applied by the optimal policy is given by

$$u_k^* \in \arg\min_{u_k \in U(x_k)} \sum_{i=1}^m b_{k,i} \Big\{ g(x_k, \theta^i, u_k) + J_{k+1}^*(I_k, f(x_k, \theta^i, u_k), u_k)) \Big\}.$$

The corresponding approximation in value space scheme with one-step lookahead minimization is given by

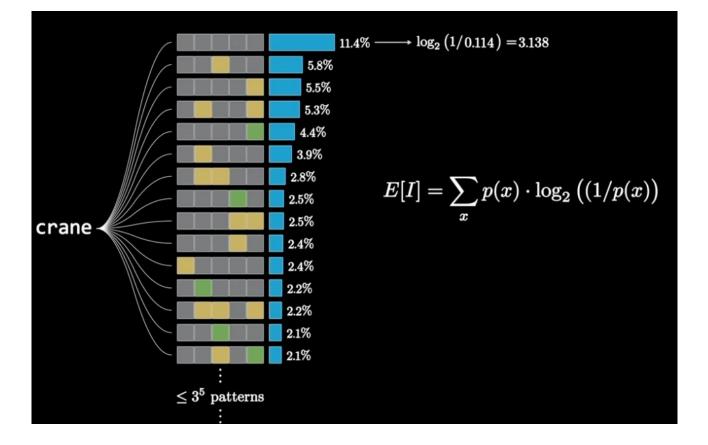
$$\tilde{u}_{k} \in \arg\min_{u_{k} \in U(x_{k})} \sum_{i=1}^{m} b_{k,i} \Big\{ g(x_{k}, \theta^{i}, u_{k}) + \tilde{J}_{k+1}^{i}(f(x_{k}, \theta^{i}, u_{k})) \Big\};$$

Bhambri, S., Bhattacharjee, A. and Bertsekas, D., 2022. Reinforcement learning methods for wordle: A pomdp/adaptive control approach. *arXiv preprint arXiv:2211.10298*.

Base Heuristic for Wordle – Information Gain!

Information gain –

calculating entropy of the distribution (roughly based on how much using a word reduces the uncertainty about the mystery word)

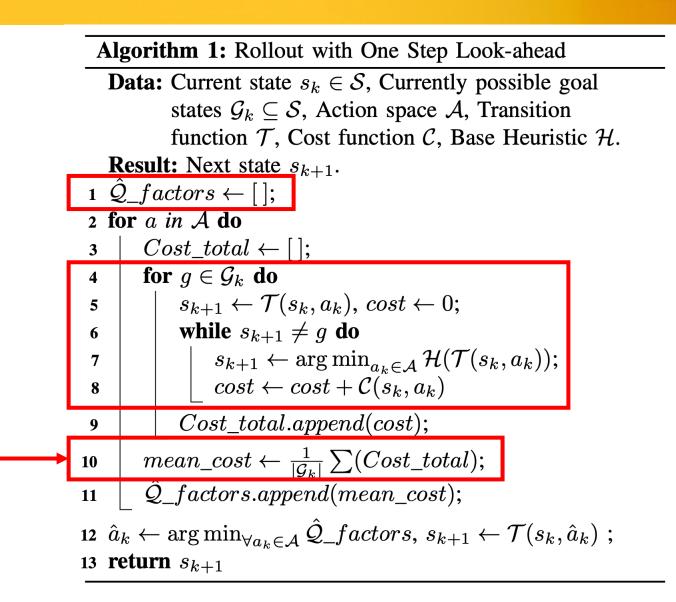


Algorithm 1: Rollout with One Step Look-ahead **Data:** Current state $s_k \in \mathcal{S}$, Currently possible goal states $\mathcal{G}_k \subset \mathcal{S}$, Action space \mathcal{A} , Transition function \mathcal{T} , Cost function \mathcal{C} , Base Heuristic \mathcal{H} . **Result:** Next state s_{k+1} . $\mathcal{Q}_{factors} \leftarrow [];$ 2 for a in A do Line 1: empty set to $Cost_total \leftarrow [];$ 3 for $q \in \mathcal{G}_k$ do 4 store the average Q $s_{k+1} \leftarrow \mathcal{T}(s_k, a_k), \ cost \leftarrow 0;$ 5 factors for each possible while $s_{k+1} \neq q$ do 6 $s_{k+1} \leftarrow \arg\min_{a_k \in \mathcal{A}} \mathcal{H}(\mathcal{T}(s_k, a_k));$ 7 action at stage k. $cost \leftarrow cost + \mathcal{C}(s_k, a_k)$ 8 $Cost_total.append(cost);$ 9 mean_cost $\leftarrow \frac{1}{|\mathcal{G}_k|} \sum (Cost_total);$ 10 $\hat{Q}_{factors.append(mean_cost)};$ 11 12 $\hat{a}_k \leftarrow \arg \min_{\forall a_k \in \mathcal{A}} \hat{\mathcal{Q}}_{factors}, s_{k+1} \leftarrow \mathcal{T}(s_k, \hat{a}_k);$ 13 return s_{k+1}

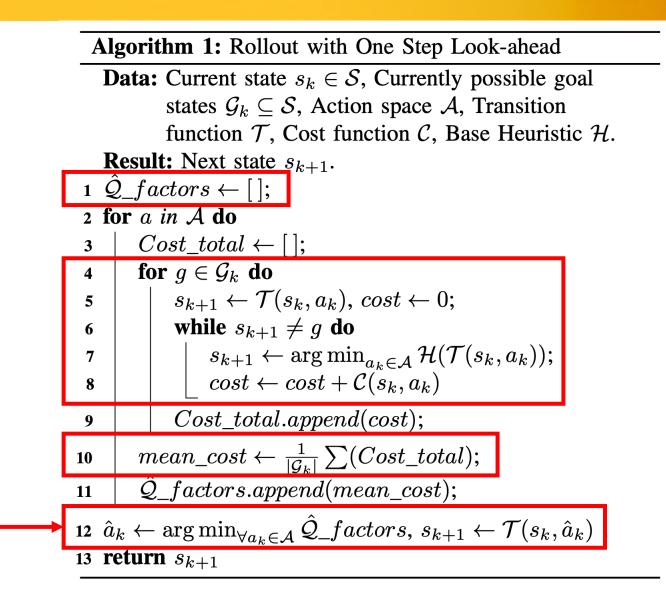
Line 4-8: for all possible $g \in G_k$, we perform the rollout by applying the next action as selected by our base heuristic cost function *H* and compute the Q-factor or cost until we reach the terminating state.

Algorithm 1: Rollout with One Step Look-ahead **Data:** Current state $s_k \in S$, Currently possible goal states $\mathcal{G}_k \subset \mathcal{S}$, Action space \mathcal{A} , Transition function \mathcal{T} , Cost function \mathcal{C} , Base Heuristic \mathcal{H} . **Result:** Next state s_{k+1} . 1 $Q_factors \leftarrow [];$ 2 for a in \mathcal{A} do $Cost_total \leftarrow [];$ for $q \in \mathcal{G}_k$ do $s_{k+1} \leftarrow \mathcal{T}(s_k, a_k), \ cost \leftarrow 0;$ 5 while $s_{k+1} \neq g$ do 6 $s_{k+1} \leftarrow \arg\min_{a_k \in \mathcal{A}} \mathcal{H}(\mathcal{T}(s_k, a_k));$ 7 $cost \leftarrow cost + \mathcal{C}(s_k, a_k)$ 8 $Cost_total.append(cost);$ 9 mean_cost $\leftarrow \frac{1}{|\mathcal{G}_k|} \sum (Cost_total);$ 10 $\hat{Q}_{factors.append(mean_cost)};$ 11 12 $\hat{a}_k \leftarrow \arg \min_{\forall a_k \in \mathcal{A}} \hat{\mathcal{Q}}_{factors}, s_{k+1} \leftarrow \mathcal{T}(s_k, \hat{a}_k);$ 13 return s_{k+1}

Line 10: find the average cost for solving the game for *g*



Line 12: we select the action \tilde{a}_k that corresponds to the minimum average cost and apply it to state s_k .

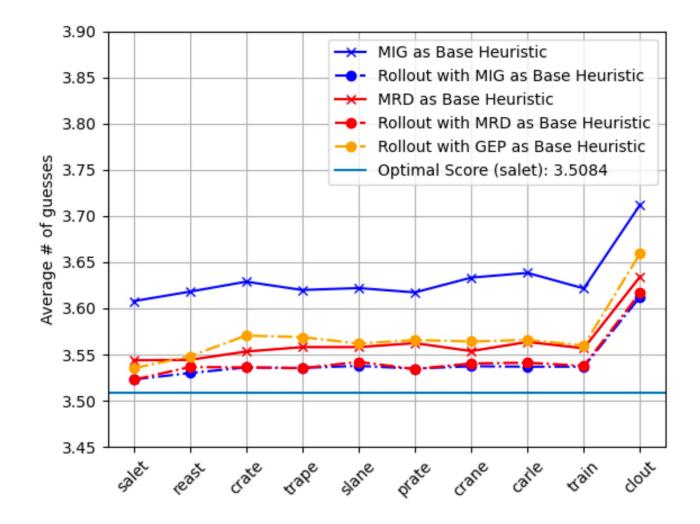


Results for Rollout vs Optimal Scores

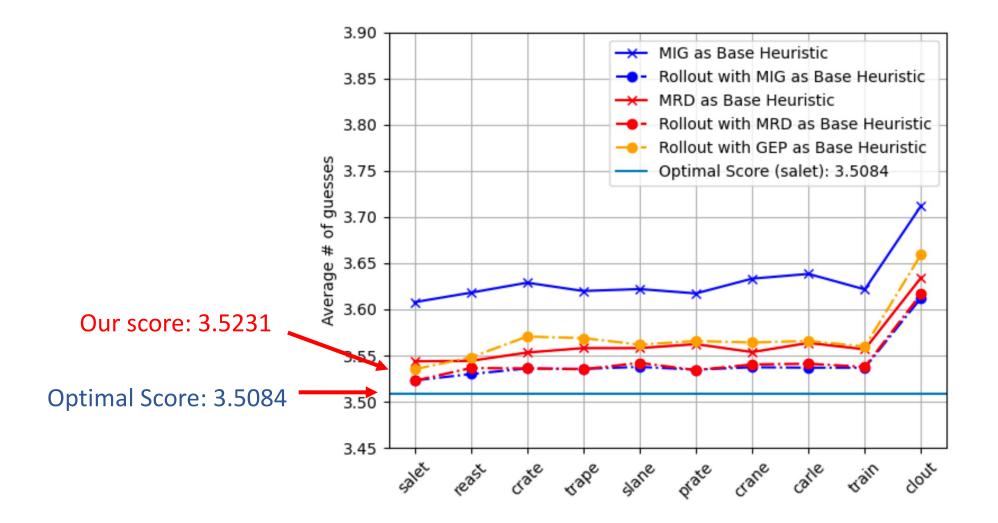
Opening Word	Easy Mode			Hard Mode		
	MIG as Base Heuristic	Rollout with MIG as Base Heuristic	Optimal Score	MIG as Base Heuristic	Rollout with MIG as Base Heuristic	Optimal Score
salet	3.6108	3.4345	3.4212	3.6078	3.5231	3.5084
reast	3.6	3.4462	3.4225	3.6181	3.53	3.5136
crate	3.6177	3.4414	3.4238	3.6289	3.5361	3.5175
trape	3.6319	3.4604	3.4454	3.6199	3.5356	3.5179
slane	3.6255	3.4444 4	3.4311	3.622	3.5378	3.5201
prate	3.6333	3.4535	3.4376	3.6173	3.5348	3.5210
crane	3.6091	3.4380	3.4255	3.6333	3.5374	3.5227
carle	3.6108	3.4419	3.4285	3.6384	3.5369	3.5261
train	3.6181	3.4622	3.4436	3.6216	3.5369	3.5248
clout	3.6955	3.5248	3.5097	3.7123	3.6125	3.5931

Table: Results using 'Maximum Information Gain' as base heuristic, and with rollout.

Advantage of Rollout vs Only Base Heuristic

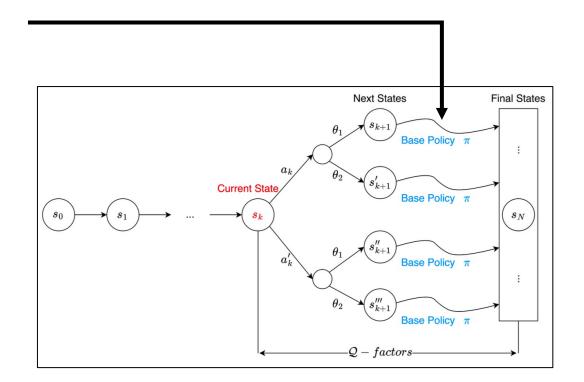


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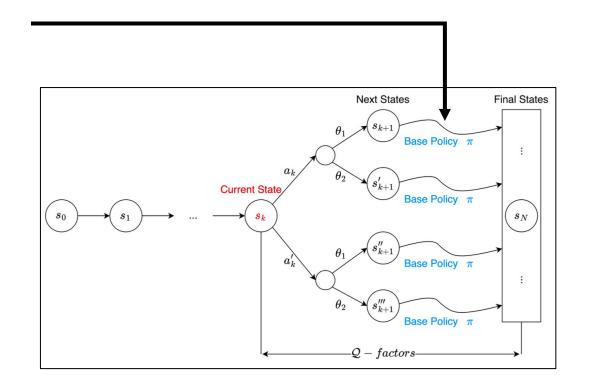
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The need for a reasonable base policy – our experience with Wordle has been that the rollout algorithm is relatively insensitive to the base policy (e.g., the GEP heuristic in the paper).



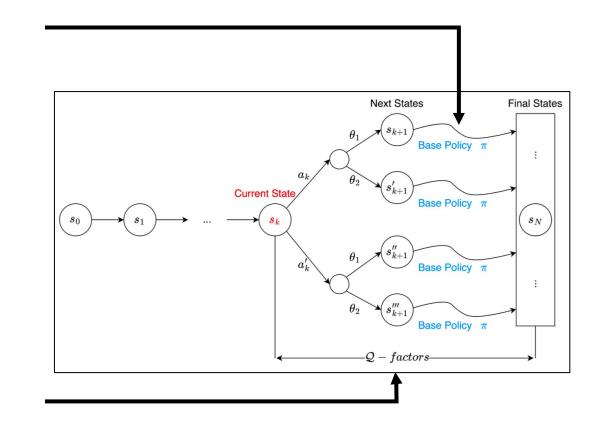
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- The number of Q-factors that need to be computed by the algorithm online, particularly for a large action space this difficulty may possibly be mitigated by intelligently pruning the action space or by offline training using a neural network.



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Bhambri, S., Bhattacharjee, A. and Bertsekas, D., 2023, August. Playing Wordle Using an Online Rollout Algorithm for Deterministic POMDPs. In *2023 IEEE Conference on Games (CoG)* (pp. 1-4). IEEE.



Access our paper: https://tinyurl.com/solving-wordle

