TD(0): $V(s_t) \leftarrow V(s_t) + \alpha(r + \gamma V(s_{t+1}) - V(s_t))$.

- 1-step bootstrap vs. multi-step ✓ ←
- on-policy data vs. off-policy data.
- tabular representation vs. function approximation.
- value prediction. vs. control

Value Prediction with Function Approximation

Reading: Algs for RL (Szepesvári), Sec 3.2

$s_1, a_1, r_1, s_2. \dots$

V^π,

Generalization for value prediction

- Major limitation of tabular RL: does not scale to large state space
  - most methods require that we run into the same state multiple times
  - when the state space is large, you might not see the same state even twice!
  - In other words: sample complexity scales with |S|
  - need generalization
- For value prediction problem, generalization requires that we have some prior knowledge about the form the value function
  - linear function approximation: design features $\phi(s) \in \mathbb{R}^d$ ("featurizing states"), and approximate $\underline{\underline{V^{\pi}}}(s) \approx \theta^{\top}\phi(s)$
  - only unknown: θ. d unknowns vs |S| unknowns!

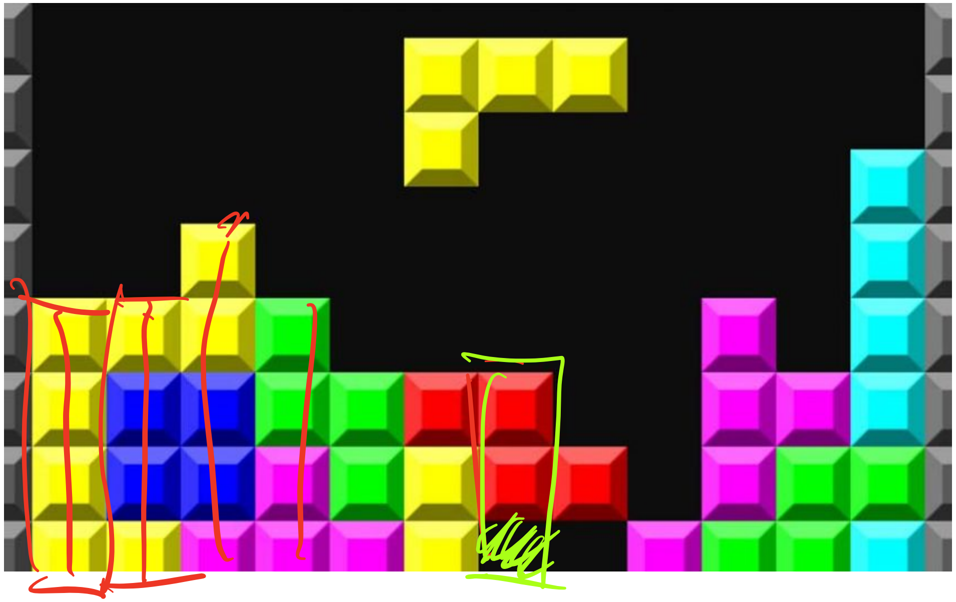
Example: linear function approximation for tetris

- An example featurization:
  - let the height of the pile in i-th column be the i-th feature
  - dimensionality of feature = #columns
  - (probably doesn't work; just an example)
- Feature engineering requires a lot of prior knowledge, domain insights, and trial and error, just as in supervised learning!

$$\begin{bmatrix}4\\4\\5\\4\\3\\\vdots\end{bmatrix}$$

$$V^{\pi} \approx \underline{\phi(s)^T\theta + b}$$

$$= [\phi(s)\ \ 1]\begin{bmatrix}\theta\\ b\end{bmatrix}$$



$\boxed{s_1^{(i)}}, a_1^{(i)}, r_1^{(i)}, \ldots, s_H^{(i)}, a_H^{(i)}, r_H^{(i)}$

Monte-Carlo Value Prediction

$p(s) > 0 \ \forall s.$

- Draw a starting state s_i from the exploratory initial distribution, roll out a trajectory using π from s_i, and let G_i be the (random) discounted return $= \sum_{t=1}^{H} \gamma^{t-1} r_t^{(i)}$

$V^\pi(s) = \mathbb{E}[G|s]$

- Collect $\{(s_i, G_i)\}$ pairs
- Least square regression: $\min_\theta \frac{1}{n} \sum_{i=1}^{n} (\theta^\top \phi(s_i) - G_i)^2$
- Why this works?

$V^\pi(s) = \mathbb{E}[G|s] = \arg\min_{f:S\to\mathbb{R}} \mathbb{E}[(f(s)-G)^2]$

  - Assume $\{(s_i, G_i)\}$ are i.i.d., let (s, G) be variables equal in distribution
  - The expected version of the objective: $\min_\theta \mathbb{E}_{s,G}[(\theta^\top \phi(s) - G)^2]$
  - If we do not restrict ourselves to linear functions, the function that minimizes this objective is $s \mapsto \mathbb{E}[G \mid s]$ $(= V^\pi(s))$!
  - If true $V^\pi(s)$ happens to take linear form, the regression will find it in the limit (of infinite data)
  - Finite sample regime: bias & variance trade-off

$$\underline{\mathbb{E}[(f(X)-Y)^2]} = \mathbb{E}[(\underline{f(X)-\mathbb{E}[Y|X]})^{2}] \leftarrow$$

$$\cancel{+\ \mathbb{E}[(\mathbb{E}[Y|X]-Y)^2]}.$$

$$s \quad \frac{1}{n}\sum_{i=1}^{n}(G_i).$$

$$\underline{V(S_t)} \leftarrow V(S_t) + \alpha(G_t - V(S_t)).$$

$$\mathbb{R}^S \ni \underline{V} \leftarrow V + \alpha(G_t - V(S_t))\begin{bmatrix}0\\0\\\vdots\\1\\0\\\vdots\\0\end{bmatrix} \overset{S_t\text{-th}}{}$$

$$\big\downarrow$$

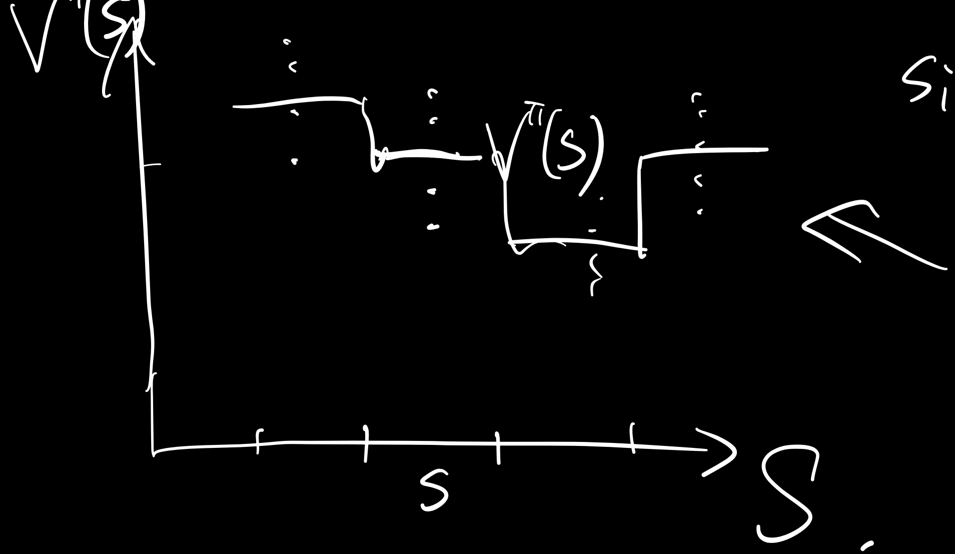
$$\theta.$$

$$[0,0,\dots,\boxed{1},0,0]\begin{bmatrix}V(s^1)\\V(s^2)\\\vdots\\V(s^{|S|})\end{bmatrix}$$

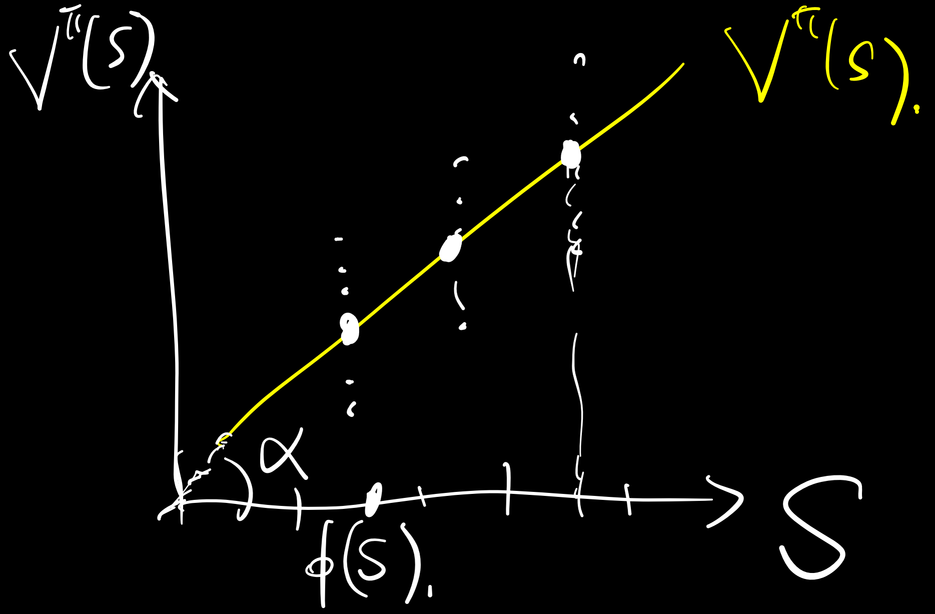
$$\Updownarrow$$

$$\phi(S_t).$$

$$\theta \leftarrow \theta + \alpha\left(G_t - \phi(S_t)^T\theta\right)\phi(S_t).$$



$s_i, G_i.$



$\underline{\theta}^T \phi(s)$

$$\boxed{\arg\min_{V_\theta \in \mathcal{F}} \mathbb{E}[(V_\theta(s) - G)^2],}$$

Monte-Carlo Value Prediction

- The same idea applies to non-linear value function approximation
- More generally & abstractly, think of function approximation as searching over a restricted **function space**, which is a set whose members are functions that map states to real values.
- Function space of linear value function approximation: $\mathscr{F} = \{V_\theta : \theta \in \mathbb{R}^d\}$, where $V_\theta(s) = \theta^\top \phi(s)$
  - typically only a small subset of all possible functions
  - Using "all possible functions" = tabular!
  - Equivalently, tabular MC value prediction can be recovered by choosing ϕ as the identity features $\phi(s) = \{\mathbb{I}[s = s']\}_{s' \in S}$

$$\phi \qquad s \rightarrow \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

- $\boxed{\min_{V_\theta \in \mathscr{F}} \frac{1}{n} \sum_{i=1}^{n} \boxed{(V_\theta(s_i) - G_i)^2}}$
- Plug in any function approximator of your choice
- SGD: uniformly sample i and $\theta \leftarrow \theta - \alpha \cdot (V_\theta(s_i) - G_i) \cdot \nabla V_\theta(s_i)$

$$\nabla_\theta(\phi(s)^T \cdot \theta) = 0 .$$

$$V(s_t) \leftarrow V(s_t) + \underbrace{\alpha}_{\boxed{V_{k+1} \leftarrow \mathcal{T}^{\pi} V_k.}} \left(r_t + \gamma V(s_{t+1}) - V(s_t)\right)$$

$$s \quad \{(r_i, s_i')\}_{i=1}^{n}$$

$$V_{k+1}(s) = \mathbb{E}_{\pi}\left[r + \gamma V_k(s') \mid s \right].$$

$$= \underset{f: S \to \mathbb{R}}{\arg\min} \; \mathbb{E}_{\pi}\left[\left(\underbrace{f(s)}_{\text{input}} - \underbrace{(r + \gamma V_k(s'))}_{\text{label}}\right)^2 \right].$$

$$\boxed{\approx \underset{V_\theta \in \mathcal{F}}{\arg\min} \; \frac{1}{n} \sum_{i=1}^{n} \left(\underline{V_\theta(s) - r_i - \gamma V_k(s_i')}\right)^2}$$

$$\text{SGD:} \quad \theta \leftarrow \theta + \alpha \left(V_\theta(s) - r_i - \gamma V_k(s_i')\right) \nabla V_\theta(s)$$

$$s_1, a_1, r_1, \cdots\cdots, s_t, a_t, r_t, \cdots.$$

$$\theta \leftarrow \theta + \alpha \left(V_\theta(s_t) - r_t - \gamma V_\theta(s_{t+1})\right) \nabla V_\theta(s_t).$$

TD(0) with function approximation

- tabular: $V(s_t) \leftarrow V(s_t) + \alpha(r_t + \gamma V(s_{t+1}) - V(s_t))$
- When we update $V(s_t)$, the target is $r_t + \gamma V(s_{t+1})$
- Batch version of the algorithm: one Bellman update can be approximated (using all data) as
$$V_{k+1} \leftarrow \arg\min_{V_\theta \in \mathscr{F}} \frac{1}{T} \sum_{t=1}^{T} (V_\theta(s_t) - r - \gamma V_k(s_{t+1}))^2$$
- SGD + "no-wait": $\theta \leftarrow \theta - \alpha \cdot (V_\theta(s_t) - r - \gamma V_\theta(s_{t+1})) \cdot \nabla V_\theta(s_t)$
- When using linear function approximation $V_\theta(s) = \phi(s)^\top \theta$, we have
$$\theta \leftarrow \theta - \alpha \cdot \underline{(\boxed{\phi(s_t)^\top}\theta - r - \gamma \phi(s_{t+1})^\top \theta)} \cdot \boxed{\phi(s_t)}$$
- When using chain rule, we only take gradient on $V_\theta(s_t)$ and ignore $V_\theta(s_{t+1})$; the latter is treated as a constant (it plays the role of V_k)

$$\underline{\theta^T \phi(s)} \approx \boxed{R(s,\pi) + \gamma \mathbb{E}_{s'|s,\pi}\left[\theta^T \phi(s') \right]}.$$

$$\theta \text{ s.t. } \phi(s)^T \theta \approx V^{\pi}(s).$$

$$s, \ a \sim \pi, \ r, \ s'.$$

$$\mathbb{E}\left[\underbrace{\left(\theta^T \phi(s) - r - \gamma \ \theta^T \phi(s') \right)^2}_{} \right]$$

$$\theta \leftarrow \theta + \underline{\underline{\alpha}} \cdot \left(\theta^T \phi(s) - r - \gamma \theta^T \phi(s') \right) \left(\phi(s) - \cancel{\gamma \phi(s')} \right).$$

What if…? (not required)

- What happens if we also differentiate $V_\theta(s_{t+1})$?
- This corresponds to $\arg\min_{V_\theta \in \mathcal{F}} \sum_{(s,r,s')} (V_\theta(s) - r - \gamma V_\theta(s'))^2$
    - no iteration anymore; a clean optimization objective
    - (most RL algorithms with bootstrapped target do not have a fixed optimization objective; objective changes over time)
- Assume for simplicity that, each data point is generated by (1) sampling s i.i.d. from some exploratory distribution, and (2) generating r and s' conditioned on $(s, \pi(s))$
- Replacing empirical objective with the population version, the objective becomes $\mathbb{E}_{s,r,s'}[(V_\theta(s) - r - \gamma V_\theta(s'))^2]$

What if…? (not required)

- $\mathbb{E}_{s,r,s'}[(V_\theta(s) - r - \gamma V_\theta(s'))^2]$ can be decomposed into two terms
  - First term: $\mathbb{E}_s[(V_\theta(s) - (\mathcal{T}^\pi V_\theta)(s))^2]$
    - This is good! measures how much V_θ violates Bellman eq
    - A version of Bellman error $\|V - \mathcal{T}^\pi V\|$
  - Second term: $\gamma^2 \mathbb{E}_s[\mathrm{Var}_{s'|s,\pi(s)}[V_\theta(s')]]$
    - (assumes deterministic rewards)
    - This is bad! An additional term that penalizes functions that has large variance w.r.t. random state transitions
    - Special case: 0 when environment is deterministic
- So it's actually a sensible algorithm for deterministic environments, but doesn't work when stochasticity is significant

Resolutions (not required)

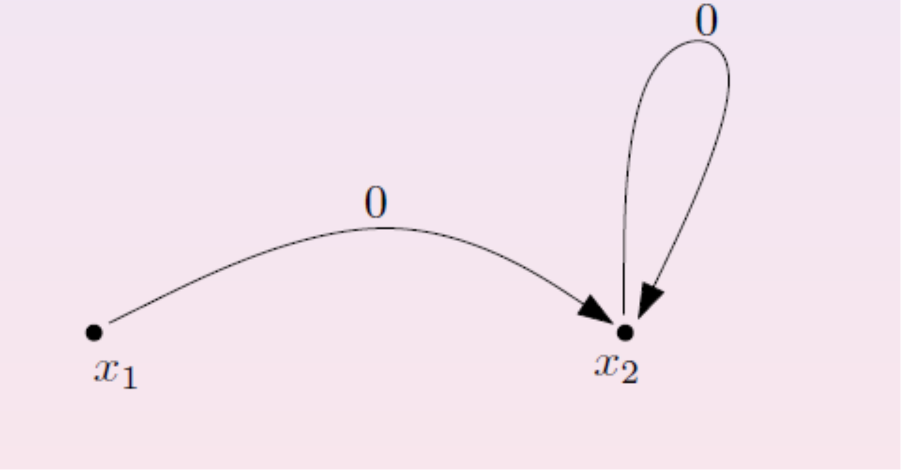
- If we have a simulator…
  - For each s in data, draw another independent state transition
  - Minimize objective $\mathbb{E}[(V_\theta(s) - r - \gamma V_\theta(s'_A))(V_\theta(s) - r - \gamma V_\theta(s'_B))]$
  - "Double sampling" and Baird's residual algorithm (Bellman residual minimization)
  - Exercise: do you need to double sample the reward if reward is stochastic?
  - The conditional variance term is eliminated by double sampling
- If we can only draw 1 next-state (as with any natural data generation process)…
  - Estimate the conditional variance term and subtract from the objective
  - A minimax formulation (not covered in this course)
  - For further readings, see 542 slides on FQI.

Convergence?

- TD with function approximation can diverge in general
- Is it because of…
  - Randomness in SGD?
    - Nope. Even the batch version doesn’t converge.
  - Sophisticated, non-linear func approx?
    - Nope. Even linear doesn’t converge.
  - That our function class does not capture V^π?
    - Nope. Even if V^π can be exactly represented in the function class (“realizable”), it still does not converge.
- 🤦

2.1 Counter-example for least-square regression [Tsitsiklis and van Roy, 1996]

An MDP with two states x_1, x_2, 1-d features for the two states: $f_{x_1} = 1, f_{x_2} = 2$. Linear Function approximation with $\tilde{V}_\theta(x) = \theta f_x$.



$$\begin{aligned}\theta_k &:= \arg\min_\theta \frac{1}{2}(\theta - \text{target}_1)^2 + (2\theta - \text{target}_2)^2 \\ &= \arg\min_\theta \frac{1}{2}(\theta - \gamma\theta^{k-1} f_{x_2})^2 + (2\theta - \gamma\theta^{k-1} f_{x_2})^2 \\ &= \arg\min_\theta \frac{1}{2}(\theta - \gamma 2\theta^{k-1})^2 + (2\theta - \gamma 2\theta^{k-1})^2\end{aligned}$$

$$(\theta - \gamma 2\theta^{k-1}) + 2(2\theta - \gamma 2\theta^{k-1}) = 0 \Rightarrow 5\theta = 6\gamma\theta^{k-1}$$

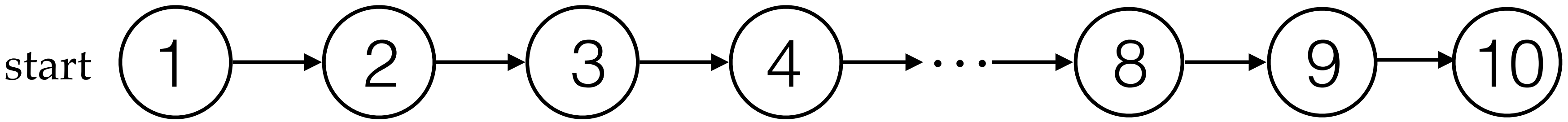
$$\theta_k = \frac{6}{5}\gamma\theta_{k-1}$$

This diverges if $\gamma \geq 5/6$.

credit: course notes
from Shipra Agrawal

A simple example (finite horizon, γ=1)

reward: Ber(0.5)



Iter #1: Data: (⑩, 1, *end*), …, (⑩, 0, *end*) ⇨ 0.501

Iter #2: Data: (⑨, 0, ⑩) ⇨ (⑨, 0+0.501) ⇨ 0.501 0.501

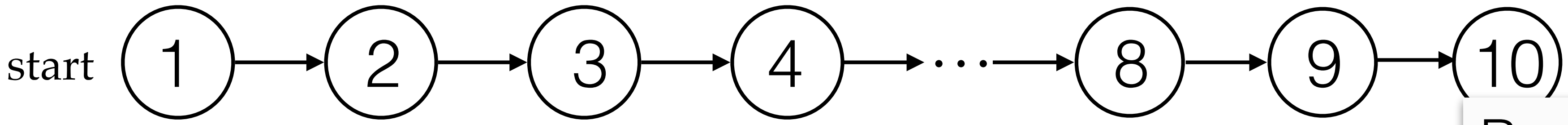
…

Iter #10: 0.501 0.501 0.501 0.501 … 0.501 0.501 0.501

- Dataset $D = \{(s, r, s')\}$ looks like:
  {(①, 0, ②), (②, 0,③), …, (⑩, 1, *end*), …, (⑩, 0, *end*)}

How things go wrong (w/ restricted class)

reward: Ber(0.5)



Realizable

Function class
0.5 × 0.5 × 0.5 × … × 0.5 × 0.5 × 0.5
1.012 0.756 0.628 0.504 0.502 0.501

Iter #1: Data: (⑩, 1, *end*), …, (⑩, 0, *end*) ⇨ 0.501

Iter #2: Data: (⑨, 0, ⑩) ⇨ (⑨, 0+0.501) ⇨ 0.502 0.501

…

!!!

Iter #10: 1.012 0.756 0.628 … 0.502 0.501

Example given in Dann et al’18

Non-convergence

- Why things go wrong?
- Bellman update is a contraction, but here we have an additional projection step: $V_{k+1} \leftarrow \Pi_{\mathscr{F}} \mathscr{T}^{\pi} V_k$, projected Bellman update may NOT be a contraction (even with linear function approximation)
  - it is still a contraction in some special cases; will see
- In other words: in each iter, we solve a regression problem where the target function is $T^{\pi}V$, where V can be arbitrary function in $\mathscr{F}$
- The fact that $V^{\pi} \in \mathscr{F}$ does not imply that $T^{\pi}V$ is in $\mathscr{F}$! We may do quite poorly in the regression problem, and the iteration does not mimic a Bellman update
- Why tabular is fine? $\mathscr{F}$ is fully expressive so $T^{\pi}V$ is always in $\mathscr{F}$.
  - Similarly for func approx, if we assume that $\mathscr{F}$ is closed under T^{π}, can prove some good properties of TD
- All alg based on bootstrapped targets suffer from this issue
  - Compare to the behavior of Monte-Carlo