Deep Reinforcement Learning

6 - Temporal Difference Learning

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Overview Lecture

For Known MDP:

General Policy Improvement Approach:

- Policy Evaluation
- Policy Improvement

In Contrast: Model-Free Approaches

- Prediction: Estimate the value function of an unknown MDP
  - Monte-Carlo Method
  - **Temporal Difference Learning**
- Model-free control (next week):
  - Optimise the policy

Big picture: Solving an MDP

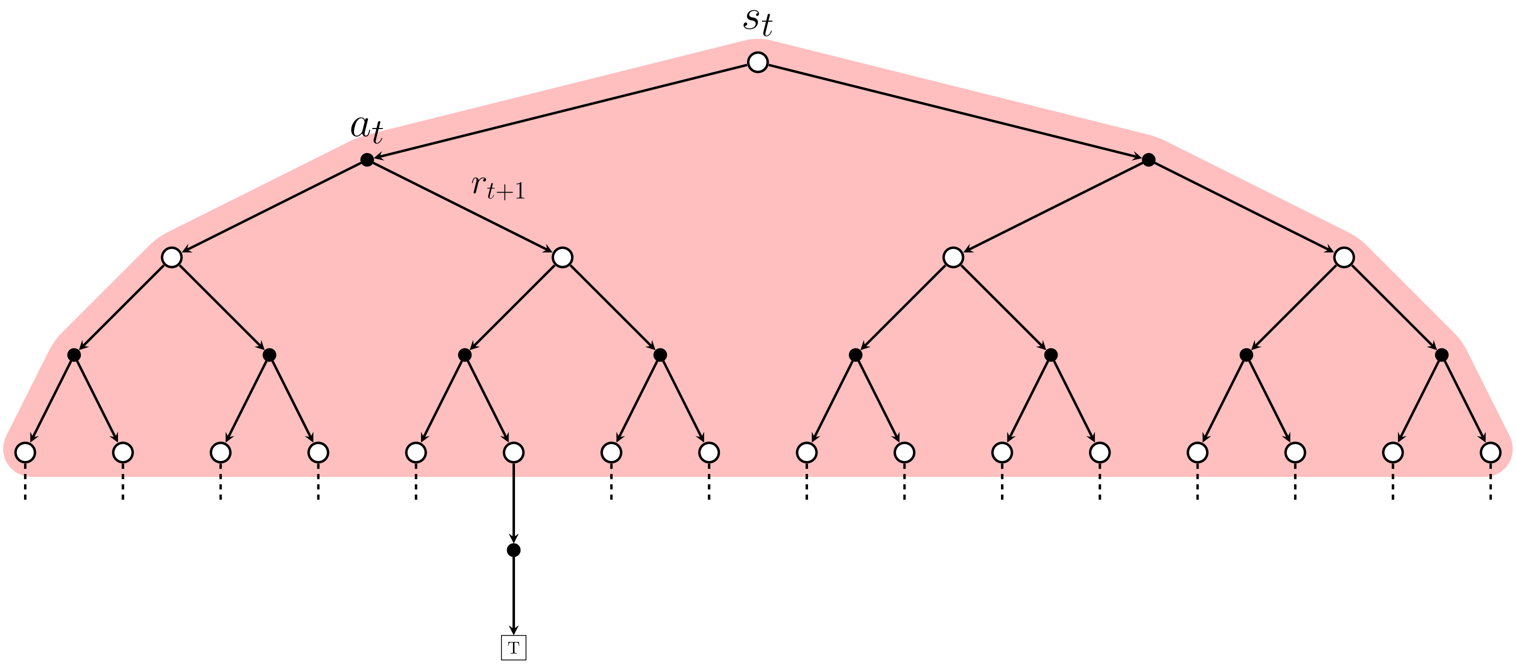
Goal: Maximize return

$$G_t = R_{t+1} + R_{t+2} + \dots$$

When MDP is fully known, joint probability $p(s', r|s, a)$:

- How environment develops and
- how reward is given.

Plus we fixed a policy how to act.



$$v_\pi(s) \leftarrow \sum_{a \in \mathcal{A}} \pi(a|s) \sum_r \sum_{s' \in \mathcal{S}} p(r, s'|s, a) \Big(r + \dots \Big)$$

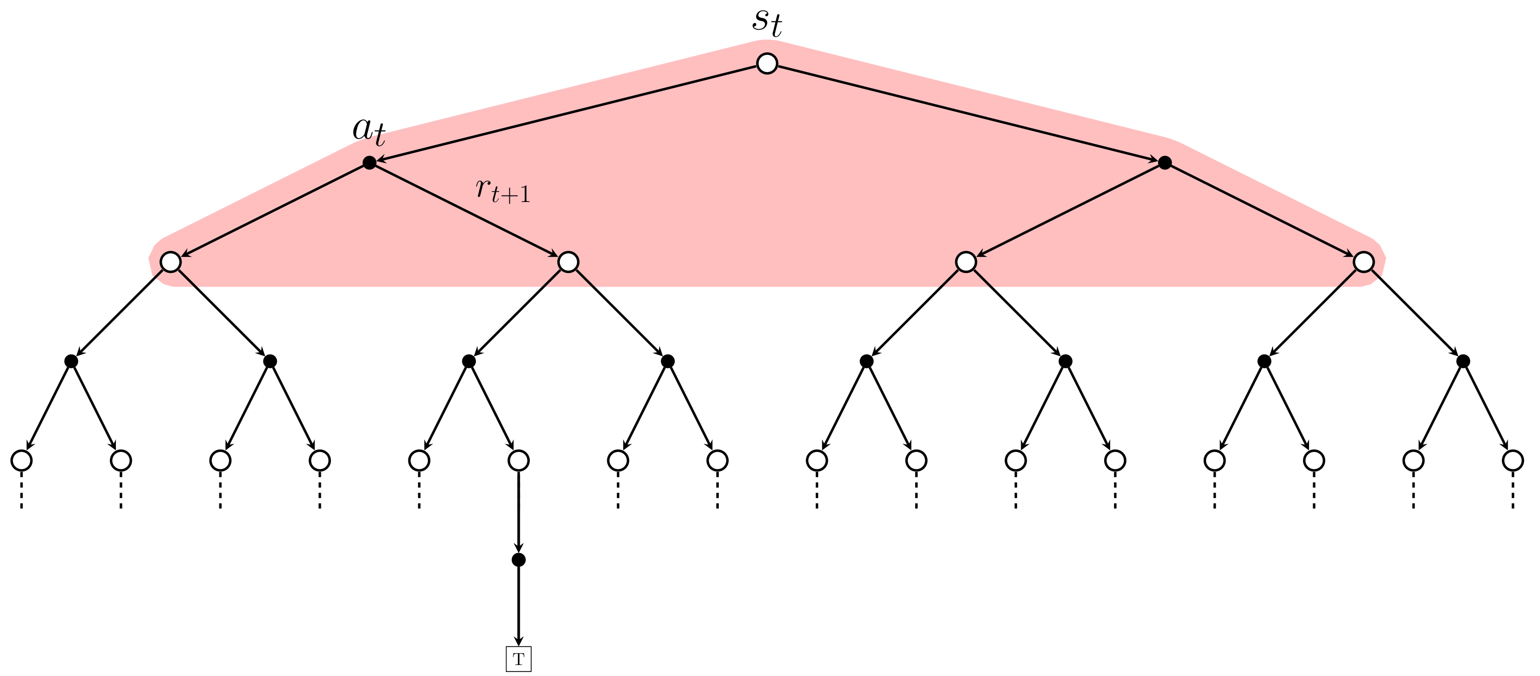
Big picture: Solving an MDP, Dynamic Programming

Goal: Maximize return

$$G_t = R_{t+1} + \gamma R_{t+2} + \ldots$$

- Use Bellman Equation for (recursive) backup.
- Model-Based Approach.
- Value function based Approach.

Called **bootstrapping**.



$$v_\pi(s) \leftarrow \sum_{a \in \mathcal{A}} \pi(a|s) \sum_r \sum_{s' \in \mathcal{S}} p(r, s'|s, a)\Big(r + \gamma v_\pi(s')\Big)$$

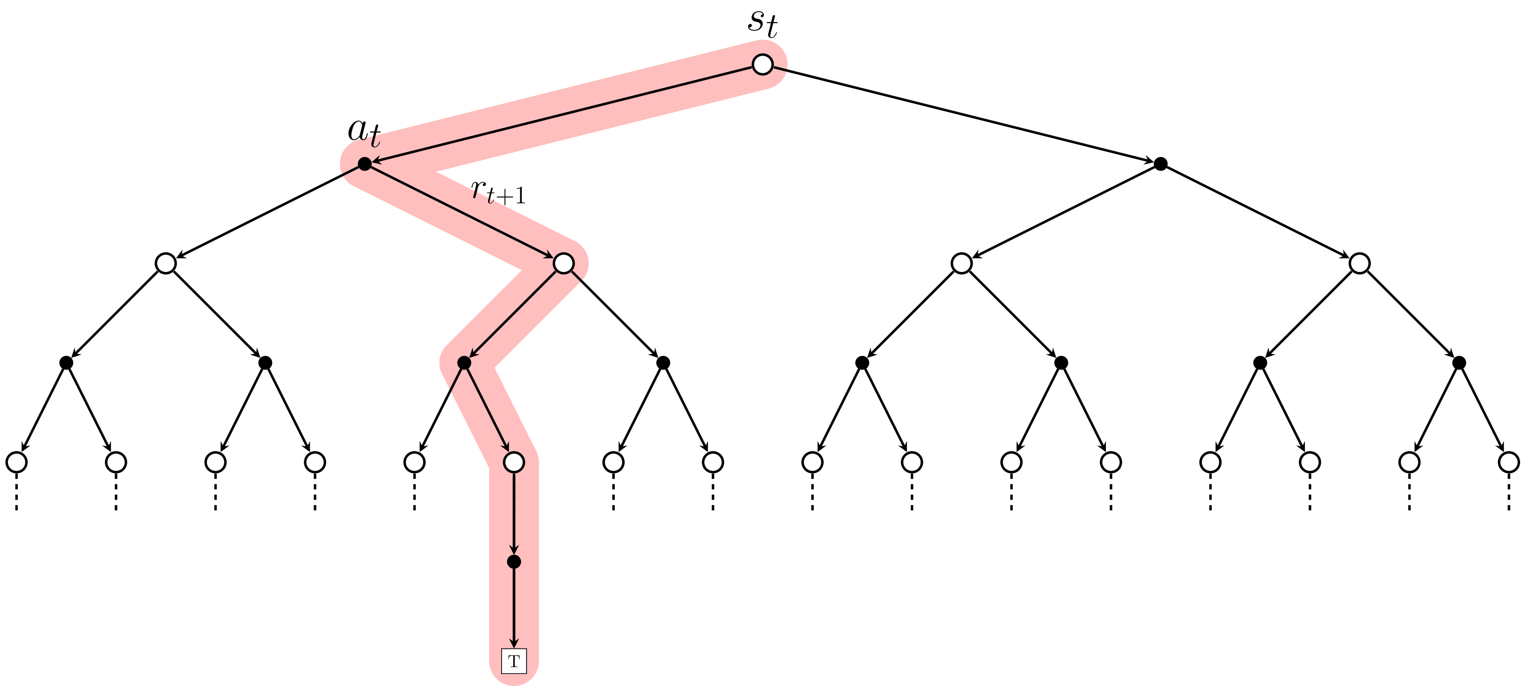
Big picture: Monte-Carlo Sampling

Goal: Maximize return

$$G_t = R_{t+1} + \gamma R_{t+2} + \ldots$$

- Model-free Approach.
- Sample from experience.
- Exploit sequential data.

Sample along path (Monte Carlo)



$$v_\pi(s) \leftarrow \mathbb{E}_\pi(G_t | S_t = s)$$

Recap – Using Monte-Carlo Method for Reinforcement Learning

Monte-Carlo:

- is a model-free approach that does not use knowledge of MDP (neither transition probabilities nor reward distribution),
- learns directly from full episodes of experience and the obtained return in these
- as it uses the straightforward idea to estimate the mean return for a state from these episodes.

One drawback: requires episodic MDPs as the episodes must terminate.

Recap – Monte-Carlo Methods

… learns from episodes of raw experience without modeling the environmental dynamics.

MC methods computes the observed mean return as an approximation of the expected return.

Computation of the empirical return G_t requires complete episodes $S_1, A_1, R_2, \dots, S_T$:

$$v(s) = \frac{\sum_{t=1}^{T} \mathbb{1}[S_t = s] G_t}{\sum_{t=1}^{T} \mathbb{1}[S_t = s]}, q(s,a) = \frac{\sum_{t=1}^{T} \mathbb{1}[S_t = s, A_t = a] G_t}{\sum_{t=1}^{T} \mathbb{1}[S_t = s, A_t = a]}$$

Recap – Incremental Monte-Carlo Updates

Update $v(s)$ incrementally after episode $S_1, A_1, R_2, \dots, S_T$

For each state S_t with return G_t

$$N(S_t) \leftarrow N(S_t) + 1$$

$$v(S_t) \leftarrow v(S_t) + \frac{1}{N(S_t)}(G_t - v(S_t))$$

In non-stationary problems, it can be useful to track a running mean, i.e. forget old episodes:

$$v(S_t) \leftarrow v(S_t) + \alpha(G_t - v(S_t))$$

(Silver 2015)

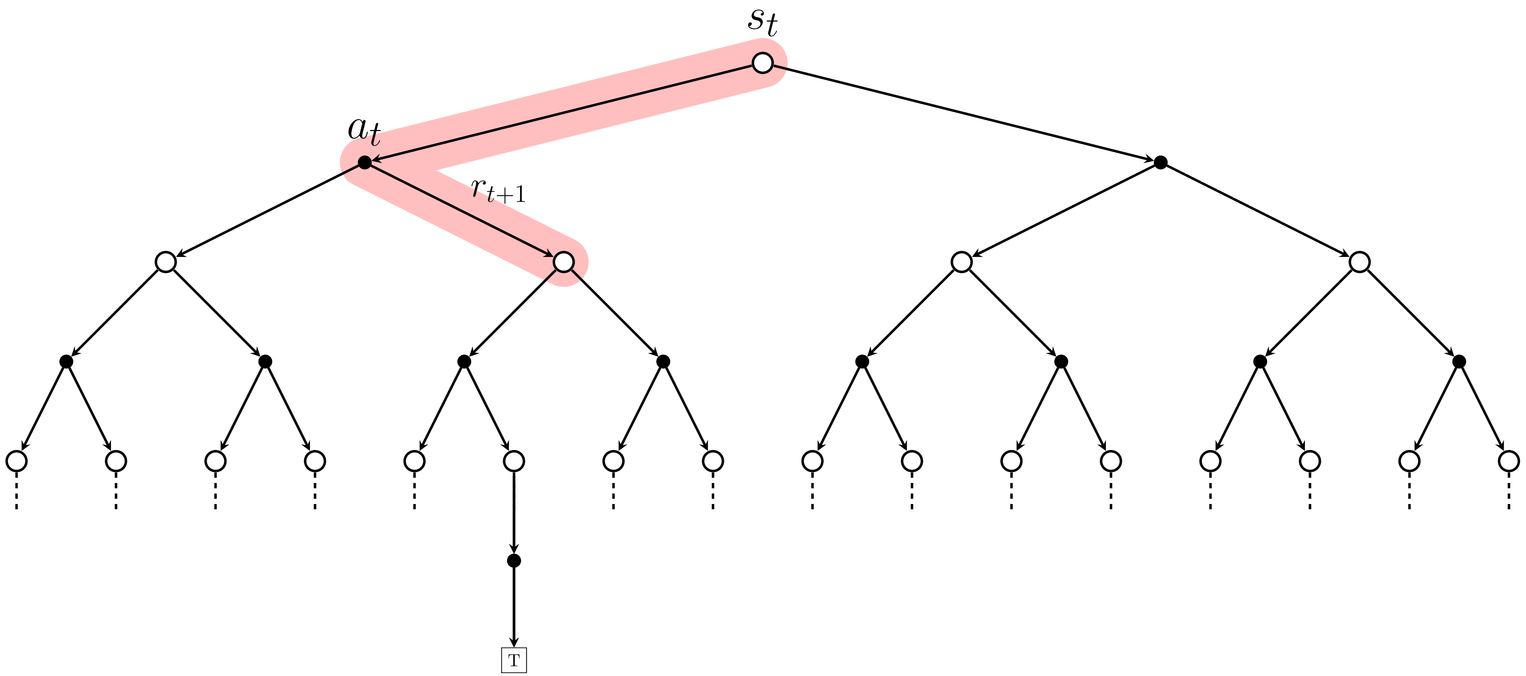
Temporal Difference Learning – Backup Diagram

Goal: Maximize return

$$G_t = R_{t+1} + \gamma R_{t+2} + \dots$$

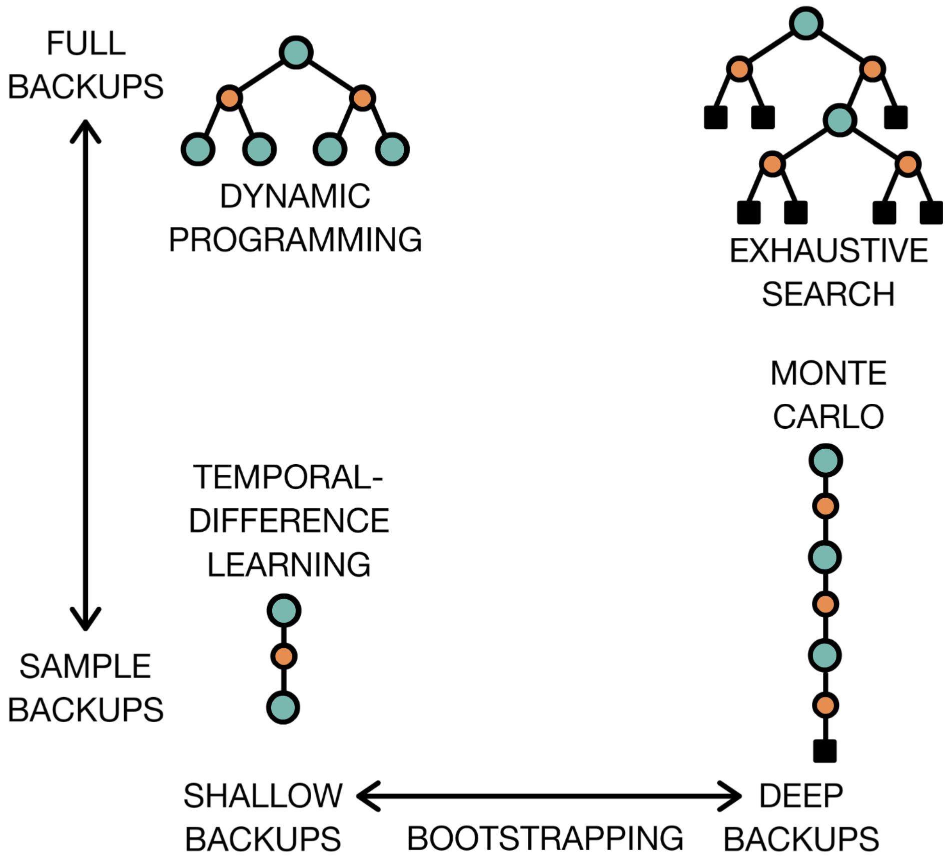
- Model-free Approach.
- Sample from experience (Monte-Carlo).
- Exploit sequential data.

But: Bootstrap as in DP (use Bellman equation).



$$v(S_t) \leftarrow v(S_t) + \alpha(R_{t+1} + \gamma v(S_t + 1) - v(S_t))$$

Reinforcement Learning Algorithms Overview



(Arulkumaran u. a. 2017)

Temporal Difference Learning

Temporal Difference Learning

Temporal Difference ...

- Learning is model-free: no knowledge on MDP transition or reward probabilities is needed
- methods also learn directly from episodes of experience

Bootstrapping

TD learning methods update targets with regard to existing estimates rather than exclusively relying on actual rewards and complete returns as in MC methods.

The key idea in TD learning is to update the value function $v(S_t)$ towards an estimated return $R_{t+1} + \gamma v(S_{t+1})$ (known as "TD target").

(Weng 2018)

From MC to Temporal Difference Learning

In both: Goal is to learn v_π online from experience under policy π

Incremental every-visit Monte-Carlo:

- Update value $v(S_t)$ towards **actual** return G_t:

$$v(S_t) \leftarrow v(S_t) + \alpha(G_t - v(S_t))$$

Simple temporal-difference learning algorithm TD(0):

- Update value $v(S_t)$ towards **estimated** return $R_{t+1} + \gamma v(S_{t+1})$:

$$v(S_t) \leftarrow v(S_t) + \alpha(R_{t+1} + \gamma v(S_{t+1}) - v(S_t))$$

(Silver 2015)

Temporal Difference Learning

$$v(S_t) \leftarrow v(S_t) + \alpha(R_{t+1} + \gamma v(S_t + 1) - v(S_t))$$

TD Target

$R_{t+1} + \gamma v(S_t + 1)$ is called the TD target.

TD Error

$\delta_t = R_{t+1} + \gamma v(S_t + 1) - v(S_t)$ is called the TD error.

TD: Value Estimation

Update of the value function is regulated by the learning rate α.

In brief: TD means update a guess (of the value function) towards a guess (experiencing a single step and a guess of what follows):

$$\text{MC: } v(S_t) \leftarrow (1-\alpha)v(S_t) + \alpha G_t$$
$$v(S_t) \leftarrow v(S_t) + \alpha(G_t - v(S_t))$$
$$\text{TD: } v(S_t) \leftarrow v(S_t) + \alpha(R_{t+1} + \gamma v(S_{t+1}) - v(S_t))$$

Similarly for the Q-function:

$$q(S_t, A_t) \leftarrow q(S_t, A_t) + \alpha(R_{t+1} + \gamma q(S_{t+1}, A_{t+1}) - q(S_t, A_t))$$

(Weng 2018)

Tabular TD(0) for estimating v_π

```
Input: The policy π to be evaluated; step size α ∈ (0, 1]
Initialize V(s), for all s ∈ S⁺, arbitrarily except that V(terminal) = 0
for each episode do
    Initialize S
    for each step in the episode, until state S is terminal do
        A ← action given by π for S
        Take action A, observe R, S'
        V(S) ← V(S) + α [R + γV(S') − V(S)]
        S ← S'
    end
end
```

Agent part of the algorithm; Environment interaction

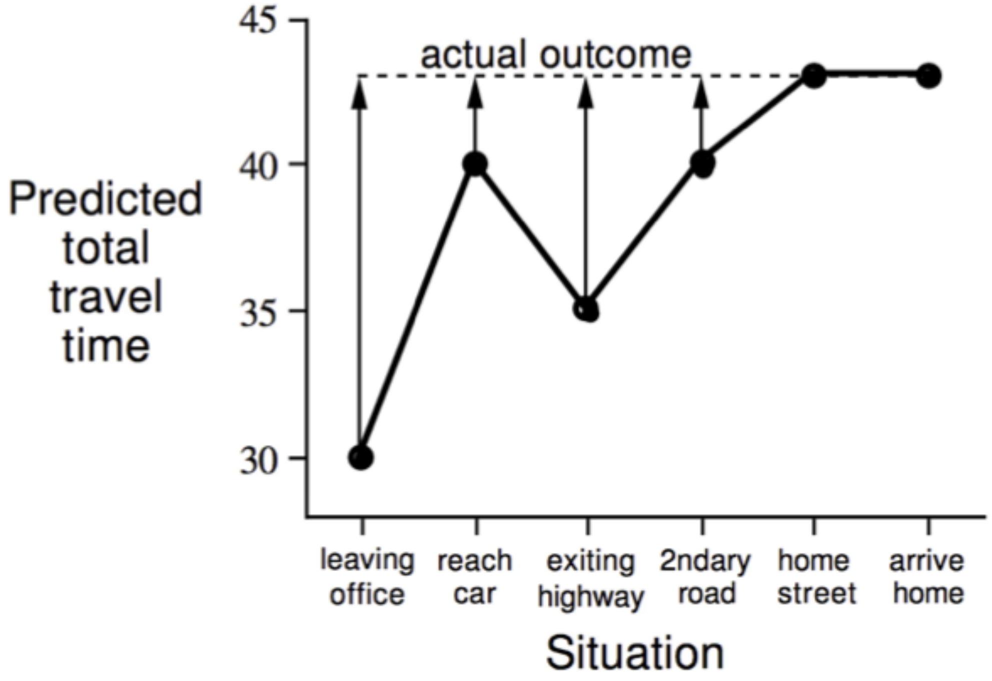
Example: Driving Home

State	Elapsed time	Predicted time to Go	Predicted total time
Leaving office, Friday at 6	0	30	30
Reach car, raining	5	35	40
Exiting highway	20	15	35
small road, behind truck	30	10	40
Entering home street	40	3	43
Arrive home	43	0	43

Example: Comparison Monte-Carlo and TD Approach

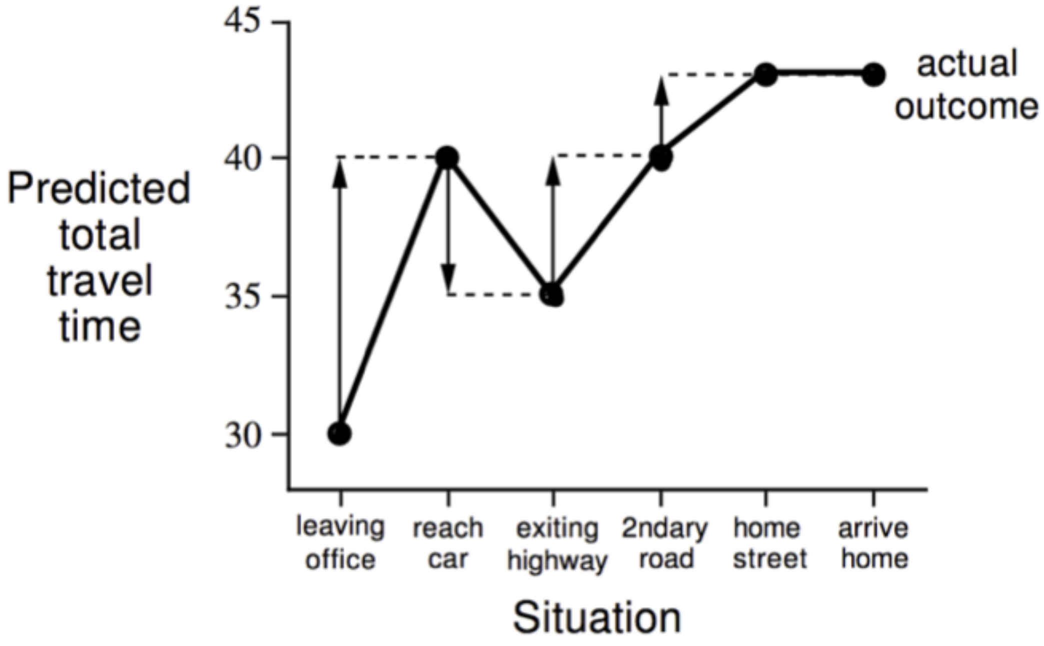
Monte-Carlo Approach

Changes recommended, MC ($\alpha = 1$):

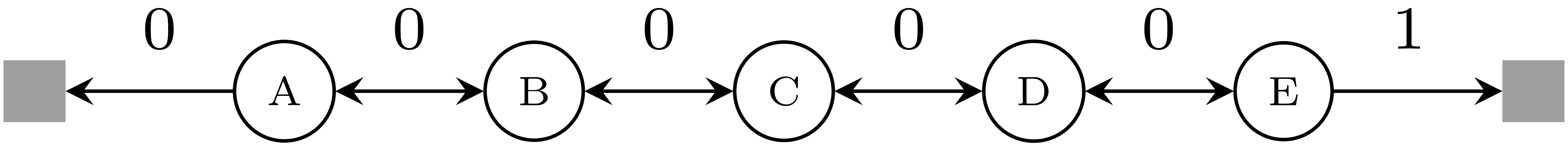


Temporal Difference Method

Changes recommended in TD ($\alpha = 1$):



Example: Random Walk



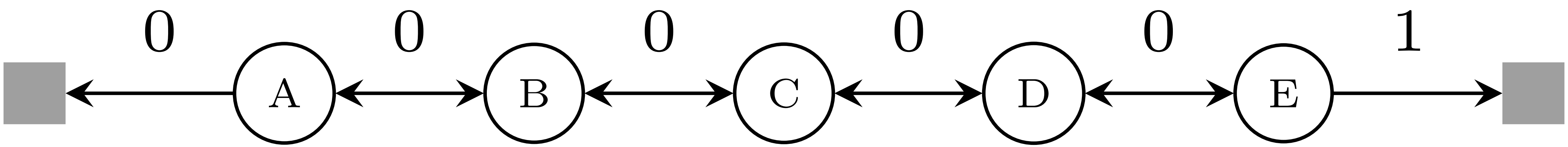
- all episodes start in the center state C,
- then proceed randomly left or right.
- Termination states are on the extreme left and extreme right.
- Reward: only given when terminating right $(+1)$.

Value of a state is the probability of terminating in the right node.

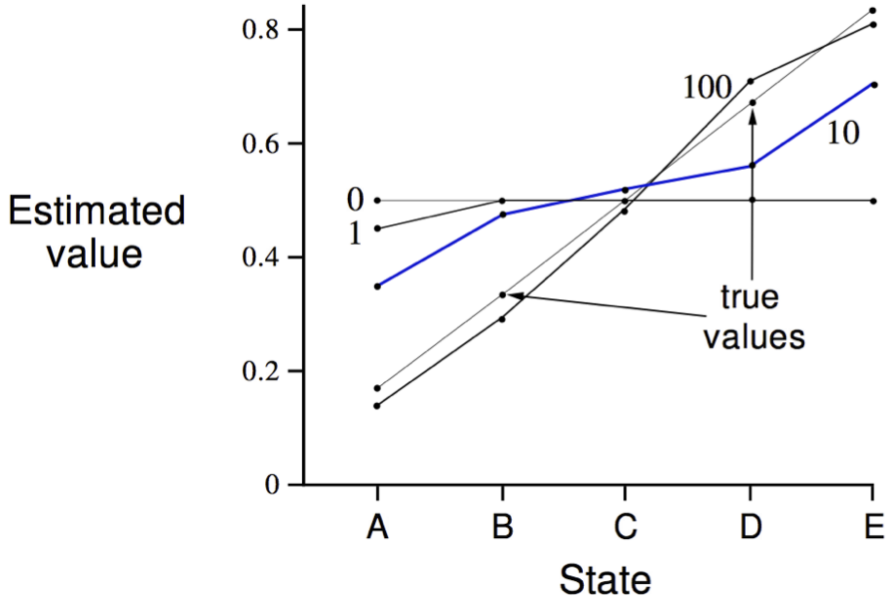
Can you derive some of the state values?

$v_\pi(C) = \frac{1}{2}$, and for states A through E these are $\frac{1}{6}, \frac{2}{6}, \frac{3}{6}, \frac{4}{6}, \frac{5}{6}$.

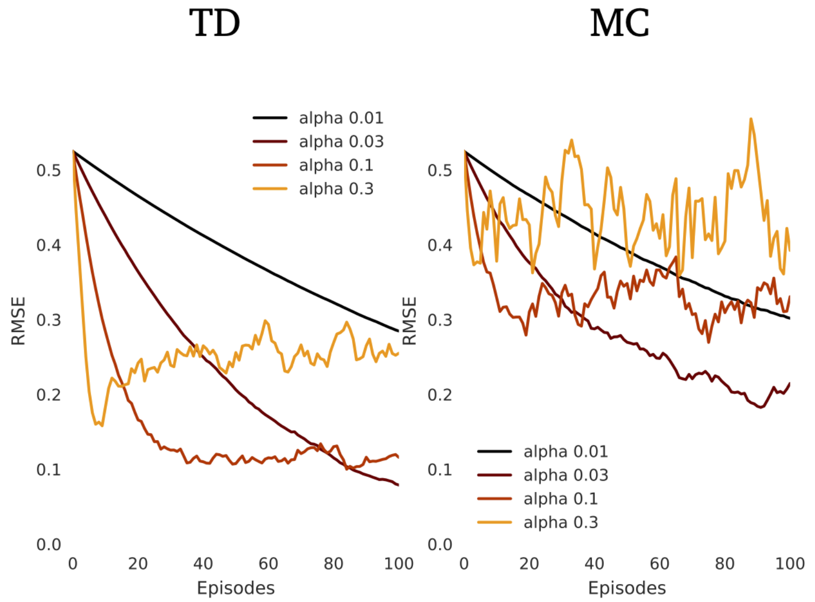
Example: Compare MC and TD empirically



TD(0) Estimates for v_π



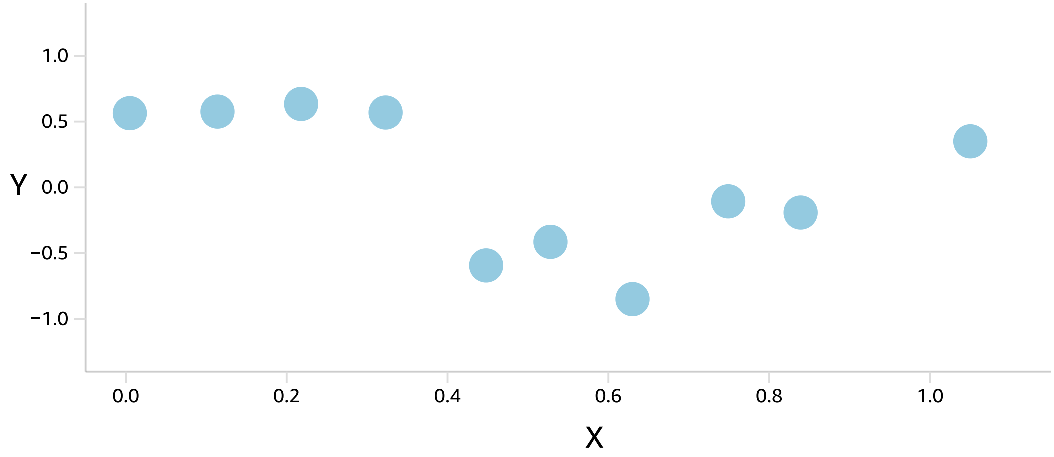
Learning Curves



(Sutton und Barto 2018; Hasselt und Borsa 2021)

ML Background: Bias-Variance Tradeoff

Bias-Variance Tradeoff – Interactive Visualization



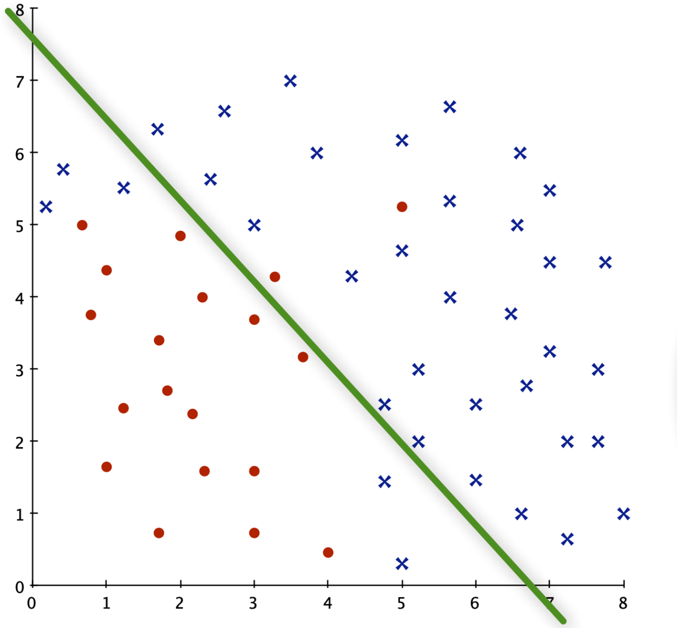
Using our wildest imagination, we can picture a dataset consisting of features X and labels Y, as on the left. Also imagine that we'd like to generalize this relationship to additional values of X - that we'd like to predict future values based on what we've already seen before.

With our imagination now undoubtedly spent, we can take a very simple approach to modeling the relationship between X and Y by just drawing a line to the general trend of the data.

(Wilber und Werness 2021)

Bias and Variance Tradeoff in ML: Classification

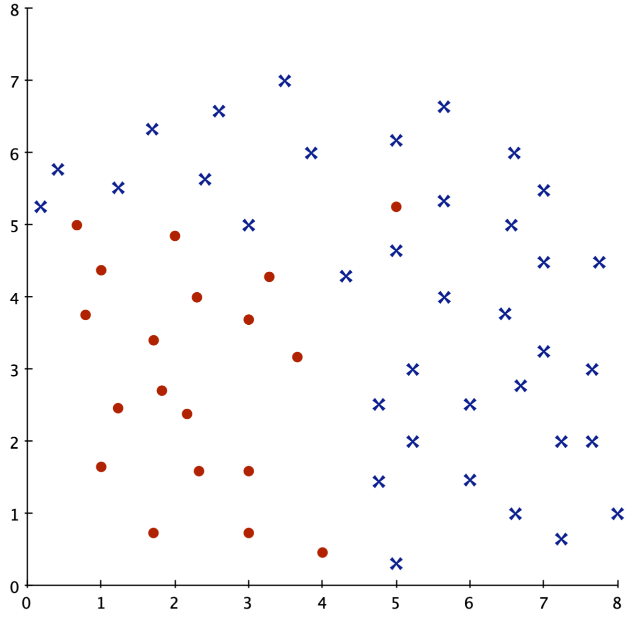
Underfitting



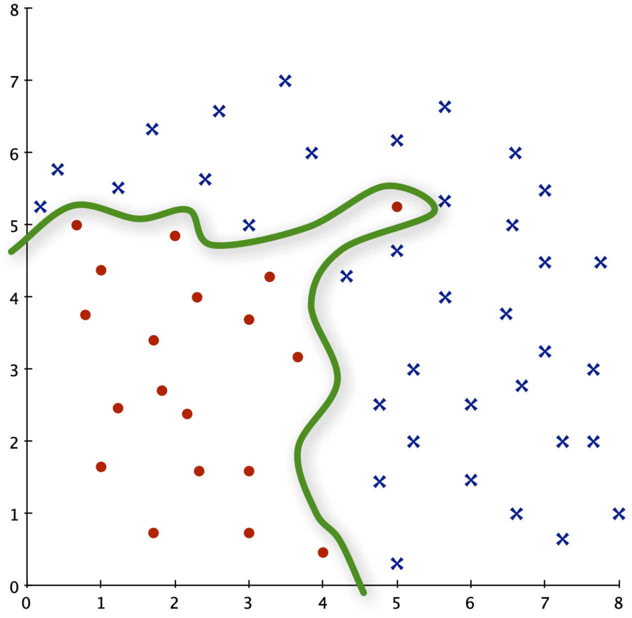
High Bias

Underfitting

Original Data



Overfitting

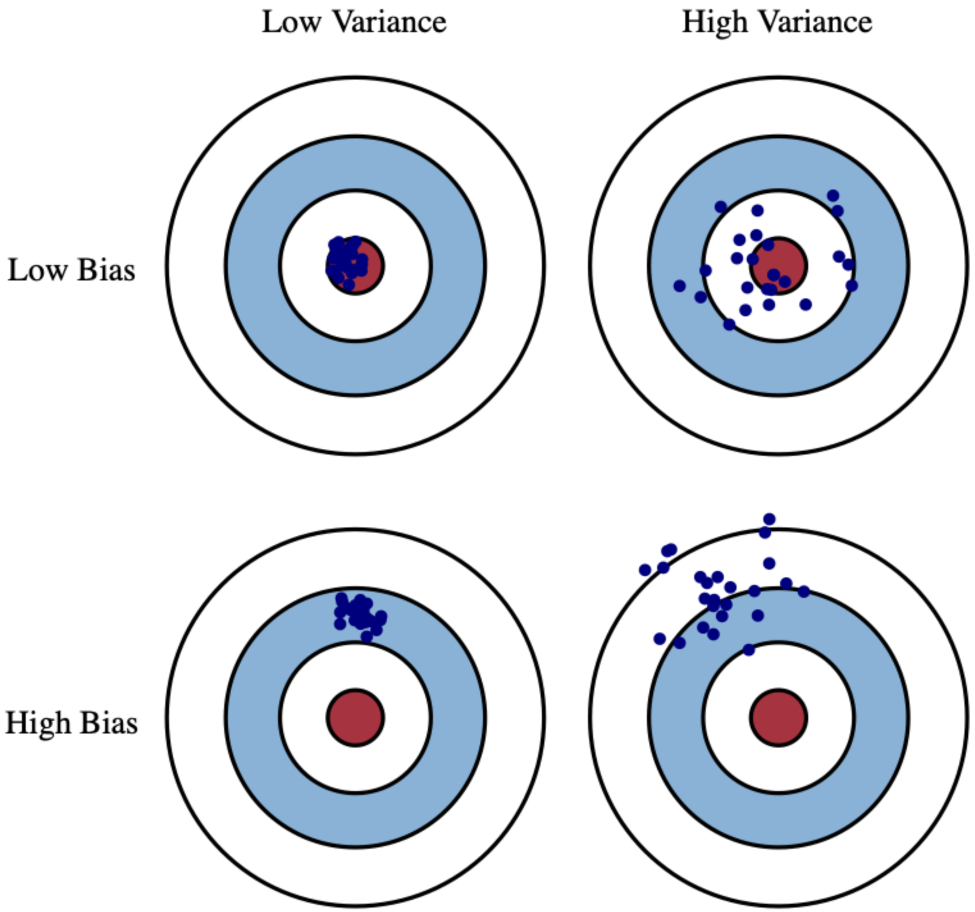


High Variance

Overfitting

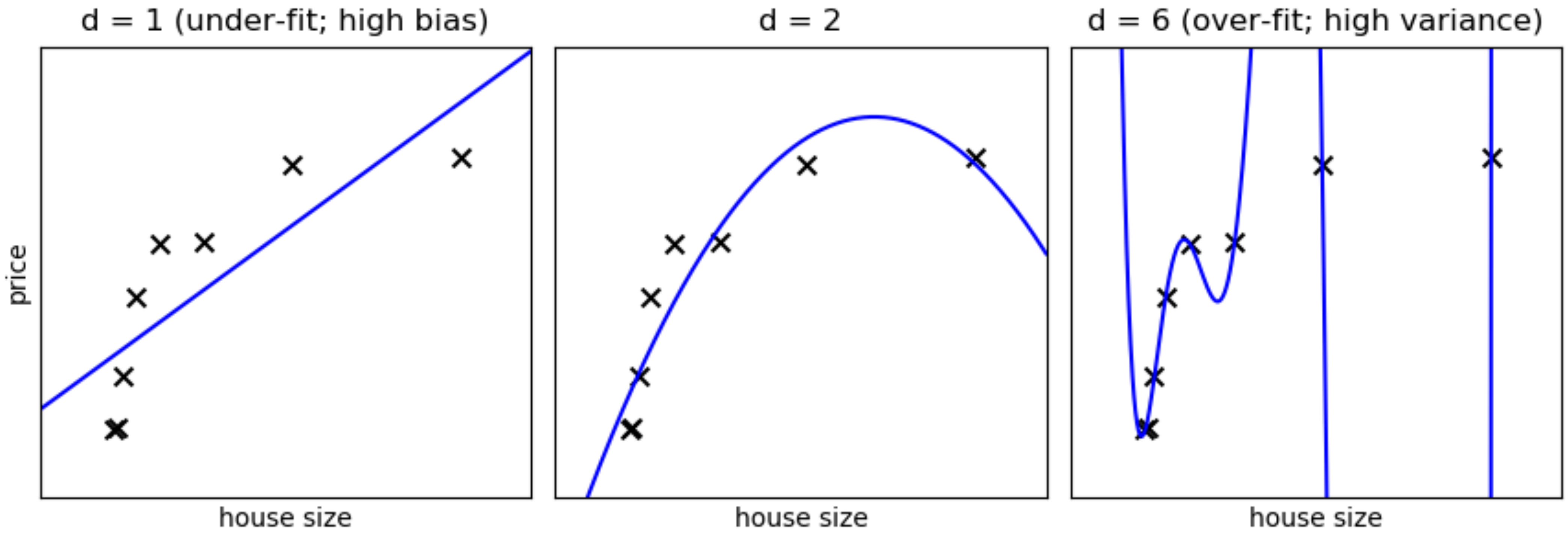
For two classes (shown as red dots and blue crosses).

Bias and Variance



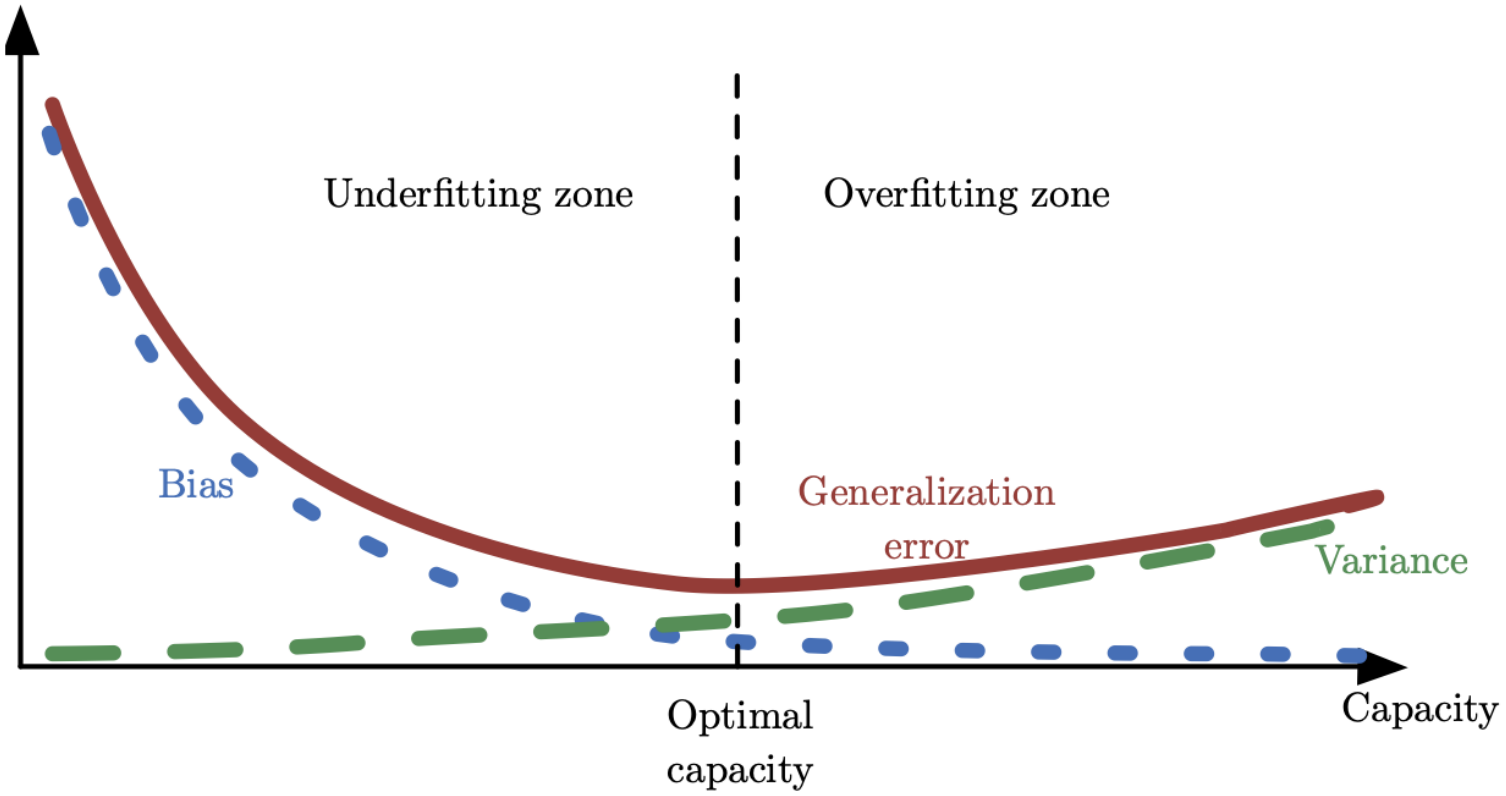
(Fortmann-Roe 2012)

Bias and Variance Tradeoff in ML: Regression Problem



(Varoquaux u. a. 2022), see as well (Bishop 2006)

Bias and Variance Tradeoff in ML



(Goodfellow, Bengio, und Courville 2016)

Task – Compare different models

For a two-class classifier model, we find the following errors during training and when testing our model afterwards. Discuss the bias and variance of the models.

Classification:
Cat?

Error on Training Set	1 %	15 %	15 %	0.1 %
Error on Dev/Test Set	11 %	16 %	30 %	1 %

Task – Solution for different models

Classification:
Cat?

Human Error?	Around 0%			
Avoidable **Bias**				
Error on Training Set	1 %	15 %	15 %	0.1 %
Variance				
Error on Dev/Test Set	11 %	16 %	30 %	1 %
	High variance	*High Bias*	*High Bias & variance*	*Low Bias & variance*

Bias and Variance

Bias

$$Bias^2(x) = \left(\mathbb{E}[\hat{f}(x)] - f(x)\right)^2$$

Variance

$$Variance(x) = \mathbb{E}\left[\hat{f}(x) - \mathbb{E}[f(x)]\right]$$

Source of Error in Bias

The error due to bias is taken as the difference between the expected (or average) prediction of our model and the correct value which we are trying to predict.

Source of Error in Variance

The error due to variance is taken as the variability of a model prediction for a given data point.

Bias measures how far off in general models' predictions are from the correct value.

The variance is how much the predictions for a given point vary between different realizations of the model.

Dealing with Variance and Bias in Neural Network Models

Classification:
Cat?

Human Error?

Avoidable **Bias**

- ▶ Train bigger model
- ▶ Train longer, use better optimization
- ▶ Change NN Architecture, Hyperparameter search

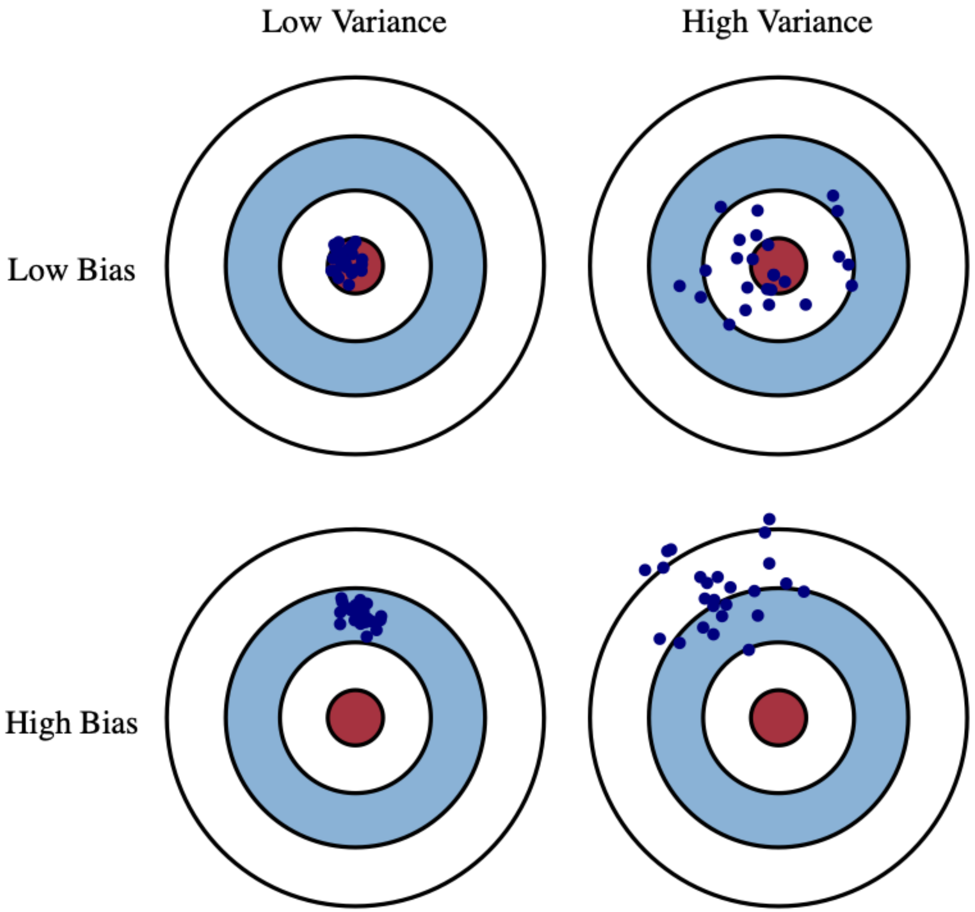
Error on Training Set

Variance

- ▶ More Data
- ▶ Regularization
- ▶ Change NN Architecture, Hyperparameter search

Error on Dev/Test Set

Bias and Variance



(Fortmann-Roe 2012)

Bias-Variance Trade-Off: Monte-Carlo

Aiming for estimated Return from that state: $v(S_t) = \mathbb{E}[G_t]$

Monte-Carlo: Update value $v(S_t)$ toward actual return G_t

$$v(S_t) \leftarrow v(S_t) + \alpha\left(G_t^{(n)} - v(S_t)\right)$$

- Return $G_t^{(n)} = R_{t+1} + \gamma R_{t+2} + \cdots + \gamma^{T-1} R_T$ is unbiased estimate of $v_\pi(S_t)$.
- MC has high variance, zero bias
  - Bias: $Bias = \mathbb{E}[G_t] - v_\pi(S_t) = 0$, as $v(S_t) = \mathbb{E}[G_t]$ as true sample from estimate
  - but following a long trajectory can possibly induce a large variance

(Satakhutdinov 2018)

Bias-Variance Trade-Off: Difference using Return or TD target

- TD target is much lower variance than the return:
  - Return depends on many random actions, transitions, rewards,
  - TD target depends on one random action, transition, reward combined with stable estimate.

(Satakhutdinov 2018)

Bias-Variance Trade-Off: TD Learning

TD: Update value $v(S_t)$ toward estimated returns $R_{t+1} + \gamma v(S_{t+1})$

$$v(S_t) \leftarrow v(S_t) + \alpha\Big(R_{t+1} + \gamma v(S_{t+1}) - v(S_t)\Big)$$

- True TD target: $R_{t+1} + \gamma v_\pi(S_{t+1})$ is unbiased estimate of $v_\pi(S_t)$
- But: TD target $R_{t+1} + \gamma v(S_{t+1})$ is biased estimate of $v_\pi(S_t)$, as

$$Bias = \mathbb{E}[R_{t+1} + \gamma v_\pi(S_{t+1})] - v_\pi(S_t)$$

  R_{t+1} and S_{t+1} are directly from sample therefore unbiased. But $v_\pi(S_{t+1})$ is an estimate and not true value function which can be biased.

- As an advantage: Estimate using value function for most part of the trajectory reduces variance.

(Satakhutdinov 2018)

Bias-Variance Trade-Off

MC has high variance, zero bias

- Good convergence properties
- Even with function approximation
- Not very sensitive to initial value
- Very simple to understand and use

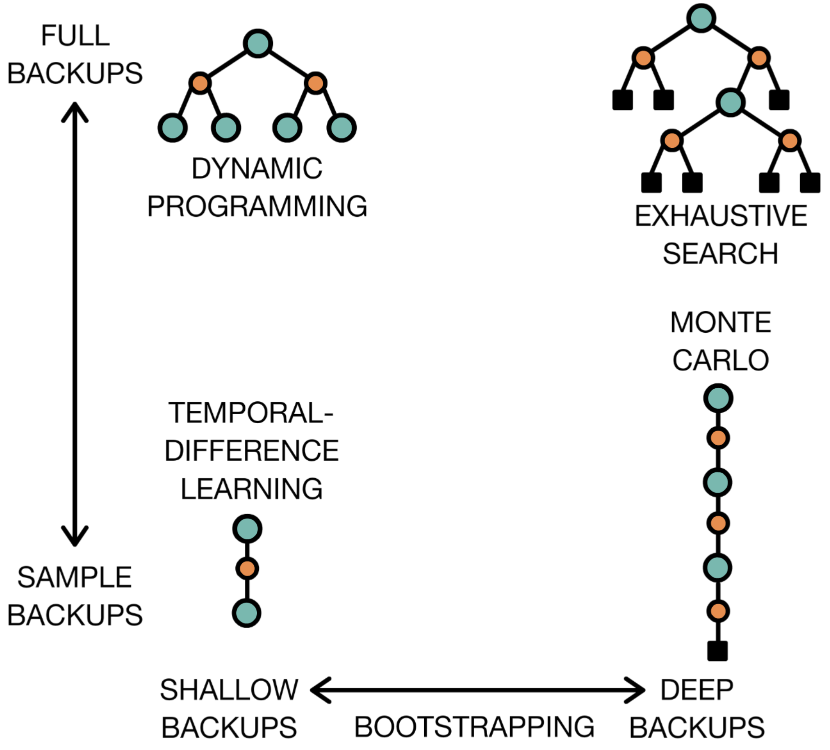
TD has low variance, some bias

- Usually more efficient than MC
- TD(0) converges to $v_\pi(s)$
- More sensitive to initial value

(Satakhutdinov 2018)

Bootstrapping and Sampling

- Bootstrapping: update involves an estimate
  - MC does not bootstrap
  - DP bootstraps
  - TD bootstraps
- Sampling: update samples an expectation
  - MC samples
  - DP does not sample
  - TD samples



(Arulkumaran u. a. 2017)

Temporal-Difference Learning

- TD is model-free (no knowledge of MDP) and learn directly from experience
- TD can learn from incomplete episodes, by bootstrapping
- TD can learn during each episode

(Hasselt und Borsa 2021)

Temporal difference learning – q-function

- We can apply the same idea to action values – when dynamics are unknown, this is much more important
- Temporal-difference learning for action values:
  - Update value $q_t(S_t, A_t)$ towards estimated return $R_{t+1} + \gamma q(S_{t+1}, A_{t+1})$

$$q(S_t, A_t) \leftarrow q(S_t, A_t) + \alpha \Big(\underbrace{R_{t+1} + \gamma q(S_{t+1}, A_{t+1} - q_t(S_t, A_t)}_{\text{TD Error}} \Big)$$

This algorithm is known as SARSA, because it uses $(S_t, A_t, R_{t+1}, S_{t+1}, A_{t+1})$.

(Hasselt und Borsa 2021)

Task – TD - MC direct Comparison

Calculate the values for the two possible states given the experience collected ($\gamma = 1$; for TD you might want to start with B – why?).

Monte-Carlo

Calculation of $v_\pi(s)$

$$v(s) = \frac{\sum_{t=1}^{T} \mathbb{1}[S_t = s] G_t}{\sum_{t=1}^{T} \mathbb{1}[S_t = s]}$$

Observed Episodes

$A \rightarrow 0, B \rightarrow 0$	$B \rightarrow 1$
$B \rightarrow 1$	$B \rightarrow 1$
$B \rightarrow 1$	$B \rightarrow 1$
$B \rightarrow 1$	$B \rightarrow 0$

Temporal Difference Learning

Update of $v_\pi(s)$

$$v(S_t) \leftarrow v(S_t) + \alpha(R_{t+1} + \gamma v(S_{t+1}) - v(S_t))$$

Task – Value Function

Episodes

$A \to 0, B \to 0; B \to 1; B \to 1; B \to 1; B \to 1; B \to 1; B \to 1; B \to 0$

Monte-Carlo

Calculation of $v_\pi(s)$

$$v(A) = \frac{0}{1} = 0$$
$$v(B) = \frac{6}{8} = 0.75$$

Temporal Difference Learning

$v(S_t) \leftarrow v(S_t) + \alpha(R_{t+1} + \gamma v(S_t + 1) - v(S_t))$

1. $v(B)$ (easier, always terminating):
$$v(B) = \frac{6}{8} = 0.75$$
2. only one episode with A, but use value estimate for ending in B:
$$v(A) = 0 + 0.75 = 0.75$$

Batch Learning – Using limited Data for Learning

Tabular MC and TD converge to v_π as we gather unlimited experience which we usually can't gather. How do these behave with limited experience?

Batch Setting

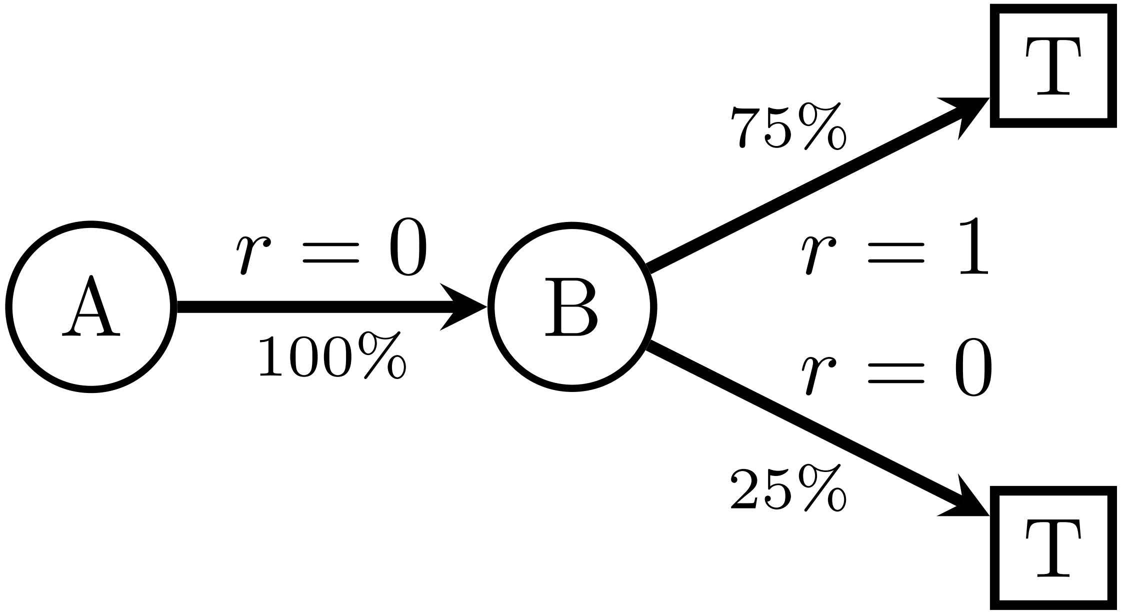
We collect multiple episodes 1 to K, :

$$\text{episode } k : S_1^k, A_1^k, R_2^k, \ldots, S_{T_k}^k$$

We can repeatedly use each episode $k \in [1, K]$ for training.

This means: we sample from an empirical model.

Underlying MDP for the example



Could be derived from experiences: Maximum-Likelihood Estimation – which is the most likely MDP producing such data?

Differences in batch solutions

Monte-Carlo

MC converges to best mean-squared fit for the observed returns:

$$\sum_{k=1}^{K}\sum_{t=1}^{T_k}\left(G_t^k - v(S_t^k)\right)^2$$

For the example: $v(A) = 0$

Temporal Difference

TD converges to solution of maximum likelihood Markov model, given the observed data.

- Solution to the empirical MDP $(\mathcal{S}, \mathcal{A}, p, \gamma)$ that best fits the data
- In the AB example: $p(S_{t+1} = B | S_t = A) = 1$, and therefore $v(A) = v(B) = 0.75$

(Hasselt und Borsa 2021)

Detail: Temporal Difference Learning

TD(0) converges to solution of maximum likelihood Markov model

Solution to the MDP $\langle \mathcal{S}, \mathcal{A}, p, \gamma \rangle$ that best fits the data

$$p(s'|s,a) = \frac{1}{N(s,a)} \sum_{k=1}^{K} \sum_{t=1}^{T_k} \mathbb{1}(s_t^k, a_t^k, s_{t+1}^k = s, a, s')$$

$$r(s,a) = \frac{1}{N(s,a)} \sum_{k=1}^{K} \sum_{t=1}^{T_k} \mathbb{1}(s_t^k, a_t^k = s, a) r_t^k$$

In the AB example, $v(A) = 0.75$

(Silver 2015)

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