CS 181 Exam 1 Notesheet

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Linear Regression

Linear regression: We usually use L1 and L2 losses; L2 loss is more convenient since it is continuously differentiable.

- L2 loss has only a single solution to $\mathbf{w}$, while L1 loss may have many equivalent solutions.
- L2 loss is not robust to outliers, but L1 loss produces unstable solutions for which small dataset changes may induce large changes in weights.

With least-squares loss, let $\mathbf{X}$ the $N \times D$ data with row n containing $\mathbf{x}_n^\top$, and $\mathbf{Y}$ the target values. We optimize

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(y_n - \mathbf{w}^\top \mathbf{x}_n\right)^2 \implies \nabla\mathcal{L}(\mathbf{w}) = \sum_{n=1}^{N}\left(y_n - \mathbf{w}^\top\mathbf{x}_n\right)(-\mathbf{x}_n) = -\left(\mathbf{X}^\top\mathbf{y} - \mathbf{X}^\top\mathbf{X}\mathbf{w}\right) \implies \mathbf{w}^* = \left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{y}.$$

Classification

Linear classification with the perceptron algorithm: We fit a discriminant function with hinge loss. We classify ±1 depending on the sign of $h(\mathbf{w}, \mathbf{w})$, and we have hinge loss

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{N}\text{ReLU}\left(-h\left(\mathbf{x}_i, \mathbf{w}\right)y_i\right) = -\sum_{y_i \neq \hat{y}_i} h\left(\mathbf{x}_i, \mathbf{w}\right)y_i = -\sum_{y_i \neq \hat{y}_i}\mathbf{w}^\top\mathbf{x}_i y_i \quad \implies \quad \frac{\partial \mathcal{L}(\mathbf{w})}{\partial \mathbf{w}} = -\sum_{y_i \neq \hat{y}_i}\mathbf{x}_i y_i.$$

which we may optimize with SGD. In contrast to other losses,

- 0/1 loss is not differentiable, and does not more heavily penalize data points that are more poorly misclassified.
- Least squares loss penalizes points that are far from the decision boundary even if they are on the correct side.

Linear classification with logistic regression: The sigmoid $\sigma(z) = 1/(1+\exp(-z))$ compresses the outputs of our discrimant function (the reals) into probabilities. Then our loss is the negative log-likelihood,

$$p\left(y^* = C_1 \mid \mathbf{x}^*\right) = \sigma\left(\mathbf{w}^\top\mathbf{x}^*\right) \quad \implies \quad \mathrm{E}(\mathbf{w}) = -\ln p\left(\{y_i\} \mid \mathbf{w}\right) = -\sum_{i=1}^{N}\left\{y_i \ln \hat{y}_i + (1-y_i)\ln\left(1-\hat{y}_i\right)\right\}.$$

With multiple classes, we squash via $\text{softmax}_i(\mathbf{z}) = \exp(z_i)/\sum_k \exp(z_i)$, and assign to the class with highest probability.

Generative classification via class-conditional distributions: We model $p(y, \mathbf{x})$. To classify $\mathbf{x}^*$, we pick C_k maximizing the conditional density $p\left(y^* = C_k \mid \mathbf{x}^*\right) \propto p\left(\mathbf{x}^* \mid y^* = C_k\right)p\left(y^* = C_k\right)$. The class prior $p(y)$ is always categorical, and the MLE of $p\left(y = C_k\right) = \pi_k$ is the proportion of the dataset belonging to C_k. We may freely choose the shape of the class-conditional feature distributions $p(\mathbf{x} \mid y)$, and then calculate the MLE of the distributions' parameters.
In Naive Bayes, we make the simplification that our features are conditionally independent on class.

Model selection

Bias-variance trade-off: Consider model $f(\cdot)$. Denote $f_{\mathbf{D}}$ its fitting on random $\mathbf{D}$ and $\bar{f}(\cdot) = \mathrm{E}_{\mathbf{D}}\left[f_{\mathbf{D}}(\cdot)\right]$. Then

$$\text{MSE} = \mathrm{E}_{\mathbf{D}, y|\mathbf{x}}\left[\left(y - f_{\mathbf{D}}(\mathbf{x})\right)^2\right] = \mathrm{E}_{y|\mathbf{x}}\left[(y-\bar{y})^2\right] + (\bar{y} - \bar{f}(\mathbf{x}))^2 + \mathrm{E}_{\mathbf{D}}\left[\left(\bar{f}(\mathbf{x}) - f_{\mathbf{D}}(\mathbf{x})\right)^2\right] = \text{noise}(\mathbf{x}) + \text{bias}(f(\mathbf{x}))^2 + \text{var}(f(\mathbf{x})).$$

Increasing dataset size does not help bias, but does decrease variance because then we have more information to learn the data distribution (reducing overfitting). Difference between train/test performance indicates variance issues.

Regularization: A convoluted overfit line won't generalize well, so we penalize the size of our weights to favor simple regression lines that focus on the most important basis functions. In linear regression settings, we introduce parameter λ

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\left(y_n - \mathbf{w}^\top\boldsymbol{\phi}_n\right)^2 + \frac{\lambda}{h}\|\mathbf{w}\|_h^h$$

- Ridge regression: We punish any individual weight from growing too large, yielding generally moderate solutions.
- Lasso: By using L1 norm, lasso yields sparser solutions by driving less informative parameters w_i to zero.

(Cross-)validation: Lets us (1) select models, and (2) tune regularization parameters to reduce overfitting. The optional cross part helps get evaluations less dependent on our training data.

NNs and SVMs

Neural nets: Hidden nodes are activations, given by a weighted sum of connected preceding nodes plus some bias term. Activations are transformed by a non-linear activation function and passed forward. In doing so, the basis transformations made by the neural network are updated along as we update the weights. Common NN losses are L2 loss for regression, and negative log-likelihood (with sigmoid or softmax) for classification. We update weights by backpropagating; output layer should not have ReLU activation since if values are mostly negative, gradients will fail to backpropagate. Activations: sigmoid ensures weights never go to infinity, tanh $\phi(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$ yields steeper gradients around 0 and is centered at 0; non-negative ouput may limit expressivity.

Hard max-margin formulation: We assume the data is linearly separable for binary classification. We classify $\mathbf{x}^*$ into classes ± 1 depending on the sign of our discriminant function, which determines some hyperplane

$$h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0 \qquad \mathbf{w}^\top \mathbf{x} + w_0 = 0.$$

Note $\mathbf{w}$ is orthogonal to the hyperplane, letting us calculate the signed distance d between $\mathbf{x}$ and the hyperplane.

$$\mathbf{x} = \mathbf{x}_p + d\frac{\mathbf{w}}{\|\mathbf{w}\|_2} \quad \Longrightarrow \quad d = \frac{\mathbf{w}^\top \mathbf{x} + w_0}{\|\mathbf{w}\|_2}.$$

The margin of the dataset is the least margin of any data point, and we may scale $\mathbf{w}, w_0$ appropriately to enforce the margin boundary $y_n\left(\mathbf{w}^\top \mathbf{x}_n + w_0\right) = 1$, so our problem is

$$y_n\left(\mathbf{w}^\top \mathbf{x}_n + w_0\right) \geq 1 \ \forall n \quad \Longrightarrow \quad \min_{\mathbf{w}, w_0} \frac{1}{2}\|\mathbf{w}\|_2^2 \quad \text{such that} \quad y_n\left(\mathbf{w}^\top \mathbf{x}_n + w_0\right) \geq 1 \forall n$$

Soft-margin formulation: We allow some data points to be within the margin boundary or on the incorrect side of the hyperplane, introducing slack variables $\xi_n \geq 0$ that give us the soft-margin training problem:

$$\xi_n = \begin{cases} = 0 & \text{if } \mathbf{x}_n \text{ is correctly classified,} \\ \in (0, 1] & \text{if } \mathbf{x}_n \text{ is correct but inside the margin,} \\ > 1 & \text{if } \mathbf{x}_n \text{ is incorrectly classified.} \end{cases}$$

$$\min_{\mathbf{w}, w_0} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N} \xi_n \quad \text{such that} \quad y_n\left(\mathbf{w}^\top \mathbf{x}_n + w_0\right) \geq 1 - \xi_n \ \forall n \qquad \text{and} \qquad \xi_n \geq 0 \ \forall n.$$

Here, the regularization parameter C determines how heavily we penalize violations of the hard margin constraints; large C yields less regularization, prioritizes less misclassifications, and favors flatter boundaries. Small C yields more regularization and behaves oppositely.

Dual formulation: The above problem formulations depend on the feature dimension, but the equivalent dual formulation only depends linearly on the dataset size N. We optimize the Lagrangian function with our margin inequalities as constraints, but introduce a subproblem on the multipliers $\boldsymbol{\alpha}$ to enforce the inequality part of our hard-margin constraint:

$$\min_{w, w_0}\left[\max_{\alpha}\left[\frac{1}{2}\|w\|_2^2 - \sum_{n=1}^{w} \alpha_n\left(y_n\left(w^\top x_n + w_0\right) - 1\right)\right]\right] \quad \text{such that} \quad \alpha_n \geq 0.$$

This encodes our hard margin constraint because if $\mathbf{w}$ violates any of our constraints, then the subproblem on $\boldsymbol{\alpha}$ becomes unbounded, with α_n on the corresponding constraints driven arbitrarily large. If all constraints are met, then $g_n(\mathbf{w}) < 0$ and thus $\alpha_n = 0$ for all n, yielding $\alpha_n g_n(\mathbf{w}) = 0$, as desired. Also using strong duality conditions, we have

$$\min_{\mathbf{w}}\left[\max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} L(\mathbf{w}, w_0, \boldsymbol{\alpha})\right] = \min_{\mathbf{w}, w_0}\left[\max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0} \frac{1}{2}\mathbf{w}^\top \mathbf{w} - \sum_{n} \alpha_n\left(y_n\left(\mathbf{w}^\top \mathbf{x}_n + w_0\right) - 1\right)\right] \quad \Longrightarrow \quad \max_{\boldsymbol{\alpha}, \boldsymbol{\alpha} \geq 0}\left[\min_{\mathbf{w}, w_0} L\left(\mathbf{w}, \boldsymbol{\alpha}, w_0\right)\right].$$

To solve this, we begin with the inner minimization problem, solving for $\mathbf{w}$ and w_0 in terms of $\boldsymbol{\alpha}$,

$$\nabla L\left(\mathbf{w}, \boldsymbol{\alpha}, w_0\right) = \mathbf{w} - \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n = 0 \qquad \frac{\partial}{\partial w_0} L\left(\mathbf{w}, \boldsymbol{\alpha}, w_0\right) = -\sum_{n=1}^{N} \alpha_n y_n = 0.$$

We do not actually a value for w_0, but another constraint on $\boldsymbol{\alpha}$. Substituting $\mathbf{w}^*$, we want to optimize the Lagrangian $L\left(\mathbf{w}, \boldsymbol{\alpha}, w_0\right)$ with some constraints, with everything entirely in terms of $\boldsymbol{\alpha}$:

$$\max_{\boldsymbol{\alpha}}\left[\sum_{n} \alpha_n - \frac{1}{2}\sum_{n, n'} \alpha_n \alpha_{n'} y_n y_{n'} \mathbf{x}_n^\top \mathbf{x}_{n'}\right] \quad \text{such that} \quad \sum_{n} \alpha_n y_n = 0, \alpha_n \geq 0 \ \forall n,$$

so we have a (convex) quadratic programming problem which we can solve for the optimal $\boldsymbol{\alpha}$. Note most of the α_i will be 0; the data points corresponding to non-zero α_i are *support vectors*, and they are the only data points informing our decision boundary so the rest can be discarded. Support vectors must be points on the margin boundary (or inside the margins or misclassified, for soft-margin). Support vectors have distance $1/\|\mathbf{w}\|_2$.

We make predictions by substituting our optimal weights $h(\mathbf{x}) = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n^\top \mathbf{x} + w_0$, and we solve for w_0 with any point $\mathbf{x}$ on the margin boundary, recognizing that $y_n\left(\mathbf{w}^\top \mathbf{x}_n + w_0\right) = 1$. To choose a point on the margin boundary, we find any example with $\alpha_i > 0$ (or for soft-margin, any with $C > \alpha_n > 0$.)

CS 181 Exam 2 Notesheet

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Clustering, Mixture Models, PCA

K-Means: Initialize centroids by selecting data points either randomly or proportionally to the squared distance from the closest cluster center (K-Means++). Then iteratively assign points to clusters and update the centroids until convergence.

- **Lloyd's:** For L2 distance, define the loss as the sum of squared distances to the cluster centers, denoted using one-hot responsibility vectors $\mathbf{r}_n$. Then the optimal centroids are the average of their data points:

$$\mathcal{L}\left(\mathbf{X}, \{\boldsymbol{\mu}\}_{c=1}^{C}, \{\mathbf{r}\}_{n=1}^{N}\right) = \sum_{n=1}^{N}\sum_{c=1}^{C} r_{nc}\left\|\mathbf{x}_n - \boldsymbol{\mu}_c\right\|_2^2 \implies \frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}_c} = -2\sum_{n=1}^{N} r_{nc}\left(\mathbf{x}_n - \boldsymbol{\mu}_c\right) \implies \boldsymbol{\mu}_c = \frac{\sum_{n=1}^{N} r_{nc}\mathbf{x}_n}{\sum_{n=1}^{N} r_{nc}}$$

- **K-Medioids:** For categorical data, we update centroids to the median since the mean may not make sense.
- **Number of clusters:** Loss strictly decreases with number of clusters C; we choose C to be the "elbow."

HAC: Beginning with N clusters for each data point, merge clusters via an intercluster distance metric (linkage criterion).

Mixture models: We wish to fit $\boldsymbol{\theta}$, the parameter for our categorical prior, and $\{\mathbf{w}_k\}_{k=1}^{K}$, the parameters for our class-conditional distributions. The complete-data log-likelihood is

$$\log L\left(\boldsymbol{\theta}, \{\beta_n\}_{k=1}^{K}\right) = \sum_{n=1}^{N} \log\left(\prod_{k=1}^{K} p\left(x_n \mid \mathbf{z}_n = C_k\right)^{I(\mathbf{z}_n = C_k)} \theta_k^{I(\mathbf{z}_n = C_k)}\right) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk}\left(\log\theta_k + \log p\left(x_n \mid \mathbf{z}_n = C_k\right)\right),$$

and we optimize our parameters iteratively with EM. In the E-step, we calculate for each data point $\mathbf{q_n} = \mathbb{E}\left[z_n \mid x_n\right]$, with $q_{nk} \propto p\left(\mathbf{x}_n \mid \mathbf{z}_n = C_k; \mathbf{w}\right) p\left(\mathbf{z}_n = C_k; \boldsymbol{\theta}\right)$. We then update our parameters to maximize the expected likelihood.

ELBO: For q some other distribution on $\mathbf{z}$, we have

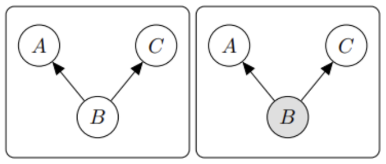
$$\sum_{n=1}^{N} \log\left[\sum_{k=1}^{K} p\left(\mathbf{x}_n \mid \mathbf{z}_n = C_k; \boldsymbol{\theta}, \mathbf{w}\right) p\left(\mathbf{z}_n = C_k \mid \boldsymbol{\theta}, \mathbf{w}\right)\right] = \sum_{n=1}^{N} \log \mathrm{E}_{\mathbf{z}_n \sim q(\mathbf{z}_n)}\left[\frac{p\left(\mathbf{x}_n \mid \mathbf{z}_n; \boldsymbol{\theta}, \mathbf{w}\right) p\left(\mathbf{z}_n \mid \boldsymbol{\theta}, \mathbf{w}\right)}{q\left(\mathbf{z}_n\right)}\right],$$

which by Jensen's is greater than the ELBO (in which we pass the log above into the expectation). So in EM, we choose q maximizing ELBO$(\mathbf{w}, q \mid \mathbf{x})$, keeping the bound tight, and then choose parameters maximizing the ELBO.

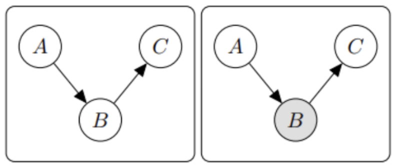
PCA: For mean-centered $\mathbf{X}$, the PCs are the eigenvectors of the empirical covariance matrix $\mathbf{S} = \frac{1}{N}\mathbf{X}\mathbf{X}^\top$. To calculate these, the SVD of a matrix is $\mathbf{X} = \mathbf{U}\mathbf{Z}\mathbf{V}^\top$, where $\mathbf{Z}$ is diagonal and $\mathbf{U}, \mathbf{V}$ are orthogonal (i.e., orthonormal columns). Then eigenvalues of $\mathbf{S}$ are the entries of $\frac{1}{N}\mathbf{Z}^2$, and the columns of $\mathbf{U}$ are the corresponding eigenvectors.

Bayesian networks & HMMs

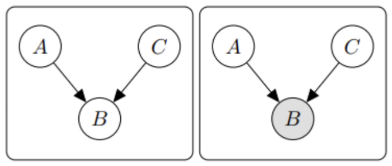
$A \not\perp C \to B$ observed $\to A \perp C$



$A \not\perp C \to B$ observed $\to A \perp C$



$A \perp C \to B$ observed $\to A \not\perp C$



HMM setup: We have N sequences of one-hot emissions, each of form $\mathbf{x}_1, \ldots, \mathbf{x}_n$, with corresponding one-hot latent states $\mathbf{s}_1, \ldots, \mathbf{s}_n$. There are K possible states and M possible observations. We model the joint distribution

$$p\left(\mathbf{s}_1, \ldots, \mathbf{s}_n, \mathbf{x}_1, \ldots, \mathbf{x}_n\right) = p\left(\mathbf{s}_1, \ldots, \mathbf{s}_n\right) p\left(\mathbf{x}_1, \ldots, \mathbf{x}_n \mid \mathbf{s}_1, \ldots, \mathbf{s}_n\right) = p\left(\mathbf{s}_1; \boldsymbol{\theta}\right) \prod_{t=1}^{n-1} p\left(\mathbf{s}_{t+1} \mid \mathbf{s}_t; \mathbf{T}\right) \prod_{t=1}^{n} p\left(\mathbf{x}_t \mid \mathbf{s}_t; \boldsymbol{\pi}\right).$$

We parameterize the categorical prior for $\mathbf{s}_1$ with $\boldsymbol{\theta} \in [0,1]^K$, the transition matrix with $\mathbf{T} \in [0,1]^{K \times K}$ where $T_{i,j}$ is the transition from i to j, and the state-conditional distribution of observations with $\boldsymbol{\pi} \in [0,1]^{K \times M}$.

Forward-backward algorithm: Factor $p\left(\mathbf{x}_1, \ldots, \mathbf{x}_n, \mathbf{s}_t\right) = p\left(\mathbf{x}_1, \ldots, \mathbf{x}_t, \mathbf{s}_t\right) p\left(\mathbf{x}_{t+1}, \ldots, \mathbf{x}_n \mid s_t\right) = \alpha_t(\mathbf{s}_t)\beta_t(\mathbf{s}_t)$, with

$$\alpha_t\left(\mathbf{s}_t\right) = \begin{cases} p\left(\mathbf{x}_1 \mid \mathbf{s}_1\right) p\left(\mathbf{s}_1\right) & \text{if } t = 1, \text{ else} \\ p\left(\mathbf{x}_t \mid \mathbf{s}_t\right) \sum_{\mathbf{s}_{t-1}} p\left(\mathbf{s}_t \mid \mathbf{s}_{t-1}\right) \alpha_{t-1}\left(\mathbf{s}_{t-1}\right). \end{cases} \qquad \beta_t\left(\mathbf{s}_t\right) = \begin{cases} 1 \text{ if } t = n, \text{ else} \\ \sum_{\mathbf{s}_{t+1}} p\left(\mathbf{s}_{t+1} \mid \mathbf{s}_t\right) p\left(\mathbf{x}_{t+1} \mid \mathbf{s}_{t+1}\right) \beta_{t+1}\left(\mathbf{s}_{t+1}\right). \end{cases}$$

After calculating all α_t and β_t, we can perform inference tasks by marginalizing (summing) over possible $\mathbf{s}_t$ or $\mathbf{s}_{t-1}$.

Viterbi: Let γ_t the likelihood of the observations if the current state is $\mathbf{s}_t$ and we already maximized over $\mathbf{s}_1, \ldots, \mathbf{s}_{t-1}$,

$$\gamma_t\left(\mathbf{s}_t\right) = \max_{\mathbf{s}_1, \ldots, \mathbf{s}_{t-1}} p\left(\mathbf{s}_1, \ldots, \mathbf{s}_t, \mathbf{x}_1, \ldots, \mathbf{x}_t\right) = \begin{cases} p\left(\mathbf{x}_1 \mid \mathbf{s}_1\right) p\left(\mathbf{s}_1\right) \text{if } t = 1, \text{ else} \\ p\left(\mathbf{x}_t \mid \mathbf{s}_t\right) \max_{\mathbf{s}_{t-1}} p\left(\mathbf{s}_t \mid \mathbf{s}_{t-1}\right) \gamma_{t-1}\left(\mathbf{s}_{t-1}\right). \end{cases}$$

To find the optimal path, we then choose $\mathbf{s_t}$ maximizing γ_t, and $\mathbf{s}_{t-1}$ maximizing $p\left(\mathbf{s}_t \mid \mathbf{s}_{t-1}\right)\gamma_{t-1}\left(\mathbf{s}_{t-1}\right)$, and so on.

Fitting HMM parameters with EM: We randomly initialize $\boldsymbol{\theta}, \mathbf{T}, \boldsymbol{\pi}$. For our current values, we compute α- and β-values using Forward-Backward. Then we compute $\{\mathbf{q}_i\}_{i=1}^n$ with $q_{t,k}^i = p\left(\mathbf{s}_t^i = k \mid \mathbf{x}_1^i, \ldots, \mathbf{x}_n^i\right)$, and $\{\mathbf{Q}_{t,t+1}^i\}_{i=1}^n$ with $Q_{t,t+1,k,\ell}^i = p\left(\mathbf{s}_t^i = k, \mathbf{s}_{t+1}^i = \ell \mid \mathbf{x}_1^i, \ldots, \mathbf{x}_n^i\right)$. This yields

$$\mathbb{E}_{\mathbf{s}^i}\left[\ln\left(p\left(\mathbf{x}^i, \mathbf{s}^i\right)\right)\right] = \sum_{k=1}^K q_{1k}^i \ln\theta_k + \sum_{t=1}^{n-1}\sum_{k=1}^K\sum_{\ell=1}^K Q_{t,t+1,k,\ell}^i \ln T_{k,l} + \sum_{t=1}^n\sum_{k=1}^K q_{t,k}^i \sum_{m=1}^M x_{t,m}^i \ln\pi_{k,m}$$

$$\implies \theta_k = \frac{\sum_{i=1}^N q_{1,k}^i}{N} \qquad T_{k,l} = \frac{\sum_{i=1}^N\sum_{t=1}^{n-1} Q_{t,t+1,k,l}^i}{\sum_{i=1}^N\sum_{t=1}^{n-1} q_{t,k}^i} \qquad \pi_{k,m} = \frac{\sum_{i=1}^N\sum_{t=1}^n q_{t,k}^i x_{t,m}^i}{\sum_{i=1}^N\sum_{t=1}^n q_{t,k}^i}$$

MDPs & Model-Free RL

Our environment has states S, actions A, reward function $r : S \times A \to [0,1]$, and transition model $p(s' \mid s,a)$. If known, we have an MDP and can both evaluate policies and learn the optimal policy π^*. If unknown, we must find π^* with RL.

Finite time horizon MDP: Let $V_T^\pi(s)$ be the expected total reward in T timesteps following π. Then for any π,

$$V_T^\pi(s) = \mathbb{E}_{s_1,\ldots,s_T}\left[\sum_{t=0}^T r\left(s_t, \pi_{(T-t)}\left(s_t\right)\right)\right] = \begin{cases} r\left(s, \pi_{(1)}(s)\right) & \text{if } t=1 \\ r\left(s, \pi_{(t)}(s)\right) + \sum_{s'\in S} p\left(s' \mid s, \pi_{(t)}(s)\right) V_{(t-1)}^\pi\left(s'\right) & \text{otherwise}\end{cases}$$

where $\pi_{(t)}$ is the policy with t timesteps left. In $O\left(|S|^2|A|T\right)$, value iteration finds the optimal policy by taking at each timestep the action maximizing the expected sum of our immediate reward and expected future reward:

$$\pi_{(1)}^*(s) = \arg\max_a[r(s,a)] \qquad \pi_{(t+1)}^*(s) = \arg\max_a\left[r(s,a) + \sum_{s'\in\mathcal{S}} p\left(s' \mid s,a\right) V_{(t)}^*\left(s'\right)\right]$$

Infinite horizon MDP: With $T \to \infty$, we evaluate a policy π by solving a system of Bellman consistency equations,

$$V^\pi(s) \coloneqq \mathbb{E}_{s_1,s_2,\ldots}\left[\sum_{t=0}^\infty \gamma^t r\left(s_t, \pi\left(s_t\right)\right)\right] \qquad V^\pi(s) = r(s,\pi(s)) + \gamma\sum_{s'\in S} p\left(s' \mid s, \pi(s)\right) V^\pi\left(s'\right).$$

Alternatively, we may find V^π by initializing $V(s)=0, \forall s$, and then iteratively updating $V \leftarrow V'$ with

$$V'(s) = r(s,\pi(s)) + \gamma\sum_{s'\in S} p\left(s' \mid s,\pi(s)\right) V\left(s'\right), \forall s \qquad \text{until} \qquad \Delta = \max\left(|V'(s) - V(s)|\right).$$

- **Value iteration:** To find π^*, we first calculate V^* by initializing $V(s)=0, \forall s$, and then iteratively updating

$$V \leftarrow V' \qquad \text{where} \qquad V'(s) = \max_{a\in A}\left[r(s,a) + \gamma\sum_{s'\in S} p\left(s' \mid s,a\right) V\left(s'\right)\right], \forall s$$

  until convergence. Then note that $V^* \triangleq V^{\pi^*}$ and that V^* satisfies Bellman optimality, so we find π^* to be

$$V^*(s) = \max_{a\in A}\left[r(s,a) + \gamma\sum_{s'\in S} p\left(s' \mid s,a\right) V^*\left(s'\right)\right] \implies \pi^*(s) = \arg\max_{a\in A}\left[r(s,a) + \gamma\sum_{s'\in S} p\left(s' \mid s,a\right) V^*\left(s'\right)\right]$$

- **Policy iteration:** Beginning with some π, we iteratively evaluate V^π (E-step) and improve π (I-step) by the update

$$\pi'(s) \leftarrow \arg\max_{a\in A}\left[r(s,a) + \gamma\sum_{s'\in S} p\left(s' \mid s,a\right) V^\pi\left(s'\right)\right], \quad \forall s \qquad \text{until } \pi \text{ converges}$$

  Policy iteration takes more computation per iteration, but tends to converge faster in practice.

Value-based methods: We try to learn optimal Q-values, which determine our optimal policy.

$$Q^*(s,a) \coloneqq r(s,a) + \gamma\sum_{s'\in S} p\left(s' \mid s,a\right) V^*\left(s'\right), \forall s,a \qquad \implies \qquad \pi^*(s) = \arg\max_a\ Q^*(s,a),$$

- **SARSA (on-policy):** Given an experience (s,a,r,s',a'), where a' is chosen by an ϵ-greedy method, we update

$$\pi(s) = \begin{cases}\text{argmax}_a\, Q(s,a) & \text{with probability } 1-\epsilon \\ \text{random} & \text{with probability } \epsilon\end{cases} \qquad Q(s,a) \leftarrow Q(s,a) + \alpha_t\left[r + \gamma Q\left(s',a'\right) - Q(s,a)\right],\ \alpha_t \in [0,1]$$

- **Q-learning (off-policy):** We update using observations (s,a,r,s'), intuitively performing SGD to bring our Q-values closer to satisfying the Bellman condition,

$$Q^*(s,a) = r(s,a) + \gamma\sum_{s'\in S} p\left(s' \mid s,a\right) \max_{a'\in A}\left[Q^*\left(s',a'\right)\right], \forall s,a \qquad Q(s,a) \leftarrow Q(s,a) + \alpha_t\left[r + \gamma\max_{a'} Q\left(s',a'\right) - Q(s,a)\right]$$

Policy learning (on-policy): We parameterize the policy space with a finite-dimensional parameter space, such that π_θ is the policy associated to parameter θ. Then we may update θ with SGD to find the optimal policy.