6.86x Machine Learning with Python

This is a cheat sheet for machine learning based on the online course given by Prof. Tommi Jaakkola and Prof. Regina Barzilay. Compiled by Janus B. Advincula.

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Linear Classifiers

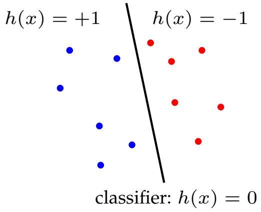
Introduction to Machine Learning

What is machine learning? Machine learning as a discipline aims to design, understand and apply computer programs that learn from experience (i.e., data) for the purpose of modeling, prediction or control.

Types of Machine Learning

- **Supervised learning:** prediction based on examples of correct behavior
- **Unsupervised learning:** no explicit target, only data, goal is to model/discover
- **Semi-supervised learning:** supplement limited annotations with unsupervised learning
- **Active learning:** learn to query the examples actually needed for learning
- **Transfer learning:** how to apply what you have learned from A to B
- **Reinforcement learning:** learning to act, not just predict; goal is to optimize the consequences of actions

Linear Classifier and Perceptron



Key Concepts

- **feature vectors, labels:**

$$x \in \mathbb{R}^d, \quad y \in \{-1, +1\}$$

- **training set:**

$$S_n = \left\{ \left(x^{(i)}, y^{(i)} \right), i = 1, \ldots, n \right\}$$

- **classifier:**

$$h : \mathbb{R}^d \to \{-1, +1\}$$
$$\chi^+ = \left\{ x \in \mathbb{R}^d : h(x) = +1 \right\}$$
$$\chi^- = \left\{ x \in \mathbb{R}^d : h(x) = -1 \right\}$$

- **training error:**

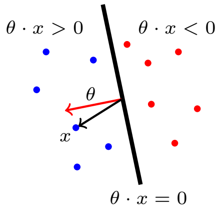
$$\mathcal{E}_n(h) = \frac{1}{n} \sum_{i=1}^{n} \left[\left[h\left(x^{(i)}\right) \neq y^{(i)} \right]\right]$$

$$\left[\left[h\left(x^{(i)}\right) \neq y^{(i)} \right]\right] = \begin{cases} 1 & \text{if error} \\ 0 & \text{otherwise} \end{cases}$$

- **test error:** $\mathcal{E}(h)$
- **set of classifiers:** $h \in \mathcal{H}$

Linear Classifiers through the Origin We consider functions of the form

$$h(x; \theta) = \text{sign}\left(\theta_1 x_1 + \cdots + \theta_d x_d\right) = \text{sign}\left(\theta \cdot x\right).$$



Linear Classifiers with Offset We can consider functions of the form

$$h(x; \theta) = \text{sign}\left(\theta \cdot x + \theta_0\right)$$

where θ_0 is the offset parameter.

Linear Separation Training examples S_n are *linearly separable* if there exists a parameter vector $\widehat{\theta}$ and offset parameter $\widehat{\theta}_0$ such that $y^{(i)} \left(\widehat{\theta} \cdot x^{(i)} + \widehat{\theta}_0 \right) > 0$ for all $i = 1, \ldots, n$.

Training Error The training error for a linear classifier is

$$\mathcal{E}_n\left(\theta, \theta_0\right) = \frac{1}{n} \sum_{i=1}^{n} \left[\left[y^{(i)} \left(\theta \cdot x^{(i)} + \theta_0 \right) \leq 0 \right]\right].$$

Perceptron Algorithm

```
procedure PERCEPTRON$\left(\{(x^{(i)}, y^{(i)}), i = 1, \ldots, n\}, T\right)$
    $\theta = 0$ (vector)
    for $t = 1, \ldots, T$ do
        for $i = 1, \ldots, n$ do
            if $y^{(i)} \left( \theta \cdot x^{(i)} \right) \leq 0$ then
                $\theta = \theta + y^{(i)} x^{(i)}$
    return $\theta$
```

Perceptron Algorithm (with offset)

```
procedure PERCEPTRON$\left(\{(x^{(i)}, y^{(i)}), i = 1, \ldots, n\}, T\right)$
    $\theta = 0$ (vector)
    for $t = 1, \ldots, T$ do
        for $i = 1, \ldots, n$ do
            if $y^{(i)} \left( \theta \cdot x^{(i)} + \theta_0 \right) \leq 0$ then
                $\theta = \theta + y^{(i)} x^{(i)}$
                $\theta_0 = \theta_0 + y^{(i)}$
    return $\theta, \theta_0$
```

Convergence Assumptions:

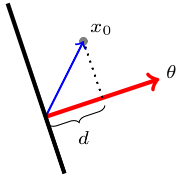
- There exists θ^* such that $\frac{y^{(i)} \left(\theta^* \cdot x^{(i)} \right)}{\left\| x^{(i)} \right\|} \geq \gamma$ for all $i = 1, \ldots, n$ for some $\gamma > 0$.
- All examples are bounded $\left\| x^{(i)} \right\| \leq R$, $i = 1, \ldots, n$.

Then the number k of updates made by the perceptron algorithm is bounded by $\frac{R^2}{\gamma^2}$.

Hinge Loss, Margin Boundaries and Regularization

Distance from a Line to a Point The perpendicular distance from a line with equation $\theta \cdot x + \theta_0 = 0$ to a point with coordinates x_0 is

$$d = \frac{\left| \theta \cdot x_0 + \theta_0 \right|}{\|\theta\|}$$

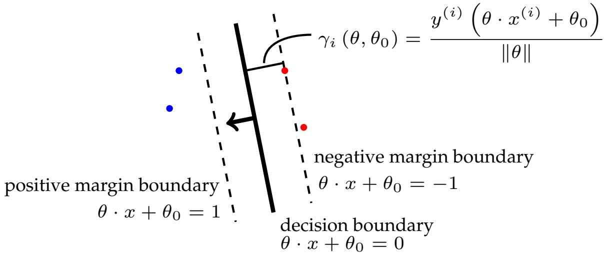


Decision Boundary The decision boundary is the set of points x which satisfy

$$\theta \cdot x + \theta_0 = 0.$$

Margin Boundary The margin boundary is the set of points x which satisfy

$$\theta \cdot x + \theta_0 = \pm 1.$$


$\gamma_i\left(\theta, \theta_0\right) = \frac{y^{(i)} \left(\theta \cdot x^{(i)} + \theta_0 \right)}{\|\theta\|}$
negative margin boundary
$\theta \cdot x + \theta_0 = -1$
positive margin boundary
$\theta \cdot x + \theta_0 = 1$
decision boundary
$\theta \cdot x + \theta_0 = 0$

Hinge Loss

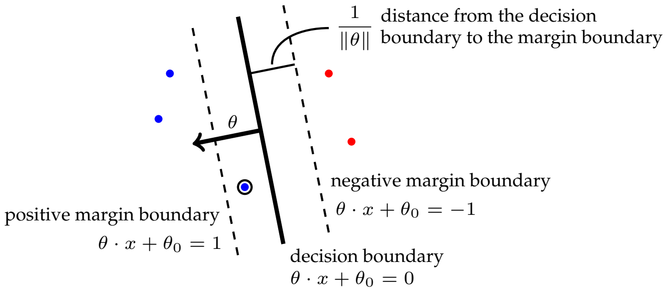
$$\text{Loss}_h\left(z\right) = \begin{cases} 0 & \text{if } z \geq 1 \\ 1 - z & \text{if } z < 1 \end{cases}$$

with $z = y^{(i)} \left(\theta \cdot x^{(i)} + \theta_0 \right)$.

Regularization Maximize margin

$$\max \frac{1}{\|\theta\|} \quad \Rightarrow \quad \min \frac{1}{2} \|\theta\|^2$$

Linear Classification and Generalization


$\frac{1}{\|\theta\|}$ distance from the decision boundary to the margin boundary
θ
negative margin boundary
$\theta \cdot x + \theta_0 = -1$
positive margin boundary
$\theta \cdot x + \theta_0 = 1$
decision boundary
$\theta \cdot x + \theta_0 = 0$

Objective function

$$J\left(\theta, \theta_0\right) = \frac{1}{n} \sum_{i=1}^{n} \left[\text{Loss}_h \left(y^{(i)} \left(\theta \cdot x^{(i)} + \theta_0 \right) \right) + \frac{\lambda}{2} \|\theta\|^2 \right]$$

λ is the regularization factor.

Stochastic Gradient Descent Select $i \in \{1, \dots, n\}$ at random

$$\theta \quad \leftarrow \quad \theta - \eta_t \nabla_\theta \left[\text{Loss}_h \left(\theta \cdot x^{(i)} + \theta_0 \right) + \frac{\lambda}{2} \|\theta\|^2 \right]$$

η_t is the learning rate which can vary at every iteration.

Support Vector Machine

- Support Vector Machine finds the maximum margin linear separator by solving the quadratic program that corresponds to $J(\theta, \theta_0)$
- In the realizable case, if we disallow any margin violations, the quadratic program we have to solve is:

  Find θ, θ_0 that minimize $\frac{1}{2}\|\theta\|^2$ subject to

  $$y^{(i)} \left(\theta \cdot x^{(i)} + \theta_0 \right) \geq 1, \quad i = 1, \dots, n$$

Nonlinear Classification, Linear Regression, Collaborative Filtering

Linear Regression

Empirical Risk

$$R_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2} \left(y^{(i)} - \theta \cdot x^{(i)} \right)^2 \qquad \text{squared error}$$

Gradient-based Approach We can use stochastic gradient descent to find the minima of the empirical risk.

Algorithm Initialize $\theta = 0$.
Randomly pick $i = \{1, \dots, n\}$.
$\theta = \theta + \eta \left(y^{(i)} - \theta \cdot x^{(i)} \right) x^{(i)}$.

η is the learning rate.

Closed Form Solution Let

$$A = \frac{1}{n} \sum_{i=1}^{n} x^{(i)} \left(x^{(i)} \right)^\intercal \quad \text{and} \quad B = \frac{1}{n} \sum_{i=1}^{n} y^{(i)} x^{(i)}.$$

Then,

$$\widehat{\theta} = A^{-1} B.$$

In matrix notation, this is

$$\widehat{\theta} = (\mathbb{X}^\intercal \mathbb{X})^{-1} \mathbb{X}^\intercal \mathbb{Y}.$$

Generalization and Regularization

Ridge Regression: The loss function is

$$J_{\lambda, n} = \frac{\lambda}{2} \|\theta\|^2 + R_n(\theta)$$

where λ is the regularization factor. We can find its minima using gradient-based approach.

Algorithm Initialize $\theta = 0$.
Randomly pick $i = \{1, \dots, n\}$.
$\theta = (1 - \eta\lambda)\theta + \eta \left(y^{(i)} - \theta \cdot x^{(i)} \right) x^{(i)}$.

Nonlinear Classification

Feature Transformation

$$x \mapsto \phi(x)$$
$$\theta \cdot x \rightarrow \theta' \cdot \phi(x)$$

Non-linear Classification

$$h(x; \theta, \theta_0) = \text{sign}(\theta \cdot \phi(x) + \theta_0)$$

Kernel Function A kernel function is simply an inner product between two feature vectors. Using kernels is advantageous when the inner products are faster to evaluate than using explicit vectors (e.g., when the vectors would be infinite dimensional).

$$K(x, x') = \phi(x) \cdot \phi(x')$$

Perceptron

```
$\theta = 0$
for $i = 1, \dots, n$ do
    if $y^{(i)} \theta \cdot \phi\left(x^{(i)}\right) \leq 0$ then
        $\theta \leftarrow \theta + y^{(i)} \phi\left(x^{(i)}\right)$
```

This algorithm gives

$$\theta = \sum_{j=1}^{n} \alpha_j y^{(j)} \phi\left(x^{(j)}\right)$$

where α_j is the number of mistakes. For the offset parameter, we get

$$\theta_0 = \sum_{j=1}^{n} \alpha_j y^{(j)}.$$

Kernel Perceptron Algorithm We can reformulate the perceptron algorithm so that we initialize and update α_j's, instead of θ.

$$\theta \cdot \phi\left(x^{(i)}\right) = \sum_{j=1}^{n} \alpha_j y^{(j)} \underbrace{\phi\left(x^{(j)}\right) \cdot \phi\left(x^{(i)}\right)}_{K\left(x^{(j)}, x^{(i)}\right)}$$

```
procedure KERNEL PERCEPTRON($\{(x^{(i)}, y^{(i)}), i = 1, \dots, n\}, T$)
    Initialize $\alpha_1, \dots, \alpha_n$ to some values
    for $t = 1, \dots, T$ do
        for $i = 1, \dots, n$ do
            if $y^{(i)} \sum_{j=1}^{n} \alpha_j y^{(j)} K\left(x^{(j)}, x^{(i)}\right) \leq 0$ then
                $\alpha_j = \alpha_j + 1$
```

The initilization $\theta = 0$ is equivalent to $\alpha_1 = \dots = \alpha_n = 0$.

Composition rules:

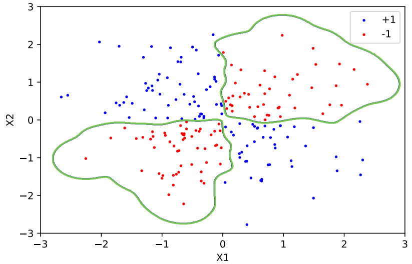
1. $K(x, x') = 1$ is a kernel function.
2. Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and $K(x, x')$ is a kernel. Then so is $\widetilde{K}(x, x') = f(x)K(x, x')f(x')$
3. If $K_1(x, x')$ and $K_2(x, x')$ are kernels, then $K(x, x') = K_1(x, x') + K_2(x, x')$ is a kernel.
4. If $K_1(x, x')$ and $K_2(x, x')$ are kernels, then $K(x, x') = K_1(x, x')K_2(x, x')$ is a kernel.

Decision Boundary The decision boundary satisfies

$$\sum_{j=1}^{n} \alpha_j y^{(j)} K\left(x^{(j)}, x\right) = 0.$$

Radial Basis Kernel

$$K(x, x') = \exp\left(-\frac{1}{2} \|x - x'\|^2 \right)$$



Other non-linear classifiers

- We can get non-linear classifiers or regression methods by simply mapping examples into feature vectors non-linearly, and applying a linear method on the resulting vectors.
- These feature vectors can be high dimensional.
- We can turn the linear methods into kernel methods by casting the computations in terms of inner products.

Recommender Systems

Problem Description We are given a matrix where each row corresponds to a user's rating of movies, for example, and each column corresponds to the user ratings for a particular movie. It can also be product ratings, etc. This matrix will be very sparse. The goal is to predict user ratings for those movies that are yet to be rated.

$$\begin{array}{cc} & m \text{ movies} \\ n \text{ users} & \begin{pmatrix} & & \\ & Y_{ai} & \\ & & \end{pmatrix} \end{array}$$

***K*-Nearest Neighbor Method** The K-Nearest Neighbor method makes use of ratings by K other *similar* users when predicting Y_{ai}. Let KNN(a) be the set of K users *similar to* user a, and let sim(a, b) be a **similarity measure** between users a and $b \in$ KNN(a). The KNN method predicts a rating Y_{ai} to be

$$\widehat{Y}_{ai} = \frac{\sum_{b \in \text{KNN}(a)} \text{sim}(a, b) Y_{bi}}{\sum_{b \in \text{KNN}(a)} \text{sim}(a, b)}$$

The similarity measure sim(a, b) could be any distance function between the feature vectors x_a and x_b.

- Euclidean distance: $\|x_a - x_b\|$
- Cosine similarity: $\cos\theta = \dfrac{x_a \cdot x_b}{\|x_a\| \|x_b\|}$

Collaborative Filtering Our goal is to come up with a matrix X that has no blank entries and whose $(a, i)^{\text{th}}$ entry X_{ai} is the prediction of user a's rating to movie i. Let D be the set of all (a, i)'s for which a user rating Y_{ai} exists. A naive approach is to minimize the objective function

$$J(X) = \sum_{(a,i)\in D} \frac{1}{2}\left(Y_{ai} - X_{ai}\right)^2 + \frac{\lambda}{2}\sum_{(a,i)} X_{ai}^2.$$

The results are

$$\begin{aligned} \widehat{X}_{ai} &= \frac{Y_{ai}}{1+\lambda} && \text{for } (a,i) \in D \\ \widehat{X}_{ai} &= 0 && \text{for } (a,i) \notin D. \end{aligned}$$

The problem with this approach is that there is no connection between the entries of X. We can impose additional constraint on X:

$$X = UV^\intercal$$

for some $n \times d$ matrix U and $d \times m$ matrix $V^\intercal$, where d is the *rank* of the matrix X.

Alternating Minimization Assume that U and V are rank k matrices. Then, we can write the objective function as

$$J(X) = \sum_{(a,i)\in D} \frac{1}{2}\left(Y_{ai} - \left[UV^\intercal\right]_{ai}\right)^2 + \frac{\lambda}{2}\left(\sum_{a,k} U_{ak}^2 + \sum_{i,k} V_{ik}^2\right).$$

To find the solution, we fix (initialize) U (or V) and minimize the objective with respect to V (or U). We plug-in the result back to the objective and minimize it with respect to U (or V). We repeat this alternating process until there is no change in the objective function.

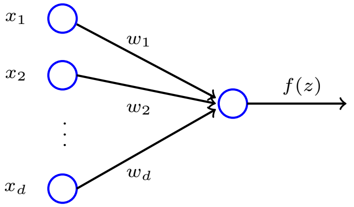
Example Consider the case $k = 1$. Then, $U_{a1} = u_a$ and $V_{i1} = v_i$. If we initialize u_a to some values, then we have to optimize the function

$$\sum_{(a,i)\in D} \frac{1}{2}\left(Y_{ai} - u_a v_i\right)^2 + \frac{\lambda}{2}\sum_i v_i^2.$$

Neural Networks

Introduction to Feedforward Neural Networks

A Unit in a Neural Network A **neural network unit** is a primitive neural network that consists of only the *input layer*, and an output layer with only one output.



A neural network unit computes a non-linear weighted combination of its input:

$$\widehat{y} = f(z) \qquad \text{where} \quad z = w_0 + \sum_{i=1}^{d} x_i w_i$$

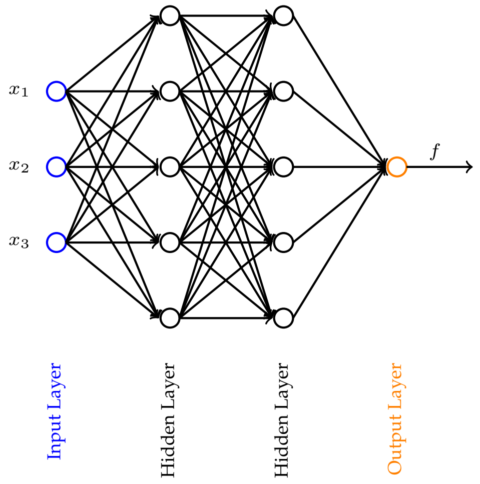
where w_i are the **weights**, z is a number and is the weighted sum of the inputs x_i, and f is generally a non-linear function called the **activation function**.

Linear Function $f(z) = z$

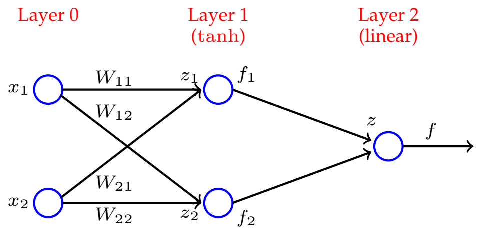
Rectified Linear Unit (ReLU) $f(z) = \max\{0, z\}$

Hyperbolic Tangent Function $\tanh(z) = \dfrac{e^z - e^{-z}}{e^z + e^{-z}} = 1 - \dfrac{2}{e^{2z}+1}$

Deep Neural Networks A **deep (feedforward) neural network** refers to a neural network that contains not only the input and output layers, but also hidden layers in between. Below is a deep feedforward neural network of 2 hidden layers, with each hidden layer consisting of 5 units:

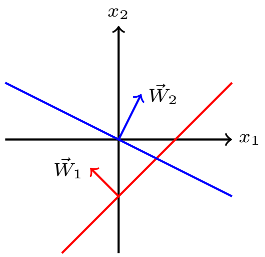


One Hidden Layer Model



$$\begin{aligned} z_1 &= \sum_{j=1}^{2} x_j W_{j1} + W_{01} & z_2 &= \sum_{j=1}^{2} x_j W_{j2} + W_{02} \\ f_1 &= f(z_1) = \tanh(z_1) & f_2 &= f(z_2) = \tanh(z_2) \\ z &= f_1 w_1' + f_2 w_2' & f &= f(z) = z \end{aligned}$$

Neural Signal Transformation We can visualize what the hidden layer is doing similarly to a linear classifier.



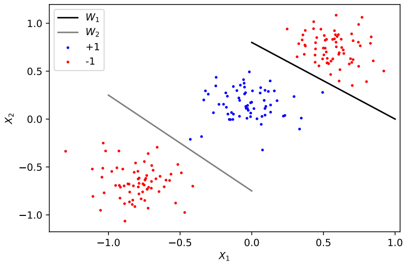
In the figure,

$$\vec{W}_1 = \begin{pmatrix} W_{11} \\ W_{21} \end{pmatrix} \qquad \text{and} \qquad \vec{W}_2 = \begin{pmatrix} W_{12} \\ W_{22} \end{pmatrix}.$$

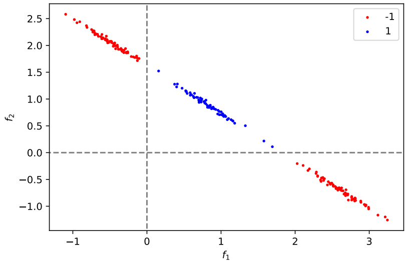
They map the input onto the f_1-f_2 axes.

Hidden Layer Representation

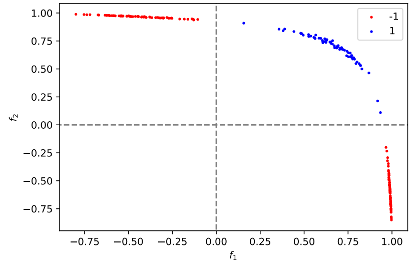
- Hidden Layer Units



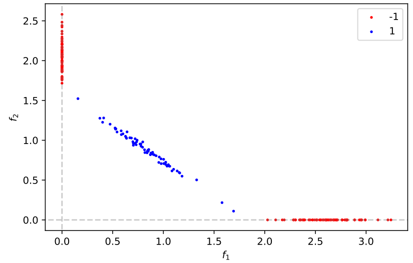
- Linear Activation



- *tanh* Activation



- ReLU Activation

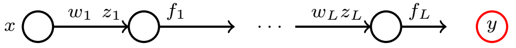


Summary

- Units in neural networks are linear classifiers, just with different output non-linearity.
- The units in feedforward neural networks are arranged in layers.
- By learning the parameters associated with the hidden layer units, we learn how to represent examples (as hidden layer activations).
- The representations in neural networks are learned directly to facilitate the end-to-end task.
- A simple classifier (output unit) suffices to solve complex classification tasks if it operates on the hidden layer representations.

Feedforward Neural Networks, Back Propagation, and Stochastic Gradient Descent (SGD)

Simple Example This simple neural network is made up of L hidden layers, but each layer consists of only one unit, and each unit has activation function f.



$$\begin{aligned} z_1 &= x w_1 \\ f_1 &= \tanh(x w_1) \\ &\vdots \\ f_L &= \tanh(f_{L-1} w_L) \\ \mathcal{L}(y, f_L) = \text{Loss}\,(y, f_L) &= \tfrac{1}{2}\,(y - f_L)^2 \end{aligned}$$

For $i = 2, \dots, L$: $z_i = f_{i-1} w_i$ where $f_{i-1} = f(z_{i-1})$. Also, y is the true value and f_L is the output of the neural network.

Gradient Descent The gradient descent update rule for the parameter w_i is

$$w_i \leftarrow w_i - \eta \cdot \boldsymbol{\nabla}_{w_i} \mathcal{L}(y, f_L)$$

where η is the learning rate. For instance, we have

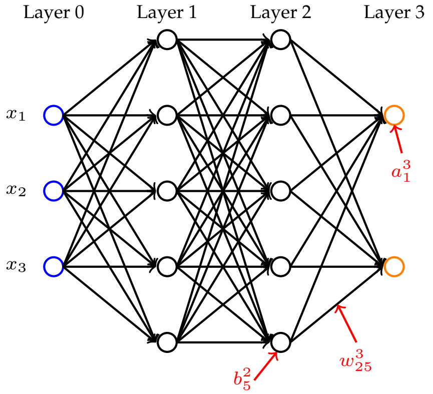
$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial w_1} &= \frac{\partial f_1}{\partial w_1} \frac{\partial \mathcal{L}}{\partial f_1} \\ \frac{\partial f_1}{\partial w_1} &= \left[1 - \tanh^2(x w_1)\right] x = \left(1 - f_1^2\right) x \\ \frac{\partial \mathcal{L}}{\partial f_1} &= \frac{\partial \mathcal{L}}{\partial f_2} \frac{\partial f_2}{\partial f_1} = \frac{\partial \mathcal{L}}{\partial f_2} \left(1 - f_2^2\right) w_2 . \end{aligned}$$

Thus, when we back-propagate, we get

$$\frac{\partial \mathcal{L}}{\partial w_1} = x \left(1 - f_1^2\right) \cdots \left(1 - f_L^2\right) w_2 \cdots w_L \cdot 2\,(f_L - y)\,.$$

Note that the above derivation applies to $\tanh$ activation.

Backpropagation Consider the L-layer neural network below.



We have the following notations:

- b_j^ℓ is the bias of the j^{th} neuron in the ℓ^{th} layer.
- a_j^ℓ is the activation of the j^{th} neuron in the ℓ^{th} layer.
- w_{jk}^ℓ is the weight for the connection from the k^{th} neuron in the $(\ell-1)^{\text{th}}$ layer to the j^{th} neuron in the ℓ^{th} layer.

If the activation function is f and the loss function we are minimizing is C, then the equations describing the network are:

$$\begin{aligned} a_j^\ell &= f\left(\sum_k w_{jk}^\ell a_k^{\ell-1} + b_j^\ell\right) \\ \text{Loss} &= C\left(a^L\right) \end{aligned}$$

Let the weighted inputs to the d neurons in layer ℓ be defined as

$$z^\ell \equiv w^\ell a^{\ell-1} + b^\ell, \quad \text{where } z^\ell \in \mathbb{R}^d.$$

Then, the activation of layer ℓ is also written as $a^\ell \equiv f(z^\ell)$. Also, let $\delta_j^\ell \equiv \frac{\partial C}{\partial z_j^\ell}$ denote the *error* of neuron j in layer ℓ. Then, $\delta^\ell \in \mathbb{R}^d$ denotes the full vector of errors associated with layer ℓ.

Equations of Backpropagation

$$\begin{aligned} \delta^L &= \boldsymbol{\nabla}_a C \odot f'\left(z^L\right) \\ \delta^\ell &= \left[\left(w^{\ell+1}\right)^{\intercal} \delta^{\ell+1}\right] \odot f'\left(z^\ell\right) \\ \frac{\partial C}{\partial b_j^\ell} &= \delta_j^\ell \\ \frac{\partial C}{\partial w_{jk}^\ell} &= a_k^{\ell-1} \delta_j^\ell \end{aligned}$$

The symbol $\odot$ represents the Hadamard product.

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \odot \begin{pmatrix} e & f \\ g & h \end{pmatrix} = \begin{pmatrix} ae & bf \\ cg & dh \end{pmatrix}.$$

Recurrent Neural Networks

Temporal/Sequence Problems

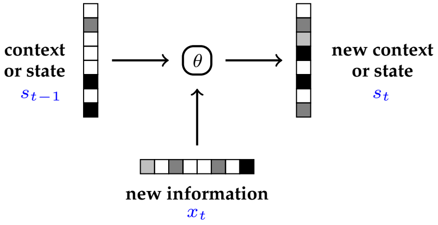
- Sequence prediction problems can be recast in a form amenable to feedforward neural networks.
- We have to engineer how *history* is mapped to a vector (representation). This vector is then fed into, e.g., a neural network.
- We would like to learn how to encode the *history* into a vector.

Key Concepts

- **Encoding** – e.g., mapping a sequence to a vector
- **Decoding** – e.g., mapping a vector to, e.g., a sequence

Example: Encoding Sentences

- Introduce adjustable *lego pieces* and optimize them for end-to-end performance.



$$s_t = \tanh(W^{s,s} s_{t-1} + W^{s,x} x_t)$$

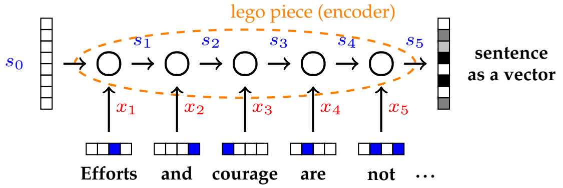
- Let's say we want to encode the incomplete sentence **Efforts and courage are not**. First, we have to represent the first word as a vector (say, a one-hot vector). This will be x_1. Then,

$$s_1 = \tanh\left(W^{s,x} x_1\right).$$

The second word will be x_2, and we compute for s_2.

$$s_2 = \tanh(W^{s,s} s_1 + W^{s,x} x_t).$$

We continue this process until we've encoded all the words in the sentence. We can visualize this as follows:



Differences from standard feedforward architecture

- Input is received at each layer (per word), not just at the beginning as in a typical feedforward network.
- The number of layers varies and depends on the length of the sentence.
- Parameters of each layer (representing an application of an RNN) are shared (same RNN at each step).

Basic RNN

$$s_t = \tanh(W^{s,s} s_{t-1} + W^{s,x} x_t)$$

Simple Gated RNN

$$\begin{aligned} g_t &= \text{sigmoid}\left(W^{g,s} s_{t-1} + W^{g,x} x_t\right) \\ s_t &= (1 - g_t) \odot s_{t-1} + g_t \odot \tanh(W^{s,s} s_{t-1} + W^{s,x} x_t) \end{aligned}$$

Long Short-Term Memory (LSTM)

$$\begin{aligned} f_t &= \text{sigmoid}\left(W^{f,h} h_{t-1} + W^{f,x} x_t\right) && \text{forget gate} \\ i_t &= \text{sigmoid}\left(W^{i,h} h_{t-1} + W^{i,x} x_t\right) && \text{input gate} \\ o_t &= \text{sigmoid}\left(W^{o,h} h_{t-1} + W^{o,x} x_t\right) && \text{output gate} \\ c_t &= f_t \odot c_{t-1} + i_t \odot \tanh\left(W^{c,h} h_{t-1} + W^{c,x} x_t\right) && \text{memory cell} \\ h_t &= o_t \odot \tanh(c_t) && \text{visible state} \end{aligned}$$

Markov Language Models Let $w \in V$ denote the set of possible words/symbols that includes

- an **UNK** symbol for any unknown word (out of vocabulary)
- $\langle$**beg**$\rangle$ symbol for specifying the start of a sentence
- $\langle$**end**$\rangle$ symbol for specifying the end of the sentence

First-order Markov Model In a first-order Markov model (**bigram model**), the next symbol only depends on the previous one. Each symbol (except ⟨beg⟩) in the sequence is predicted using the same condition probability table until an ⟨end⟩ symbol is seen. The probability associated to the sentence is

$$\prod_{i=1} \mathbb{P}\left(w_i | w_{i-1}\right).$$

Maximum Likelihood Estimation The goal is to maximize the probability that the model can generate all the observed sentences (corpus S)

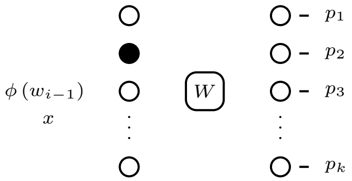
$$s \in S, s = \left\{w_1^s, w_2^s, \ldots, w_{|s|}^s\right\}$$

$$\ell = \log\left\{\prod_{s \in S}\left[\prod_{i=1}^{|s|} \mathbb{P}\left(w_i^s | w_{i-1}^s\right)\right]\right\}$$

The maximum likelihood estimate is obtained as normalized counts of successive word occurrences (matching statistics)

$$\widehat{\mathbb{P}}\left(w' | w\right) = \frac{\text{count}\left(w', w\right)}{\sum_{\tilde{w}} \text{count}\left(w, \tilde{w}\right)}$$

Feature-based Markov Model We can also represent the Markov model as a feedforward neural network (very extendable). We define a one-hot vector, $\phi\left(w_{i-1}\right)$, corresponding to the previous word. This will be an input to the feedforward neural network.



In the figure,

$$p_k = \mathbb{P}\left(w_i = k | w_{i-1}\right)$$

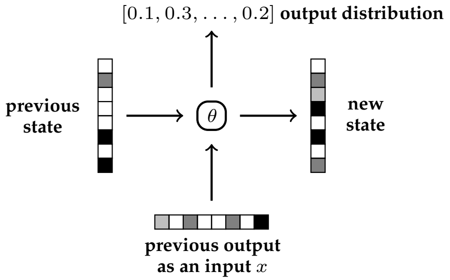
is the probability of the next word, given the previous word. The aggregate input to the k^{th} output unit is

$$z_k = \sum_k x_j W_{jk} + W_{0k}.$$

These input values are not probabilities. A typical transformation is the **softmax transformation**:

$$p_k = \frac{e^{z_k}}{\sum_j e^{z_j}}.$$

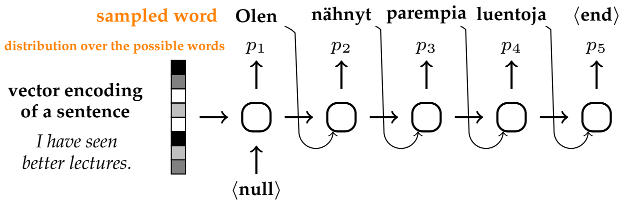
RNNs for Sequences Our RNN now also produces an output (e.g., a word) as well as update its state


$[0.1, 0.3, \ldots, 0.2]$ **output distribution**
previous state
θ
new state
previous output as an input x

$$s_t = \tanh\left(W^{s,s} s_{t-1} + W^{s,x} x_t\right) \quad \text{state}$$

$$p_t = \text{softmax}\left(W^o s_t\right) \quad \text{output distribution}$$

Decoding

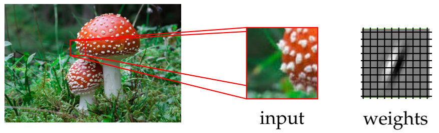

sampled word
distribution over the possible words
vector encoding of a sentence
I have seen better lectures.
Olen
nähnyt
parempia
luentoja
⟨end⟩
p_1
p_2
p_3
p_4
p_5
⟨null⟩

Convolutional Neural Networks

Problem Image classification

- The presence of objects may vary in location across different images.

Patch classifier/filter



The patch classifier goes through the entire image. We can think of the weights as the image that the unit prefers to see.

Convolution The convolution is an operation between two functions f and g:

$$(f * g)(t) \equiv \int_{-\infty}^{+\infty} f(\tau) g(t-\tau) d\tau.$$

Intuitively, convolution *blends* the two functions f and g by expressing the amount of overlap of one function as it is shifted over another function.

Discrete Convolution For discrete functions, we can define the convolution as

$$(f * g)[n] \equiv \sum_{m=-\infty}^{m=+\infty} f[m] g[n-m].$$

Pooling We wish to know whether a feature was there but not exactly where it was.

Pooling (Max) Pooling region and *stride* may vary.

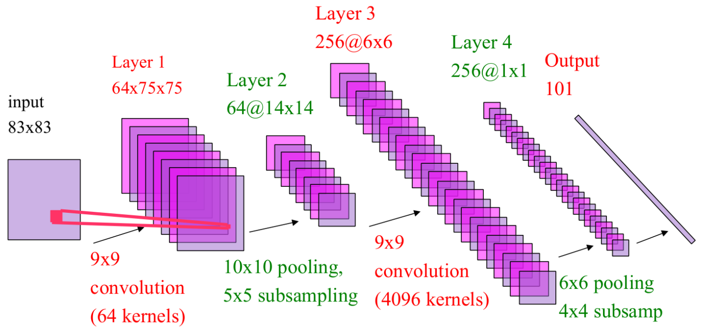
- Pooling induces translation invariance at the cost of spatial resolution.
- Stride reduces the size of the resulting feature map.

original

feature map

feature map after max pooling

Example of CNN From LeCun (2013)



Unsupervised Learning

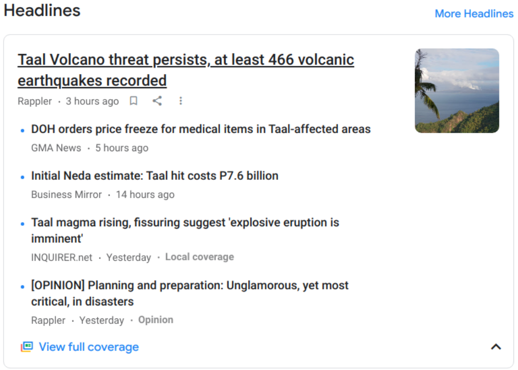
Clustering

Training set We are provided a training set but with no labels

$$S_n = \left\{x^{(i)} \middle| i = 1, \ldots, n\right\}$$

and the goal is to find structure in the data.

Example: Google News



Headlines

More Headlines

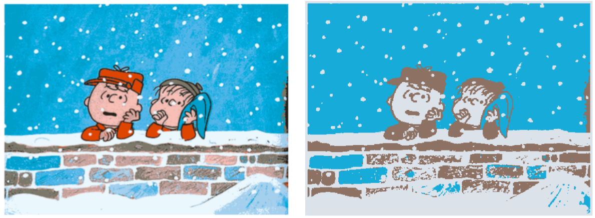
Taal Volcano threat persists, at least 466 volcanic earthquakes recorded

Rappler · 3 hours ago

- DOH orders price freeze for medical items in Taal-affected areas
  GMA News · 5 hours ago
- Initial Neda estimate: Taal hit costs P7.6 billion
  Business Mirror · 14 hours ago
- Taal magma rising, fissuring suggest 'explosive eruption is imminent'
  INQUIRER.net · Yesterday · Local coverage
- [OPINION] Planning and preparation: Unglamorous, yet most critical, in disasters
  Rappler · Yesterday · Opinion

View full coverage

Example: Image Quantization



original

compressed

Partition A partition of a set is a grouping of the set's elements into non-empty subsets, in such a way that **every** element is included in one and only one of the subsets. In other words, $C_1, \ldots, C_K$ is a partition of $\{1, \ldots, n\}$ if and only if

$$C_1 \cup \cdots \cup C_K = \{1, \ldots, n\} \quad \text{and}$$

$$C_i \cap C_j = \emptyset \quad \text{for any} \quad i \neq j \quad \text{in} \quad \{1, \ldots, K\}.$$

Clustering: Input

- Set of feature vectors $S_n = \left\{ x^{(i)} \middle| i = 1, \ldots, n \right\}$
- The number of clusters K

Clustering: Output

- A partition of indices $\{1, \ldots, n\}$ into K sets, $C_1, \ldots, C_K$
- *Representatives* in each of the K partition sets, given as $z_1, \ldots, z_K$

Cost We can calculate the total cost by summing the cost of each cluster:

$$\text{Cost}\left(C_1, \ldots, C_K\right) = \sum_{j=1}^{K} \text{Cost}\left(C_j\right)$$

Similarity Measure We use the Euclidean distance between the elements of a cluster and its representative to calculate the cost for each cluster. Then, the total cost is

$$\text{Cost}\left(C_1, \ldots, C_K, z_1, \ldots, z_K\right) = \sum_{j=1}^{K} \sum_{i \in C_j} \left\| x^{(i)} - z_j \right\|^2.$$

K-Means Algorithm

1. Randomly select $z_1, \ldots, z_K$.
2. Iterate:
   (a) Given $z_1, \ldots, z_K$, assign each data point $x^{(i)}$ to the closest z_j so that

   $$\text{Cost}\left(z_1, \ldots, z_K\right) = \sum_{i=1}^{n} \min_{j=1,\ldots,K} \left\| x^{(i)} - z_j \right\|^2.$$

   (b) Given $C_1, \ldots, C_K$, find the best representatives $z_1, \ldots, z_K$, i.e., find $z_1, \ldots, z_K$ such that

   $$z_j = \operatorname*{argmin}_{z} \sum_{i \in C_j} \left\| x^{(i)} - z \right\|^2 = \frac{1}{|C_j|} \sum_{i \in C_j} x^{(i)}.$$

K-Medoids Algorithm The K-Medoids algorithm is a variation of the K-Means algorithm that addresses some of the K-Means algorithm's limitations.

1. Randomly select $\{z_1, \ldots, z_K\} \subseteq \{x_1, \ldots, x_n\}$.
2. Iterate:
   (a) Given $z_1, \ldots, z_K$, assign each $x^{(i)}$ to the closest z_j so that

   $$\text{Cost}\left(z_1, \ldots, z_K\right) = \sum_{i=1}^{n} \min_{j=1,\ldots,K} \text{dist}\left(x^{(i)}, z_j\right)$$

   (b) Given $C_j \in \{C_1, \ldots, C_K\}$, find the best representative $z_j \in \{x_1, \ldots, x_n\}$ such that

   $$\sum_{x^{(i)} \in C_j} \text{dist}\left(x^{(i)}, z_j\right)$$

   is minimal.

Generative Models

Generative vs. Discriminative Models *Generative models* work by explicitly modeling the probability distribution of each of the individual classes in the training data. *Discriminative models* learn explicit decision boundary between classes.

Simple Multinomial Generative Model Consider a multinomial model M to generate text documents. Assume that M has a fixed vocabulary W and we generate a document by sampling one word at a time from this vocabulary. Furthermore, all the words that are generated by M are independent of each other. We denote the probability that M generates certain word $w \in W$ is

$$\mathbb{P}\left(w|\theta\right) = \theta_w, \quad \theta_w \geq 0, \sum_{w \in W} \theta_w = 1.$$

Then, the probability of generating the document D is

$$\mathbb{P}\left(D|\theta\right) = \prod_{i=1}^{n} \theta_{w_i} = \prod_{w \in W} \theta_w^{\text{count}(w)}.$$

Maximum Likelihood Estimate The log-likelihood for the model is

$$\ell = \log \mathbb{P}(D|\theta) = \sum_{w \in W} \text{count}(w) \log \theta_w$$

and the maximum likelihood estimate is

$$\widehat{\theta}_w = \frac{\text{count}(w)}{\sum_{w' \in W} \text{count}(w')}.$$

Prediction Consider using a multinomial generative model M for the task of binary classification consisting of two classes: $+$ (positive class) and $-$ (negative class).

- θ^+: parameter for the positive class
- θ^-: parameter for the negative class

Suppose that we classify a new document D to belong to the positive class if and only if

$$\log \frac{\mathbb{P}(D|\theta^+)}{\mathbb{P}(D|\theta^-)} \geq 0.$$

The generative classifier is equivalent to a linear classifier:

$$\log \frac{\mathbb{P}(D|\theta^+)}{\mathbb{P}(D|\theta^-)} = \sum_{w \in W} \text{count}(w) \log \frac{\theta_w^+}{\theta_w^-} = \sum_{w \in W} \text{count}(w)\, \theta'_w.$$

Prior, Posterior and Likelihood In the above discussion, there is an assumption that the likelihood of being in one of the classes is the same. However, we may have some prior knowledge and we want to incorporate it into our model. The posterior distribution for the positive class is then

$$\mathbb{P}\left(y = +|D\right) = \frac{\mathbb{P}(D|\theta^+)\, \mathbb{P}(y = +)}{\mathbb{P}(D)}.$$

The generative classifier becomes

$$\log \frac{\mathbb{P}\left(y = +|D\right)}{\mathbb{P}\left(y = -|D\right)} = \sum_{w \in W} \text{count}(w)\, \theta'_w + \theta'_0$$

where $\theta'_w = \log \dfrac{\theta_w^+}{\theta_w^-}$ and $\theta'_0 = \log \dfrac{\mathbb{P}(y = +)}{\mathbb{P}(y = -)}$.

Gaussian Generative Models The likelihood of $\mathbf{x} \in \mathbb{R}^d$ being generated by a Gaussian with mean μ and standard deviation σ is

$$f_X\left(\mathbf{x}|\mu, \sigma^2\right) = \frac{1}{\left(2\pi\sigma^2\right)^{d/2}} \exp\left(-\frac{1}{2\sigma^2} \|\mathbf{x} - \mu\|^2\right).$$

MLE for the Mean

$$\widehat{\mu} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}^{(i)}$$

MLE for the Variance

$$\widehat{\sigma}^2 = \frac{1}{nd} \sum_{i=1}^{n} \left\| \mathbf{x}^{(i)} - \mu \right\|^2$$

Mixture Models; EM Algorithm

Gaussian Mixture Models Instead of just a single Gaussian, we have a mixture of Gaussian components. Assume that there are K Gaussians with known means and variances. Assume also that the mixture weights $p_1, \ldots, p_K$ are known. The likelihood for an observation $\mathbf{x}$ obtained from the model is

$$p(\mathbf{x}|\theta) = \sum_{j=1}^{K} p_j \mathcal{N}\left(\mathbf{x}; \mu^{(j)}, \sigma_j^2 \mathbf{I}\right).$$

For the training set

$$S_n = \left\{ \mathbf{x}^{(i)}, i = 1, \ldots, n \right\},$$

the likelihood is

$$\mathbb{P}\left(S_n|\theta\right) = \prod_{i=1}^{n} \sum_{j=1}^{K} p_j \mathcal{N}\left(\mathbf{x}^{(i)}; \mu^{(j)}, \sigma_j^2 \mathbf{I}\right).$$

Observed Case Consider the case of hard clustering, i.e., a point either belongs to a cluster or not. Let

$$\delta(j|i) = \begin{cases} 1, & \mathbf{x}^{(i)} \text{ is assigned to } j \\ 0, & \text{otherwise.} \end{cases}$$

Also, let $\widehat{n}_j = \sum_{i=1}^{n} \delta(j|i)$ denote the number of points belonging to cluster j.

Maximizing the likelihood gives

$$\widehat{p}_j = \frac{\widehat{n}_j}{n}$$

$$\widehat{\mu}^{(j)} = \frac{1}{\widehat{n}_j} \sum_{i=1}^{n} \delta(j|i)\, \mathbf{x}^{(i)}$$

$$\widehat{\sigma}_j^2 = \frac{1}{\widehat{n}_j d} \sum_{i=1}^{n} \delta(j|i) \left\| \mathbf{x}^{(i)} - \mu^{(j)} \right\|^2.$$

The EM Algorithm Instead of hard clustering, the data can actually be generated from different clusters with different probabilities. We have soft clustering. We can maximize the likelihood through the EM algorithm.

Randomly initialize θ: $\mu^{(1)}, \ldots, \mu^{(K)}, \sigma_1^2, \ldots, \sigma_K^2, p_1, \ldots, p_K$.

1. **E-step:**

   $$p(j|i) = \frac{p_j \mathcal{N}\left(\mathbf{x}^{(i)}; \mu^{(j)}, \sigma_j^2 \mathbf{I}\right)}{p\left(\mathbf{x}|\theta\right)}$$

   where $p(\mathbf{x}|\theta) = \sum_{j=1}^{K} p_j \mathcal{N}\left(\mathbf{x}^{(i)}; \mu^{(j)}, \sigma_j^2 \mathbf{I}\right)$

2. **M-step:**

   $$\widehat{n}_j = \sum_{i=1}^{n} p(j|i)$$

   $$\widehat{p}_j = \frac{\widehat{n}_j}{n}$$

   $$\widehat{\mu}^{(j)} = \frac{1}{\widehat{n}_j} \sum_{i=1}^{n} p(j|i)\, \mathbf{x}^{(i)}$$

   $$\widehat{\sigma}_j^2 = \frac{1}{\widehat{n}_j d} \sum_{i=1}^{n} p(j|i) \left\| \mathbf{x}^{(i)} - \mu^{(j)} \right\|^2.$$

Reinforcement Learning

Objectives of RL The goal of RL is to learn a good policy with no or limited supervision.

Markov Decision Processes

Definition A **Markov decision process (MDP)** is defined by

- a set of **states** $s \in S$ (may be observed or unobserved);
- a set of **actions** $a \in A$;
- action-dependent **transition probabilities** $T(s, a, s') = \mathbb{P}(s'|s, a)$ so that, for each state s and action a,

$$\sum_{s' \in S} T(s, a, s') = 1$$

.

- **reward functions** $R(s, a, s')$, representing the reward for starting in state s, taking action a and ending up in state s' after one step. (The reward function may also depend only on s, or only s and s.)

Property MDPs satisfy the **Markov property** in that the transition probabilities and rewards depend only on the current state and action, and remain unchanged regardless of the history (i.e., past states and actions) that leads to the current state.

Utility Function The main problem for MDPs is to optimize the agent's behavior. We first need to specify the criterion that we are trying to maximize in terms of accumulated rewards. We define a **utility function** and maximize its expectation.

- **Finite horizon based utility:** The utility function is the sum of rewards after acting for a fixed number n of steps. When the rewards depend only on the states, the utility function is

$$U[s_0, s_1, \ldots, s_n] = \sum_{i=0}^{n} R(s_i.)$$

- **(Infinite horizon) discounted reward based utility:** In this setting, the reward one step into the future is discounted by a factor γ, the reward two steps ahead by γ^2, and so on. The goal is to continue acting (without an end) while maximizing the expected discounted reward. The discounting allows us to focus on near term rewards, and control this focus by changing γ. If the rewards depend only on the states, the utility function is

$$U[s_0, s_1, \ldots] = \sum_{k=0}^{\infty} \gamma^k R(s_k).$$

Optimal Policy A **policy** is a function $\pi : S \to A$ that assigns an action $\pi(s)$ to any state s. Given an MDP and a utility function $U[s_0, s_1, \ldots, s_n]$, our goal is to find an **optimal policy** function that maximizes the expectation of the utility. We denote the optimal policy by π^*.

Bellman Equations

Value Function Denote by $Q^*(s, a)$ the expected reward starting at s, taking action a and acting optimally. The *value function* $V^*(s)$ is the expected reward starting at state s and acting optimally.

The Bellman Equations These equations connect the notion of the value of a state and the value of policy.

$$V^*(s) = \max_a Q^*(s, a) = Q^*(s, \pi^*(s))$$

$$Q^*(s, a) = \sum_{s'} T(s, a, s') \left[R(s, a, s') + \gamma V^*(s')\right]$$

We can define the $V^*(s)$ recursively to get

$$V^*(s) = \max_a \left\{ \sum_{s'} T(s, a, s') \left[R(s, a, s') + \gamma V^*(s')\right] \right\}$$

Value Iteration Algorithm

Definition *Value iteration* is an iterative algorithm that computes the values of states indexed by k. Let $V_k^*(s)$ be the expected reward from state s after k steps:

$$V_k^*(s) \to V^*(s) \quad \text{as} \quad k \to \infty.$$

1. Initialization: $V_0^*(s) = 0$
2. Iterate until $V_k^*(s) \simeq V_{k+1}^*(s)\ \forall s$

$$V_{k+1}^*(s) \leftarrow \max_a \left\{ \sum_{s'} T(s, a, s') \left[R(s, a, s') + \gamma V_k^*(s')\right] \right\}$$

3. Compute $Q^*(s, a)$ and $\pi^*(s, a) = \operatorname*{argmax}_a Q^*(s, a)$.

Convergence This algorithm will converge as long as $\gamma < 1$.

Q-Value Iteration

Definition We can directly operate at the level of Q-values. Q-value iteration is a reformulation of value iteration algorithm.

Update Rule

$$Q_{k+1}^*(s, a) \leftarrow \sum_{s'} T(s, a, s') \left[R(s, a, s') + \gamma \max_{a'} Q_k^*(s', a')\right]$$

Reinforcement Learning

MDP vs. RL In MDPs, we are given 4 quantities $\langle S, A, T, R \rangle$. In reinforcement learning, we are given only the states and actions $\langle S, A \rangle$. In the real world, transitions and rewards might not be directly available and they need to be estimated.

Estimation Consider a random variable X. The goal is to estimate

$$\mathbb{E}\left[f(X)\right] = \sum_x p(x) f(x).$$

We have access to K samples: $x_i, i = 1, \ldots, K$.

Model-based Learning

$$\widehat{p}(x_i) = \frac{1}{K} \operatorname{count}(x_i)$$

$$\mathbb{E}\left[f(X)\right] \approx \sum_{i=1}^{K} \widehat{p}(x_i) f(x_i)$$

Model-free Learning

$$\mathbb{E}\left[f(X)\right] \approx \frac{1}{K} \sum_{i=1}^{K} f(x_i)$$

Q-Value Iteration for RL

1. Initialization: $Q(s, a) = 0\ \forall s, a$
2. Iterate until convergence:
   (a) Collect sample: $s, a, s', R(s, a, s')$
   (b) Update:

$$Q_{i+1}(s, a) \leftarrow \alpha \left[R(s, a, s') + \gamma \max_{a'} Q_i(s', a')\right] + (1 - \alpha)\, Q_i(s, a)$$

$$= Q_i(s, a) + \alpha \left[R(s, a, s') + \gamma \max_{a'} Q_i(s', a') - Q_i(s, a)\right]$$

Recommended Resources

- Introduction to Machine Learning with Python (Müller and Guido)
- Machine Learning with Python – From Linear Models to Deep Learning [Lecture Slides] (`http://www.edx.org`)
- LaTeX File (`github.com/mynameisjanus/686xMachineLearning`)

Please share this cheatsheet with friends!