Machine Learning Notes

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Contents

1 Machine Learning Introduction

A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.

1.1 Supervised Learning

Supervised learning algorithms build a mathematical model of a set of data that contains both the inputs and the desired outputs.

In supervised learning, each example is a pair consisting of an input object (typically a vector) and a desired output value (also called the supervisory signal).

1.1.1 Regression

Regression analysis is a set of statistical processes for estimating the relationships between a dependent variable (often called the 'outcome variable') and one or more independent variables (often called 'predictors', 'covariates', or 'features').

Training(Learning) Process:
observed data(training set) $\rightarrow$ *learning algorithm* $\rightarrow$ *h(hypothesis)*

Predicting Process:
independent variable $\rightarrow$ *h(hypothesis)* $\rightarrow$ *dependent variable*

1.1.2 Classification

Classification is the problem of identifying to which of a set of categories (sub-populations) a new observation belongs, on the basis of a training set of data containing observations (or instances) whose category membership is known.

1.2 Unsupervised Learning

Unsupervised learning algorithms take a set of data that contains only inputs, and find structure in the data, like grouping or clustering of data points.

Draw inferences from data sets consisting of input data without labeled responses.

1.3 Reinforcement learning

Reinforcement learning is an area of machine learning concerned with how software agents ought to take actions in an environment so as to maximize some notion of cumulative reward.

2 Regression

2.1 Linear Regression(from Wikipedia)

Given a data set $\{y_i, x_{i1}, ..., x_{ip}\}_{i=1}^n$ of n statistical units, a linear regression model assumes that the relationship between the dependent variable y and the p-vector of regressors x is linear.

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i,\ i = 1, \ldots, n$$
$$y = X\beta + \epsilon$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, X = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1p} \\ 1 & x_{21} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \dots & x_{np} \end{bmatrix}, \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}, \epsilon = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

y is a vector of observed values y_i $(i = 1, \dots, n)$ of the variable called the regressand, endogenous variable, response variable, measured variable, criterion variable, or dependent variable.

X may be seen as a matrix of row-vectors x_i or of n-dimensional column-vectors X_j, which are known as regressors, exogenous variables, explanatory variables, covariates, input variables, predictor variables, or independent variables. Usually a constant is included as one of the regressors. In particular, $x_{i0} = 1$ for $i = 1, \dots, n$. The corresponding element of β is called the intercept.

β is a $(p + 1)$-dimensional parameter vector, where β_0 is the intercept term (if one is included in the model—otherwise β is p-dimensional). Its elements are known as effects or regression coefficients (although the latter term is sometimes reserved for the estimated effects).

ϵ is a vector of values ϵ_i. This part of the model is called the error term, disturbance term, or sometimes noise (in contrast with the "signal" provided by the rest of the model).

Matrix Concepts

identity matrix I(or $I_{n\times n}$):

$$A \cdot I = I \cdot A = A$$

$$I = \begin{bmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix}$$

inverse matrix A^{-1}: If A is an $m \times m$ matrix, and if it has an inverse.

$$A \cdot A^{-1} = A^{-1} \cdot A = I$$

transpose matrix A^T: Let A be an $m \times n$ matrix. Then A^T is an $n \times m$ matrix.

$$A^T_{ij} = A_{ji}$$

2.1.1 Linear Regression Learning (from Machine Learning course)

For convenience reasons, define $x_0 = 1$

$$x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}, \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$$

hypothesis:

$$y = h_\theta(x) = \theta^T x = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_n x_n$$

training data:

$$(x^{(i)}, y^{(i)})\ for\ i = 1, \dots, m$$

cost function:
convex: second derivative (hessian matrix) is non-negative definite.

goal: $\underset{\theta}{\text{minimize}}\, J(\theta)$

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2$$

gradient descent:
repeat until convergence {

$$\theta_j =: \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta) = \theta_j - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

simultaneously update θ_j for $j = 0, \ldots, n$

}

vectorized implementation:
repeat until convergence {

$$\theta =: \theta - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x^{(i)}$$

}

batch size:
The number of training samples to use in a training action.

epoch:
The number of times of training which uses all the training samples.

Feature scaling:
The range of all features should be normalized so that each feature contributes approximately proportionately to the result. Also it helps gradient descent converge much faster.

mean normalization: (don't apply to x_0)

$$x_i = \frac{x_i - mean(x_i)}{max(x_i) - min(x_i)}$$

standardization: (don't apply to x_0)
Feature standardization makes the values of each feature in the data have zero-mean (when subtracting the mean in the numerator) and unit-variance.

μ : mean, σ^2 : variance, σ : standard deviation

$$\mu_i = \frac{1}{m}\sum_{j=1}^{m}x_i^{(j)}$$

$$\sigma_i^2 = \frac{1}{m}\sum_{j=1}^{m}(x_i^{(j)} - \mu_i)^2$$

$$x_i = \frac{x_i - \mu_i}{\sigma_i}$$

learning rate α:
If α is too small: slow convergence.
If α is too large: may not decrease on every iteration and thus may not converge.
try a range of learning rate to find a good one:

$$\alpha = \ldots, 0.001, \ldots, 0.01, \ldots, 0.1, \ldots$$

Feature choosing:
Choose the right features to fit the data set.
housing price example, choose from:

$$h_\theta(x) = \theta_0 + \theta_1 \times frontage + \theta_2 \times depth$$
$$h_\theta(x) = \theta_0 + \theta_1 \times area$$

polynomial regression:
Use the polynomial model with the machinery of multivariant linear regression.
housing price example, choose from:

$$h_\theta(x) = \theta_0 + \theta_1 \times area + \theta_2 \times area^2$$
$$h_\theta(x) = \theta_0 + \theta_1 \times area + \theta_2 \times \sqrt{area}$$

2.1.2 Normal Equation

Let:

$$X = \begin{bmatrix} (x^{(1)})^T \\ (x^{(2)})^T \\ \vdots \\ (x^{(m)})^T \end{bmatrix}, y = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(m)} \end{bmatrix}$$

Calculate best θ: * maths derivation needed

$$\theta = (X^T X)^{-1} X^T y$$

If $X^T X$ is noninvertible, the common causes might be having:
1. Redundant features, where two features are very closely related (i.e. they are linearly dependent)
2. Too many features (e.g. $m < n$). In this case, delete some features or use "regularization".

Gradient Descent vs **Normal Equation**:

Gradient Descent	**Normal Equation**
Need to choose α	No need to choose α
Needs many iterations	No need to iterate
$O(kn^2)$	$O(n^3)$. Need to calculate $(X^T X)^{-1}$
Works well when n is large	Slow if n is very large

Vectorized Cost Function:

$$J(\theta) = \frac{1}{2m}(X\theta - y)^T (X\theta - y)$$

2.2 Logistic Regression

sigmoid function: (Logistic Function)
Maps any real number from $(-\infty, +\infty)$ to the $(0, 1)$ interval.

$$g(z) = \frac{1}{1 + e^{-z}}$$

hypothesis:

$$h_\theta(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$$

$h_\theta(x)$ will give us the probability that our output is 1. Our probability that our prediction is 0 is just the complement of our probability that it is 1.

$$h_\theta(x) = P(y = 1 \mid x; \theta) = 1 - P(y = 0 \mid x; \theta)$$
$$P(y = 1 \mid x; \theta) + P(y = 0 \mid x; \theta) = 1$$

decision boundary:
In order to get our discrete 0 or 1 classification, we can translate the output of the hypothesis function as follows:

$$h_\theta(x) \geq 0.5 \rightarrow y = 1$$
$$h_\theta(x) < 0.5 \rightarrow y = 0$$

Decision is made when:

$$g(\theta^T x) \geq 0.5, \text{ when } \theta^T x \geq 0$$
$$g(\theta^T x) < 0.5, \text{ when } \theta^T x < 0$$

Now we get:

$$\theta^T x \geq 0 \rightarrow y = 1$$
$$\theta^T x < 0 \rightarrow y = 0$$

The decision boundary is the line that separates the area where $y = 0$ and where $y = 1$:

$$\theta^T x = 0$$

cost function:
If we use the the same cost function that we use for linear regression for logistic regression, the cost function will have many local optima. It will not be a convex function. Instead, we construct logistic regression cost function as follows:

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} Cost(h_\theta(x^{(i)}), y^{(i)})$$
$$Cost(h_\theta(x), y) = -log(h_\theta(x)), \text{ if } y = 1$$
$$Cost(h_\theta(x), y) = -log(1 - h_\theta(x)), \text{ if } y = 0$$

We can find it guarantees that $J(\theta)$ is convex for logistic regression:

$$Cost(h_\theta(x), y) = 0 \text{ if } h_\theta(x) = y, \text{ at } h_\theta(x) = y = 0 \text{ and } h_\theta(x) = y = 1$$

$$Cost(h_\theta(x), y) \rightarrow +\infty \text{ if } y = 0 \text{ and } h_\theta(x) \rightarrow 1$$
$$Cost(h_\theta(x), y) \rightarrow +\infty \text{ if } y = 1 \text{ and } h_\theta(x) \rightarrow 0$$

We can compress our cost function's two conditional cases into one case:

$$Cost(h_\theta(x), y) = -ylog(h_\theta(x)) - (1 - y)log(1 - h_\theta(x))$$

simplified cost function:

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} [y^{(i)} log(h_\theta(x^{(i)})) + (1 - y^{(i)}) log(1 - h_\theta(x^{(i)}))]$$

vectorized cost function:

$$h = g(X\theta)$$

$$J(\theta) = \frac{1}{m}(-y^T log(h) - (1-y)^T log(1-h))$$

gradient descent:
repeat until convergence {

$$\theta_j =: \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta) = \theta_j - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

$$\text{simultaneously update } \theta_j \text{ for } j = 0, \dots, n$$

}

vectorized implementation:
repeat until convergence {

$$\theta =: \theta - \alpha\frac{1}{m}X^T(g(X\theta) - y)$$

}

advanced optimization methods:
With the same cost function, we can choose different optimization method to optimize θ:

- gradient descent
- conjugate gradient
- BFGS
- L-BFGS
- ...

multiclass classification: (one vs all)
Instead of $y = \{0, 1\}$, we will expand our definition so that $y = \{0, 1, ..., n\}$. Then we divide our problem into n+1 binary classification problems, by constructing n + 1 hypothesis functions; in each one, we choose one class and then lump all the others into a single second class, then predict the probability that y is a member of the chosen class.

To summarize:
Train a logistic regression classifier $h_\theta^{(i)}(x)$ for each class to predict the probability that $y = i$. On a new input x, to make a prediction, pick the class i that maximizes $h_\theta^{(i)}(x)$.

$$y \in \{0, 1...n\}$$
$$h_\theta^{(0)}(x) = P(y = 0 \mid x; \theta)$$
$$h_\theta^{(1)}(x) = P(y = 1 \mid x; \theta)$$
$$\cdots$$
$$h_\theta^{(n)}(x) = P(y = n \mid x; \theta)$$
$$\text{prediction} = \max_i(h_\theta^{(i)}(x))$$

2.3 Overfitting Problem

underfitting:
High bias, which means hypothesis fits training data poorly, is usually caused by a function that is too simple or using too few features.

overfitting:
High variance, which means hypothesis fits training data well, but does not generalize well to predict new data. It is usually caused by a complicated function with too many features.

address overfitting:

1. Reduce the number of features:
   - Manually select which features to keep.
   - Use a model selection algorithm (studied later in the course).
2. Regularization:
   - Keep all the features, but reduce the magnitude of parameters θ_j.
   - Regularization works well when we have a lot of slightly useful features.

2.3.1 Linear Regression Regularization

regularized cost function:
We can reduce(penalize) the weight of the features in our function carry by increasing their cost. The λ is the regularization parameter. It determines how much the costs of our theta parameters are inflated.

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

Using the above cost function with the extra summation, we can smooth the output of our hypothesis function to reduce overfitting. If λ is too small, it would be hard to see a difference. If λ is too large, it may smooth out the function too much and cause underfitting.

regularized gradient descent:
repeat until convergence {

$$\theta_0 =: \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

$$\theta_j =: \theta_j - \alpha((\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}) + \frac{\lambda}{m}\theta_j)$$

$$= \theta_j(1 - \alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}$$

$$\text{simultaneously update } \theta_0 \text{ and } \theta_j \text{ for } j = 1, \ldots, n$$

}

The first term in the above equation, $1 - \alpha\frac{\lambda}{m}$ will always be less than 1. Intuitively you can see it as reducing the value of θ_j by some amount on every update.

regularized normal equation: * maths derivation needed

$$\theta = (X^TX + \lambda L)^{-1}X^Ty$$

$$L = \begin{bmatrix} 0 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 \end{bmatrix}$$

L has a dimension of $(n+1) \times (n+1)$. Intuitively, this is the identity matrix (though we are not including x_0), multiplied with a single real number λ.

Recall that if $m < n$, then $X^T X$ is non-invertible. However, when we add the term λL ($\lambda > 0$), the term $X^T X + \lambda L$ becomes invertible.

2.3.2 Logistic Regression Regularization

regularized cost function:

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)} log(h_\theta(x^{(i)})) + (1-y^{(i)}) log(1-h_\theta(x^{(i)}))] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

regularized gradient descent:
repeat until convergence {

$$\theta_0 =: \theta_0 - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_0^{(i)}$$

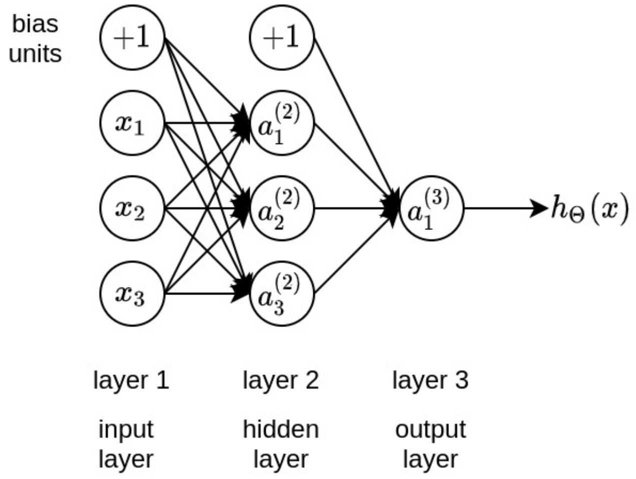
$$\begin{aligned} \theta_j =: \theta_j &- \alpha((\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)}) + \frac{\lambda}{m}\theta_j) \\ &= \theta_j(1-\alpha\frac{\lambda}{m}) - \alpha\frac{1}{m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})x_j^{(i)} \end{aligned}$$

simultaneously update θ_0 and θ_j for $j = 1, \dots, n$

}

3 Neural Network

3.1 Basic Structure

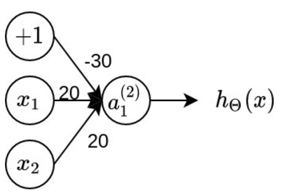


$$a_i^{(j)} = \text{"activation" of unit i in layer j}$$
$$\Theta^{(j)} = \text{matrix of weights (edges) from layer j to j + 1}$$

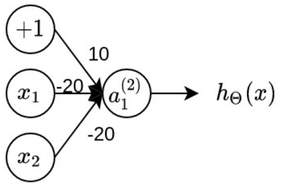
$$a_1^{(2)} = g(\Theta_{10}^{(1)}x_0 + \Theta_{11}^{(1)}x_1 + \Theta_{12}^{(1)}x_2 + \Theta_{13}^{(1)}x_3)$$
$$a_2^{(2)} = g(\Theta_{20}^{(1)}x_0 + \Theta_{21}^{(1)}x_1 + \Theta_{22}^{(1)}x_2 + \Theta_{23}^{(1)}x_3)$$
$$a_3^{(2)} = g(\Theta_{30}^{(1)}x_0 + \Theta_{31}^{(1)}x_1 + \Theta_{32}^{(1)}x_2 + \Theta_{33}^{(1)}x_3)$$
$$h_\Theta(x) = a_1^{(3)} = g(\Theta_{10}^{(2)}a_0^{(2)} + \Theta_{11}^{(2)}a_1^{(2)} + \Theta_{12}^{(2)}a_2^{(2)} + \Theta_{13}^{(2)}a_3^{(2)})$$

If network has s_j units in layer j, s_{j+1} units in layer $j+1$, then $\Theta^{(j)}$ will be of dimension $s_{j+1} \times (s_j + 1)$.

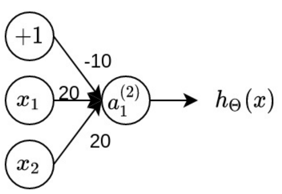
3.2 Simple Applications



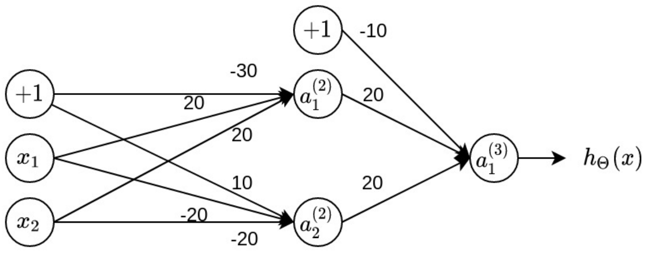
x_1 AND x_2



(NOT x_1) AND (NOT x_2)

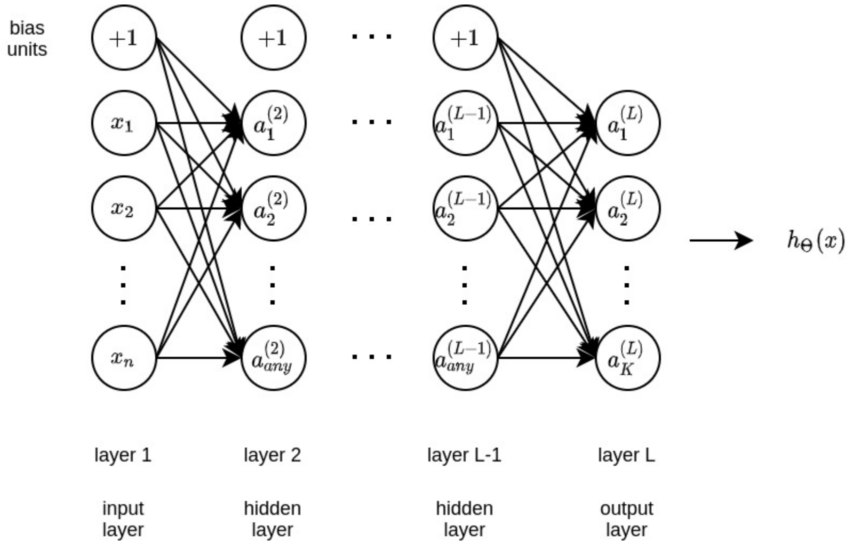


x_1 OR x_2



x_1 XNOR x_2

3.3 Generalized Model (one vs all)



For a neural network that has:

$$L = \text{total number of layers in the network}$$
$$s_l = \text{number of units (not counting bias unit) in layer } l$$
$$K = \text{number of output units/classes}$$

assume $a^{(1)} = x, a^{(L)} = h_\Theta(x)$, let:

$$z^{(l)} = \Theta^{(l-1)} a^{(l-1)}$$
$$a^{(l)} = g(z^{(l)})$$
$$h_\Theta(x) = a^{(L)} = g(z^{(L)})$$

Notice that bias units ($a_0^{(l)} = 1$) are considered as input only when calculating the next layer. They are not included in the output generated by previous layer.

regularized cost function:

$$J(\Theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K}[y_k^{(i)} log(h_\Theta(x^{(i)})_k) + (1 - y_k^{(i)}) log(1 - h_\Theta(x^{(i)})_k)] + \frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_{j,i}^{(l)})^2$$

3.4 Backpropagation Preliminary

matrix calculus: see Wikipedia
chaine rule:
Suppose the variable J depends on the variables $\theta_1, \dots, \theta_p$ via the intermediate variable $z_1, \dots, z_k$.

$$z_j = z_j(\theta_1, \dots, \theta_p), \forall j \in \{1, \dots, k\}$$
$$J = J(z_1, \dots, z_k)$$

Expand J, we can find:

$$\frac{\partial J}{\partial \theta_i} = \sum_{j=1}^{k} \frac{\partial J}{\partial z_j}\frac{\partial z_j}{\partial \theta_i}, \forall i \in \{1, \dots, p\}$$

chain rule derivation for matrix:
Suppose J is a real-valued output variable, $z \in \mathbb{R}^m$ is the intermediate variable and $\Theta \in \mathbb{R}^{m \times d}$, $a \in \mathbb{R}^d$ are the input variables. Suppose they satisfy:

$$z = \Theta a$$
$$J = J(z)$$

Then we can get:

$$\frac{\partial J}{\partial a} = \begin{bmatrix} \frac{\partial J}{\partial a_1} \\ \vdots \\ \frac{\partial J}{\partial a_d} \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^m \frac{\partial J}{\partial z_j} \frac{z_j}{a_1} \\ \vdots \\ \sum_{j=1}^m \frac{\partial J}{\partial z_j} \frac{z_j}{a_d} \end{bmatrix} = \begin{bmatrix} \frac{\partial z_1}{\partial a_1} & \dots & \frac{\partial z_m}{\partial a_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_1}{\partial a_d} & \dots & \frac{\partial z_m}{\partial a_d} \end{bmatrix} \begin{bmatrix} \frac{\partial J}{\partial z_1} \\ \vdots \\ \frac{\partial J}{\partial z_m} \end{bmatrix} = \frac{\partial z}{\partial a}\frac{\partial J}{\partial z} = \Theta^T \frac{\partial J}{\partial z}$$

$$\frac{\partial J}{\partial \Theta_{ij}} = \sum_{k=1}^{m} \frac{\partial J}{\partial z_k}\frac{\partial z_k}{\partial \Theta_{ij}} = \frac{\partial J}{\partial z_i}\frac{\partial z_i}{\partial \Theta_{ij}} = \frac{\partial J}{\partial z_i} a_j$$

$$\frac{\partial J}{\partial \Theta} = \begin{bmatrix} \frac{\partial J}{\partial z_1} \\ \vdots \\ \frac{\partial J}{\partial z_m} \end{bmatrix} \begin{bmatrix} a_1 & \dots & a_d \end{bmatrix} = \frac{\partial J}{\partial z} a^T$$

element-wise chain rule:
Assume $z, a \in \mathbb{R}^d$:

$$a = \sigma(z), \text{ where } \sigma \text{ is an element-wise activation}$$
$$J = J(a)$$

Then we have:

$$\frac{\partial J}{\partial z} = \frac{\partial J}{\partial a} \odot \sigma'(z)$$

Where σ' is the element-wise derivative of the activation function σ.

3.5 Backpropagation

To train the model, we need to update Θ for each epoch: (gradient decent)

$$\Theta := \Theta - \alpha \frac{\partial}{\partial \Theta} J(\Theta)$$

We can see $\frac{\partial}{\partial \Theta} J(\Theta)$ is hard to get directly. There is an easier way to calculate it. For each training example $(x^{(q)}, y^{(q)}), q \in \{1, \ldots, m\}$, define **loss function**:

$$J = -\sum_{k=1}^{K} [y_k^{(q)} log(h_\Theta(x^{(q)})_k) + (1 - y_k^{(q)}) log(1 - h_\Theta(x^{(q)})_k)]$$

Apply chain rule we have:

$$\begin{aligned}
\frac{\partial J}{\partial \Theta^{(l)}} &= \frac{\partial J}{\partial z^{(l+1)}} (a^{(l)})^T \\
\frac{\partial J}{\partial a^{(l)}} &= (\Theta^{(l)})^T \frac{\partial J}{\partial z^{(l+1)}} \\
\frac{\partial J}{\partial z^{(l)}} &= \frac{\partial J}{\partial a^{(l)}} \odot g'(z^{(l)}) \\
&= (\Theta^{(l)})^T \frac{\partial J}{\partial z^{(l+1)}} \odot g'(z^{(l)}) \\
&= (\Theta^{(l)})^T \frac{\partial J}{\partial z^{(l+1)}} \odot (a^{(l)} \odot (1 - a^{(l)}))
\end{aligned}$$

For $p \in \{1, ..., K\}$:

$$\begin{aligned}
\frac{\partial J}{\partial z_p^{(L)}} &= \frac{\partial}{\partial z_p^{(L)}} \sum_{k=1}^{K} -[y_k^{(q)} log(h_\Theta(x^{(q)})_k) + (1 - y_k^{(q)}) log(1 - h_\Theta(x^{(q)})_k)] \\
&= \frac{\partial}{\partial z_p^{(L)}} \{-[y_p^{(q)} log(\frac{1}{1 + e^{-z_p^{(L)}}}) + (1 - y_p^{(q)}) log(1 - \frac{1}{1 + e^{-z_p^{(L)}}})]\} \\
&= -[y_p^{(q)} (1 + e^{-z_p^{(L)}}) \frac{0 - (-e^{-z_p^{(L)}})}{(1 + e^{-z_p^{(L)}})^2} + (1 - y_p^{(q)}) \frac{1 + e^{-z_p^{(L)}}}{e^{-z_p^{(L)}}} \frac{(-e^{-z_p^{(L)}})(1 + e^{-z_p^{(L)}}) - e^{-z_p^{(L)}}(-e^{-z_p^{(L)}})}{(1 + e^{-z_p^{(L)}})^2}] \\
&= -[y_p^{(q)} \frac{e^{-z_p^{(L)}}}{1 + e^{-z_p^{(L)}}} + (1 - y_p^{(q)}) \frac{-1}{1 + e^{-z_p^{(L)}}}] \\
&= -\frac{y_p^{(q)} e^{-z_p^{(L)}} + y_p^{(q)} - 1}{1 + e^{-z_p^{(L)}}} \\
&= \frac{1}{1 + e^{-z_p^{(L)}}} - y_p^{(q)} \\
&= a_p^{(L)} - y_p^{(q)}
\end{aligned}$$

Then we get:

$$\frac{\partial J}{\partial z^{(L)}} = \begin{bmatrix} \frac{\partial J}{\partial z_1^{(L)}} \\ \vdots \\ \frac{\partial J}{\partial z_K^{(L)}} \end{bmatrix} = a^{(L)} - y^{(q)}$$

For convenience, define **error term**:

$$\delta^{(l)} = \frac{\partial J}{\partial z^{(l)}}$$

Then we get:

$$\frac{\partial J}{\partial \Theta^{(l)}} = \delta^{(l+1)} (a^{(l)})^T$$
$$\delta^{(l)} = (\Theta^{(l)})^T \delta^{(l+1)} \odot (a^{(l)} \odot (1 - a^{(l)}))$$
$$\delta^{(L)} = a^{(L)} - y^{(q)}$$

backpropagation algorithm: (compute $\frac{\partial}{\partial \Theta} J(\Theta)$)

```
training set: $(x^{(q)}, y^{(q)}), q \in \{1, \ldots, m\}$
set $\Delta_{ij}^{(l)} = 0, l \in \{1, \ldots, L-1\}$
for $q \in \{1, \ldots, m\}$:
    forward propagation: compute $a^{(l)}$ for $l \in \{2, \ldots, L\}$
    compute $\delta^{(L)} = a^{(L)} - y^{(q)}$
    for $l \in \{L-1, \ldots, 2\}$:
        compute $\delta^{(l)} = (\Theta^{(l)})^T \delta^{(l+1)} \odot (a^{(l)} \odot (1 - a^{(l)}))$
    for $l \in \{1, \ldots, L-1\}$:
        compute $\Delta^{(l)} := \Delta^{(l)} + \frac{\partial J}{\partial \Theta^{(l)}} = \Delta^{(l)} + \delta^{(l+1)} (a^{(l)})^T$
compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = D_{ij}^{(l)} = \begin{cases} \frac{1}{m}\Delta_{ij}^{(l)} + \frac{\lambda}{m}\Theta_{ij}^{(l)}, & \text{if } j \neq 0 \\ \frac{1}{m}\Delta_{ij}^{(l)}, & \text{if } j = 0 \end{cases}$
```

3.6 Backpropagation in Practice

unrolling parameters:
We can concat flattened matrices into a single vector for the convenience of some calculations. Also after slice and reshape on the vector we can get matrices back.

$$thetaVector = concat(\Theta^{(1)}.flatten(), \ldots, \Theta^{(L-1)}.flatten())$$
$$deltaVector = concat(D^{(1)}.flatten(), \ldots, D^{(L-1)}.flatten())$$

gradient checking:
We can approximate the derivative of $J(\Theta)$ with respect to $\Theta_{ij}^{(l)}$ as:

$$\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) \approx \frac{J(\ldots, \Theta_{ij}^{(l)} + \epsilon, \ldots) - J(\ldots, \Theta_{ij}^{(l)} - \epsilon, \ldots)}{2\epsilon}$$

A small value for ϵ such as $\epsilon = 10^{-4}$, guarantees that the math works out properly. If the value for ϵ is too small, we can end up with numerical problems. Then we can check if $gradApprox \approx deltaVector$. Once you have verified once that your backpropagation algorithm is correct, you don't need to compute gradApprox again. The code to compute gradApprox can be very slow.

random initialization: (symmetry breaking)
Initializing all the weights to zero does not work with neural networks, because all hidden units will be completely identical (symmetric) - compute exactly the same function. When we backpropagate, all nodes

will update to the same value repeatedly. Instead we can randomly initialize our weights for our Θ matrices using the following method: (here ϵ is a value selected for random initialization)

$$\text{initialize each } \Theta_{ij}^{(l)} \text{ to a random value in } [-\epsilon, +\epsilon]$$

One effective strategy for choosing ϵ is to base it on the number of units in the network: (Xavier normalized initialization)

$$\epsilon^{(l)} = \frac{\sqrt{6}}{\sqrt{s^{(l)} + s^{(l+1)}}}$$

in summary:
First, pick a network architecture; choose the layout of your neural network, including how many hidden units in each layer and how many layers in total you want to have.

- Number of input units = dimension of features $x^{(i)}$
- Number of output units = number of classes
- Number of hidden units per layer = usually more the better (must balance with cost of computation as it increases with more hidden units)
- Defaults: 1 hidden layer. If you have more than 1 hidden layer, then it is recommended that you have the same number of units in every hidden layer.

Training a Neural Network

1. Randomly initialize the weights
2. Implement forward propagation to get $h_\Theta(x^{(i)})$ for any $x^{(i)}$
3. Implement the cost function
4. Implement backpropagation to compute partial derivatives
5. Use gradient checking to confirm that your backpropagation works. Then disable gradient checking.
6. Use gradient descent or a built-in optimization function to minimize the cost function with the weights in theta.

This will minimize our cost function. However, keep in mind that $J(\Theta)$ is not always convex and thus we can end up in a local minimum instead.

4 Evaluating a Learning Algorithm

4.1 Concepts

Possible methods to improve the performance of model:

- Getting more training examples.
- Trying smaller sets of features.
- Trying additional features.
- Trying polynomial features.
- Increasing or decreasing λ.

Break down our dataset into the three sets:

- Training set: 60%. A set of examples used for learning the optimal weights with backpropagation.
- Cross validation set: 20%. A set of examples used to tune the hyper parameters including the number of layers and hidden units, and find a stopping point for the backpropagation algorithm to avoid over-fitting.
- Test set: 20%. A set of examples used only to assess the performance of a fully-trained model.

The estimate of the final model on validation data will be biased (smaller than the true error rate) since the validation set is used to select the final model. So we need to use test set to to assess the performance of the final model.

We can now calculate three separate error values for the three different sets using the following method:

1. Optimize the parameters in Θ using the training set for each polynomial degree.
2. Find the polynomial degree d with the least error using the cross validation set.
3. Estimate the generalization error using the test set with $J_{test}(\Theta^{[d]})$.

This way, the degree of the polynomial d has not been trained using the test set.

The test error:

1. For linear regression:

$$J(\Theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\Theta(x^{(i)}) - y^{(i)})^2 + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2$$

$$J_{train}(\Theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\Theta(x^{(i)}) - y^{(i)})^2$$

$$J_{cv}(\Theta) = \frac{1}{2m_{cv}}\sum_{i=1}^{m_{cv}}(h_\Theta(x_{cv}^{(i)}) - y_{cv}^{(i)})^2$$

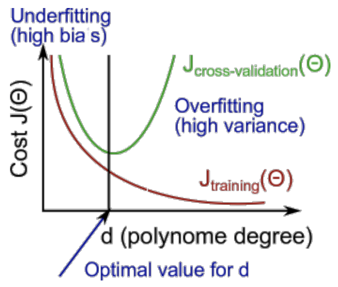
$$J_{test}(\Theta) = \frac{1}{2m_{test}}\sum_{i=1}^{m_{test}}(h_\Theta(x_{test}^{(i)}) - y_{test}^{(i)})^2$$

2. For classification: (misclassification error, aka 0/1 misclassification error)

$$err(h_\Theta(x), y) = \begin{cases} 1, & \text{if } h_\Theta(x) \geq 0.5 \text{ and } y = 0 \text{ or } h_\Theta(x) < 0.5 \text{ and } y = 1 \\ 0, & \text{otherwise} \end{cases}$$

$$\text{test error} = \frac{1}{m_{test}}\sum_{i=1}^{m_{test}} err(h_\Theta(x_{test}^{(i)}), y_{test}^{(i)})$$

Bias and Variance:
The training error will tend to decrease as we increase the degree d of the polynomial. At the same time, the cross validation error will tend to decrease as we increase d up to a point, and then it will increase as d is increased, forming a convex curve.



High bias(underfitting): both $J_{train}(\Theta)$ and $J_{cv}(\Theta)$ will be high. Also, $J_{cv}(\Theta) \approx J_{train}(\Theta)$.
High variance(overfitting): $J_{train}(\Theta)$ will be low and $J_{cv}(\Theta)$ will be high. Also, $J_{cv}(\Theta) \gg J_{train}(\Theta)$.

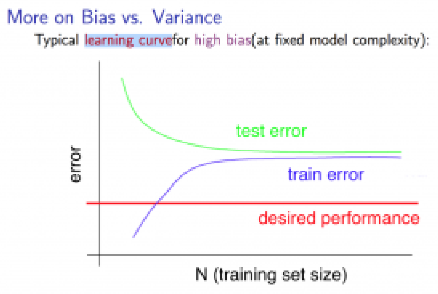
Regularization:
$\lambda = 0$ causes overfitting. λ too large causes underfitting. To find a good λ:

1. Create a list of lambdas (i.e. $\lambda \in \{0, 0.1, 0.2, 0.4, 0.8, ..., 6.4\}$).
2. Create a set of models with different degrees or any other variants.
3. Iterate through the λs and for each λ go through all the models to learn some Θ.
4. Compute the cross validation error using the learned Θ(computed with λ) on the $J_{cv}(\Theta)$.
5. Select the best combo that produces the lowest error on the cross validation set.
6. Using the best combo Θ and λ, apply it on $J_{test}(\Theta)$ to see if it has a good generalization of the problem.

Learning curves:
Training an algorithm on a very few number of data points (such as 1, 2 or 3) will easily have 0 errors because we can always find a quadratic curve that touches exactly those number of points. Hence:

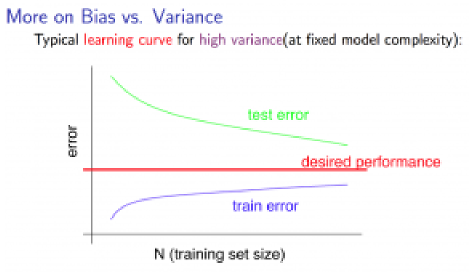
- As the training set gets larger, the error for a quadratic function increases.
- The error value will plateau out after a certain m, or training set size.

When Experiencing high bias:



Low training set size: $J_{train}(\Theta)$ will be low and $J_{cv}(\Theta)$ will be high.
Large training set size: both $J_{train}(\Theta)$ and $J_{cv}(\Theta)$ will be high, with $J_{train}(\Theta) \approx J_{cv}(\Theta)$.
If a learning algorithm is suffering from high bias, getting more training data will not (by itself) help much.

When Experiencing high variance:



Low training set size: $J_{train}(\Theta)$ will be low and $J_{cv}(\Theta)$ will be high.
Large training set size: $J_{train}(\Theta)$ will increase and $J_{cv}(\Theta)$ will decrease, with $J_{train}(\Theta) < J_{cv}(\Theta)$ significantly.
If a learning algorithm is suffering from high variance, getting more training data is likely to help.

Optimizing approaches:

- Getting more training examples: Fixes high variance.
- Trying smaller sets of features: Fixes high variance.
- Adding features: Fixes high bias.
- Adding polynomial features: Fixes high bias.
- Decreasing λ: Fixes high bias.
- Increasing λ: Fixes high variance.

Diagnosing Neural Networks:

- A neural network with fewer parameters is prone to underfitting. It is also computationally cheaper.
- A large neural network with more parameters is prone to overfitting. It is also computationally expensive. In this case you can use regularization (increase λ) to address the overfitting.

Using a single hidden layer is a good starting default. You can train your neural network on a number of hidden layers using your cross validation set. You can then select the one that performs best.

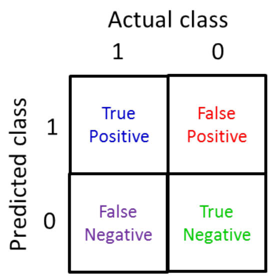
Model Complexity Effects:

- Lower-order polynomials (low model complexity) have high bias and low variance. In this case, the model fits poorly consistently.
- Higher-order polynomials (high model complexity) fit the training data extremely well and the test data extremely poorly. These have low bias on the training data, but very high variance.
- In reality, we would want to choose a model somewhere in between, that can generalize well but also fits the data reasonably well.

Recommended approach:

- Start with a simple algorithm, implement it quickly, and test it early on your cross validation data.
- Plot learning curves to decide if more data, more features, etc. are likely to help.
- Manually examine the errors on examples in the cross validation set and try to spot a trend where most of the errors were made.

Precision & Recall: (deal with skewed classes)
High $F_{score} \in [0,1]$ (high precision and high recall) represents a good prediction model.



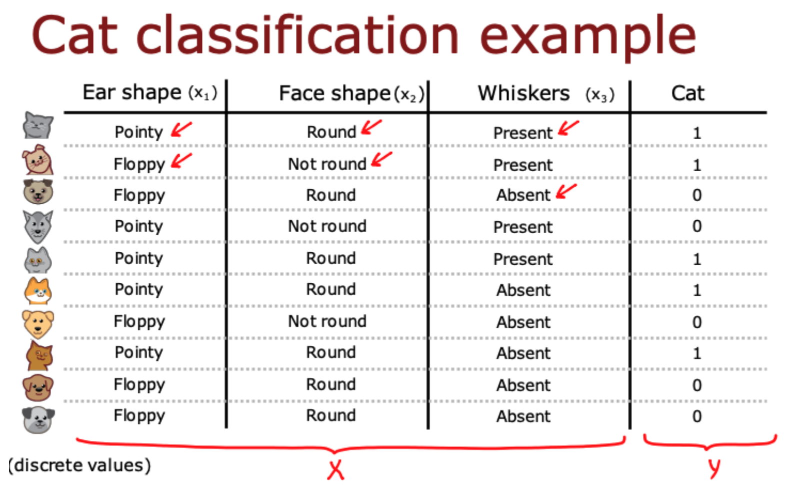
$$\text{Precision} = \frac{\text{True positives}}{\text{predicted as positive}} = \frac{\text{True positives}}{\text{True positives} + \text{False positives}}$$

$$\text{Recall} = \frac{\text{True positives}}{\text{actual positives}} = \frac{\text{True positives}}{\text{True positives} + \text{False negatives}}$$

$$F_{score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

5 Decision Tree

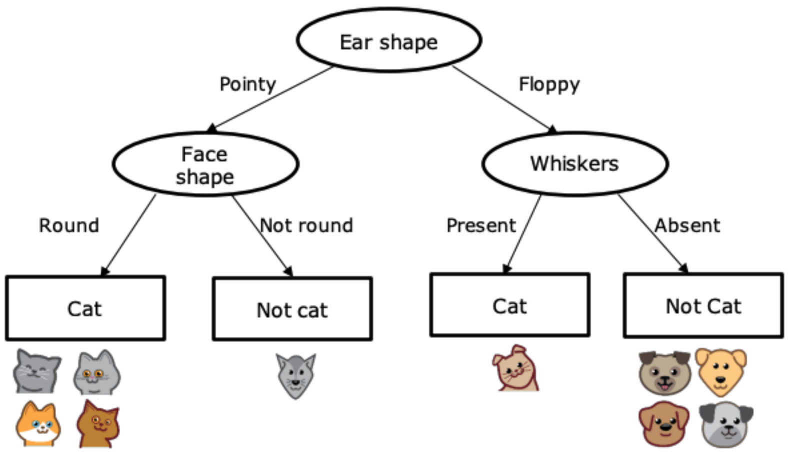
5.1 Classification



Cat classification example

Ear shape (x_1)	Face shape (x_2)	Whiskers (x_3)	Cat
Pointy	Round	Present	1
Floppy	Not round	Present	1
Floppy	Round	Absent	0
Pointy	Not round	Present	0
Pointy	Round	Present	1
Pointy	Round	Absent	1
Floppy	Not round	Absent	0
Pointy	Round	Absent	1
Floppy	Round	Absent	0
Floppy	Round	Absent	0

(discrete values) X y



root node: The node on the top.

decision node: The node used to split data.

leaf node: The node on the bottom.

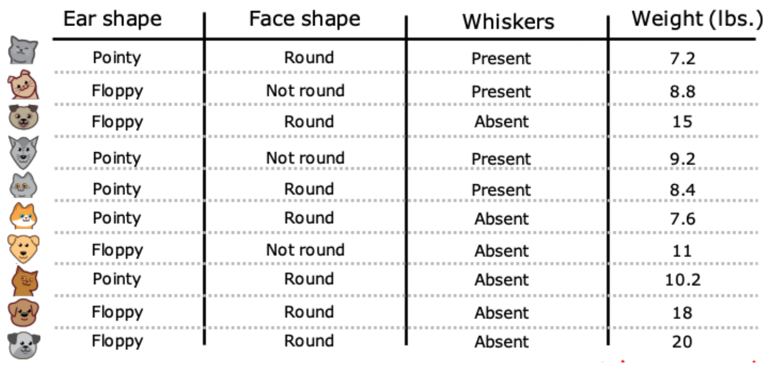
node entropy: Measure of the purity of the split data on nodes. Large if the data is not pure. Small if data is pure. Assume decision tree has K output classes. For $i \in \{1, \ldots, K\}$, p_k is the proportion of class k of all the data examples this node has.

$$H(node) = -\sum_{i=1}^{K} p_k \log_2 p_k$$

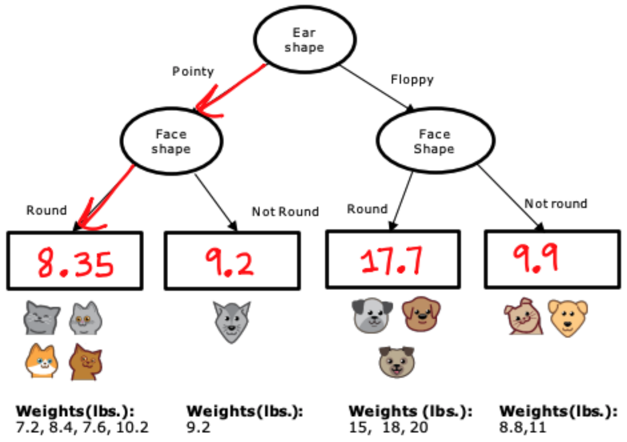
information gain: Reduce of entropy from parent to children nodes. Assume parent node has C children, m_p data examples, entropy $H(p)$. Each child for $c \in \{1, \ldots, C\}$ has m_c data examples, entropy $H(c)$.

$$IG(parent, children) = H(p) - \sum_{c=1}^{C} \frac{m_c}{m_p} H(c)$$

5.2 Regression



Ear shape	Face shape	Whiskers	Weight (lbs.)
Pointy	Round	Present	7.2
Floppy	Not round	Present	8.8
Floppy	Round	Absent	15
Pointy	Not round	Present	9.2
Pointy	Round	Present	8.4
Pointy	Round	Absent	7.6
Floppy	Not round	Absent	11
Pointy	Round	Absent	10.2
Floppy	Round	Absent	18
Floppy	Round	Absent	20



node entropy.: For regression problem, we can use variance of the outputs of the examples on node $\sigma^2(node)$ as the entropy.

$$H(node) = \sigma^2(node)$$

information gain: Same expression as classification problem, just with different entropy.

$$IG(parent, children) = H(p) - \sum_{c=1}^{C} \frac{m_c}{m_p} H(c)$$

5.3 Decision Tree Learning

Notice that the decision tree splitting is a recursive process. Each of the children splits in the same way like their parents.

- Start with all examples at the root node
- Calculate information gain for all possible features, and pick the one with the highest information gain
- Split dataset according to selected feature, and create branches of the tree
- Keep repeating splitting process until stopping criteria is met:
  - When a node is 100% one class
  - When splitting a node will result in the tree exceeding a maximum depth
  - Information gain from additional splits is less than threshold
  - When number of examples in a node is below a threshold

What if feature has multiple possible values?
Use one-hot encoding to build training set. For example, if **Ear shape** has 3 possible values: **Pointy**, **Floppy**, **Oval**. We can add three features for each of the possible values to the training set, instead of adding **Ear shape** as a feature.

What if feature is continuous?
Use ranges of the feature to build training set. For example, **Weight** has a continuous value. We can add ranges: $Weight \leq 0.8$, $0.8 < Weight < 0.9$, $Weight \geq 0.9$ as features to the training set.

5.4 Decision Tree Prediction

Feed an example to the root node. After the processing, the example will reach the leaf node.

- **Classification**: The class k of the largest proportion p_k on leaf node on training examples is the prediction of decision tree.
- **Regression**: The average value of the outputs of training examples on the leaf node is the prediction of decision tree.

5.5 Tree Ensembles

Depending on the given training set, trained decision trees can be totally different and the performance can be unstable. Tree ensembles samples the training set randomly (sampling with replacement) to create multiple training sets with same size. With these training sets we can train multiple decision trees, and use them to do prediction. And take the final prediction based on the votes generated from different decision tree models.

5.6 Random Forest Algorithm

Given training set of size m, for $b \in \{1, \dots, B\}$ (B means "bags", the number of training sets we want to generate): use sampling with replacement to create a new training set of size m, then train a decision tree on the new dataset.

Randomizing the feature choice: at each node, when choosing a feature to use to split, if n features are available, pick a random subset of $k < n$ features (can use $k = \sqrt{n}$ when n is large) and allow the algorithm to only choose from that subset of features. This is to prevent the first a few level of tree using the same features at nodes even when the training set is randomly sampled. This helps to generate more different decision tree models.

5.7 XGBoost (Extreme Gradient Boosting)

Given training set of size m, for $b \in \{1, \dots, B\}$ (B means "bags", the number of training sets we want to generate): use sampling with replacement to create a new training set of size m. **(But instead of picking from all examples with equal $\frac{1}{m}$ probability, make it more likely to pick examples that the previously trained trees misclassify.)** Then train a decision tree on the new dataset. (* The sampling approach is complicated and not covered in this section.)

This helps to make the training process focus on the training data that the decision tree currently cannot do well on.

5.8 Decision Trees vs Neural Networks

Decision Trees and Tree ensembles:

- Works well on tabular (structured) data

- Not recommended for unstructured data (images, audio, text)
- Fast
- Small decision trees may be human interpretable

Neural Networks:

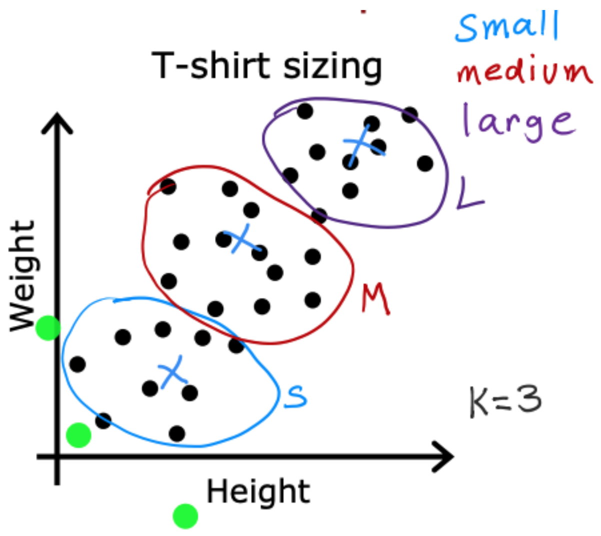
- Works well on all types of data, including tabular (structured) and unstructured data
- May be slower than a decision tree
- Works with transfer learning
- When building a system of multiple models working together, it might be easier to string together multiple neural networks

6 Unsupervised Learning

6.1 Clustering

Clustering is the task of grouping a set of objects in such a way that objects in the same group (called a cluster) are more similar (in some sense) to each other than to those in other groups (clusters).

6.1.1 K-means



K: number of clusters we want to get.
$c^{(i)}$: index of cluster $\{1,\ldots,K\}$ to which example $x^{(i)}$ is currently assigned.
μ_k: cluster centroid of cluster $k \in \{1,\ldots,K\}$.
$\mu_{c^{(i)}}$: cluster centroid of cluster to which example $x^{(i)}$ has been assigned.
cost function:

$$J(c^{(1)},\ldots,c^{(m)},\mu_1,\ldots,\mu_K) = \frac{1}{m}\sum_{i=1}^{m} ||x^{(i)} - \mu_{c^{(i)}}||^2$$

Random initialization: (reduce the chance of getting local optimum)

```
repeat 50 - 1000 times: {
    pick $K$ random examples from the dataset as $\{\mu_1,\ldots,\mu_K\}$
    for $i \in \{1,\ldots,m\}$, $c^{(i)}$ := index of cluster centroid closest to $x^{(i)}$
    compute $J(c^{(1)},\ldots,c^{(m)},\mu_1,\ldots,\mu_K)$
}
```

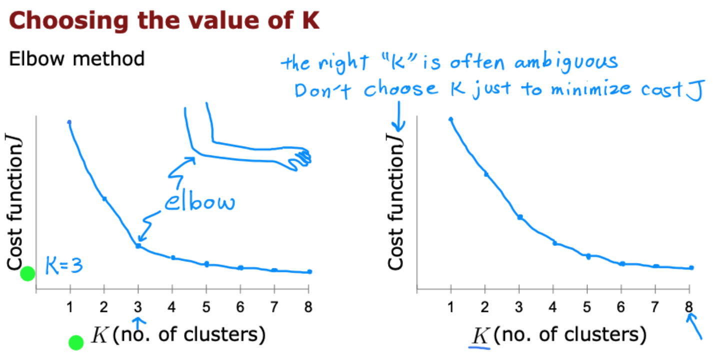
then pick the set of clusters that gave lowest cost J

Clustering process:

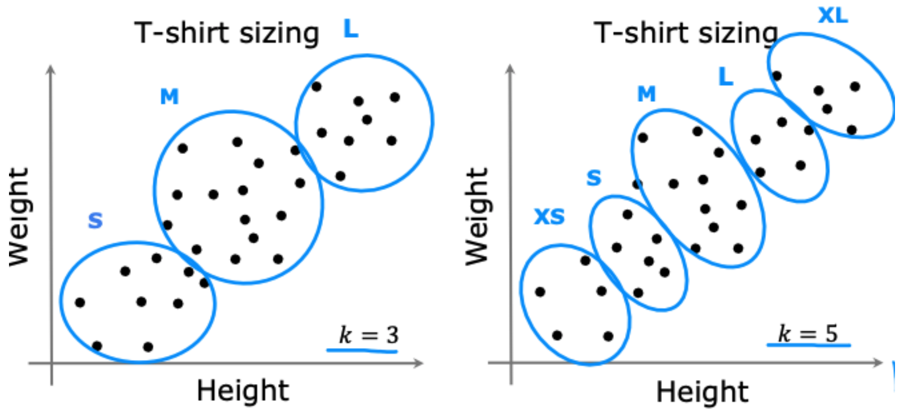
```
repeat until convergence {
    # assign points to cluster centroids
    for $i \in \{1, \dots, m\}$, $c^{(i)}$ := index of cluster centroid closest to $x^{(i)}$
    # move cluster centroids
    for $k \in \{1, \dots, K\}$, $\mu_k$ := average (mean) of points assigned to cluster $k$
}
```

How to choose K?

We can use elbow method to pick the value of K.



Often, you want to get clusters for some later (downstream) purpose. Evaluate K-means based on how well it performs on that later purpose to choose the value of K.



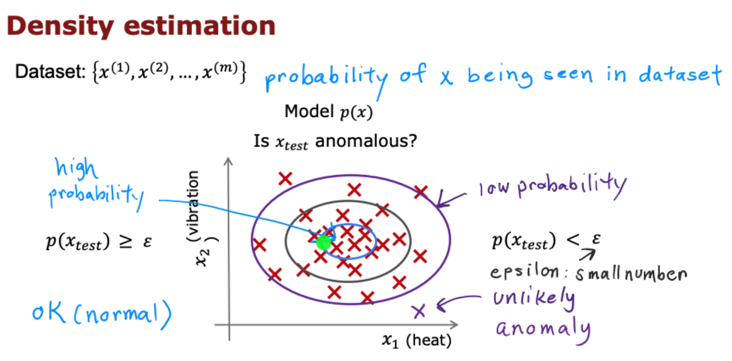
6.2 Anomaly Detection

Anomaly detection is generally understood to be the identification of rare items, events or observations which deviate significantly from the majority of the data and do not conform to a well defined notion of normal behaviour.

Gaussian (Normal) Distribution:

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

Anomaly Detection Algorithm:



Model normal distribution $p(x)$ from data. Identify unusual data by checking which have $p(x) < \epsilon$.

$$\mu = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$$

$$\sigma^2 = \frac{1}{m}\sum_{i=1}^{m} ||x^{(i)} - \mu||^2$$

$$p(x) = \prod_{j=1}^{n} p(x_j; \mu_j; \sigma_j^2) = \prod_{j=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_j} e^{\frac{-(x_j-\mu_j)^2}{2\sigma_j^2}}$$

$$y = \begin{cases} 1, & \text{if } p(x) < \epsilon \text{ (anomaly)} \\ 0, & \text{if } p(x) \geq \epsilon \text{ (normal)} \end{cases}$$

training set: m training examples with $y = 0$ (non-anomalous).

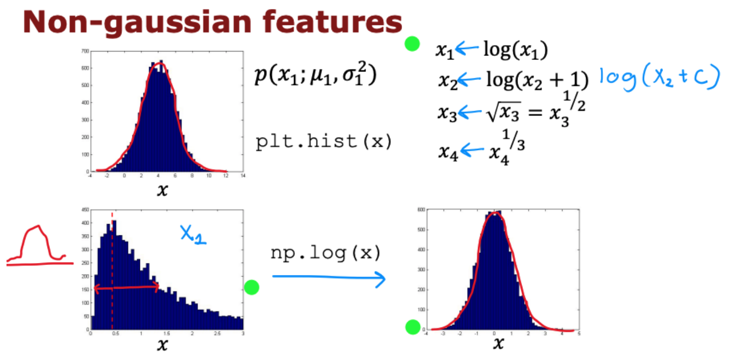
cross validation set: m_{cv} examples with mostly $y = 0$ (non-anomalous) and some $y = 1$ (anomalous).

test set: m_{test} examples with mostly $y = 0$ (non-anomalous) and some $y = 1$ (anomalous).

evaluation: use F_1 score for skewed dataset.

Training Process:
Fit model $p(x)$ on training set. (get μ, σ^2)
On cross validation/test set, do evaluation and tune ϵ, x_j to minimize F_1 score. (choose the right threshold and features)

Non-gaussian Features:



We want the features fit gaussian distribution well. But features are not always normally distributed. We can process the features to make them normally distributed, for example: use $log(x_j + c)$, $x_j^{\frac{1}{c}}$ instead of x_j.

The most common problem in anomaly detection is $p(x)$ is similar for normal and anomalous examples. To solve this problem, we can choose features that might take on unusually large or small values in the event of an anomaly. These features can distinct anomalous examples from the normal ones.

Choose features based on $p(x)$: large for normal examples, small for anomaly examples in the cross validation set.

For example: x_3 is CPU load, x_4 is network traffic. We can construct:

$$x_5 = \frac{(\text{CPU load})^2}{\text{network traffic}}$$

Anomaly Detection vs. Supervised Learning:
Use Anomaly detection if:

- Very small number (0 to 20) of positive examples $y = 1$; large number of negative examples $y = 0$; Model $p(x)$ with just negative examples. Use positive examples for cv and test sets.
- Many different "types" of anomalies. Hard for any algorithm to learn (from just positive examples) what the anomalies look like. Future anomalies may look nothing like any of the anomalous examples seen so far.
- e.g. Fraud detection; Manufacturing finding new previously unseen defects; Monitoring machines in a data center; Security applications.

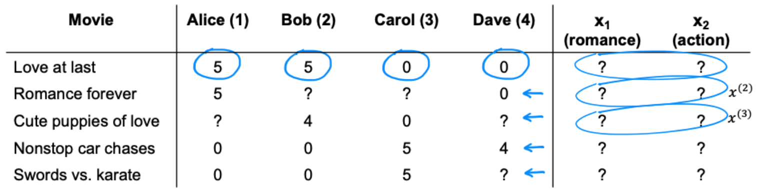
Use Supervised Learning if:

- Large number of positive and negative examples.
- Enough positive examples for algorithm to get a sense of what positive examples are like. Future positive examples likely to be similar to ones in training set.
- e.g. Email spam classification; Manufacturing finding known, previously seen defects; Weather prediction; Diseases classification.

7 Recommender System

7.1 Collaborative Filtering

collaborative filtering is a method of making automatic predictions (filtering) about the interests of a user by collecting preferences or taste information from many users (collaborating).



Movie	Alice (1)	Bob (2)	Carol (3)	Dave (4)	x_1 (romance)	x_2 (action)
Love at last	5	5	0	0	?	?
Romance forever	5	?	?	0	?	?
Cute puppies of love	?	4	0	?	?	?
Nonstop car chases	0	0	5	4	?	?
Swords vs. karate	0	0	5	?	?	?

$r(i,j)$: if user j has rated movie i (1 or 0)
$y^{(i,j)}$: rating given by user j on movie i
$w^{(j)}, b^{(j)}$: parameters for user j
$x^{(i)}$: feature vector for movie i
$m^{(j)}$: number of movies rated by user j
n_m: number of movies
n_u: number of users
n: number of features

predict rating: (user j on movie i)

$$f_{(w,b,x)}(x^{(i)}) = w^{(j)} \cdot x^{(i)} + b^{(j)}$$

cost function to learn: $\{w^{(1)}, b^{(1)}, \ldots, w^{(n_u)}, b^{(n_u)}\}$

$$J(w,b) = \frac{1}{2}\sum_{j=1}^{n_u} \sum_{i:r(i,j)=1} (w^{(j)} \cdot x^{(i)} + b^{(j)} - y^{(i,j)})^2 + \frac{\lambda}{2}\sum_{j=1}^{n_u}\sum_{k=1}^{n}(w_k^{(j)})^2$$

cost function to learn: $\{x^{(1)}, \ldots, x^{(n_m)}\}$

$$J(x) = \frac{1}{2}\sum_{i=1}^{n_m} \sum_{j:r(i,j)=1} (w^{(j)} \cdot x^{(i)} + b^{(j)} - y^{(i,j)})^2 + \frac{\lambda}{2}\sum_{i=1}^{n_m}\sum_{k=1}^{n}(x_k^{(i)})^2$$

cost function: (combined)

$$J(w,b,x) = \frac{1}{2} \sum_{(i,j):r(i,j)=1} (w^{(j)} \cdot x^{(i)} + b^{(j)} - y^{(i,j)})^2 + \frac{\lambda}{2}\sum_{j=1}^{n_u}\sum_{k=1}^{n}(w_k^{(j)})^2 + \frac{\lambda}{2}\sum_{j=1}^{n_m}\sum_{k=1}^{n}(x_k^{(i)})^2$$

Training Process:
repeat until convergence {

$$w_i^{(j)} = w_i^{(j)} - \alpha \frac{\partial}{\partial w_i^{(j)}} J(w,b,x)$$

$$b^{(j)} = b^{(j)} - \alpha \frac{\partial}{\partial b^{(j)}} J(w,b,x)$$

$$x_k^{(i)} = x_k^{(i)} - \alpha \frac{\partial}{\partial x_k^{(i)}} J(w,b,x)$$

}

Binary Labels:
predict like/unlike: (user j on movie i)

$$f_{(w,b,x)}(x^{(i)}) = g(w^{(j)} \cdot x^{(i)} + b^{(j)})$$

cost function:

$$J(w,b,x) = \sum_{(i,j):r(i,j)=1} -y^{(i,j)} log(f_{(w,b,x)}(x^{(i)})) - (1 - y^{(i,j)}) log(1 - f_{(w,b,x)}(x^{(i)}))$$

Finding Related Items:
Find item k with $x^{(k)}$ similiar to $x^{(i)}$ with smallest distance:

$$||x^{(k)} - x^{(i)}||^2 = \sum_{l=1}^{n}(x_l^{(k)} - x_l^{(i)})^2$$

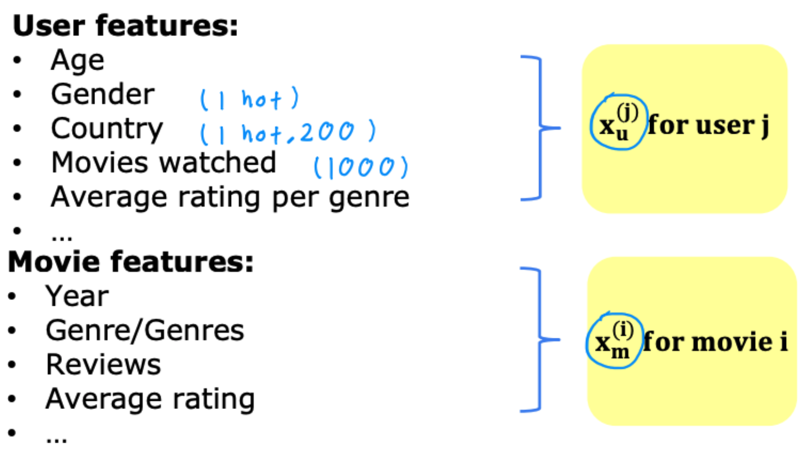
Limitations of Collaborative Filtering:

- Cold start problem
  - How to rank new items that few users have rated?
  - How to show something reasonable to new users who have rated few items?
- Use side information about items or users
  - Item: Genre, movie stars, studio, ...
  - User: Demographics(age, gender, location), expressed preferences, ...

7.2 Content-based Filtering

Content-based filtering uses item features to recommend other items similar to what the user likes, based on their previous actions or explicit feedback.

We can construct 2 neural networks: user network, movie network. And then combine them, train them and make predictions.

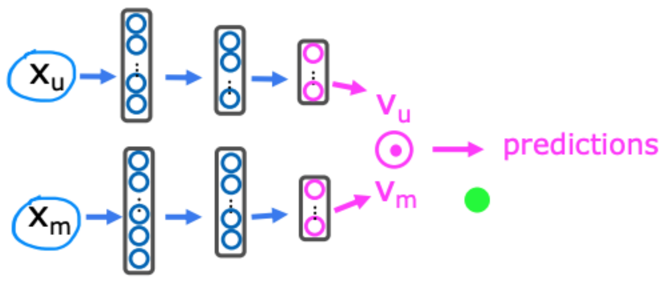


User features:
- Age
- Gender (1 hot)
- Country (1 hot, 200)
- Movies watched (1000)
- Average rating per genre
- ...

$x_u^{(j)}$ **for user j**

Movie features:
- Year
- Genre/Genres
- Reviews
- Average rating
- ...

$x_m^{(i)}$ **for movie i**



x_u: user features.
x_m: movie features.
v_u: learned user vector.
v_m: learned movie vector.

cost function:

$$J = \sum_{(i,j):r(i,j)=1} (v_u^{(j)} \cdot v_m^{(i)} - y^{(i,j)})^2 + \text{NN regularization term}$$

Finding Related Items:
To find movies similar to movie i with small distance:

$$||v_m^{(k)} - v_m^{(i)}||^2$$

How to efficiently find recommendation from a large set of items?

- Retrieval:
  - Generate large list of plausible item candidates. For example:
    - For each of the last 10 movies watched by the user, find 10 most similar movies
    - For most viewed 3 genres, find the top 10 movies
    - Top 20 movies in the country
  - Combine retrieved items into list, removing duplicates and items already watched/purchased
- Ranking:
  - Take list retrieved and rank using learned model
  - Display ranked items to user

Trade-off:

- Retrieving more items results in better performance, but slower recommendations.
- To analyse/optimize the trade-off, carry out offline experiments to see if retrieving additional items results in more relevant recommendations (i.e., $p(y^{(i,j)}) = 1$ of items displayed to user are higher).

7.3 Ethical Use of Recommender Systems

The goal of the recommender system. Recommend:

- Movies most likely to be rated 5 stars by user
- Products most likely to be purchased
- Ads most likely to be clicked on
- Products generating the largest profit
- Video leading to maximum watch time

However, sometimes we get recommender systems like:

- Maximizing user engagement (e.g. watch time) has led to large social media/video sharing sites to amplify conspiracy theories and hate/toxicity
- Maximizing profit rather than users' welfare

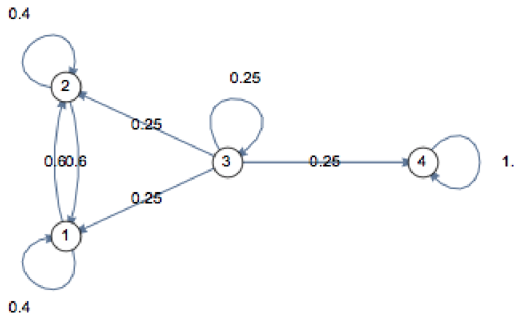
The ameliorations we can take:

- Do not accept ads from exploitative businesses
- Filter out problematic content such as hate speech, fraud, scams and violent content
- Be transparent with users

8 Reinforcement Learning

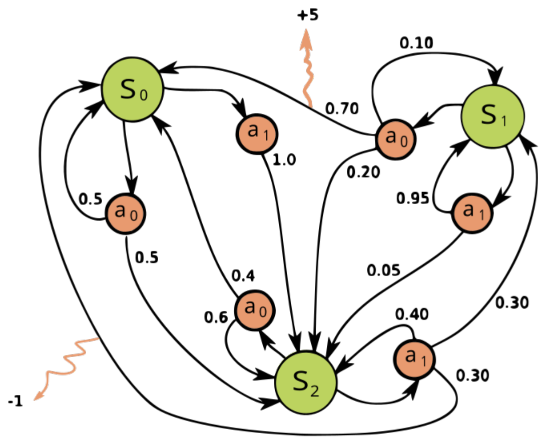
Reinforcement learning (RL) is an area of machine learning concerned with how intelligent agents ought to take actions in an environment in order to maximize the notion of cumulative reward.

8.1 Markov Chain



A Markov chain is a mathematical system that experiences transitions from one state to another according to certain probabilistic rules. The defining characteristic of a Markov chain is that no matter how the process arrived at its present state, the possible future states are fixed. In other words, the probability of transitioning to any particular state is dependent solely on the current state and time elapsed.

8.2 Markov decision process



A Markov decision process is a 4-tuple (S, A, P_a, R_a), where:

S: a set of states called the state space. The state space may be discrete or continuous, like the set of real numbers.
A: a set of actions called the action space (alternatively, A_s is the set of actions available from state s). As for state, this set may be discrete or continuous.
$P_a(s, s')$: on an intuitive level, the probability that action a in state s at time t will lead to state s' at time $t + 1$. In general, this probability transition is defined to satisfy: $Pr(s_{t+1} \in S' \mid s_t = s, a_t = a) = \int_{S'} P_a(s, s')ds', S' \subseteq S$. In case the state space is discrete, the integral is intended with respect to the counting measure, so that the latter simplifies as $P_a(s, s') = Pr(s_{t+1} = s' \mid s_t = s, a_t = a)$.
$R_a(s, s')$: the immediate reward (or expected immediate reward) received after transitioning from state s to state s', due to action a.

A policy function π is a (potentially probabilistic) mapping from state space S to action space A.

8.3 Q-learning

For any finite Markov decision process (FMDP), Q-learning finds an optimal policy in the sense of maximizing the expected value of the total reward over any and all successive steps, starting from the current state. Q-learning can identify an optimal action-selection policy for any given FMDP, given infinite exploration time and a partly-random policy.

s: current state.
a: current action.
s': new state after taking action a.
a': action chosen on state s'.
γ: discount factor.
η: soft update factor.
episode: a sequence of states, from an initial state to a terminal state.
experience: agent's experience on a state $(s, a, R(s), s')$.
M: number of episodes.
T: maximum episode length (time steps) if episode doesn't terminate.
N: memory buffer capacity to store experiences.
C: number of time steps for update.
B: batch size.
$R(s)$: reward from state s.
ϵ: greedy policy during training - with probability ϵ, pick an action randomly; with probability $1-\epsilon$, pick the action that maximizes $Q(s,a)$. (can start high and reduce gradually during the training process)

$Q(s,a)$: The expected cumulative reward for taking action a on state s, then choosing actions for the following states that maximizes cumulative reward.

$$Q(s,a) = R(s) + \gamma \max_{a'} Q(s', a')$$

$\pi(s)$: a policy that given state s, returns best action that maximizes the cumulative reward from state s onward.

$$\pi(s) = \underset{a}{argmax}\ Q(s,a)$$

Training data: get $(s_i, a_i, R(s_i), s_{i+1})$ experience tuple from environment.

$$x^{(i)} = s_i$$

$$y^{(i)} = \begin{cases} R(s_i), & \text{for terminal } s_{i+1} \\ R(s_i) + \gamma \underset{a_{i+1}}{max}\ Q(s_{i+1}, a_{i+1}), & \text{for non-terminal } s_{i+1} \end{cases}$$

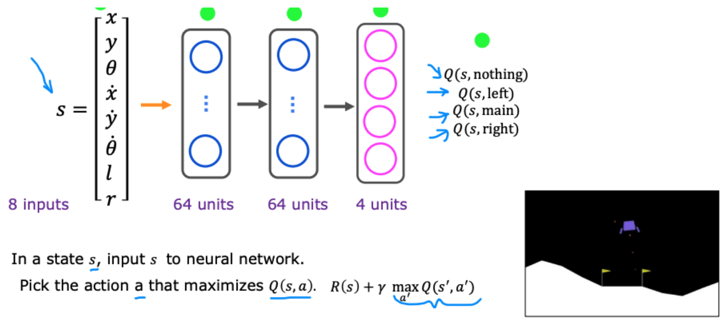
Cost function:

$$J(w,b) = \frac{1}{2m} \sum_{i=1}^{m} (Q(s_i, a_i) - y^{(i)})^2$$

Random (stochastic) environment?
In a stochastic environment, after taking an action, the next state can have multiple possibilities. For example, after taking action a, there is 0.1 chance that we get state s_1, 0.2 chance to get state s_2, and 0.7 chance to get state s_3. To solve this problem, we can take the expectation of following cumulative reward:

$$Q(s,a) = R(s) + \gamma E[\max_{a'} Q(s', a')]$$

Learning Process:



In a state s, input s to neural network.
Pick the action a that maximizes $Q(s,a)$. $R(s) + \gamma \max_{a'} Q(s',a')$

```
Initialize memory buffer with capacity $N$.
Initialize Q-network with random $w, b$ as a guess of $Q(s,a)$.
for $i \in \{1, \dots, M\}$:
    Receive initial state $s_1$.
    for $t \in \{1, \dots, T\}$:
        Choose $a_t$ for $s_t$ with greedy policy $\epsilon$.
        Get $(s_t, a_t, R(s_t), s_{t+1})$ experience tuple from environment.
        Store experience tuple in memory buffer, first in first out.

        Every $C$ time steps perform a learning update:
        Sample $B$ random experiences from memory buffer.
        For $(s_j, a_j, R(s_j), s_{j+1})$, $j \in \{1, \dots, B\}$, construct training sample:
```

$$x^{(j)} = s_j$$

$$y^{(j)} = \begin{cases} R(s_j), & \text{for terminal } s_{j+1} \\ R(s_j) + \gamma \underset{a_{j+1}}{max}\ Q(s_{j+1}, a_{j+1}), & \text{for non-terminal } s_{j+1} \end{cases}$$

```
        Train $Q_{new}$ such that $Q_{new}(s,a) \approx y$:
        Perform a gradient descent with mini batch and implement soft update:
```

$$w = (1-\eta)w + \eta w_{new}$$
$$b = (1-\eta)b + \eta b_{new}$$

```
        Start a new episode if $s_{t+1}$ terminates, else continue.
```

8.4 Policy Gradient

On-policy vs Off-policy learning:
The key difference lies in how these methods approach learning:

- On-policy:
  - Training data is only generated from the exact same policy. e.g. Policy Gradient
  - Learn from your own current strategy (even if it's not the best one yet).
- Off-policy:
  - Training data can originate from other sources that are not from the exact same policy. e.g. Q-learning, with greedy policy ϵ in training, without ϵ in prediction
  - Learn from a different strategy (potentially better or more informed) than what you're currently using.

- The primary distinction lies in how they approach exploration and exploitation, which affects their convergence properties and practical performance in different types of environments.

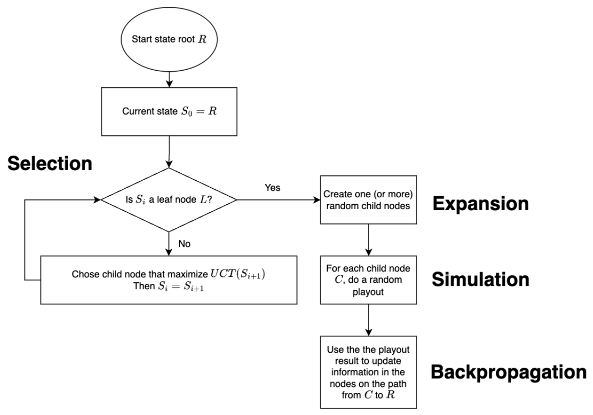
Policy Gradient Algorithms:
TBD: https://lilianweng.github.io/posts/2018-04-08-policy-gradient/

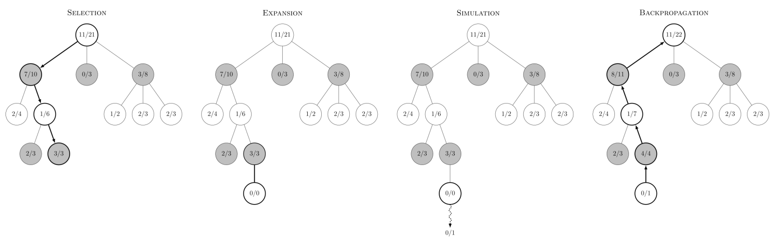
8.5 Monte Carlo tree search (MCTS)

The focus of MCTS is on the analysis of the most promising moves, expanding the search tree based on random sampling of the search space. The application of Monte Carlo tree search in games is based on many playouts, also called roll-outs. In each playout, the game is played out to the very end by selecting moves at random. The final game result of each playout is then used to weight the nodes in the game tree so that better nodes are more likely to be chosen in future playouts.

The most basic way to use playouts is to apply the same number of playouts after each legal move of the current player, then choose the move which led to the most victories. The efficiency of this method—called Pure Monte Carlo Game Search—often increases with time as more playouts are assigned to the moves that have frequently resulted in the current player's victory according to previous playouts. Each round of Monte Carlo tree search consists of four steps:

- Selection: Start from root R and select successive child nodes until a leaf node L is reached. The root is the current game state and a leaf is any node that has a potential child from which no simulation (playout) has yet been initiated. $L = R$ at the beginning of the search. The section below says more about a way (UCT) of biasing choice of child nodes that lets the game tree expand towards the most promising moves, which is the essence of Monte Carlo tree search.
- Expansion: Unless L ends the game decisively (e.g. win/loss/draw) for either player, create one (or more) child nodes. Child nodes are any valid moves from the game position defined by L.
- Simulation: For each node C from the expanded nodes, complete one random playout from node C. This step is sometimes also called playout or rollout. A playout may be as simple as choosing uniform random moves until the game is decided (for example in chess, the game is won, lost, or drawn).
- Backpropagation: Use the result of the playout to update information in the nodes on the path from C to R.


Start state root R
Current state $S_0 = R$
Selection
Is S_i a leaf node L?
Yes
No
Chose child node that maximize $UCT(S_{i+1})$ Then $S_i = S_{i+1}$
Create one (or more) random child nodes
Expansion
For each child node C, do a random playout
Simulation
Use the the playout result to update information in the nodes on the path from C to R
Backpropagation



This graph shows the steps involved in one decision, with each node showing the ratio of wins to total playouts from that point in the game tree for the player that the node represents. In the Selection diagram, black is about to move. The root node shows there are 11 wins out of 21 playouts for white from this position so far. It complements the total of 10/21 black wins shown along the three black nodes under it, each of which represents a possible black move. Note that this graph does not follow the UCT algorithm described below.

If white loses the simulation, all nodes along the selection incremented their simulation count (the denominator), but among them only the black nodes were credited with wins (the numerator). If instead white wins, all nodes along the selection would still increment their simulation count, but among them only the white nodes would be credited with wins. In games where draws are possible, a draw causes the numerator for both black and white to be incremented by 0.5 and the denominator by 1. This ensures that during selection, each player's choices expand towards the most promising moves for that player, which mirrors the goal of each player to maximize the value of their move.

Rounds of search are repeated as long as the time allotted to a move remains. Then the move with the most simulations made (i.e. the highest denominator) is chosen as the final answer.

DeepMind's AlphaZero replaces the simulation step with an evaluation based on a neural network.

UCT (Upper Confidence Bound 1 applied to trees):

The main difficulty in selecting child nodes is maintaining some balance between the exploitation of deep variants after moves with high average win rate and the exploration of moves with few simulations. The first formula for balancing exploitation and exploration in games is called UCT. UCT recommends to choose in each node of the game tree the move for which the following expression has the highest value:

$$\frac{w_i}{n_i} + c\sqrt{\frac{lnN_i}{n_i}}$$

- w_i stands for the number of wins for the node considered after the i-th move
- n_i stands for the number of simulations for the node considered after the i-th move
- N_i stands for the total number of simulations after the i-th move run by the parent node of the one considered
- c is the exploration parameter—theoretically equal to $\sqrt{2}$; in practice usually chosen empirically

The first component of the formula above corresponds to exploitation; it is high for moves with high average win ratio. The second component corresponds to exploration; it is high for moves with few simulations.