Learning theory for classification

g is the *classifier*.

$$g : \mathcal{X} \to \mathcal{Y}$$
$$\mathbb{R}^d \to \{0, 1\}$$

To model the learning problem, we use the pair (X, Y) described by (μ, η) where μ is the probability measure:

$$\mu(A) = \mathbb{P}(X \in A)$$

And η is the regression of Y on X:

$$\eta(X) = \mathbb{P}(Y = 1|X = x) = \mathbb{E}[Y|X = x]$$

η is also called the *a posteriori probability*.
The Bayes classifier is:

$$\begin{cases} 1 & \text{if } \eta(x) > 1/2 \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

Or, if $\mathcal{Y}$ is $\{-1, 1\}$, we write the classifier as such: $g(x) = 2\mathbb{1}\{\eta(x) > 1/2\} - 1$.

Theorem:

For any classifier g: $\mathbb{R}^d \to \{0, 1\}$,

$$\mathbb{P}(g^*(X) \neq Y) \leq \mathbb{P}(g(X) \neq Y)$$

In other words, the Bayes classifier is theorically **the best classifier**.

Proof: express $\mathbb{P}(g(X) \neq Y) - \mathbb{P}(g^*(X) \neq Y)$ in terms of dummies (use complementaries) and show that it is superior to 0.

Logistic regression

Logistic regression is used for binary classification.
It is quite similar to a simple linear regression in the sense that the objective is to find optimal weights ω to predict a variable. However, in the logistic regression we use a sigmoïd function.

Rem: "logistic" because the logistic law has a sigmoïd function as a repartition function.

Rationale behind the use of the sigmoïd function:
We look for the *à posteriori* probability $\mathbb{P}(y = 1|x) = \pi(x) = \hat{y}$.
The predicted variable $\hat{y}$ is thus a probability.

The sigmoïd function: $\sigma : z \to \frac{1}{1+e^{-z}}$ is well adapted because of two reasons:

1) We want an output variable that is included in $[0, 1]$
2) $\frac{\pi(z)}{1-\pi(z)}$ represents the relationship between a distribution and its complementary (good in binary case), and it is just a transformation of $\sigma(z) = \frac{1}{1+e^{-z}} = \frac{e^z}{1-e^z}$

Thus, we have:
$\hat{y} = \mathbb{P}(y = 1|x) = \sigma(\omega^T x + b) = \frac{1}{1-e^{-(\omega^T x+b)}}$

Estimation
Estimation is done using maximum likelihood. Maximum likelihood is finding the parameter that maximizes the probability to have a specific event (x_i, y_i) but in our case, it is a *conditional* maximum likelihood since we want to maximize the *à posteriori* probability that depends on x.

$L(\omega, b) = \prod_{i=1}^{n} \pi(x_i)^{y_i}(1 - \pi(x_i))^{1-y_i}$

This equation has no analytic solution. We use a numeric method to find the optimal parameters (see optimizaton algorithms).
See *Neural Network* section for more details on optimization.

Note: logistic regression is really a linear model since the objective is to find ω that is the slope of the line $\omega^T x + b$.

Linear discriminant analysis

We focus on the binary case, that is when $Y = +1$ or $Y = -1$, that is to sets of variables.
These two conditional laws need to be gaussians with same covariance:
$X|Y = +1 \sim \mathcal{N}(\mu_+, \Sigma)$ with density f_+
$X|Y = -1 \sim \mathcal{N}(\mu_-, \Sigma)$ with density f_-
Let π_+, π_- be the simple probabilities $P(Y = +1)$, $P(Y = -1)$

$\mathbb{P}\{Y = +1|X = x\} = \frac{\mathbb{P}\{Y=+1, X=x\}}{\mathbb{P}\{X=x\}}$
$\mathbb{P}\{Y = +1|X = x\} = \frac{\mathbb{P}\{X=x|Y=+1\}\mathbb{P}\{Y=+1\}}{\mathbb{P}\{X=x\}}$
$\mathbb{P}\{Y = +1|X = x\} = \frac{f_+\pi_+}{\mathbb{P}\{X=x\}}$
$\mathbb{P}\{Y = +1|X = x\} = \frac{f_+\pi_+}{(\mathbb{P}\{X=x|Y=+1\}\mathbb{P}\{Y=+1\}+\mathbb{P}\{X=x|Y=-1\}\mathbb{P}\{Y=-1\})}$
$\mathbb{P}\{Y = +1|X = x\} = \frac{f_+\pi_+}{(f_+\pi_+ + f_-\pi_-)}$
Similarly,
$\mathbb{P}\{Y = -1|X = x\} = \frac{f_-(1-\pi_+)}{\mathbb{P}\{X=x\}}$
$\mathbb{P}\{Y = -1|X = x\} = \frac{f_-(1-\pi_+)}{(f_+\pi_+ + f_-\pi_-)}$

The result shows us that we can express the two conditionnal probabilities in terms of conditionnal densities and "simple" probabilities (π_+, π_-).
Recall that multivariable gaussian density is: $f(x) = \frac{1}{\sqrt{2\pi|\Sigma|}} e^{-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}$
In practice, μ_+, μ_-, π_+ and Σ are unknown. Thus we use empiric values:
$\widehat{\pi}_+ = m/n$
$\widehat{\mu}_+ = \frac{1}{m}\Sigma\mathbb{1}_{\{y_i=+1\}}x_i$
$\widehat{\mu}_- = \frac{1}{n-m}\Sigma\mathbb{1}_{\{y_i=-1\}}x_i$

$\widehat{\Sigma} = \frac{1}{n-2}((m-1)\widehat{\Sigma}_+ + (n-m-1)\widehat{\Sigma}_-)$
$\widehat{\Sigma}_+ = \frac{1}{m-1}\Sigma \mathbb{1}_{\{y_i=+1\}}(x_i - \widehat{\mu}_+)(x_i - \widehat{\mu}_+)^T$
$\widehat{\Sigma}_- = \frac{1}{n-m-1}\Sigma \mathbb{1}_{\{y_i=-1\}}(x_i - \widehat{\mu}_-)(x_i - \widehat{\mu}_-)^T$

Classification
We predict class = 1 when $\mathbb{P}(Y=+1|X) > \mathbb{P}(Y=-1|X)$
$=> \frac{\mathbb{P}(Y=+1|X)}{\mathbb{P}(Y=-1|X)} > 1$
$=> \log(\frac{\mathbb{P}(Y=+1|X)}{\mathbb{P}(Y=-1|X)}) > 0$
=>
Using previous conditional probability expressions, we end up with the following prediction rule:

$$\begin{cases} 1 & \text{if } x^T\widehat{\Sigma}^{-1}(\widehat{\mu}_+ - \widehat{\mu}_-) > \frac{1}{2}\widehat{\mu}_+^T\widehat{\Sigma}\widehat{\mu}_+ - \frac{1}{2}\widehat{\mu}_-^T\widehat{\Sigma}\widehat{\mu}_- + \log(1-m/n) - \log(m/n) \\ -1 & \text{otherwise} \end{cases} \tag{2}$$

$\widehat{\mu}_+$, $\widehat{\mu}_-$, $\widehat{\pi}_+$ and $\widehat{\Sigma}$ will be computed with *train data*.
x is the *test data*.

Note: $\widehat{\Sigma}^{-1}(\widehat{\mu}_+ - \widehat{\mu}_-)$ is the **Fisher function** (Saporta).

Listing 1: LDA algorithm

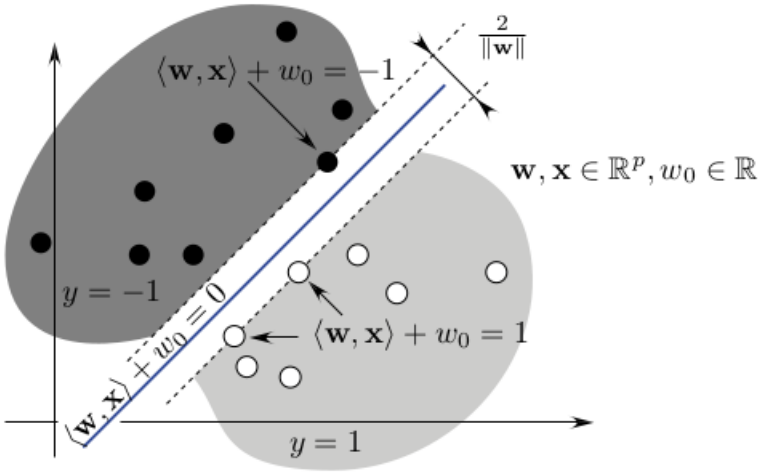
```
class LDAClassifier():

    def fit(self, X, y):

        X_p = X[y == 1, :]
        X_m = X[y == -1, :]

        X_p_x1 = X_p[:,0]
        X_p_x2 = X_p[:,1]
        X_m_x1 = X_m[:,0]
        X_m_x2 = X_m[:,1]

        n = len(X)
        m = len(X_p)

        mean_p_x1 = np.mean(X_p_x1)
        mean_p_x2 = np.mean(X_p_x2)
        mean_p = np.array([mean_p_x1,mean_p_x2]) # mu_plus (estimated)
        cov_p = np.cov(np.transpose(X_p))


        mean_m_x1 = np.mean(X_m_x1)
        mean_m_x2 = np.mean(X_m_x2)
        mean_m = np.array([mean_m_x1,mean_m_x2]) # mu_minus (estimated)
        cov_m = np.cov(np.transpose(X_m))

        cov_est = (1/(n-2))*( (m-1)* cov_p + (n-m-1)* cov_m) # sigma (estimated)
        inv_cov_est = np.linalg.inv(cov_est)

        a1 = np.dot(np.transpose(mean_p),inv_cov_est)
        a2 = np.dot(np.transpose(mean_m),inv_cov_est)
```

```
        # 2nd term in inequality
        self.alpha = 0.5*(np.dot(a1,mean_p)  - 0.5*np.dot(a2,mean_m)) + np.log(1- m/n) - np.log
        # 1st term in inequality
        self.beta =  np.dot(inv_cov_est,mean_p-mean_m)

        return self

    def predict(self, X):

        y_=[]

        for i in range(len(X)):
            X_pred = X[i]
            beta = np.dot(np.transpose(X_pred), self.beta)
            if (beta>self.alpha):
                Y_pred = 1
            else:
                Y_pred = -1
            y_.append(Y_pred)
        return np.array(y_)
```

SVM

Margin

This idea of SVM is to separate data as best as possible using a margin.



Three planes:
- $H_1 : \omega^T x + b = 1$
- $H : \omega^T x + b = 0$
- $H_{-1} : \omega^T x + b = -1$

Computing $H_1 - H_{-1}$ we get:
$(x_1 - x_{-1})\omega^T = 2$
$=> ||x_1 - x_{-1}|| = \frac{2}{||\omega||}$

The SVM problem starts with a **margin maximization**. We want to maximize the distance between x_1 and x_{-1} (**to be double checked**) and it is equivalent to minimizing $||\omega||$. Thus the optimization problem is written as such:

$$min_{\omega,b}\ \frac{1}{2}||\omega||^2$$
$$s.t.\ y_i(\omega^T x_i + b) \geq 1\ i = 1, ..., n$$

Primal formulation

The above problem reflects the case where all data are perfectly separable, this is not true in practice. We thus add an error term ξ_i for each observation. This leads to the **primal formulation** of the problem:

$$min_{\omega,b,\xi}\ \frac{1}{2}||\omega||^2 + C\Sigma_{i=1}^n \xi_i$$
$$s.t.\ y_i(\omega^T x_i + b) \geq 1 - \xi_i\ i = 1, ..., n$$
$$\xi_i \geq 0\ i = 1, ..., n$$

Note: the problem can be rewritten with the hinge loss function
$y_i(\omega^T x_i + b) \geq 1 - \xi_i => \xi_i \geq 1 - y_i(\omega^T x_i + b)$
$=> \xi_i \geq 1 - y_i(\omega^T x_i + b) \geq 0$ since $\xi_i \geq 0$
$=> \xi_i = max(0, 1 - y_i(\omega^T x_i + b))$
$=> \xi_i = (0, 1 - y_i(\omega^T x_i + b))_+$
$=> \xi_i = hinge(f(x))$ where *hinge* is the *Hinge loss* function
$hinge(f(x)) = (1 - yf(x))_+$

$$min_{\omega,b}\ \frac{1}{2}||\omega||^2 + C\Sigma_{i=1}^n (0, 1 - y_i(\omega^T x_i + b))_+$$

Lagrange

We can write this problem using Lagrange formulation, that is, integrating the constraints into the main formula:
$\mathcal{L}(\omega, b, \xi, \alpha, \mu) = \frac{1}{2}\omega^T\omega + C\Sigma\xi_i + \Sigma\alpha_i(1 - \xi_i - y_i(\omega^T x_i + b)) - \Sigma\mu_i\xi_i$
$\alpha_i, \mu_i \geq 0$

First order conditions:
$\frac{\partial\mathcal{L}}{\partial\omega} = 0 => \omega - \Sigma\alpha_i y_i x_i = 0 => \omega = \Sigma\alpha_i y_i x_i$
$\frac{\partial\mathcal{L}}{\partial b} = 0 => -\Sigma\alpha_i y_i = 0$
$\frac{\partial\mathcal{L}}{\partial\xi_i} = 0 => C - \alpha_i - \mu_i = 0 => \alpha_i = C - \mu_i$
Since $\alpha_i, \mu_i \geq 0$ we have $C \geq \alpha_i \geq 0$

Dual formulation

We can rewrite the problem using the first order conditions above:
$\mathcal{L}(\omega, b, \xi, \alpha, \mu) = \frac{1}{2}(\Sigma\alpha_i y_i x_i)^T(\Sigma\alpha_i y_i x_i) + C\Sigma\xi_i + \Sigma\alpha_i - \Sigma\alpha_i\xi_i - \Sigma\alpha_i y_i(\Sigma\alpha_i y_i x_i)^T x_i - \Sigma\alpha_i y_i b - \Sigma\mu_i\xi_i$
$= -\frac{1}{2}(\Sigma\alpha_i y_i x_i)^T(\Sigma\alpha_i y_i x_i) + \Sigma(C - \alpha_i - \mu_i)\xi_i + \Sigma\alpha_i - \Sigma\alpha_i y_i b$

$$= -\frac{1}{2}\Sigma_{i,j}\alpha_i\alpha_j y_i y_j x_i^T x_j + \Sigma\alpha_i$$

The problem is convex with lineary inequality constraints, we can apply the saddle point theorem.
Note: a point is saddle if it's a maximum w.r.t. one axis and a minimium w.r.t. another axis
The saddle theorem allows us to solve the problem $min_\omega max_\alpha$ as $max_\alpha min_\omega$

This leads to the problem in its **dual formulation**:

$$\begin{array}{c} max_\alpha \quad -\frac{1}{2}\Sigma_{i,j}\alpha_i\alpha_j y_i y_j x_i^T x_j + \Sigma\alpha_i \\ s.t. \;\; 0 \leq \alpha_i \leq C \quad i = 1, ..., n \\ \Sigma\alpha_i y_i = 0 \quad i = 1, ..., n \end{array}$$

Using the above expression of ω (optimal condition), the classification function is:

$$f(x) = sign(\Sigma\alpha_i y_i x_i^T x + b)$$

Kernel

Kernels are used when separation is non linear.
Recall the primal formulation:

$$\begin{array}{c} min_{\omega,b,\xi} \;\; \frac{1}{2}||\omega||^2 + C\Sigma_{i=1}^n \xi_i \\ s.t. \;\; y_i(\omega^T x_i + b) \geq 1 - \xi_i \;\; i = 1, ..., n \\ \xi_i \geq 0 \;\; i = 1, ..., n \end{array}$$

When separation is non linear, we set ϕ as a non linear transformation. The constraint becomes: $y_i(\omega^T \phi(x_i) + b) \geq 1 - \xi_i \quad i = 1, ..., n$

Dual formulation is now:

$$\begin{array}{c} max_\alpha \quad -\frac{1}{2}\Sigma_{i,j}\alpha_i\alpha_j y_i y_j \phi(x_i)^T \phi(x_j) + \Sigma\alpha_i \\ s.t. \;\; 0 \leq \alpha_i \leq C \quad i = 1, ..., n \\ \Sigma\alpha_i y_i = 0 \quad i = 1, ..., n \end{array}$$

The classification becomes:

$$f(x) = sign(\Sigma\alpha_i y_i \phi(x_i)^T \phi(x) + b)$$

To classify a new point, we thus need to be able to compute $\phi(x_i)^T \phi(x)$.

Kernel trick: there is no need to know an explicit expression of ϕ (i.e. knowing the coordinates of points in new set) since we are only looking at distances and angles, that is scalar product.

Kernel functions implement those scalar products: $K(x, x') = \phi(x)^T \phi(x')$ where ϕ is a transformation function into a Hilbertian set $\phi : \mathcal{X} \to \mathcal{F}$

Note: an Hilbertian is a set with scalar product: $\mathcal{F} = (\mathcal{H}, < ., . >)$

Most used kernels:
Linear kernel: $K(x, x') = x^T x'$ (we often call this setup a "no-kernel SVM")
Polynomial kernel: $K(x, x') = (x^T x' + c)^d$
Gaussian kernel: $K(x, x') = exp(-\gamma ||x - x'||^2)$

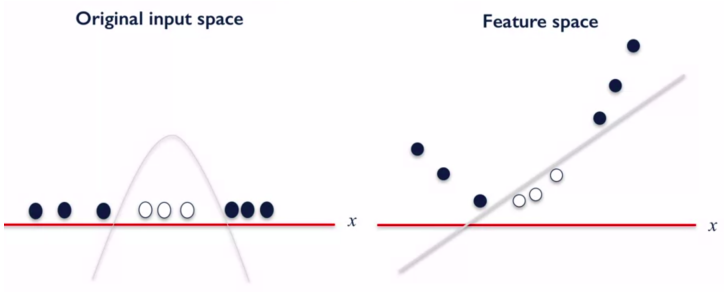
The optimisation problem can be written with kernel:

$$\begin{array}{c} max_\alpha \quad -\frac{1}{2}\Sigma_{i,j}\alpha_i\alpha_j y_i y_j K(x_i, x_j) + \Sigma\alpha_i \\ s.t. \;\; 0 \leq \alpha_i \leq C \quad i = 1, ..., n \\ \Sigma\alpha_i y_i = 0 \quad i = 1, ..., n \end{array}$$

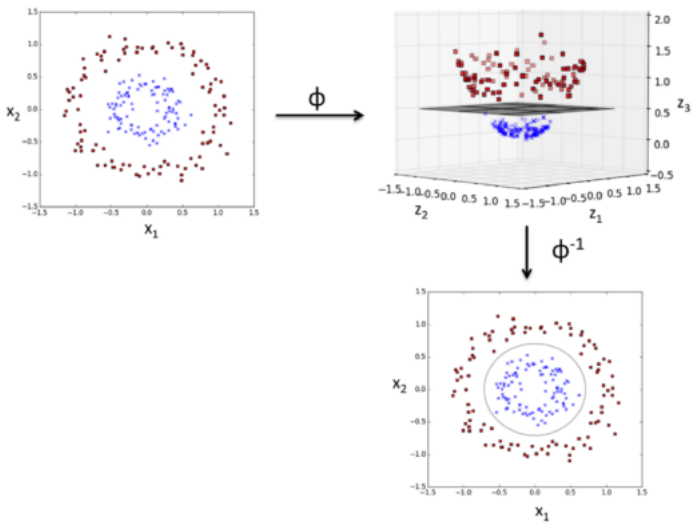
Summary

SVM allows to find complex non linear separations in transforming the problem into a higher dimension where data are linearly separable.

From 1D to 2D:



From 2D to 3D:



Expectation-Maximization (EM) in the case of GMM (Gaussian Mixture Model)

(for more details, see document *gmm.pdf* in Cloud folder)

GMM problem aims at estimating parameters of a sample distribution. It is part of the unsupervised learning where the goal is to **learn some underlying hidden structure of the data** ("Generative models" p. 295 Understanding Machine Learning)

A GMM sample is composed of j Gaussian variables (*clusters*) distributed with proportions $(\pi_1, ..., \pi_k)$ $(\Sigma\pi_i = 1)$
We can write:

$$X \sim \mathcal{N}(\mu_Z, \Sigma_Z) \qquad with \;\; Z \sim \pi$$

π is not really a law but more the proportions of each Gaussian categories.
Thus, X has a density which is a weighted-average of all Gaussian densities:

$$p_\theta(x) = \Sigma_{j=1}^k \pi_j f_j(x) \qquad (*)$$

Estimation
We want to estimate $\theta = (\pi, \mu, \Sigma)$ where:
$\pi = (\pi_1, ..., \pi_k)$, $\mu = (\mu_1, ..., \mu_k)$, $\Sigma = (\Sigma_1, ..., \Sigma_k)$

To do so, we use the maximum likelihood method (product of densities across all samples):

$$p_\theta(x) = \Pi_{i=1}^n p_\theta(x_i)$$

$$l(\theta) = log(\Pi_{i=1}^n p_\theta(x_i)) = \Sigma_{i=1}^n log(p_\theta(x_i))$$

We thus need to find $argmax(l(\theta))$
Problem: the likelihood function is not convex!

The expectation-maximization problem is used when we have *latent variables* (= variables for which we don't know their associated distribution).
Let $z = (z_1, ..., z_k)$ be the vector of latent variables. We can express the density $(*)$ as a joint function with respect to z:

$$p_\theta(x, z) = p_\theta(z) p_\theta(x|z)$$

$$l(\theta, z) = ... = \Sigma(log\pi_{z_i}) + \Sigma(log f_{z_i}(x_i))$$

A classic optimization (in case of Gaussians) give us empirical values as solutions e.g. $\hat{\pi_j} = \frac{n_j}{n}$
Problem: we don't know j!

We will thus use the *expected* log-likelihood method.
Let us find another expression of the likelihood:

$$p_\theta(x, z) = p_\theta(x) p_\theta(z|x)$$

As seen previously: $p_\theta(x,z) = \Pi\pi_{z_i} f_{z_i}(x_i)$
$p_\theta(z|x) = \Pi p_\theta(z_i|x_i) = \frac{\Pi\pi_{z_i} f z_i(x_i)}{p_\theta(x_i)} \propto \Pi\pi_{z_i} f z_i(x_i)$

Given an initial parameter θ_0, the *expected* log-likelihood is written as such:

$$\mathbb{E}_{\theta_0}[l(\theta;z)] = \Sigma p_{\theta_0}(z|x) l(\theta;z)$$
$$\mathbb{E}_{\theta_0}[l(\theta;z)] = \Sigma_j \Sigma_i p_{ij}(log\pi_j + log f_j(x_i))$$

We now have an expression that doesn't depend on z but only on p_{ij} and we know that $n_j = \Sigma_i p_{ij}$

K-means

(see kmeans.pdf from OneDrive folders for more details)

Objective: group data into k clusters so that samples in the same cluster are close to each other w.r.t. the Euclidean distance.

The cost function minimization is written as such:

$$\underset{C_1,\ldots,C_k;\mu_1,\ldots,\mu_k}{\operatorname{argmin}} \Sigma_{j=1}^{k} \Sigma_{i \in C_j} ||x_i - \mu_j||^2$$

Where μ_j is the mean, also called gravity center or cluster center:

$$\mu_j = \frac{1}{|C_j|} \Sigma_{i \in C_j} x_i$$

The quality of the clustering strongly depends on the initial center values. This is why the algorithm is generally run multiple times for different initial values. The best clustering (i.e., that of minimum cost) is returned.

K-means++
To improve the quality of the clustering, we choose the initial cluster centers far from each other:
- select the first cluster center uniformly at random among the n data samples
- select the following cluster centers at random, with a probability proportional to the square distance to the closest current cluster center

Listing 2: K-means++ initial centers selection

```
centers = []
centers.append(X[np.random.randint(X.shape[0])]) # inital center = one random sample
distance = np.full(X.shape[0], np.inf) # a vector (n,1) with only infinity terms
for j in range(1, self.n_clusters):
    distance = np.minimum(np.linalg.norm(X - centers[-1], axis=1), distance) # size (n,1);
# distance = the smallest distance associated with
# the last added center
    p = np.square(distance) / np.sum(np.square(distance)) # probability vector [p1,...,pn]
# the highest probability in p is associated
# with the biggest distance w.r.t the last added center
    sample = np.random.choice(X.shape[0], p = p) # one sample is
                                                 # selected according to probabilities
    centers.append(X[sample])
```

Algorithm 1 K-means

Input: $x_1, ..., x_n$
Output: clusters $C_1, ..., C_k$
Random values for $\mu_1, ..., \mu_k$
while no convergence **do**
  // Step 1: Update clusters
  $C_1, ..., C_k \leftarrow \emptyset$
  for $i = 1$ to n **do**
    $j \leftarrow argmin_l ||x_i - \mu_l||$
    $C_j \leftarrow C_j + \{i\}$ // We add observation i to the cluster C_j
  end for
  // Step 2: Update cluster centers
  for $j = 1$ to k **do**
    $\mu_j \leftarrow 0$
    $n_j \leftarrow 0$
    for i in C_j **do** // We loop on all observations of each cluster
      $\mu_j \leftarrow \mu_j + x_i$
      $n_j \leftarrow n_j + 1$
    end for
    $\mu_j \leftarrow \mu_j / n_j$
  end for
end while

Note: this problem is called *NP-hard problem*. It means that its complexity is at least equal to the complexity of an NP-problem
NP-problem: a problem is NP if it can be determined by a non-deterministic Turing machine in polynomial time. Intuitively, a problem is NP if we can quickly verify if one candidate is a solution of the problem. E.g. "travelling salesman problem" = let d be a distance and n be a number of cities. Is there an itinerary with distance $\geq d$ stopping by every city? -> easy to check...

Turing machine (1936)

"non-deterministic turing machine": itinerary can be represented by a tree...

Neural network

Logistic regression with a neural network mindset
Based on the example from coursera (*deeplearning.ai*)
Let us take the example of an image that we want to classify in a **binary** way: man/woman
The picture is vectorized as a vector of pixels : $\begin{pmatrix} x_1 \\ ... \\ x_p \end{pmatrix}$
We use a regression to predict if it's a man/woman:
$y = \omega^T x + b$
Note: x are all the pixels of **one** image.

We want a probability in output (if it's ≥ 0.5 then we say it's a man).
We thus want the output to be $\widehat{y} = \sigma(\omega^T x + b) = \mathbb{P}(y|x) \in [0, 1]$
(see regression part to get more details on the sigmoid)

Now since it's a binary classification, we want the y (real value) to be 0 or 1.
Thus, the loss function is:

$$\mathcal{L}(y, \widehat{y}) = -y \log(\widehat{y}) + (1 - y) \log(1 - \widehat{y})$$

Proof: TODO from binary law (Bernoulli) to cross-entropy

The cost function is the empiric loss on all examples:

$$J(\omega, b) = \frac{1}{m} \Sigma_{i=1}^{m} \mathcal{L}(\widehat{y}^{(i)}, y^i)$$

Forward propagation

$$x_1, x_2, \omega_1, \omega_p, b \rightarrow z = \omega_1 x_1 + \omega_2 x_2 + b \rightarrow \widehat{y} = a = \sigma(z) \rightarrow \mathcal{L}(a, y)$$

- First arrow: regression
- Second arrow: probability
- Third arrow: error

Backward propagation
The idea is: with the error computed on the last step, we go backward in order to correct the parameters ω and b.

$$x_1, x_2, \omega_1, \omega_p, b \leftarrow z = \omega_1 x_1 + \omega_2 x_2 + b \leftarrow \widehat{y} = a = \sigma(z) \leftarrow \mathcal{L}(a, y)$$

Example: we want to find ω_1 that minimizes the cost function:
$\frac{d\mathcal{L}}{d\omega_1} = "d\omega_1" = \frac{d\mathcal{L}}{da} \frac{da}{dz} \frac{dz}{d\omega_1} = ... = (a - y) x_1 = dz x_1$
Steps:
We compute all the derivatives, then we apply the gradient descent

Listing 3: Gradient descent (logistic regression with a NN mindset)

```
for i in range(num_iterations):

    # Cost and gradient calculation
    grads, cost = propagate(w, b, X_train, Y_train) # propagation on ALL the training sample

    # Retrieve derivatives from grads
    dw = grads["dw"]
    db = grads["db"]

    # update parameters
    w = w - learning_rate * dw
    b = b - learning_rate * db

    # Record the costs
    costs.append(cost)
```

Listing 4: Propagation (logistic regression with a NN mindset)

```
def propagate(w, b, X, Y):

    m = X.shape[1]

    # FORWARD PROPAGATION (FROM X TO COST)
    A = sigmoid(np.dot(w.T,X)+b)
    cost = (- 1 / m) * np.sum(Y * np.log(A) + (1 - Y) * (np.log(1 - A)))

    # BACKWARD PROPAGATION (TO FIND GRAD)
    dw = (1/m)*np.dot(X,(A-Y).T)
    db = (1/m)*np.sum(A-Y)
```

Gradient descent

ℓ the loss function to minimize:
$\theta_{t+1} = \theta_t - \alpha \nabla \ell$
More details in Jupyter Notebook ML_GS.ipynb.
Proof of the formula:

Taylor series by definition

$$C(\theta_{new}) = C(\theta_{old}) + \nabla C \cdot [\theta_{new} - \theta_{old}] + ..$$

Here $\Delta\theta = [\theta_{new} - \theta_{old}]$, $\nabla C = \frac{\partial C}{\partial \theta}$

$$C(\theta_{new}) \approx C(\theta_{old}) + \frac{\partial C}{\partial \theta} \cdot \Delta\theta \qquad (1)$$

If we set $\Delta\theta = -\eta \frac{\partial C}{\partial \theta}$ with η a small positive learning rate

equation (1) becomes:

$$C(\theta_{new}) \approx C(\theta_{old}) + \frac{\partial C}{\partial \theta} \cdot \left(-\eta \frac{\partial C}{\partial \theta}\right) = C(\theta_{old}) - \eta \left(\frac{\partial C}{\partial \theta}\right)\left(\frac{\partial C}{\partial \theta}\right)$$

$C(\theta_{new}) \leq C(\theta_{old})$, since $\eta \left(\frac{\partial C}{\partial \theta}\right)\left(\frac{\partial C}{\partial \theta}\right)$ is always positive

Conclusion: if we set $\Delta\theta = -\eta \frac{\partial C}{\partial \theta}$ it will decrease C

(Idemia courses "DeepLearningTPT2018S1S2.pdf")

Learning rate optimization

Note:
- one epoch = one forward pass and one backward pass of all the training examples.
- batch size = the number of training examples in one forward/backward pass. The higher the batch size, the more memory space needed.
- number of iterations = number of passes, each pass using [batch size] number of examples. To be clear, one pass = one forward pass + one backward pass.

Learning rate decay
Simple idea: reduce the learning rate progressively.
E.g. $1/t$ decay:

$$\alpha_t = \frac{1}{(t+1)}$$

Momentum
Momentum is a method that helps accelerate SGD in the relevant direction and reduce oscillations.
General idea:
$0 \leq \gamma \leq 1$
$M_{t_0} = x_0$
$M_{t_1} = \gamma M_{t_0} + x_1$
$M_{t_2} = \gamma M_{t_1} + x_2$
Let's develop M_{t_2} to have a better view of momentum effect:
$M_{t_2} = \gamma(\gamma M_{t_0} + x_1) + x_2 = \gamma^2 x_0 + \gamma x_1 + x_2$
We can see that more importance is given to the most recent value (x_2) and the least to the past values.

In practice, $\gamma = 0.9$ gives good results.
Advantage: less dependent on noise

Adagrad - Adaptive Gradient Algorithm (2011)
Divide the learning rate by "average" gradient:
$\theta_t = \theta_{t-1} - \frac{\alpha}{\sqrt{\Sigma_{i=0}^{t}(\nabla f_i^2)}} \nabla f$

RMSProp - Root Mean Squared Propagation
Same as AdaGrad, but with an exponentially decaying average of past squared gradients.
$\theta_t = \theta_{t-1} - \frac{\alpha}{\sigma_{t-1}} \nabla f$
Where:
$\sigma_t = \sqrt{\alpha(\sigma_{t-1})^2 + (1-\alpha)(\nabla f_t)^2}$

Adam - Adaptive moment estimation

Adam = RMS + momentum => use of a exponential decaying average of past squared gradients and past gradients