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Support Vector Machines

We have a space with negative and positive examples. The problem is to separate the samples using a straight line. And then line is drawn with the view of putting the widest street that separates the positive from the negative examples. (The margin that I drawn is the smallest distance to the closest point)

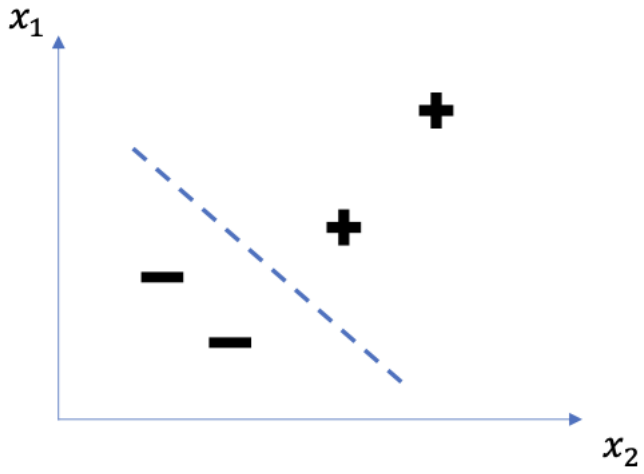


Figure 1: image

We want to create a decision rules that use that decision boundary

Imagine a vector $\vec{w}$ constraint to be perpendicular to the medium line of the street. And the we have an unkown vector $\vec{u}$ and we are interested in understanding if that vector is on the right side or on the left side of the steet. We can project $\vec{u}$ down to the one that is perpendicular to the street because then, we will have the distance in the $\vec{w}$ direction and the further out we go the closer we'll get to being on the right side of the street. So we can say

$$\vec{w} \cdot \vec{u} \geq c$$

The dot product take the projection onto w and the bigger that projection is, the further out along this projection will lie and eventually it will be so big that the projection crosses the median line of the street, and we'll say it must be a positive sample. Without loss of generality we can say that

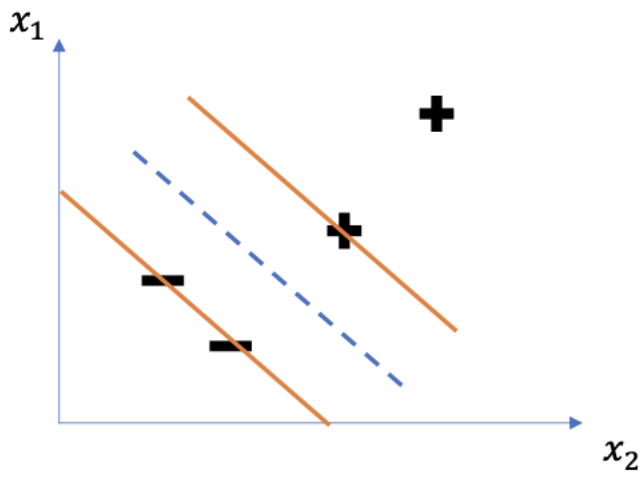


Figure 2: image

$$\vec{w} \cdot \vec{u} + b \geq c \text{THEN} +$$

$$c = -b$$

That's our decision rule.

So we define that for a positive sample this equation is true

$$\vec{w} \cdot \vec{x_+} + b \geq 1$$

Likewise for a negative sample

$$\vec{w} \cdot \vec{x_-} + b \leq -1$$

Let's introduce another variable for mathematical convenience

y_i such that $y_i = 1$ for positive samples and $y_i = -1$ for negative samples.

So:

$$y_i(\vec{w} \cdot x_i + b) \geq 1 y_i(\vec{w} \cdot x_i + b) - 1 \geq 0$$

And $y_i(\vec{w} \cdot x_i + b) - 1 = 0$ for x_i in the GUTTER

The goal is to arrange for the line to be such at the street separating the pluses from the minuses as wide as possible. So we need to express the distance between the two gutters.

We can consider the difference between the two vectors $\vec{x_+} - \vec{x_-}$ and project the difference to a unit vector that is perpendicular to the straight line.

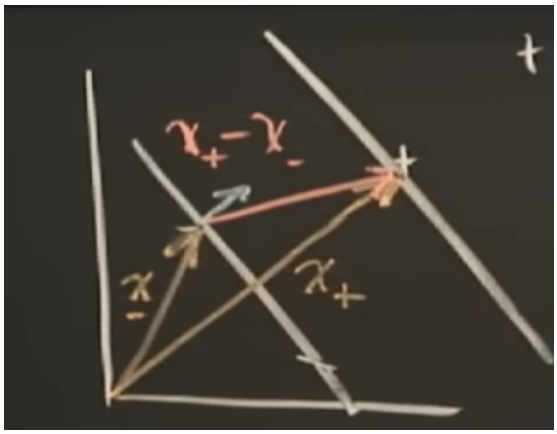


Figure 3: image

$$\text{WIDTH} = (\vec{x_+} - \vec{x_-}) \cdot \frac{\vec{w}}{||w||})$$

$$\frac{(1-b)+(1+b)}{||w||} = \frac{2}{||w||}$$

And this represent the width of the street and we want to maximize that quantity $\text{MAX}\frac{2}{||w||}$ equals to $\text{MIN}||w||$ equals to $\text{MIN}\frac{1}{2}||w||^2$. We have also a contraint that is:

$$y_i(\vec{w} \cdot x_i + b) \geq 1$$

We've now transformed the problem into a form that can be efficiently solved. The above is an optimization problem with a convex quadratic objective and only linear constraints. Its solution gives us the optimal margin classifier.

Lagrange duality

Consider a problem of the following form:

$$min_w f(w) \text{s.t} h_i(w) = 0, i = 1, ..., l$$

This problem can be solved with a method called the Lagrange multipliers. The Langrangian is defined to be:

$$L(w, \beta) = f(w) + \sum_{i}^{l} \beta_i h_i(w)$$

Here, the β_i's are called the **Lagrange multipliers**. We would then find and set L's partial derivatives to zero

$$\frac{\partial L}{\partial w_i} = 0; \frac{\partial L}{\partial \beta_i} = 0$$

and solve for w and β. ### Primal optimization problem

In this section, we will generalize this to constrained optimization problems in which we may have inequality as well as equality contraints. Due to In order to maximize the size of the street we're going to maximize the following quantity (lagrange multipliers)

$$min_w f(w) \text{s.t} g_i(w) \leq 0, i = 1, ..., k h_i(w) = 0, i = 1, ..., l.$$

To solve it, we start by defining the **generalized Lagrangian**

$$L(w, \alpha, \beta) = f(w) + \sum_{i=1}^{k} \alpha_i g_i(w) + \sum_{i=1}^{l} (\beta_i h_i(w))$$

Here, the α_i's and β_i's are the Lagrange multipliers. The generalized Lagrangian correspond to the dual problem

$$\text{maximize} L(w, \alpha, \beta) \text{s.t} \alpha \geq 0$$

In our case we have that:

$$L = \frac{1}{2}||\vec{w}||^2 - \sum \alpha_i [y_i(\vec{w} \cdot \vec{x_i} + b) - 1]$$

So we're going to compute the partial derivative

$$\frac{\partial L}{\partial \vec{w}} = \vec{w} - \sum \alpha_i y_i x_i = 0 \Rightarrow \vec{w} = \sum_{i} \alpha_i y_i \vec{x_i}$$

This tells us that the vector w is a linear sum of the samples. **BUT NOT ALL** the samples, because some alphas could be zero. We can differentiate also for b

$$\frac{\partial L}{\partial b} = -\sum \alpha_i y_i = 0 \Rightarrow \sum \alpha_i y_i = 0$$

If we compute the differentation also for alpha

$$L = \frac{1}{2}||\vec{w}||^2 - \sum \alpha_i [y_i(\vec{w} \cdot \vec{x_i} + b) - 1] \frac{\partial L}{\partial \alpha} = [y_i(\vec{w} \cdot \vec{x_i} + b) - 1] = 0$$

Now that we got a value for w we can substitute the formula in L

$$L = \frac{1}{2}\left(\sum \alpha_i y_i \vec{x_i}\right)\left(\sum \alpha_i y_j \vec{x_j}\right) - \sum \alpha_i y_i x_i \left(\sum \alpha_j y_j x_j\right) - \sum \alpha_i y_i b + \sum \alpha_i$$

And $\sum \alpha_i y_i b = 0$ because of the partial derivative with the respect of b

The Lagrangian can be rewrited as

$$L = \sum \alpha_i - \frac{1}{2} \sum_i \sum_j \alpha_i \alpha_j y_i y_j \vec{x_i} \cdot \vec{x_j}$$

We're trying to find a maximum of L and what I discovered that the optimization depends only on the dot product of pairs of samples $x_i \cdot x_j$ So now, my decision rule with this expression for w is going to be

$$\sum \alpha_i y_i \vec{x_i} \cdot \vec{u} + b \geq 0 \rightarrow +$$

So we discovered that the decison rules depends only on the dot product of those sample vectors and the unknown.

Non Linear separable data

The derivation of the SVM as presented so far assumed that the data is linearly separable. When data are non-linearly separable, we may get a separation between classes with a hyperplane only allowing that, after having defined the separating hyperplane, some pattern of the training set with positive label are classified as negative and viceversa. We must accept that some constraints are **violated**

We introduce a **slack** variable ξ_i for each constraint, in order to allow an error tolerance:

$$y^{(i)}(w^T \cdot x^i + b) \geq 1 - \xi^i$$

An additional term C is introduced in the cost function to penalize misclassification errors.

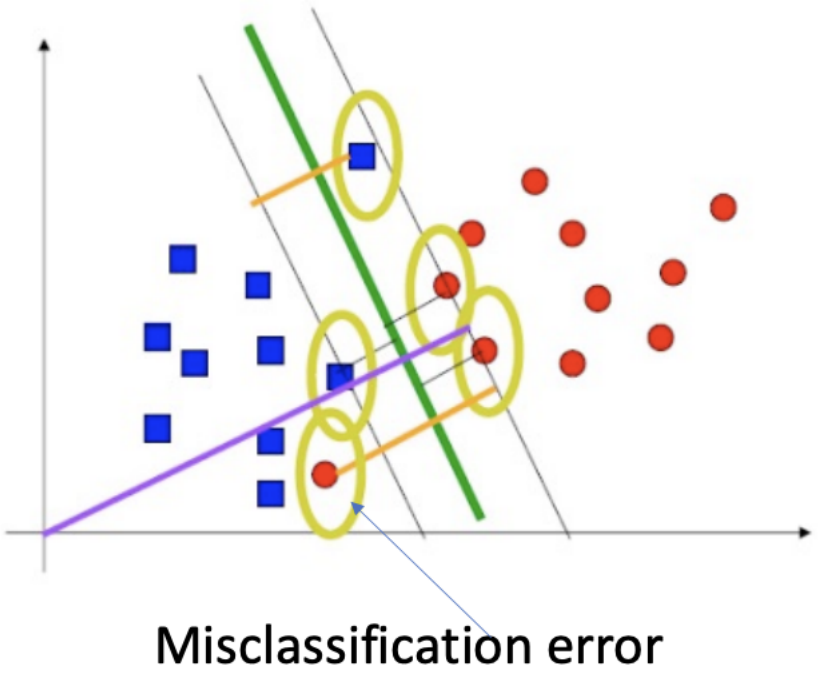


Figure 4: image

$$\frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi^{(i)}$$

The ξ_i are cost variables proportional to how far the misclassified pattern is from the hyperplane. $\xi_i > 1$ indicates a misclassification error.

C (**regularization** parameter) lets to control the trade-off between hypothesis space complexity and the admissible number of errors. A big value for C gives a stronger penalization to errors. The optimization problem to solve becomes:

Minimize:

$$\frac{1}{2}||w||^2 + C\sum_{i=1}^{m}\xi^{(i)}\text{s.t}y^i(w^T \cdot x^i + b) \geq 1 - \xi^{(i)}\xi^{(i)} \geq 0$$

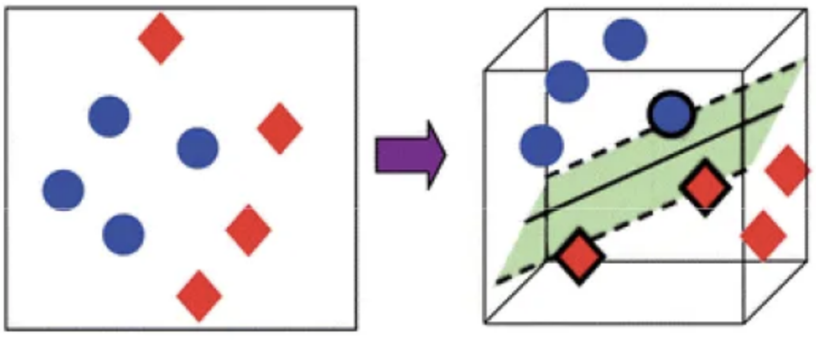
The dual problem now becomes:

$$max_\alpha \sum_{i=1}^{m}\alpha_i - \frac{1}{2}\sum \alpha_i\alpha_j y_i y_j x_i^T x_j \text{s.t. } 0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^{m}\alpha_i y_i = 0$$

The dual variables are now bounded with C. The proposed solution could not be enough. It does not guarantee good performances since a hyperplane can only represent a dichotomy in the space of instances/patterns.

Cover's theorem

Cover's theorem state that, a complex pattern classification problem, cast in a high dimensional space nonlinearly, is more likely to be linearly separable than in a low dimensional space, provided that the space is not densely populated. Or in simple terms, given a set of training data that is not linearly separable, one can transform it into a training set that is linearly seperable by mapping it into a possibly higher dimensional space via some non linear transformation.



1. Patterns (input space) are mapped into a space with (much) higher dimension (feature space) through kernel functions;
2. The optimal hyperplane is defined within this feature space

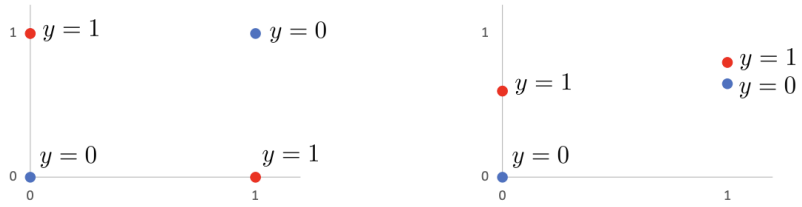


Figure 5: image

In this case the samples are not linearly separable and we are not able to find a solution for our problem, but we can move to another space that is more convenient for our purposes:

$$\vec{x} \Rightarrow \phi(\vec{x})$$

For our optimization problem now all we need is a function K that corresponds to the dot product between the samples in the new space.

This function K is called **kernel function** and we have no need to compute the transformation function $\phi(\vec{x_i})$

$$K(x_i, x_j) = \phi(\vec{x_i}) \cdot \phi(\vec{x_j})$$

Kernel trick

To solve the optimization problem, the product $\phi(\vec{x_i}) \cdot \phi(\vec{x_j})$ does not have to be explicitly computed in the feature space once we find a kernel function (specifically a positive definite kernel).

$$K(x_i, x_j) = \phi(\vec{x_i}) \cdot \phi(\vec{x_j})$$

The kernel is a function that returns the (scalar) product of projections: it avoids you to explicitly compute the projection and make the product between the projected vectors. The explicit form of the transformation function may be ignored.

If a kernel function is defined, that is a function such that:

$$K(x_i, x_j) = \phi(\vec{x_i}) \cdot \phi(\vec{x_j}) = \sum_{k=1}^{m} \phi(\vec{x_i}) \cdot (\phi(\vec{x_j}))$$

The optimization problem becomes:

$$max_\alpha \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j k(x_i, x_j)$$

Such that:

$$0 \leq \alpha_i \leq C \text{ and } \sum_{i=1}^{m} \alpha_i y_i = 0$$

The projection $\phi(\vec{x_i})$ into the feature space must not be explicitly computed. I should compute the scalar product $\phi(\vec{x_i}) \cdot (\phi(\vec{x_j}))$, but I don't have to, since I can indirectly obtain it with the kernel function.

Kernel examples

Linear kernel

$$(\vec{u} \cdot \vec{v})$$

Polinomial kernel

$$(\vec{u} \cdot \vec{v} + 1)^d$$

Multi-Layer Perceptron tanh

$$tanh(b(\vec{u} \cdot \vec{v} - c))$$

Radial basis function (RBF) kernel

$$e^{-\frac{||x_i - x_j||}{\sigma}}$$

Gaussian Radial basis function kernel

$$e^{-\frac{(x_i - x_j)^2}{2\sigma^2}}$$

Parameters tuning

To use Support Vector Machines you have to define - the kernel function; - potential parameter of the kernel function; - The value for the regularization parameter C.

General rules for the set up do not exist, but you should make your choice on a validation set, usually through cross validation.

Advantages of SVMs

- There are no local minima (the optimization problem is quadratic -> $\exists$! optimal solution)
- The optimal solution can be found in polynomial time.
- There are few parameters to set up (C, type of kernel and specific kernel parameters)
- Solution is stable (ex. there is no problem of randomly initializing of weights just as in Neural Networks)
- Solution is sparse: it just involves support vectors

SVM Online resources

- https://www.youtube.com/watch?v=_PwhiWxHK8o
- https://www.youtube.com/watch?v=xpHQ6UhMlx4

Generalized Linear Models

Basic functions

It is usual that our data cannot be approximated to a linear function. What we need is to find a way to model non linear relations without increasing too much the complexity of the algorithm.

The main limiting characteristics of linear regression is the linearity of parameters

$$h(x) = \sum_{i=0}^{n} \theta_i \cdot x_i = \theta^T x$$

h(x) keeps a linear relation w.r.t the features space X. This linearity represents a limitation of the expressiveness of the model because the hypothesis is only able to approximate linear functions of the input. GLMs represent an extension to linear models that allow non linear transformations of the input

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$$h(x) = \sum_{i=0}^{n} \theta_i \cdot \psi(x_i) = \theta^T \psi(x)$$

Phi are called basic functions Example $x_i, x_2, x_3 \rightarrow x_1, x_2, x_3, x_1x_2, x_1x_3, x_1^2, x_2^2, x_3^2$

SVM notes from Waterloo lecture

Support vector machines will find a linear separator such that we have the same distance for point on one side and point of the other side and line is gonna be right in the middle. The point that are the closest are called support vector. And support vector tells us where to put the line such as it has the same distance and distance is the maximum we can obtain.

Unsupervised Learning (Stanford CS229 Notes)

K-Means

In the supervised setting we get points with labels that we can separate with a line and with a supervised learning algorithm. In unsupervised we have the points but we don't have the labels. Unsupervised learning is harder so we have to allow stronger assumptions and we're gonna have to assume that there are some kind of latent or hidden structure and we're gonna have to allow weaker guarantees. (Guess number of cluster for example and assume that there is some cluster in our data).

So we have some data and set up the number of cluster e.g $K = 2$ and our goal is to find the cluster. So given a dataset with points $x^{(1)}$ ... $x^{(n)} \in \mathbb{R}$ and K # of cluster, we find an assignment to point to cluster in this way $C^{(i)} = j$ means that the point i belong to cluster j. Where i = 1 ... n and j = 1 ... k.

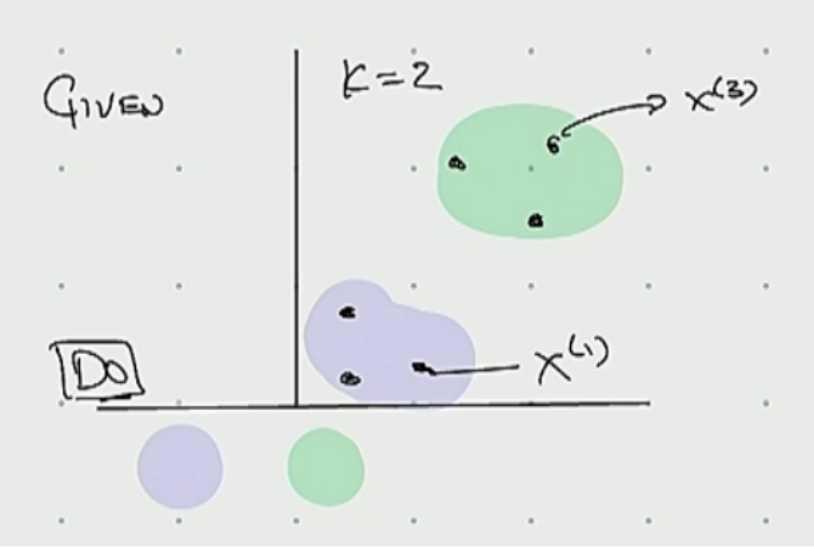


Figure 6: image

So we start assigning points to cluster, for example $C^{(3)} = 2$ means that point 3 is in cluster 2.

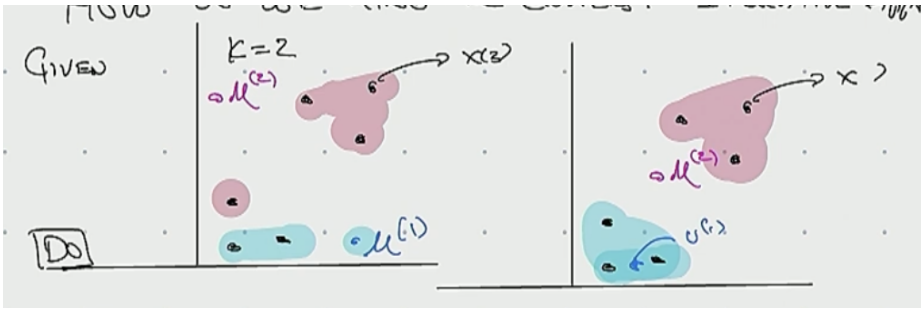


Figure 7: image

How do we find the clusters? We use and iterative approach. So we're going to start by randomly picking cluster centers for each cluster and find the optimal one in which all the points belonging to the cluster are closer to the center than they are to any other center. So the first step of the algorith is 1. Randomly initialize center cluster points $\mu^{(1)}$ and $\mu^{(2)}$ (They don't have to be point in the dataset) 2. Assign each point to a cluster by considering the distance to each center cluster $C^{(i)} = argmin_{j=1...k}||\mu^{(j)} - x^{(i)}||^2$ 3. I compute new cluster centers

And I repeat the step 2 and step 3 until there are no more changes. The cluster center can be computed in this way

$$\mu^{(j)} = \frac{1}{|\Omega_j|} \sum_{i \in \Omega_j} x^{(i)} \text{ s.t } \Omega_j = i : C^{(i)} = j$$

Notice that if the point assignment doesn't change in step 2 the center will not change (step 3).

The first question is: Does it terminate? and the answer is yes.

$$J(C, \mu) = \sum_{i=1}^{N} ||x^{(i)} - \mu^{C^{(i)}}||^2$$

That is, the distance between a point and its cluster center is actually monotonically decreasing. So the oscillation can happen (you can basically do grandient descent on this) but it converges to something but it does not converge necessarily to a global minimizer

How do you choose k? There is no one right answer (modeling question).

Professor slide Objective Function(L) The K-means algorithm aims to minimize the within-cluster sum of squares, which measures the distance between

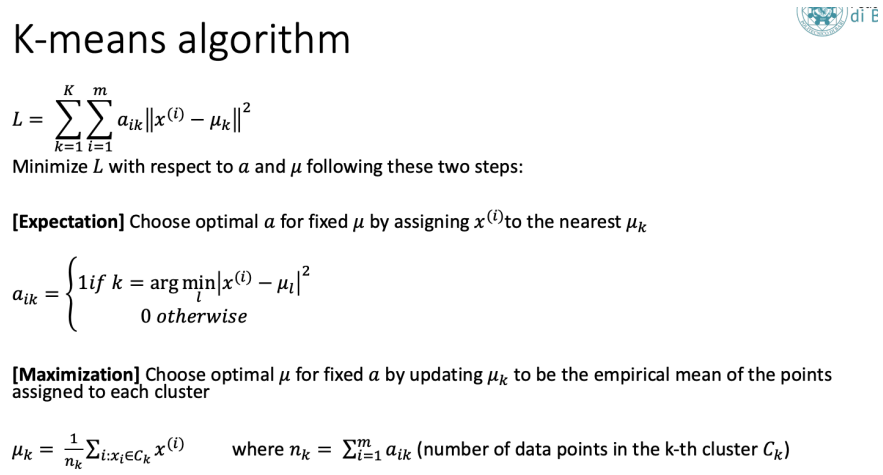


Figure 8: image

each data point $x^{(i)}$ and the centroid μ_k of the cluster it belongs to. The objective function is defined as:

$$L = \sum_{k=1}^{K}\sum_{i=1}^{m} a_{ik}||x^{(i)} - \mu_k||^2$$

- K: The number of clusters.
- m: The number of data points.
- a_{ik}: A binary variable, which is 1 if data point $x^{(i)}$ is assigned to cluster k, and 0 otherwise.
- $x^{(i)}$: The i-th data point in the dataset
- μ_k: The centroid (mean) of the k-th cluster

The algorithm attempts to minimize L, which is the total sum of squared distances between each data point and the centroid of the cluster of which it belongs.

Expectation Step

In this step, the algorithm assigns each data point $x^{(i)}$ to the nearest cluster centroid μ_k. Mathematically, it computes the binary assignment variable a_{ik}:

$$a_{ik} = \begin{cases} 1 \text{ if k} = \arg\min_l ||x^{(i)} - \mu_l||^2 \\ 0 \text{ otherwise} \end{cases}$$

This means that for each data point, the cluster index k is chosen such that the distance between the point $x^{(i)}$ and the centroid μ_k is minimized. The variable a_{ik} will be 1 if the point is assigned to cluster k, and 0 otherwise.

Maximization Step

Once the assignments are made, the centroids of the clusters are updated to reflect the new mean position of the points in each cluster. The update for the $k-th$ cluster centroid μ_k is given by:

$$\mu_k = \frac{1}{n_k} \sum_{i:x_i \in C_k} x^{(i)}$$

- $n_k = \sum_{i=1}^{m} a_{ik}$: The number of points assigned to cluster k.
- C_k: The set of points assigned to cluster k.

The new centroid μ_k is the average of all the points currently assigned to cluster k. This update ensures that the centroid moves towards the center of the points assigned to it.

Iteration The algorithm repeats the Expectation Step and the Maximization step alternately: 1. In the Expectation Step it assigns points to the nearest cluster. 2. In the M-step, it updates the cluster centroids to the mean of the assigned points.

This process continues until the assignments no longer change, meaning the algorithm has

Multivariate Gaussian

A **Multivariate Gaussina distribution** extends the concept of a normal distribution to multiple dimension. It is characterized by a **mean vector** and a **covariance matrix**. #### Gaussian (Normal) distribution

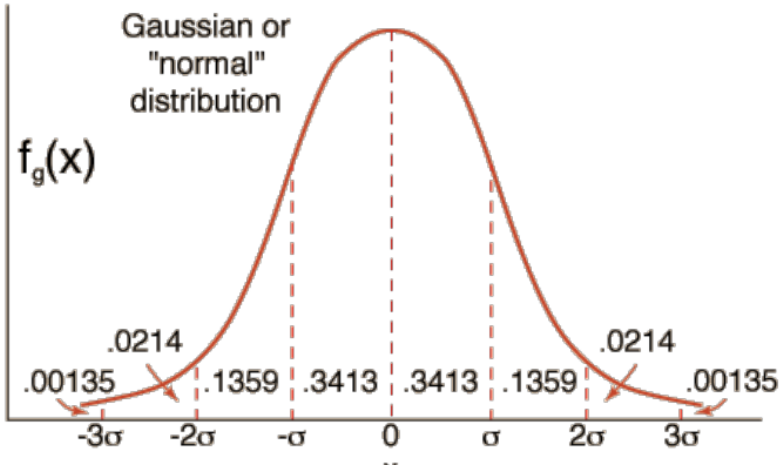


Figure 9: image

In a Gaussian (Normal) distribution we have $x \in \mathbf{R}$ that is our random variable and x has a Gaussina distribution with mean μ and variance σ^2. We can express this fact with this notation $x \sim \mathcal{N}(\mu, \sigma^2)$. The formula for the probability is

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

Parameters estimation Given a dataset : $x^{(1)}, x^{(2)}, ..., x^{(m)}$ We can compute the empirical mean and variance by:

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

Multivariate Gaussian (Normal) distribution For the multivariate case we define the following quantities

$$x \in \mathbf{R^n} \mu \in \mathbf{R^n} \sum \in \mathbf{R^{nxn}} \text{ covariance matrix}$$

And our probability will be:

$$p(x; \mu; \sum) = \frac{e^{\left(-\frac{1}{2}(x-\mu)^T \sum^{-1} (x-\mu)\right)}}{\sqrt{(2\pi)^n |\sum|}}$$

Example: Height and Weight in a Population (Optional Reading) Let's assume we want to model the height and weight of individuals in a population using a 2D multivariate Gaussian distribution. We'll desribe the joint distribution of these two variables using: - A mean vector representing the average height and weight - A covariance matrix representing the variance in height, variance in weight, and how the two variables are correlated.

1. Mean Vector

The mean vector μ consist of the mean of the two variables:

$$\mu = \begin{bmatrix} \mu_{height} \\ \mu_{weight} \end{bmatrix}$$

For example:

$$\mu = \begin{bmatrix} 170 \text{ cm (average height)} \\ 70 \text{ kg (average weight)} \end{bmatrix}$$

2. Covariance Matrix

The covariance matrix $\sum$ contains information about the variances of each variable and their covariance:

$$\sum = \begin{bmatrix} \sigma_{height^2} & Cov(height, weight) \\ Cov(height, weight) & \sigma^2_{weight} \end{bmatrix}$$

- $\sigma^2_{height} = 100cm^2$ that is the variance of height, so standard deviation of height $\sigma_{height} = 10cm$
- $\sigma^2_{weight} = 225kg^2$ that is the variance of weight, so standard deviation of height $\sigma_{weight} = 50$

Interpretation

- The covariance matrix indicates that height and weight are positively correlated (Covariance = 50). Taller individuals tend to weigh more. A positive covariance means that when one variable (height) increases, the other variable (weight) also tends to increase.

For a population described by this bivariate Gaussian distribution:

- Average height = 170 cm
- Average weight = 70 kg
- Height standard deviation = 10 cm
- Weight standard deviation = 15 kg
- Positive correlation between height and weight (Covariance = 50).

If you plot a 2D contour of this distribution, it would look like elliptical contours centered around the mean vector (170 cm, 70 kg), with the major axis of the ellipse tilted due to the positive correlation between height and weight.

The major axis of the elliptical contours in a Multivariate Gaussian distribution is determined by the direction of the greatest variance (or spread) of the data. To determine whether the major axis is aligned more with weight or height, we need to look at both the variances and the covariance between the two variables.

In our example we have that

$$\sum = \begin{bmatrix} 100 & 50 \\ 50 & 225 \end{bmatrix}$$

1. Variance Comparison: The variance in weight (225) is larger than the variance in height (100). This suggests that there is more spread in the weight data than in the height data, which is an initial clue that the major axis might be aligned more with weight.
2. Covariance: The positive covariance (50) between height and weight indicates that the two variables are positively correlated. This means that when height increases, weight tends to increase as well. The ellipse is tilted upward due to this correlation.

Eigenvalues and Eigenvectors

To rigorously determine the direction of the major axis, we would compute the eigenvalues and eigenvectors of the covariance matrix Σ . The eigenvectors give the direction of the principal axes (major and minor), and the eigenvalues indicate the magnitude of variance along these axes.

1. Larger eigenvalue: Corresponds to the major axis (the direction of maximum variance).
2. Smaller eigenvalue: Corresponds to the minor axis (the direction of minimum variance).

Since the variance in weight is larger than the variance in height, we can reasonably expect that the major axis will be closer to the direction of weight. However, because of the positive covariance, the major axis will be tilted, not perfectly aligned with either height or weight. The direction of the tilt would be somewhere between the two, leaning more toward the weight axis because the variance in weight is higher

In the context of the covariance matrix, the eigenvalue problem is solved by finding the eigenvalues and eigenvectors of the matrix. This allows us to determine the principal axes of the ellipse and how spread out the data is along these axes.

The eigenvalue equation is given by:

$$\Sigma v = \lambda v$$

Where:

- v is an eigenvector, representing the direction of one of the principal axes.
- λ is an eigenvalue, representing the variance along that direction.

The characteristic equation to find the eighenvalues is:

$$det(\Sigma - \lambda I) = 0$$

Where I is the identity matrix.

After solving for the eigen values, we use them to find the eigenvectors, which tell us the direction of the major axes of the ellipse.

Resources - Alexander Ihler

Mixture Model

The probability of a point (sample) in the mixture is the sum of the probability (the marginal probability) of the same point in each k Gaussians

$$p(x) = \sum_{j=1}^{k} p(x \wedge z = j)$$

The probability can be explicitly rewritten using the Bayes rules as:

$$p(x) = \sum_{j=1}^{k} p(x|z = j)p(z = j)$$

We can set:

- $p_j(x) = p(x|z = j)$ the probability density fo the jth gaussian in the point x
- $\pi_j = p(z = j)$ the probability of the jth gaussian among all gaussian, called mixing coefficient. (Sample probability)

We can rewrite

$$p(x) = \sum_{j=1}^{k} \pi_j p_j(x)$$

We can further make explicit the parameter of the gaussians (mean and variance), through a theta parameter.

$$p(x|\theta) = \sum_{j=1}^{k} \pi_j p_j(x|\theta_j)$$

- θ_j represents the parameters of the jth gaussian
- θ represents the parameters of all gaussians

A multivariate gaussian under the mixture perspective can be defined as:

$$p(x; \mu_j, \Sigma_j) = \frac{e^{\left(-\frac{1}{2}(x-\mu_j)^T \Sigma^{-1}(x-\mu_j)\right)}}{\sqrt{(2\pi)^n |\sigma_j|}}$$

Where: - μ_j is the vector of the means of the jth gaussian - Σ_j is the covariance matrix of the jth gaussian - n is the number of features

What we want to know are the parameters of the Gaussians:

μ_j and Σ_j $j = 1..., k$

Let us define C_j as the jth cluster, and $|C_j|$ the number of the points that belong to it. If we knew which point belongs to which cluster, we would compute the paramters as:

Univariate

$$\hat{\mu_j} = \frac{1}{|C_j|} \sum_{x^{(i)} \in C_j} x^{(i)} \hat{\sigma_j}^2 = \frac{1}{|C_j| - 1} \sum_{x^{(i)} \in C_j} (x^{(i)} - \hat{\mu_j})^2$$

Multivariate

$$\hat{\mu}_j = \frac{1}{|C_j|} \sum_{x^{(i)} \in C_j} x^{(i)} \hat{\Sigma}_j = \frac{1}{|C_j| - 1} \sum_{x^{(i)} \in C_j} (x^{(i)} - \hat{\mu}_j)(x^{(i)} - \hat{\mu}_j)^T$$

Expectation-Maximization Algorithm (EM)

1. Randomly set the parameters (μ_j,Σ_j, and π_j) for each of the K gaussians.
2. Repeat {
    1. (E) Expectation step: for each cluster-point pair the "responsability" coefficient is computed. This coefficient gives an idea of how much the point is generated from the gaussian that is pared with it at the moment, w.r.t the entire mixture.
    2. (M) Maximization step: the parameters (means, variances and mixing coefficient) are recomputed as a function of the responsibility coefficient to maximize the Likelihood. } until convergence.

Expectation step For each cluster-point pair, the "responsability" coefficient is computed. This coefficient shows how much the point is generated from the Gaussian that is paired with it at the moment, w.r.t the entire mixture.

$$r_{ij} := p(z = j | x^{(i)}, \theta^{(t-1)})$$

$\theta_j^{(t-1)}$ are the parameters set in the previous iteration. We can make the formula more explicit:

$$r_{ij} = \frac{\pi_j p_j(x^{(i)} | \theta_j^{(t-1)})}{\sum_{j=1}^{k} \pi_j p_j(x^i | \theta_j^{(t-1)})}$$

The numerator represents the probability that the data point x is generated by the j-th Gaussian component (with his mean and coveriance). And the coefficient is averaged with the sum of the probability that the point has been generated by the i-th gaussian with his distribution paramters

Maximization step The parameters (means, variances and mixing coefficient) are recomputed as a function of the responsibility coefficient to maximize the likelihood.

$$\pi_j = \frac{1}{m}\sum_{i=1}^{m} r_{ij}\mu_j = \frac{\sum_i r_{ij}x^{(i)}}{\sum_i r_{ij}}\Sigma_j = \frac{\sum_i r_{ij}(x^{(i)}-\mu_j)(x^{(i)}-\mu_j)^T}{\sum_i r_{ij}}$$

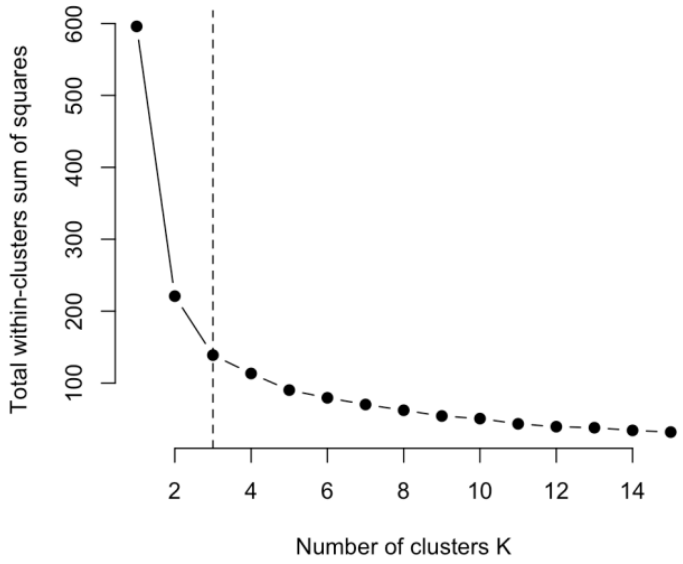
PROS/CONS Pros - It is a flexible algorithm that is able to approximate multivariate gaussian to fit data maximing the likelihood - It is not affected by bias approaching zero means - Less sensible to outliers

Cons - The algorithm can diverge if there are only few points w.r.t. the overall mixture - All the flexibility of the model is always used, even if it is not needed

Resources

- [Alexander Ihler] https://www.youtube.com/watch?v=qMTuMa86NzU&list=PLaXDtXvwY-oDvedS3f4HW0b4KxqpJ_imw&index=34
- [Stanford Lecture] https://www.youtube.com/watch?v=LMZZPneTcP4&list=PLoROMvodv4rNyWOpJg_
- [Stanford 2019 Very clean so far] https://www.youtube.com/watch?v=LmpkKwsyQj4&t=2896s

Choosing the value of K



Elbow Method
Is a visual approach used to determine the ideal 'K' (number of clusters) in K-means clustering. It operates by calculating the Total Within Cluster Sum of Squares, which is the total of the squared idstances between data points and their cluster center. However, there is a point where increasing K no longer leads to a significant decrease in WCSS and the rate of decrease slows down.

This point is often referred to as the elbow. In ordere to measure the distance we can use for example Euclidian distance

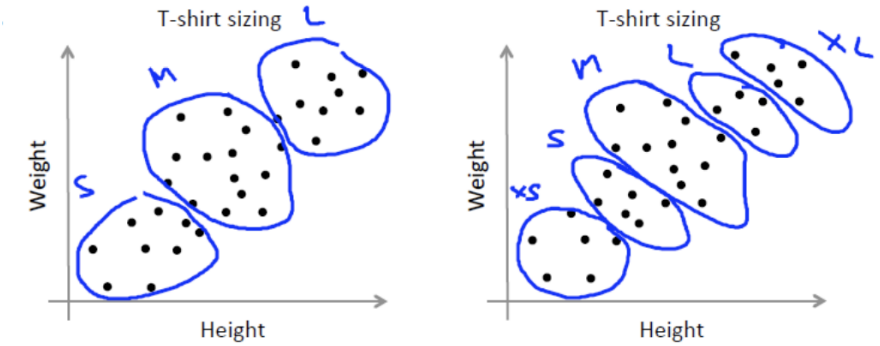


Figure 10: image

External constraints Sometimes our ML systems must fit some external constraints, in those cases the number of clusters depends on how well the clusters performs on an external task.

Kullback-Leibler divergence It can be used to measures how the "true" probability distribution $P(i)$ diverges from the expected probability distribution that is the distribution fo the model $Q(i)$. It can assume values from 0 (when the two distributions behave in the same way) to 1 (when their behaviour is completely different)

$$D_{KL}(P||Q) = -\sum_i P(i) log \frac{Q(i)}{P(i)} = \sum_i P(i) log \frac{P(i)}{Q(i)}$$

It can be for example used to compare two models (GMM models) if the two models produce very similar probability distributions, the KL divergence will be close to 0, indicating that adding an extra cluster does not improve the model much

Information criterion approach

- AIC: Akaike information criterion
- BIC: Bayesian information criterion
- DIC: Deviance information criterion
- BF: Bayes factors
- MDL: Minimum Description Length
- FIA: Fisher Information Aproximation

Likelihood Given a probabilistic model and come observed data the likelihood is the probability of the observed data $X = x_1, x_2, ..., x_n$, given a model with parameters θ. Formally, the likelihood function id defined as:

$$L(\theta; X) = P(X|\theta)$$

Akaike information criterion (AIC) AIC derived as asymptotic approximation of Kullback-Liebler information distance between the model of interest and the truth

$$AIC = 2k - 2ln(\hat{L})$$

Where k is the number of parameters. An alternative is AICc, in which a correction related to the number of samples is considered:

$$AICc = AIC + \frac{2k \cdot (k+1)}{m-k-1}$$

The model that minimizes AIC is selected

AIC (Wikipedia) Given a collection of models for the data, AIC estimates the quality of each model, relative to each of the other models. Thus, AIC provides a means for model selection.

Given a set of candidate models for the data, the preferred model is the one with the minimum AIC value

Suppose that the data is generated by some unknown process f. We consider two candidate models to represent f: $g1$ and $g2$. If we knew f, then we could find the information lost from using g1 to represent f by calculating the Kullback–Leibler divergence, $DKL(f$Ę$g1)$; similarly, the information lost from using $g2$ to represent f could be found by calculating $DKL(f$Ę$g2)$. We would then, generally, choose the candidate model that minimized the information loss.

We cannot choose with certainty, because we do not know f. Akaike (1974) showed, however, that we can estimate, via AIC, how much more (or less) information is lost by $g1$ than by $g2$. The estimate, though, is only valid asymptotically.

Note that AIC tells nothing about the absolute quality of a model, only the quality relative to other models. Thus, if all the candidate models fit poorly, AIC will not give any warning of that.

Bayesian information criterion BIC is the aymptotic approximation under the assumption that the model can result in an exponential distribution

$$BIC = ln(m) \cdot k - 2ln(\hat{L})$$

Where m is the number of samples and k is the number of parameters

The model that minimizes BIC is selected.

Deviance information criterion It represents an asymptotic approximation of the deviance under the assumption that the posterior distribution is a multivariate normal

????

Information criterions comparison

- AIC lacks the finite samples correction in its base form
- AIC is asymptotically equivalent to k-folds cross-validation on linear regression models with a least squares optimization
- BIC is able to detect the true model (if present in the comparison)
- BIC is only valid if n is much greater than k
- BIC penalizes complex models more than AIC
- DIC tends to suggest overfitted models

Silhoutte Coefficient Silhoutte Coefficient combines the ideas of cohesion and separation for single samples, clusters, and clusterings

For an individual sample, $x^{(i)}$ - coh = average distance of $x^{(i)}$ to the samples in the same cluster. - sep = min (average distance of xˆ{(i)}) to samples in another cluster - silhoutte coefficient fo xˆ{(i)}: - $s_i = 1 - \frac{coh}{sep}$ if $coh < sep$ The closer to 1 the better Can calculate the Average Silhouette width for a cluster or a clustering

Hierarchical Clustering

Hierarchical cluster involves builing a hierarchy of (potentially overlapping) clusters. We have two categories of hierarchical cluster: - Agglomerative: This is a "bottom-up" approach: Each observation starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy. - Divisive: This is a "top-down" approach: All observations start in one cluster, and splits are performed recursively as one moves down the hierarchy

The Hierarchical clustering technique can be visualized using a Dendogram.

A Dendogram is a tree like diagram that records the sequences of merges or splits

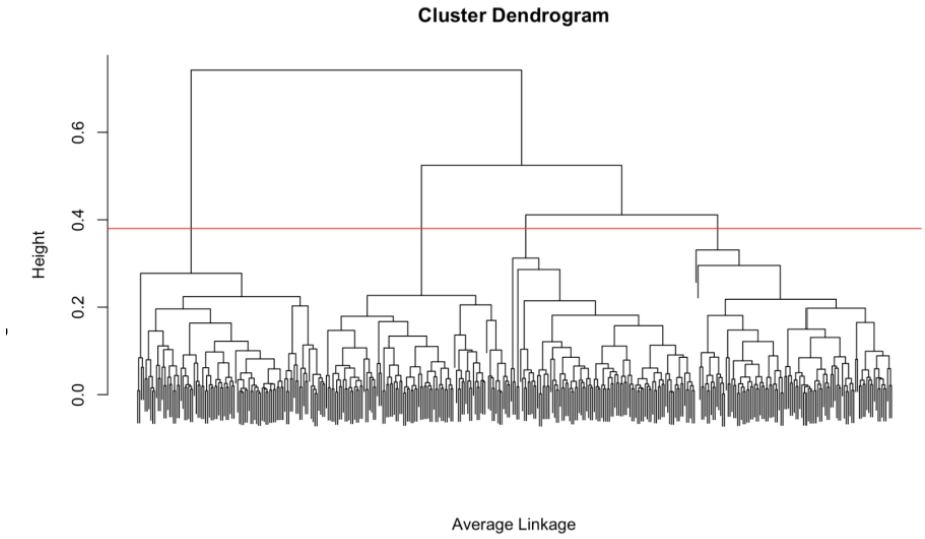


Figure 11: image

Once the hierarchy is built, cluster extraction is done by selecting some height to 'cut' For example in the image above we ends up with 4 clusters.

In order to merge two cluster (agglomerative) we need to calculate the similarity between two cluster. So we have to define the 1. **Similarity meause/metric**: For example Euclidean Distance, Mahalanobis distance, etc. 2. **Linkage Criterion** - Distance Based: Max/min/mean distance (complete/single/ average linkage) - Probability based: the probability that the candidate clusters come from the same distribution - The product of the in-and-out degree of a node (graph degree linkage) - Instance-based constraints

Single Linkage The most well-known hierarchical clustering algorithm is called the Single Linkage algorithm.

1. Each point belongs to a separate cluster so we would have n cluster for n points
2. The two closest points form a new cluster
3. The steps are repeated so each time we merge the two closest pair of points The similarity metric is Euclidean distance and the linkage criterion is the (pairwise) minimum distance.

Wards Criterion Rather than use distance metrics as measures of similarity, why not merge based on a more statistically intuitive notion Perhaps its fair to assume observations come from an approximately elliptically-shaped distribution Ward proposed agglomeration where observations are merged in such as way

that minimizes the total squared error (maximizes r^2 at each merge) So to give a concrete Idea 1. Compute SSR for cluster A: - For a cluster A, the sum of squared residuals (SSR) is the sum of squared distances between each point in A and the centroid (mean) of A. - This is calculated as:

$$SSR_A = \sum_{x \in A} ||x_A - \mu_a||^2$$

where x is a point in cluster A and μ_A is the centroid of cluster A. 2. Compute SSR for Cluster B: - Similarly, for a cluster B, the SSR is:

$$SSR_B = \sum_{x \in B} ||x - \mu_B||^2$$

3. Compute SSR for the Merged Cluster AB - Now, if you merge clusters A and B, the new merged cluster AB will have a new centroid μ_{AB}, and you compute the SSR for the merged cluster AB:

```
$$
SSR_{AB} = \sum_{x \in A \cup B}||x - \mu_{AB}||^{2}
$$
```

4. Calculate the increase in SSR:
    - The key decision in Ward's method is to minimize the increase in SSR when merging two clusters. This increase is calculated as:

$$\Delta SSR = SSR_{AB} - (SSR_A + SSR_B)$$

Cluster distance measures

- Single link: We compute the distance between closest elements in cluster and merge cluster based on this minimum distance, this method produces long chains a –>b—>c. . .
- Complete link: The distance between two clusters is defined by the maximum distance between any pair of points from the two clusters
    1. Initialize: Treat each data point as its own cluster
    2. Distance calculation: Compute the distance between all pairs of clusters. For two clusters C_1 and C_2, the distance is the maximum distance between any point in C_1 and any point in C_2. Mathematically $D(c_1, c_2) = max_{x_1 \in C_1, x_2 \in C_2} D(x_1, x_2)$
    3. Merge clusters: Find the two clusters that have the smallest maximum distance between them, and merge them together
    4. Repeat: Continue calculating distances and merging clusters until all points are in a single cluster or until a stopping criterion is met.
- Average link: We take two cluster and we compute the distance between of all pair of points and we compute the average of all pairwise distances between points from the two clusters.

1. Initialize: Each data point starts as its own cluster.
2. Distance Calculation: For each pair of clusters, calculate the average distance between all points in one cluster and all points in the other cluster. Mathematically, if you have two cluster C_1 and C_2, the distance between them is computed as:

$$D(c_1, c_2) = \frac{1}{|C_1|}\frac{1}{|C_2|}\sum_{x_1 \in c_1}\sum_{x_2 \in c_2} D(x_1, x_2)$$

   where $|C_1|$ and $|C_2|$ represent the number of points in cluster C_1 and C_2 respectively, and $D(x_1, x_2)$ is the euclidean distance between the point from C_1 and point from C_2
3. Merge Clusters: Find the two clusters with the smallest average distance and merge them toghether
4. Repeat: Continue calculating the distances between the new merged cluster and all other cluster, then merge the cosest clusters until all points are in a single cluster or a stopping condition is met.

- Centroid: Is another hierarichal clustering technique, where the distance between two clusters is defined as the distance between their centroids (i.e the mean points of the clusters)

1. Initialize: Each data point starts as its own cluster
2. Compute Centroid: For each cluster, calculate the centroid (mean point), which is the average of all points in the cluster. For a cluster C with points $x_1, ...x_n$, the centroid μ_C is given by:

$$\mu_C = \frac{1}{|C|}\sum_{i=1}^{|C|} x_i$$

   where $|C|$ is the number of points in the cluster.

3. Distance Between Centroids: The distance between two clusters C_1 and C_2 is calculated as the distance between their centroids.

$$d(C_1, C_2) = ||\mu_{C_1} - \mu_{C_2}||$$

4. Merge Clusters: Find the pair of clusters whose centroids are closest together and merge them into a new cluster.
5. Update Centroid: After merging two clusters, the centroid of the new merged cluster is recalculated as the mean of all points in the merged cluster.
6. Repeat: Continue this process, recalculating the centroids after each merge and merging the cluster with the closest centroids, until all points are in a single cluster or a stopping condition is met.

- Ward's method: The idea is when two cluster are joined together how does it change the total distance (TD) from centroids? (Variance). Mathematically

$$TD_{C_1 \cup C_2} = \sum_{x \in C_1 \cup C_2} D(x, \mu_{c_1 \cup c_2})^2$$