Mahalanobis Distance

Neuroinformatics Tutorial 4

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Content

- Revision: Naive Bayes Classifer
- Revision: Lecture
- Mahalanobis Distance

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Revision: Naive Bayes Classifier

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B: 2,4

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$$\underset{k=0,\ldots,N}{\operatorname{argmax}}[P(C_k|x_1,\ldots x_n)]$$

$$= \underset{k=0,\ldots,K}{\operatorname{argmax}}[P(C_k)\cdot P(x_1|C_k)\cdot P(x_2|C_k,x_1)\cdots P(x_n|C_k,x_1,\ldots,x_{n-1})]$$

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Naive Bayes Classifier

- Given a labeled training set, how do we get these probabilities?

$$\underset{k=0,\ldots,K}{\operatorname{argmax}}[P(C_k)\cdot P(x_1|C_k)\cdot P(x_2|C_k)\cdots P(x_n|C_k)]$$

Prior of class C_k:
Number of class occurences in data set divided by number of all samples in data set

Likelihoods of all features, given class C_k

For each feature/class combination, we need a (gaussian) distribution model!
This way we can calculate the probability during inference!

Estimation of Likelihood

- In practice quite important:
  - Estimation of Likelihood P(feature | class)
  - Easy for categorical features:
  - But what about continuous features?

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

Temp.	Class
19°C	Rainy
18°C	Rainy
20°C	Rainy
21°C	Sunny
22°C	Sunny
24°C	Sunny

  - P(Temp=19.5°C | Class = Rainy) = 0% ?

  - => Need to estimate underlying distribution!
  - Assume Gaussian
    => Mean Temp (Given Class = Rainy) = 19°C
    => Variance (Given Class = Rainy) = $\frac{2}{3}$

    => P(Temp=19.5°C | Class = Rainy) = $\frac{1}{\sqrt{2\pi\frac{2}{3}}} e^{-\frac{(19.5-19)^2}{2\cdot\frac{2}{3}}}$

Naive Bayes Classifier: Jupyter

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$$\underset{k}{\operatorname{argmax}}\{d^k(x)\}$$

$$d^k(x) := \ln P(x|c^k)$$

$$d^k(x) := -||x - \mu_k||_2$$

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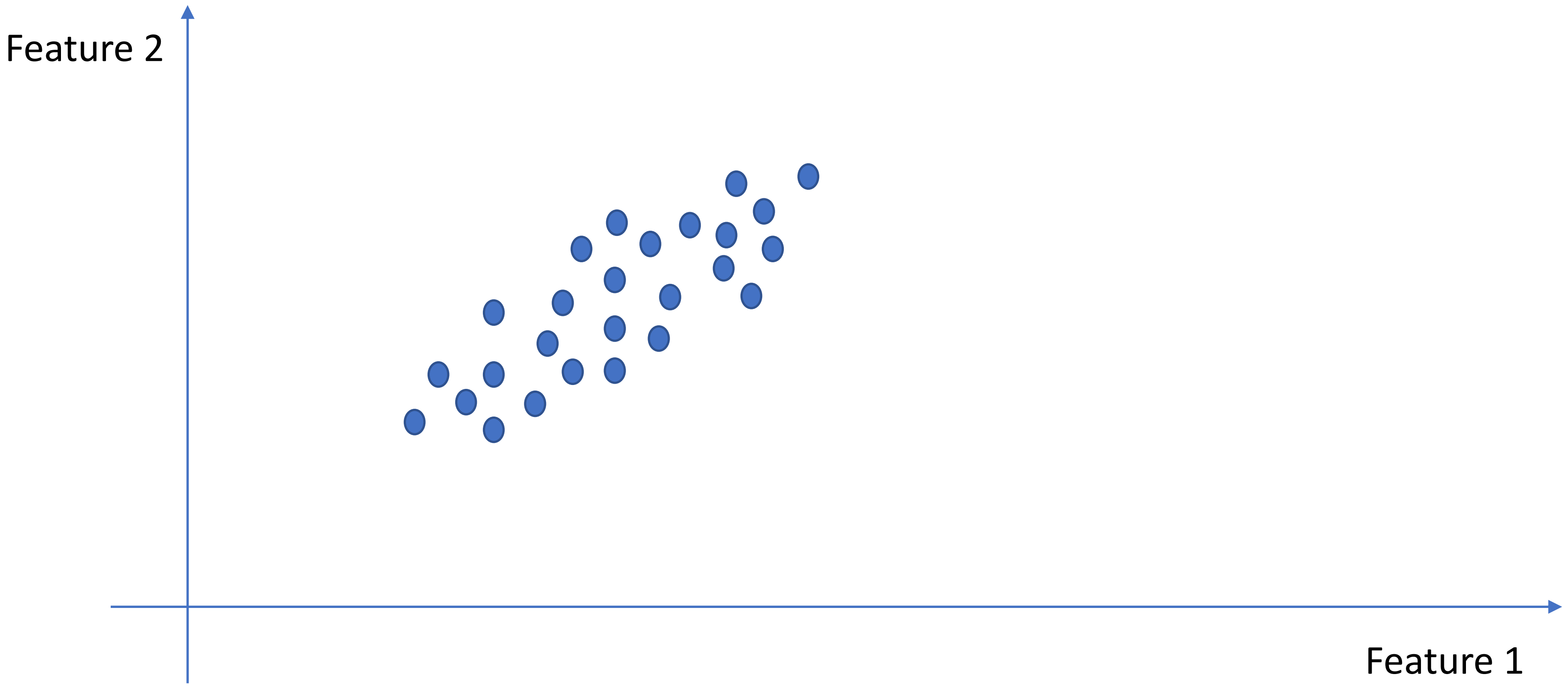
Mahalanobis Distance: Motivation



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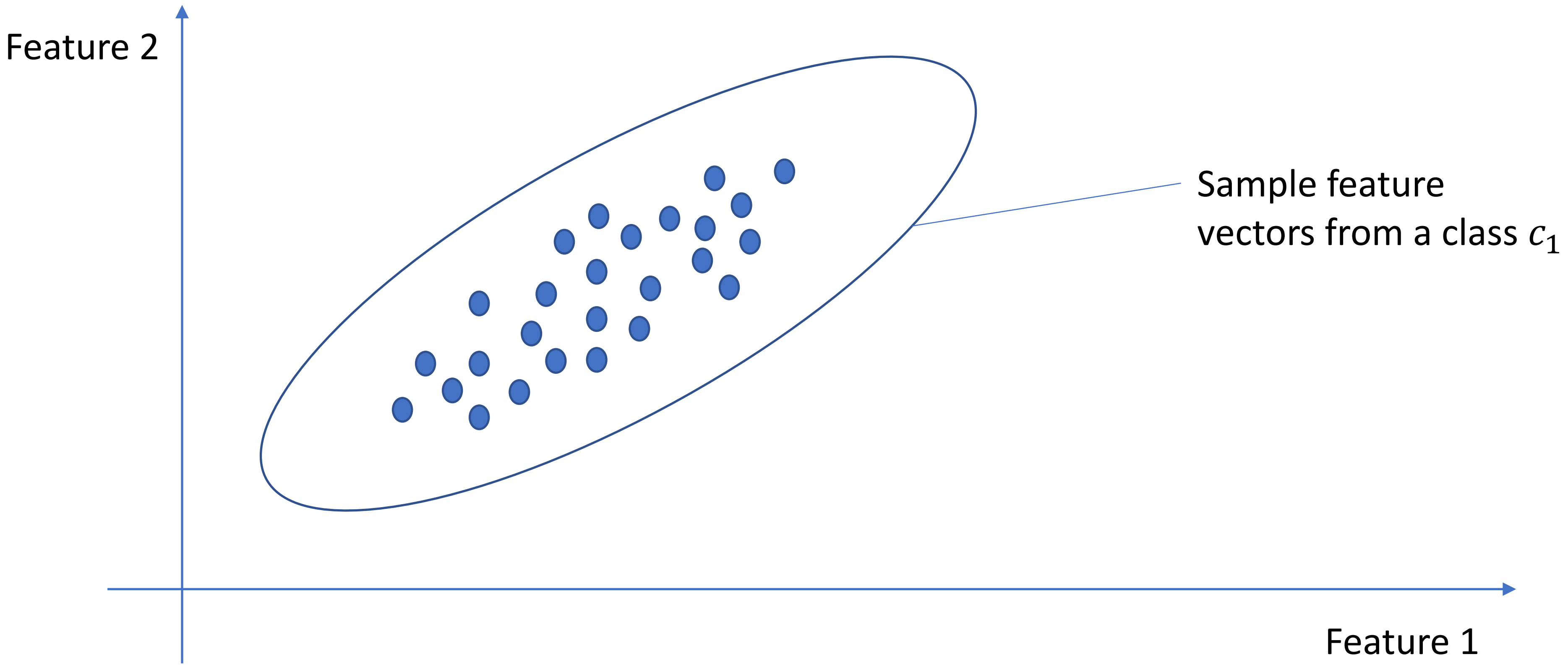

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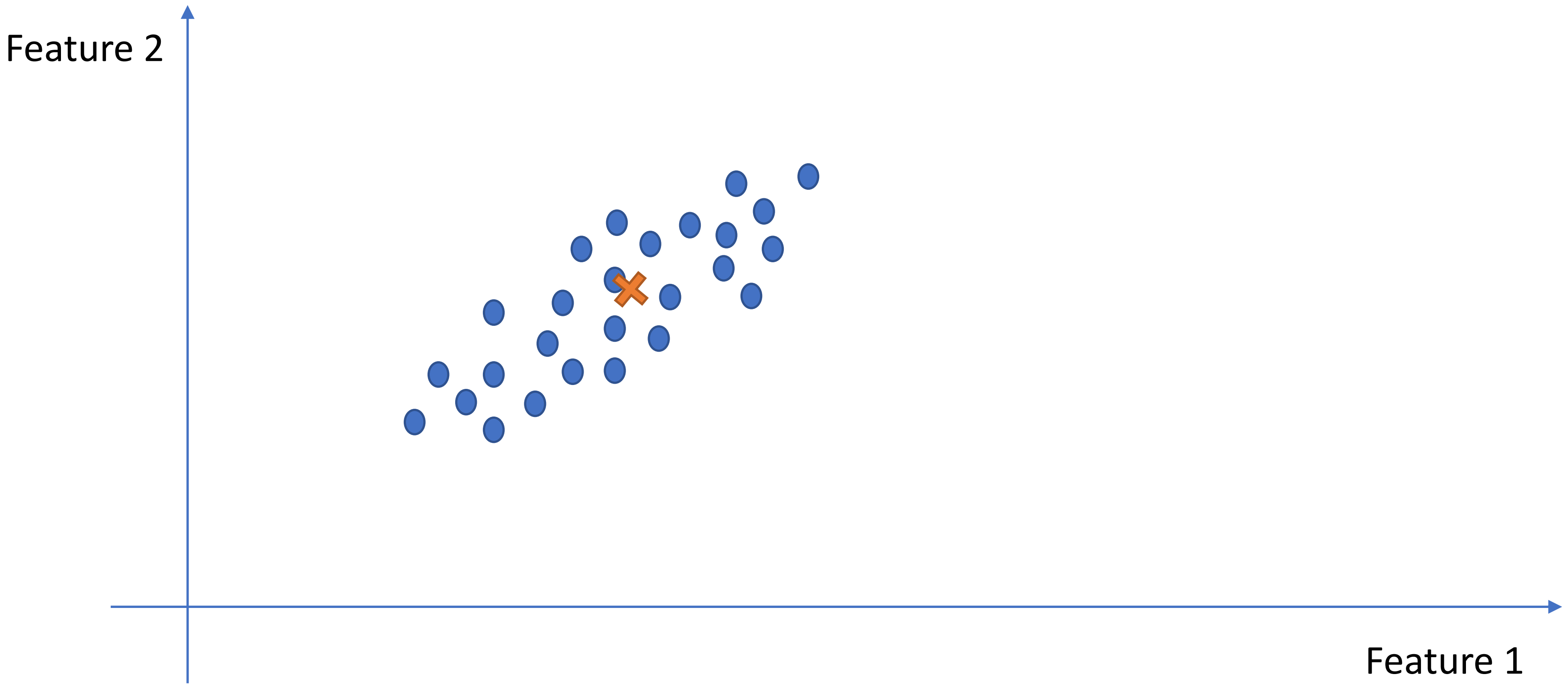

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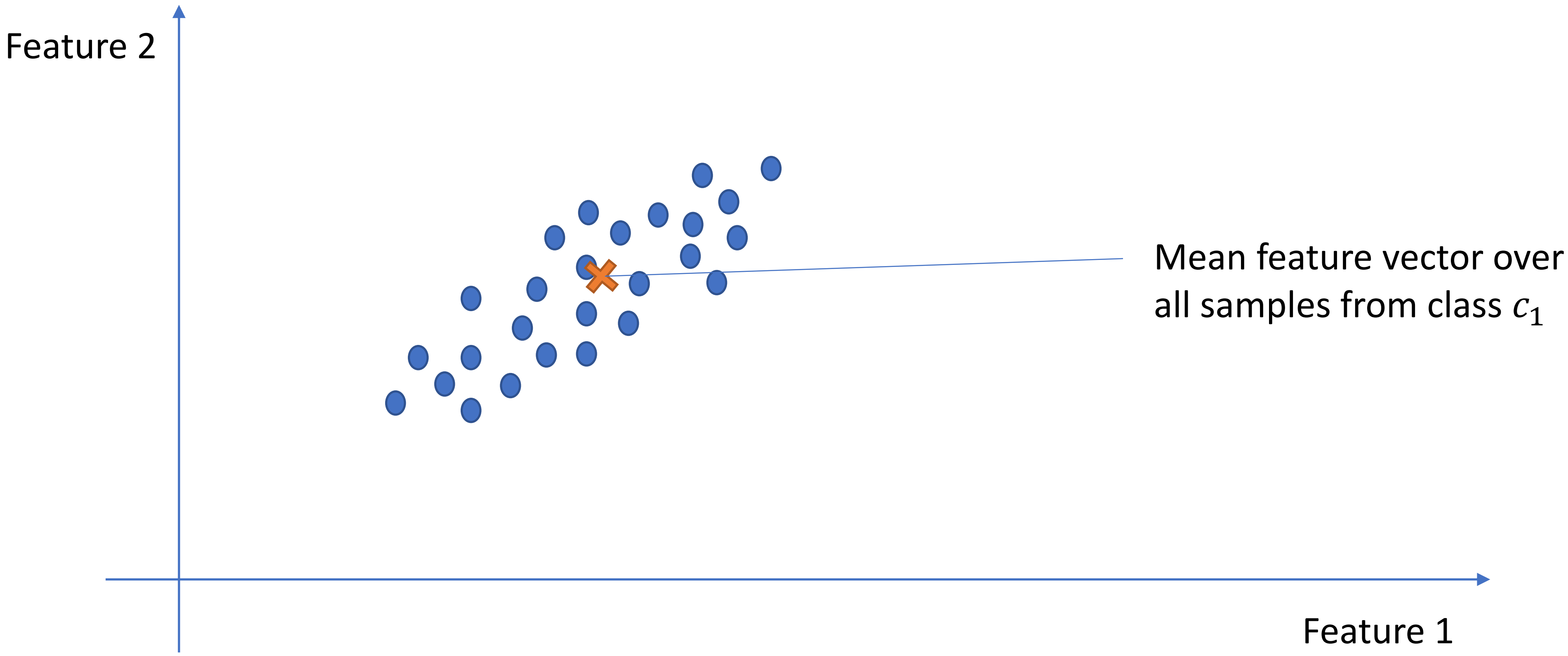

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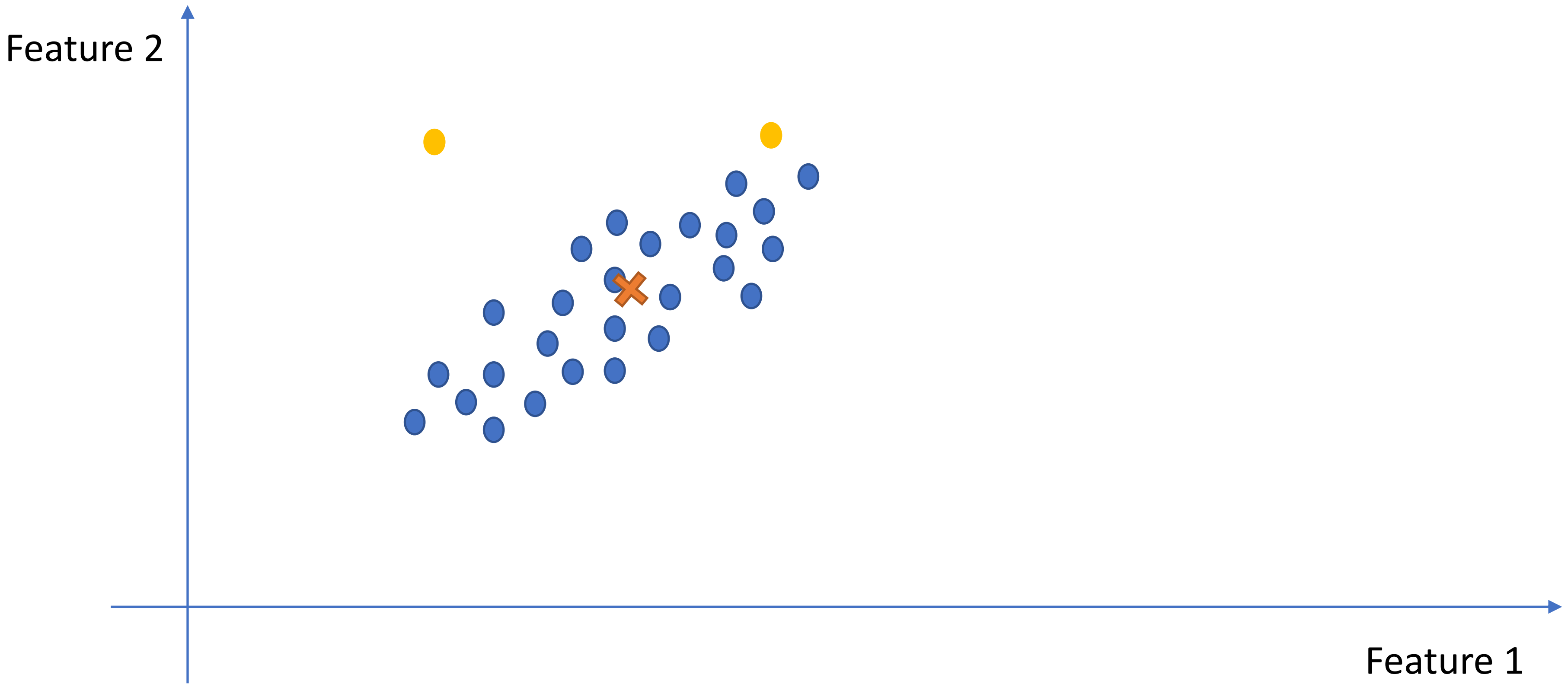

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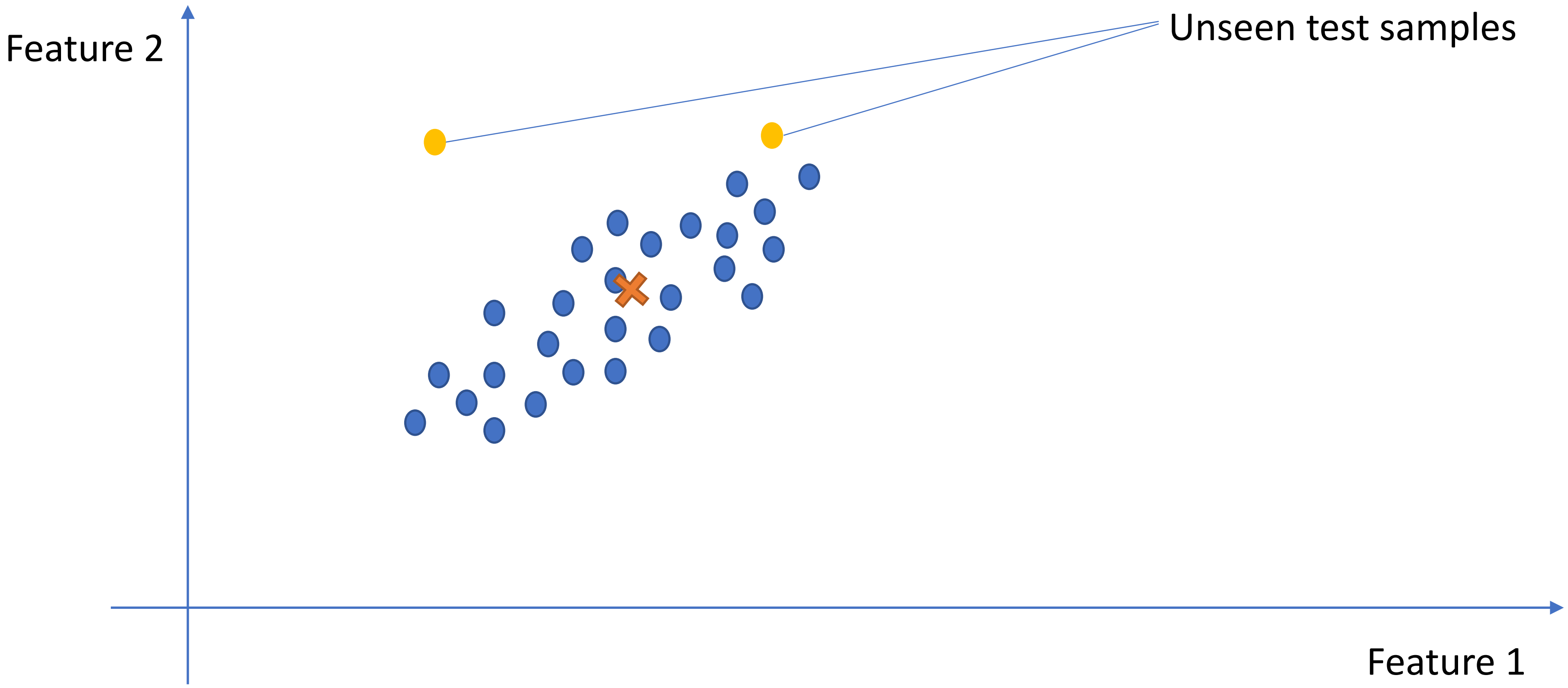

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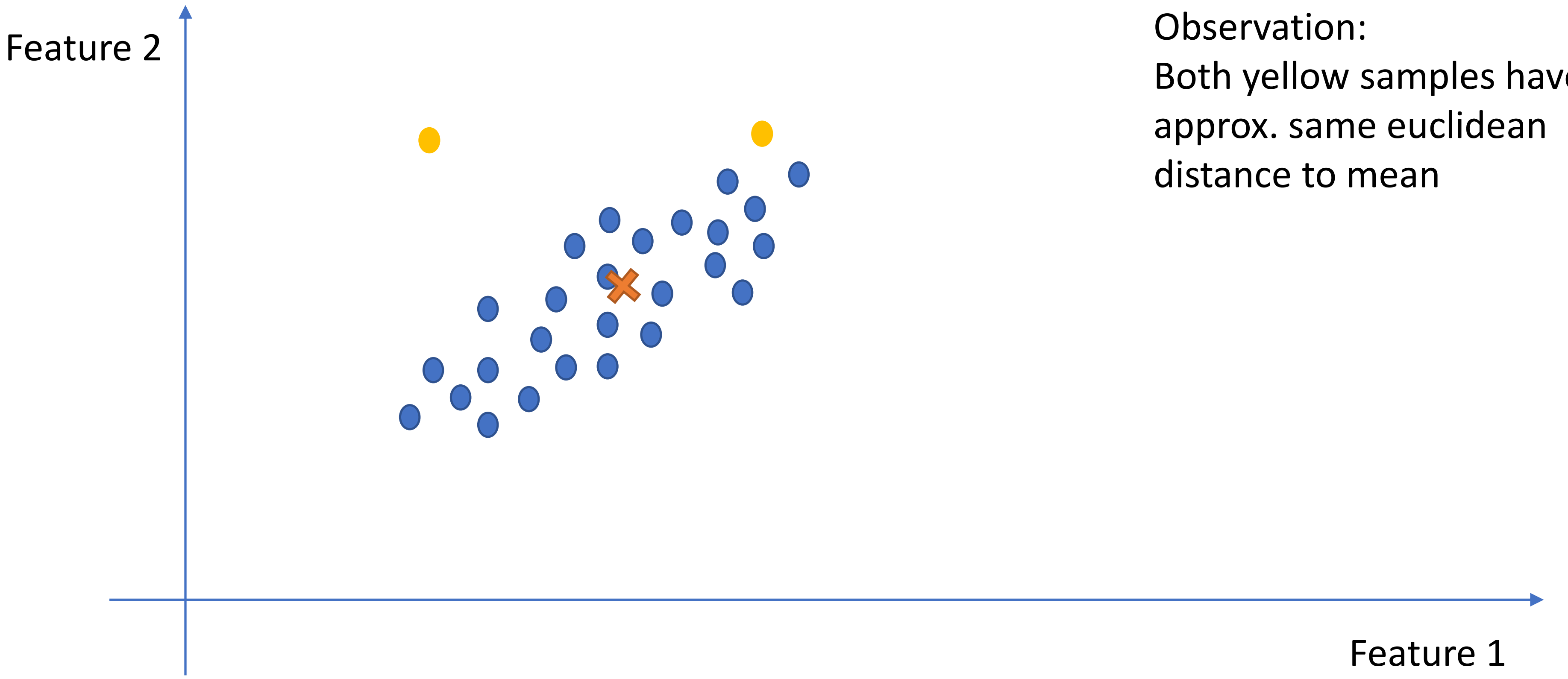

Observation:
Both yellow samples have approx. same euclidean distance to mean

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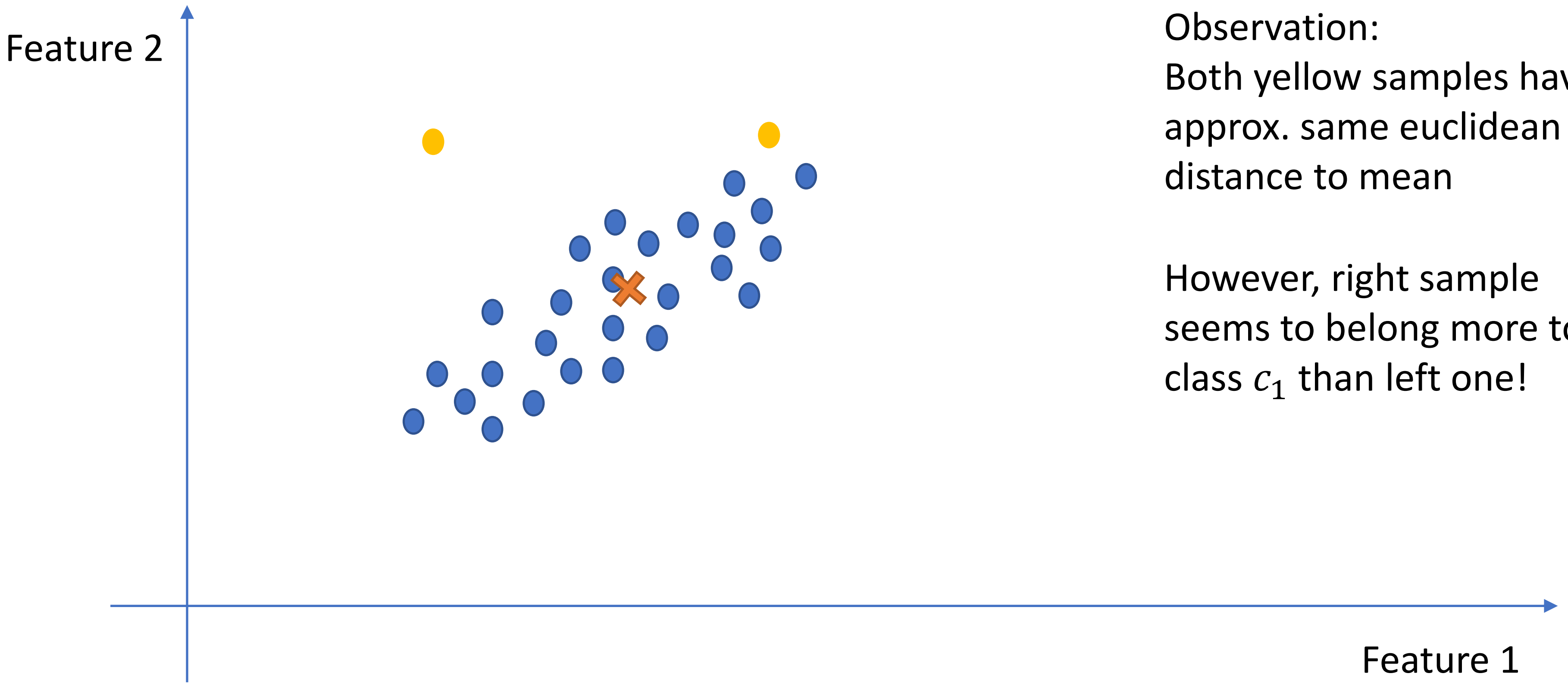

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However, right sample seems to belong more to class c_1 than left one!

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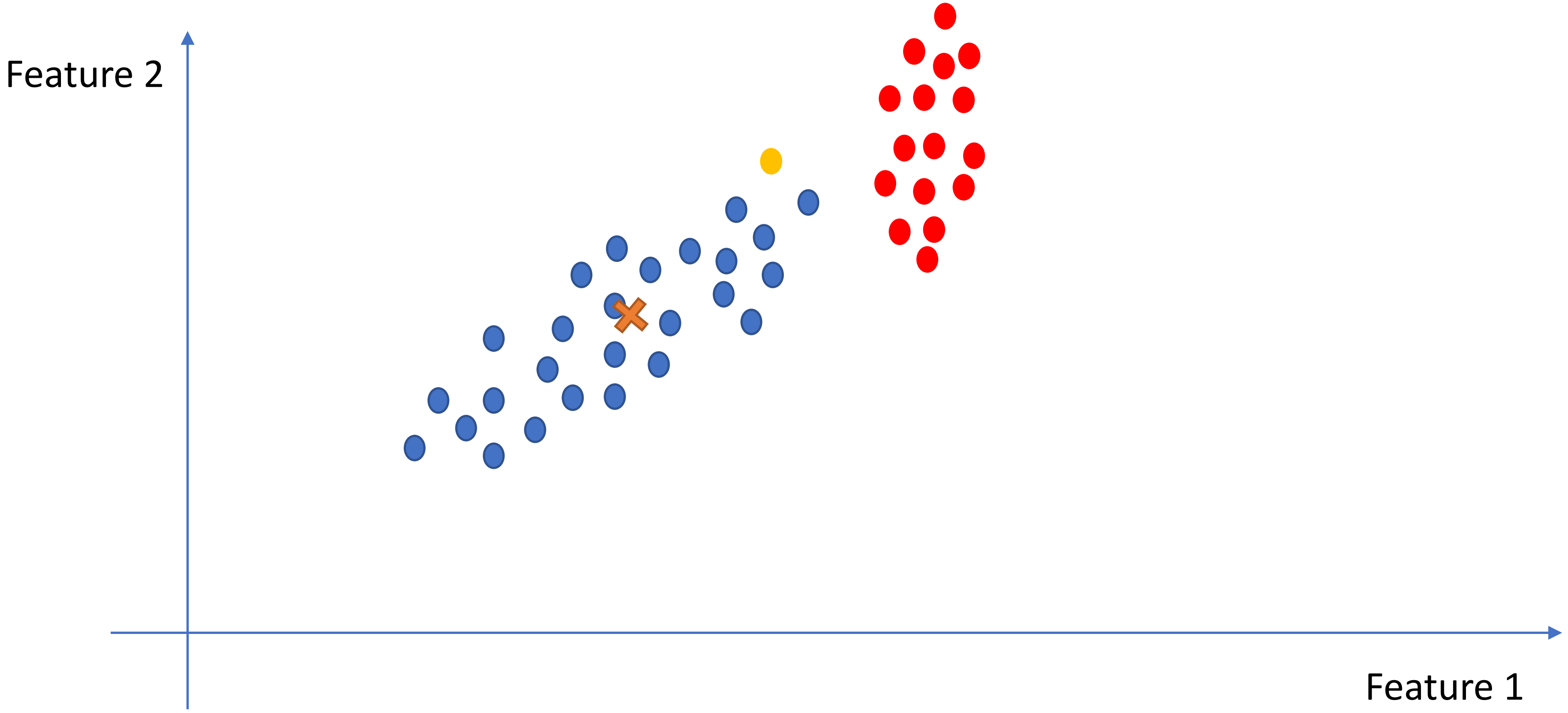

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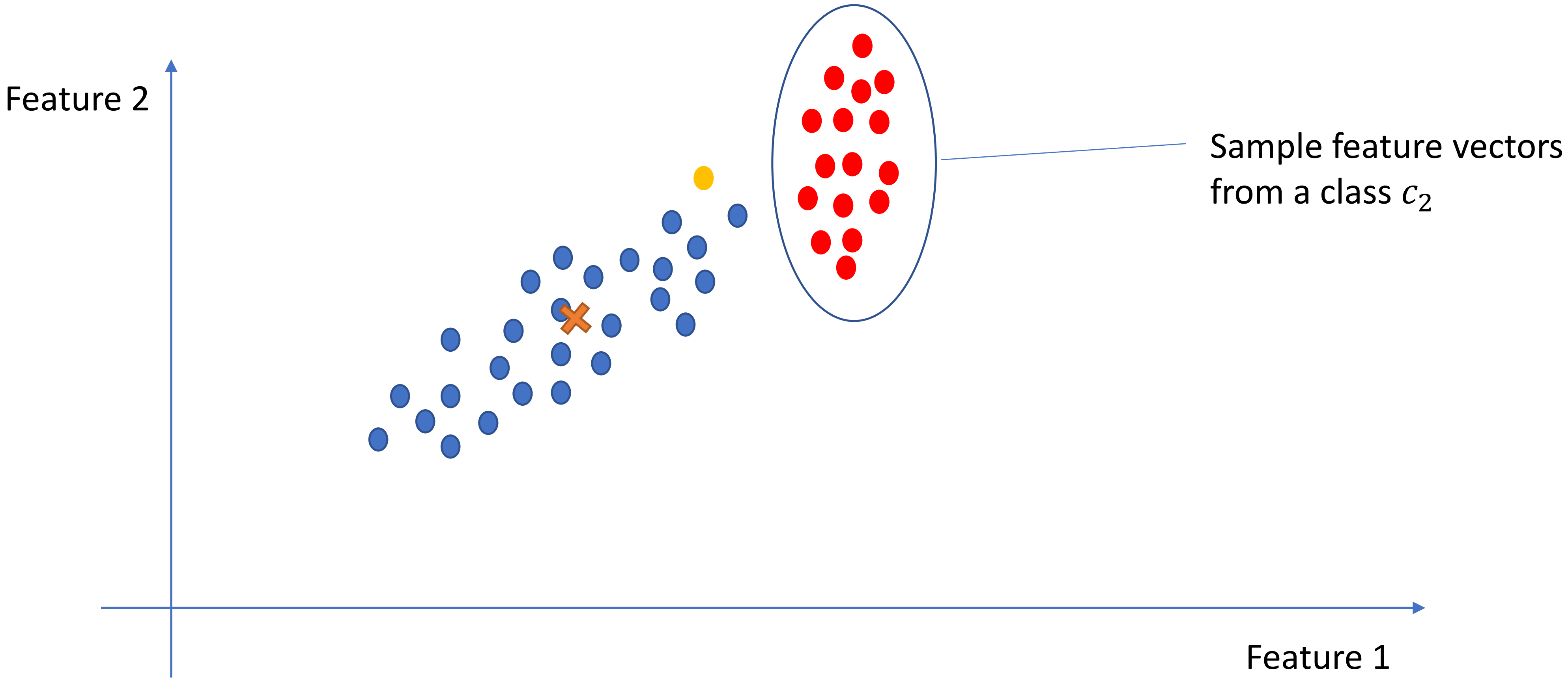

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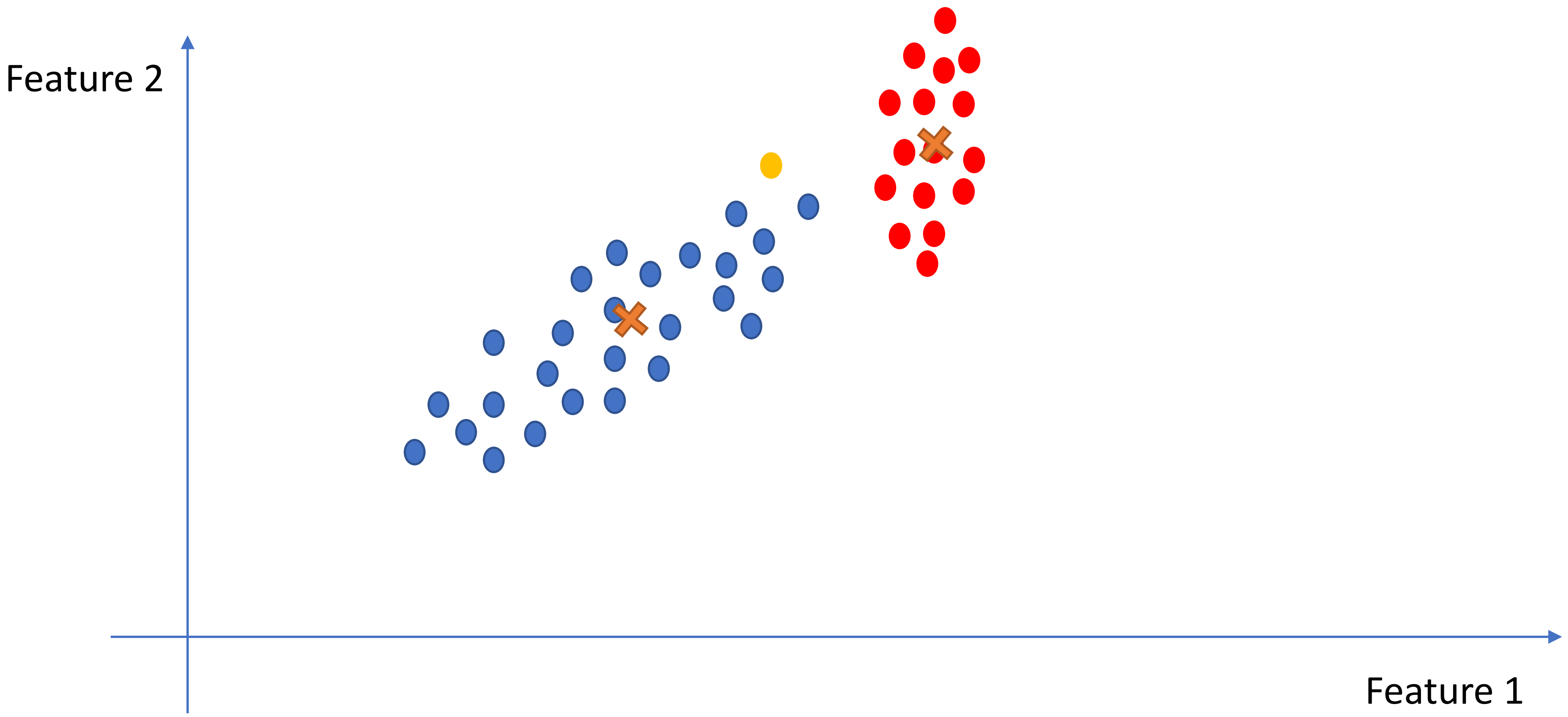

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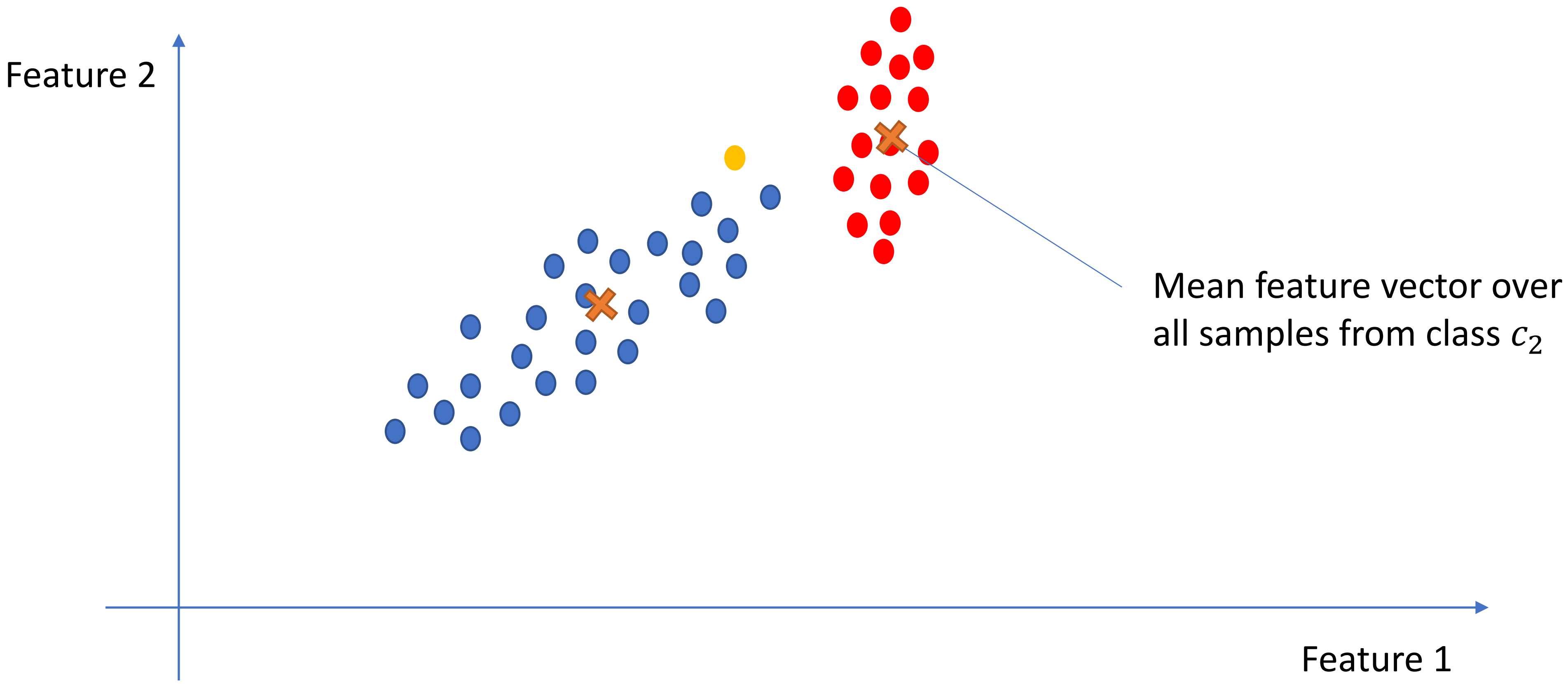

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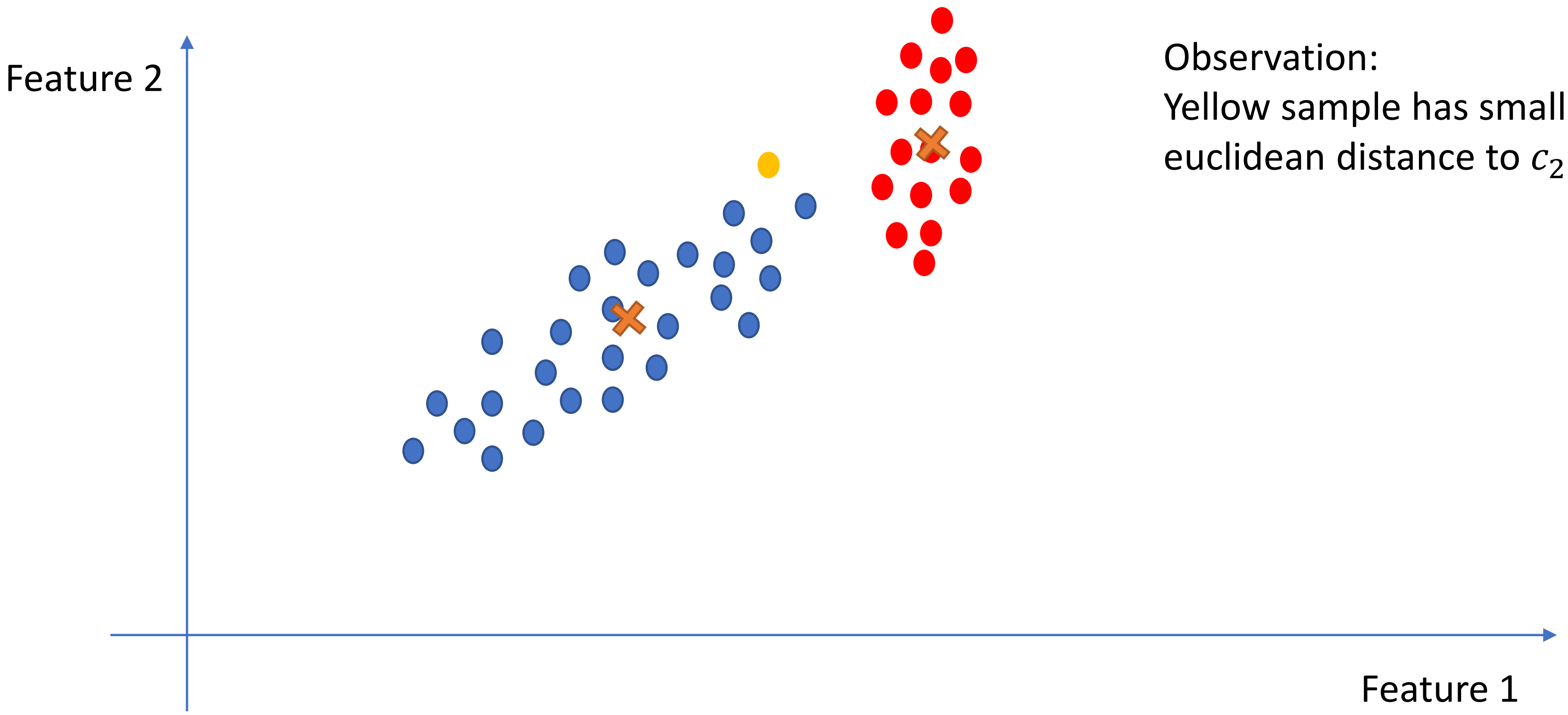

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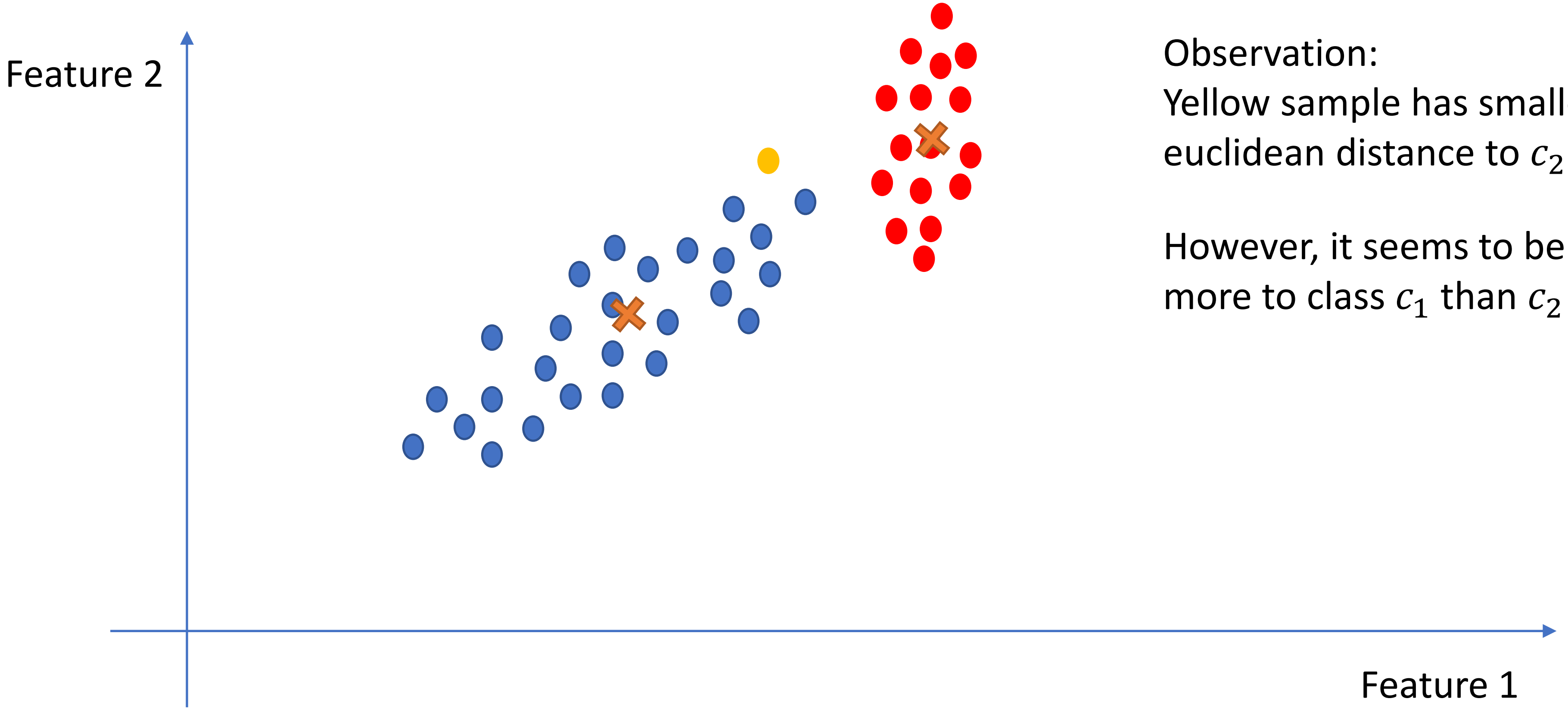

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However, it seems to belong more to class c_1 than c_2 !

Prerequisites: Covariance

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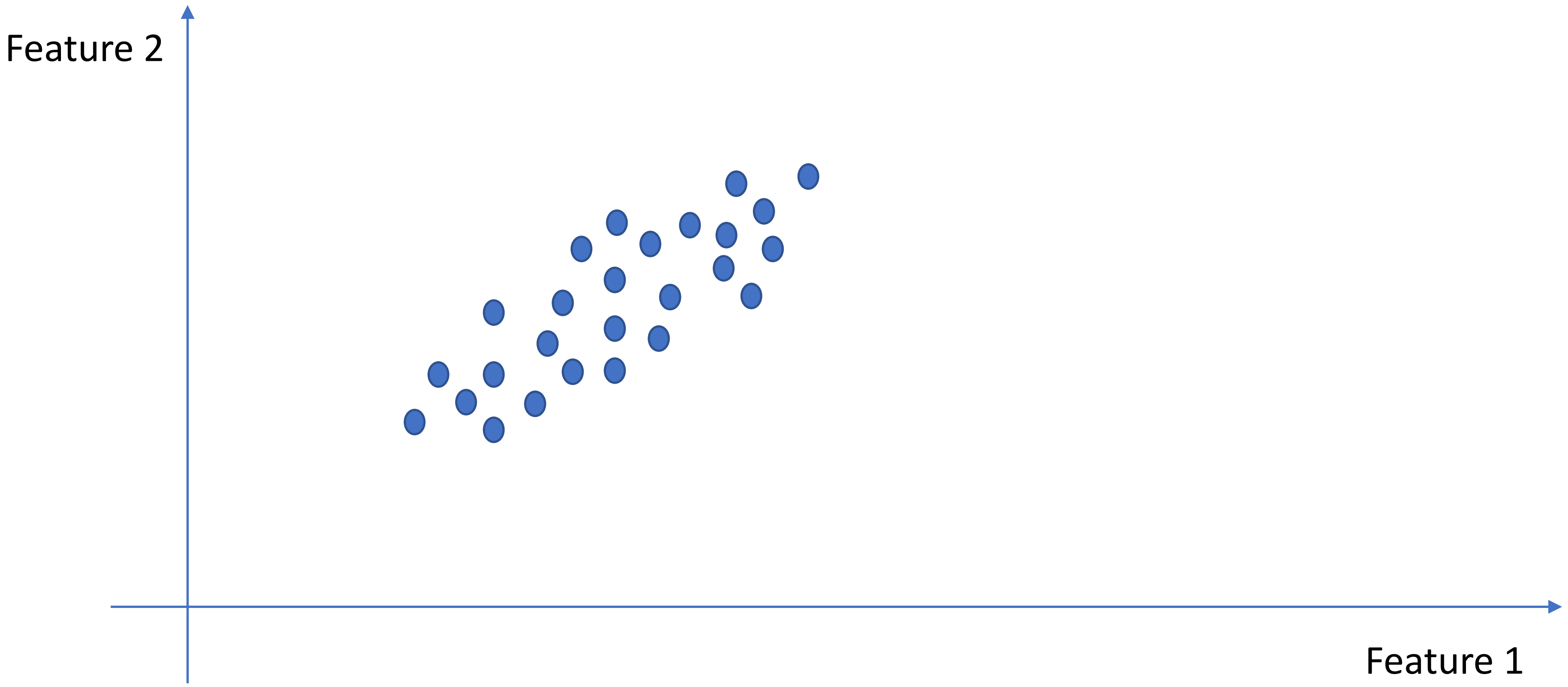
  (But there can be a non-linear dependency!)
- Features/Measurements can be statistically represented by random variables!
  (Random variables map a value to probabilistic events!)

Positive Covariance



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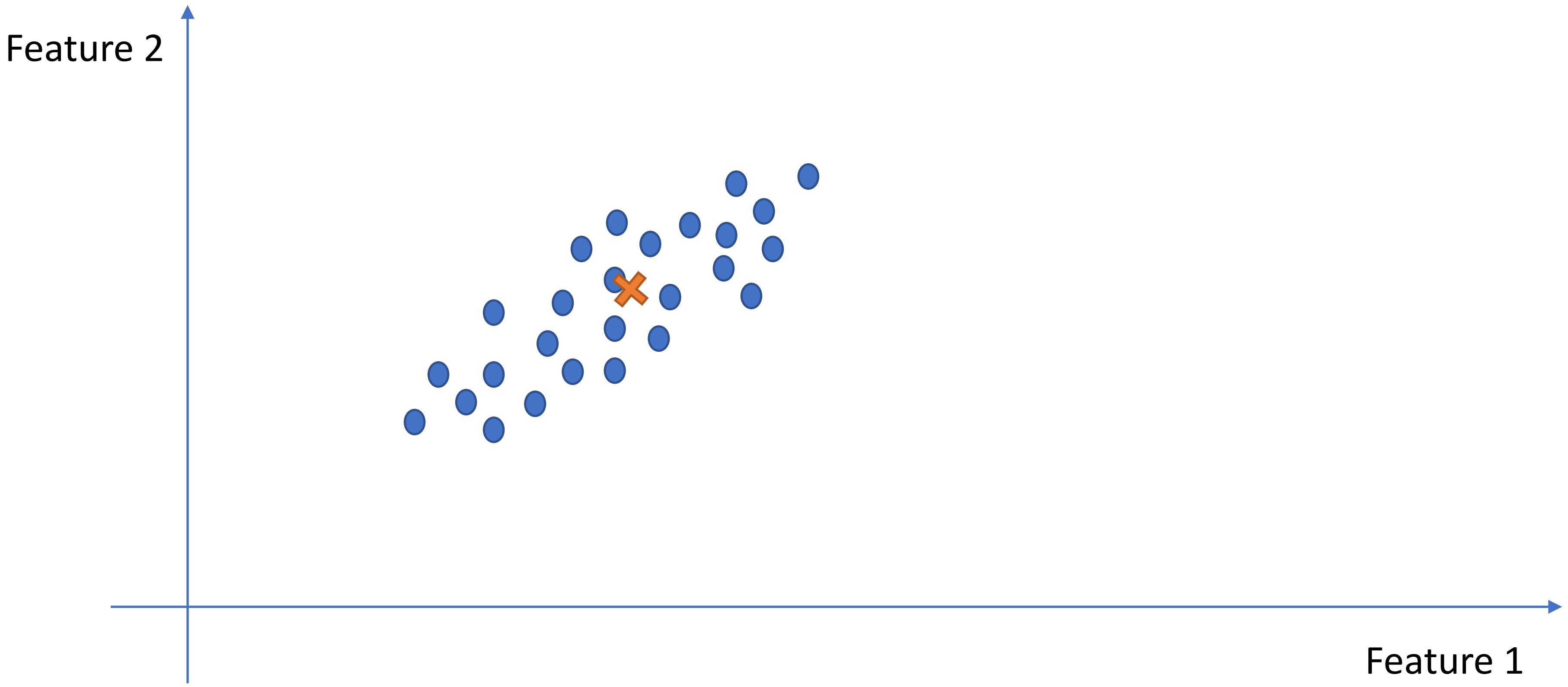
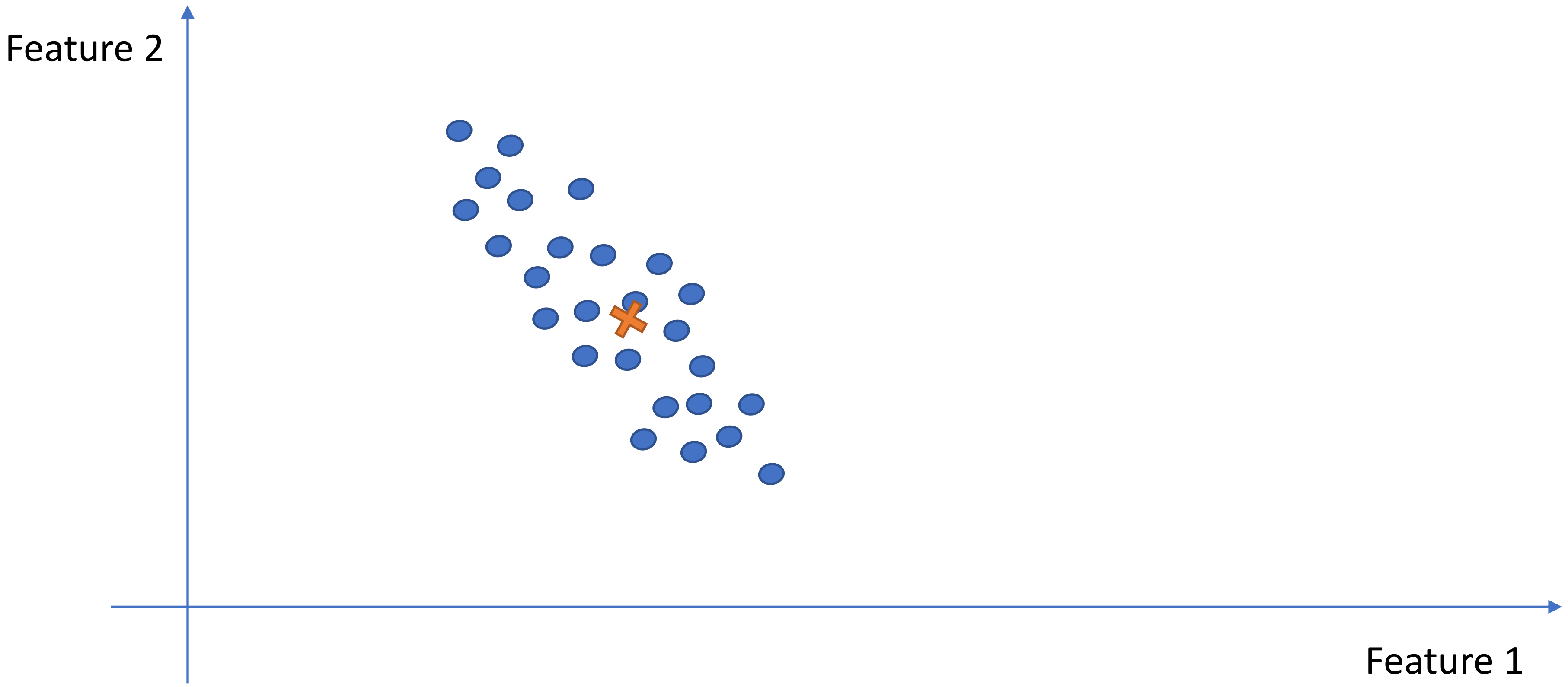
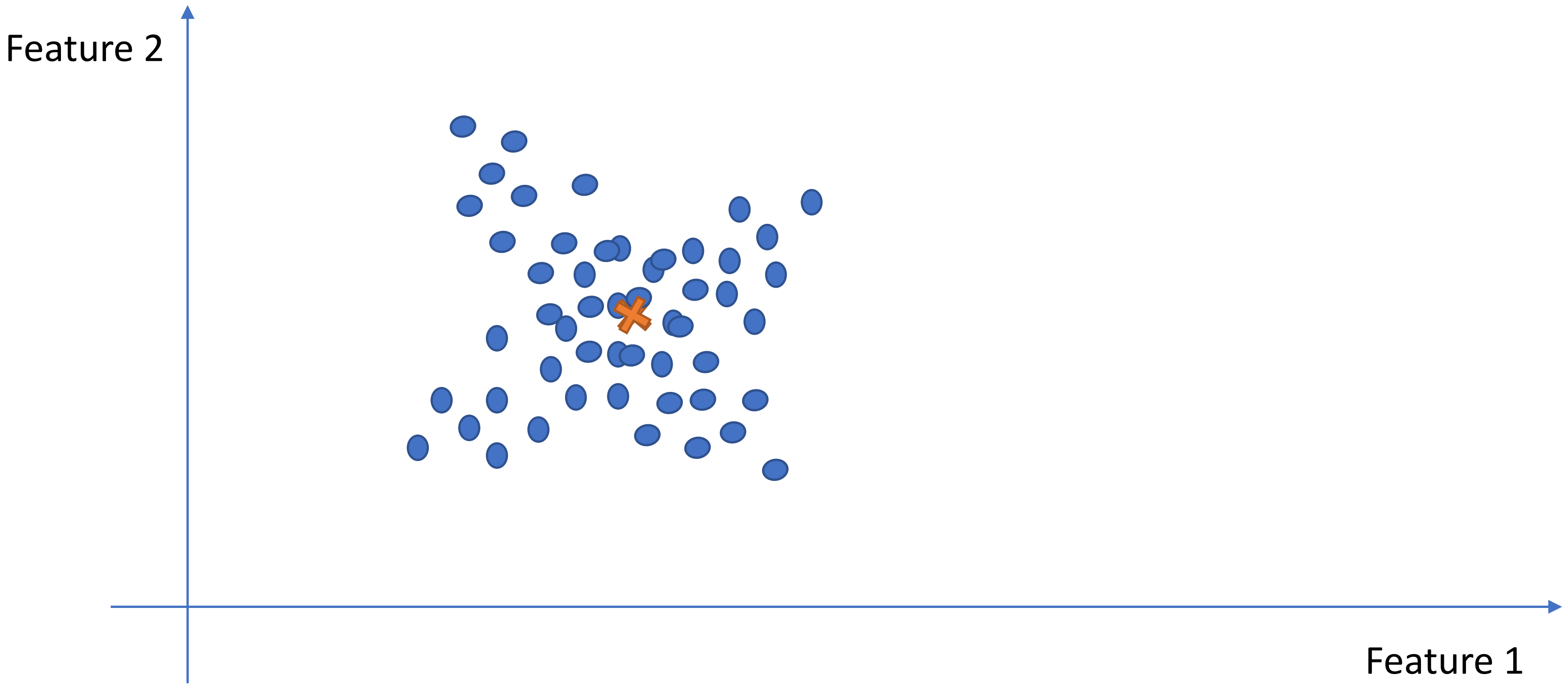


Negative Covariance



Zero Covariance



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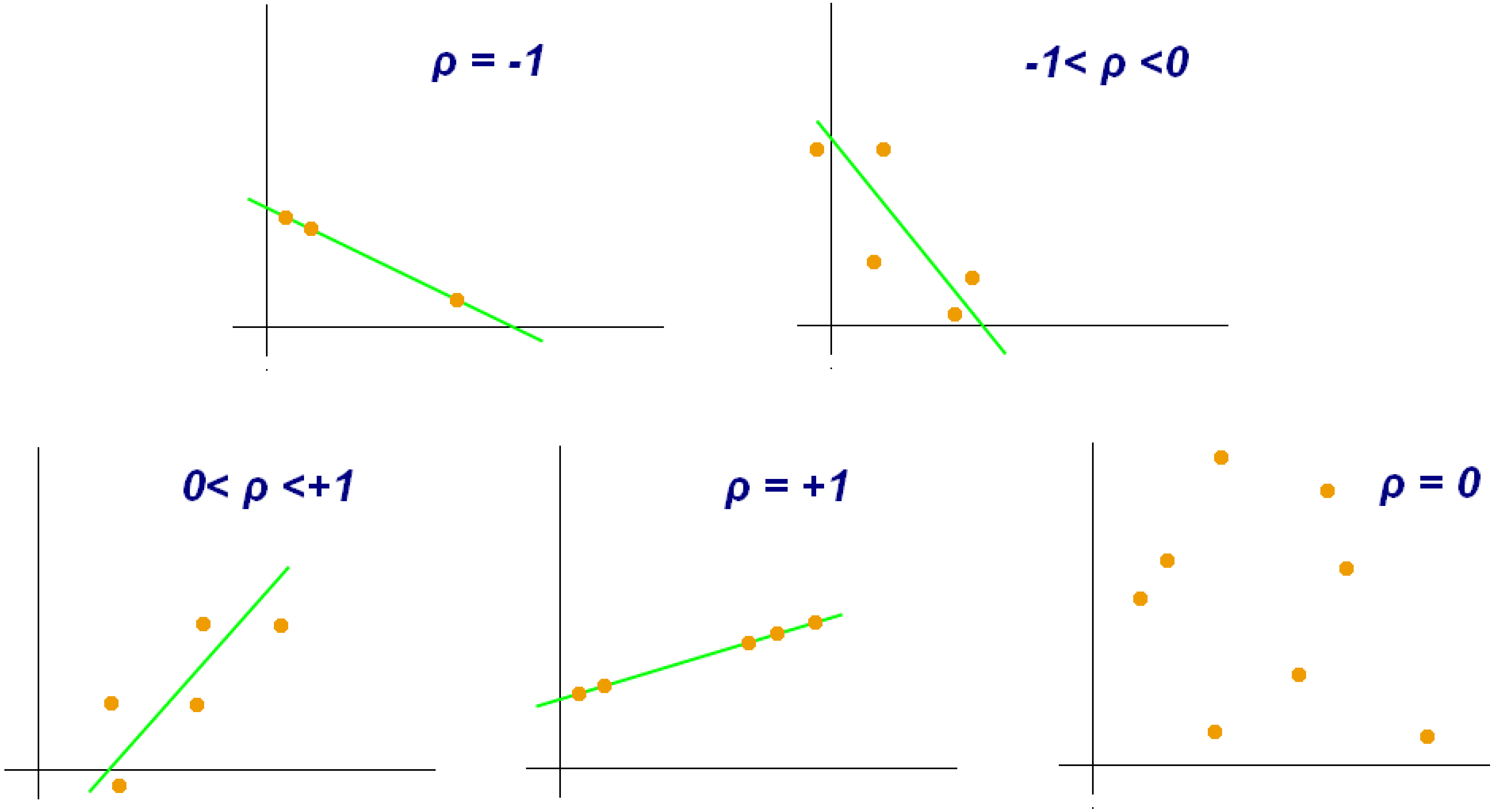
Standard deviations

Excursion: Pearson Correlation Coefficient



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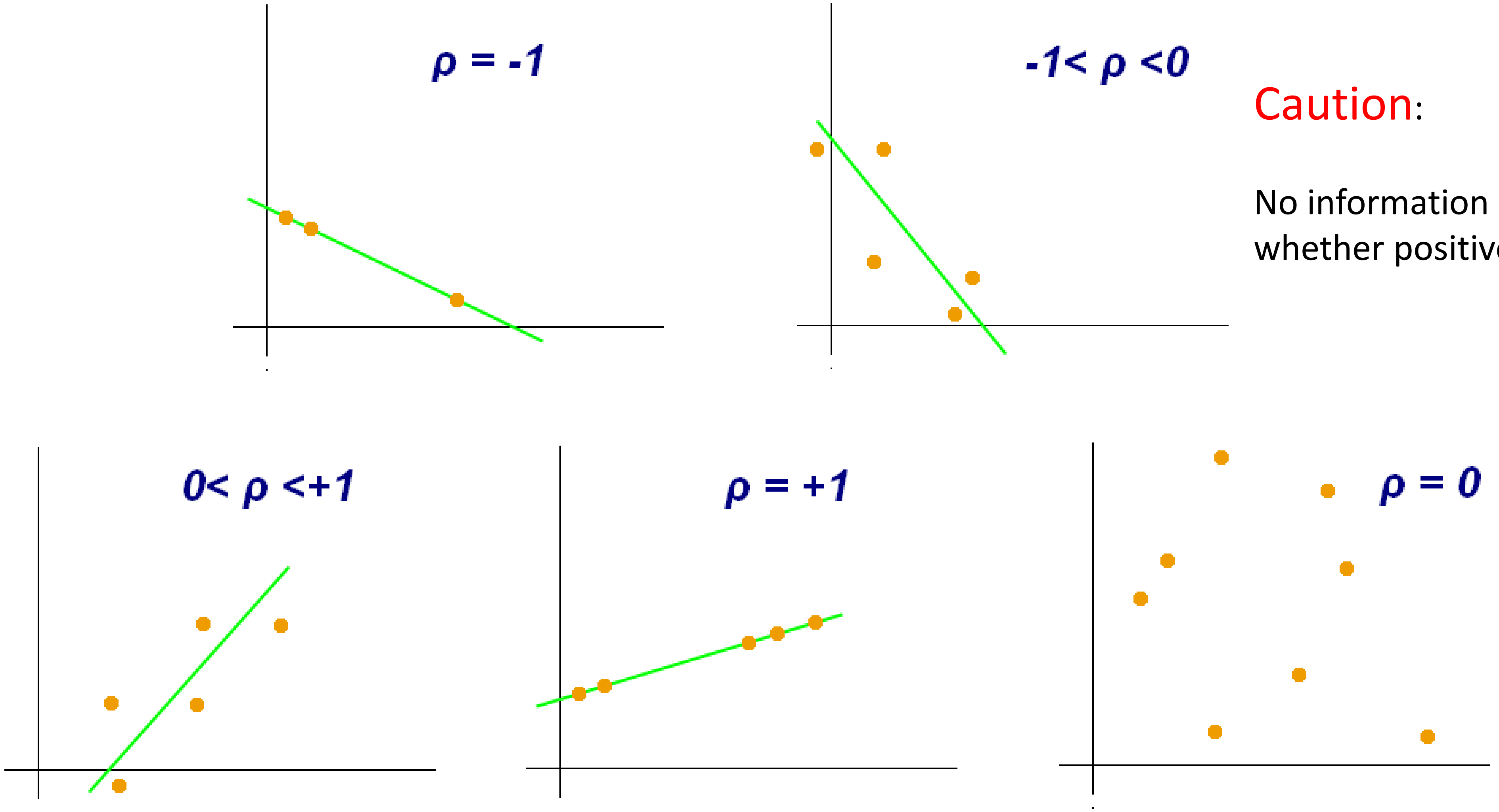

Caution:

No information about slope except whether positive or negative!

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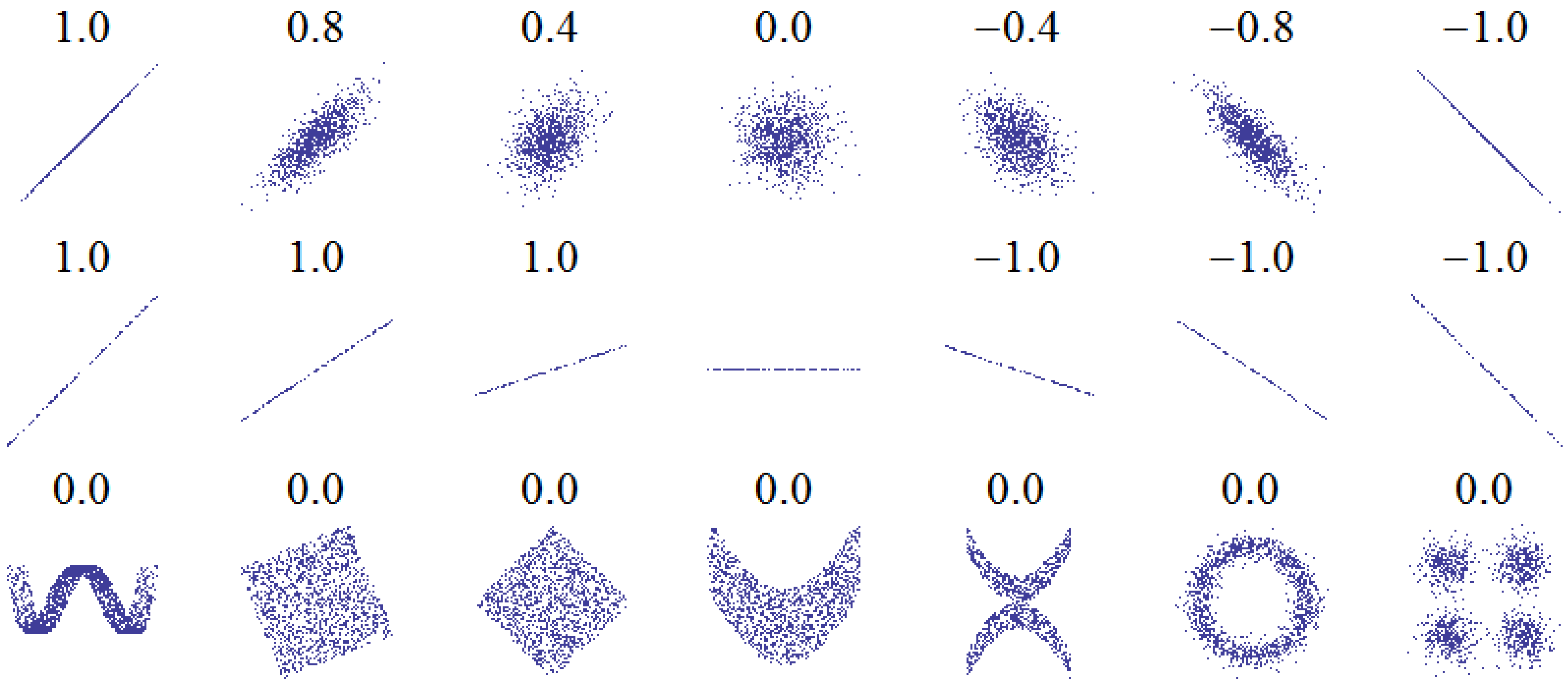

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Prerequisites: Covariance Matrix

- Multidimensional feature vectors can be represented by multivariate random variables!

$$\mathrm{X} := \begin{pmatrix} X_1 \\ X_2 \\ \cdots \\ X_N \end{pmatrix}$$

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$$\mathrm{Cov}(\mathrm{X}) = \mathbb{E}[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T]$$

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Mean feature vector over
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Number of samples belonging to class k

Sample feature vector from class k

Mean feature vector over all samples from class k

Prerequisites: Cholesky Matrix

- A covariance matrix Σ can be uniquely decomposed into:

$$\boldsymbol{\Sigma} = \boldsymbol{U}^{\boldsymbol{T}}\boldsymbol{U}$$

- U is an upper triangular matrix
- This matrix is called Cholesky matrix

Inverse Cholesky Transform

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$$\frac{1}{N_k}\sum_{i=1}^{N_k}(U^{T^{-1}}x_i - U^{T^{-1}}\mu_k)(U^{T^{-1}}x_i - U^{T^{-1}}\mu_k)^T$$

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$$=\frac{1}{N_k}\sum_{i=1}^{N_k}U^{T^{-1}}(x_i-\mu_k)(x_i-\mu_k)^T U^{T^{-1^T}}$$

$$=\frac{1}{N_k}\sum_{i=1}^{N_k}U^{T^{-1}}(x_i-\mu_k)(x_i-\mu_k)^T U^{-1}$$

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$$=U^{T^{-1}}\Sigma U^{-1} \quad =U^{T^{-1}}(U^T U)U^{-1}$$

Inverse Cholesky Transform

$$\frac{1}{N_k}\sum_{i=1}^{N_k}({U^T}^{-1}x_i - {U^T}^{-1}\mu_k)({U^T}^{-1}x_i - {U^T}^{-1}\mu_k)^T$$

$$=\frac{1}{N_k}\sum_{i=1}^{N_k}{U^T}^{-1}(x_i-\mu_k)(x_i-\mu_k)^T{{U^T}^{-1}}^T$$

$$=\frac{1}{N_k}\sum_{i=1}^{N_k}{U^T}^{-1}(x_i-\mu_k)(x_i-\mu_k)^T U^{-1}$$

$$={U^T}^{-1}[\frac{1}{N_k}\sum_{i=1}^{N_k}(x_i-\mu_k)(x_i-\mu_k)^T]U^{-1}$$

$$={U^T}^{-1}\Sigma U^{-1} \quad ={U^T}^{-1}(U^T U)U^{-1} \quad =({U^T}^{-1}U^T)(UU^{-1})$$

Inverse Cholesky Transform

$$\frac{1}{N_k}\sum_{i=1}^{N_k}(U^{T^{-1}}x_i - U^{T^{-1}}\mu_k)(U^{T^{-1}}x_i - U^{T^{-1}}\mu_k)^T$$

$$=\frac{1}{N_k}\sum_{i=1}^{N_k}U^{T^{-1}}(x_i - \mu_k)(x_i - \mu_k)^T U^{T^{-1^T}}$$

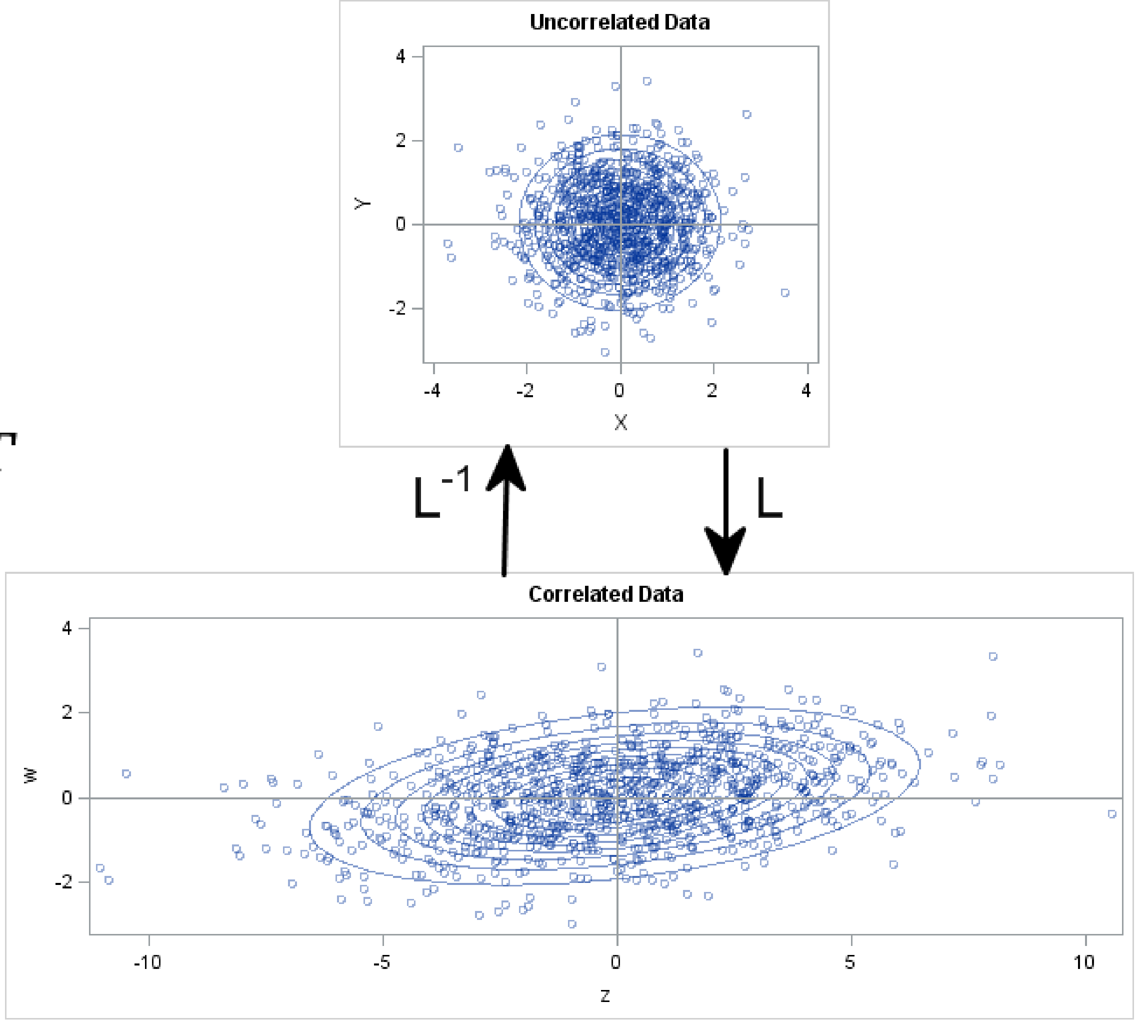
$$=\frac{1}{N_k}\sum_{i=1}^{N_k}U^{T^{-1}}(x_i - \mu_k)(x_i - \mu_k)^T U^{-1}$$

$$=U^{T^{-1}}[\frac{1}{N_k}\sum_{i=1}^{N_k}(x_i - \mu_k)(x_i - \mu_k)^T]U^{-1}$$

$$=U^{T^{-1}}\Sigma U^{-1} \quad =U^{T^{-1}}(U^T U)U^{-1} \quad =(U^{T^{-1}}U^T)(UU^{-1}) =I$$

Inverse Cholesky Transform

$$L := U^T$$



Mahalanobis Distance

- Distance measure, that takes into account the correlations of the data set

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- Main idea:
  - Transform data into uncorrelated space with inverse cholesky transform

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- Main idea:
    - Transform data into uncorrelated space with inverse cholesky transform
    - Measure euclidean distance to mean in transformed space

Mahalanobis Distance

$$d(x, \mu) := \sqrt{({U^T}^{-1}x - {U^T}^{-1}\mu)^T({U^T}^{-1}x - {U^T}^{-1}\mu)}$$

Mahalanobis Distance

$$d(x,\mu) := \sqrt{({U^T}^{-1}x - {U^T}^{-1}\mu)^T({U^T}^{-1}x - {U^T}^{-1}\mu)}$$

$$= \sqrt{(x-\mu)^T {{U^T}^{-1}}^T {U^T}^{-1}(x-\mu)}$$

Mahalanobis Distance

$$
\begin{aligned}
d(x,\mu) &:= \sqrt{(U^{T^{-1}}x - U^{T^{-1}}\mu)^T (U^{T^{-1}}x - U^{T^{-1}}\mu)} \\
&= \sqrt{(x-\mu)^T U^{T^{-1}T} U^{T^{-1}} (x-\mu)} \\
&= \sqrt{(x-\mu)^T U^{-1} U^{T^{-1}} (x-\mu)}
\end{aligned}
$$

Mahalanobis Distance

$$
\begin{aligned}
d(x,\mu) &:= \sqrt{({U^T}^{-1}x - {U^T}^{-1}\mu)^T({U^T}^{-1}x - {U^T}^{-1}\mu)} \\
&= \sqrt{(x-\mu)^T {{U^T}^{-1}}^T {U^T}^{-1}(x-\mu)} \\
&= \sqrt{(x-\mu)^T U^{-1} {U^T}^{-1}(x-\mu)} \\
&= \sqrt{(x-\mu)^T (U^T U)^{-1}(x-\mu)}
\end{aligned}
$$

Mahalanobis Distance

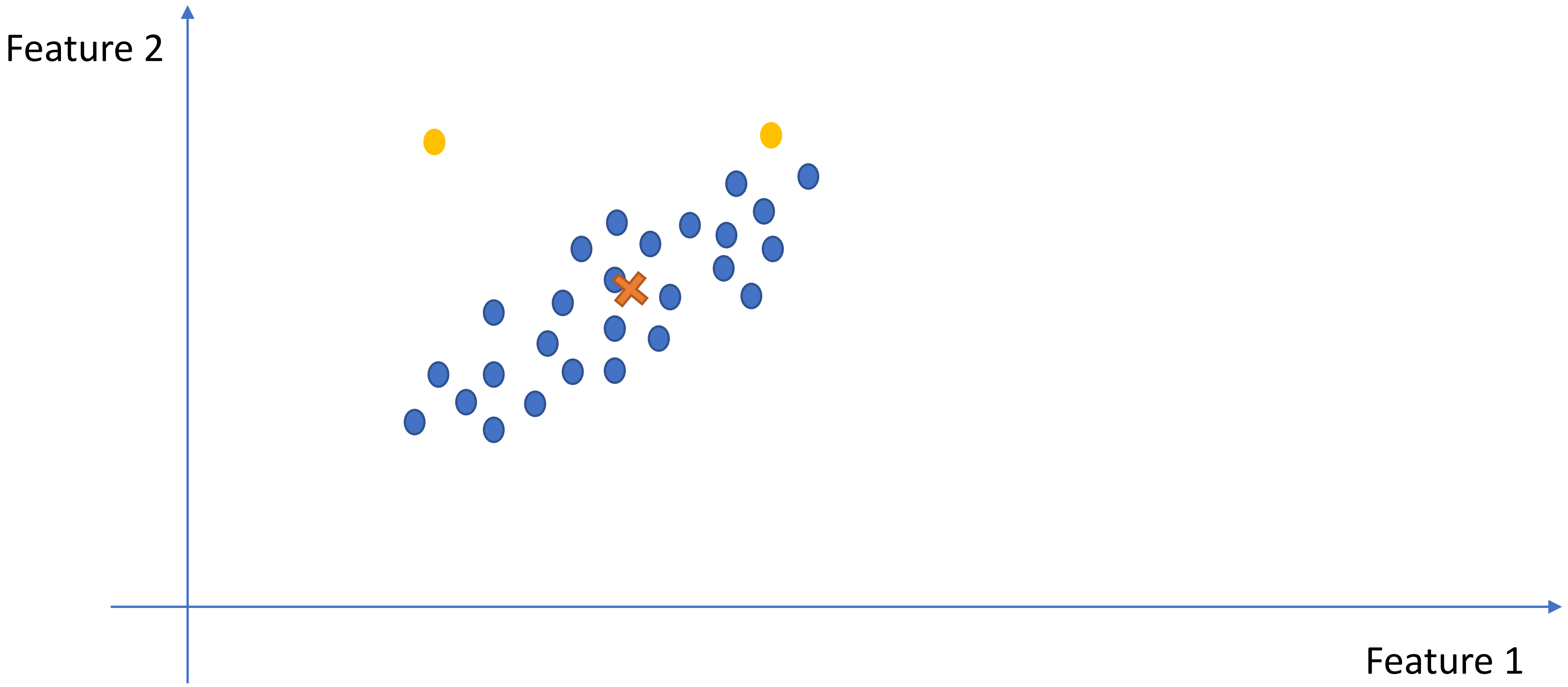
$$\begin{aligned} d(x,\mu) &:= \sqrt{({U^T}^{-1}x - {U^T}^{-1}\mu)^T({U^T}^{-1}x - {U^T}^{-1}\mu)} \\ &= \sqrt{(x-\mu)^T {{U^T}^{-1}}^T {U^T}^{-1}(x-\mu)} \\ &= \sqrt{(x-\mu)^T U^{-1} {U^T}^{-1}(x-\mu)} \\ &= \sqrt{(x-\mu)^T (U^T U)^{-1}(x-\mu)} \\ &= \sqrt{(x-\mu)^T \Sigma^{-1}(x-\mu)} \end{aligned}$$

Mahalanobis Distance

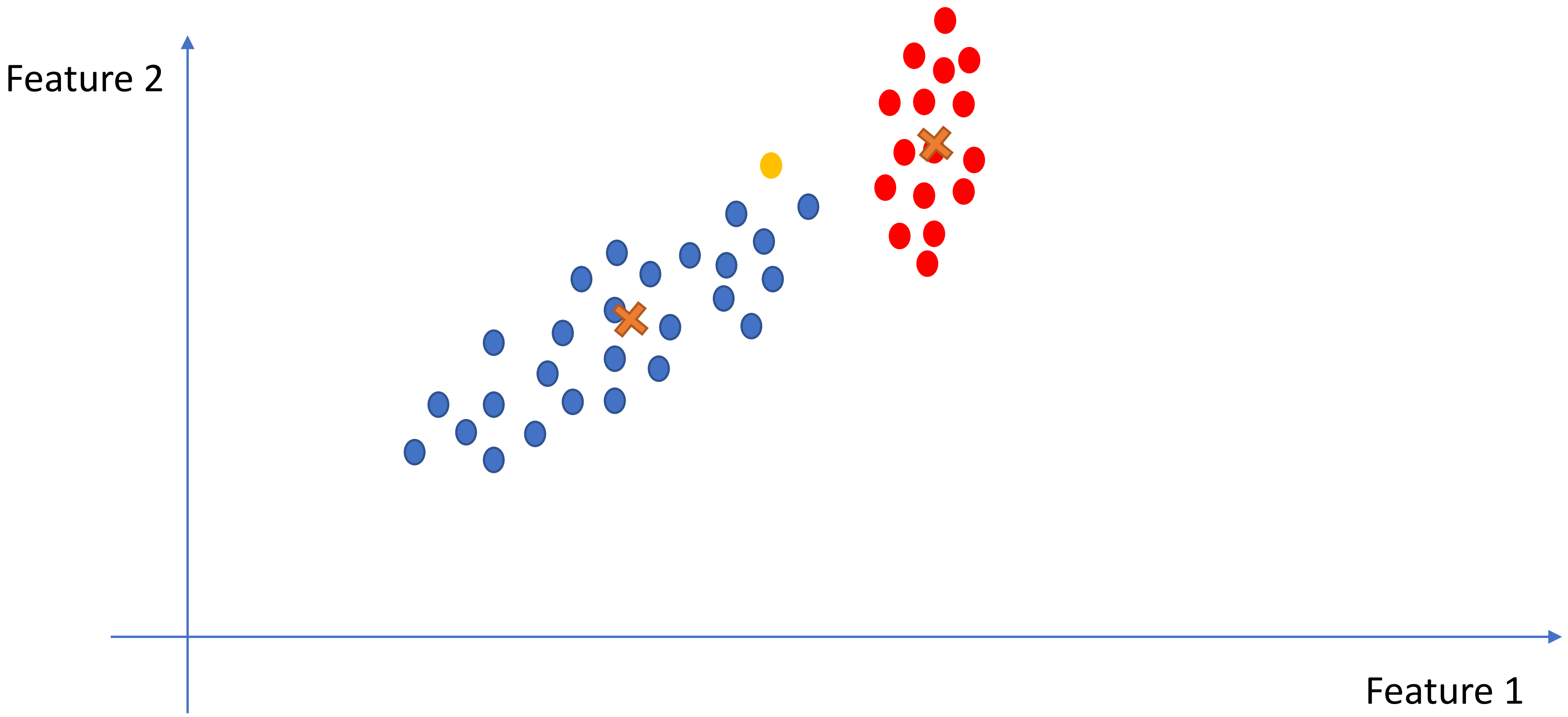
$$d(x, \mu) := \sqrt{(x-\mu)^T \Sigma^{-1} (x-\mu)}$$

- To calculate the distance:
  - No need for cholesky matrix
  - Only need inverse of covariance!

Likelihood Estimation



Classification via Likelihood Estimation



Mahalanobis Classifier

- „Training “:
  - Calculate mean feature vectors for each class

Mahalanobis Classifier

- „Training“:
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  - Calculate inverse covariance matrix for each class

Mahalanobis Classifier

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  - Calculate mean feature vectors for each class
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- Inference:
  - For each class calculate (sqaured) Mahalanobis distance to its mean feature vector

Mahalanobis Classifier

- „Training ":
  - Calculate mean feature vectors for each class
  - Calculate inverse covariance matrix for each class

- Inference:
  - For each class calculate (squared) Mahalanobis distance to its mean feature vector
  - Return class with lowest Mahalanobis distance

$$d(x, \mu) := \sqrt{(x-\mu)^T \Sigma^{-1} (x-\mu)}$$