Fondamenti di IA

05 - Unsupervised Learning

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Deck of slides borrowed from

Big Data Computing

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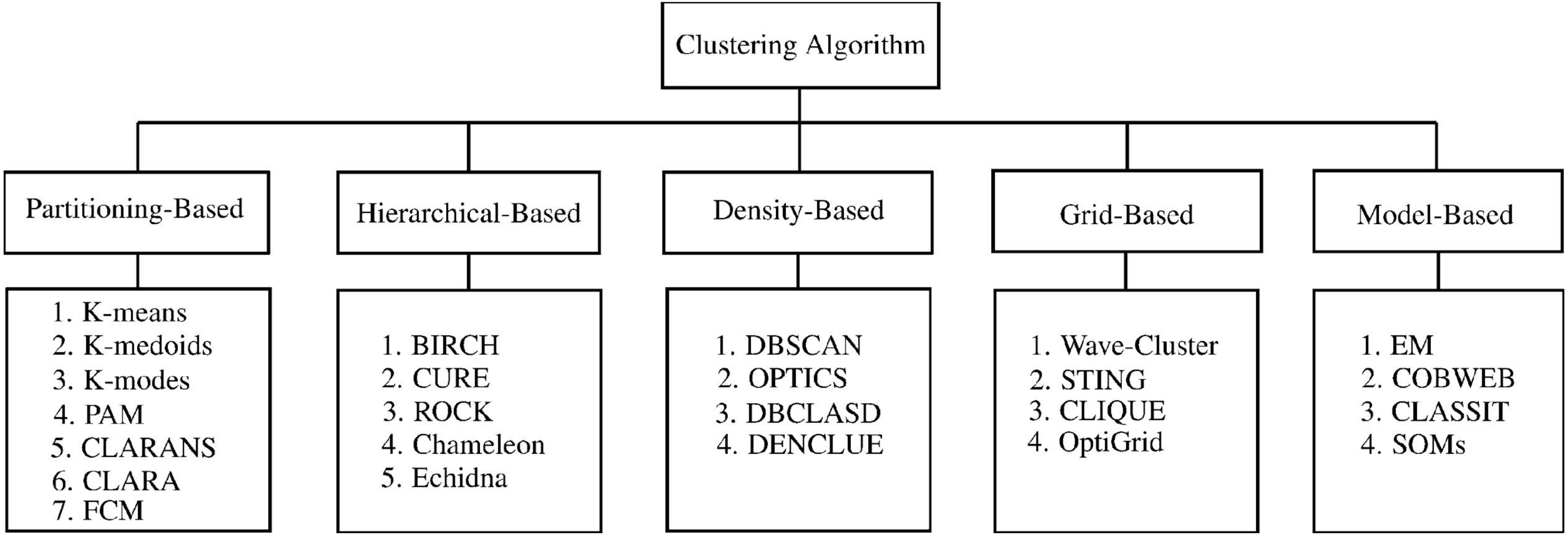
Clustering Algorithms

Clustering Algorithms: Taxonomy



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https://www.computer.org/csdl/journal/ec/2014/03/06832486/13rRUEgs2xB

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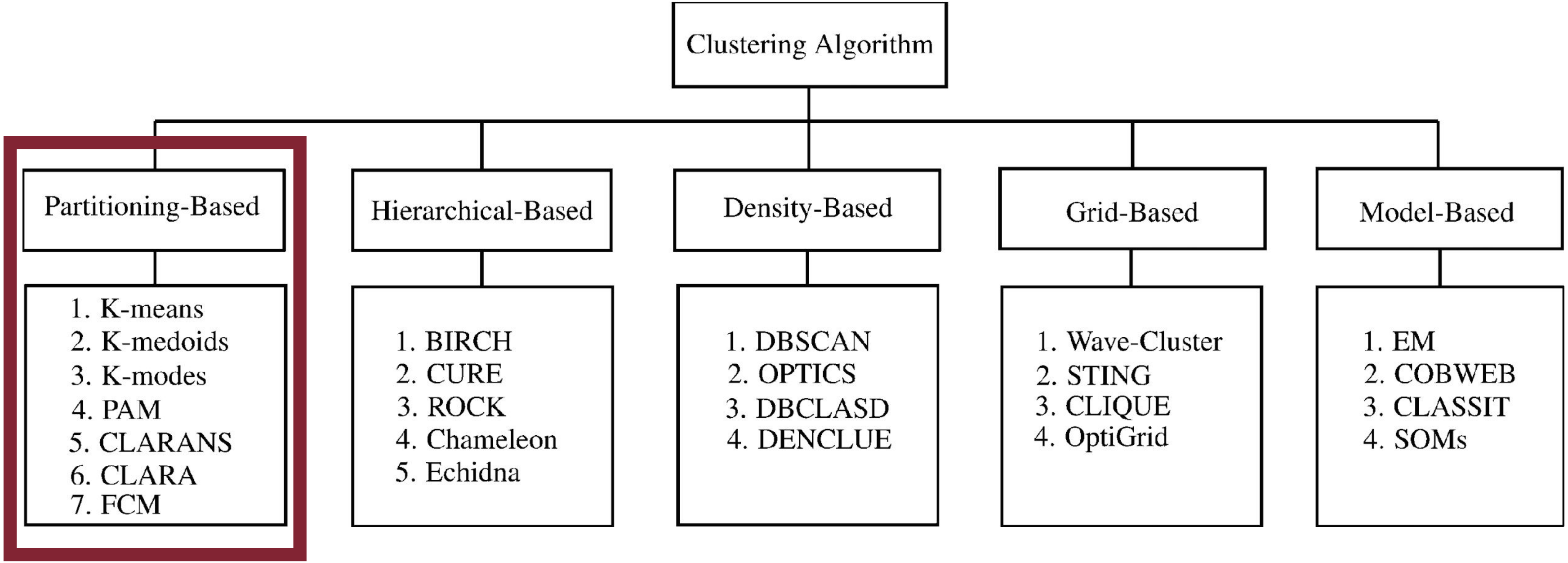

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Partitioning: Hard Clustering

- **Input:** A set of N data points and a number K (K < N)

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  - $S(K, N) \sim K^N/K! = O(K^N)$ K-way non-empty partitions of N elements
  - Effective heuristics → K-means, K-medoids, K-means++, etc.

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Flat Hard Clustering: General Framework

$\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ the set of N input data points

$\{C_1, \ldots, C_K\}$ the set of K output clusters

C_k the generic k-th cluster

$\boldsymbol{\theta}_k$ is the *representative* of cluster C_k

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$\boldsymbol{\theta}_k$ is the *representative* of cluster C_k

Note:

At this stage we haven't yet specified what a cluster representative actually is

Objective Function

$$L(A, \mathbf{\Theta}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} \delta(\mathbf{x}_n, \boldsymbol{\theta}_k)$$

where:

- A is an $N \times K$ matrix s.t. $\alpha_{n,k} = 1$ iff $\mathbf{x}_n$ is assigned to cluster C_k, 0 otherwise
- $\mathbf{\Theta} = \{\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_K\}$ are the cluster representatives
- $\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)$ is a function measuring the distance between $\mathbf{x}_n$ and $\boldsymbol{\theta}_k$

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hard clustering

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$$\boxed{A^*, \boldsymbol{\Theta}^* = \text{argmin}_{A, \boldsymbol{\Theta}} \underbrace{\sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} \delta(\mathbf{x}_n, \boldsymbol{\theta}_k)}_{L(A, \boldsymbol{\Theta})}}$$

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exact solution must explore exponential search space
S(K, N) ~ O(K^N)

⇒

NP-hard

Objective Function

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exact solution must explore exponential search space **S(K, N) ~ O(K^N)** ⇒ **NP-hard**

non-convex due to the discrete assignment matrix *A* ⇒ **multiple local minima**

Iterative Solution: Lloyd-Forgy Algorithm

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- **Lloyd-Forgy Algorithm:** 2-step **iterative** approximated solution
  - **Assignment step**
  - **Update step**

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- **Lloyd-Forgy Algorithm:** 2-step **iterative** approximated solution
  - **Assignment step**
  - **Update step**

Does not guarantee to find the global optimum as it may stuck to a local optimum or a saddle point

2-Step Optimization: Assignment Step

Minimize L w.r.t. A by fixing $\boldsymbol{\Theta}$

$$L(A|\boldsymbol{\Theta}) = L(A;\boldsymbol{\Theta}) = L \text{ is a function of } A \text{ parametrized by } \boldsymbol{\Theta}$$

2-Step Optimization: Assignment Step

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Note:
Can't take the gradient of L w.r.t. A
since A is discrete!

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Intuitively, given a set of fixed representatives, L is minimized if each data point is assigned to the closest cluster representative according to δ

(L is just the summation of all the distances from each data point to its assigned representative)

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$$\alpha_{n,k} = \begin{cases} 1 & \text{if } \delta(\mathbf{x}_n, \boldsymbol{\theta}_k) = \min_{1 \leq j \leq K}\{\delta(\mathbf{x}_n, \boldsymbol{\theta}_j)\} \\ 0 & \text{otherwise} \end{cases}$$

2-Step Optimization: Update Step

$\boxed{\text{Minimize } L \text{ w.r.t. } \boldsymbol{\Theta} \text{ by fixing } A}$

$$L(\boldsymbol{\Theta}|A) = L(\boldsymbol{\Theta}; A) = L \text{ is a function of } \boldsymbol{\Theta} \text{ parametrized by } A$$

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Minimize L w.r.t. $\mathbf{\Theta}$ by fixing A

$$L(\mathbf{\Theta}|A) = L(\mathbf{\Theta}; A) = L \text{ is a function of } \mathbf{\Theta} \text{ parametrized by } A$$

We can minimize L by taking the **gradient** of L w.r.t $\mathbf{\Theta}$
(i.e., the vector of partial derivatives), set it to 0 and solve it for $\mathbf{\Theta}$

2-Step Optimization: Update Step

$$\nabla L(\boldsymbol{\Theta}; A) = \left(\frac{\partial L(\boldsymbol{\Theta}; A)}{\partial \boldsymbol{\theta}_1}, \ldots, \frac{\partial L(\boldsymbol{\Theta}; A)}{\partial \boldsymbol{\theta}_K} \right)$$

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$$\boxed{\frac{\partial L(\boldsymbol{\theta}_1 \ldots \boldsymbol{\theta}_K; A)}{\partial \boldsymbol{\theta}_j}}$$

The general *j*-th partial derivative

2-Step Optimization: Update Step

$$\nabla L(\boldsymbol{\Theta}; A) = \mathbf{0} \Leftrightarrow \frac{\partial L(\boldsymbol{\theta}_1, \ldots, \boldsymbol{\theta}_K; A)}{\partial \boldsymbol{\theta}_j} = 0 \; \forall j \in \{1, \ldots, K\}$$

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$$\downarrow$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_j}$$

To make the notation easier!

2-Step Optimization: Update Step

$$\frac{\partial L}{\partial \boldsymbol{\theta}_j} = \frac{\partial}{\partial \boldsymbol{\theta}_j}\left[\sum_{n=1}^{N}\sum_{k=1}^{K}\alpha_{n,k}\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)\right] = 0$$

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When computing the partial derivative w.r.t. $\boldsymbol{\theta}_j$ any other term $\boldsymbol{\theta}_k$ of the inner summation is treated as constant!

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Solve for each $\boldsymbol{\theta}_j$ independently

Depends on the distance function δ

A Special Case: K-means

- Each cluster representative is its center of mass (i.e., **centroid**)

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A Special Case: K-means

- Each cluster representative is its center of mass (i.e., **centroid**)
- The centroid of a cluster is the **mean** of the instances assigned to that cluster
- (Re)Assignment of instances to clusters is based on distance/similarity to the current cluster centroids
- The basic idea is constructing clusters so that the total within-cluster **Sum of Square Distances** (**SSD**) is minimized

K-means: Setup

$\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ the set of N input data points

$\{C_1, \ldots, C_K\}$ the set of K output clusters

C_k the generic k-th cluster

$$\boldsymbol{\theta}_k = \frac{\sum_{n=1}^{N} \alpha_{n,k} \mathbf{x}_n}{\sum_{n=1}^{N} \alpha_{n,k}} = \boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{n \in C_k} \mathbf{x}_n$$

$$\text{where } |C_k| = \sum_{n=1}^{N} \alpha_{n,k}$$

K-means: Objective Function

$$L(A, \boldsymbol{\Theta}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} \underbrace{(||\mathbf{x}_n - \boldsymbol{\theta}_k||_2)^2}_{\delta(\mathbf{x}_n, \boldsymbol{\theta}_k)}$$

Euclidean space

K-means: Objective Function

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$$\delta(\mathbf{x}_n, \boldsymbol{\theta}_k) = (||\mathbf{x}_n - \boldsymbol{\theta}_k||_2)^2 =$$

$$= \left[\sqrt{(\mathbf{x}_n - \boldsymbol{\theta}_k)^2}\right]^2 = (\mathbf{x}_n - \boldsymbol{\theta}_k)^2$$

Sum of Square Distances (SSD)

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Sum of Square Distances (SSD)

$$\boxed{L(A, \boldsymbol{\Theta}) = \sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} (\mathbf{x}_n - \boldsymbol{\theta}_k)^2}$$

K-means: Assignment Step

Minimize *L* w.r.t. *A* by fixing $\boldsymbol{\Theta}$

Intuitively, given a set of fixed centroids, *L* is minimized if each data point is assigned to the centroid with the smallest SSD

(*L* is just the SSD from each data point to its assigned centroid)

$$\alpha_{n,k} = \begin{cases} 1 & \text{if } (\mathbf{x}_n - \boldsymbol{\theta}_k)^2 = \min_{1 \le j \le K}\{(\mathbf{x}_n - \boldsymbol{\theta}_j)^2\} \\ 0 & \text{otherwise} \end{cases}$$

K-means: Update Step

Minimize *L* w.r.t. $\mathbf{\Theta}$ by fixing *A*

$$\mathbf{\Theta}^* = \mathrm{argmin}_{\mathbf{\Theta}} \left\{ \underbrace{\sum_{n=1}^{N} \sum_{k=1}^{K} \alpha_{n,k} (\mathbf{x}_n - \boldsymbol{\theta}_k)^2}_{L(\mathbf{\Theta};A)} \right\}$$

Compute the gradient w.r.t. $\mathbf{\Theta}$, set it to 0 and solve it for $\mathbf{\Theta}$

K-means: Update Step

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \frac{\partial}{\partial \boldsymbol{\theta}_k}\left[\sum_{n=1}^{N} \alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k)^2\right] = 0 \qquad \forall k \in \{1, \ldots, K\}$$

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$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \frac{\partial}{\partial \boldsymbol{\theta}_k}\left[\sum_{n=1}^{N} \alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k)^2\right] = 0 \quad \forall k \in \{1, \ldots, K\}$$

$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \sum_{n=1}^{N} -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k)$$

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$$\frac{\partial L}{\partial \boldsymbol{\theta}_k} = \sum_{n=1}^{N} -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k)$$

$$\text{Find } \boldsymbol{\theta}_k^* \text{ s.t. } \sum_{n=1}^{N} -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k^*) = 0$$

K-means: Update Step

$$\sum_{n=1}^{N} -2\alpha_{n,k}(\mathbf{x}_n - \boldsymbol{\theta}_k^*) = 0 \Leftrightarrow$$

$$2\sum_{n=1}^{N} \alpha_{n,k}\boldsymbol{\theta}_k^* = 2\sum_{n=1}^{N} \alpha_{n,k}\mathbf{x}_n$$

$$\boldsymbol{\theta}_k^* \sum_{n=1}^{N} \alpha_{n,k} = \sum_{n=1}^{N} \alpha_{n,k}\mathbf{x}_n$$

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$\boldsymbol{\theta}^*_k$ does not depend on N, therefore it can be factored out

K-means: Update Step

$$\boldsymbol{\theta}_k^* \sum_{n=1}^{N} \alpha_{n,k} = \sum_{n=1}^{N} \alpha_{n,k} \mathbf{x}_n$$

$$\boldsymbol{\theta}_k^* = \frac{\sum_{n=1}^{N} \alpha_{n,k} \mathbf{x}_n}{\sum_{n=1}^{N} \alpha_{n,k}} = \boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{n \in C_k} \mathbf{x}_n$$

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The cluster centroid (i.e., **mean**) minimizes the objective (for a fixed assignment *A*)

K-means: Lloyd-Forgy Algorithm

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5. Iteratively repeat steps 3-4 until a **stopping criterion** is met

Stopping Criterion

- Several options to choose from:
  - Fixed number of iterations
  - Cluster assignments stop changing (beyond some threshold)
  - Centroid doesn't change (beyond some threshold)

Lloyd-Forgy's Convergence

- How/Why are we guaranteed the K-means algorithm ever reaches a fixed point?
  - A state in which clusters do not change

Lloyd-Forgy's Convergence

- How/Why are we guaranteed the K-means algorithm ever reaches a fixed point?
  - A state in which clusters do not change
- Intuitively, in both steps we either improve the objective or not

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- Computing centroids [M-step]: O(Nd) as there are O(N) average computations since each data point is added to a cluster exactly once *at each iteration*, each one taking O(d)
- Overall: O(RKNd) assuming the 2 steps above are repeated R times

K-means: Seed Choice

- Convergence (rate) and clustering quality depends on the selection of **initial centroids**
  - Forgy method **randomly** chooses K data points as the initial means
  - Random Partition method **randomly** assigns a cluster to each observation

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- Randomness may result in convergence to **sub-optimal** clusterings

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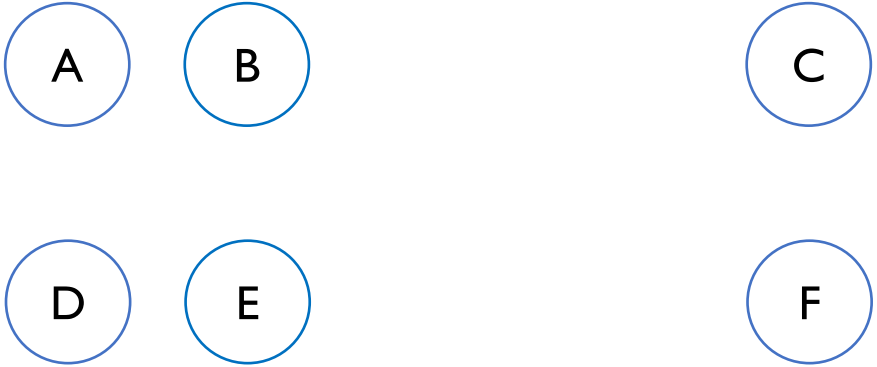
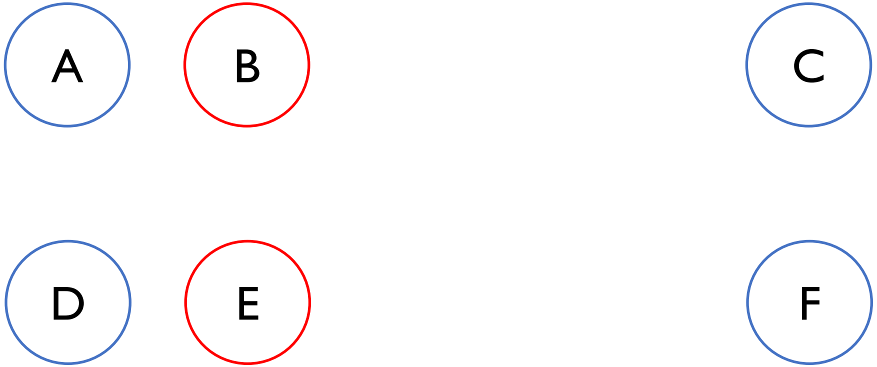
Problem Mitigation:

Execute several runs of the Lloyd-Forgy algorithm with multiple random initialization seeds

K-means: Seed Choice



K-means: Bad (Unlucky) Seed Choice



If B and E are randomly chosen as initial centroids…

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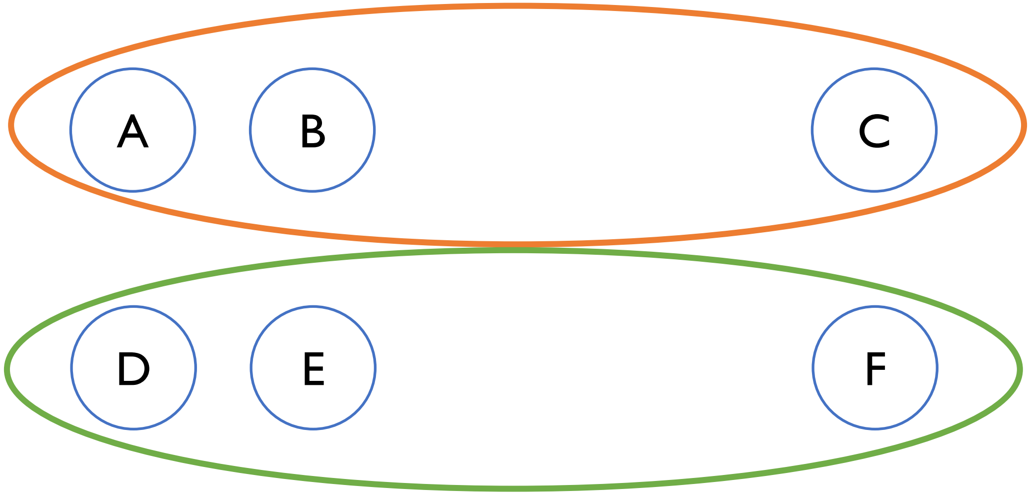
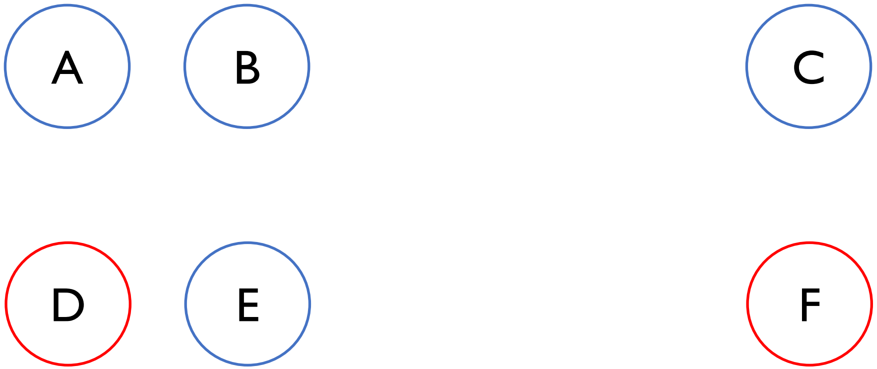


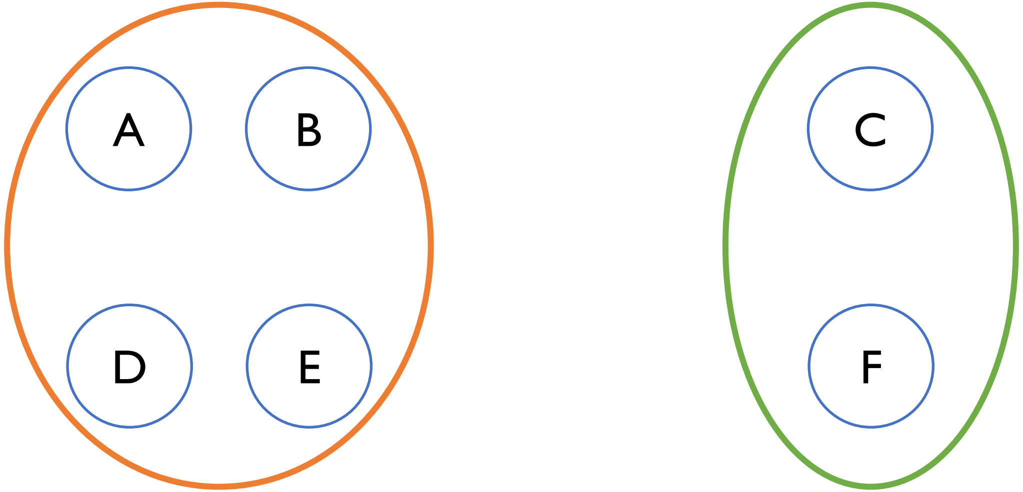
The algorithm converges to the sub-optimal clustering above

K-means: Good (Lucky) Seed Choice



If D and F are randomly chosen as initial centroids instead…

K-means: Good (Lucky) Seed Choice



The algorithm converges to a better clustering

K-means: How Many Clusters?

- Number of clusters K is given
  - Great! Partition N data points into a predetermined number K of clusters
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  - Unfortunately, it is very uncommon to know K in advance
- Finding the "right" number K of clusters is part of the problem!
  - Trade-off between having too few and too many clusters
  - Total benefit vs. Total cost

K-means: Total Benefit

- Given a clustering, define the benefit b_i for a data point $\mathbf{x}_\mathrm{i}$ to be the similarity to its assigned centroid

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B increases with larger values of K, but P allows to stop that

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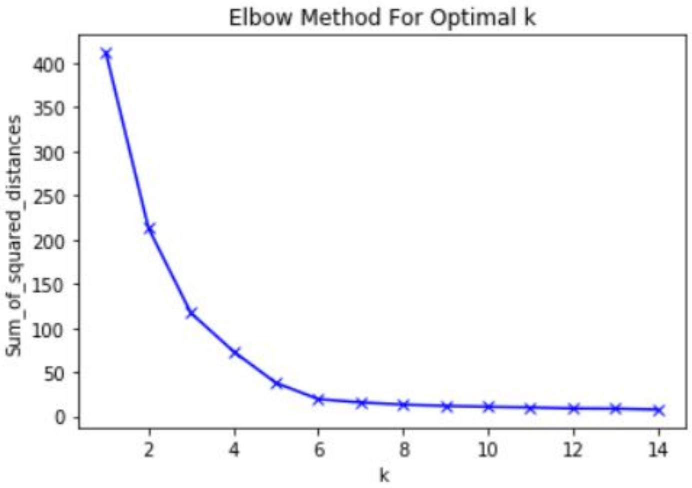

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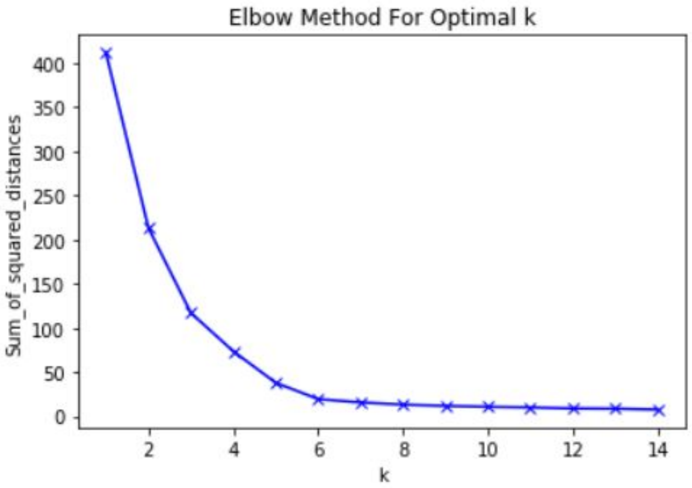

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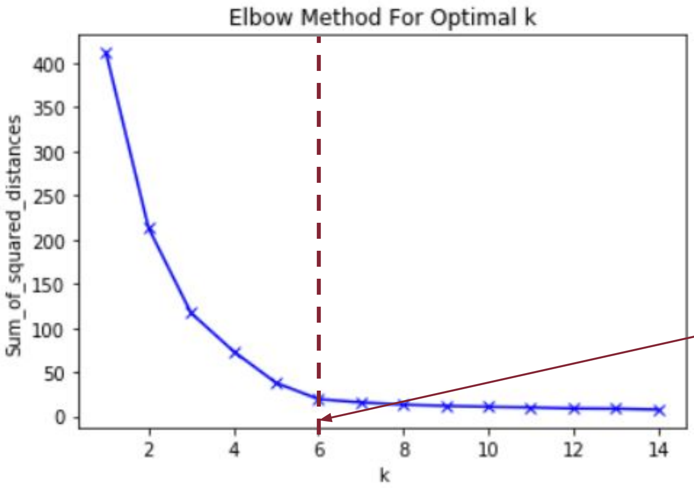

As K increases, SSD sharply decreases

up to a certain value

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- Others, require specific minimizers
  - δ = **Manhattan distance** (L^1-Norm) □ median is the minimizer (**K-medians**)

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- Similar to K-means yet chooses input data points as centers (**medoids**)

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- **PAM** (**P**artitioning **A**round **M**edoids) greedy Algorithm, introduced by Kaufman and Rousseeuw in 1987 [paper] vs. Lloyd-Forgy
- Robust to outliers yet computationally expensive $O(K(N-K)^2)$

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Measures of Clustering Quality

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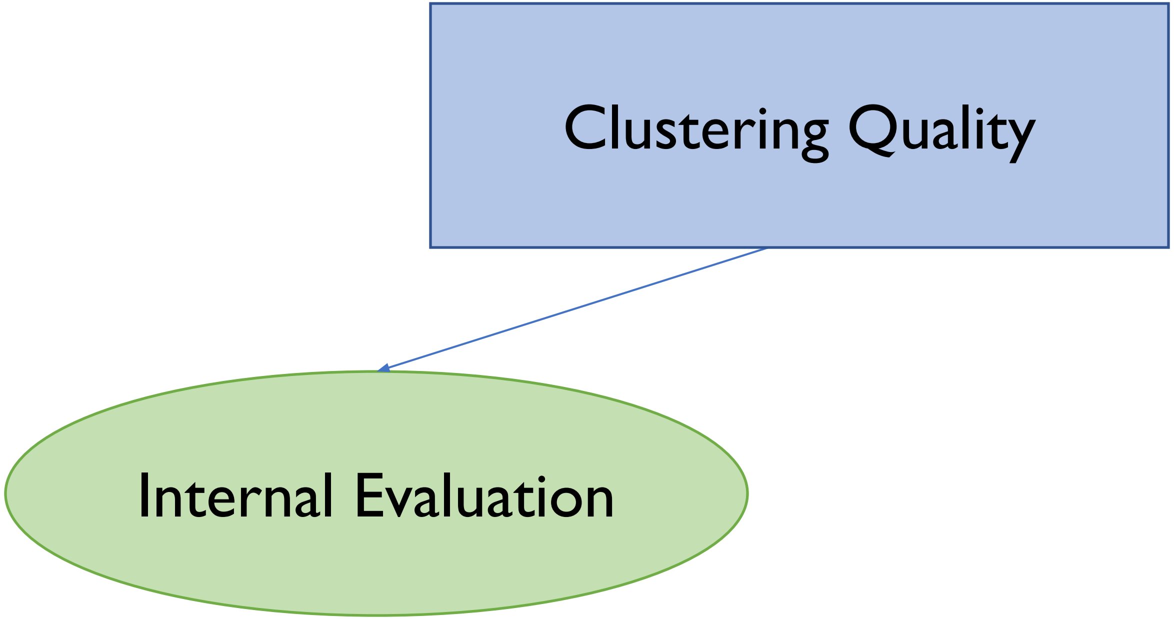

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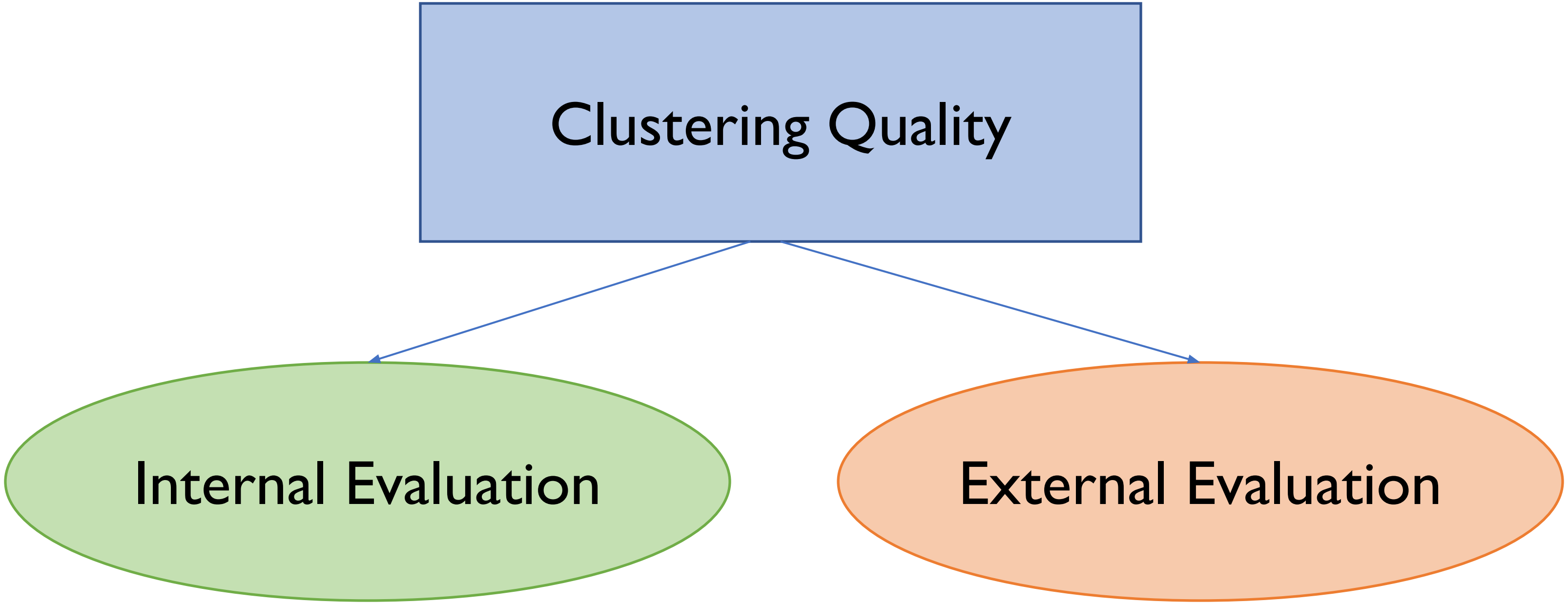

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- A good clustering will produce high quality clusters with:
  - **high intra-cluster similarity**
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- The measured quality of a clustering depends on
  - **data representation**
  - **similarity measure**

Internal Evaluation: Davies-Bouldin Index

$$DB = \frac{1}{K} \sum_{i=1}^{K} \max_{j \neq i} \left(\frac{\sigma_i + \sigma_j}{\delta(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j)} \right)$$

$$K = \text{number of clusters}$$

$$\boldsymbol{\mu}_k = \text{centroid of cluster } C_k$$

$$\sigma_k = \text{avg. distance of all elements of cluster } C_k \text{ from its centroid } \boldsymbol{\mu}_k$$

$$\delta(\boldsymbol{\mu}_i, \boldsymbol{\mu}_j) = \text{distance between centroids of } C_i \text{ and } C_j$$

The smaller the better

Internal Evaluation: Dunn Index

$$D = \frac{\min_{1 \leq i < j \leq K} \delta(C_i, C_j)}{\max_{1 \leq k \leq K} \delta'(C_k)}$$

K = number of clusters
$\delta(C_i, C_j)$ = distance between cluster C_i and C_j
$\delta'(C_k)$ = intra-cluster distance of cluster C_k

Distance between centroids

Max distance between any pair of objects

The higher the better

Internal Evaluation: Silhouette Coefficient

mean distance between *i* and all other data points in the same cluster C_i

$$a(i) = \frac{1}{|C_i| - 1} \sum_{j \in C_i, j \neq i} \delta(i, j)$$

smallest mean distance of *i* to all points in any other cluster C_k != C_i

$$b(i) = \min_{k \neq i} \frac{1}{|C_k|} \sum_{j \in C_k} \delta(i, j)$$

$$s(i) = \begin{cases} 1 - a(i)/b(i) & \text{if } a(i) < b(i) \\ 0 & \text{if } a(i) = b(i) \\ b(i)/a(i) - 1 & \text{if } a(i) > b(i) \end{cases}$$

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- Quality measured by the ability to discover some or all of the hidden patterns in gold standard data
- Hard as it requires labeled data typically provided by human experts

External Evaluation: Purity

$$C_1 \ldots, C_K = \text{set of } K \text{ clusters}$$

$$L_1 \ldots, L_J = \text{set of } J \text{ labels}$$

$$n_{i,j} = \text{number of items with label } L_j \text{ clustered in } C_i$$

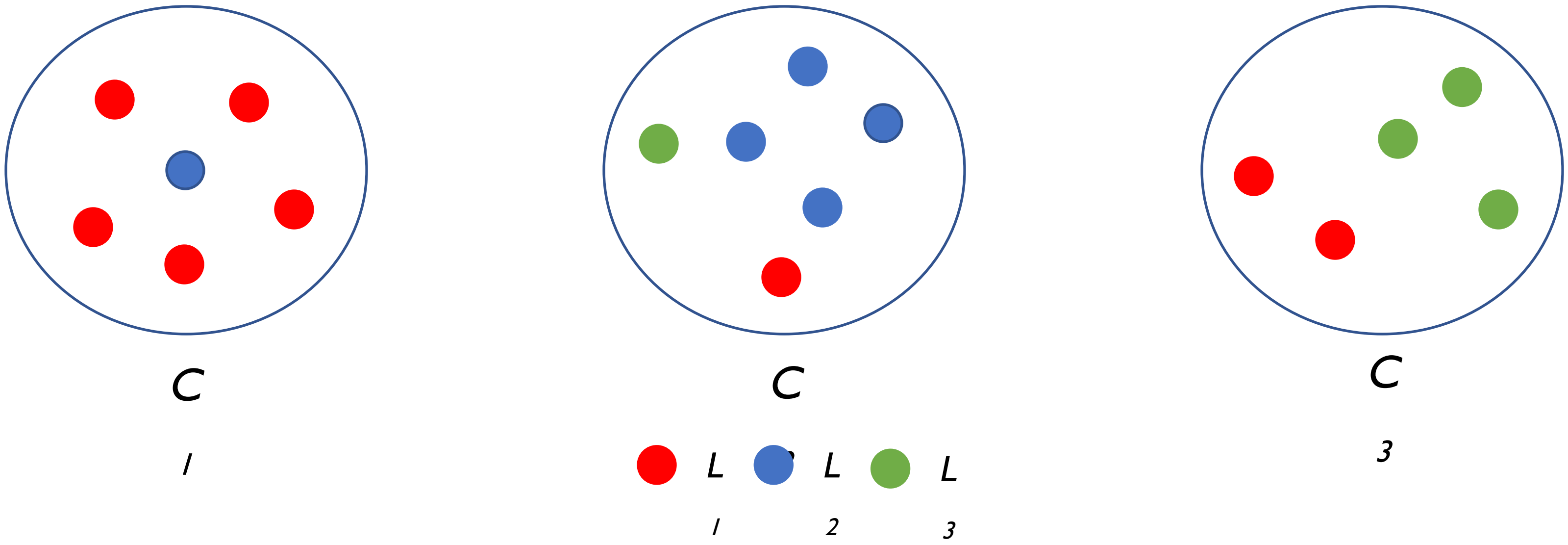
$$n_i = \sum_{j=1}^{J} n_{i,j} \text{ number of items clustered in } C_i$$

$$\text{purity}(C_i) = \frac{1}{n_i} \max_{j \in \{1,\ldots,J\}} n_{i,j}$$

$$\text{purity} = \frac{1}{K} \sum_{i=1}^{K} \text{purity}(C_i)$$

Biased because having as many clusters as items maximizes purity

External Evaluation: Purity Example



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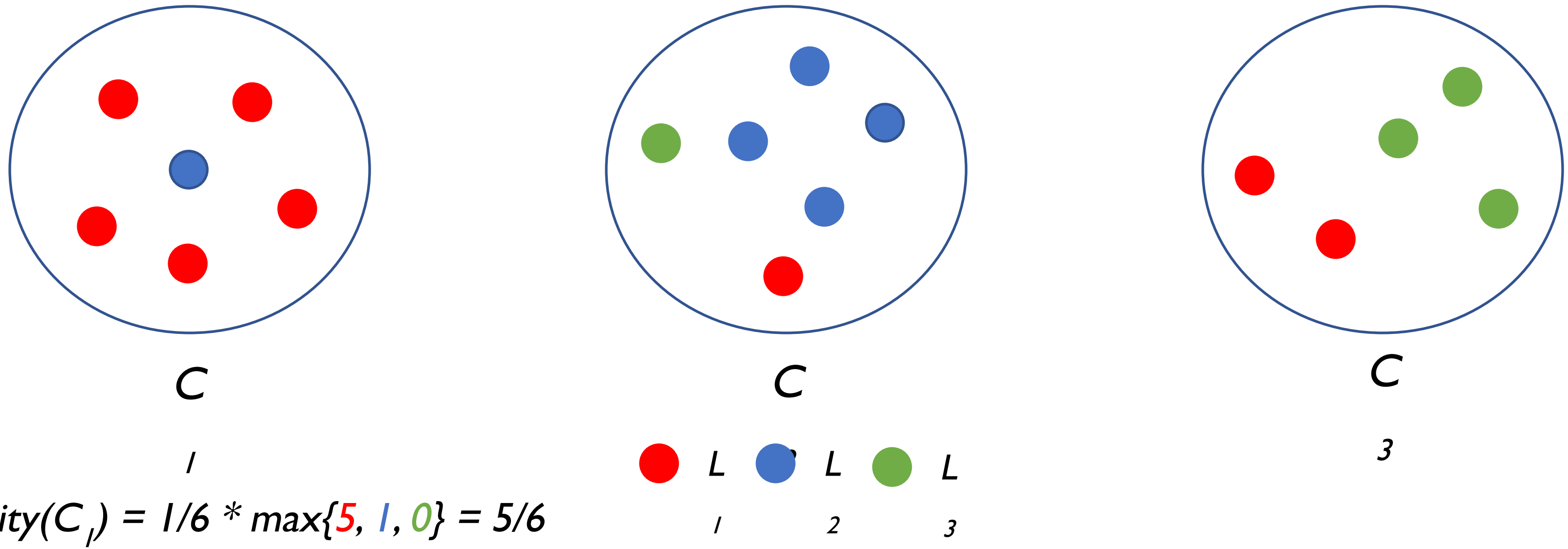
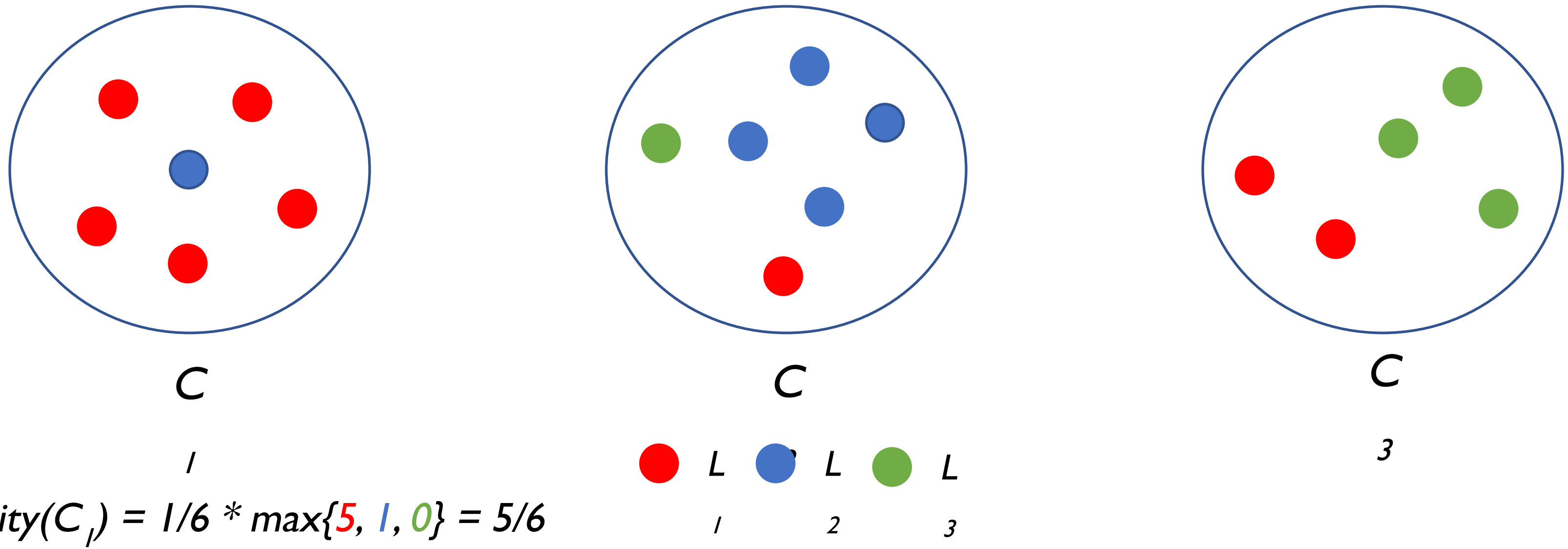


$purity(C_1) = 1/6 * max\{5, 1, 0\} = 5/6$

External Evaluation: Purity Example



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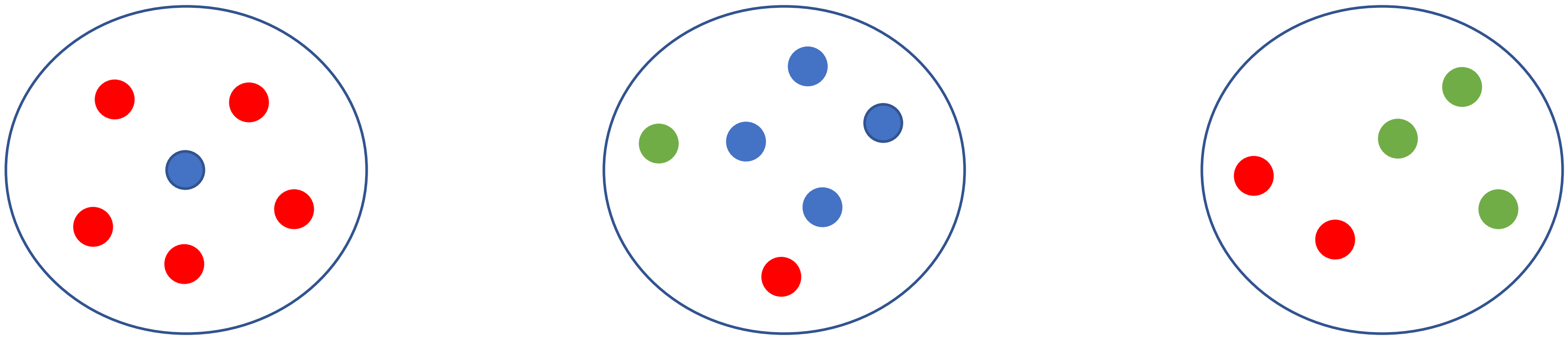

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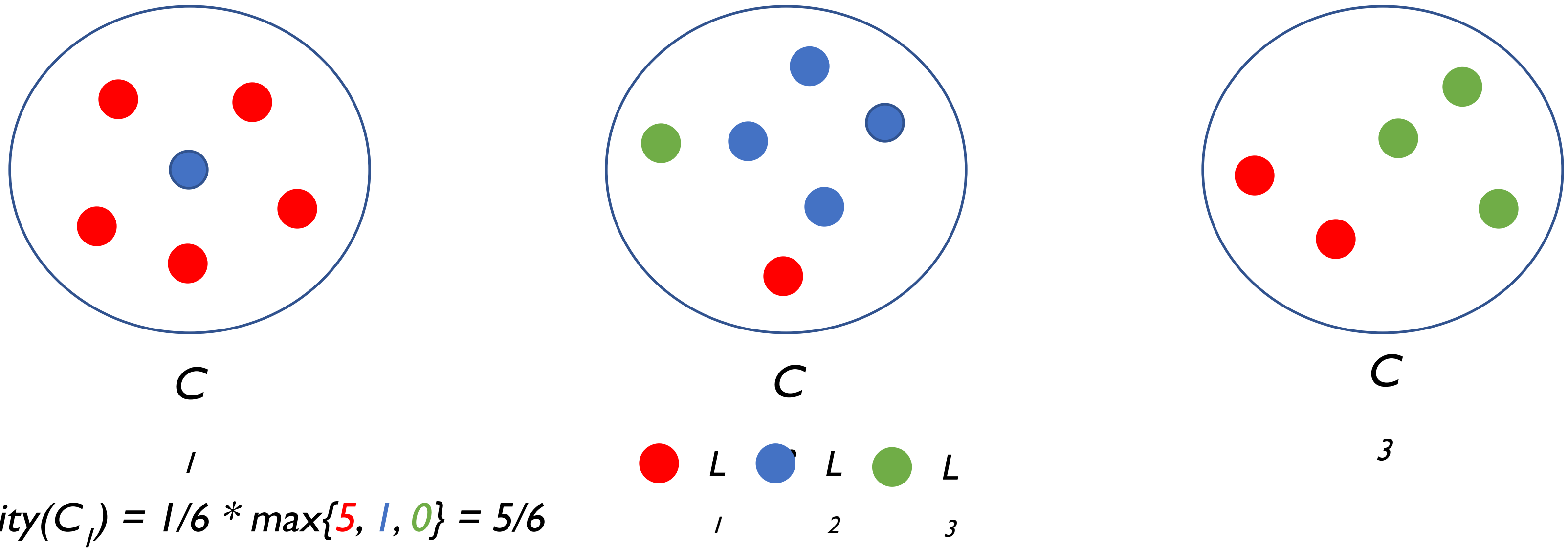

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$\boxed{\textbf{purity} = 1/3 * purity(C_1)+purity(C_2)+purity(C_3) = \mathbf{7/10}}$

External Evaluation: Rand Index

$$\text{Rand} = \frac{TP + TN}{TP + TN + FP + FN}$$

$$\left.\begin{aligned} TP &= \text{number of } \textit{true positives} \\ TN &= \text{number of } \textit{true negatives} \\ FP &= \text{number of } \textit{false positives} \\ FN &= \text{number of } \textit{false negatives} \end{aligned}\right\}$$

All computed from **pairs** of elements

Measures the level of agreement between clustering and ground truth

External Evaluation: Rand Index

n. of pairs	Same Cluster in Clustering	Different Clusters in Clustering
Same Cluster in Ground-Truth		
Different Clusters in Ground-Truth		

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Same Cluster in Ground-Truth	TRUE POSITIVES (TP)	FALSE NEGATIVES (FN)
Different Clusters in Ground-Truth	FALSE POSITIVES (FP)	TRUE NEGATIVES (TN)

Confusion

External Evaluation: Precision, Recall, F-measure

$$P = \frac{TP}{TP + FP} \quad R = \frac{TP}{TP + FN}$$

$$F_\beta = \frac{(\beta^2 + 1) \cdot P \cdot R}{\beta^2 \cdot P + R}$$

$$F_1 = \frac{2 \cdot P \cdot R}{P + R}$$

Balances the contribution of false negatives by weighting recall through a parameter β

External Evaluation: Many Other Measures

- Jaccard index
- Dice index
- Fowlkes-Mallows index
- Mutual information
- etc.

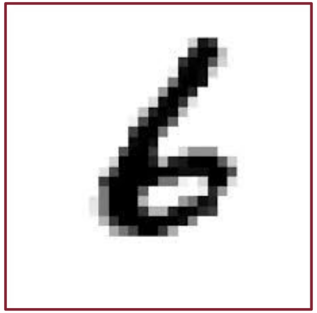
DIMENSIONALITY REDUCTION

Modeled vs. True Dimensionality

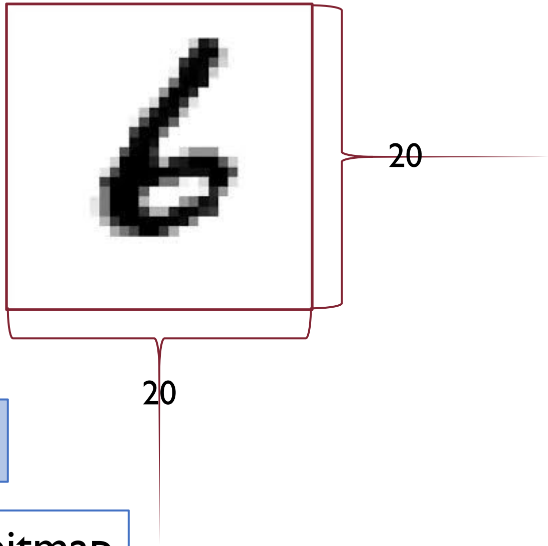
Example

Handwritten digit recognition

Modeled vs. True Dimensionality



Modeled vs. True Dimensionality

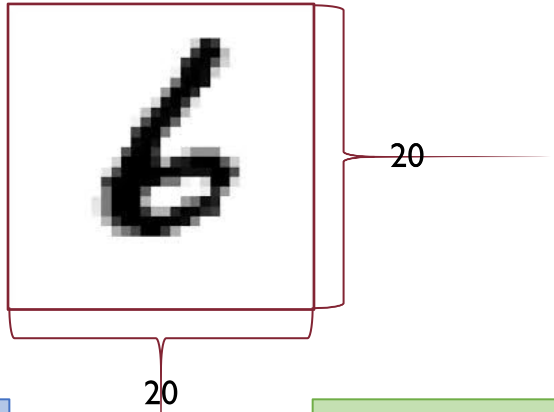


Modeled dimensionality

Each digit represented by **20x20** bitmap

400-dimensional binary vector

Modeled vs. True Dimensionality



Modeled dimensionality

Each digit represented by **20x20** bitmap

400-dimensional binary vector

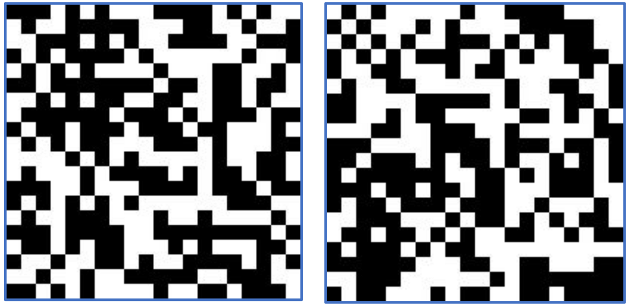
True dimensionality

Actual digits just cover a tiny fraction of all this huge space

Small variations of the pen-stroke

Modeled vs. True Dimensionality

Random samples from 400-d space



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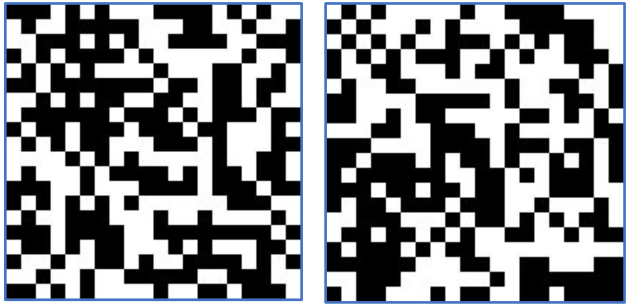

True digits living in a 400-d space

Modeled vs. True Dimensionality

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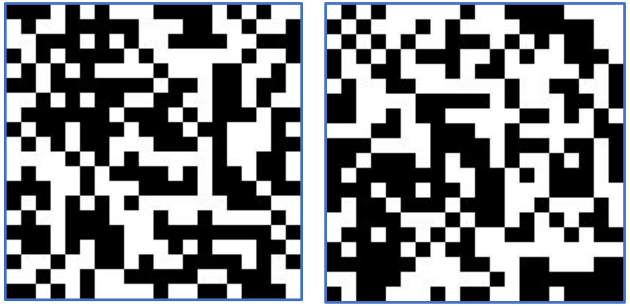

True digits living in a 400-d space

We model data (i.e., digits) as very high dimensional…

… In fact, they are not so

The Curse of Dimensionality

As dimensionality grows fewer examples in each region of the feature space (assuming # examples is constant)

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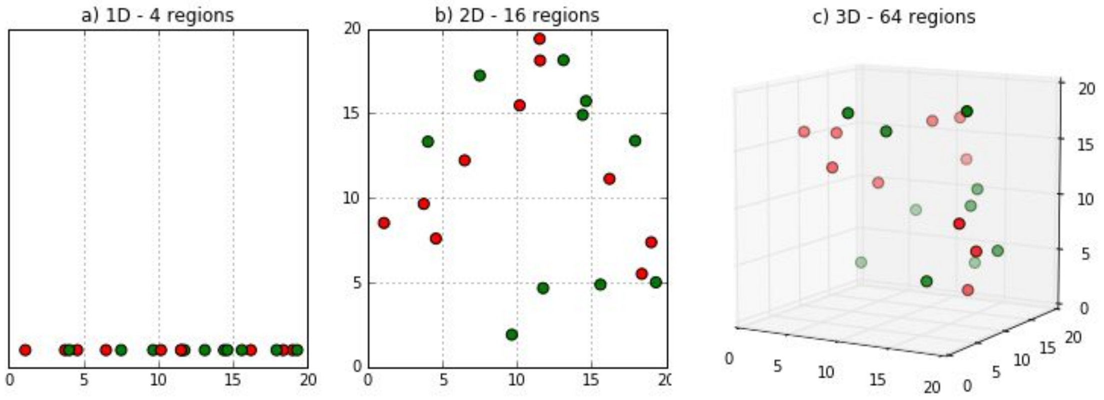

Dealing with High Dimensionality

3 possible approaches

Feature Engineering
(using domain knowledge)

e.g., SIFT in computer vision

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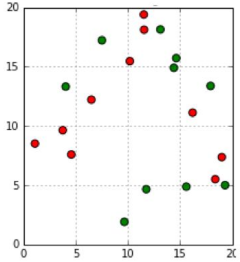
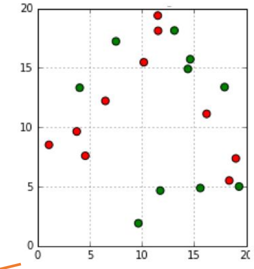
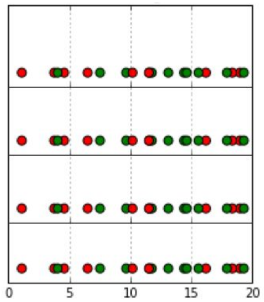
Making Assumptions



Dealing with High Dimensionality: Assumptions

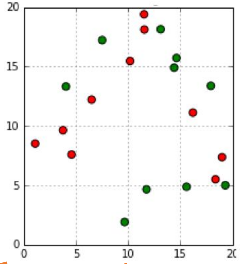


independence



Count along each dimension separately

Dealing with High Dimensionality: Assumptions



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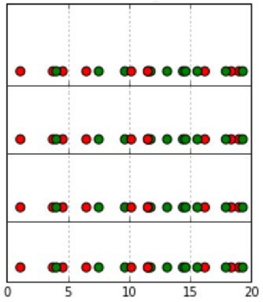
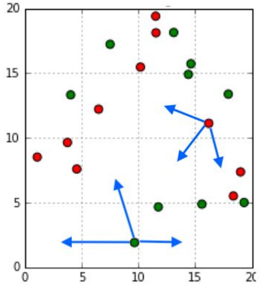


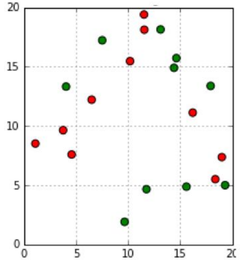
Count along each dimension separately

smoothness



Propagate counts to neighboring regions

Dealing with High Dimensionality: Assumptions



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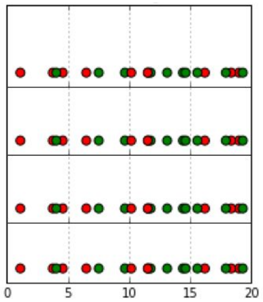

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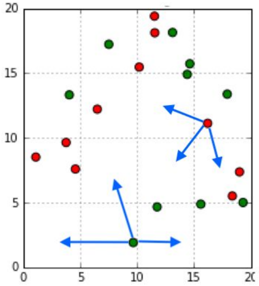
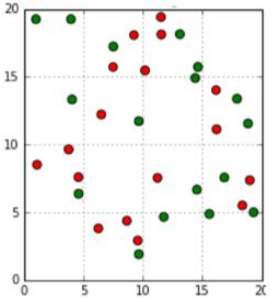


Propagate counts to neighboring regions

simmetry



Invariance to the order of dimensions

Dealing with High Dimensionality

3 possible approaches

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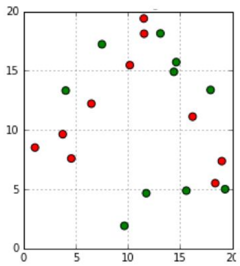
(using domain knowledge)

e.g., SIFT in computer vision

Making Assumptions



Reduce Dimensionality

Create a new set of dimensions (i.e., variables)

Dimensionality Reduction

- A technique to unveil the actual (i.e., meaningful) dimensions of data
- A pre-processing step for representing data with fewer features
- Preserve as much "structure" of the data as possible
- Retained structure must be discriminative affecting data separability

"structure" here means
variance

Dimensionality Reduction

2 main approaches

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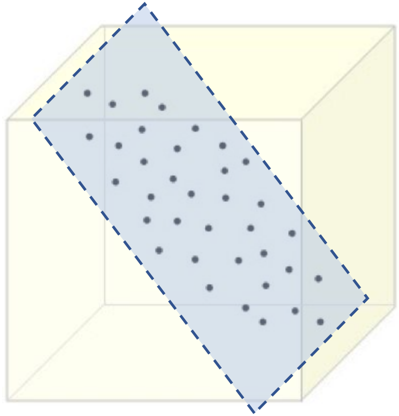
Example

A 3-d set of points embedded into a 2-d hyperplane



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- 1st: direction of the greatest variance of data
- 2nd: perpendicular to 1st and greatest variance of what's left
- … and so on until d

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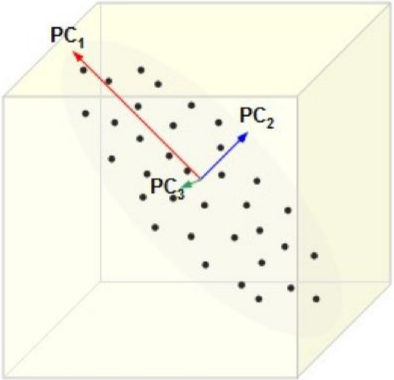
The top k < d components become the new dimensions



e.g., k = 2

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PC_1 and **PC_2** are the top-2 principal components

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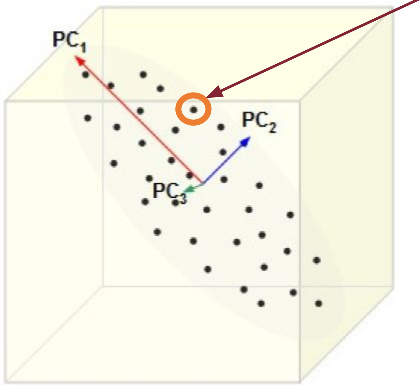
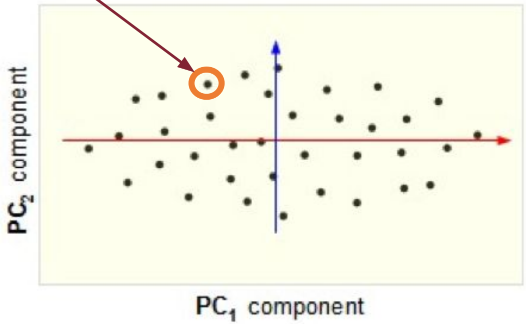
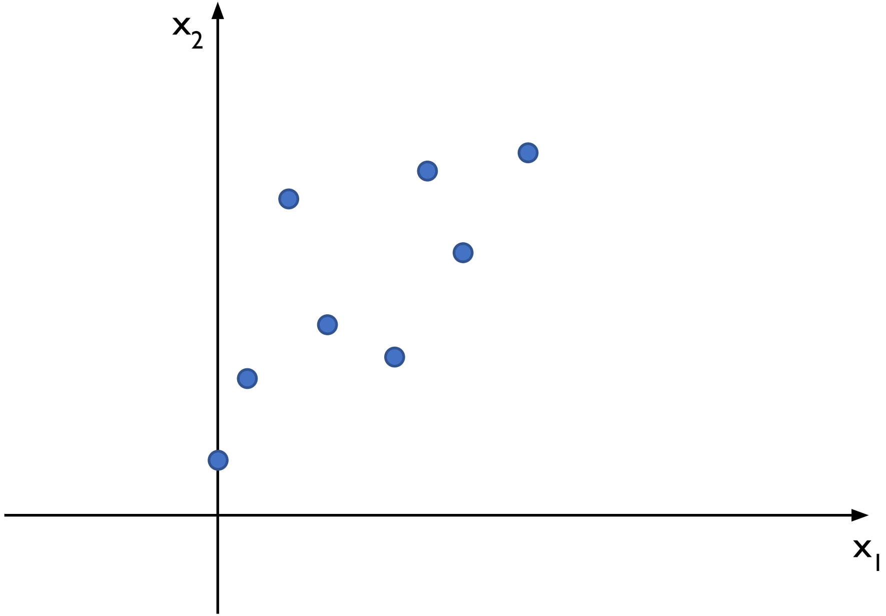
Change the coordinates of every point according to the new dimensions





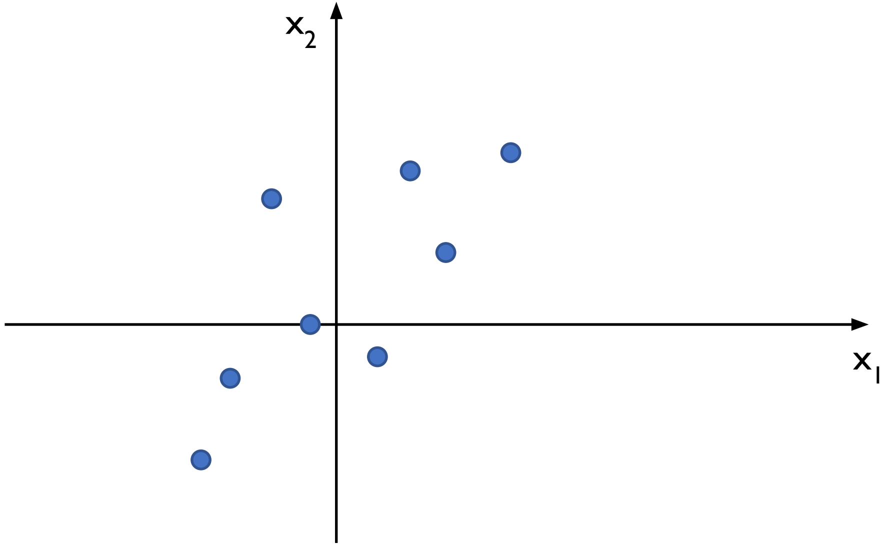
Why Do We Look for Greatest Variance?

Example: Reduce 2-dimensional data to 1-d



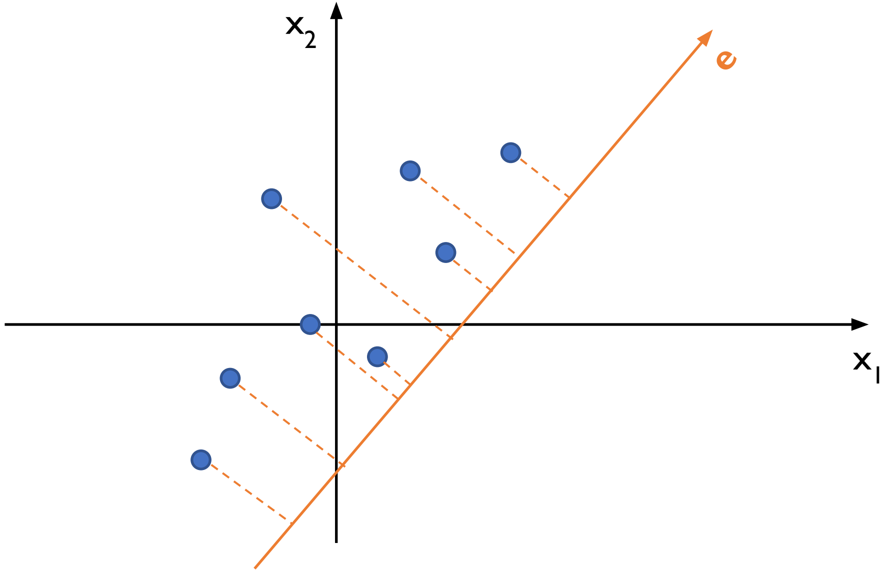
Why Do We Look for Greatest Variance?

First of all, let's center the points around the mean along x_1 and x_2



Why Do We Look for Greatest Variance?

Map, i.e., project (x_1, x_2) to a new single dimension axis **e**



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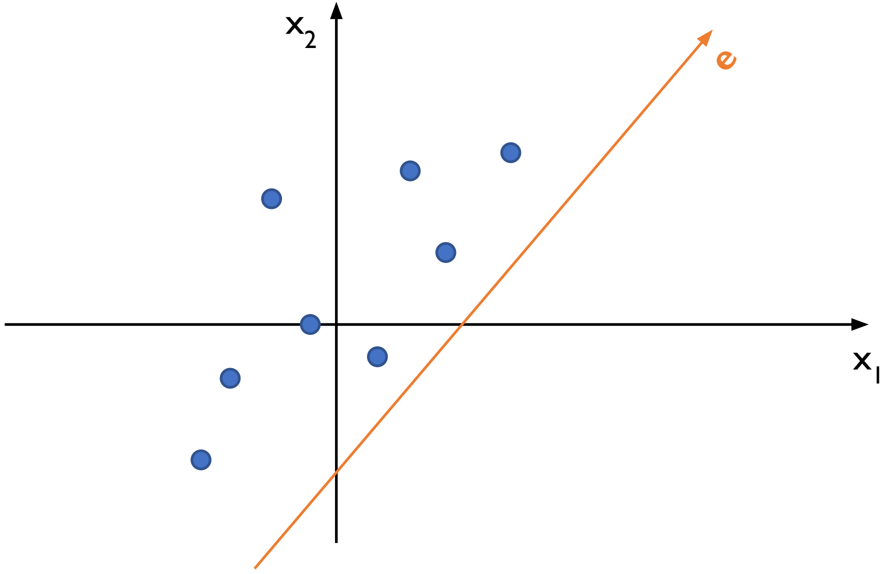

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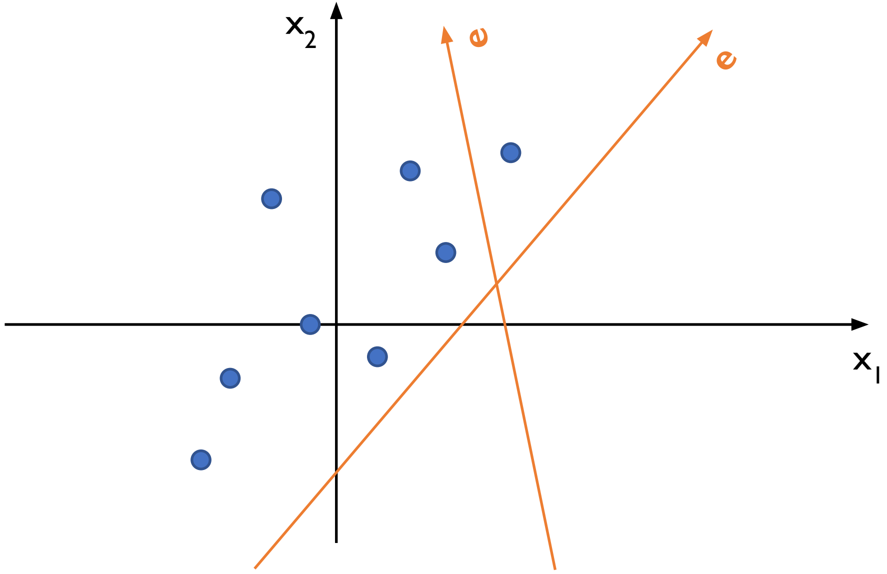

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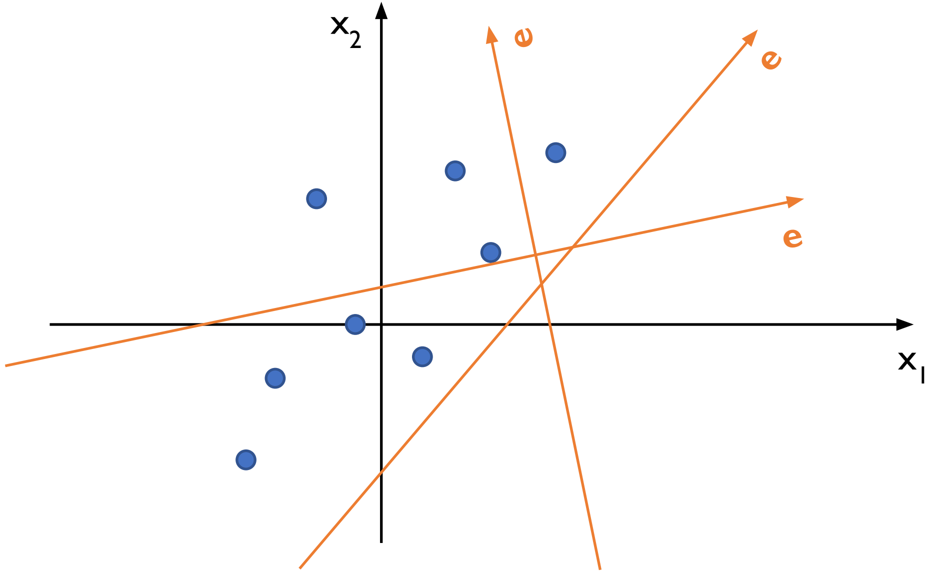

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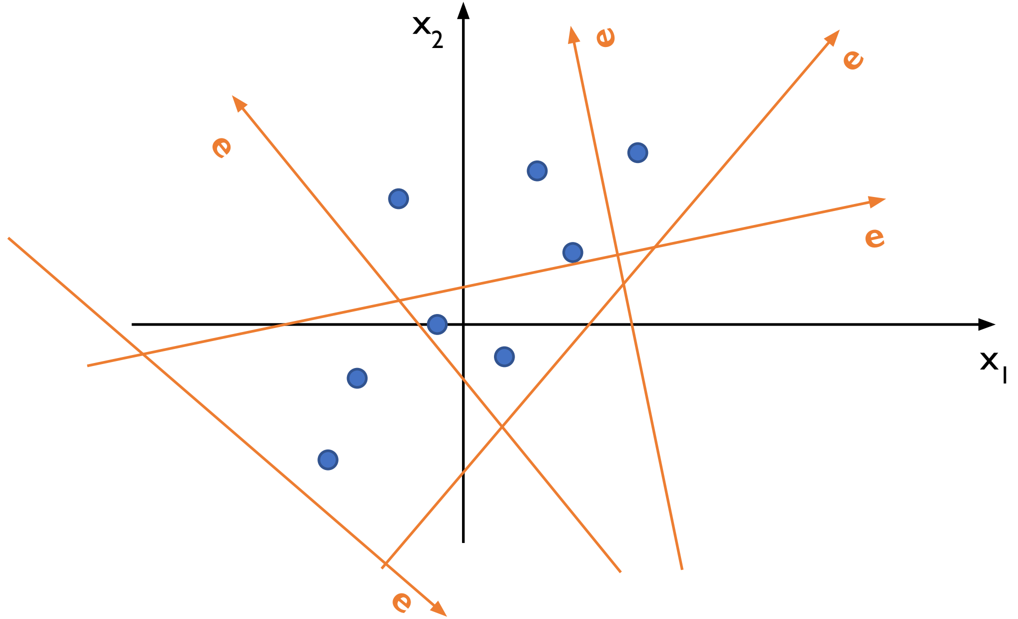
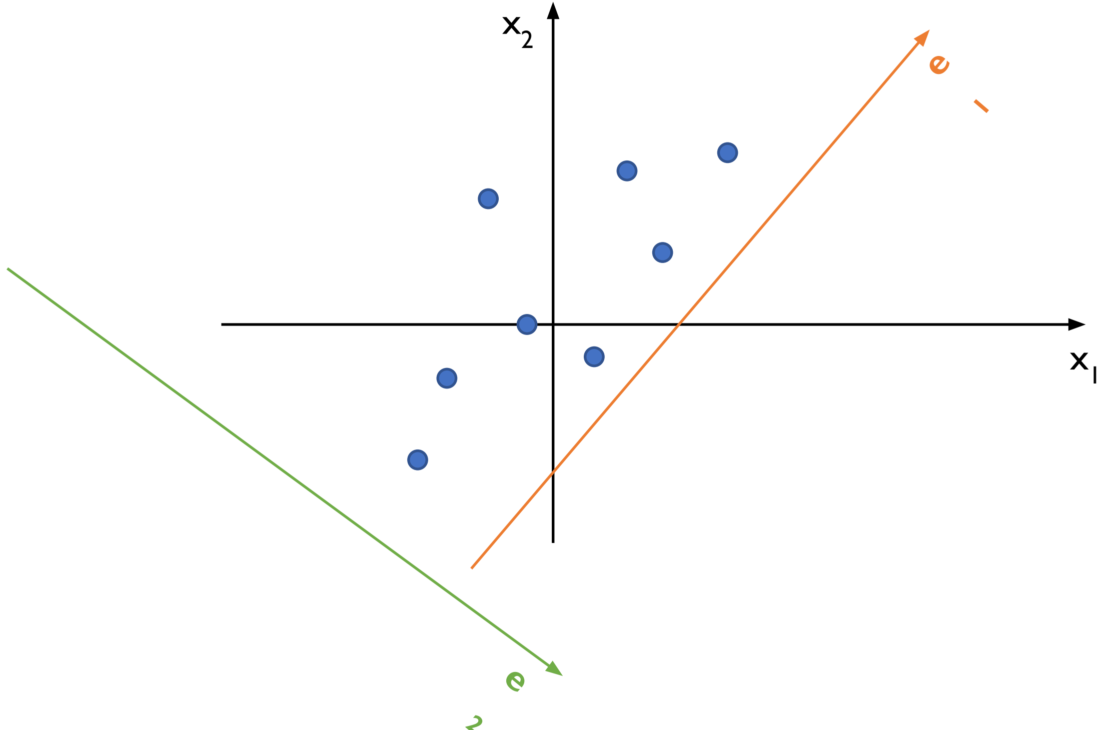


infinitely many mappings from (x_1, x_2) to a new axis **e**

Why Do We Look for Greatest Variance?

Let's consider 2 different mappings e_1 and e_2



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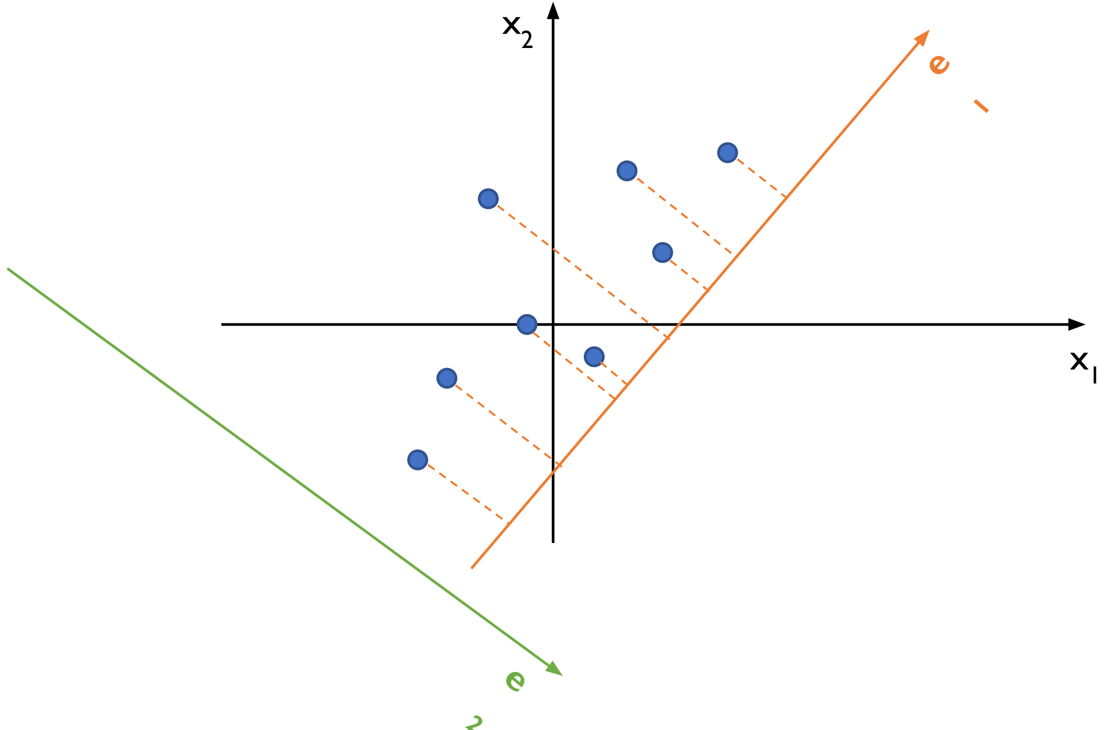

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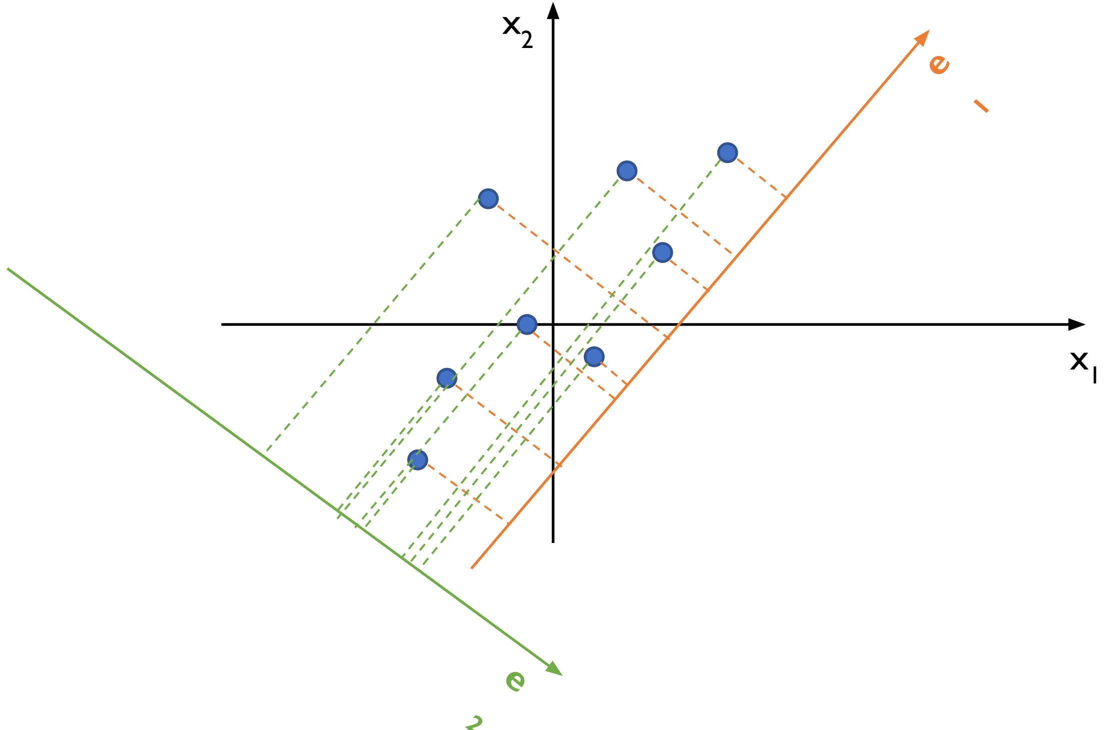
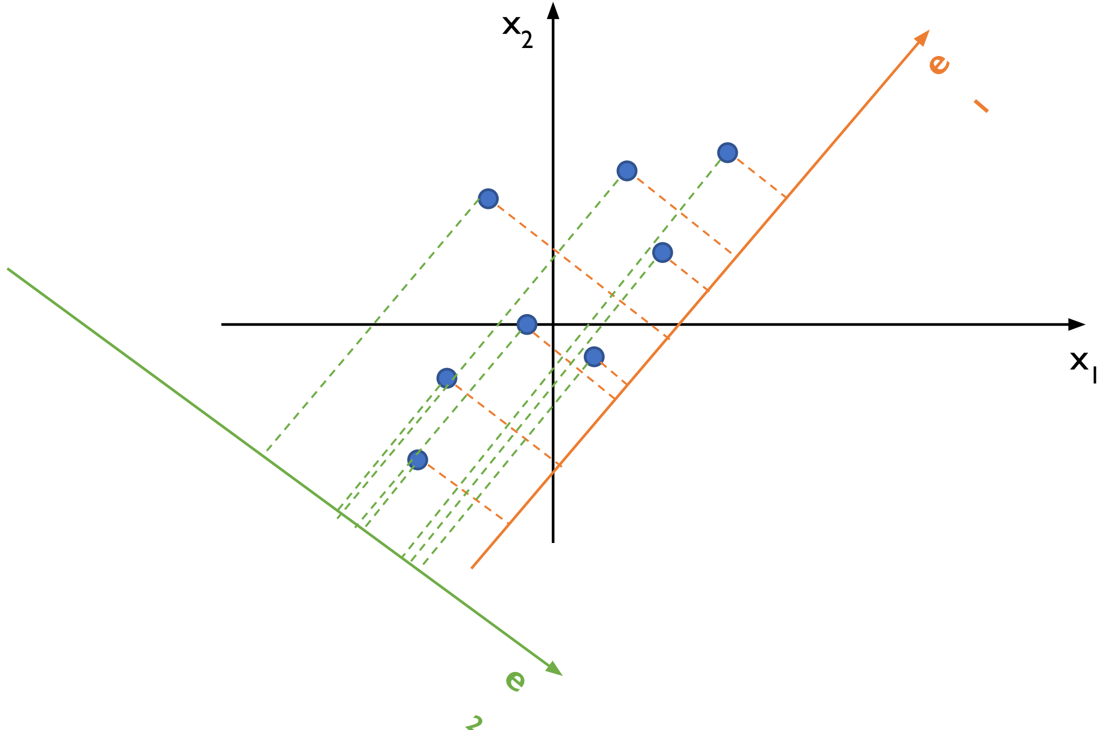


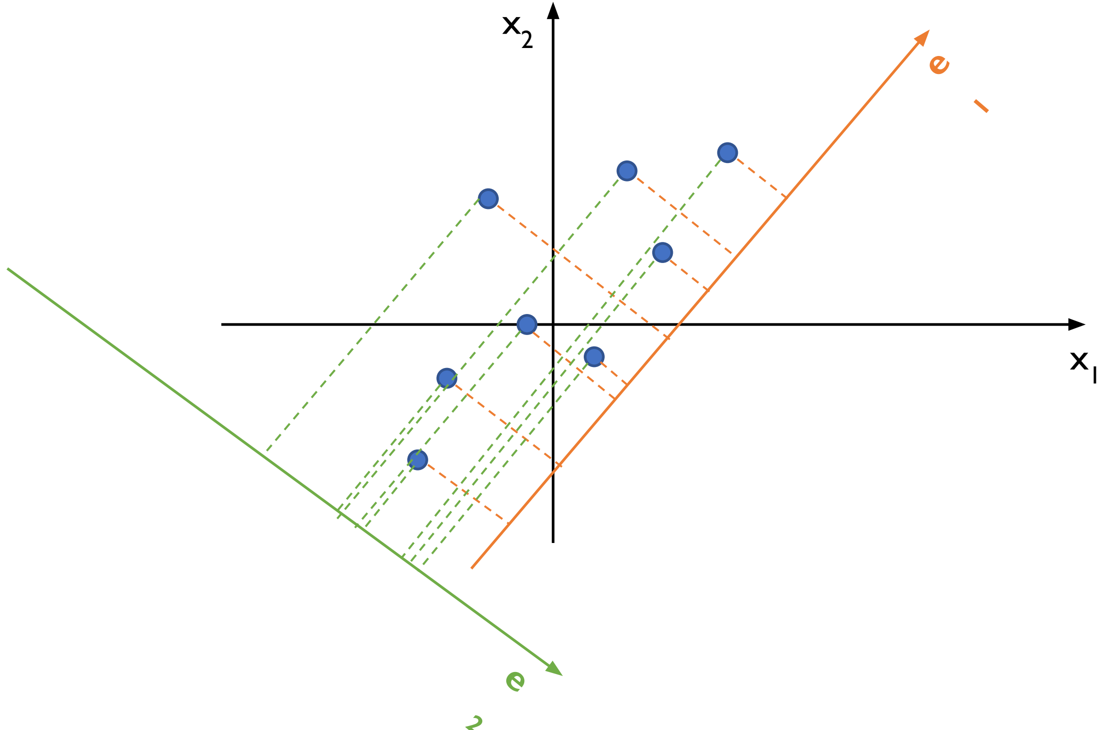
Why Do We Look for Greatest Variance?

Which one is better?



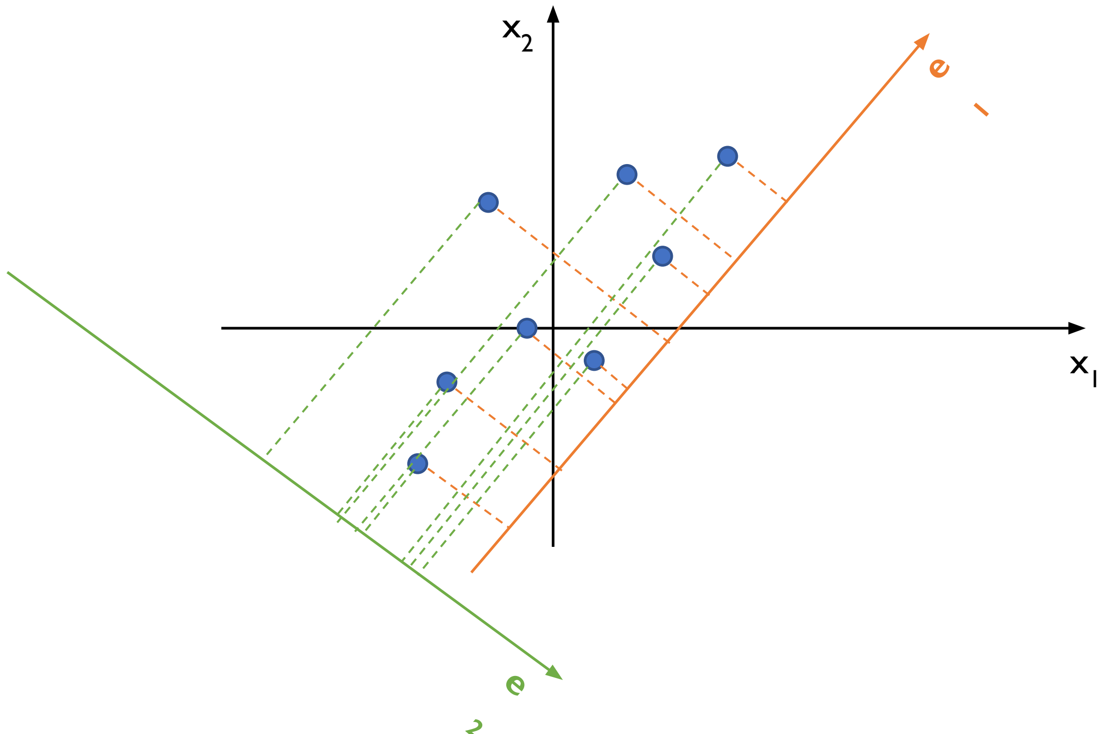
Why Do We Look for Greatest Variance?

Points projected onto $\mathbf{e_1}$ look more **spread-out** than onto $\mathbf{e_2}$



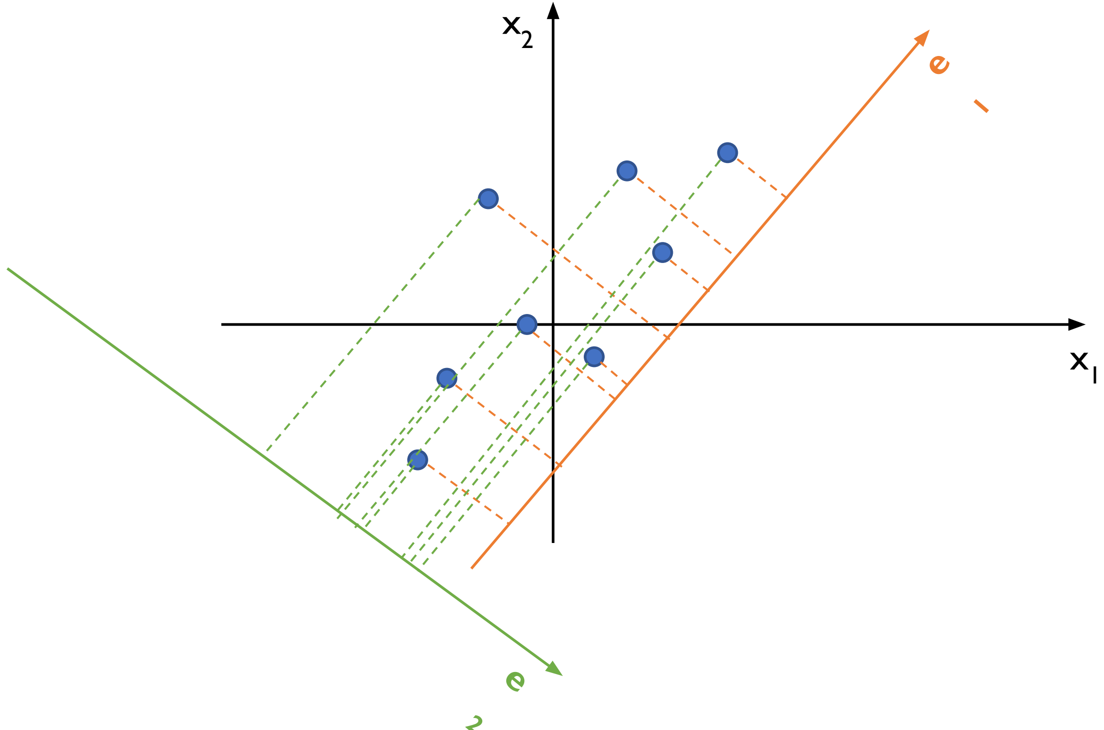
Why Do We Look for Greatest Variance?

The **variance** along $\mathbf{e_1}$ is larger than along $\mathbf{e_2}$



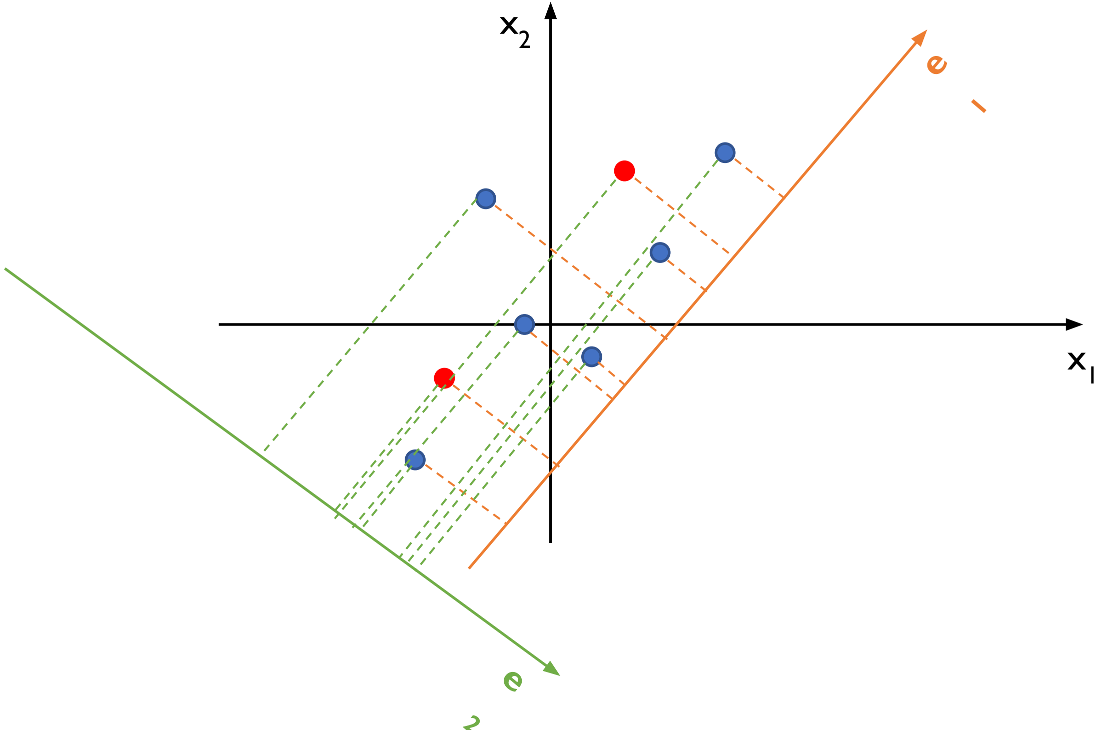
Why Do We Look for Greatest Variance?

Why is that good?



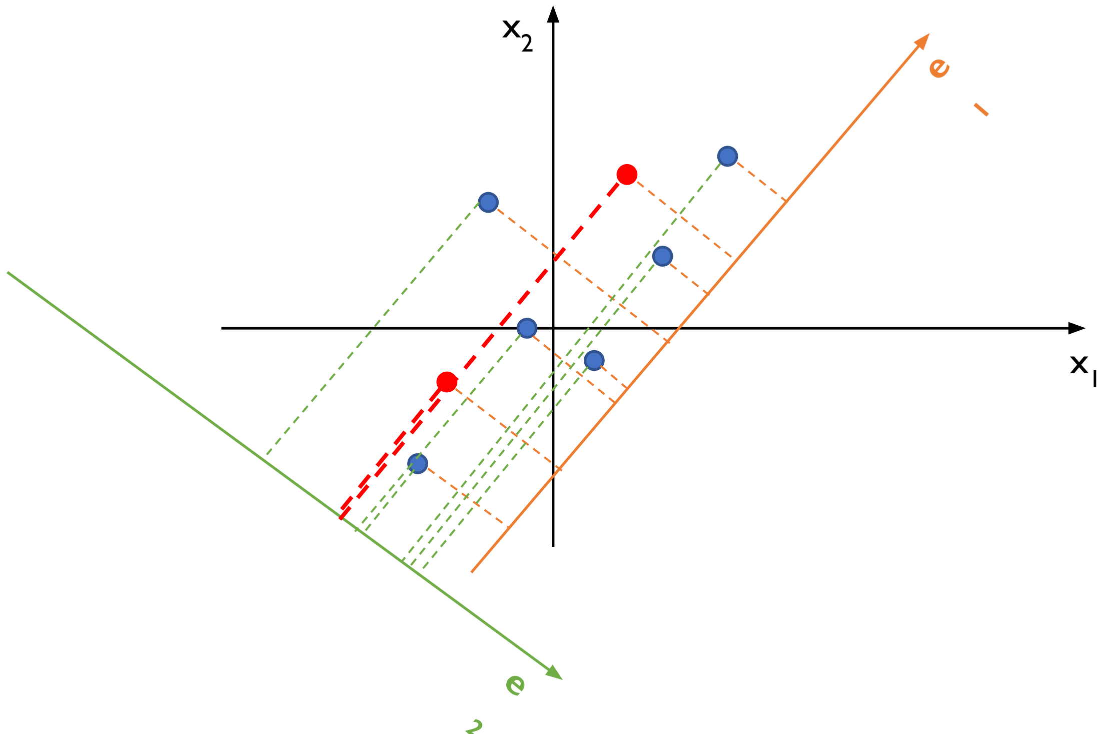
Why Do We Look for Greatest Variance?

Consider the 2 red points below



Why Do We Look for Greatest Variance?

On (x_1, x_2) far away from each other, end up close if projected onto $\mathbf{e_2}$



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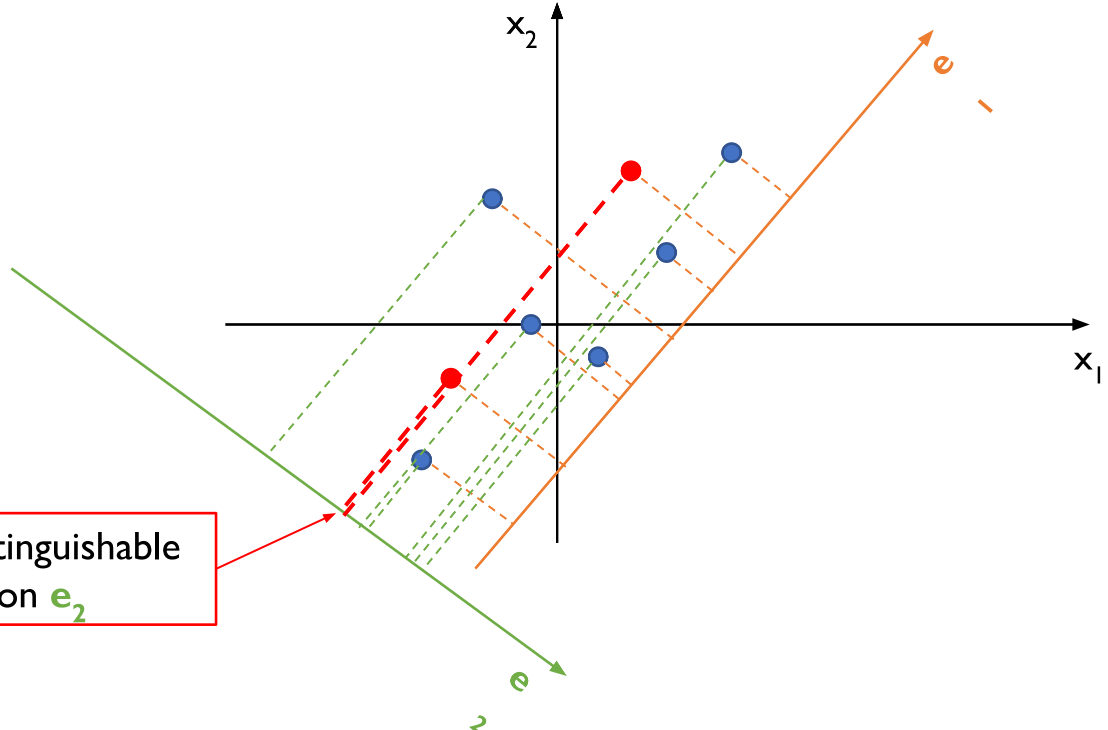
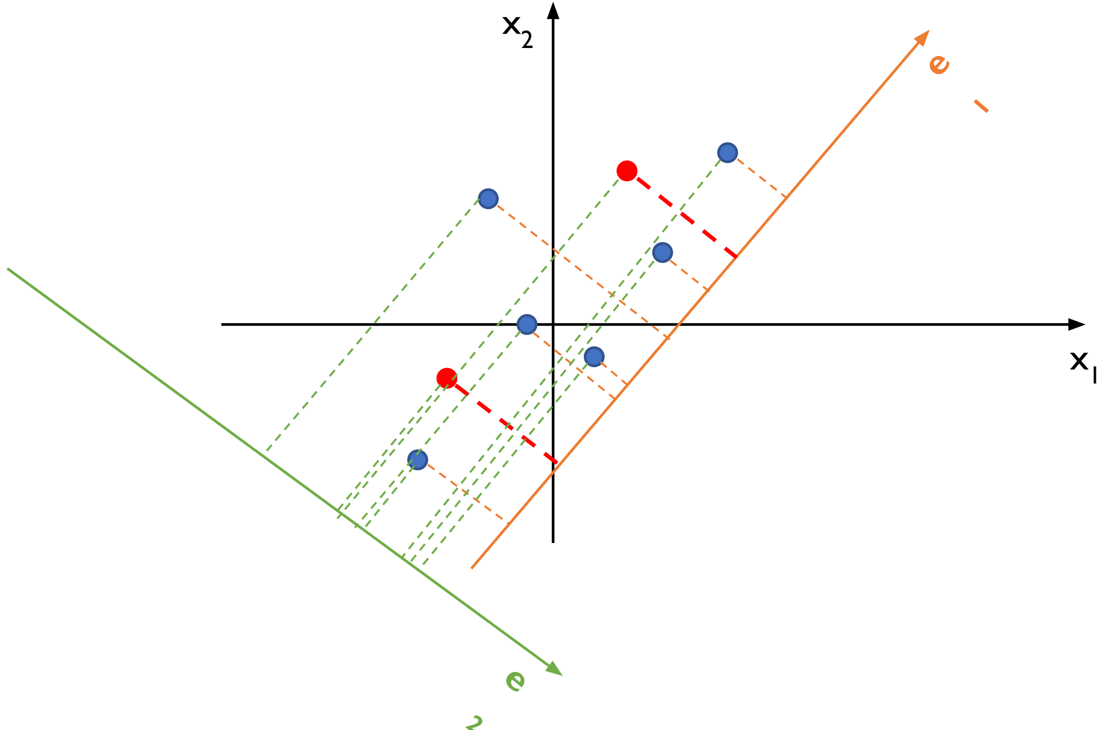


Almost indistinguishable points on e_2

Why Do We Look for Greatest Variance?

If projected onto e_1 they better preserve their distance



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$\Downarrow$

Solution

Pick **e** so as to **maximize variance** of projected data

Variance of a Random Variable

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- Formally, it is the expected value of the squared deviation from its mean

$$\mathrm{Var}(X) = \mathrm{E}[(X - \mu)^2]$$

$$\text{where } \mu = \mathrm{E}[X]$$

Covariance of Two Random Variables

- A measure of the joint variability of two random variables X and Y
  - Do X and Y increase/decrease together, or when one increases/decreases the other decreases/increases?

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$$\mathrm{Cov}(X, Y) = \mathrm{E}[(X - \mu_X)(Y - \mu_Y)]$$

$$\boxed{\mathrm{Cov}(X, X) = \mathrm{Var}(X)}$$

$$\text{where } \mu_X = \mathrm{E}[X] \text{ and } \mu_Y = \mathrm{E}[Y]$$

Covariance Matrix

- Given a random vector $\mathbf{X} = (X_1, \ldots, X_d)$ its covariance matrix K is a dxd square matrix with the covariance between each pair of elements

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- In the matrix diagonal there are variances, i.e., the covariance of each element with itself

$$\mathrm{K}[i, j] = \mathrm{Cov}(X_i, X_j)$$

Covariance Matrix of Original Dimensions

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- In our example, d = 2 and $\mathbf{X} = (X_1, X_2)$
- The covariance matrix K is a 2-by-2 matrix
- To ease the covariance computation, we center each data point at zero
  - Subtracting the mean of each attribute/dimension
  - The mean of each dimension becomes then 0

Covariance Matrix of Original Dimensions

Let n be the total number of data points: $\mathbf{x}_1, \ldots, \mathbf{x}_n$

Each data point is represented by a (x_1, x_2) pair

$\mathbf{x}_i = (x_{i,1}, x_{i,2})$

We associate 2 random variables X_1, X_2 to each dimension, and we compute:

$$\mu_1 = \mathrm{E}[X_1] = \frac{1}{n}\sum_{i=1}^{n} x_{i,1}$$

$$\mu_2 = \mathrm{E}[X_2] = \frac{1}{n}\sum_{i=1}^{n} x_{i,2}$$

$$\mathbf{x}_i = (x_{i,1} - \mu_1, x_{i,2} - \mu_2)$$

Covariance Matrix of Original Dimensions

Let us rewrite each data point $\mathbf{x}_i$ as follows:

$\mathbf{x}_i = (x'_{i,1}, x'_{i,2})$ where:

$x'_{i,1} = x_{i,1} - \mu_1; x'_{i,2} = x_{i,2} - \mu_2$

$$\mu_1^{\text{new}} = \text{E}[X_1] = \frac{1}{n}\sum_{i=1}^{n} x'_{i,1} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,1} - \mu_1)$$

$$\mu_2^{\text{new}} = \text{E}[X_2] = \frac{1}{n}\sum_{i=1}^{n} x'_{i,2} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,2} - \mu_2)$$

Covariance Matrix of Original Dimensions

$$\mu_1^{\text{new}} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,1}-\mu_1) = \frac{1}{n}\left(\underbrace{\sum_{i=1}^{n} x_{i,1}}_{n\mu_1} - \underbrace{\sum_{i=1}^{n} \mu_1}_{n\mu_1}\right) = 0$$

$$\mu_2^{\text{new}} = \frac{1}{n}\sum_{i=1}^{n}(x_{i,2}-\mu_2) = \frac{1}{n}\left(\underbrace{\sum_{i=1}^{n} x_{i,2}}_{n\mu_2} - \underbrace{\sum_{i=1}^{n} \mu_2}_{n\mu_2}\right) = 0$$

0-mean

Covariance Matrix of Original Dimensions

Scaling data so as to have 0-mean on all dimensions allow computing covariance much easily

$$\mathrm{Cov}(X_1, X_2) = \mathrm{E}[(X_1 - \underbrace{\mu_1^{\text{new}}}_{=0})(X_2 - \underbrace{\mu_2^{\text{new}}}_{=0})] = \mathrm{E}[X_1 X_2]$$

Covariance Matrix of Original Dimensions

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As a consequence, the covariance matrix is also easier to compute!

Covariance Matrix of Original Dimensions

Let's assume the following is our 2-by-2 covariance matrix

$$
\begin{array}{c c}
 & \begin{array}{cc} x_1 & x_2 \end{array} \\
\begin{array}{c} x_1 \\ x_2 \end{array} & \begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix}
\end{array}
$$

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$$\boxed{\operatorname{Cov}(X_1, X_2) = \frac{1}{n} \sum_{i=1}^{n} x'_{i,1} * x'_{i,2}}$$

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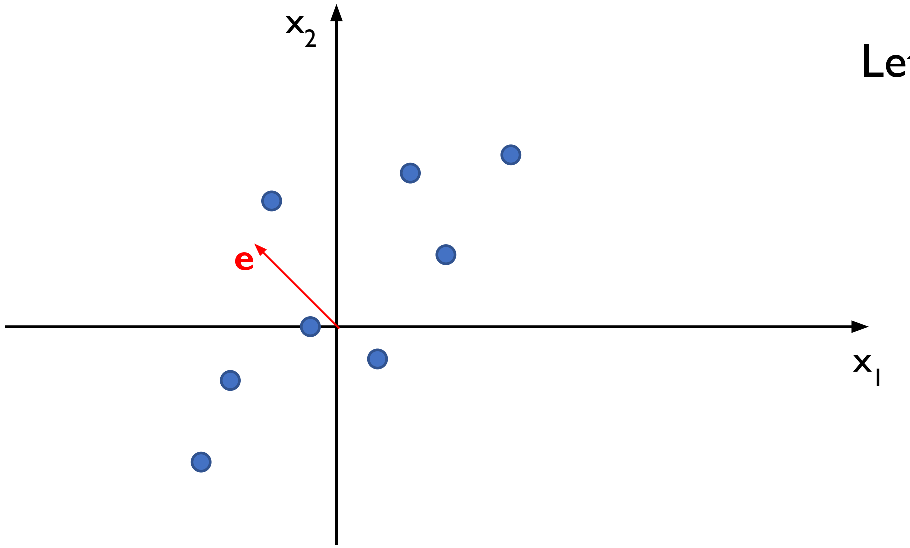
$$\boxed{\mathrm{Cov}(X_2, X_2) = \mathrm{Var}(X_2) = \frac{1}{n}\sum_{i=1}^{n} (x'_{i,2})^2}$$

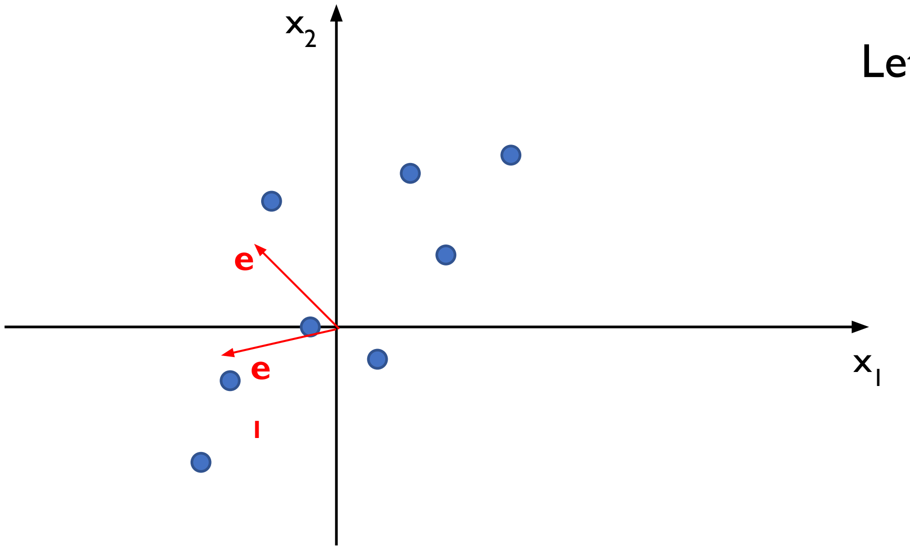
Covariance Matrix of Original Dimensions



Let's multiply our 2-by-2 covariance matrix K by a **random** vector **e** = (-1,1)

$$\underbrace{\begin{bmatrix} 2 & 4/5 \\ 4/5 & 3/5 \end{bmatrix}}_{K} \underbrace{\begin{bmatrix} -1 \\ 1 \end{bmatrix}}_{\mathbf{e}} =$$

Covariance Matrix of Original Dimensions



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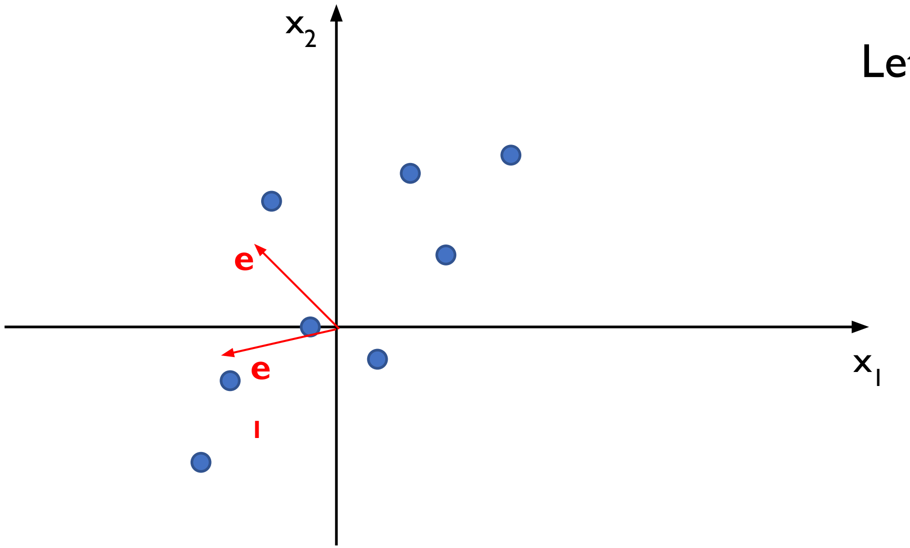
Covariance Matrix of Original Dimensions



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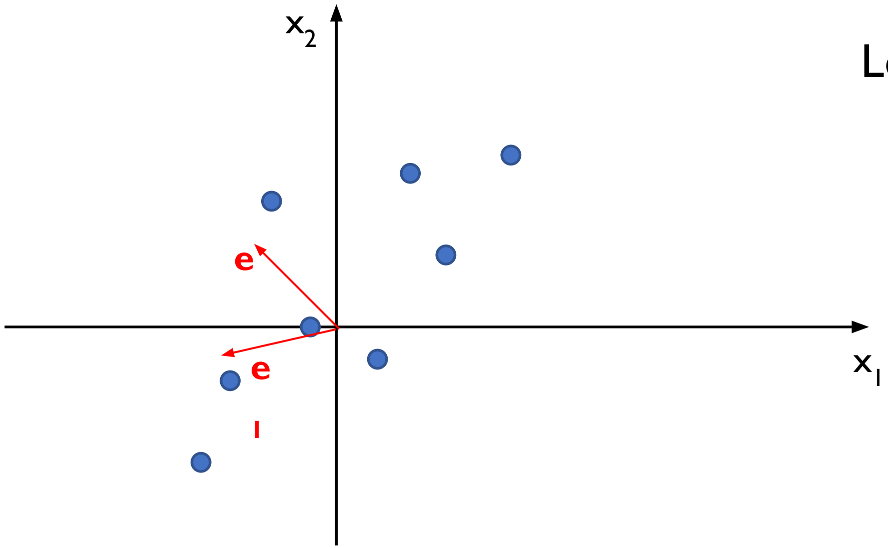
slope = 1/-1 = -1

Covariance Matrix of Original Dimensions



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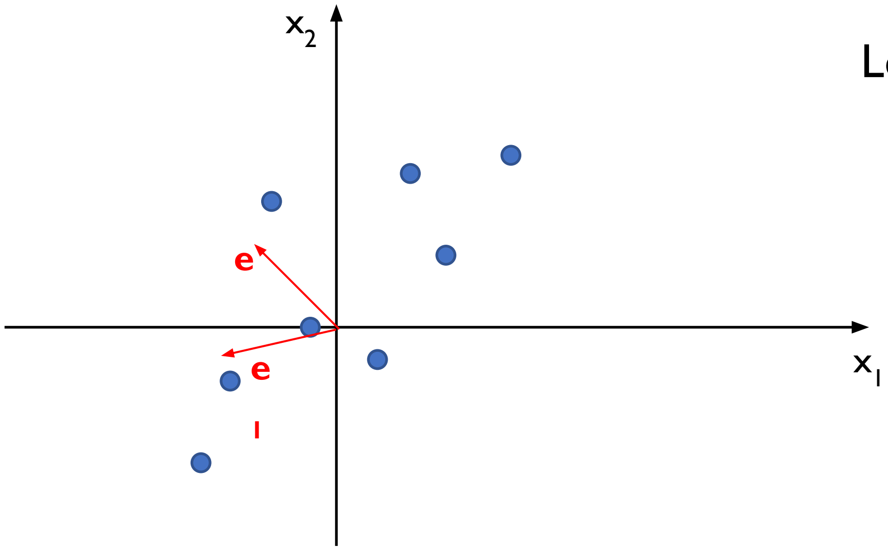
slope = 1/-1 = -1

new slope = -(1/5)/-(6/5) = 1/6

Covariance Matrix of Original Dimensions



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Turns towards the direction of the greatest variance

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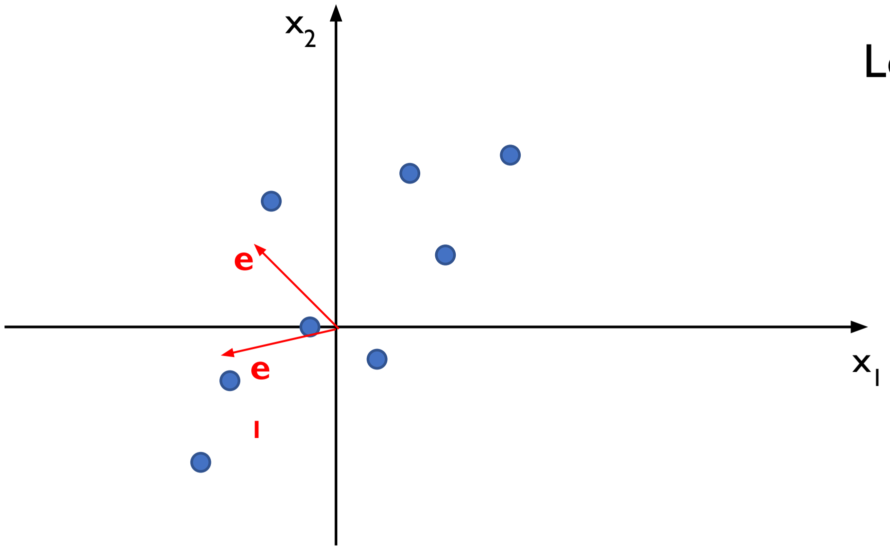
Covariance Matrix of Original Dimensions



Let's repeat the previous step multiplying the covariance matrix K by $\mathbf{e}_1$ = (-6/5,-1/5)

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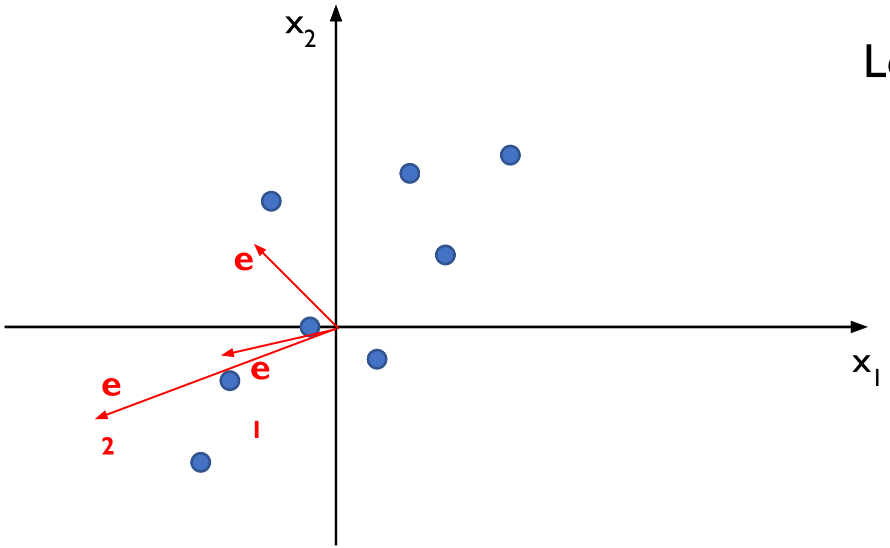
Covariance Matrix of Original Dimensions



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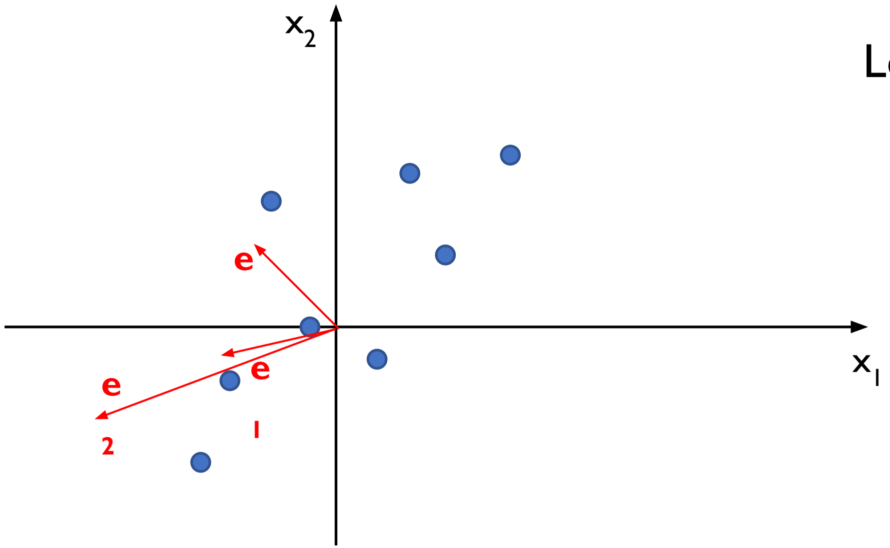
Covariance Matrix of Original Dimensions



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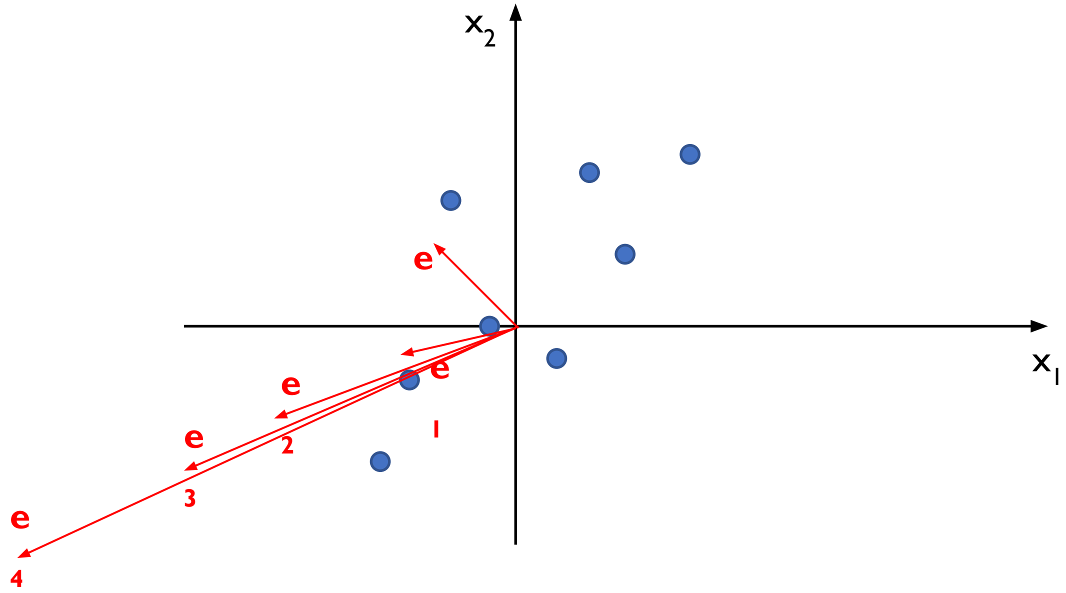
slope = 1/6

Turns towards the direction of the greatest variance

new slope = 27/64

Covariance Matrix of Original Dimensions

If we keep doing this the resulting vector is getting **longer** and **turns** towards the direction of the **largest variance**



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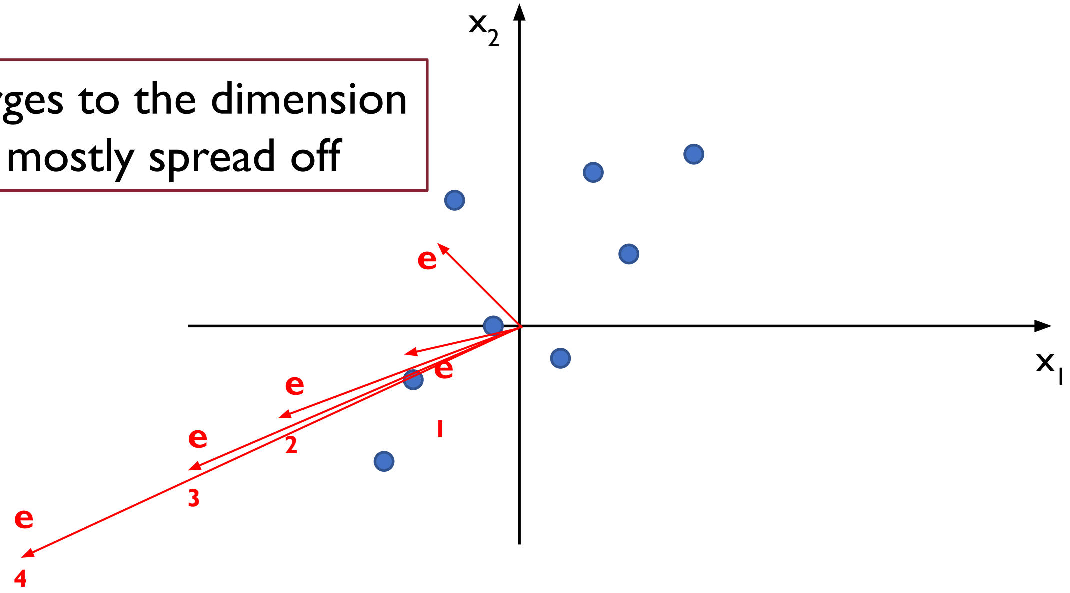
The slope converges to the dimension where data is mostly spread off



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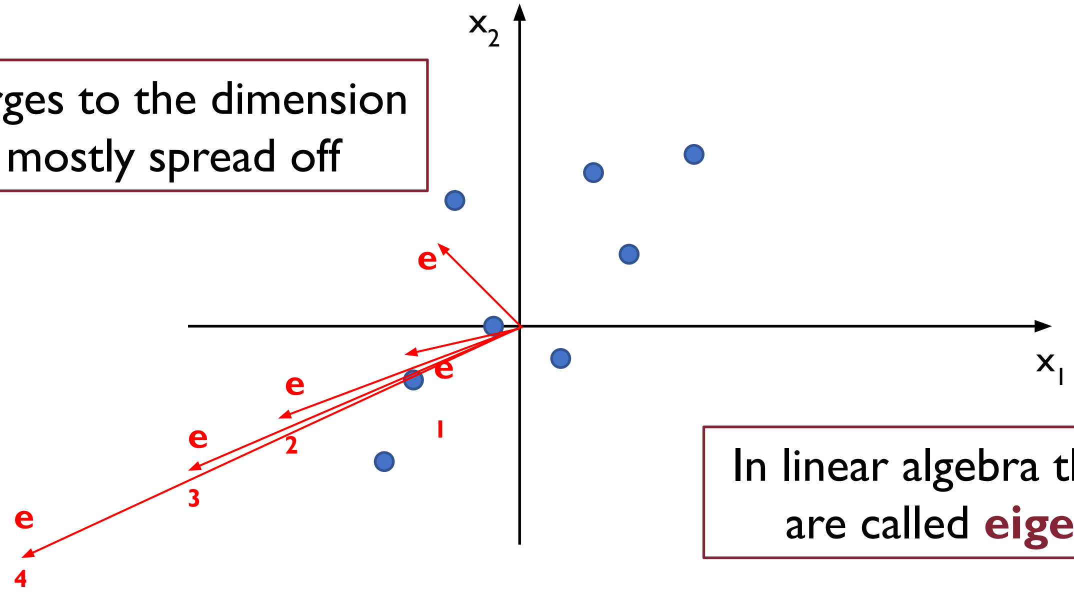
If we keep doing this the resulting vector is getting **longer** and **turns** towards the direction of the **largest variance**

The slope converges to the dimension where data is mostly spread off



In linear algebra those vectors are called **eigenvectors**

Take-Home Message of Today

- Formulate clustering as a (**non-convex**) optimization problem
  - Focus on flat partitioning (hard)

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Take-Home Message of Today

- Raw data are often embedded within high-dimensional spaces
- Dimensionality reduction techniques allow to extract "important" features
- PCA is a dimensionality reduction technique which tries to represent high-dimensional data into a low-dimensional **linear subspace**
- The intuition behind PCA is to find a change of basis so that the first component maximizes the preserved **variance** of the data
- Suggested video: https://www.youtube.com/watch?v=PFDu9oVAE-g

Fondamenti di IA

End of Lecture

04 - Unsupervised Learning

SAPIENZA
UNIVERSITÀ DI ROMA

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