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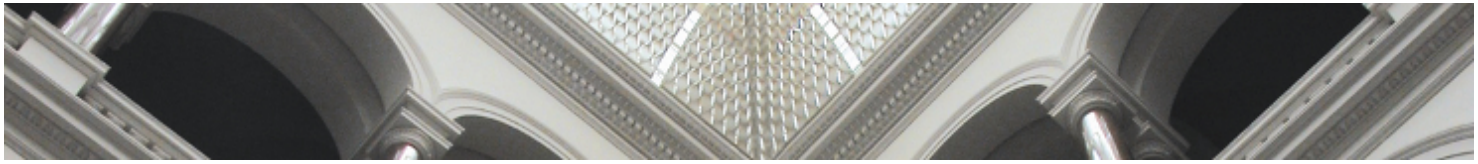
Unsupervised Learning

Malte Esders, Christopher Anders, Wojciech Samek
Technische Universität Berlin - Machine Learning Group



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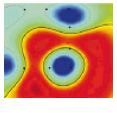
This presentation

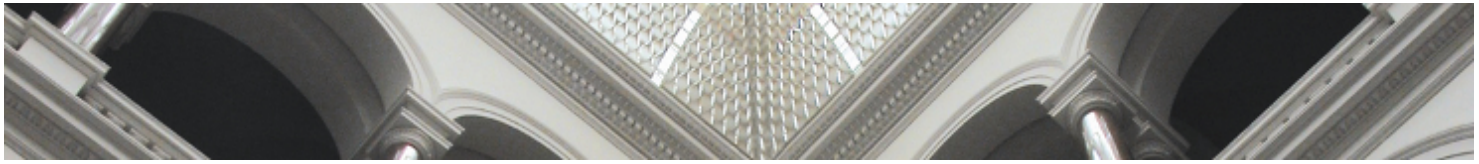
Presentation repository:

`https://github.com/Maltimore/unsupervised_learning_lecture`

Contains code to generate plots

Parts not otherwise marked: BSD licensed





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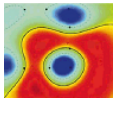

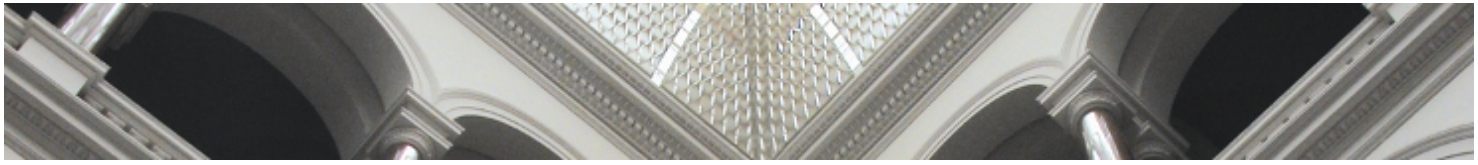

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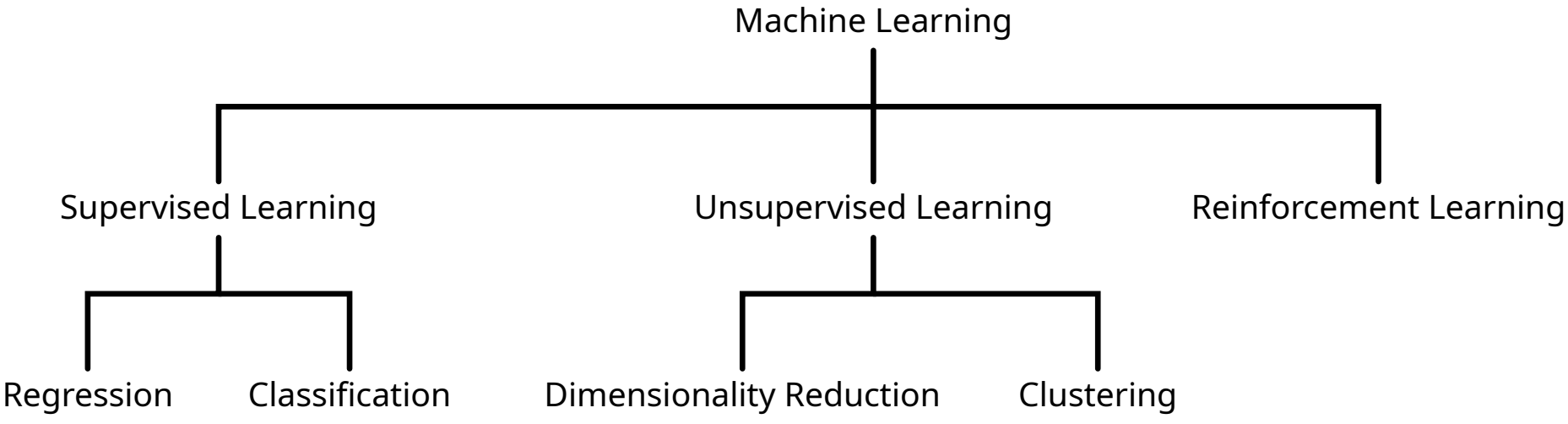

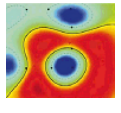

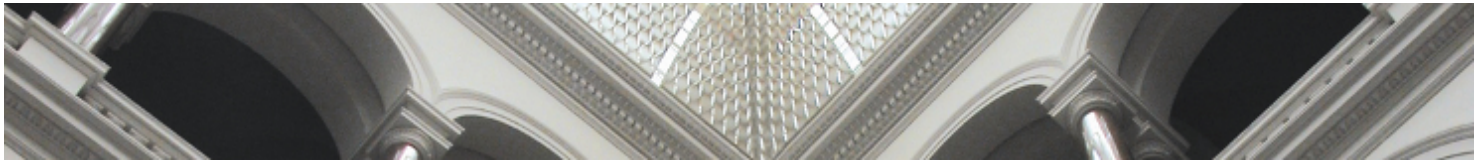

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Unsupervised Learning Motivation

> *When we're learning to see, nobody's telling us what the right answers are - we just look. Every so often, your mother says 'that's a dog', but that's very little information. You'd be lucky if you got a few bits of information - even one bit per second - that way. The brain's visual system has* 10^{14} *neural connections. And you only live for* 10^{9} *seconds. So it's no use learning one bit per second. You need more like* 10^{5} *bits per second. And there's only one place you can get that much information: from the input itself.*
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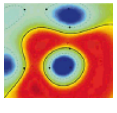
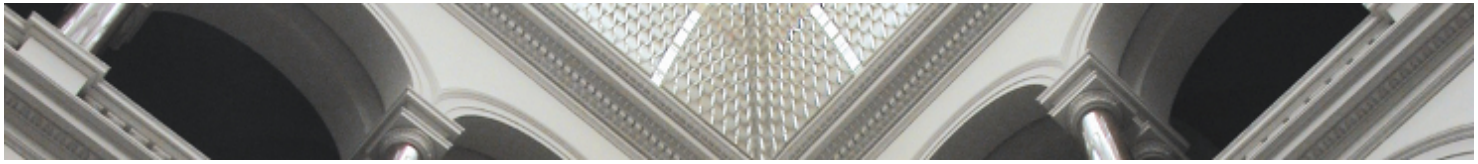
Genome: $3 * 10^{9}$ base-pairs (A, T, C, G), with 2 bits per location has $6 * 10^{9}$ bits.





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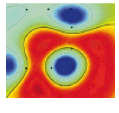
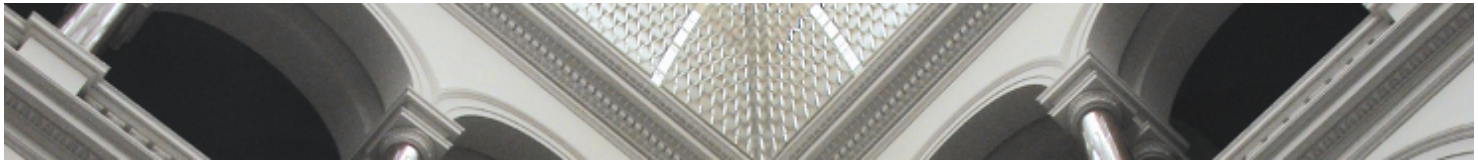
Yann LeCun's cake analogy (2016):

- Unsupervised learning is the cake itself
- Supervised learning is the icing
- Reinforcement Learning is the cherry on top





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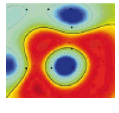
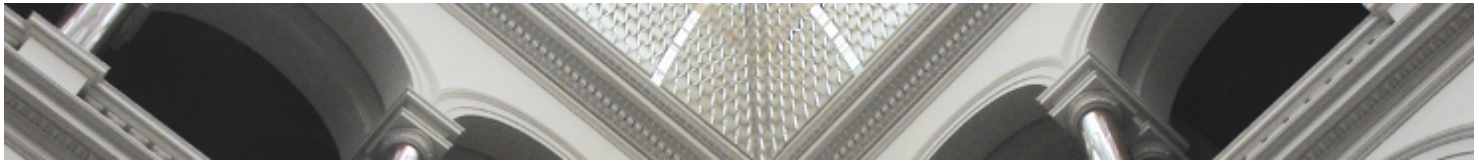
ChatGPT is unsupervised learning!





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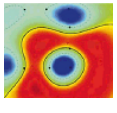

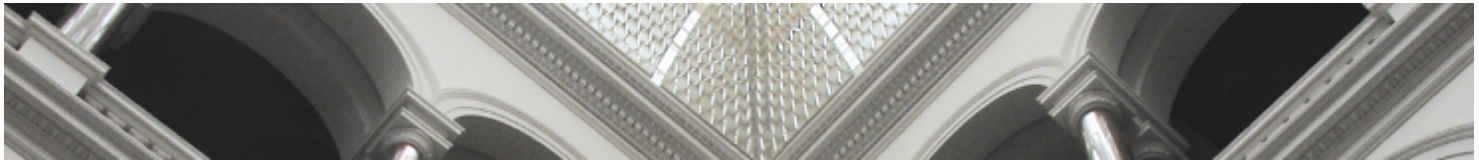

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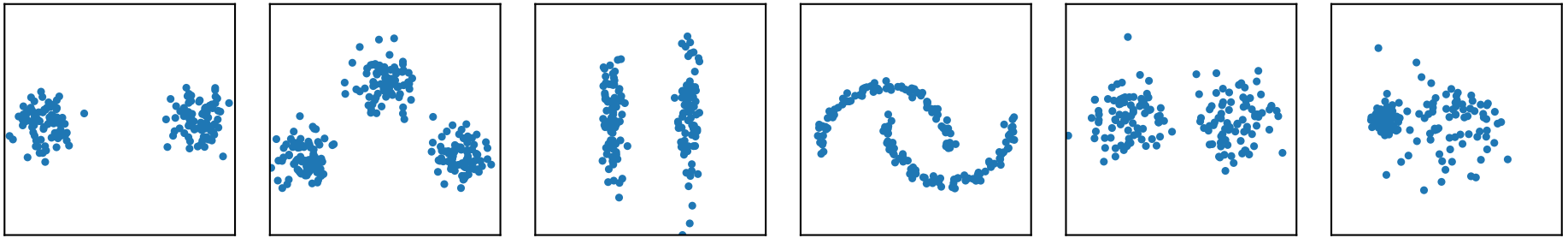
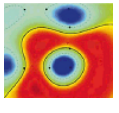
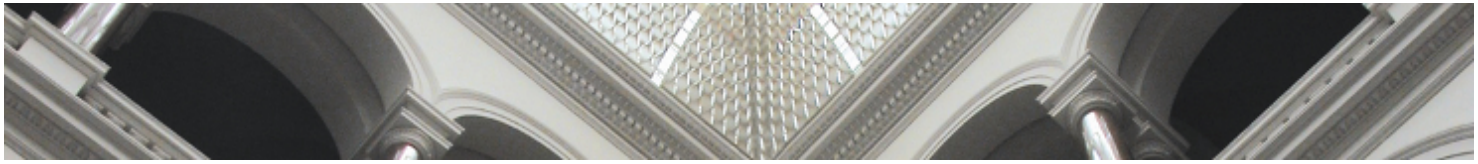
Clusters - Intuition

Without labels:







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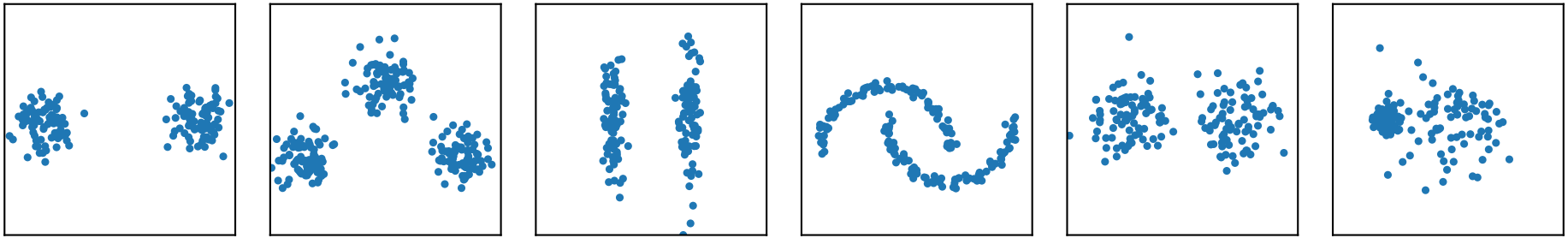
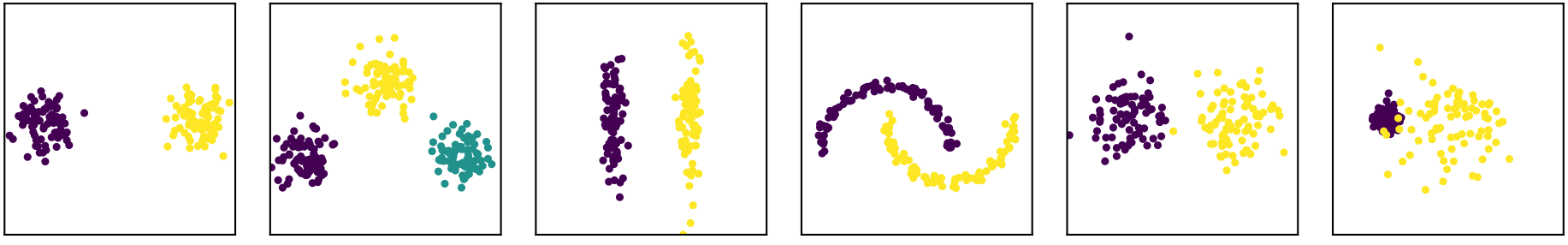
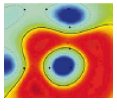
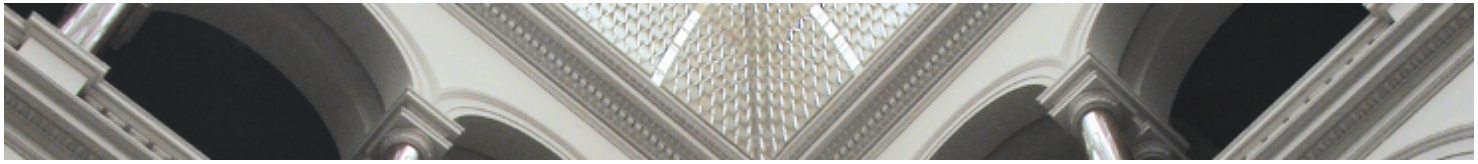


"True" clusters:



We do not have the "true" clusters with real data!





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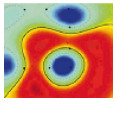
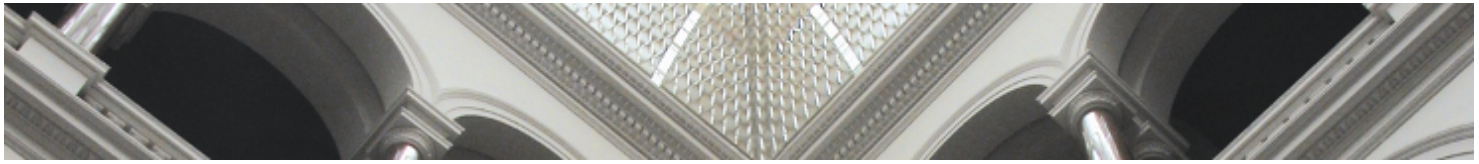
Clusters - Intuition

Clustering is an ill-posed problem: no definition of a cluster.

Some approaches:

- samples within a cluster should be “similar”, samples between clusters “different”
- clusters are regions of densely populated feature space
- samples in the same cluster come from the same underlying process





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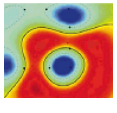

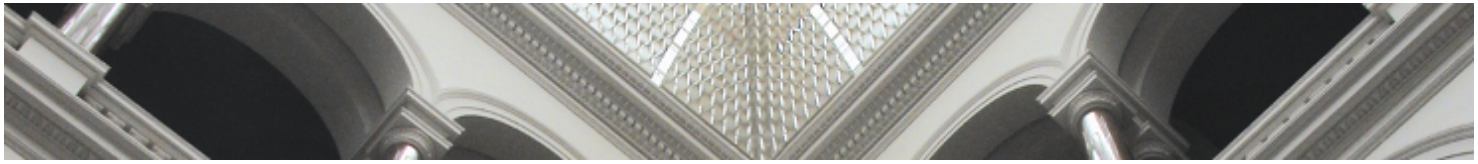

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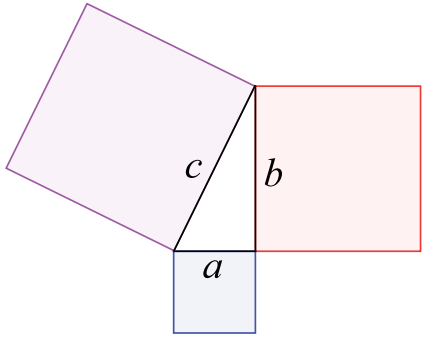
Euclidean distance

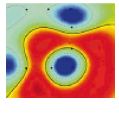
Pythagoras formula:

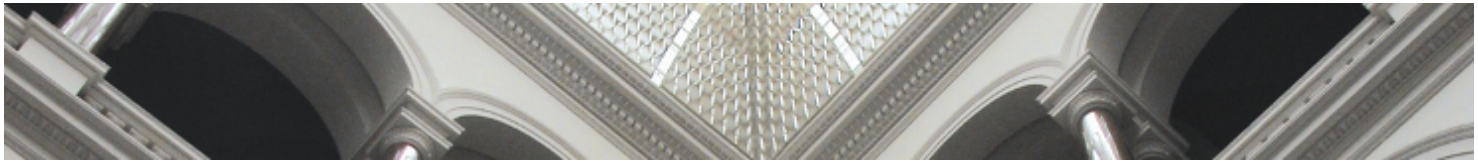
$$c^2 = a^2 + b^2$$

$$c = \sqrt{a^2 + b^2}$$



Wikipedia Pythagorean theorem





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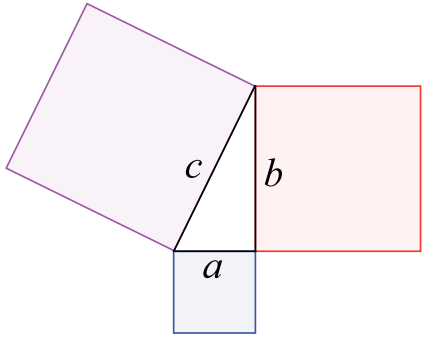

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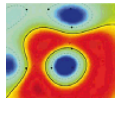

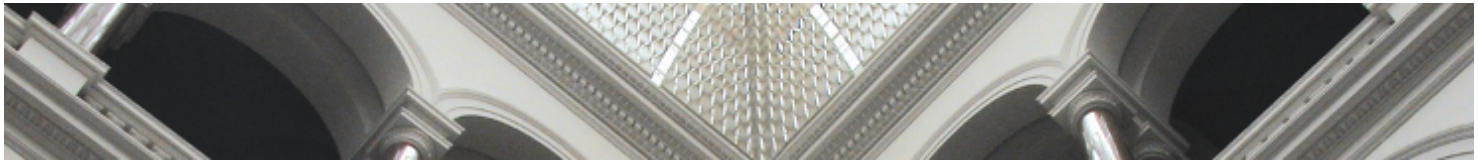

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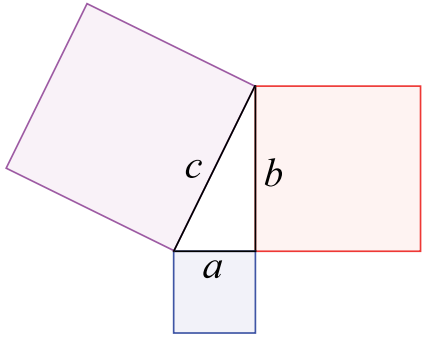

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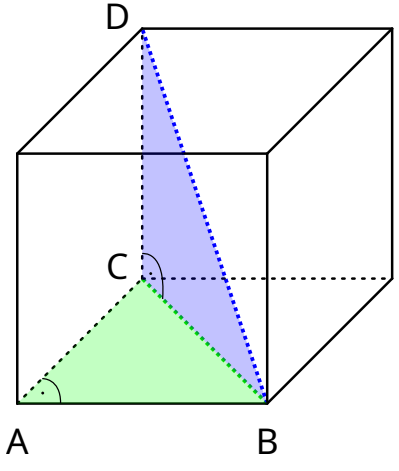

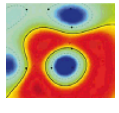

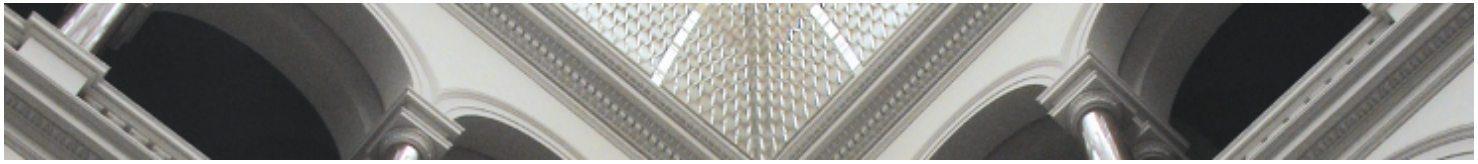

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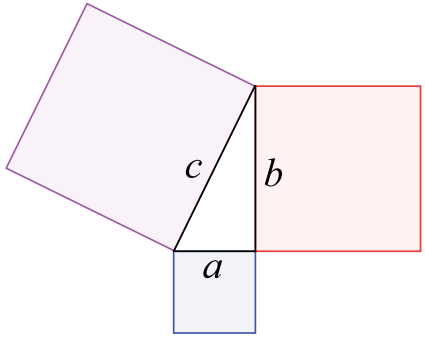

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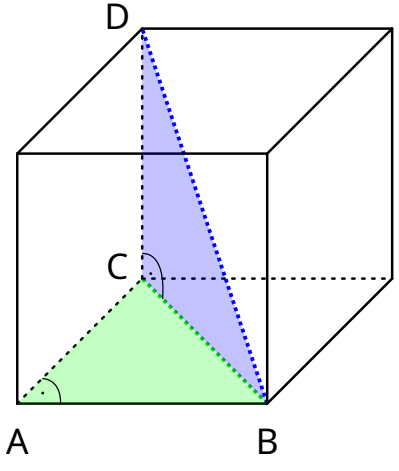

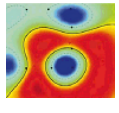

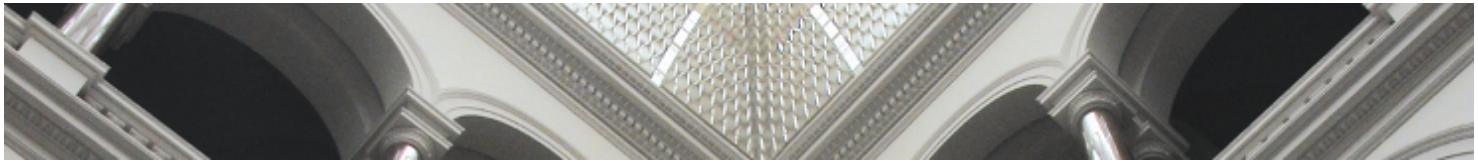

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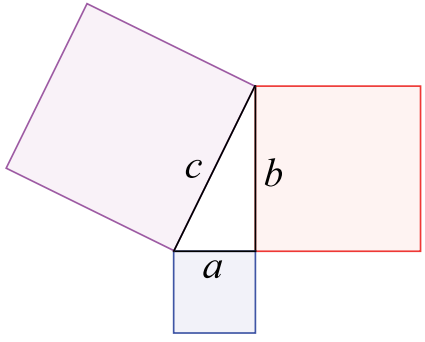

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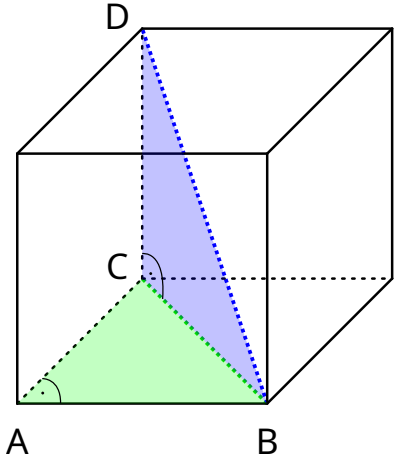

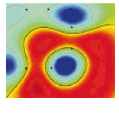

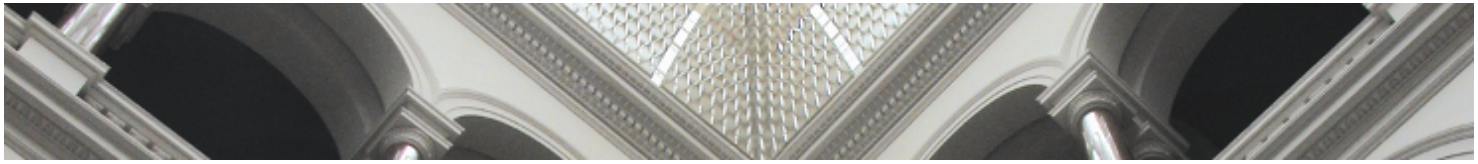

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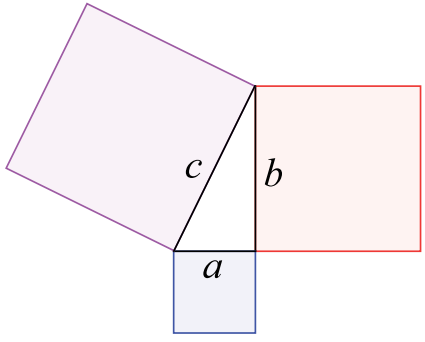
Euclidean distance

Pythagoras formula:

$$c^2 = a^2 + b^2$$

$$c = \sqrt{a^2 + b^2}$$



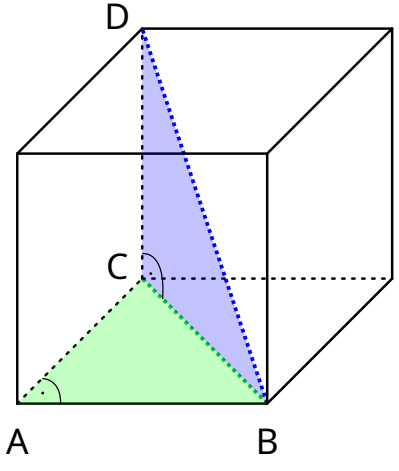
Wikipedia Pythagorean theorem

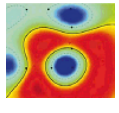
Euclidean distance notation:

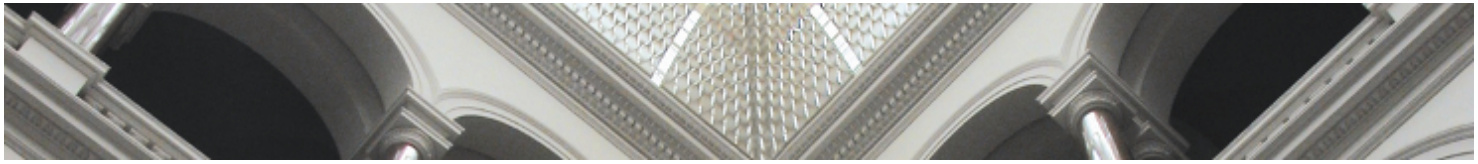
$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\Delta x_1^2 + \Delta x_2^2}$$

Euclidean distance d-D:

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\sum_{i=1}^{d} \Delta x_i^2}$$







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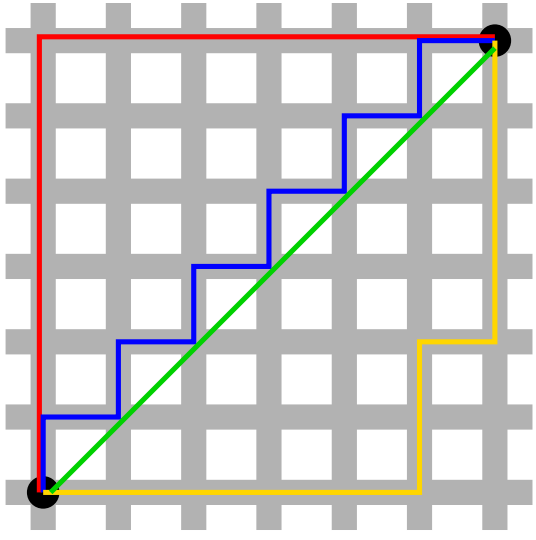
Manhattan distance

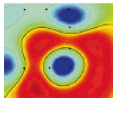
"Manhattan" / "Taxicab" distance

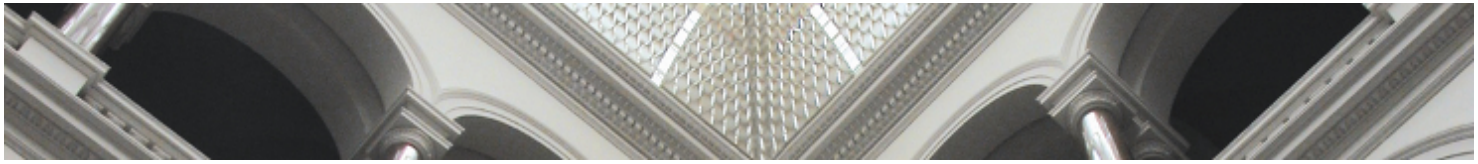
$$d(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{d} |\Delta x_i|$$

Usage: LASSO regularization



Wikipedia Manhattan distance





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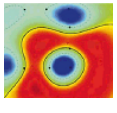
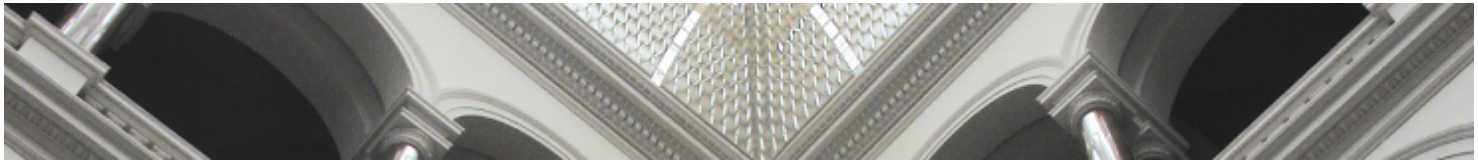
Minkowski distance

Minkowski distance generalizes Euclidean and Manhattan distance:

$$d(\boldsymbol{x}, \boldsymbol{y}) = \left(\sum_{i=1}^{d} |\Delta x_i|^p \right)^{1/p}$$





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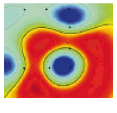
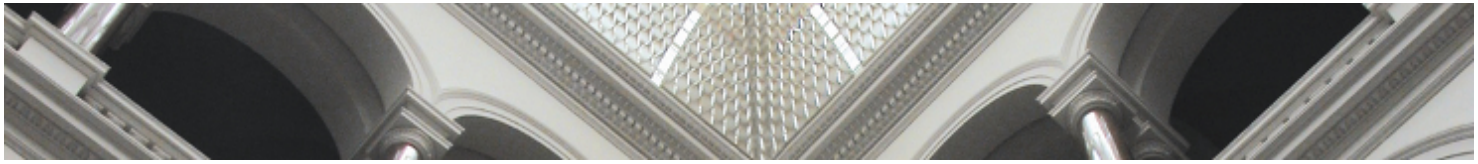
$p = 1$: Manhattan distance

$p = 2$: Euclidean distance





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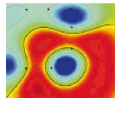

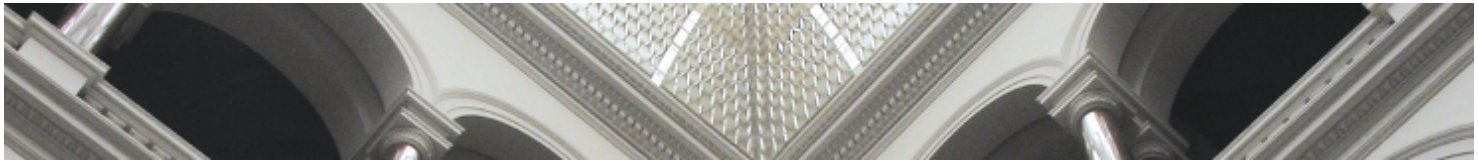

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$p = \infty$:

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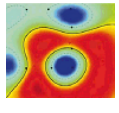
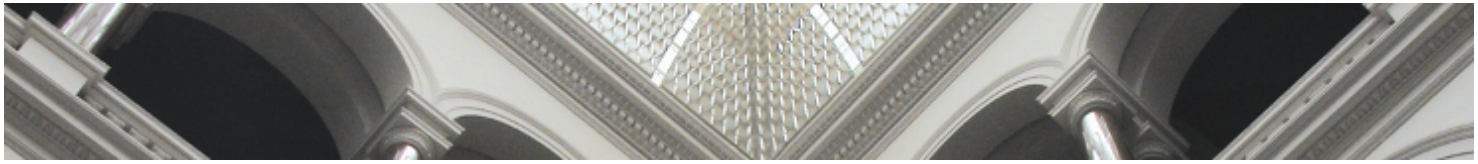
$p \to 0$:

$$d(\boldsymbol{x}, \boldsymbol{y}) = \min_i |\Delta x_i|$$





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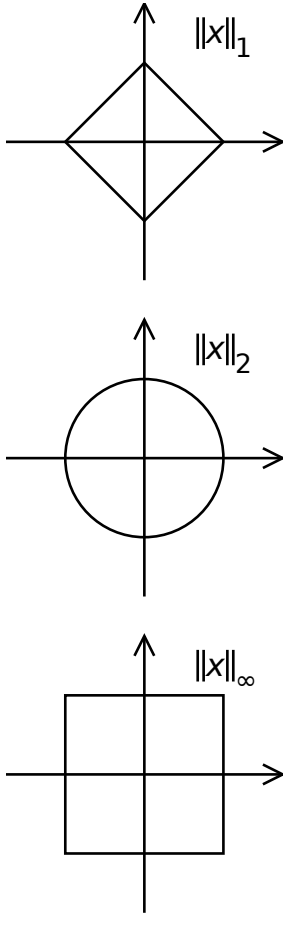
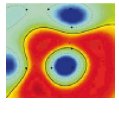
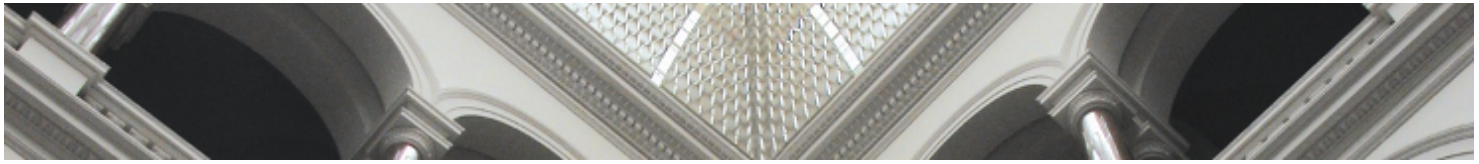


Wikipedia Norm (mathematics)





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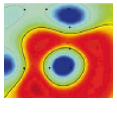

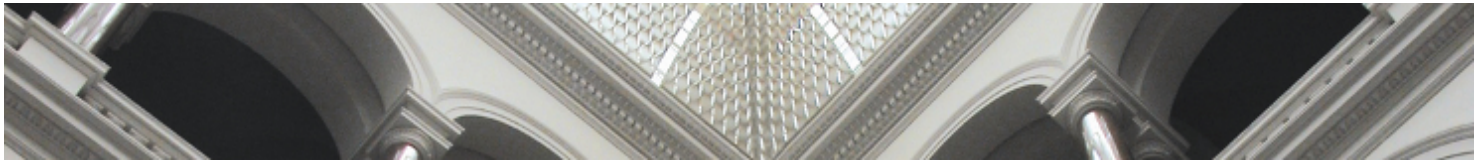

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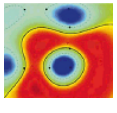
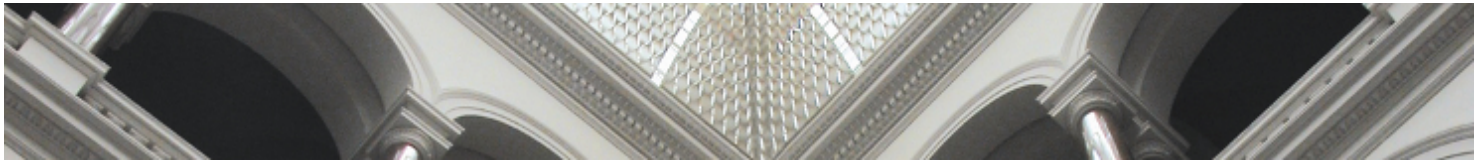
Vector norm

The distance between vectors is the vector-norm of their difference:

$$d(\boldsymbol{x}, \boldsymbol{y}) = \left(\sum_{i=1}^{d} |\Delta x_i|^p \right)^{1/p} = ||\boldsymbol{x} - \boldsymbol{y}||_p$$





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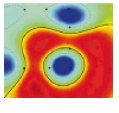
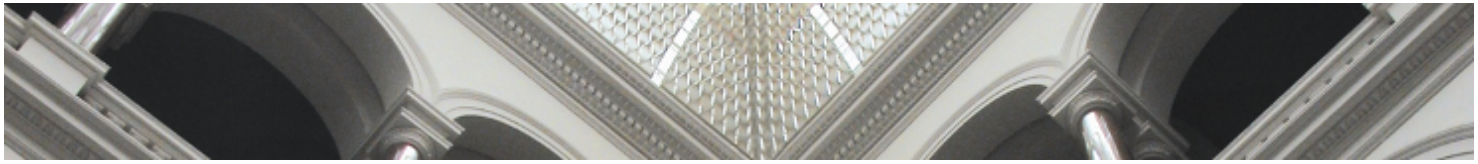
For $p = 2$, the shorthand is:

$$||\boldsymbol{x} - \boldsymbol{y}||_2 = ||\boldsymbol{x} - \boldsymbol{y}||$$





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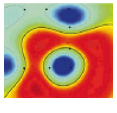
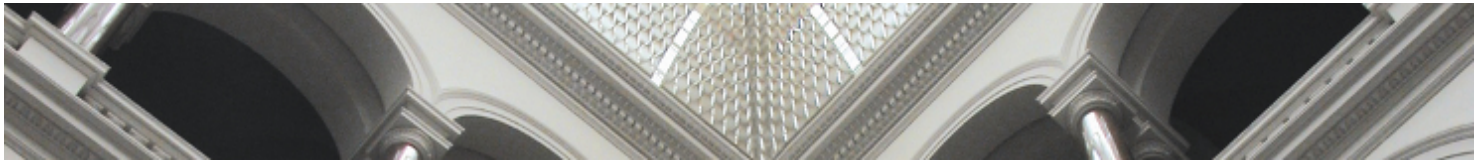
Squared euclidean distance

Squared euclidean distance:

$$||\boldsymbol{x} - \boldsymbol{y}||_2^2 = \sum_{i=1}^{d} |\Delta x_i|^2$$





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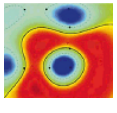
Squared euclidean distance

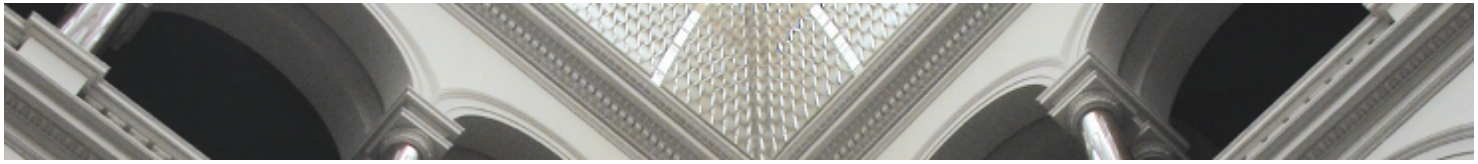
Squared euclidean distance:

$$||\boldsymbol{x} - \boldsymbol{y}||_2^2 = \sum_{i=1}^{d} |\Delta x_i|^2$$

Do not confuse

$$||\boldsymbol{x} - \boldsymbol{y}|| = ||\boldsymbol{x} - \boldsymbol{y}||_2 \neq ||\boldsymbol{x} - \boldsymbol{y}||^2 = ||\boldsymbol{x} - \boldsymbol{y}||_2^2$$





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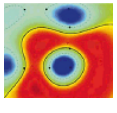
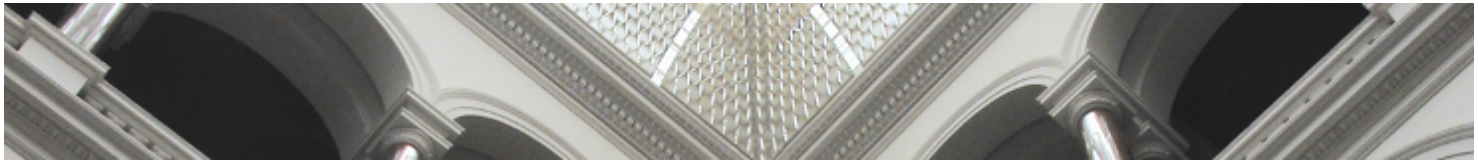
Squared Euclidean distance:

- not a true metric (no triangle inequality)
- overemphasizes big distances (and vice versa)
- makes some optimization problems converge better





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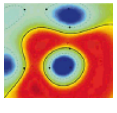

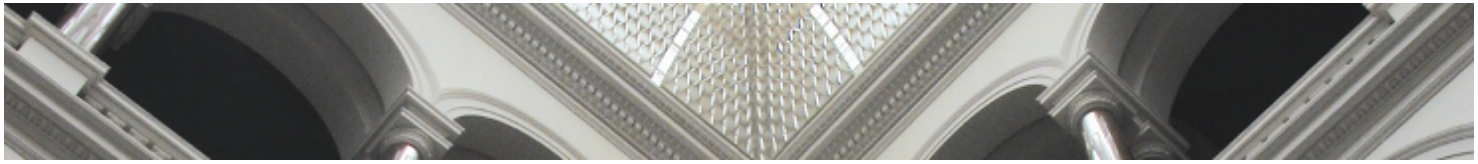

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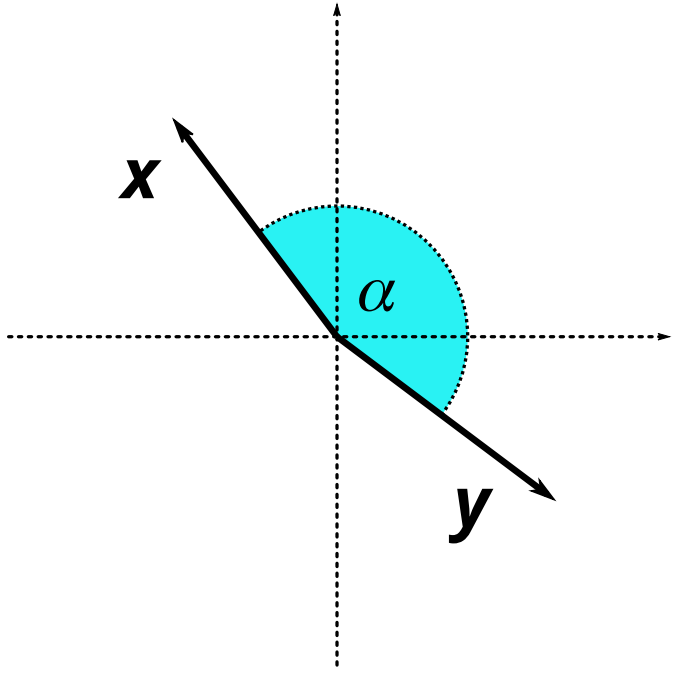
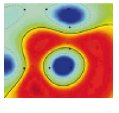
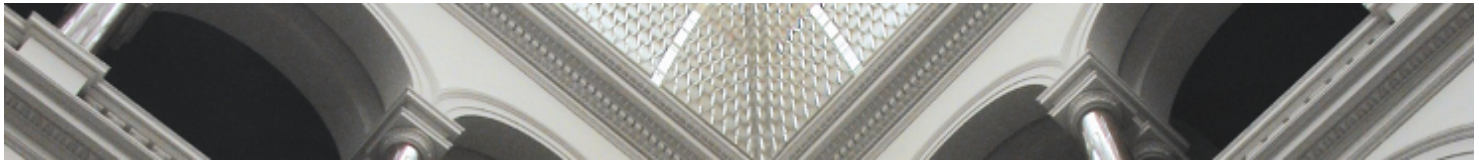
Cosine distance

Cosine distance only compares angles between vectors.







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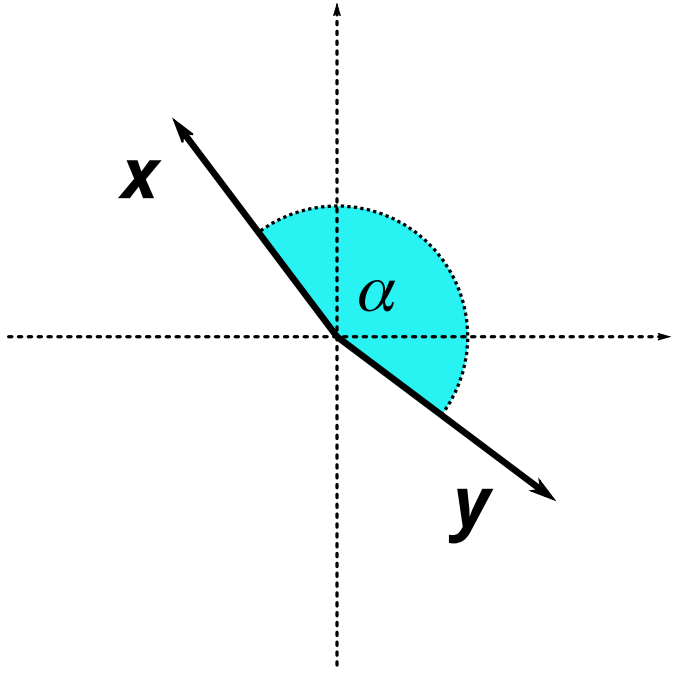
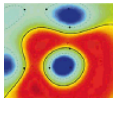
Cosine distance only compares angles between vectors.

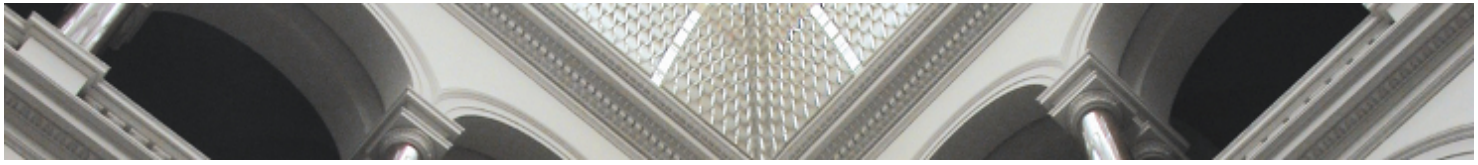
Cosine definition:

$$\boldsymbol{x}^\mathsf{T}\boldsymbol{y} = |\boldsymbol{x}||\boldsymbol{y}|cos(\alpha)$$

$$cos(\alpha) = \frac{\boldsymbol{x}^\mathsf{T}\boldsymbol{y}}{|\boldsymbol{x}||\boldsymbol{y}|}$$







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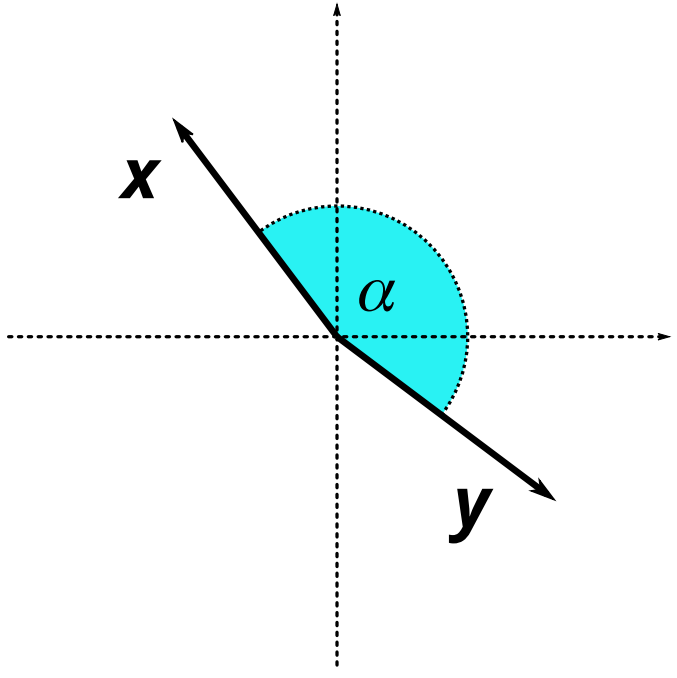
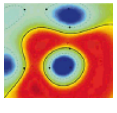
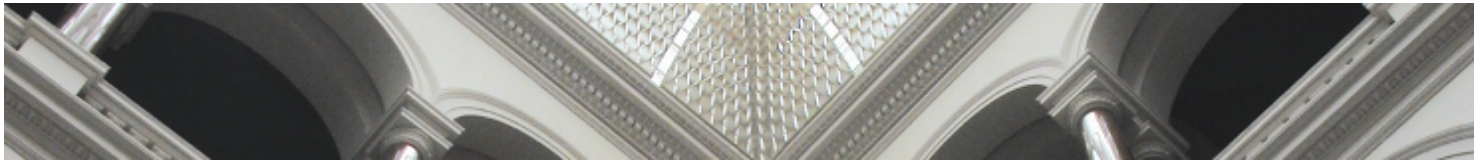
Cosine distance:

$$d(\boldsymbol{x}, \boldsymbol{y}) = 1 - \frac{\boldsymbol{x}^\mathsf{T}\boldsymbol{y}}{|\boldsymbol{x}||\boldsymbol{y}|}$$







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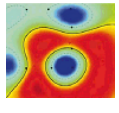

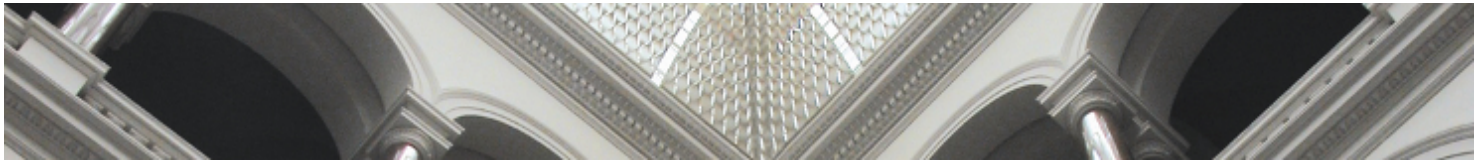

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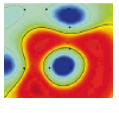
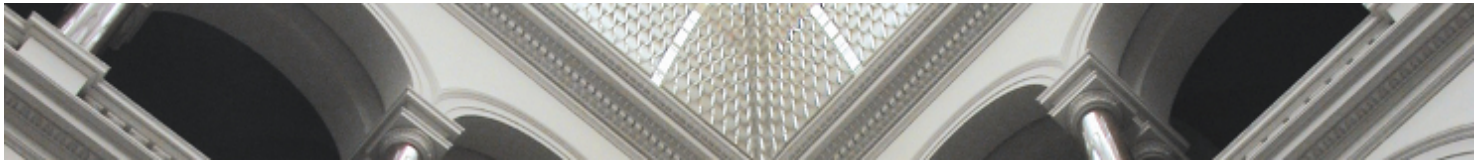
Different scales

Measurements can be at different scales (for instance cm, kg etc.)

We can normalize:

$$z = \frac{x - \mu}{\sigma}$$





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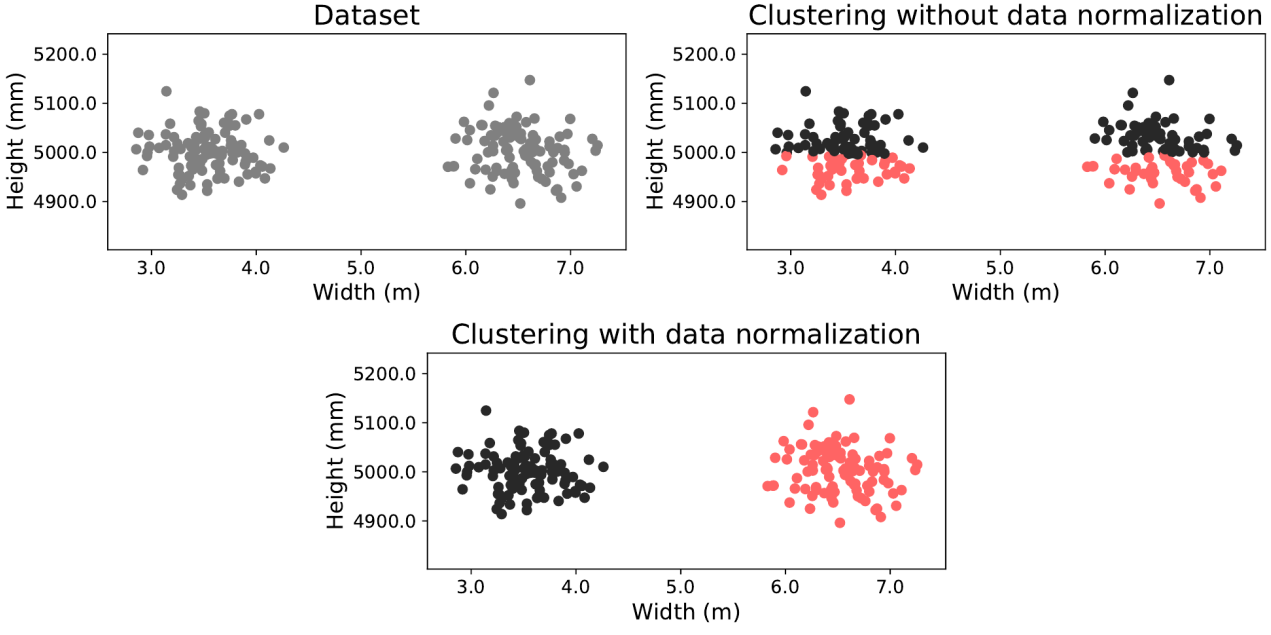
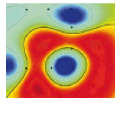
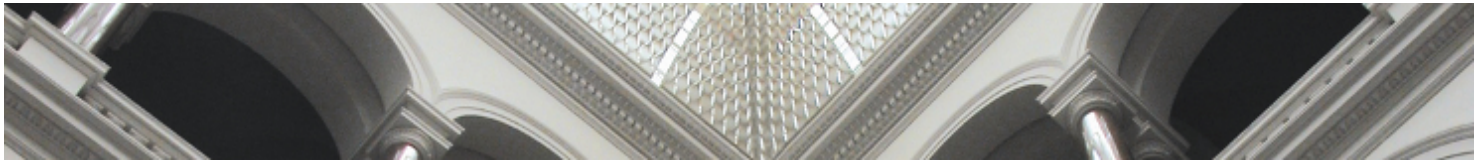
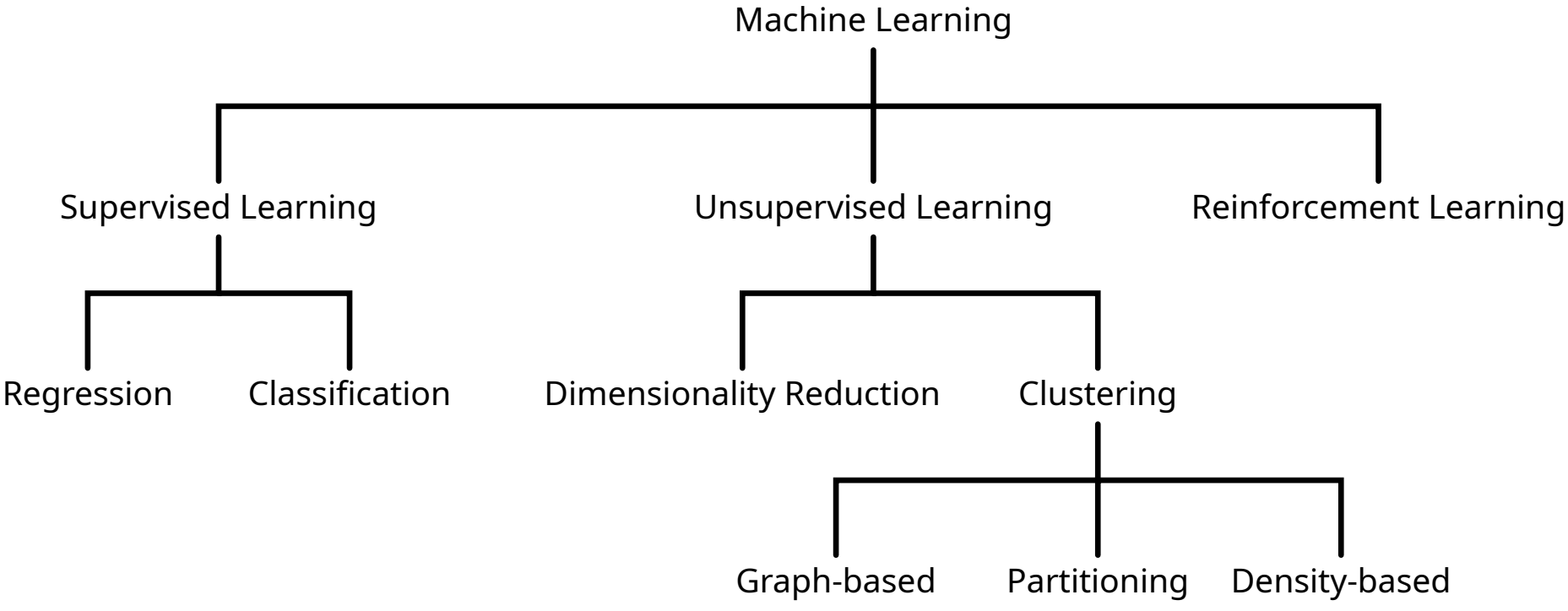
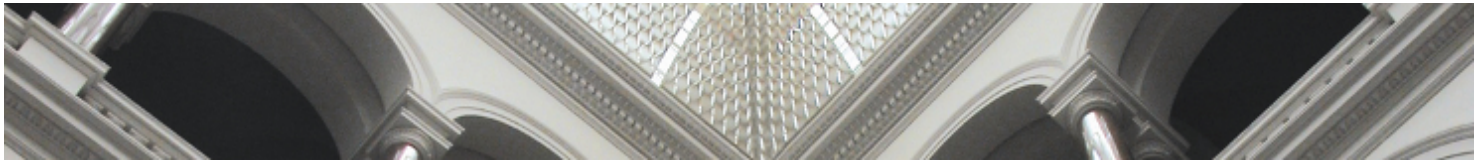


Guérin et al. 2017






Machine Learning
Supervised Learning
Unsupervised Learning
Reinforcement Learning
Regression
Classification
Dimensionality Reduction
Clustering
Graph-based
Partitioning
Density-based



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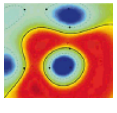

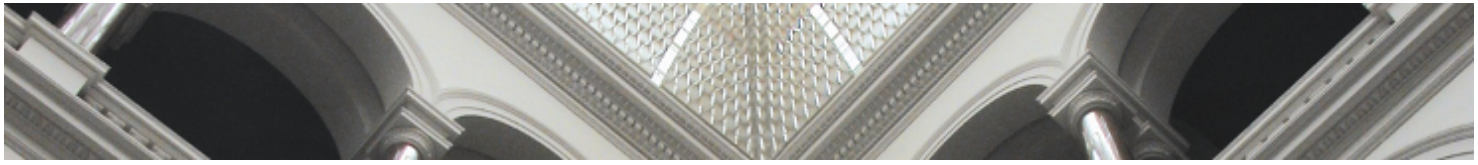

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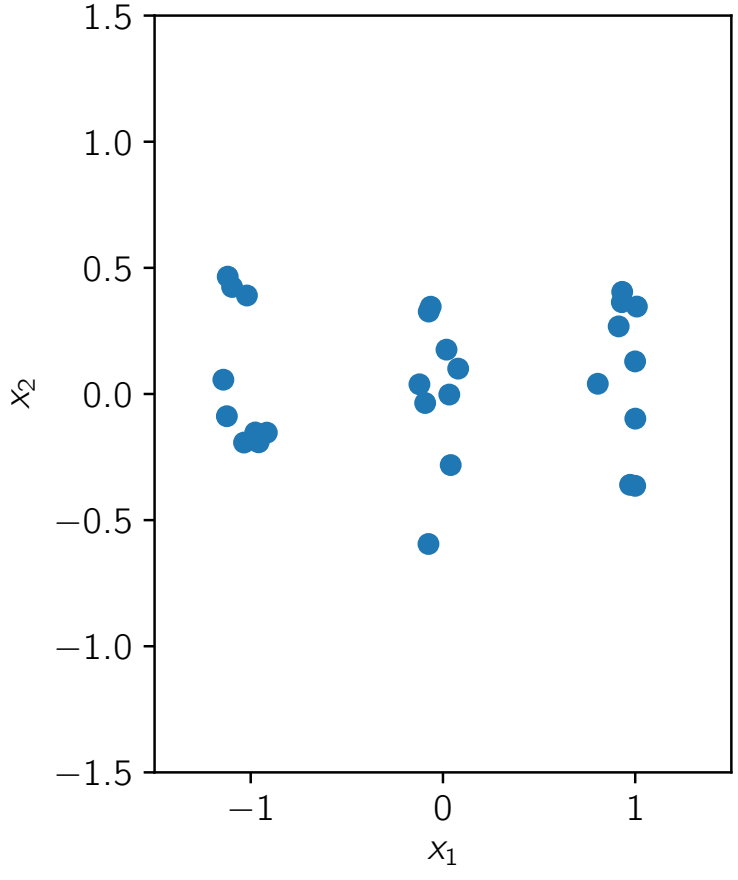
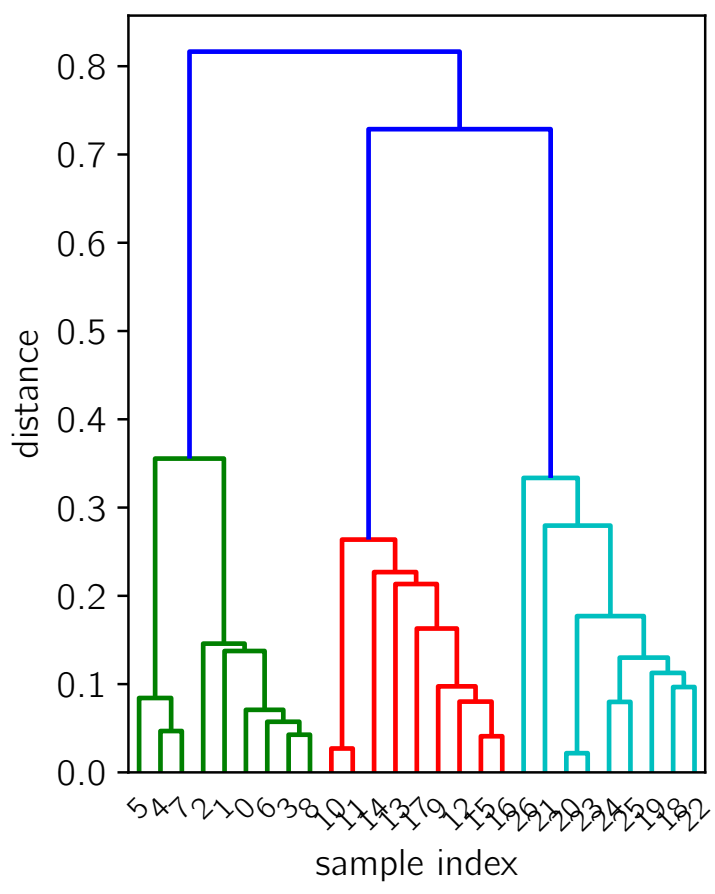
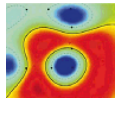
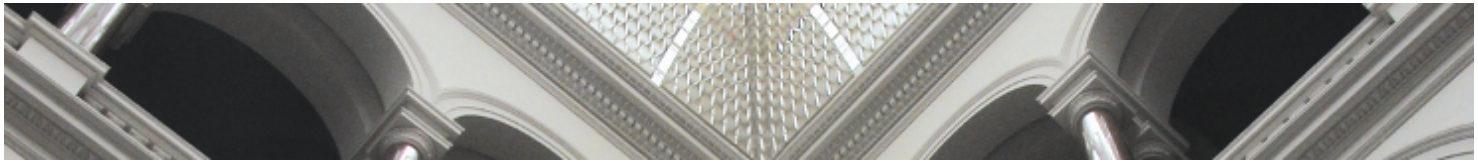
Dendrogram with Euclidean distance









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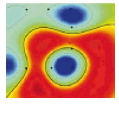
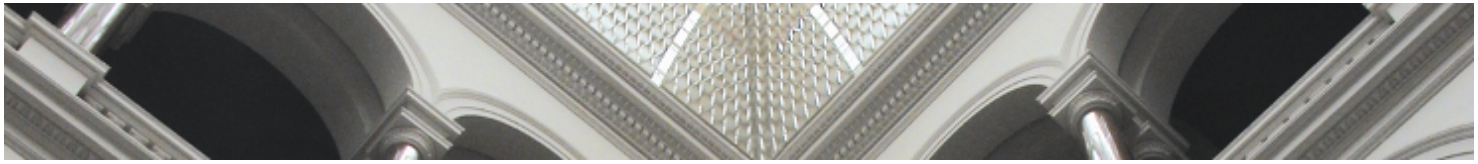
Hierarchical Clustering

– graph-based (no embedding needed!)





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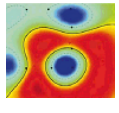
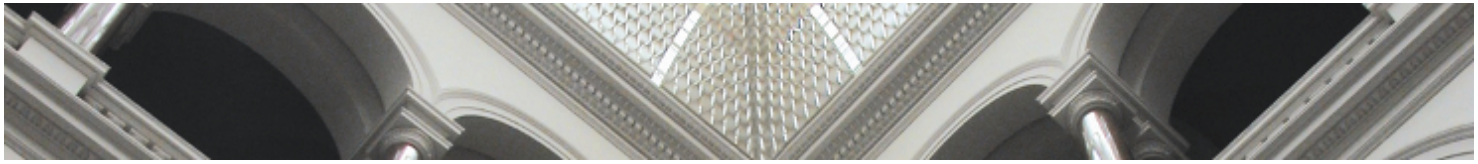
Hierarchical Clustering

- graph-based (no embedding needed!)
- builds a hierarchy of clusters, either top down (“divisive”) or bottom up (“agglomerative”)





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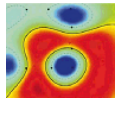
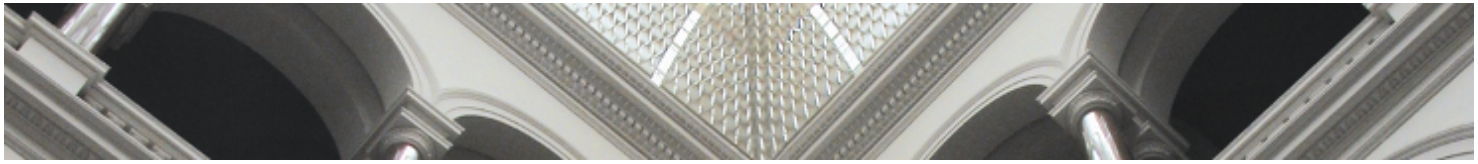
Hierarchical Clustering

- graph-based (no embedding needed!)
- builds a hierarchy of clusters, either top down (“divisive”) or bottom up (“agglomerative”)
- intuitive





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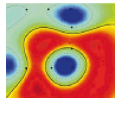
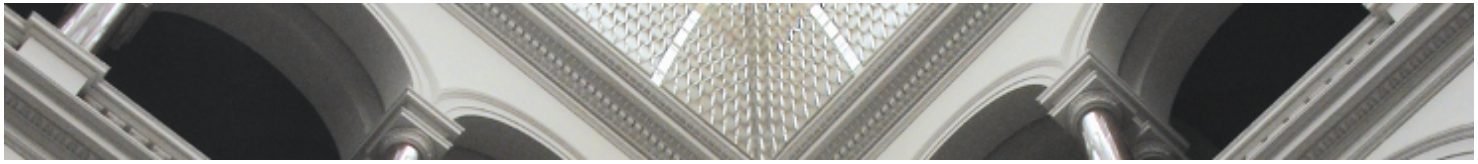
Hierarchical Clustering

- graph-based (no embedding needed!)
- builds a hierarchy of clusters, either top down (“divisive”) or bottom up (“agglomerative”)
- intuitive
- suggests numbers of clusters





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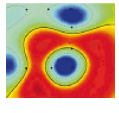
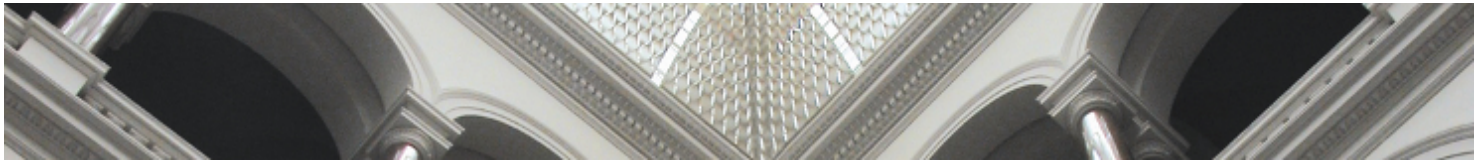
- intuitive
- suggests numbers of clusters
- arbitrary cluster shapes





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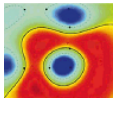
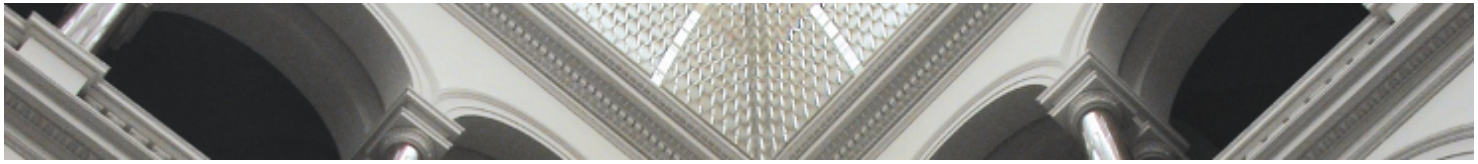
Hierarchical Clustering

- graph-based (no embedding needed!)
- builds a hierarchy of clusters, either top down (“divisive”) or bottom up (“agglomerative”)
- intuitive
- suggests numbers of clusters
- arbitrary cluster shapes
- sensitive to noise





Agglomerative clustering algorithm:

Let $\mathcal{D}_i$ be the sets containing the samples in cluster i.

choose n_{final} clusters

initialize $\mathcal{D}_i$ as singleton clusters

initialize $n_{clusters} = n_{samples}$

while $n_{clusters} > n_{final}$ **do**

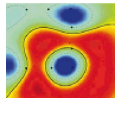
  find clusters i and j with smallest distance

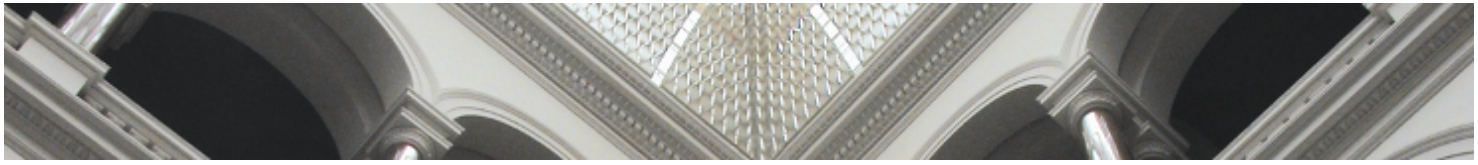
  merge $\mathcal{D}_i$ and $\mathcal{D}_j$

  $n_{clusters} \leftarrow n_{clusters} - 1$

end

return clusters





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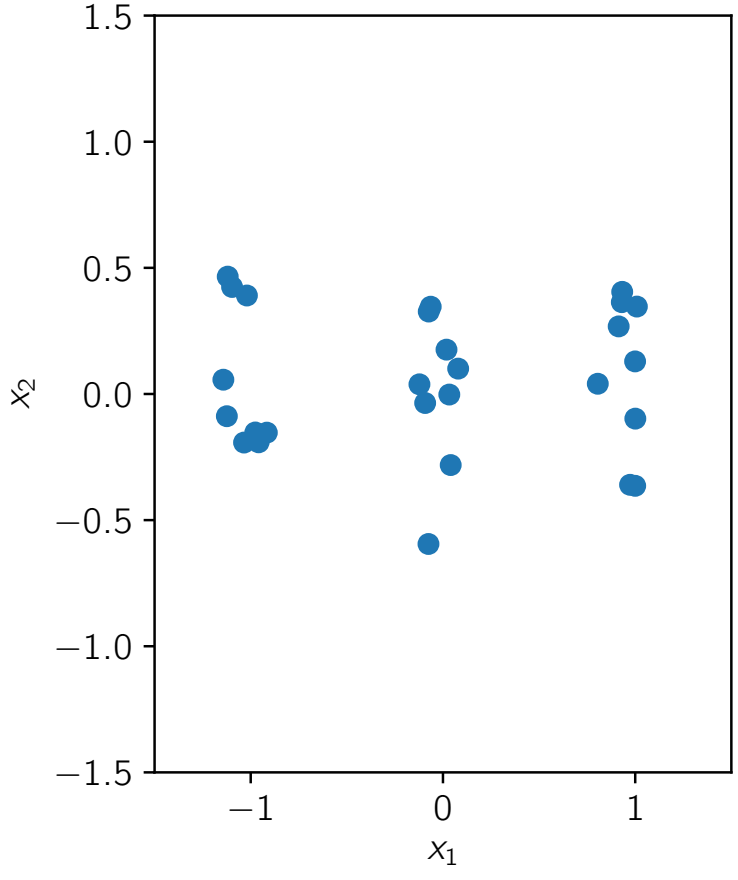

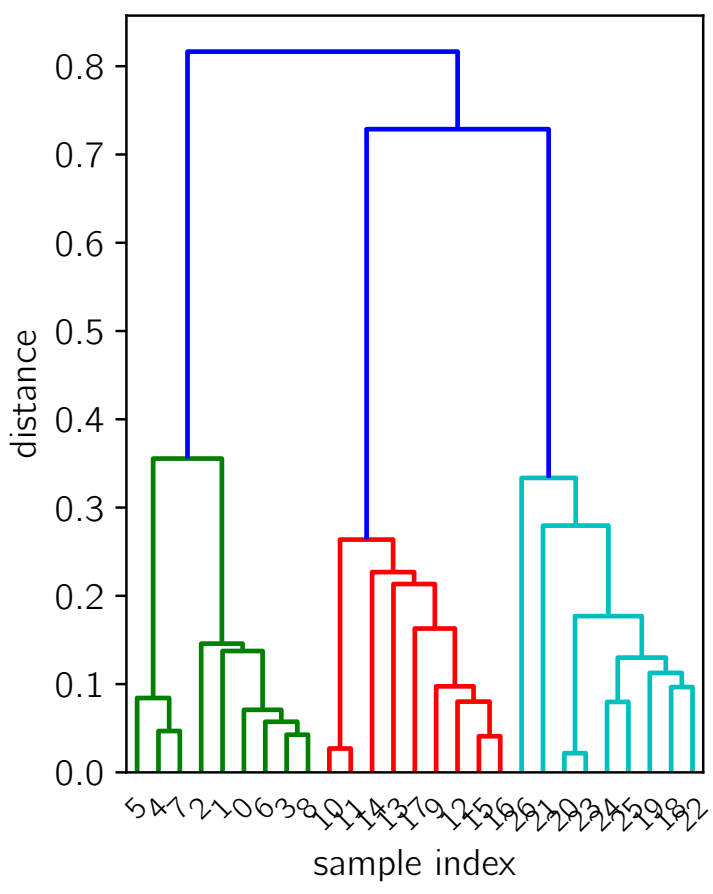

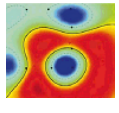

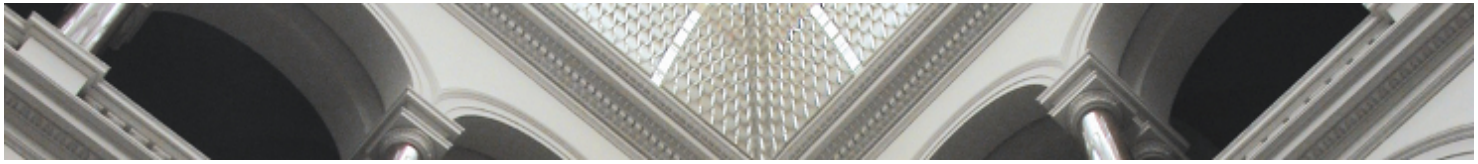

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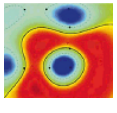
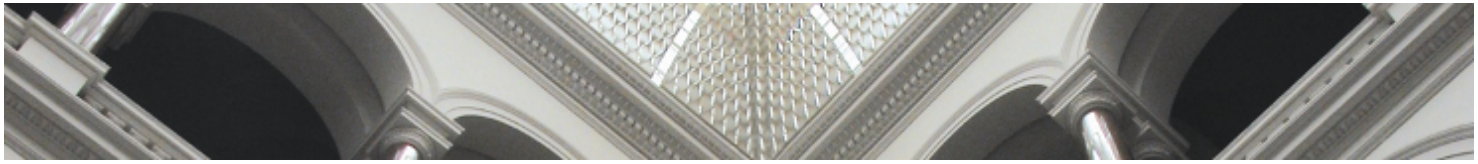
Cluster distance measures

Let $\mathcal{D}_i$, $\mathcal{D}_j$ be the sets containing the samples in clusters *i* and *j*.

Minimum linkage:

$$d_{min}(\mathcal{D}_i, \mathcal{D}_j) = \min_{\boldsymbol{x} \in \mathcal{D}_i, \boldsymbol{x}' \in \mathcal{D}_j} ||\boldsymbol{x} - \boldsymbol{x}'||$$





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Maximum or “complete” linkage:

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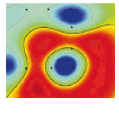

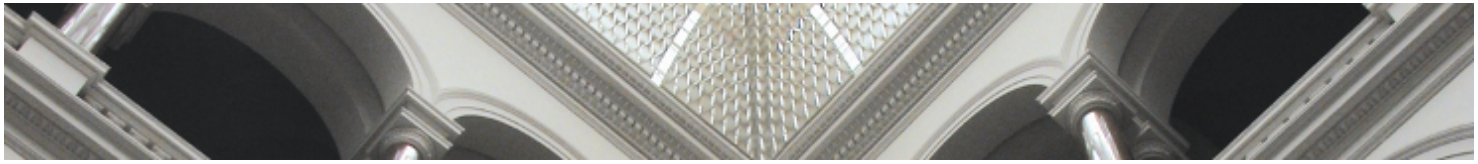

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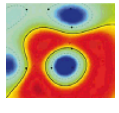
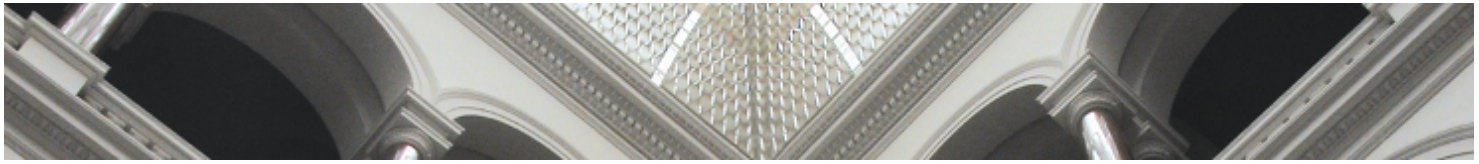
Average linkage:

$$d_{avg}(\mathcal{D}_i, \mathcal{D}_j) = \frac{1}{n_i n_j} \sum_{\boldsymbol{x} \in \mathcal{D}_i} \sum_{\boldsymbol{x}' \in \mathcal{D}_j} ||\boldsymbol{x} - \boldsymbol{x}'||$$

Notation from Duda, Hart, and Stork 2012





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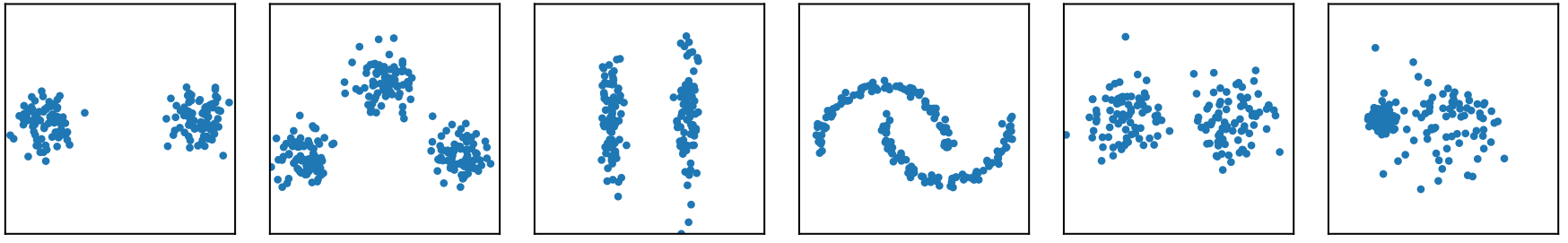
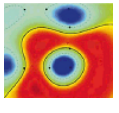
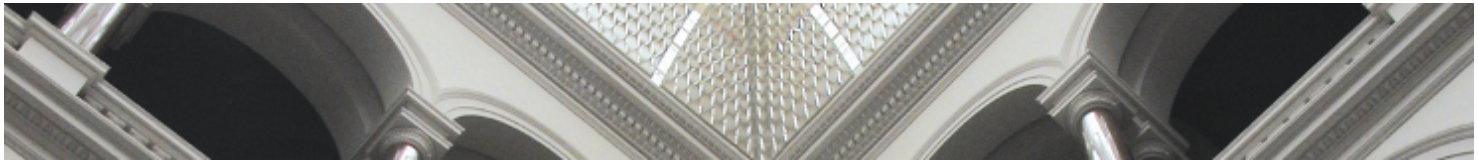
Original data

After clustering, assignments can seem “natural”, good to compare original data:







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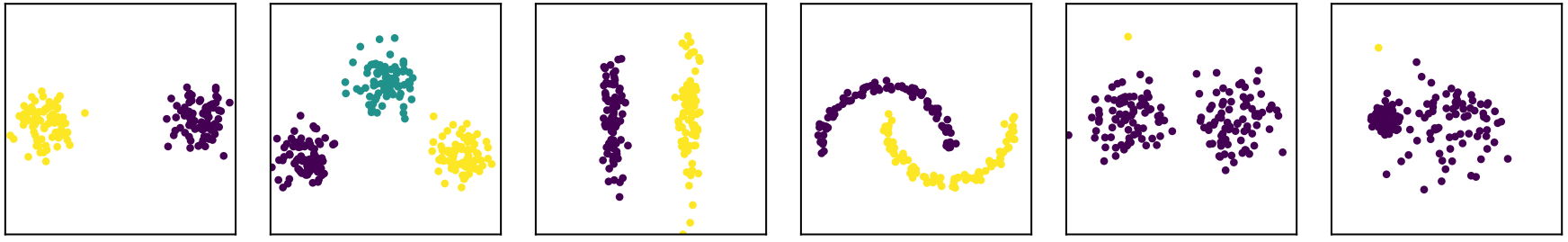
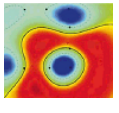
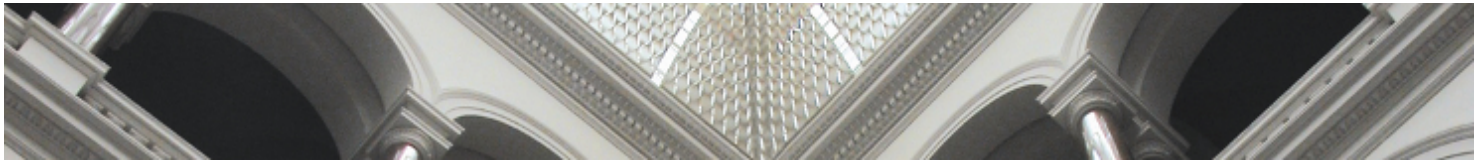
Agglomerative clustering results

Minimum







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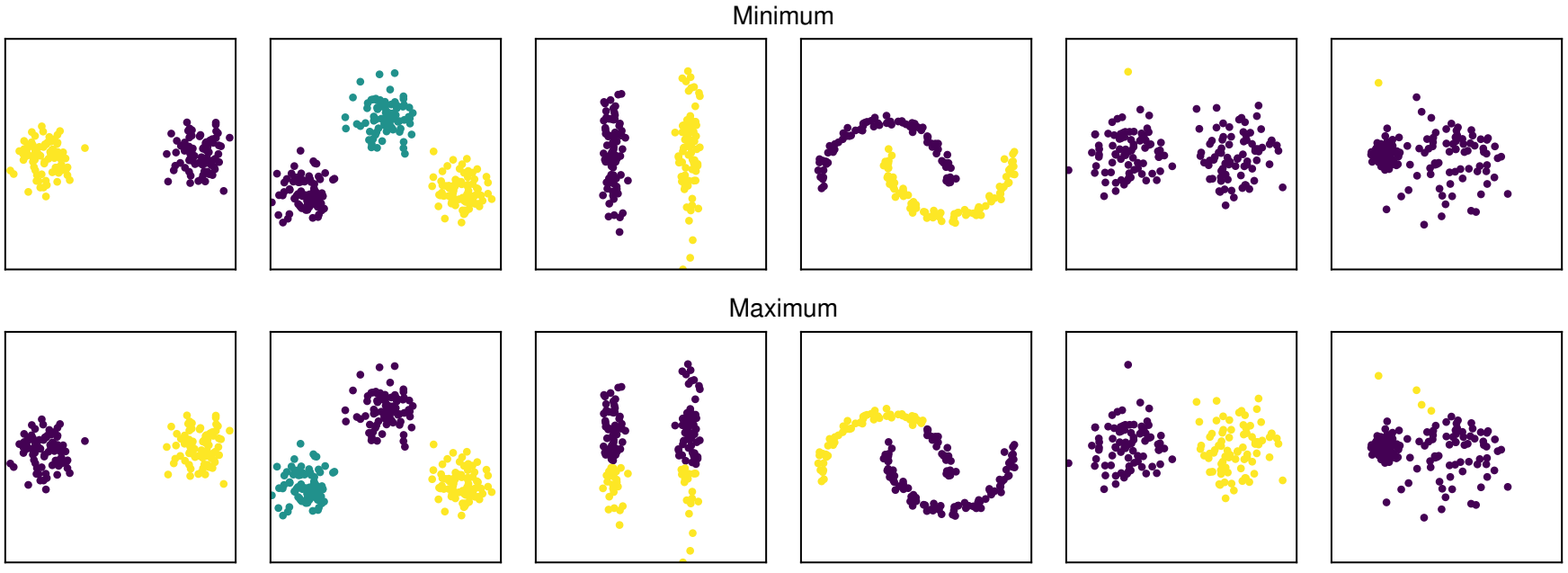
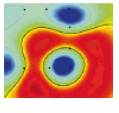
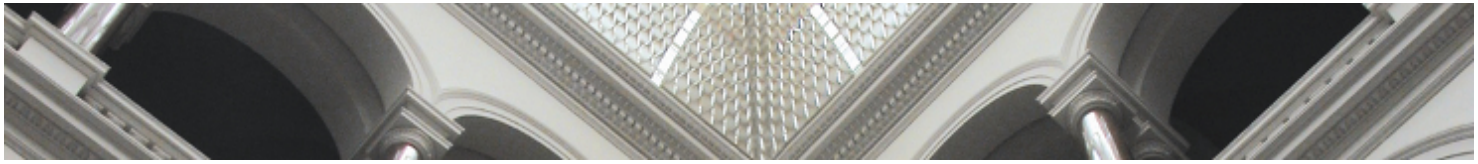
Agglomerative clustering results







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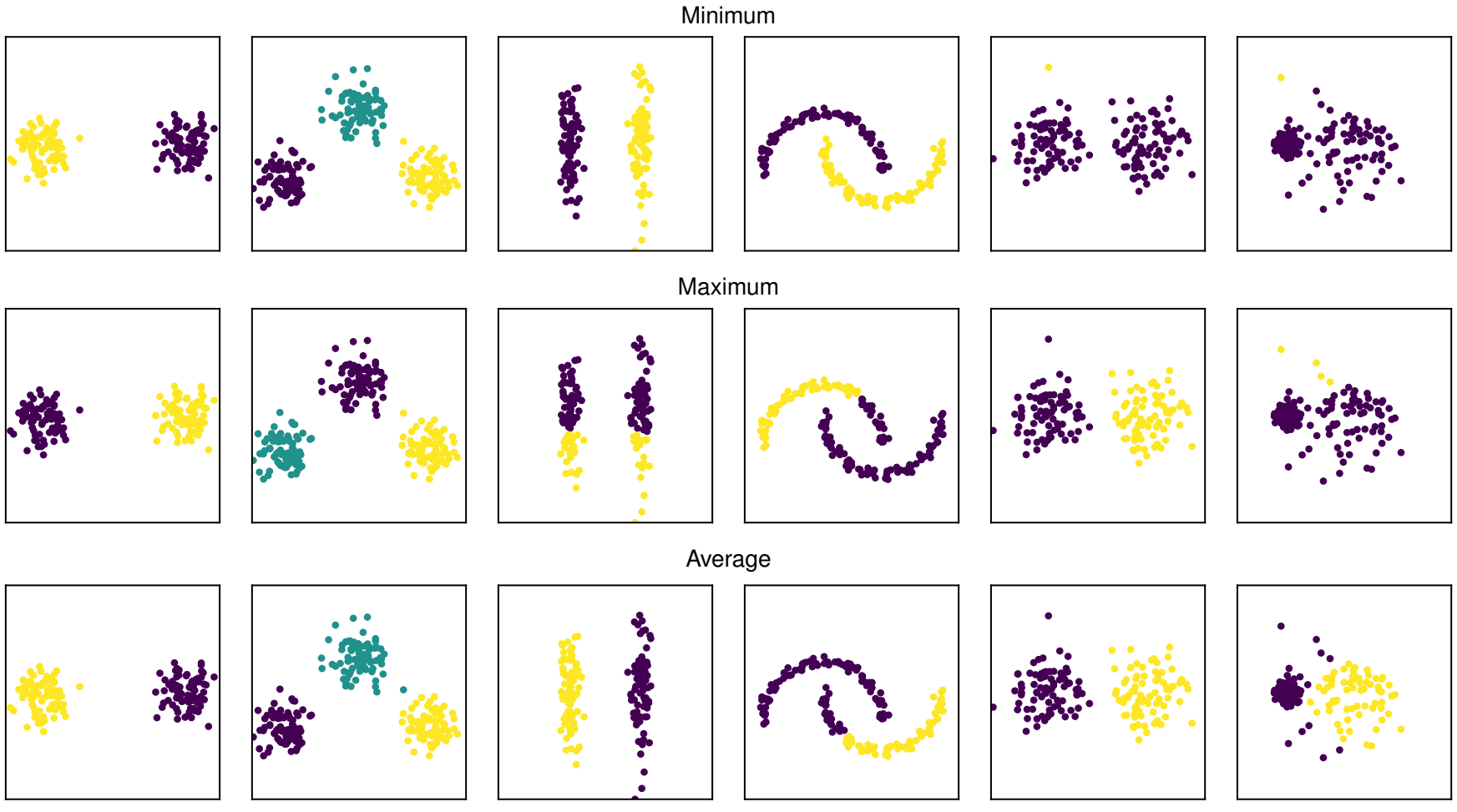

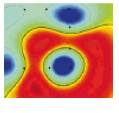

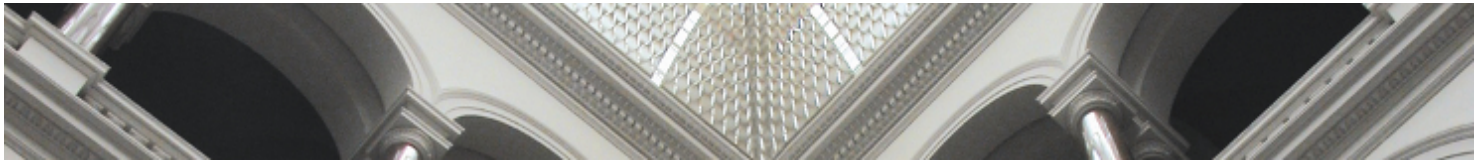

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Tips and tricks

class `sklearn.cluster.` **`AgglomerativeClustering`** (*n_clusters=2, affinity='euclidean', memory=None, connectivity=None, compute_full_tree='auto', linkage='ward', pooling_func=<function mean>*) [source]

Agglomerative Clustering

Recursively merges the pair of clusters that minimally increases a given linkage distance.

Read more in the User Guide.

Parameters: **n_clusters** : int, default=2

The number of clusters to find.

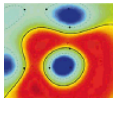
affinity : string or callable, default: "euclidean"

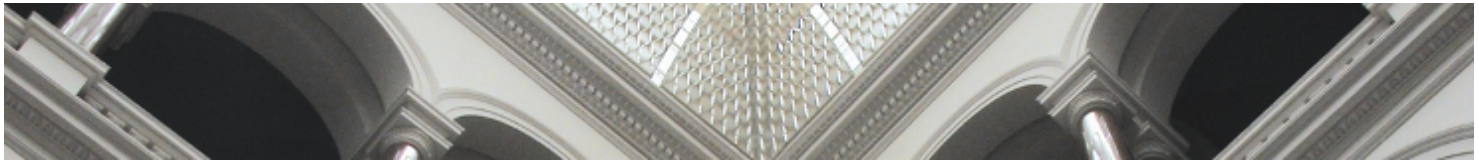
Metric used to compute the linkage. Can be "euclidean", "l1", "l2", "manhattan", "cosine", or 'precomputed'. If linkage is "ward", only "euclidean" is accepted.

Sometimes, documentation can be confusing:

What is the difference between "l2" and "euclidean"?

Or "l1" and "manhattan"?





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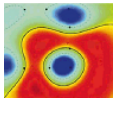
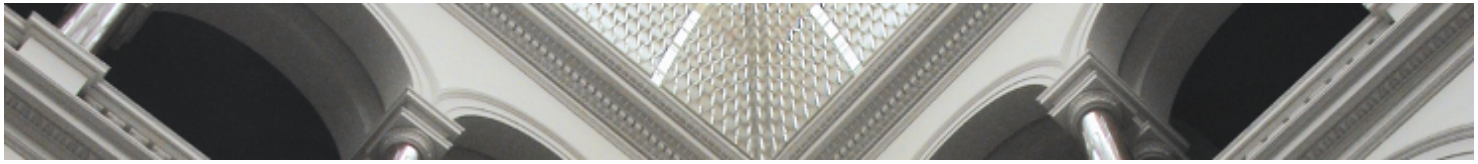
Tips and tricks

Looking into the code:

```
408             elif affinity == 'l2':
409                 # Translate to something understood by scipy
410                 affinity = 'euclidean'
411             elif affinity in ('l1', 'manhattan'):
412                 affinity = 'cityblock'
```

In the background it does exactly the same.





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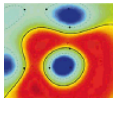
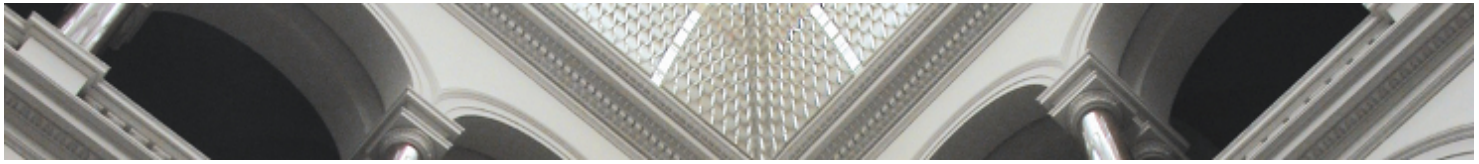
Agenda





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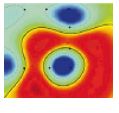
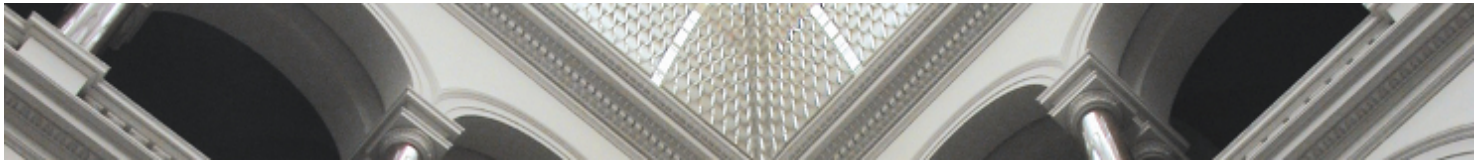
K-Means

Idea: prototype for every cluster

Prototype is mean of all samples in cluster c, $\mathcal{D}_c$:

$$\mu_c = \frac{1}{n_c} \sum_{i \in \mathcal{D}_c} x_i$$





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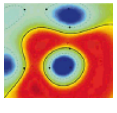
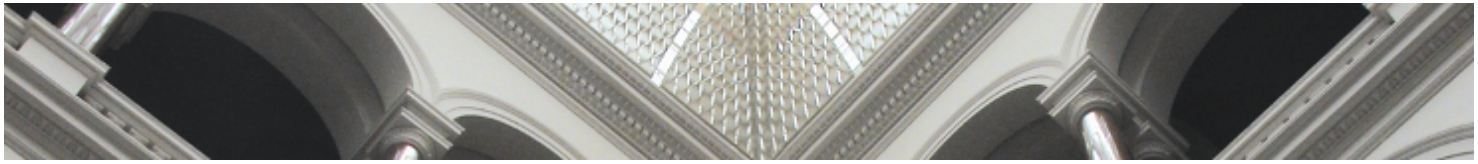
Minimize distance from prototype to each member in the cluster:

$$\mathcal{L} = \sum_c \sum_{i \in \mathcal{D}_c} d(\boldsymbol{x}_i, \mu_c)$$





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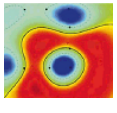
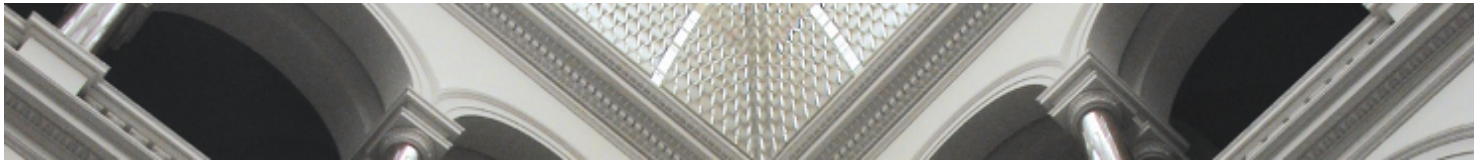
Finding a solution is NP-hard, but in practice straightforward

K-means cannot work with pairwise data such as user ratings





K-Means algorithm

initialize μ_c to random samples

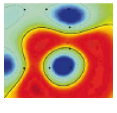
while clusters change do

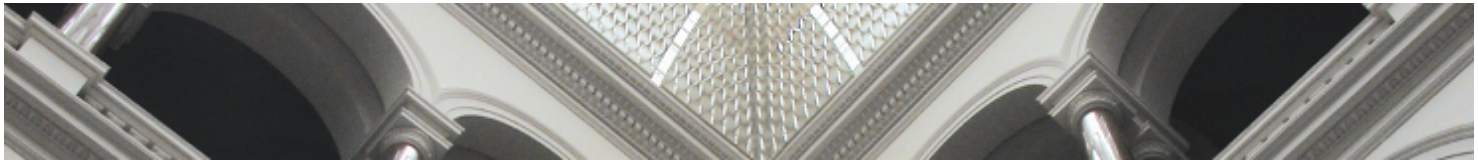
    assign μ_c to cluster means

    assign samples to clusters

end

return clusters





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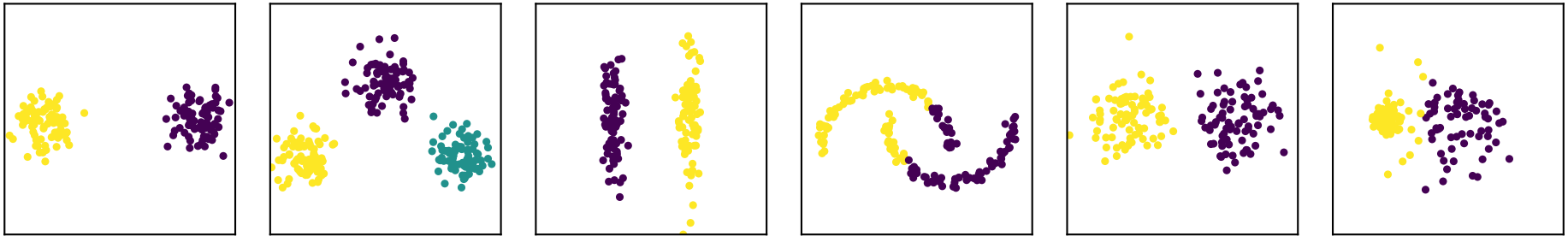
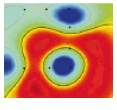
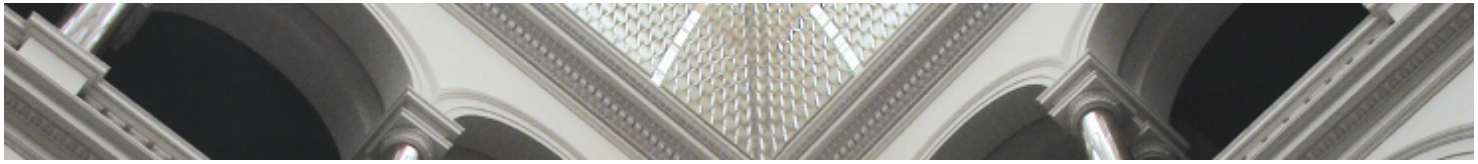
K-Means clusters

K-Means assignment:







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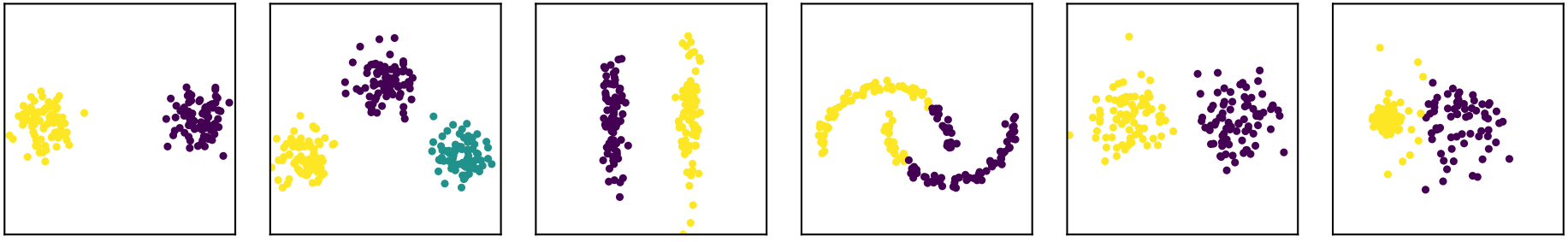
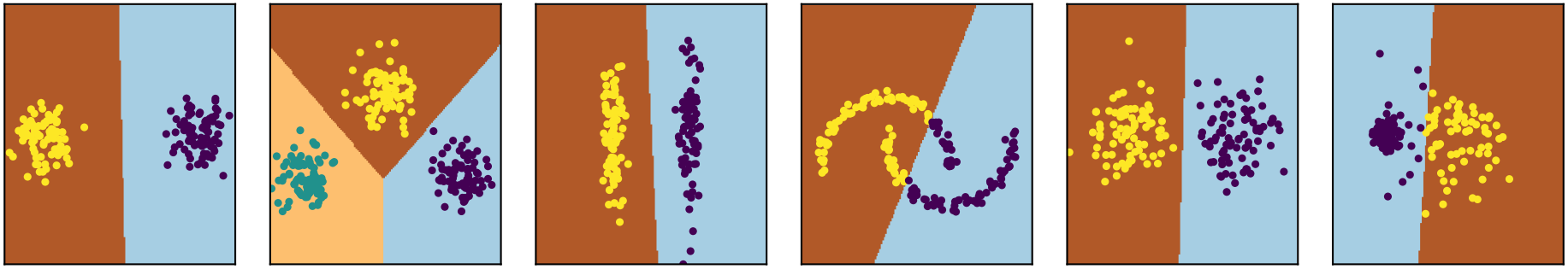
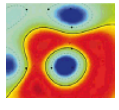
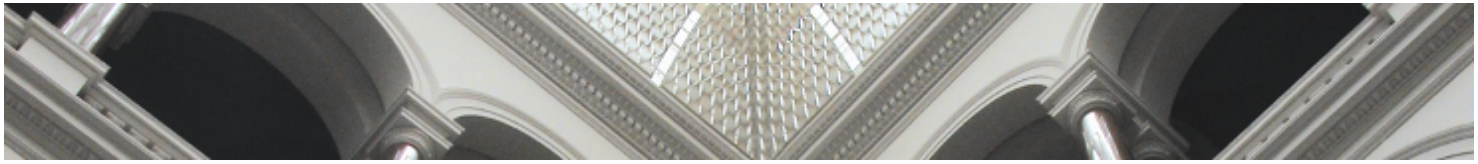


Voronoi tesselation:



Voronoi diagram not possible with hierarchical clustering!





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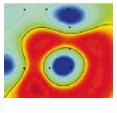

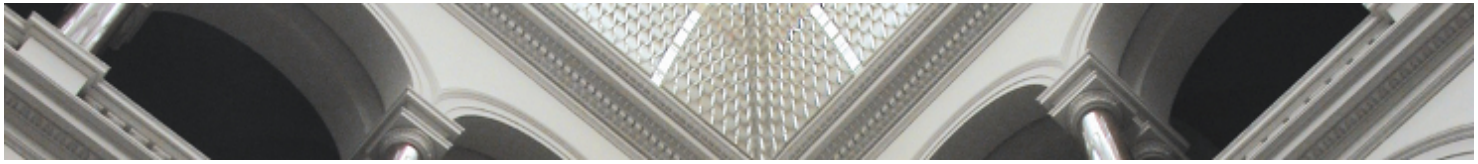

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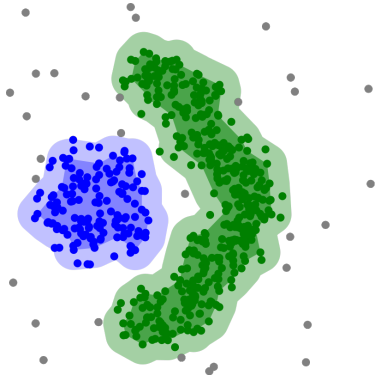
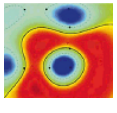
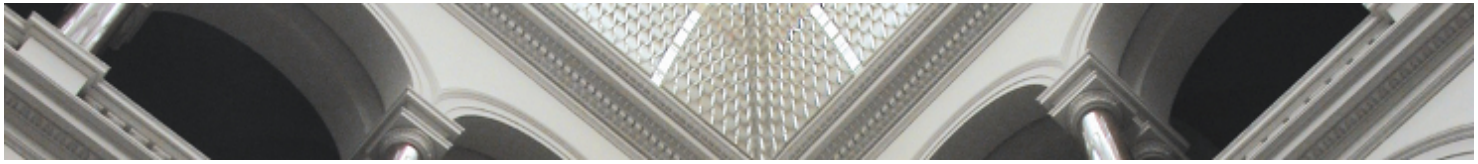
DBSCAN

- clusters are regions of high density separated by regions of low density
- arbitrary cluster shapes



(Wikipedia ”DBSCAN”)





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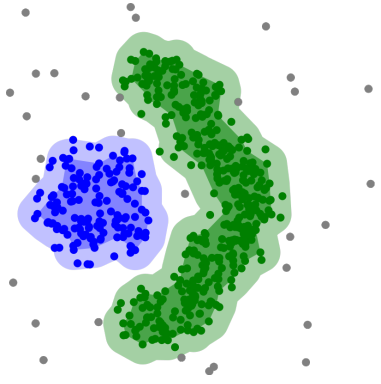
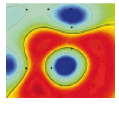
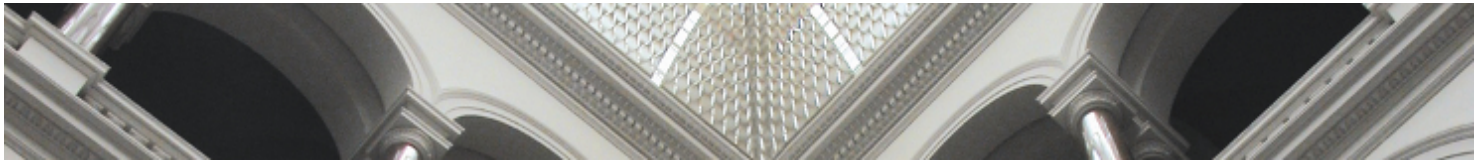


(Wikipedia ”DBSCAN”)

- very simple, but effective (2014 SIGKDD test-of-time award (Schubert et al. 2017))
- explicit noise point modeling





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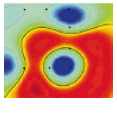
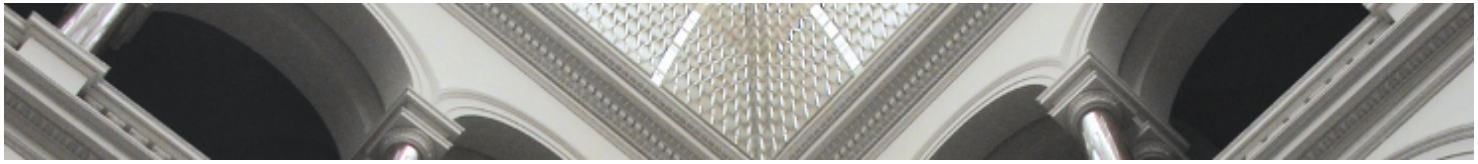
DBSCAN

Two parameters:

- ϵ: distance, defines a neighborhood
- MinPts: amount of neighbors to be a core point





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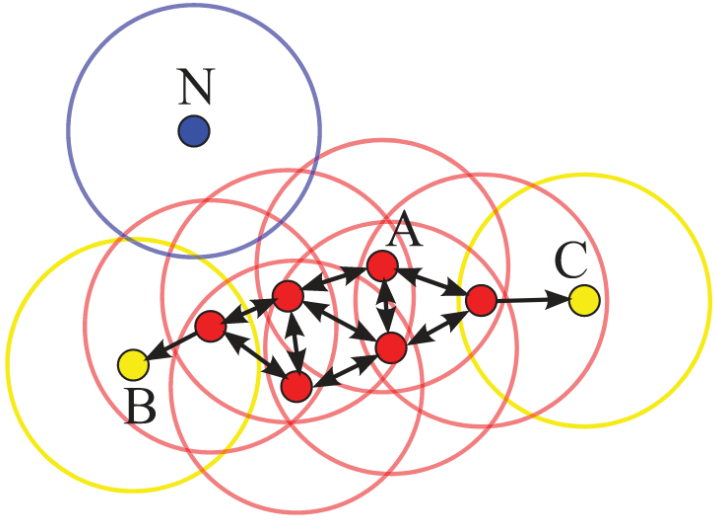

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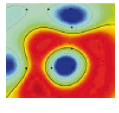

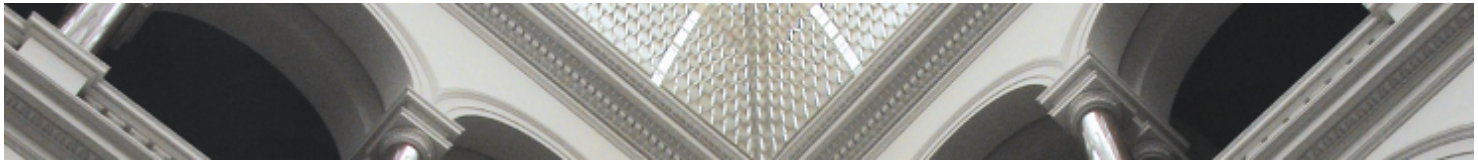

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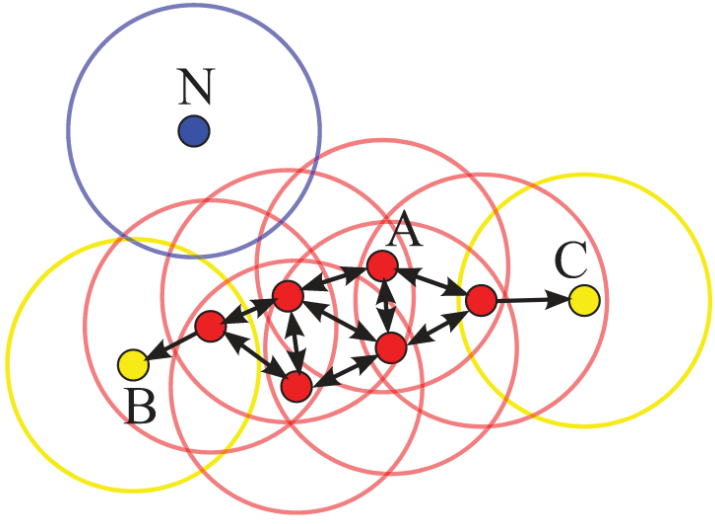
Three types of points:

- core: has MinPts points in its epsilon-neighborhood
- border: within epsilon-neighborhood of core point
- noise: all other points



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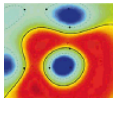

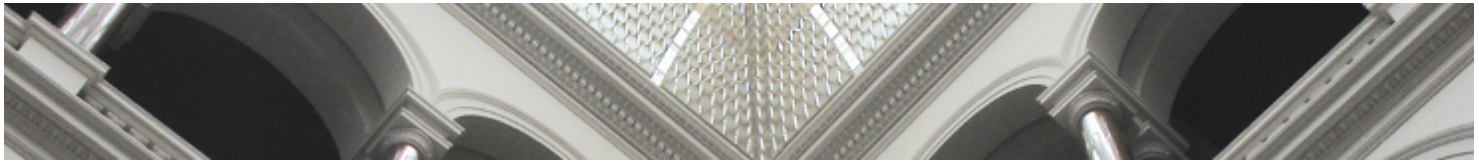

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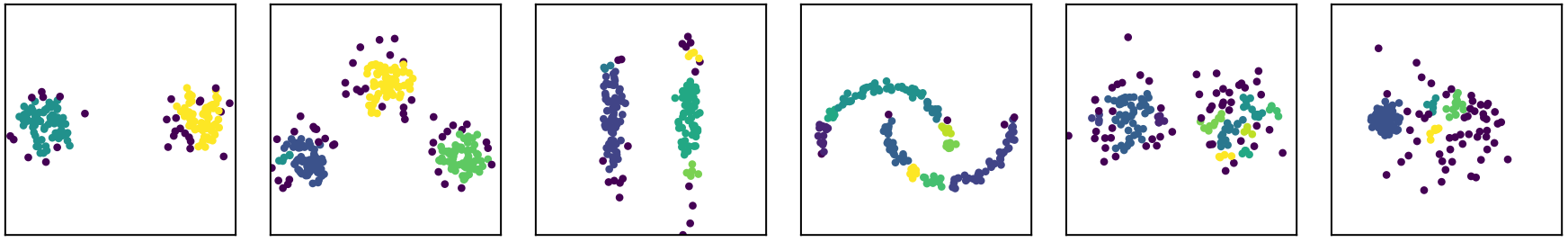
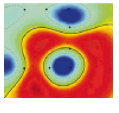
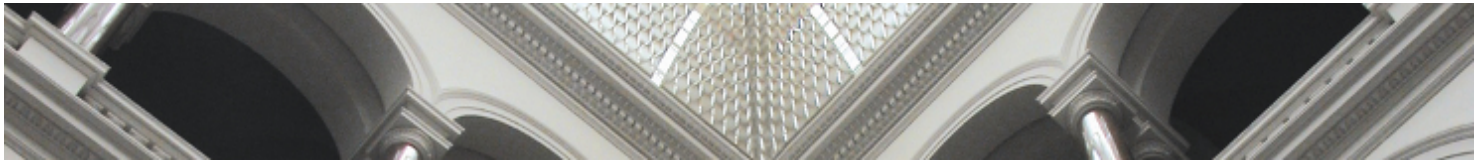
DBSCAN clustering results

$\epsilon = 0.1$, MinPts $= 4$







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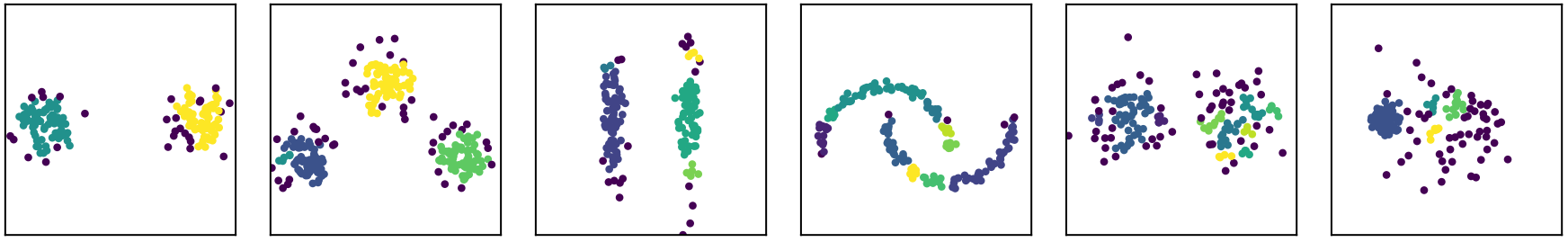
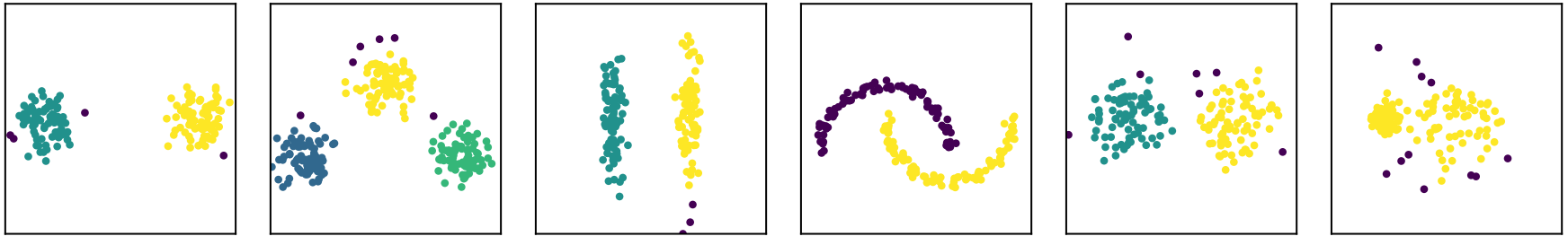
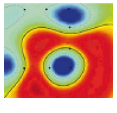
DBSCAN clustering results

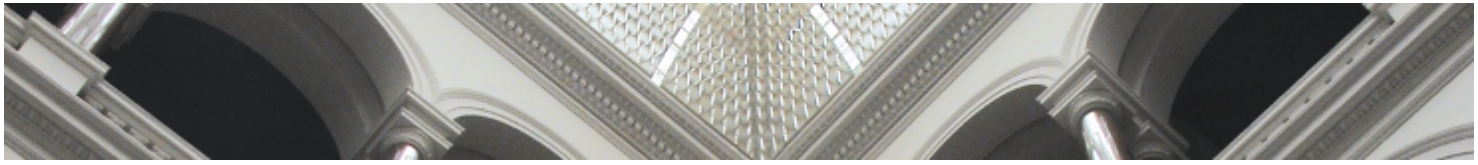
$\epsilon = 0.1$, MinPts $= 4$



$\epsilon = 0.2$, MinPts $= 4$







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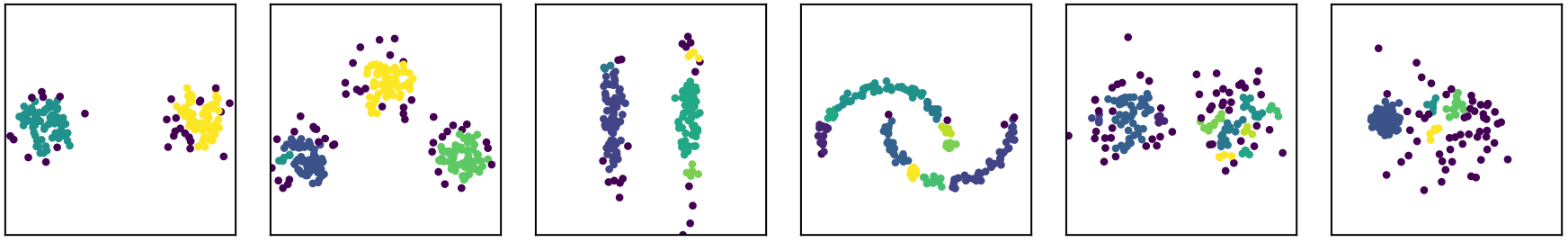
$\epsilon = 0.1$, MinPts $= 4$



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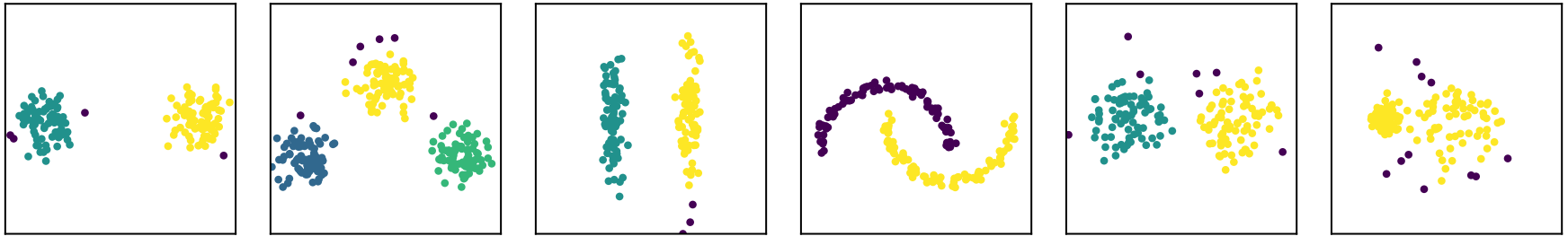
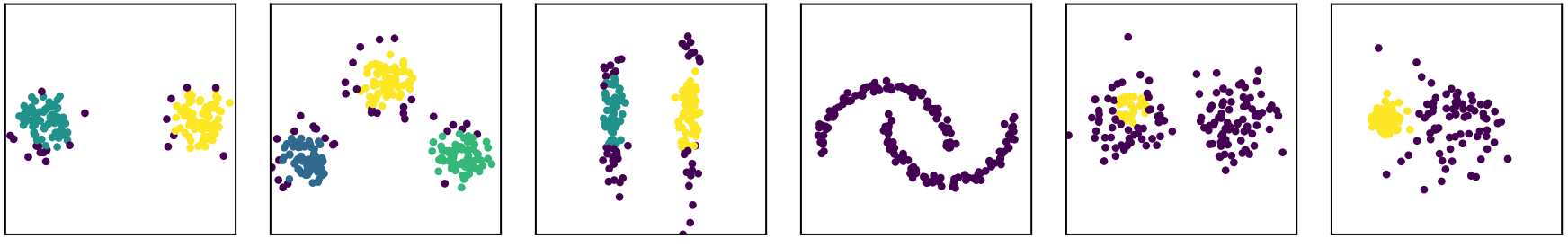
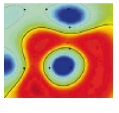
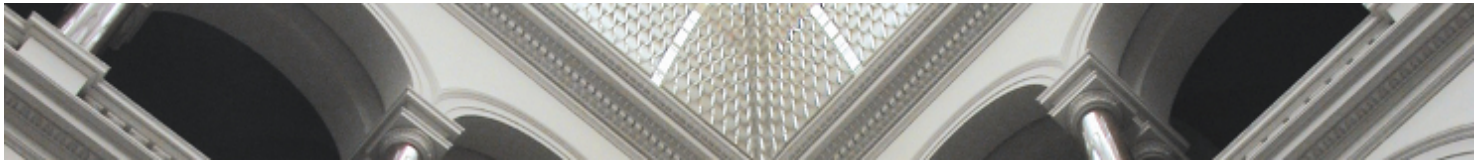


$\epsilon = 0.2$, MinPts $= 20$







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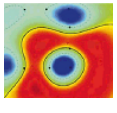

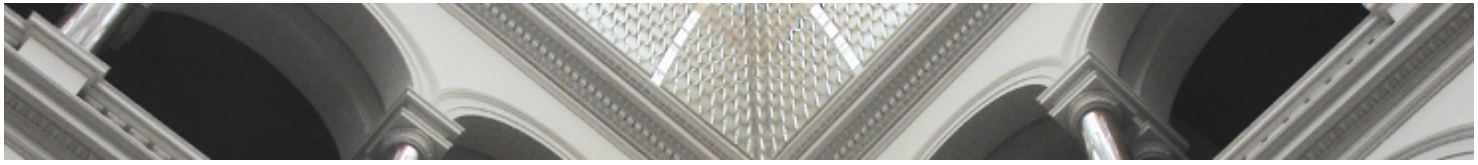

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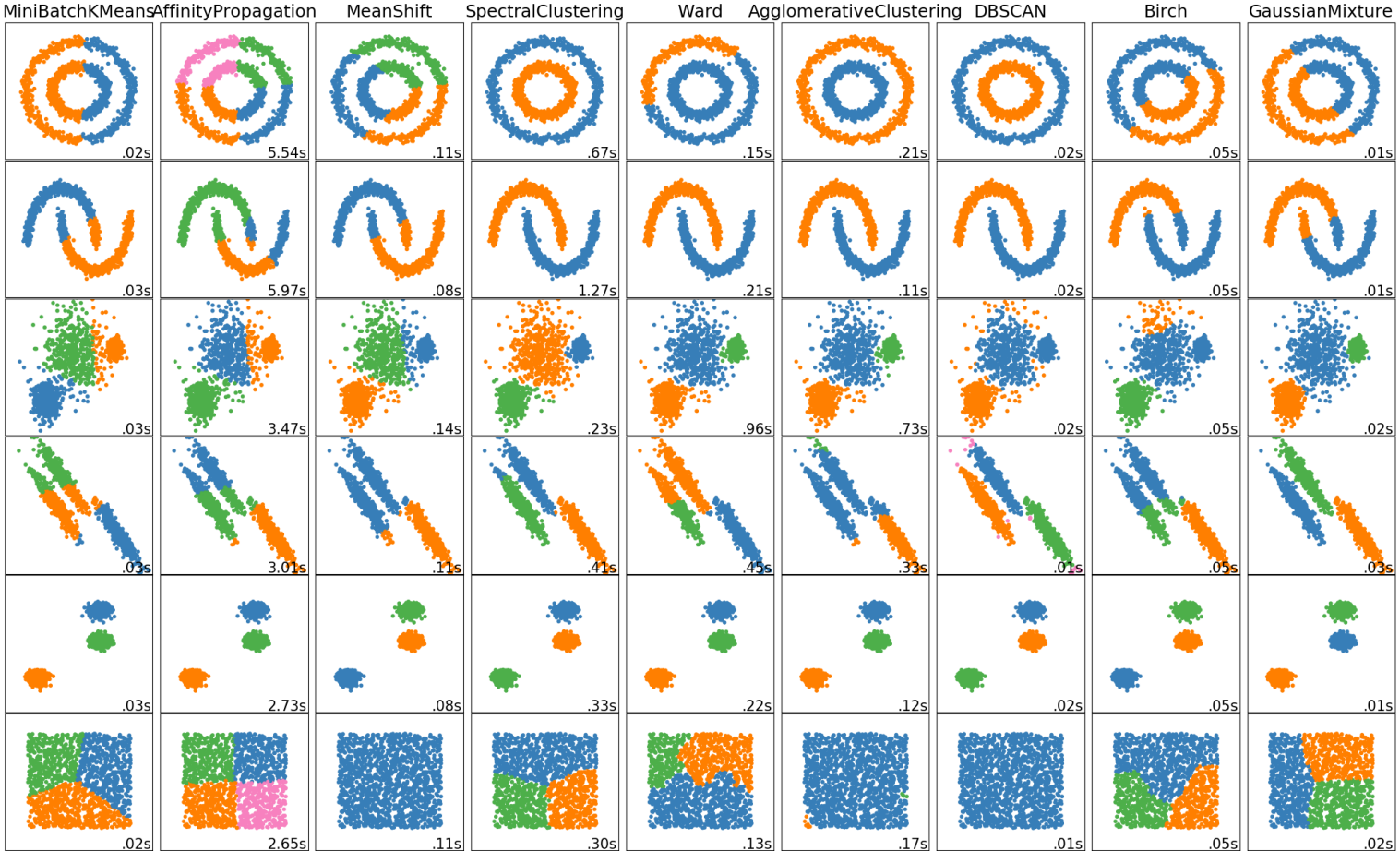
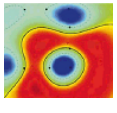
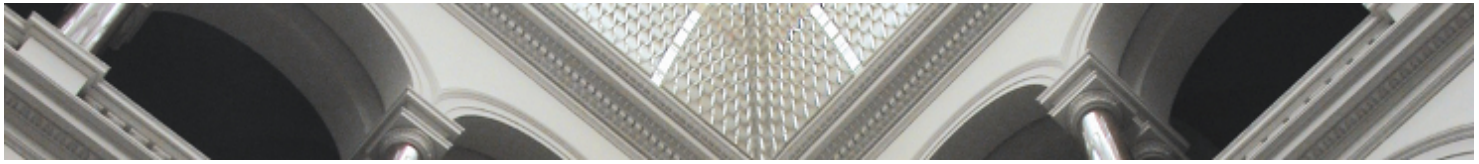
Overview of clustering algorithms



http://scikit-learn.org/stable/modules/clustering.html Pedregosa et al. 2011





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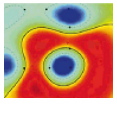

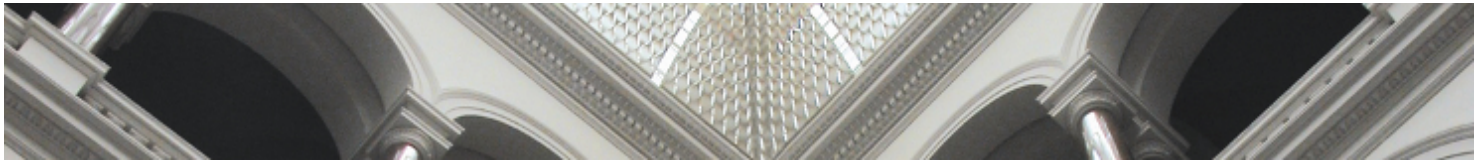

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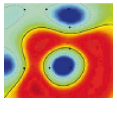
Dimensionalty Reduction - Motivation

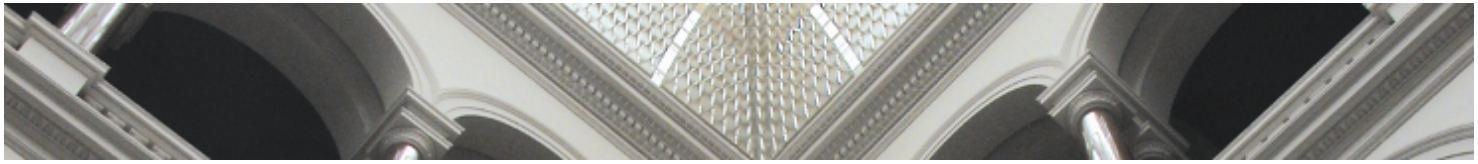
In many applications, we have

- high-dimensional data
- reason to believe they lie close to a lower dimensional subspace

$\rightarrow$ Fewer parameters needed to account for the data properties

hidden causes or *latent variables*





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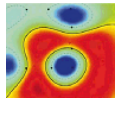
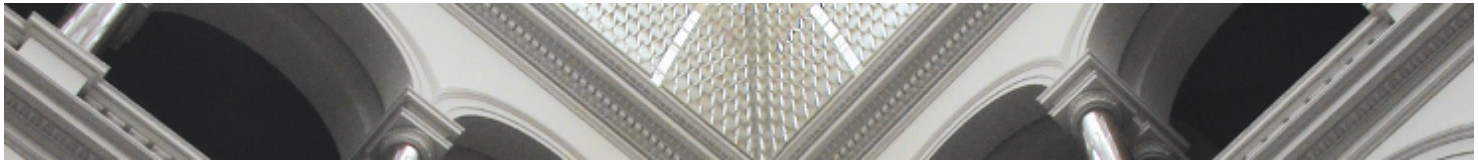
Examples:

- classify high resolution images
- make a predictive model based on hundreds of customer attributes
- analyse high dimensional neural data
- detect trends in news data





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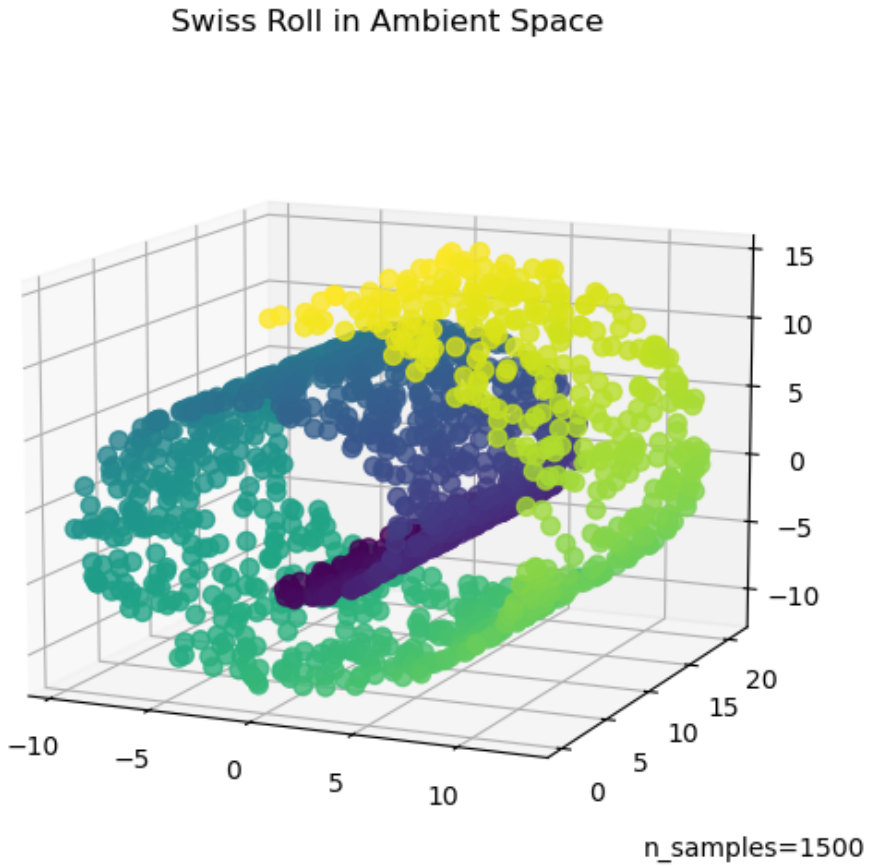
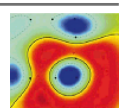
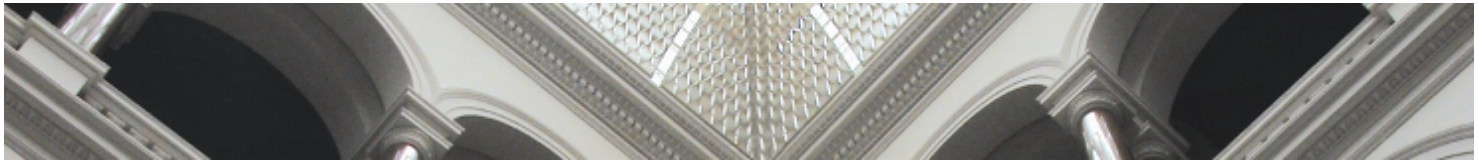
Swiss roll data



Scikit-Learn swiss roll dataset





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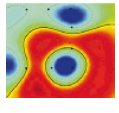
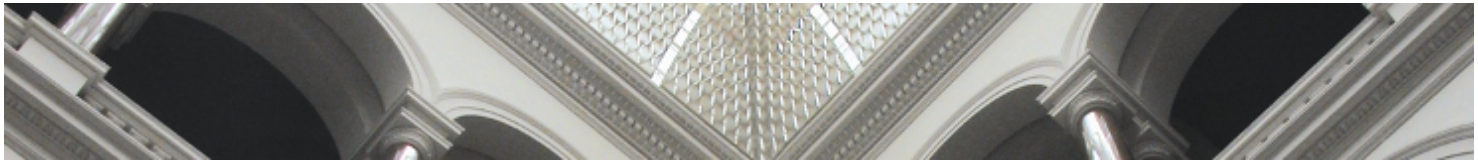
Why Dimensionalty Reduction

- **Visualization**:
  Insights into high-dimensional structures in the data
- **Better Generalization**:
  Fewer dimensions $\rightarrow$ less chances of overfitting
- **Speeding up** learning algorithms:
  Most algorithms scale badly with increasing data dimensionality
- **Data compression**:
  Less storage requirements





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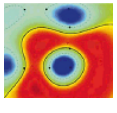

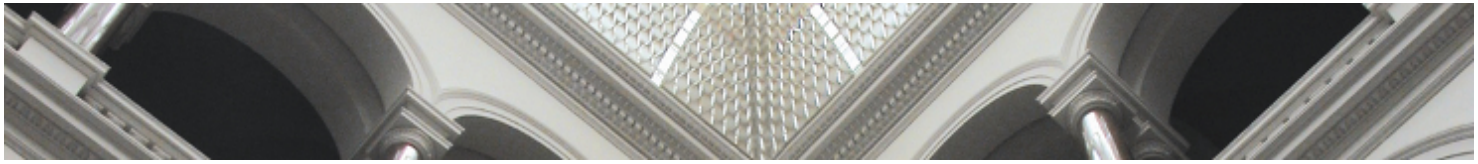

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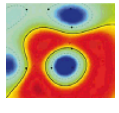
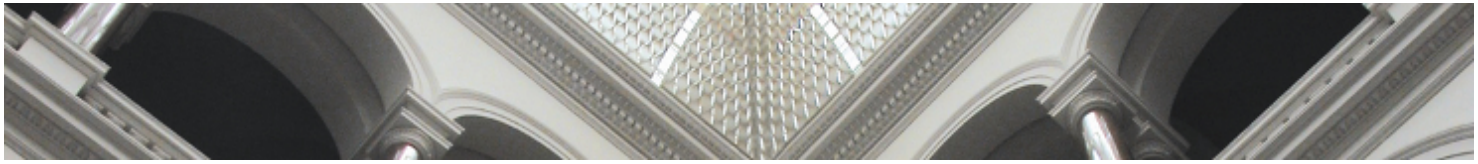
The mathematical model for dimensionalty reduction

We have

- high-dimensional data $X = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N] \in \mathbb{R}^{D \times N}$
- reason to believe they lie close to a lower dimensional subspace

$\rightarrow$ $k < D$ parameters needed to account for the data properties
hidden causes or *latent variables* $H \in \mathbb{R}^{k \times N}$





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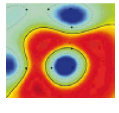
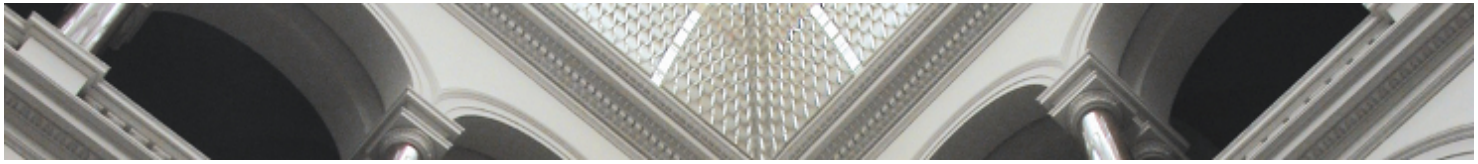
Goal: Find $k < D$ hidden causes $H \in \mathbb{R}^{k \times N}$, that explain the observed data via a mixing $W \in \mathbb{R}^{D \times k}$:

$$X \approx WH$$





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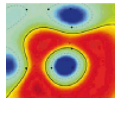
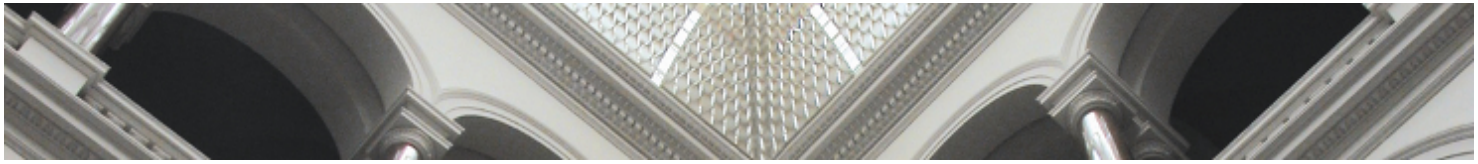
Principal Component Analysis

We obtained some data $X = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N] \in \mathbb{R}^{D \times N}$

PCA finds a direction $\mathbf{w} \in \mathbb{R}^D$ such that the variance of the projected data $\mathbf{w}^\top X$ is maximal





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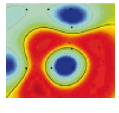
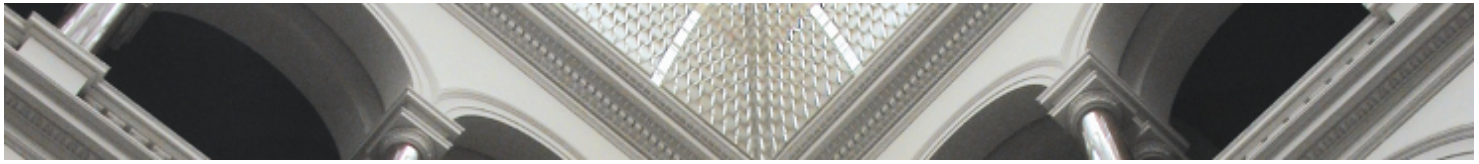
$$\mathrm{Var}(\mathbf{w}^T X) \quad = \quad \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^\top \mathbf{x}_n - \mathrm{E}(\mathbf{w}^\top \mathbf{x}))^2$$





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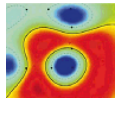
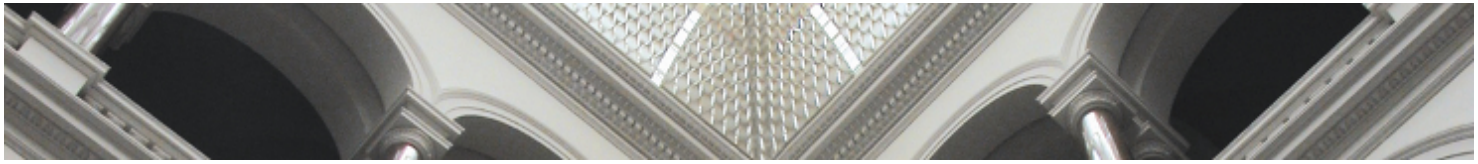
$$\begin{aligned} \mathrm{Var}(\mathbf{w}^T X) &= \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^\top \mathbf{x}_n - \mathrm{E}(\mathbf{w}^\top \mathbf{x}))^2 \\ &= \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^\top \mathbf{x}_n - \mathbf{w}^\top \mathrm{E}(\mathbf{x}))^2 = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^\top (\mathbf{x}_n - \mathrm{E}(\mathbf{x})))^2 \end{aligned}$$





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\begin{aligned}
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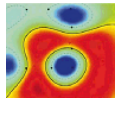
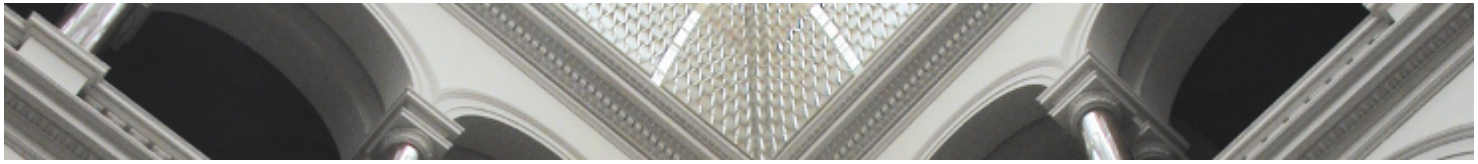
&= \frac{1}{N} \sum_{n=1}^{N} \mathbf{w}^\top (\mathbf{x}_n - \mathrm{E}(\mathbf{x})) \cdot (\mathbf{x}_n - \mathrm{E}(\mathbf{x}))^\top \mathbf{w}
\end{aligned}
$$





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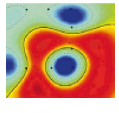
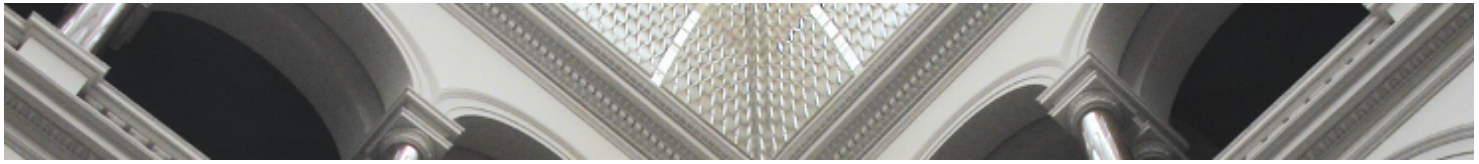
\begin{aligned}
\mathrm{Var}(\mathbf{w}^T X) &= \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^\top \mathbf{x}_n - \mathrm{E}(\mathbf{w}^\top \mathbf{x}))^2 \\
&= \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^\top \mathbf{x}_n - \mathbf{w}^\top \mathrm{E}(\mathbf{x}))^2 = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^\top (\mathbf{x}_n - \mathrm{E}(\mathbf{x})))^2 \\
&= \frac{1}{N} \sum_{n=1}^{N} \mathbf{w}^\top (\mathbf{x}_n - \mathrm{E}(\mathbf{x})) \cdot (\mathbf{x}_n - \mathrm{E}(\mathbf{x}))^\top \mathbf{w} \\
&= \mathbf{w}^\top \underbrace{\left(\frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \mathrm{E}(\mathbf{x})) \cdot (\mathbf{x}_n - \mathrm{E}(\mathbf{x}))^\top \right)}_{\text{Covariance matrix S}} \mathbf{w}
\end{aligned}
$$





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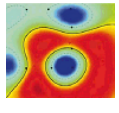
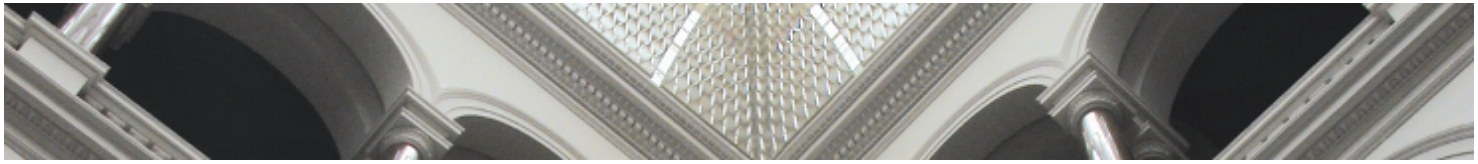
Principal Component Analysis

We obtained some data $X = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N] \in \mathbb{R}^{D \times N}$

PCA finds a direction $\mathbf{w} \in \mathbb{R}^D$ such that the variance of the projected data $\mathbf{w}^\top X$ is maximal

$$\mathrm{Var}(\mathbf{w}^T X) = \mathbf{w}^\top \underbrace{\left(\frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \mathrm{E}(\mathbf{x})) \cdot (\mathbf{x}_n - \mathrm{E}(\mathbf{x}))^\top \right)}_{\text{Covariance matrix S}} \mathbf{w}$$





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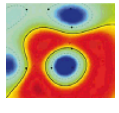
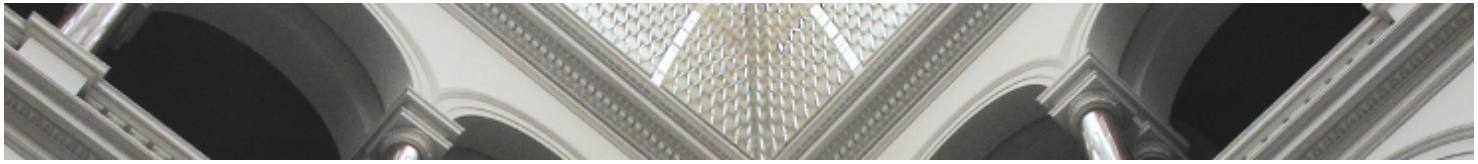
where we assume centered data





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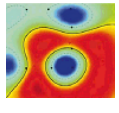
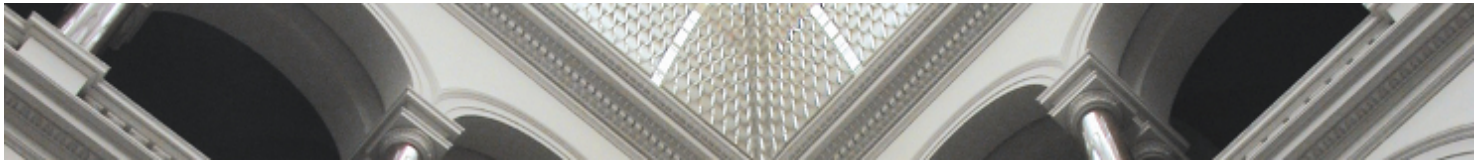
where we assume centered data

And: we need to constrain $\mathbf{w}$





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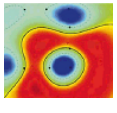
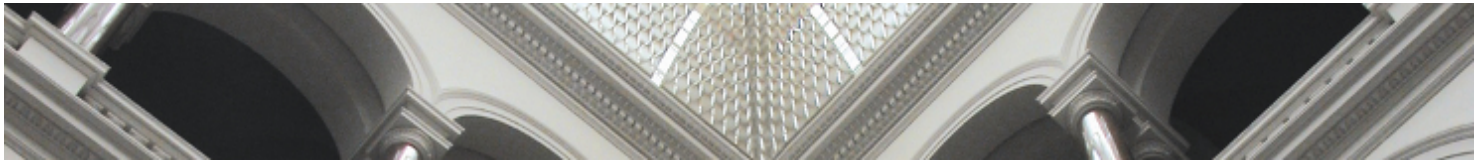
Principal Component Analysis

PCA finds a direction $\mathbf{w} \in \mathbb{R}^D$ such that the variance of the projected data $\mathbf{w}^T X$ is maximal

$$\arg\max_{w} \frac{\mathbf{w}^\top S \mathbf{w}}{\mathbf{w}^\top \mathbf{w}}$$

This objective function is independent of the scaling of $\mathbf{w}$.





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Principal Component Analysis

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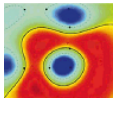
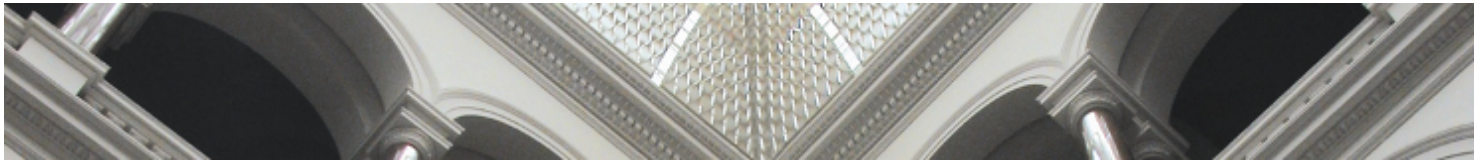
This objective function is independent of the scaling of $\mathbf{w}$.

Note the similarity to the objective of Linear Discriminant Analysis!

$\rightarrow$ Different covariance matrices, different problem, but: same maths solve it





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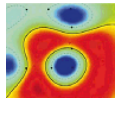
Principal Component Analysis

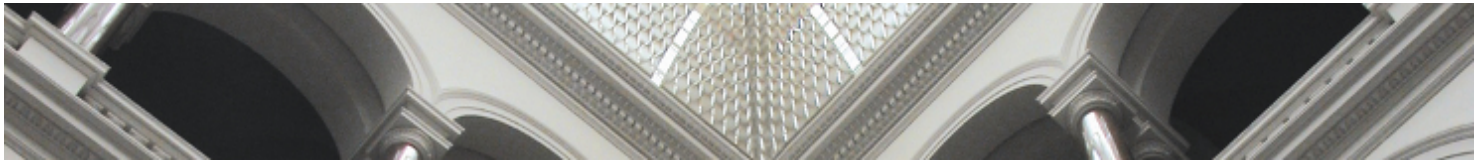
$$\arg\max_{\mathbf{w}} \frac{\mathbf{w}^\top S\mathbf{w}}{\mathbf{w}^\top \mathbf{w}}$$

Set the derivative w.r.t $\mathbf{w}$ to zero:

$$\begin{aligned}
\frac{(\mathbf{w}^\top \mathbf{w})2S\mathbf{w} - (\mathbf{w}^\top S\mathbf{w})2\mathbf{w}}{(\mathbf{w}^\top \mathbf{w})^2} &= 0 \\
(\mathbf{w}^\top S\mathbf{w})\mathbf{w} &= (\mathbf{w}^\top \mathbf{w})S\mathbf{w} \\
\mathbf{w} &= S\mathbf{w} \cdot \underbrace{\frac{\mathbf{w}^\top \mathbf{w}}{\mathbf{w}^\top S\mathbf{w}}}_{\textit{scalar}} \\
S\mathbf{w} &= \lambda \mathbf{w}
\end{aligned}$$

This is the standard eigenvalue problem.





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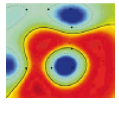
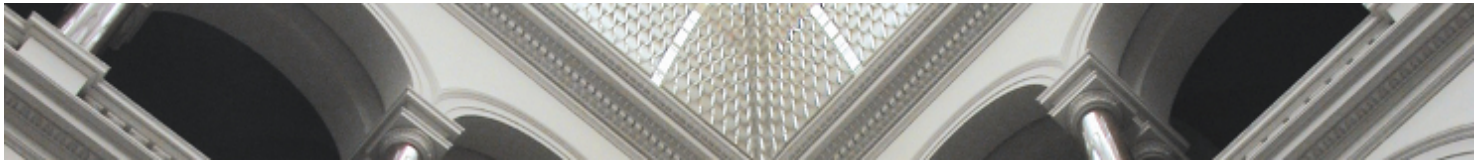
Principal Component Analysis

For $S\mathbf{w} = \lambda\mathbf{w}$, we see that the variance in direction $\mathbf{w}$ is given by:

$$\arg\max_{\mathbf{w}} \frac{\mathbf{w}^\top S\mathbf{w}}{\mathbf{w}^\top\mathbf{w}} = \frac{\mathbf{w}^\top \lambda\mathbf{w}}{\mathbf{w}^\top\mathbf{w}} = \lambda$$

The variance of the projected data in an eigendirection $\mathbf{w}$ is given by the corresponding eigenvalue!





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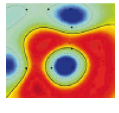
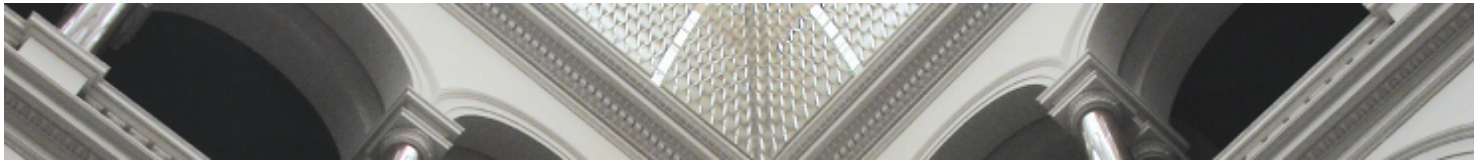
The variance of the projected data in an eigendirection $\mathbf{w}$ is given by the corresponding eigenvalue!

The direction of maximal variance in the data is equal to the eigenvector having the largest eigenvalue.





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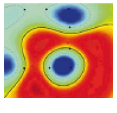
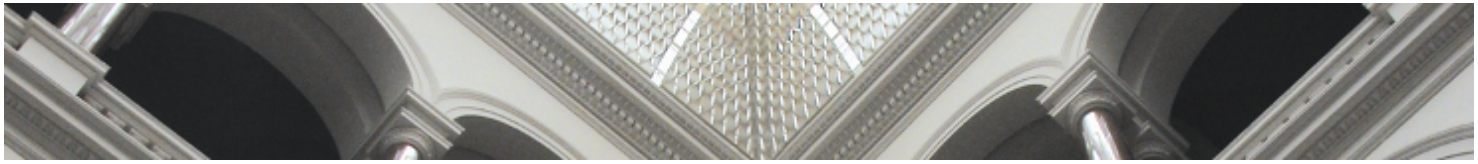
Principal Component Analysis

Require: data $x_1, \ldots, x_N \in \mathbb{R}^d$, number of principal components k

1: # Center Data
2: $X = X - 1/N \sum_i x_i$
3: # Compute Covariance Matrix
4: $C = 1/N \, XX^\top$
5: # Compute eigenvectors corresponding to the k largest eigenvalues
6: $W = \text{eig}(C)$
7: # Project data onto W
8: $H = W^\top X$
9: **return** W, H

Algorithm 1: Principal Component Analysis





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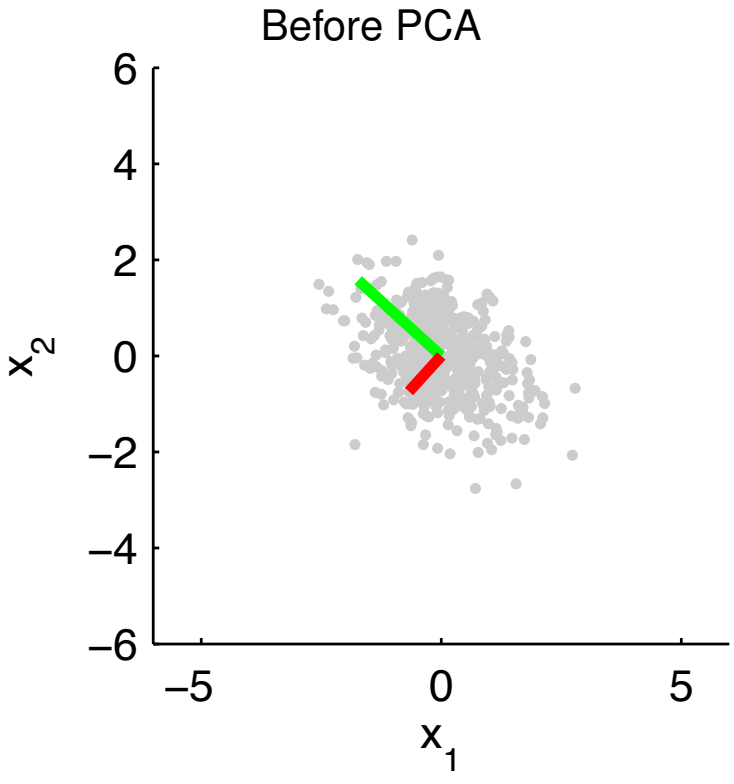
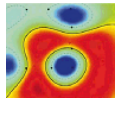
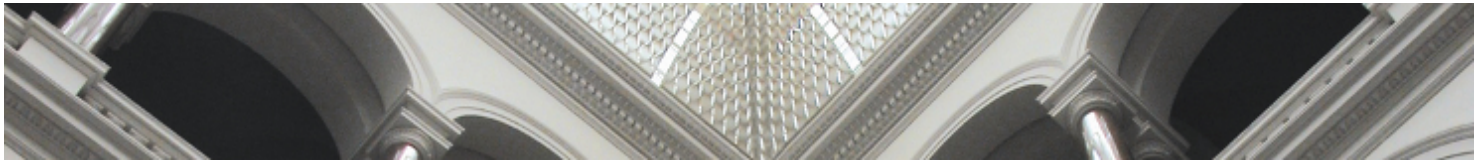
Principal Component Analysis







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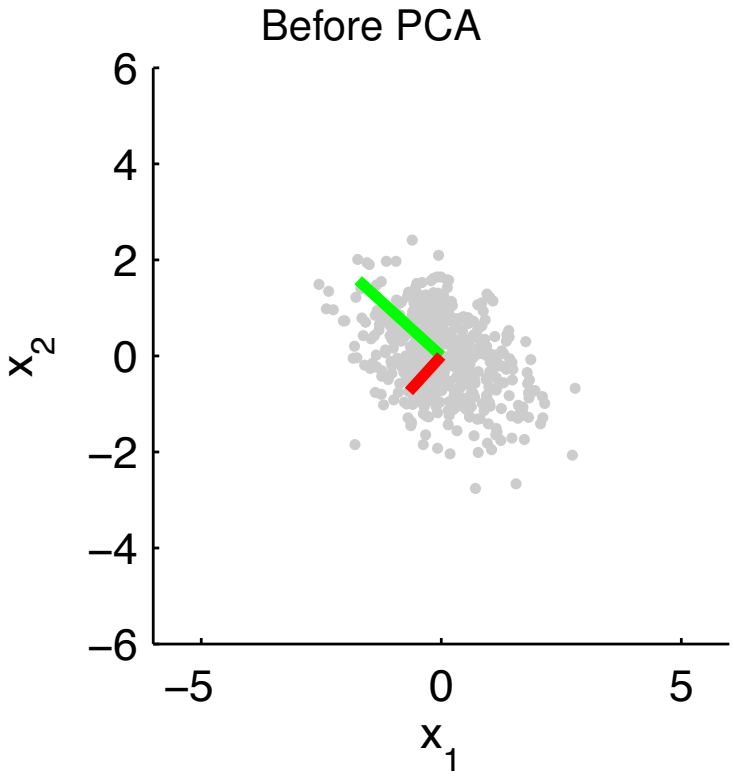

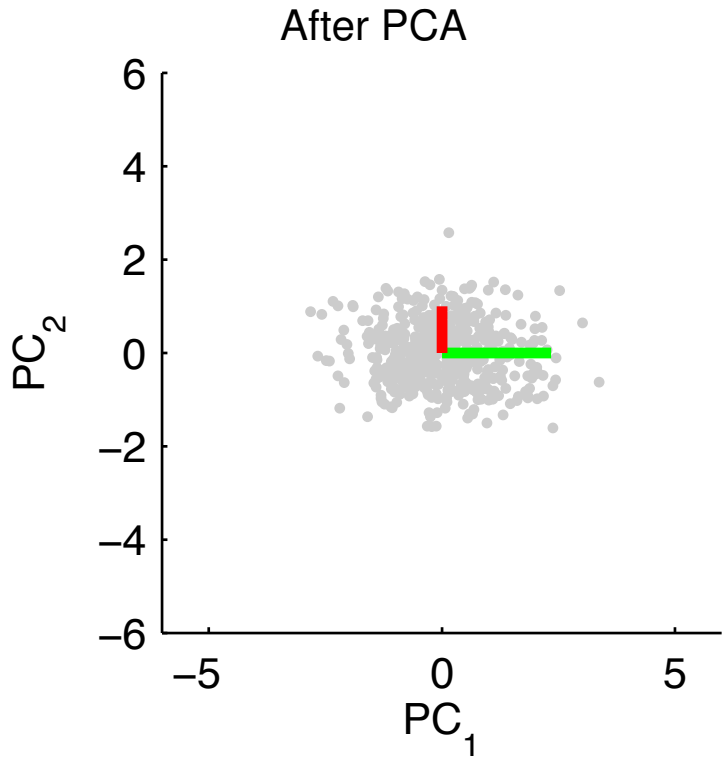

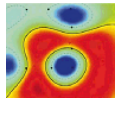

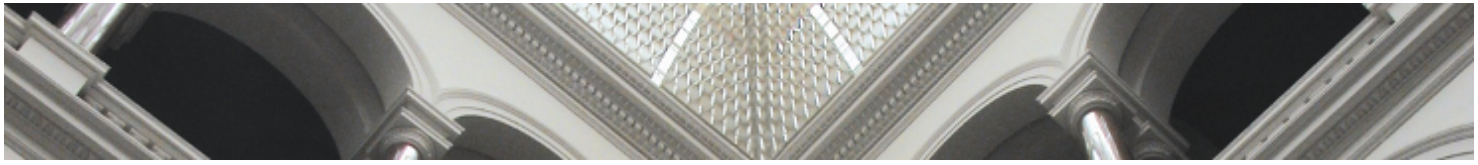

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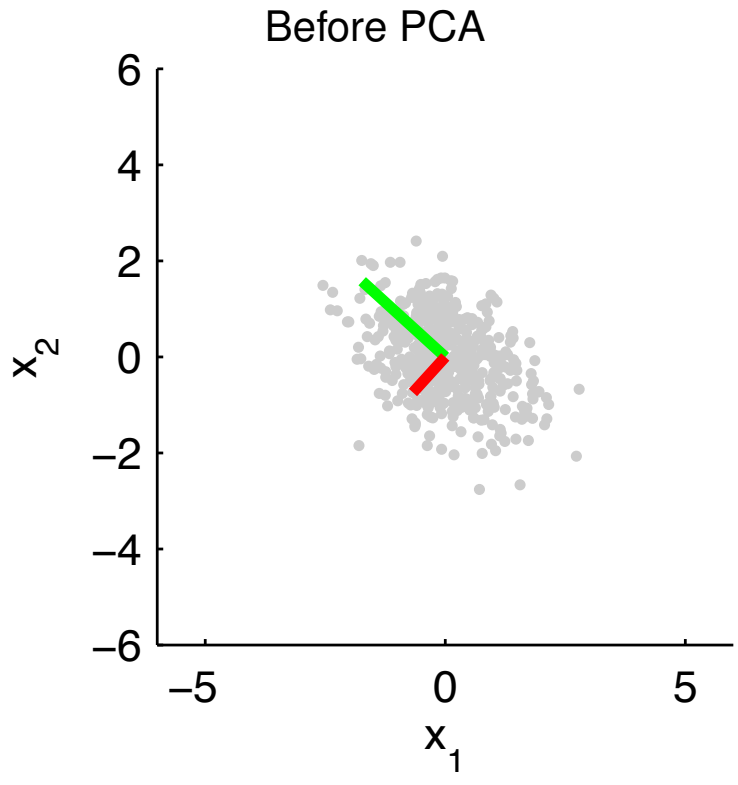
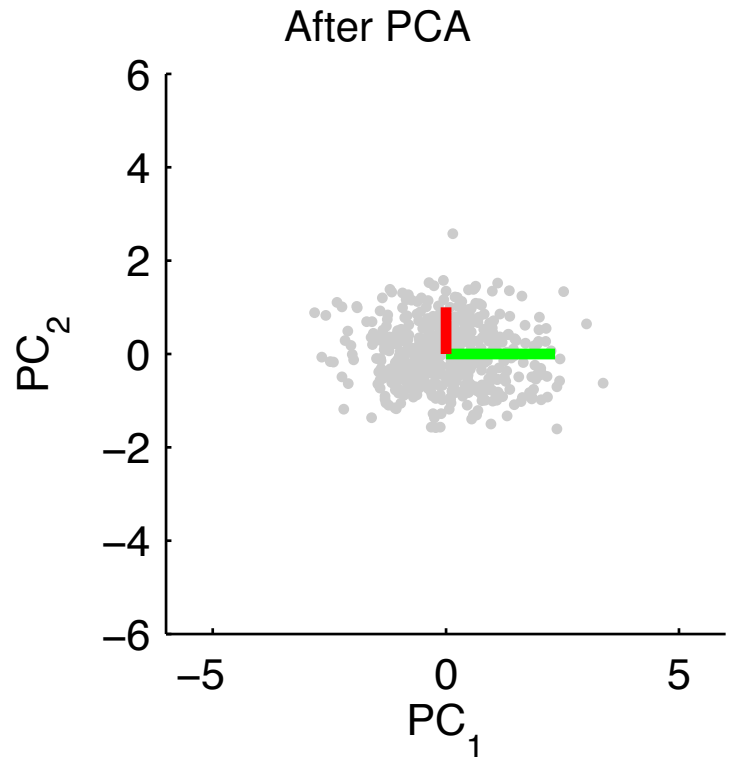
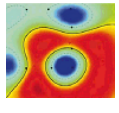


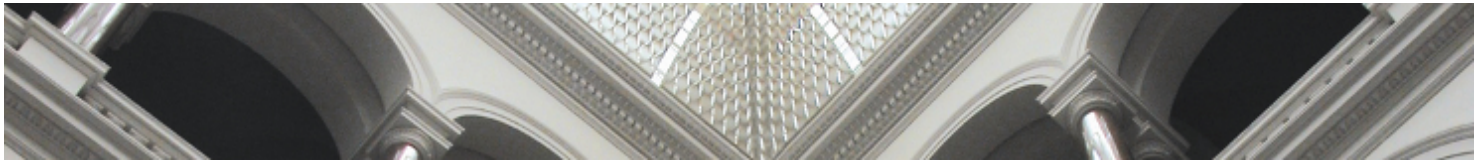


PCA aligns maximum variance directions with standard basis

$\rightarrow$ Variance along each dimension is **uncorrelated**

$\rightarrow$ Now we can remove each dimension separately





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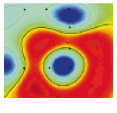
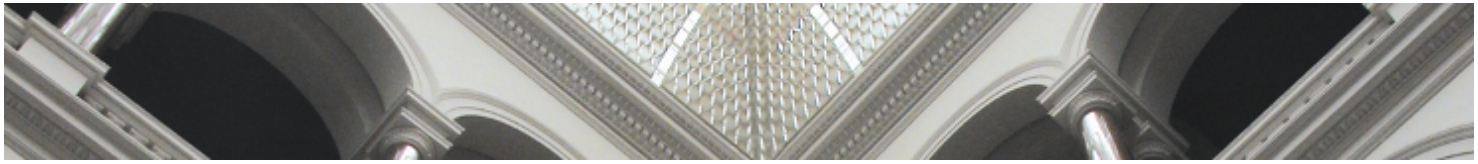
Agenda





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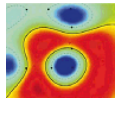
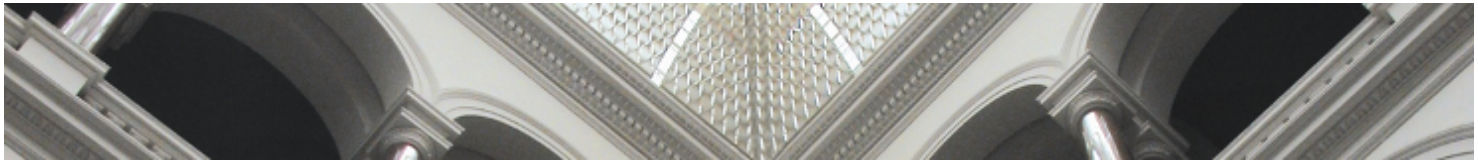
Non-Negative Matrix Factorization

- For some data PCA does not make sense
- Example: Non-negative data
  - Principal directions will have negative entries
  - This can be hard to interpret
- Many data sets are strictly positive
  - Text data
  - Image data
  - Probabilistic data
- Very easy to implement

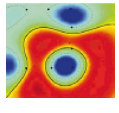


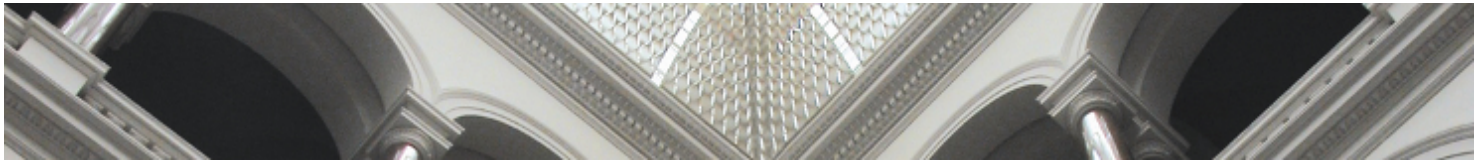


Non-Negative Matrix Factorization

Given non-negative data $X \in \mathbb{R}_+^{D \times N}$ we want to find $W \in \mathbb{R}_+^{D \times C}$, $H \in \mathbb{R}_+^{C \times N}$ such that

$$\arg\min_{W,H} ||X - WH||_{\text{Fro}}^2 = \arg\min_{W,H} \sum_{d=1}^{D} \sum_{n=1}^{N} (X_{dn} - (WH)_{dn})^2$$





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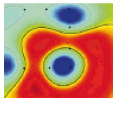
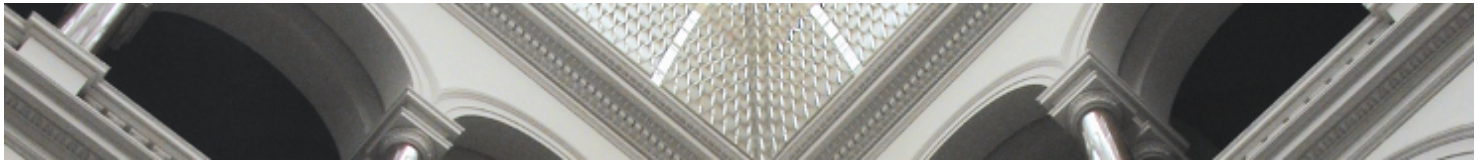
Non-Negative Matrix Factorization

– Local minima





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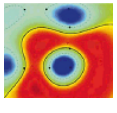
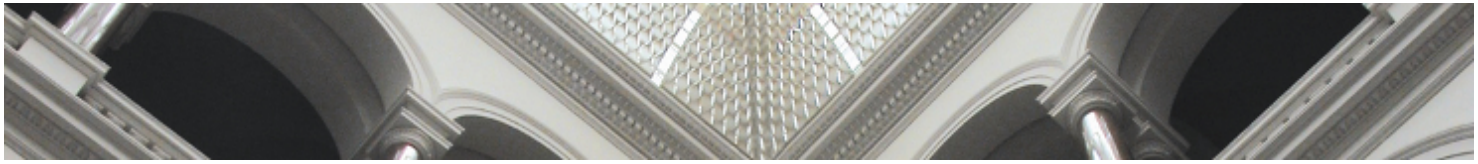
Non-Negative Matrix Factorization

- Local minima
- Gradient descent finds an optimal solution by iterating

$$H \leftarrow H + \eta \left(W^\top WH - X^\top W \right)$$

$$W \leftarrow W + \eta \left(WHH^\top - XH^\top \right)$$





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Non-Negative Matrix Factorization

- Local minima
- Gradient descent finds an optimal solution by iterating

$$H \leftarrow H + \eta \left(W^\top WH - X^\top W \right)$$

$$W \leftarrow W + \eta \left(WHH^\top - XH^\top \right)$$

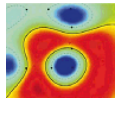
- By choosing η wisely one can transform the additive updates into multiplicative ones:

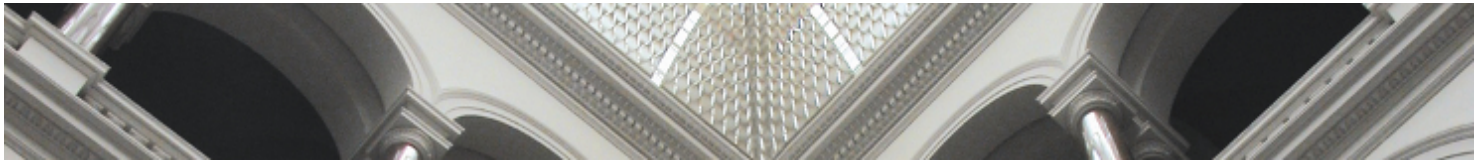
$$H = H \odot W^\top X \oslash W^\top WH$$

$$W = W \odot XH^\top \oslash WHH^\top$$

where

- $\odot$ is *element-wise* multiplication (in python '*')
- $\oslash$ is *element-wise* division (in python '/')



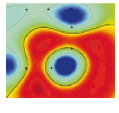


NMF Algorithm

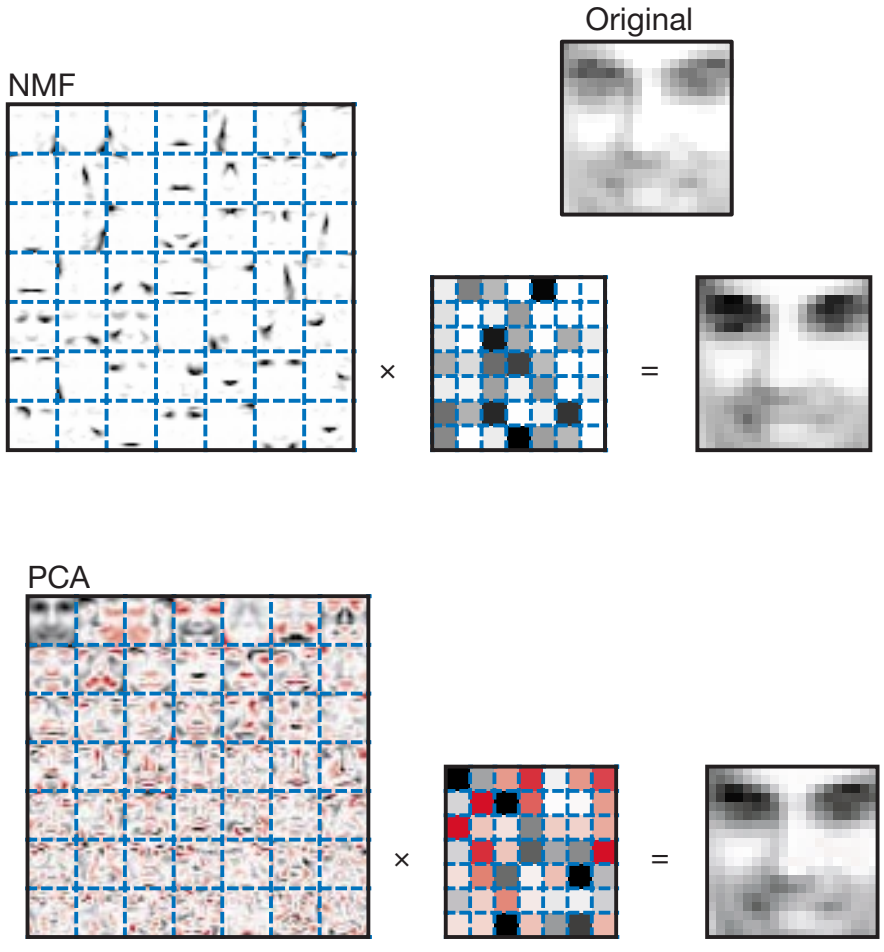
Require: data $X = [x_1, \ldots, x_N] \in \mathbb{R}_+^{D \times N}$, number of factors k

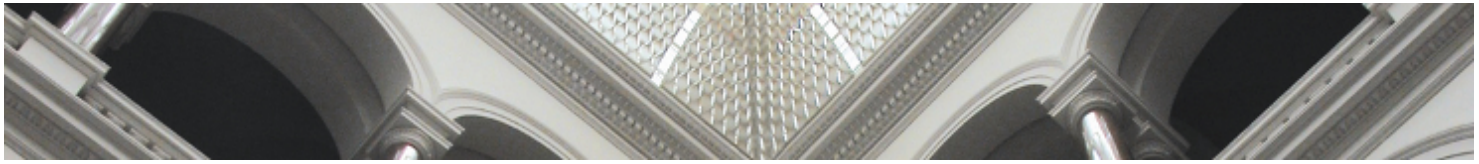
1: # Initialize $W \in \mathbb{R}_+^{D \times k}$, $H \in \mathbb{R}_+^{k \times N}$ randomly
2: # Add a small constant $\epsilon = 10^{-19}$ to X to avoid zero-divisions
3: **for** it $\leq$ Iterations **do**
4: $\quad H = H \odot W^\top X \oslash W^\top WH$
5: $\quad W = W \odot XH^\top \oslash WHH^\top$
6: **end for**
7: **return** W, H

Algorithm 2: Non-negative Matrix Factorization



NMF Applications - Face Parts





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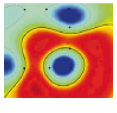
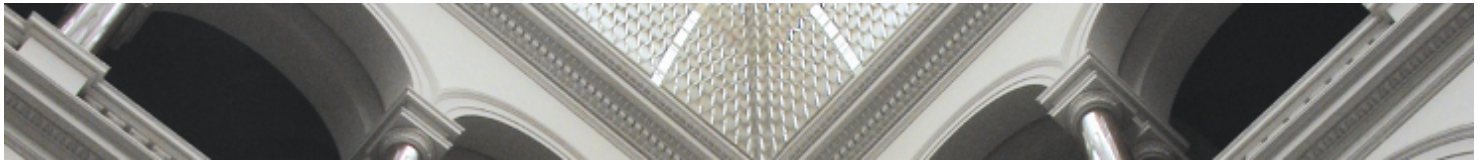
Agenda





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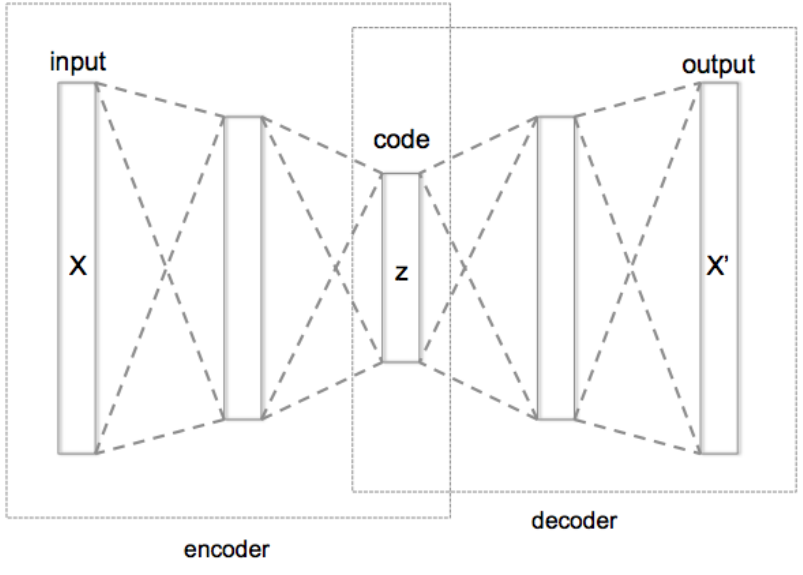
Autoencoder

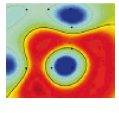
Two parts:

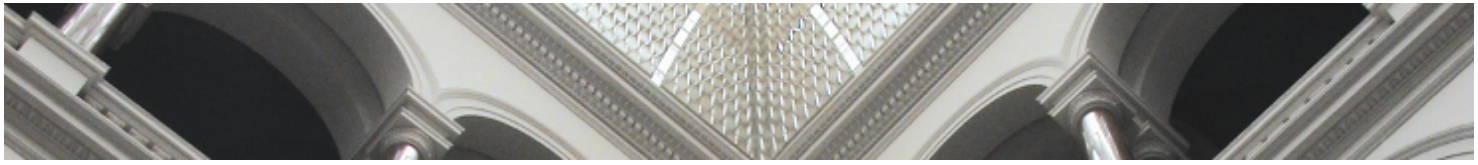
Encoder: A neural network that forces the input into a low-dimensional ”code”

Decoder: A neural network that tries to reconstruct the input from the ”code”



Wikipedia autoencoder





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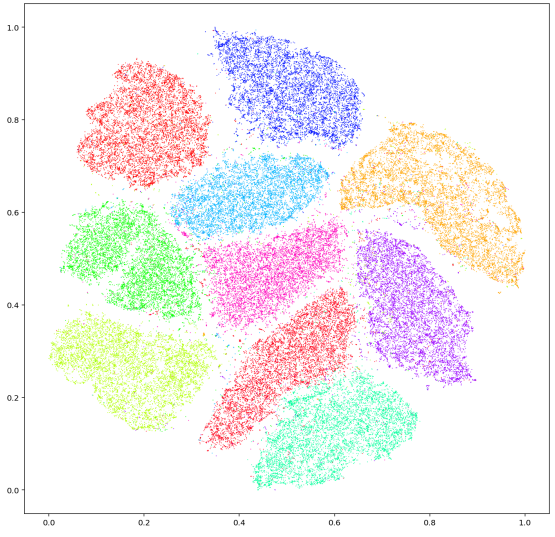
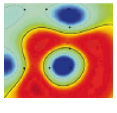
t-SNE (t-distributed Stochastic Neighbor Embedding)

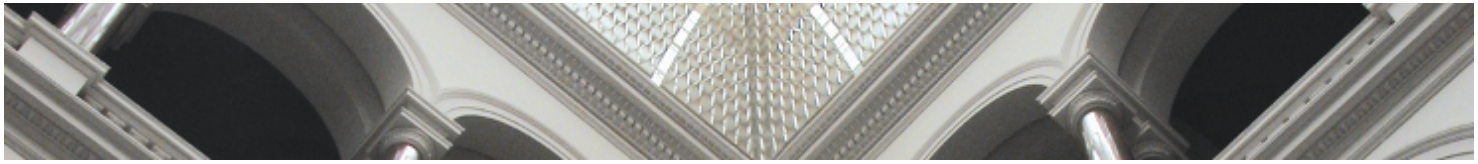
Unlike Autoencoder, non-parametric, i.e. can not easily embed new points.

Local similarities in the data preserved, higher distances not preserved.



Wikipedia t-SNE. A visualization of MNIST in two t-SNE dimensions.





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References

Duda, Richard O, Peter E Hart, and David G Stork (2012). **Pattern classification**. John Wiley & Sons.

Guérin, Joris et al. (Mar. 2017). "Clustering for Different Scales of Measurement - the Gap-Ratio Weighted K-means Algorithm". en. In: **arXiv:1703.07625 [cs, stat]**. arXiv: 1703.07625. URL: http://arxiv.org/abs/1703.07625 (visited on 08/29/2018).

Pedregosa, Fabian et al. (2011). "Scikit-learn: Machine learning in Python". In: **Journal of machine learning research** 12.Oct, pp. 2825–2830.

Schubert, Erich et al. (2017). "DBSCAN revisited, revisited: why and how you should (still) use DBSCAN". In: **ACM Transactions on Database Systems (TODS)** 42.3, p. 19.