Unsupervised Machine Learning

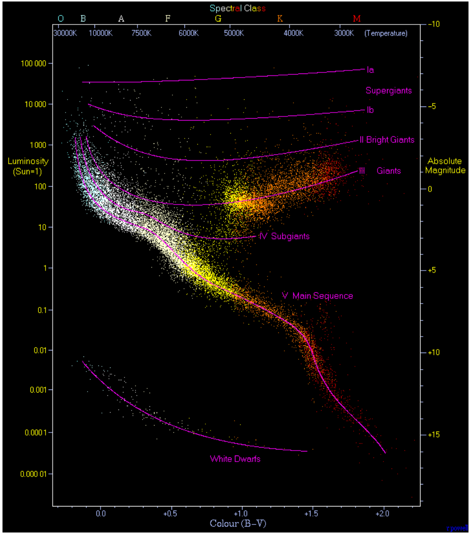
Martin Žonda and Pavel Baláž

Seminář Astronomického ústavu UK

Supervised Learning

Supervised

- Typical tasks: classification, target predictions, regression



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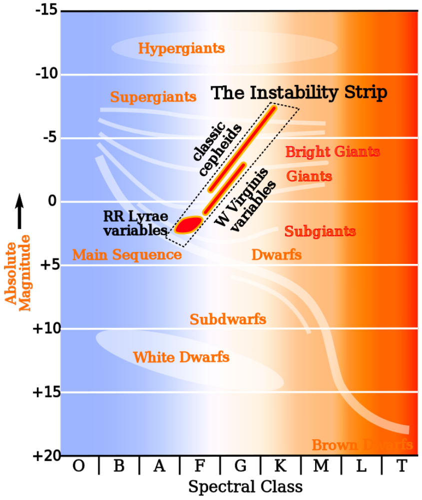

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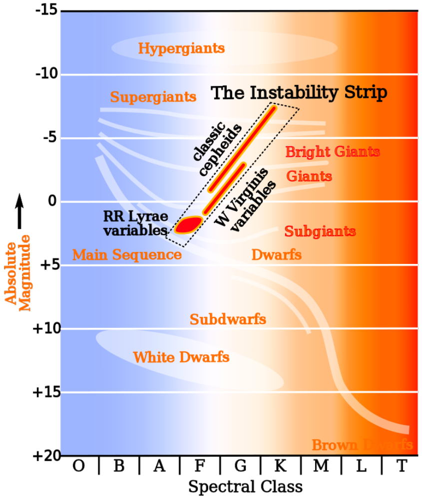

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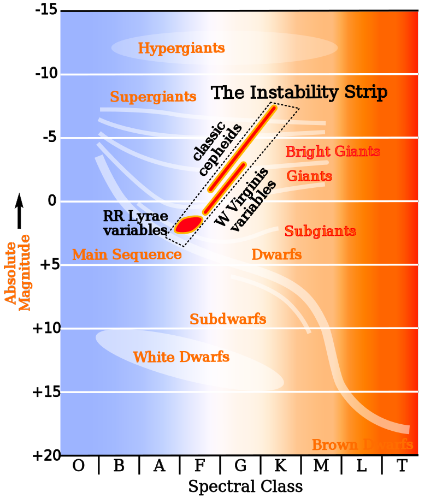
- All of the above are used for **Stellar Classification**



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The main ideas behind unsupervised learning

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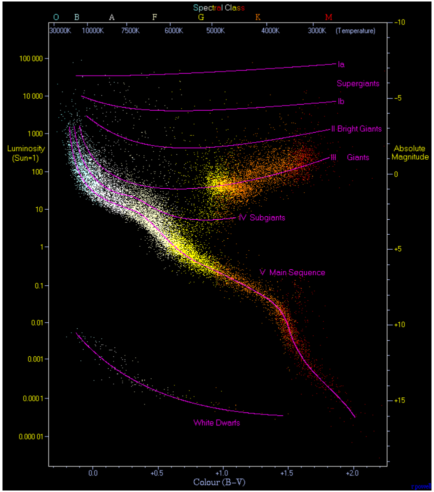

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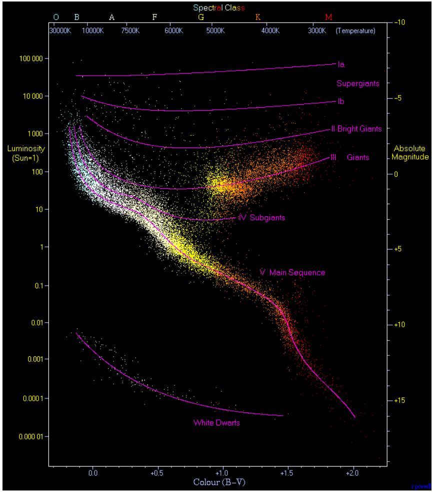

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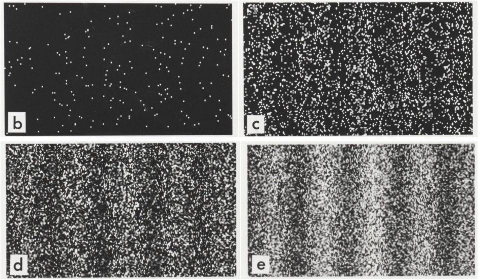

Dr. Tonomura

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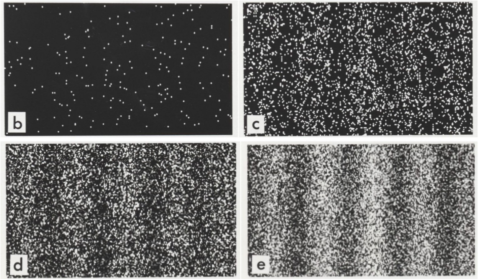

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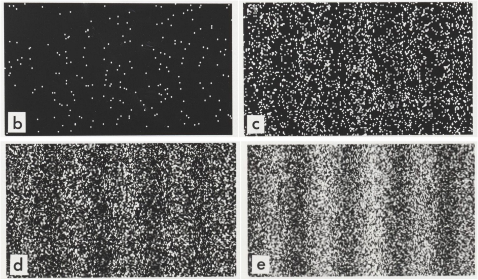

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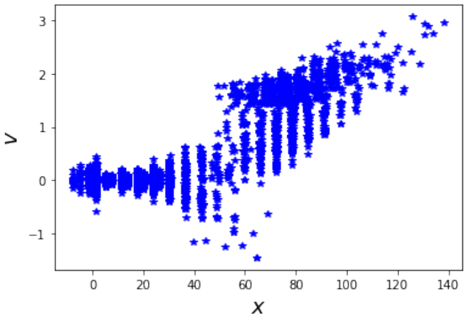

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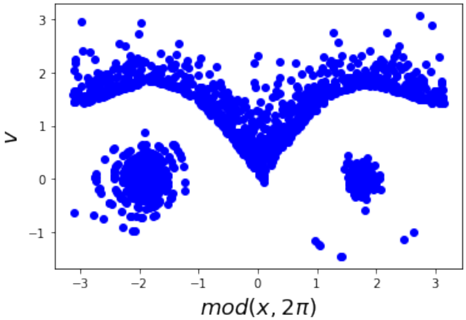

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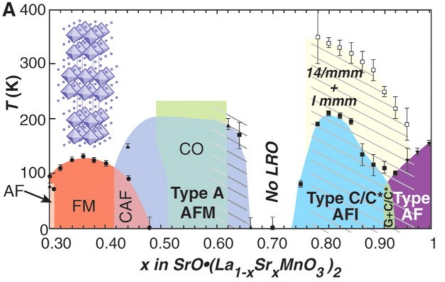
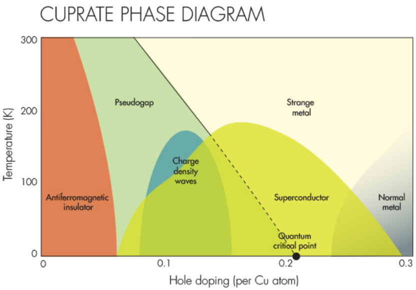
Unsupervised phase classification

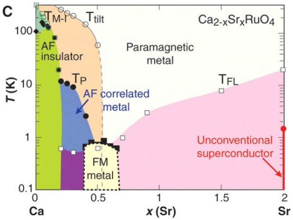
Bilayer Manganites [Dagotto, Science (2005)]



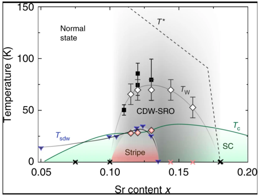
Cuprates [Shmahalo, Quanta Magazine, (2016)]



Single layered Ruthenates [Dagotto, Science (2005)]



LASCO [Wen at al.,Nature Comm. (2019)]



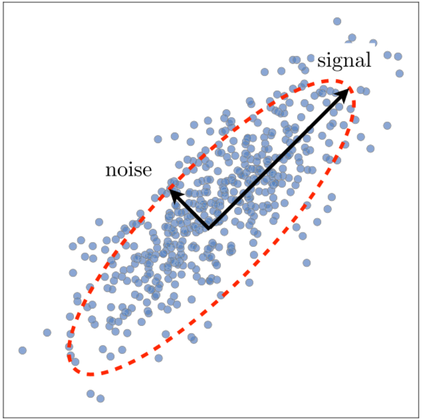
Outline

- **Principal Component Analysis (PCA)**
  - Dimensional reduction and visualization
  - Unsupervised phase classification
  - Kernel PCA
- **Clustering**
  - K-Means
  - Density-based (DB) clustering
- **Unsupervised phase classification**
  - Complicated phase diagrams
  - *Interpretability*

Dimensional reduction, data visualization and phase transitions

Why to reduce dimensionality

- By dimension we mean measured property



Physics Reports 810,1 (2019)

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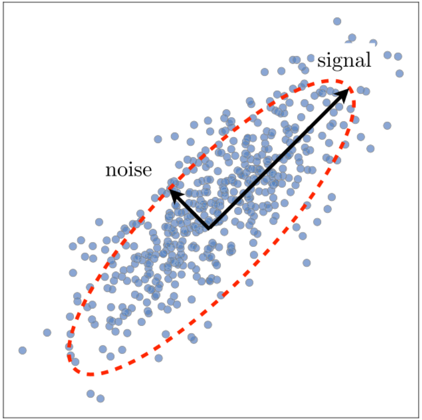

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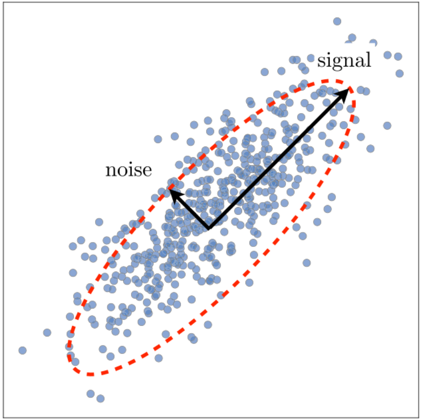

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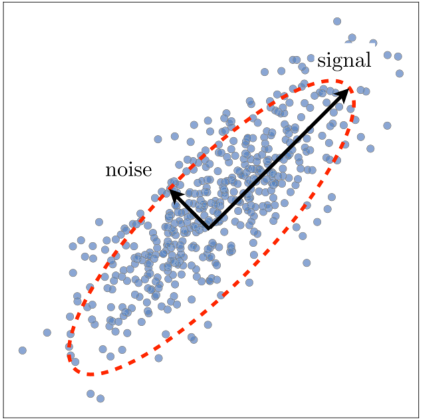

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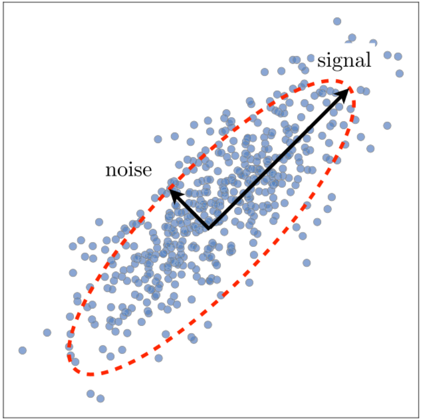
- **Intrinsic dimensionality** - a minimum number of dimensions required to capture the signal



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Singular Value Decomposition (SVD)

$$\boldsymbol{X} = \boldsymbol{U}\Sigma\boldsymbol{V}^T = \begin{bmatrix} \check{\boldsymbol{U}} & \check{\boldsymbol{U}}^{\perp} \end{bmatrix} \begin{bmatrix} \check{\Sigma} \\ \mathbf{0} \end{bmatrix} \boldsymbol{V}^T = \check{\boldsymbol{U}}\check{\Sigma}\boldsymbol{V}^T$$

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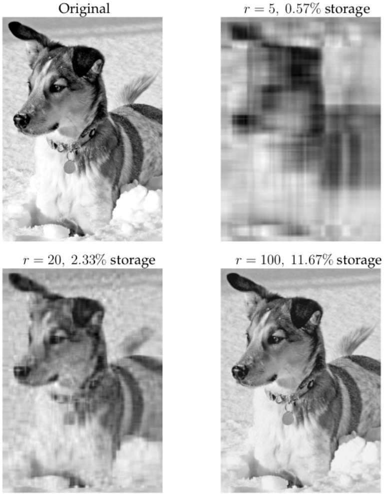
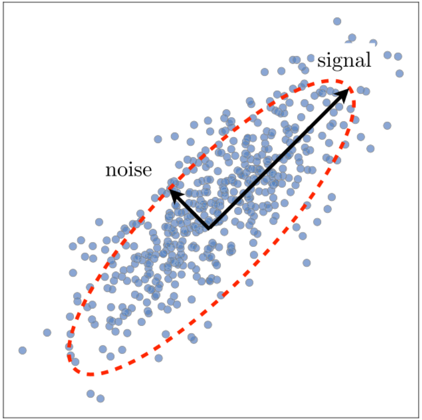


Original image resolution is 2000 × 1500

Brunton and Kutz, Data Driven Science & Engineering

Principal component analysis (PCA)

- **PCA** is the most important application of the SVD in ML
  (SVD is related to eigenvalue problem of the covariance matrix matrix $\frac{1}{n-1}\boldsymbol{X_c}\boldsymbol{X_c}^\dagger = \boldsymbol{V}\frac{\Sigma^2}{l-1}\boldsymbol{V}^\dagger$)



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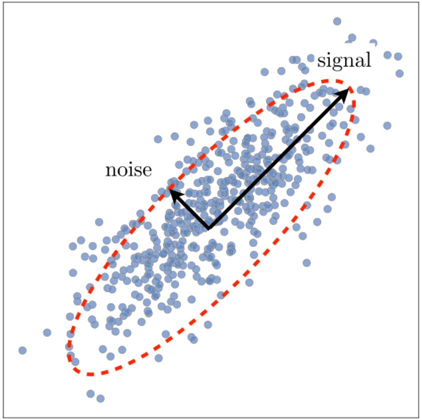

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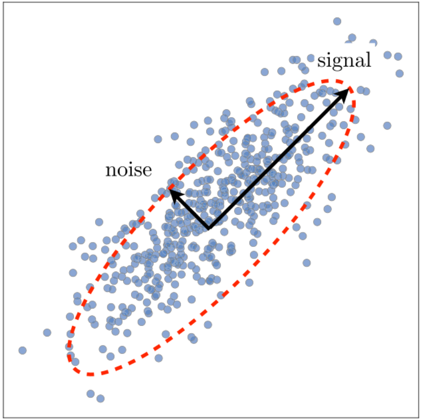

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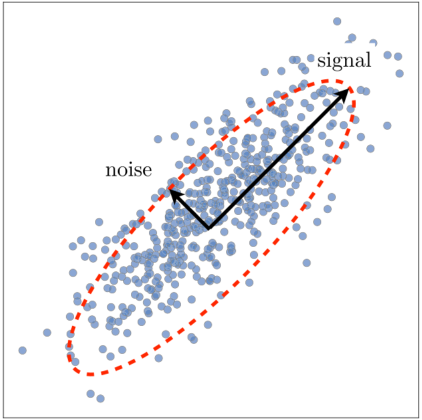

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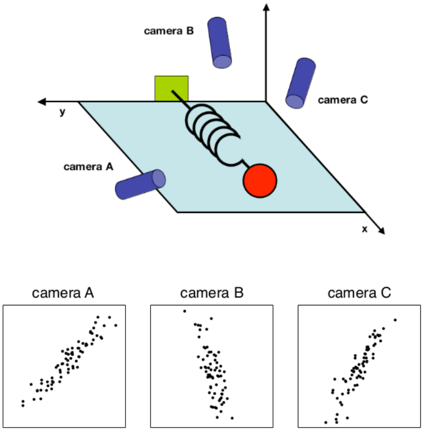
- Let me explain [Check notebook pca_blobs]



J. Shlens: A Tutorial on Principal Component Analysis

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  - profit

Why does PCA work and when it does not?

PCA assumptions:

Linearity

The new basis is build as a linear combination of the components of the original one.

Large Signal to Noise ratio

Principal components with larger associated variances represent the droids we are looking.

The principal components are ortogonal

This allows us to use SVD and we can be sure that we will get the optimal result (If the three assumptions are true!)

Check notebook pca_blobs on Kernel PCA.

PCA and phase transitions

- The PCA is in physics usually used as a first step towards supervised learning.
- But (for me) there is a much more exciting application of PCA.
- Automatic identification of phase-boundaries without a supervision.

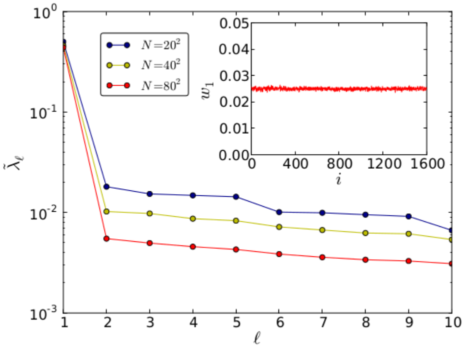
Test case the Ising model:

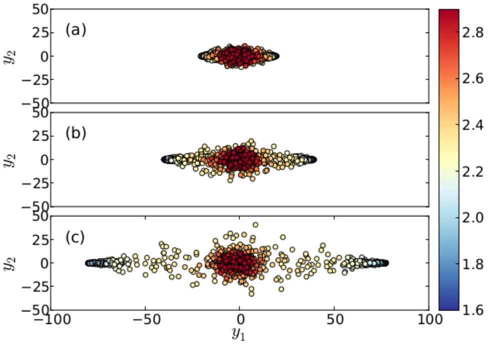
$$H = -J \sum_{\{ij\}} S_i S_j + h \sum_j S_j \tag{1}$$

Its a paradigmatic model for phase transitions and defines its universality class.

PCA and phase transitions in Ising model

Let's say that we don't know what we should measure. Therefore we will store snapshots of spin configurations. They contain all the information necessary for investigation of order and phase transitions. PCA can be used to extract it.





Wang, Phys. Rev. B **94**, 195105 (2016)

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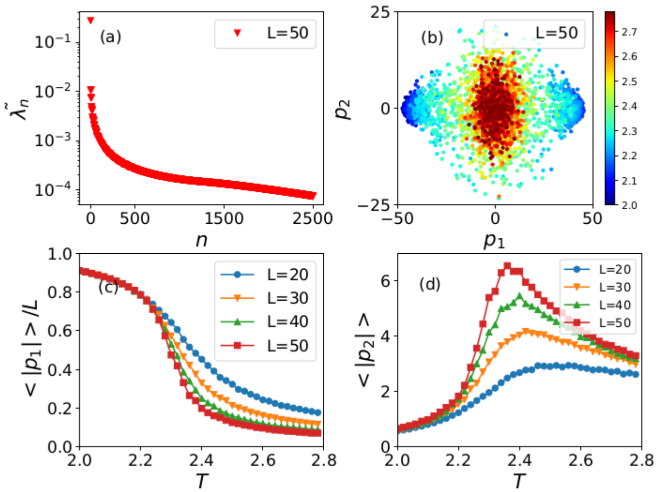
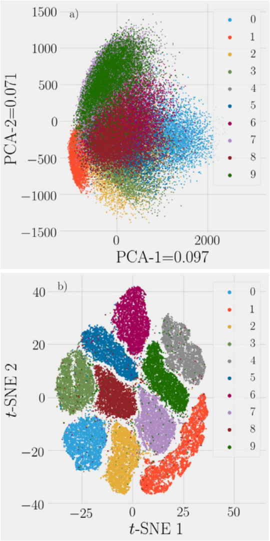


Hu et al., Phys. Rev. E **95**, 062122 (2017)

Other dimension reduction techniques

- t-SNE The basic idea is to associate a probability distribution to the neighborhood of each data point and keep similar instances together.



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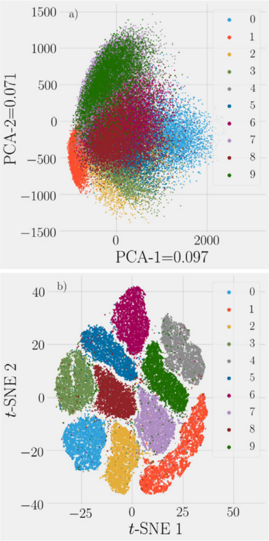

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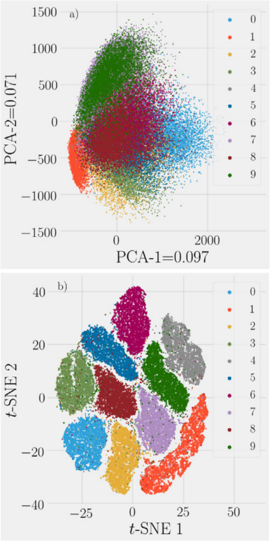

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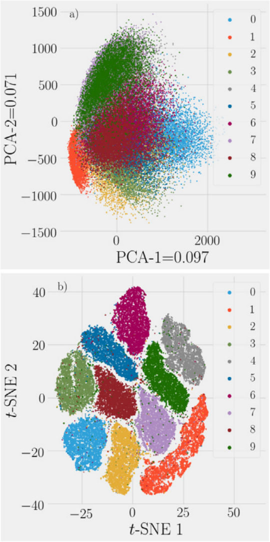

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Clustering

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- Probably the simplest way to seek a hidden structure
- Lots of methods

Basic concepts

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Basic concepts

- The aim of clustering is to group unlabeled data into clusters according to some similarity or distance measure
- Probably the simplest way to seek a hidden structure
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- We will talk about more standard ones: K-means and DB-clustering
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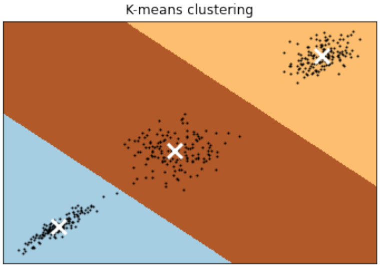
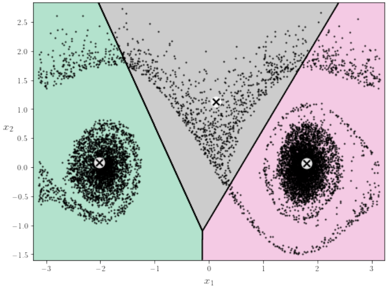
K-Means

- Let's have N unlabeled measurements $\boldsymbol{x}_i$, where $\boldsymbol{x}_i \in \mathbb{R}^p$





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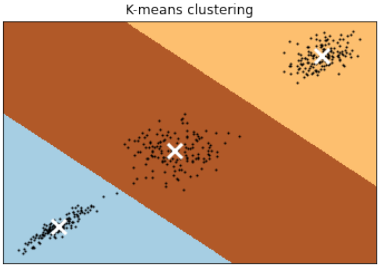

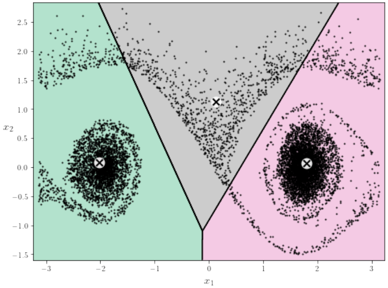

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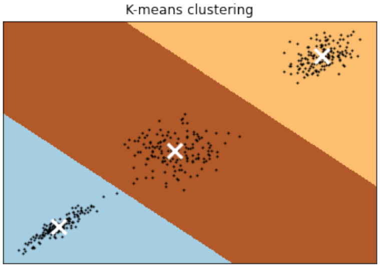

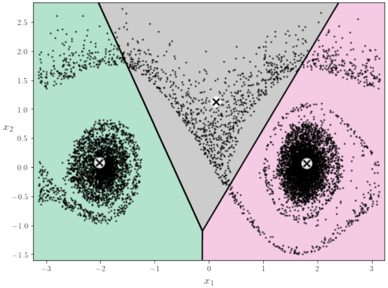

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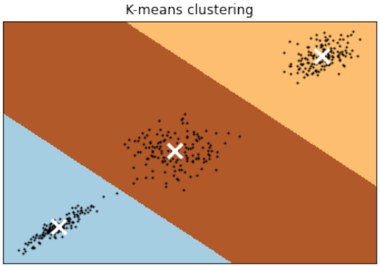

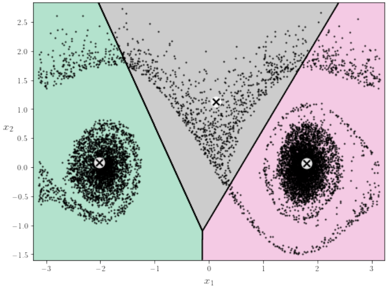

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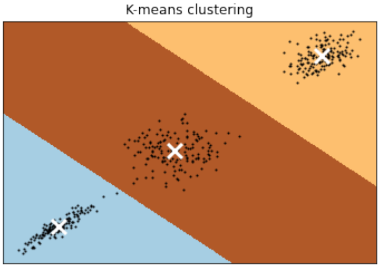
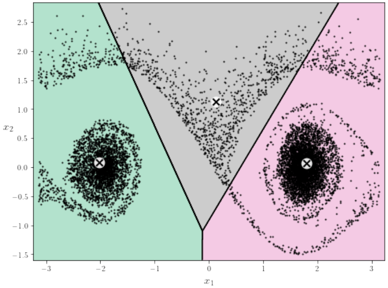
  Find the cluster means (positions) and the data point assignments to them in order to minimize the following cost function:

$$\mathcal{C}(\{\mathbf{x}, \boldsymbol{\mu}\}) = \sum_{k=1}^{K} \sum_{i=1}^{N} r_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)^2 \text{, where } r_{ik} \in \{0, 1\}$$

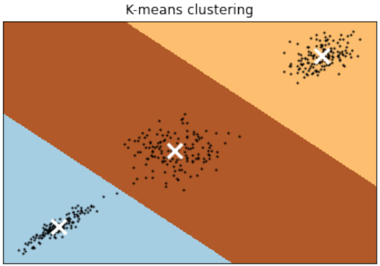


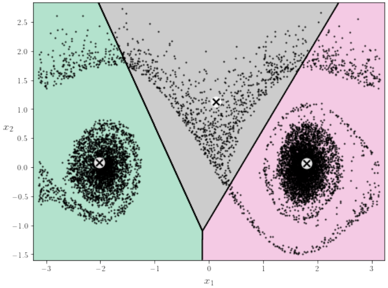


K-Means : optimization procedure

- Take assignments r, minimize $\mathcal{C}$ with respect to μ_k

$$\mu_k = \frac{1}{N_k} \sum_i r_{ik} \mathbf{x}_i$$





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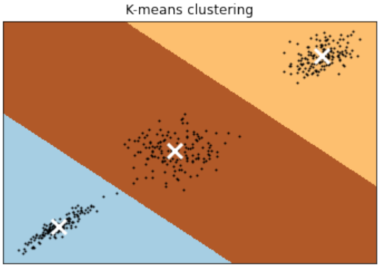

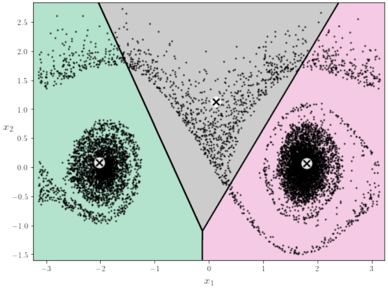

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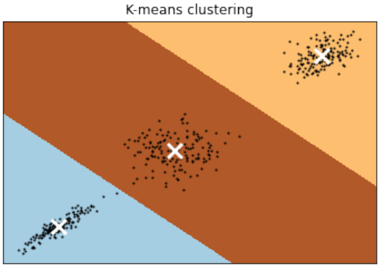

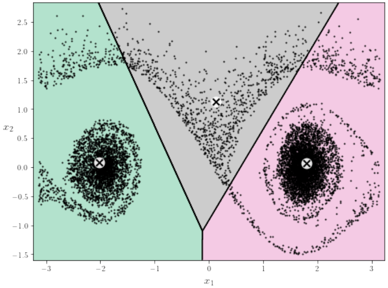

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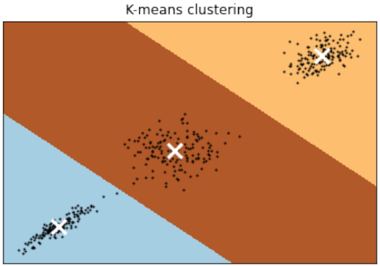

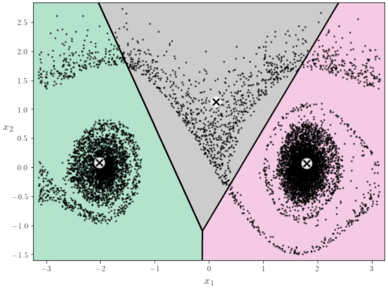

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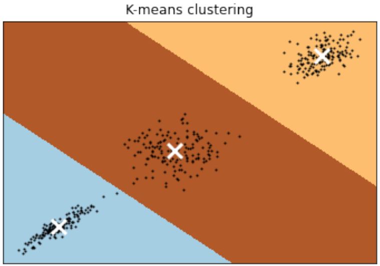
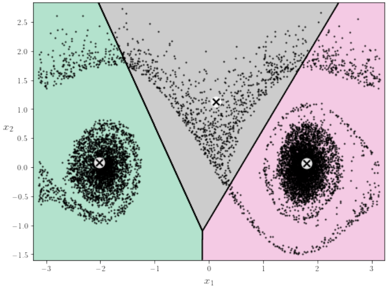
- Repeat! K-means algorithm is guaranteed to converge.
- Be aware that K-means can lead to spurious results





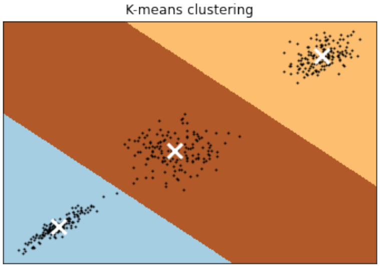
K-Means: Pros. and Cons.

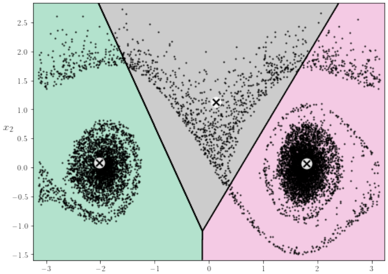
Advantages

- It is fast and scalable
- It converges (it will finish)
- Can be improved

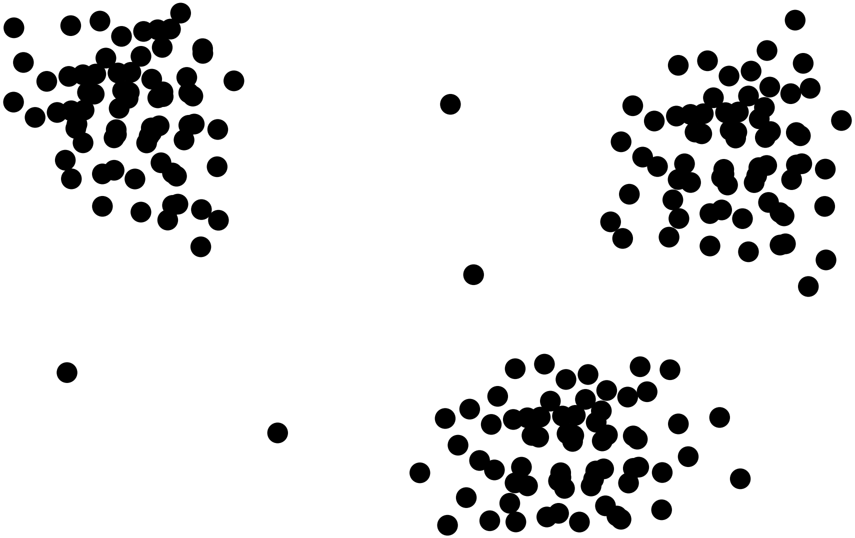
Disadvantages

- It must be run several times
- The number of clusters must be specify
- Does not behave well when the clusters have significantly
    - different size,
    - different densities,
    - nonspherical shapes





Density-based (DB) clustering DBSCAN



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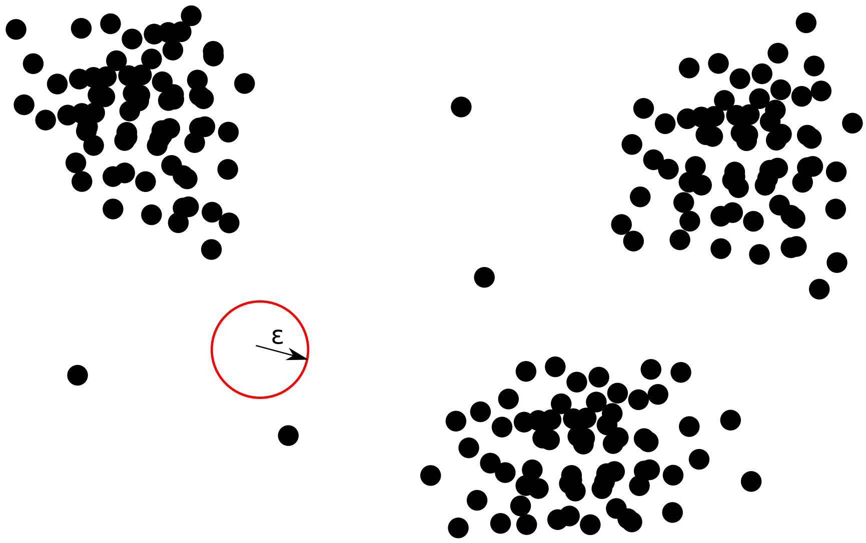

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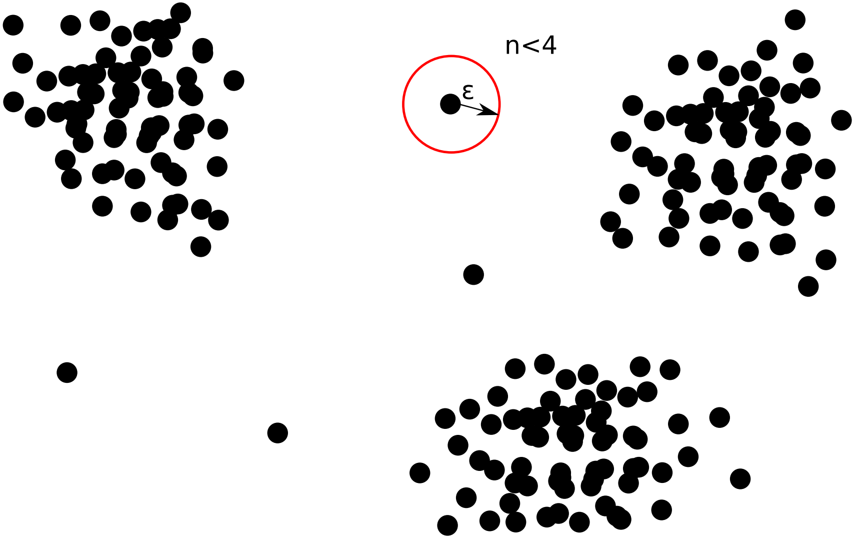

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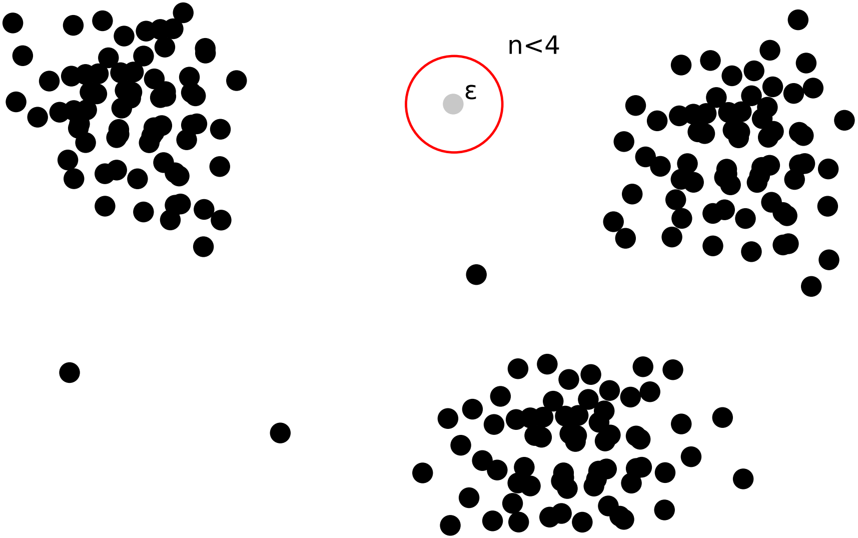

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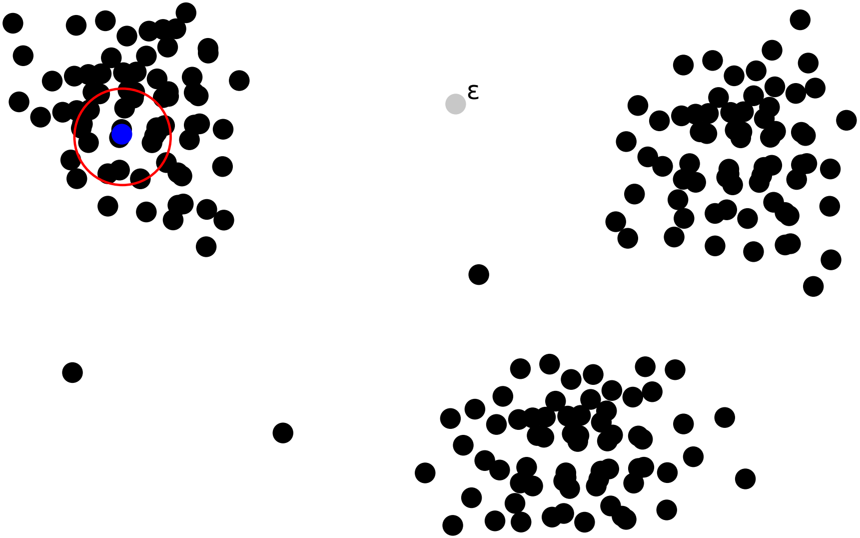

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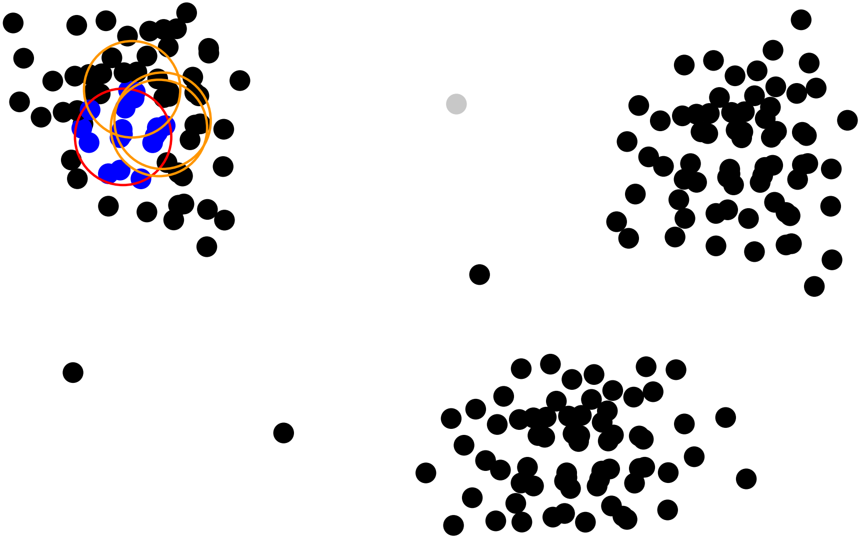

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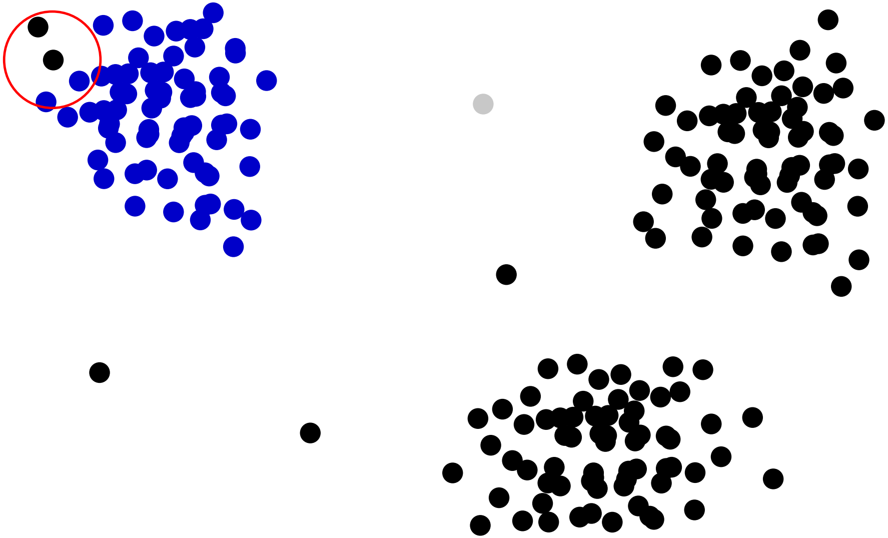

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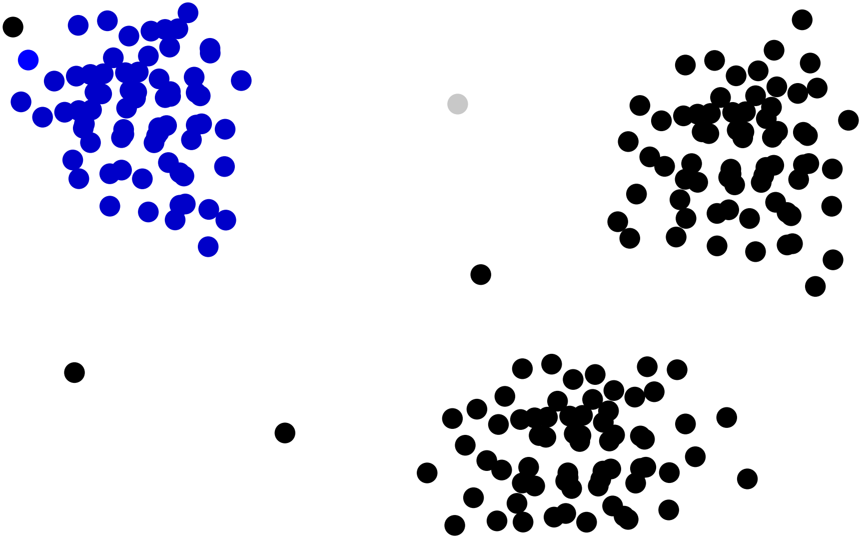

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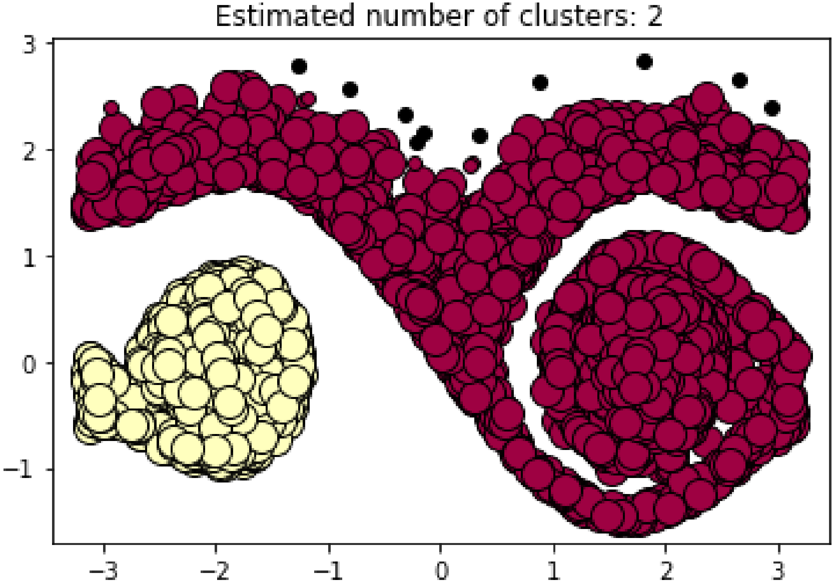

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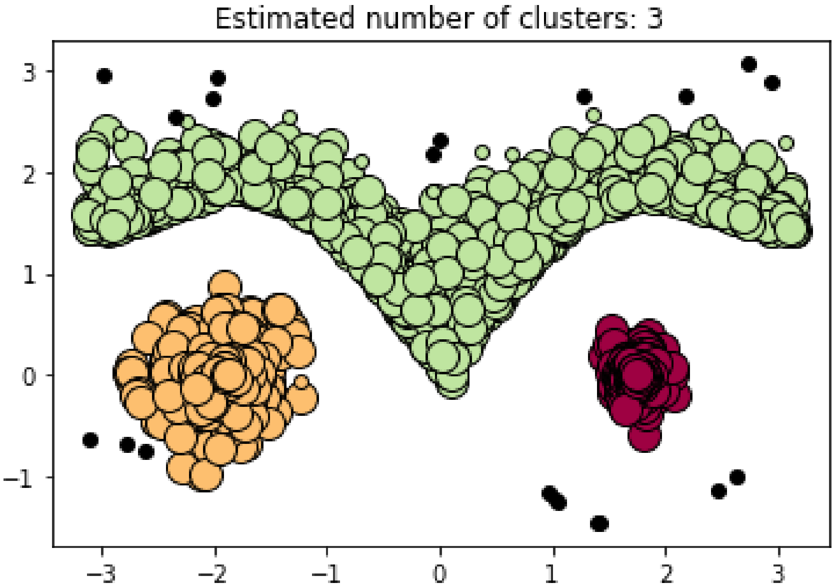
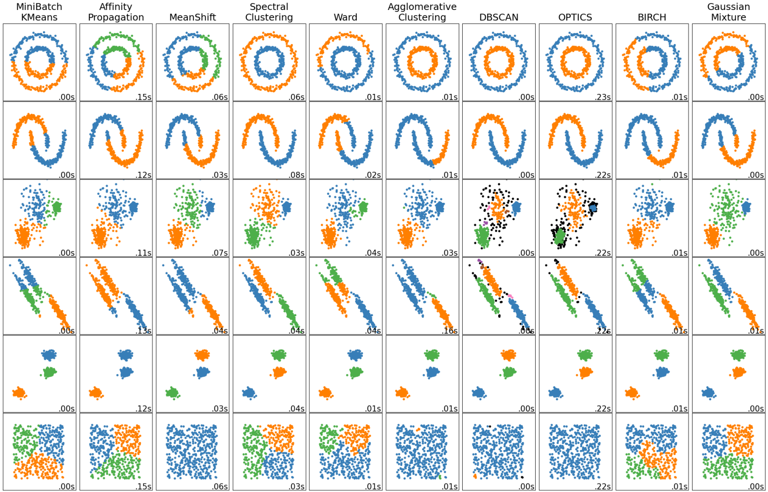


Other clustering techniques

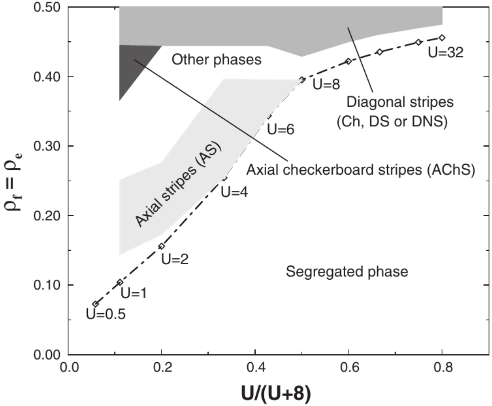


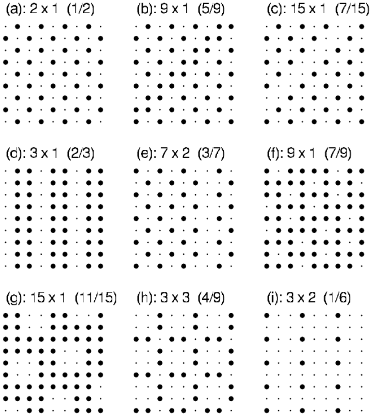
Comparing different clustering algorithms in sklearn

Unsupervised phase classification

More complicated systems, e.g., Phase diagram of correlated electrons

$$H_{FK} = -t \sum_{\langle i,j \rangle} \hat{d}_i^\dagger \hat{d}_j + U \sum_i \hat{f}_i^\dagger \hat{f}_i \, \hat{d}_i^\dagger \hat{d}_i$$





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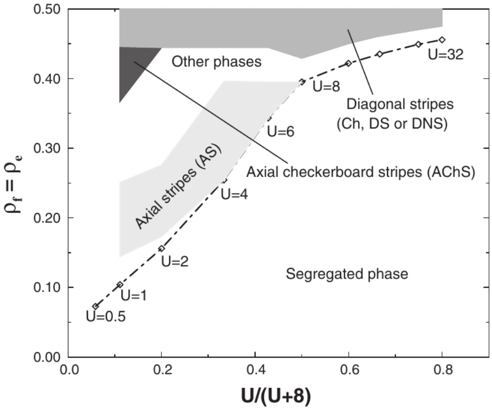

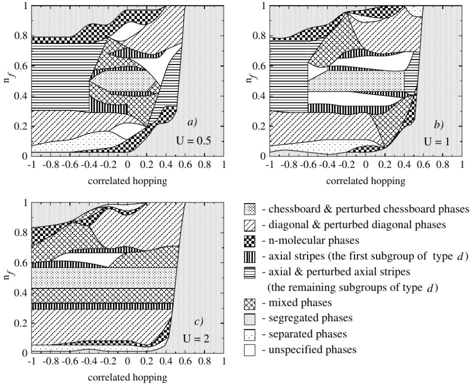

Phase diagram of generalized FKM [Čenčariková et al., (2011)]

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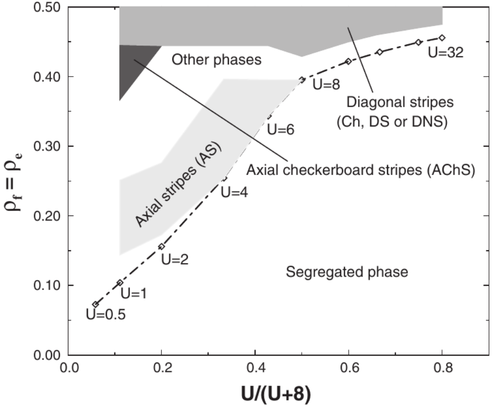
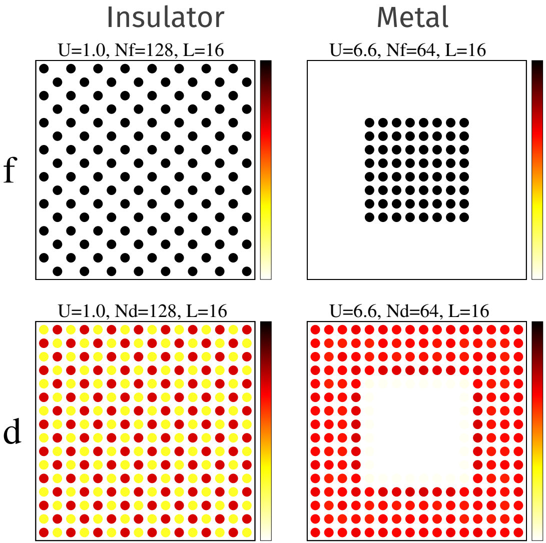


- The classification of GS phases in the FKM was for years a manual, lengthy and cumbersome task
- Yet, it seems to be suited for the modern Machine learning (ML) techniques
- But we need something better then standard techniques

Different ordering (phases) have different physical properties



Automatic classification - basic principles

We want to construct the phase diagram without supervision!

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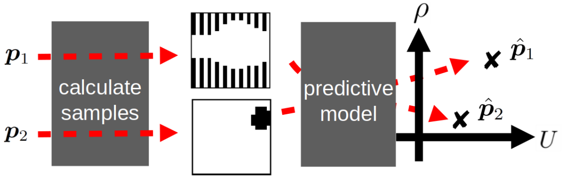

We can train neural network to infer $\overline{\boldsymbol{p}} \equiv (\overline{U}, \overline{\rho})$ by minimizing $\delta \boldsymbol{p} = ||\boldsymbol{p} - \overline{\boldsymbol{p}}||$

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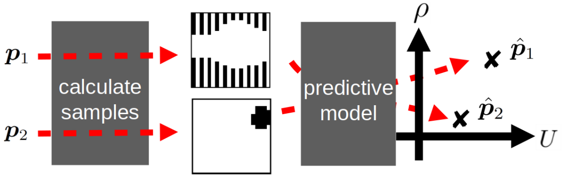

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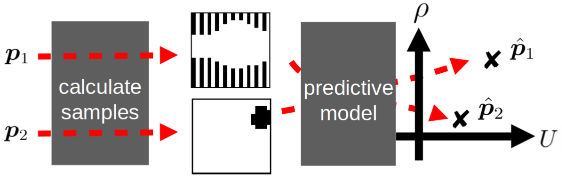

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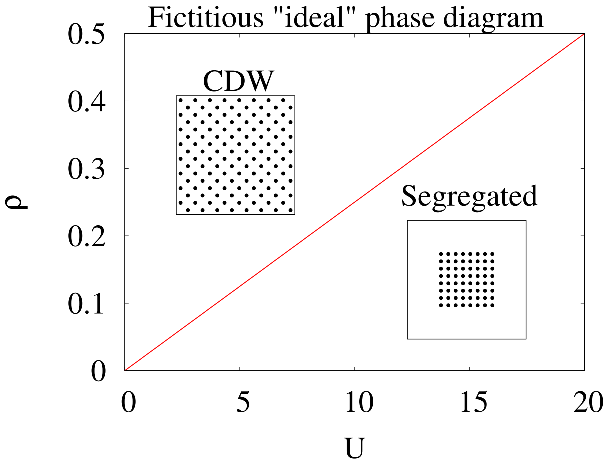
- We needed DNN (namely CNN), but other predictive models can be used
- The MSE loss function is defined as

$$\mathcal{L}_{\mathrm{MSE}} = \frac{1}{N_{\mathrm{p}} N_{\mathrm{x}}} \sum_{\boldsymbol{p}} \sum_{\boldsymbol{x}} \left|\left| \boldsymbol{p} - \overline{\boldsymbol{p}(x)} \right|\right|^2$$

Automatic classification - basic principles



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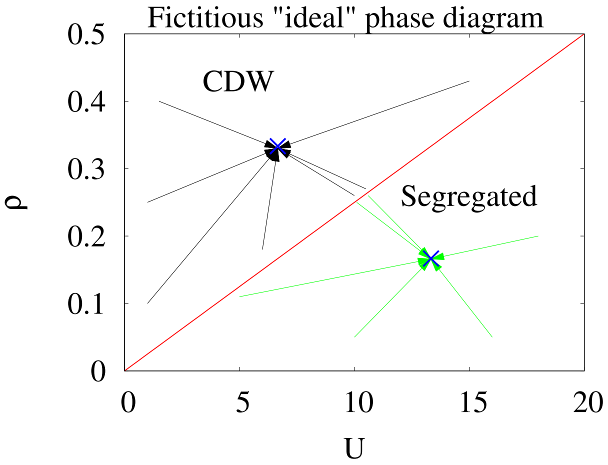

When is MSE loss function minimal?

$$\mathcal{L}_{\mathrm{MSE}} = \frac{1}{N_{\mathrm{p}} N_{\mathrm{x}}} \sum_{\boldsymbol{p}} \sum_{\boldsymbol{x}} \left|\left|\delta \boldsymbol{p}(x)\right|\right|^2$$

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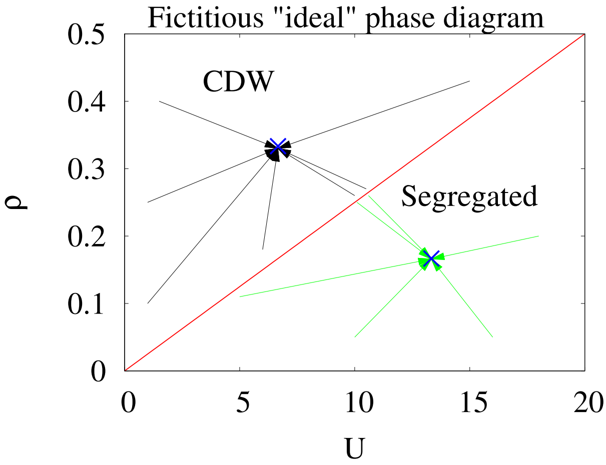

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The vector-field divergence signals phase boundaries

$$\nabla_{\boldsymbol{p}} \cdot \delta \boldsymbol{p} = \frac{\partial \delta U}{\partial U} + \frac{\partial \delta \rho}{\partial \rho}$$

Final phase diagram