Lecture 6:
More tricks of the trade

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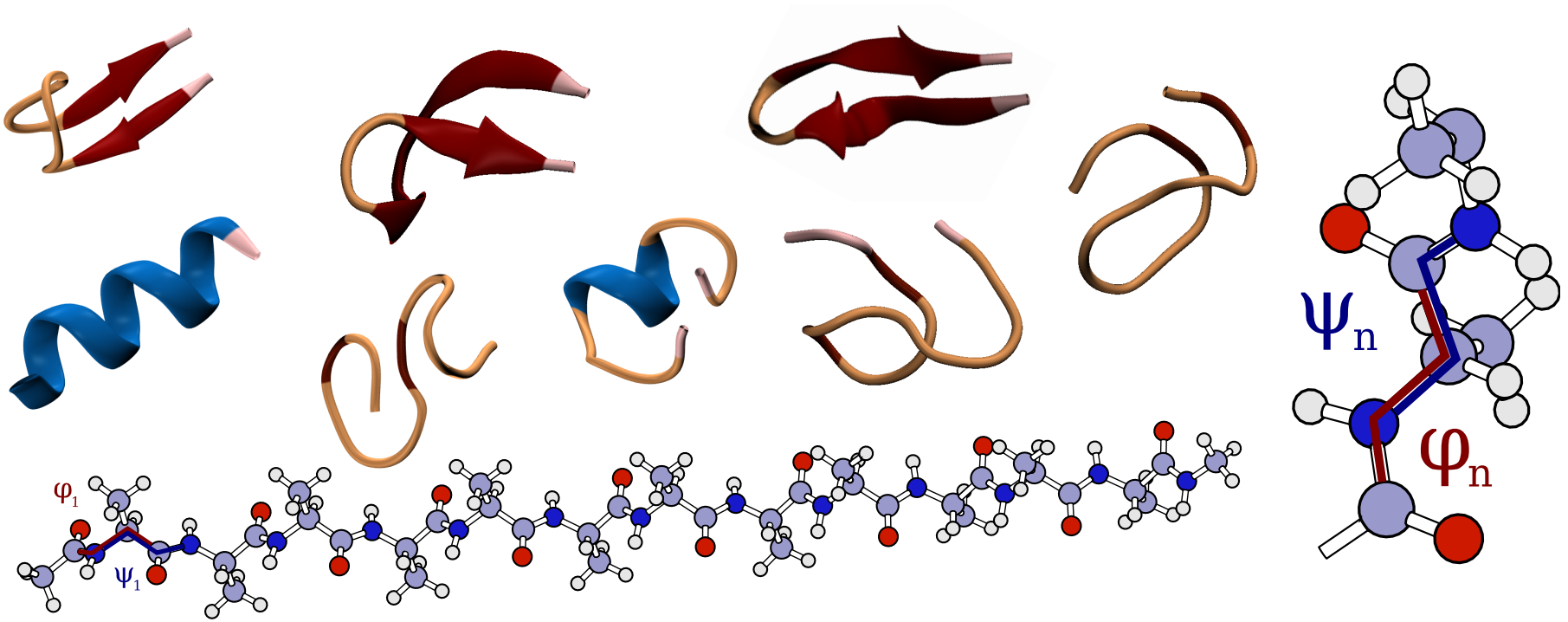
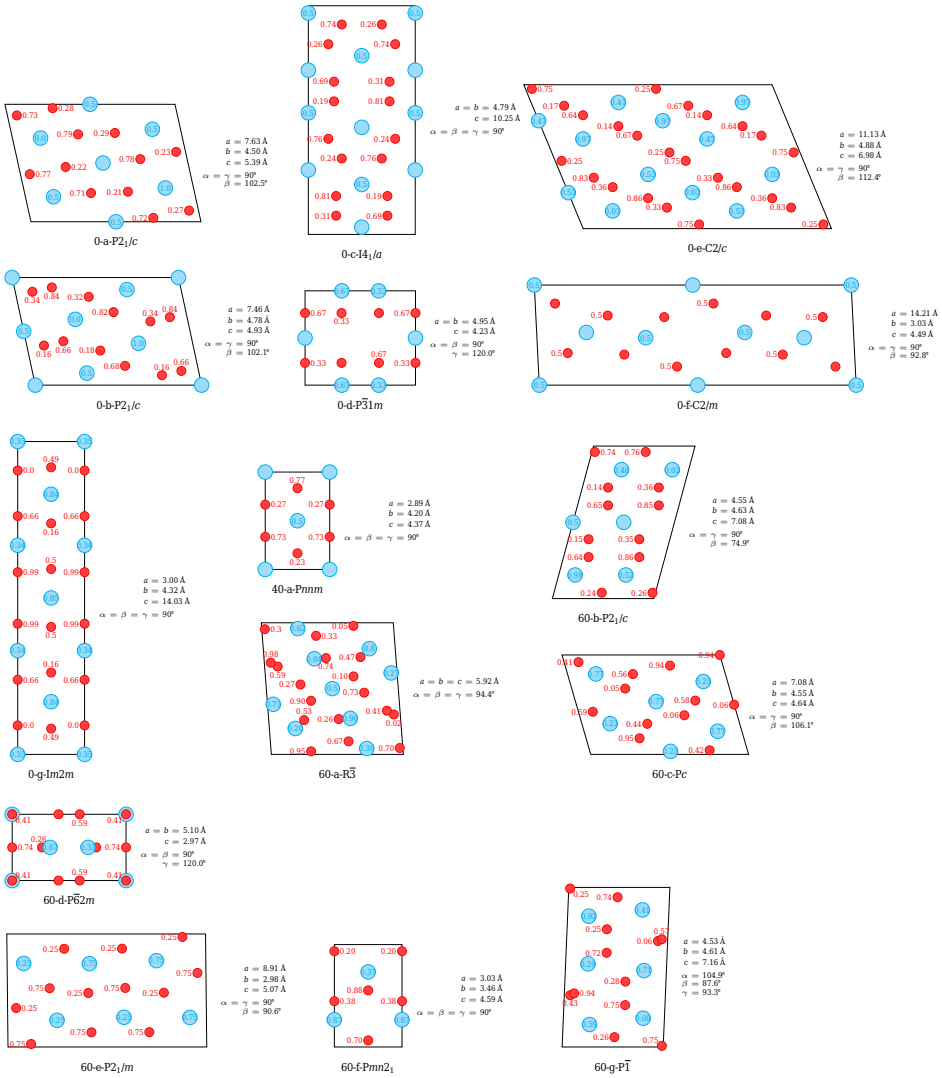
Recap

- The basic concept in machine learning
- Linear regression, nonlinear regression, kernel regression
- Neural networks, deep learning
- Representations of molecules
- Dimensionality reduction

Dimensionality reduction for chemical data



Dimensionality reduction for chemical data



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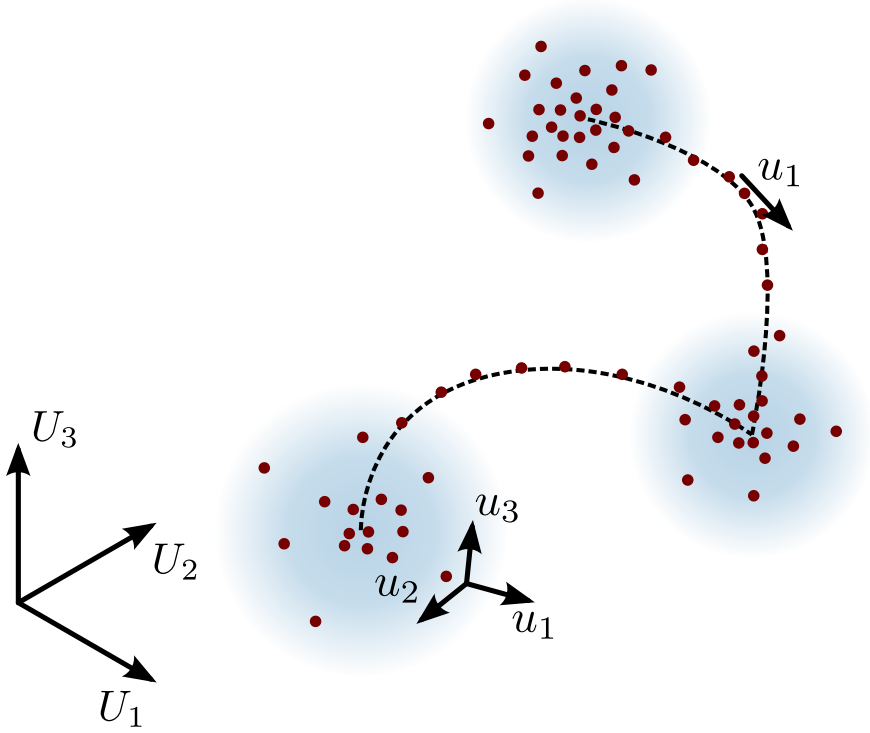
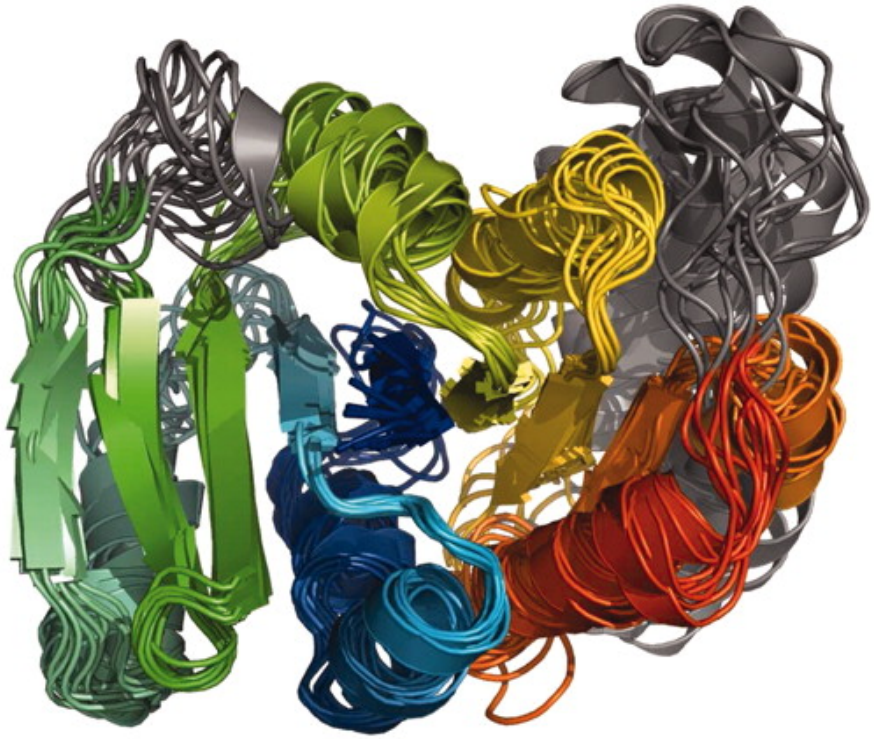




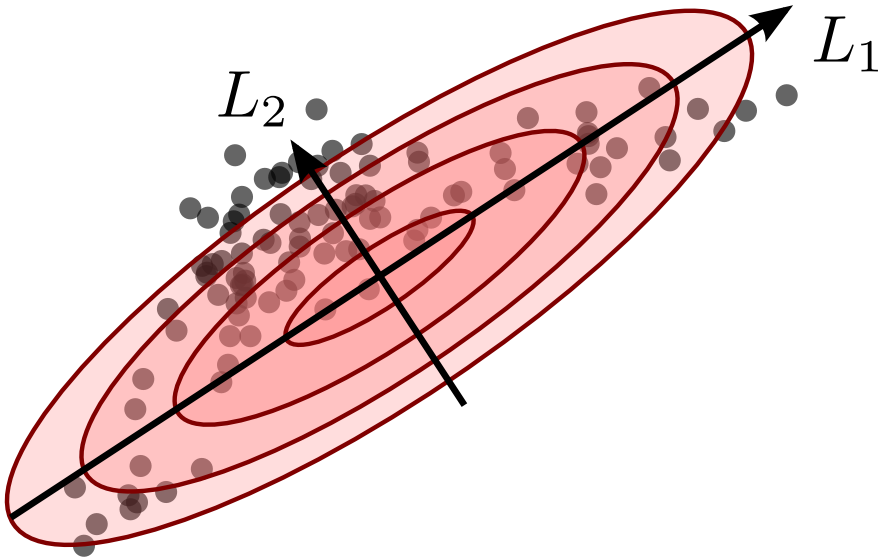
Outline

- More tricks of the trade
  - Sparsification
    - Single value decomposition (SVD)
    - CUR decomposition
    - Farthest Point Sampling (FPS)
  - Clustering
    - Gaussian mixture model (GMM)
    - K-means
    - DBSCAN
- Representing structual data

Principal component analysis

Question:
What is preserved during PCA?

Principal component analysis



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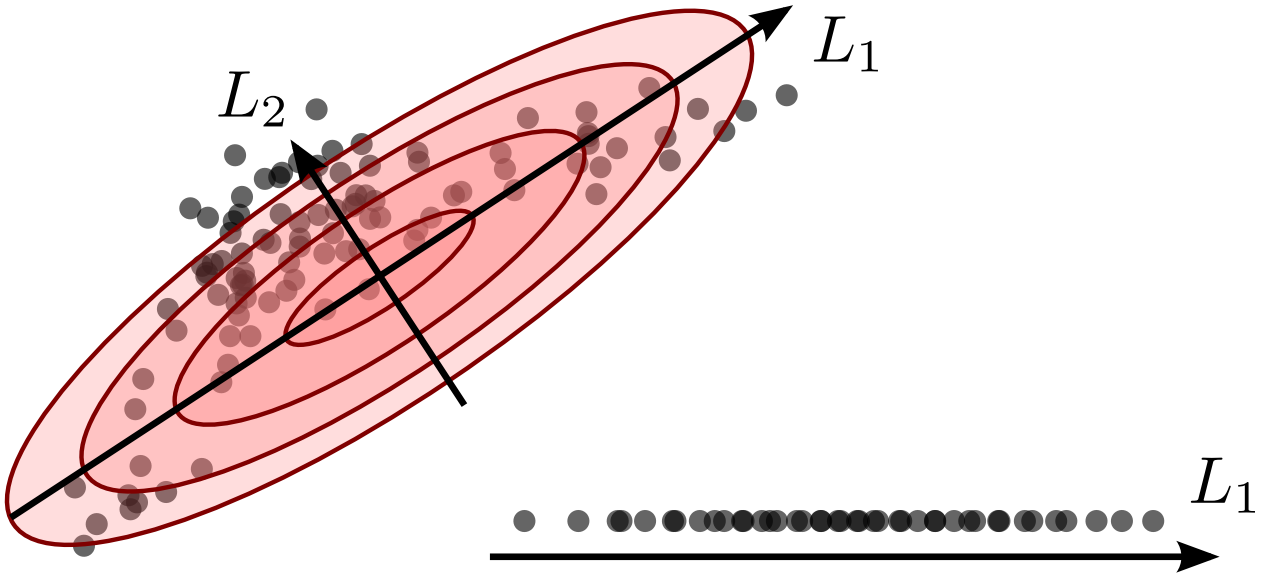
Principal component analysis



Question:
What is preserved during PCA?

Principal component analysis

PCA identifies the axis that accounts for the largest amount of variance in the data set.

- $\{\mathbf{X}_i\}^D$: data in the D-dimensional space
- $\{\mathbf{x}_i\}^d$: linear projection in the low d dimensional space
- $\mathbf{c}$: normalized projection matrix

$$\mathbf{x}_i = \mathbf{X}_i \mathbf{c}$$

- Covariance of the data: $\mathbf{C} = \mathbf{X}^T \mathbf{X}$
- Covariance of the projected data: $\mathbf{x}^T \mathbf{x}$

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Given d , how to reserve the largest amount of variance?

Principal component analysis

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Keep the first d eigenvectors of the covariance matrix $\mathbf{C} = \mathbf{X}^T\mathbf{X}$

Eigenvalues and eigenvectors

- The covariance matrix $\mathbf{C} = \mathbf{X}^T\mathbf{X}$: $D \times D$ form.
- Eigenvalues $\{\lambda^j\}$
- Corresponding eigenvectors $\{\mathbf{v}^j\}$ of the matrix

Eigenvalues and eigenvectors fulfills

$$\mathbf{C}\mathbf{v}^j = \lambda^j\mathbf{v}^j$$

for $j = 1 \ldots D$.
One can find the eigenvalues $\{\lambda^j\}$ by solving

$$det(\mathbf{C} - \lambda\mathbf{I}) = 0$$

Eigenvalues and eigenvectors

- The covariance matrix $\mathbf{C} = \mathbf{X}^T\mathbf{X}$: $D \times D$ form.
- Eigenvalues $\{\lambda^j\}$.Diagonal matrix $\Sigma = \mathbf{diag}(\lambda^1, \lambda^2, \ldots, \lambda^d)$
- Corresponding eigenvectors $\mathbf{V} = [\mathbf{v}^1, \mathbf{v}^2, \ldots, \mathbf{v}^d]$ of the matrix.
- Normalization condition $\mathbf{V}\mathbf{V}^T = \mathbf{I}$

The covariance matrix can be expressed as

$$\mathbf{C} = \mathbf{V}\Sigma\mathbf{V}^T$$

equalvalently

$$\Sigma = \mathbf{V}^T\mathbf{C}\mathbf{V}$$

Singular value decomposition (SVD)

a general matrix $\mathbf{M} \in \mathcal{R}^{m \times n}$ can be represented in the SVD form:

$$\mathbf{M} = \mathbf{U}\Sigma\mathbf{V}^T$$

- $\mathbf{U} = [\mathbf{u}_2, \mathbf{u}_2, \ldots, \mathbf{u}_m]$
- $\mathbf{V} = [\mathbf{v}_2, \mathbf{v}_2, \ldots, \mathbf{v}_n]$
- $\Sigma = \mathbf{diag}(\sigma_1, \sigma_2, \ldots, \sigma_p)$

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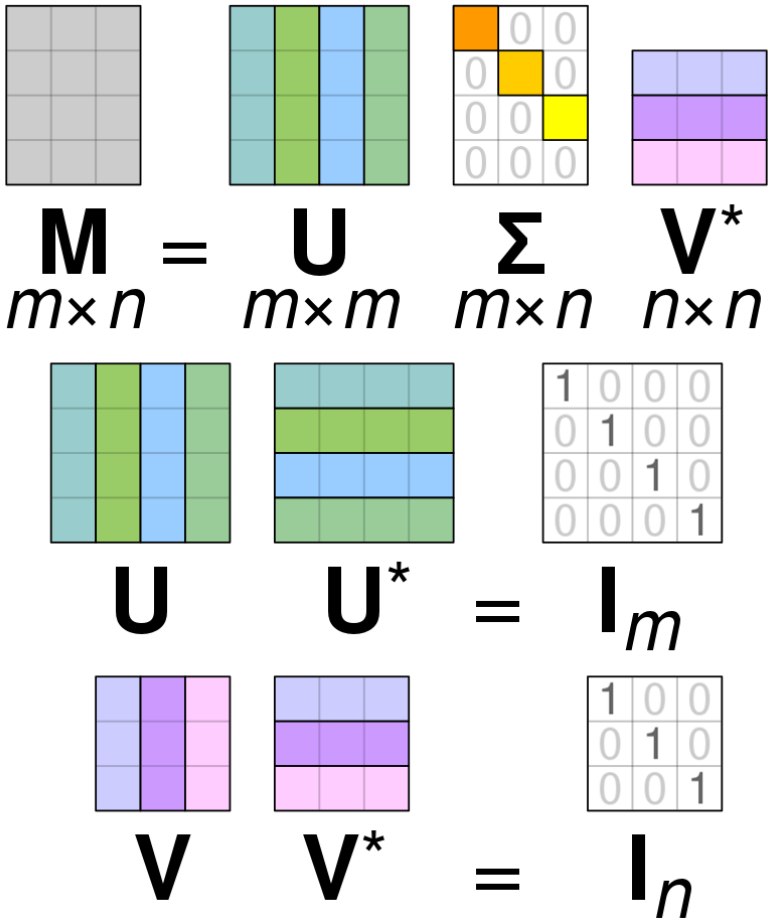

Singular value decomposition (SVD)

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$$\mathbf{M} = \mathbf{U}\Sigma\mathbf{V}^T$$

Problem: each vector $\mathbf{v}_i$ and $\mathbf{u}_i$ a linear combination of the original rows and columns of the design matrix, so they may not be particularly informative or meaningful.

Example: gene expression data, the eigenvector of images, and a linear combination of atomic environments.

CUR Decomposition

Similar with SVD, but using the actual rows and columns for the design matrix for the decomposition.

$$\mathbf{X} \approx \mathbf{C}\,\mathbf{U}\,\mathbf{R}$$

- $\mathbf{C} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_k]$
- $\mathbf{R} = [\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_k]^T$
- $\mathbf{U}$: a $k \times k$ matrix

Many ways of selecting $\mathbf{C}$ and $\mathbf{R}$:

- deterministic
- probabilistic

"CUR matrix decompositions for improved data analysis" PNAS 2009

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Q: What is the physical significance of CUR decomposition?

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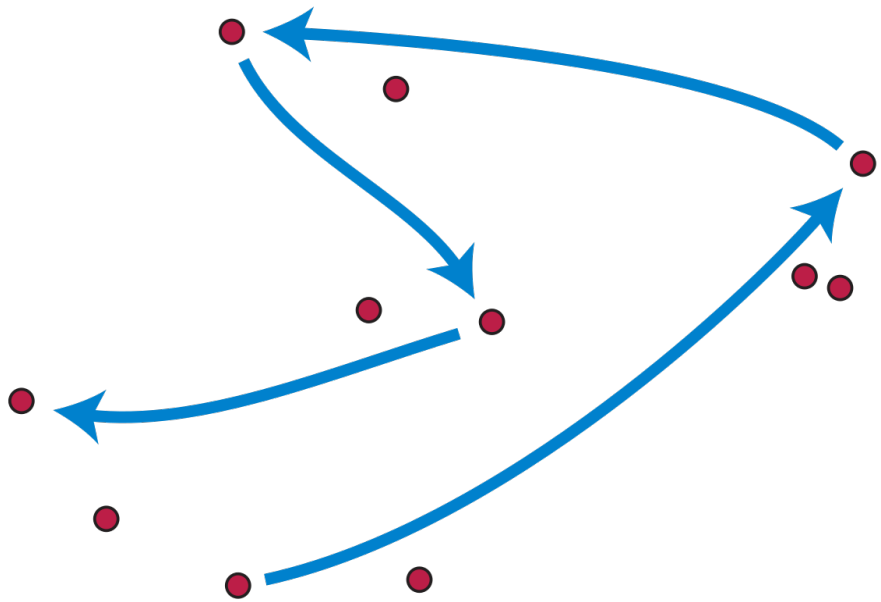
A: feature selection and data sparsification

"CUR matrix decompositions for improved data analysis" PNAS 2009

Farthest point sampling (FPS)

- Aim to select uniformly-spaced reference points
- Successive points are chosen so as to maximize the Euclidean distance between them.
  - Arbitrarily selecting the first fingerprint,
  - each subsequent one is chosen as
    $k = \text{argmax}(\min_j |\mathbf{x}_k - \mathbf{x}_j|)$



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    - DBSCAN
- Representing structual data

The IRIS dataset

- Measures of four morphological features (petal/sepal width/length) of a total of 150 samples of three species of iris
- 4D dataset, strong correlation between the indicators, but also spread within one species

Iris Setosa

Iris Versicolor

Iris Virginica

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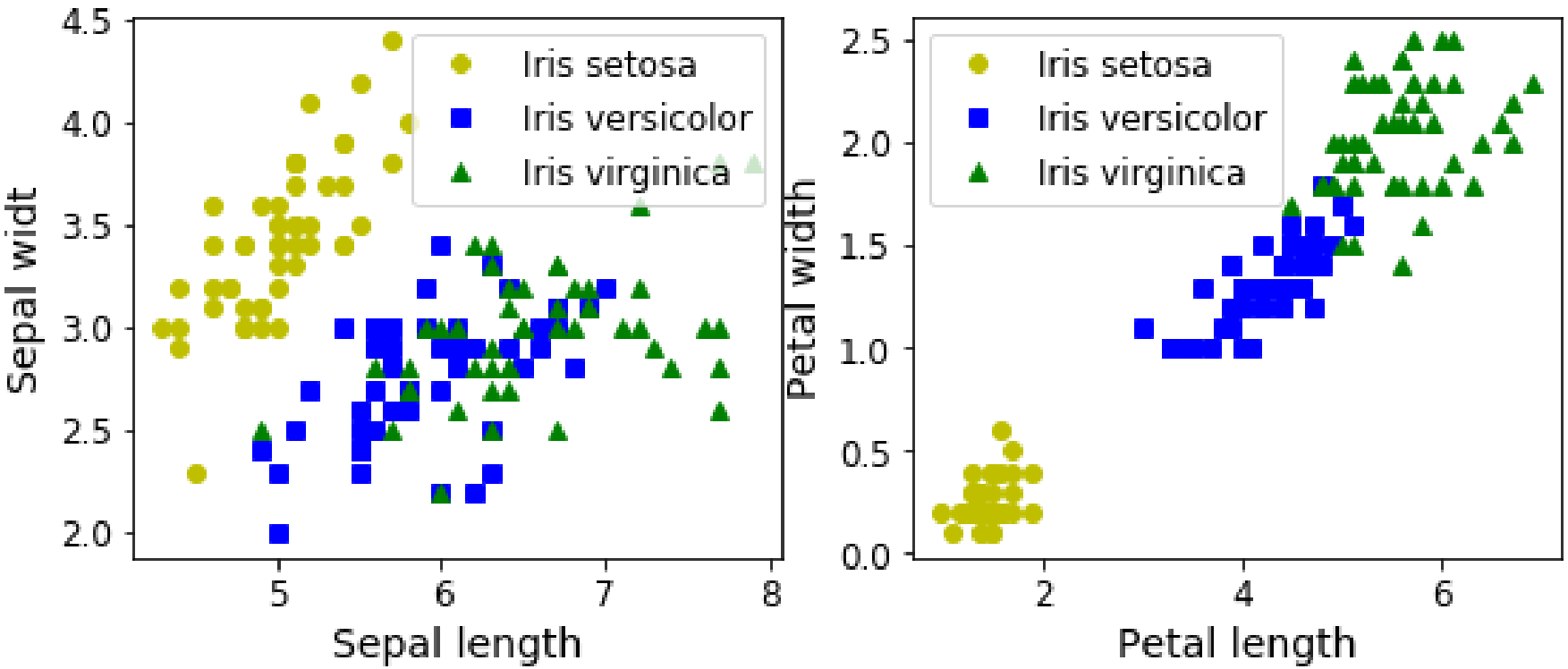


The IRIS dataset

- Clearly clustered in 2D.
- Versicolor and Virginica are pretty close... and they look quite similar!

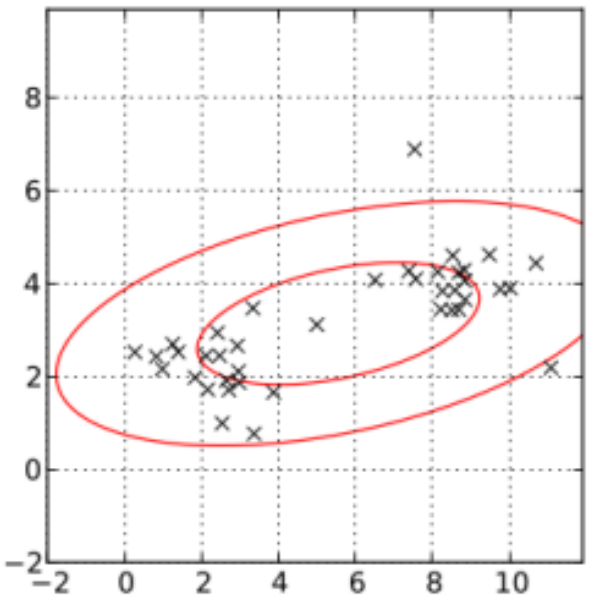
Iris Setosa

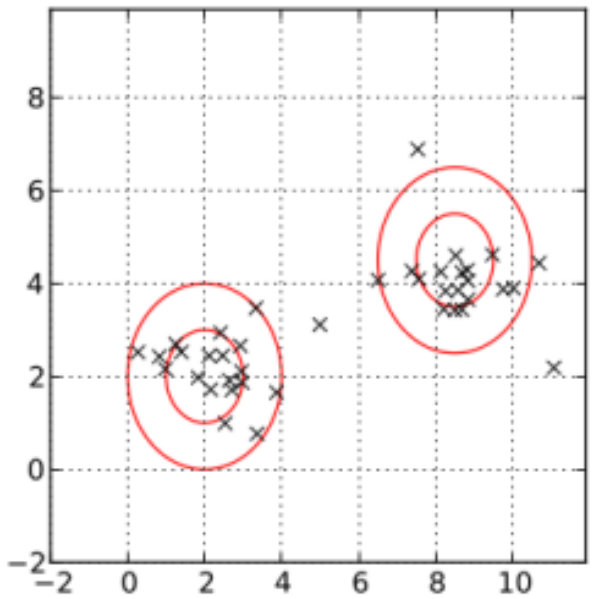
Iris Versicolor

Iris Virginica

Gaussian mixture model (GMM)

- good for multimodal distribution, and each blob is Gaussian-like
- K components:
  - a mean of μ_k and a covariance matrix of $\mathbf{C}_k$





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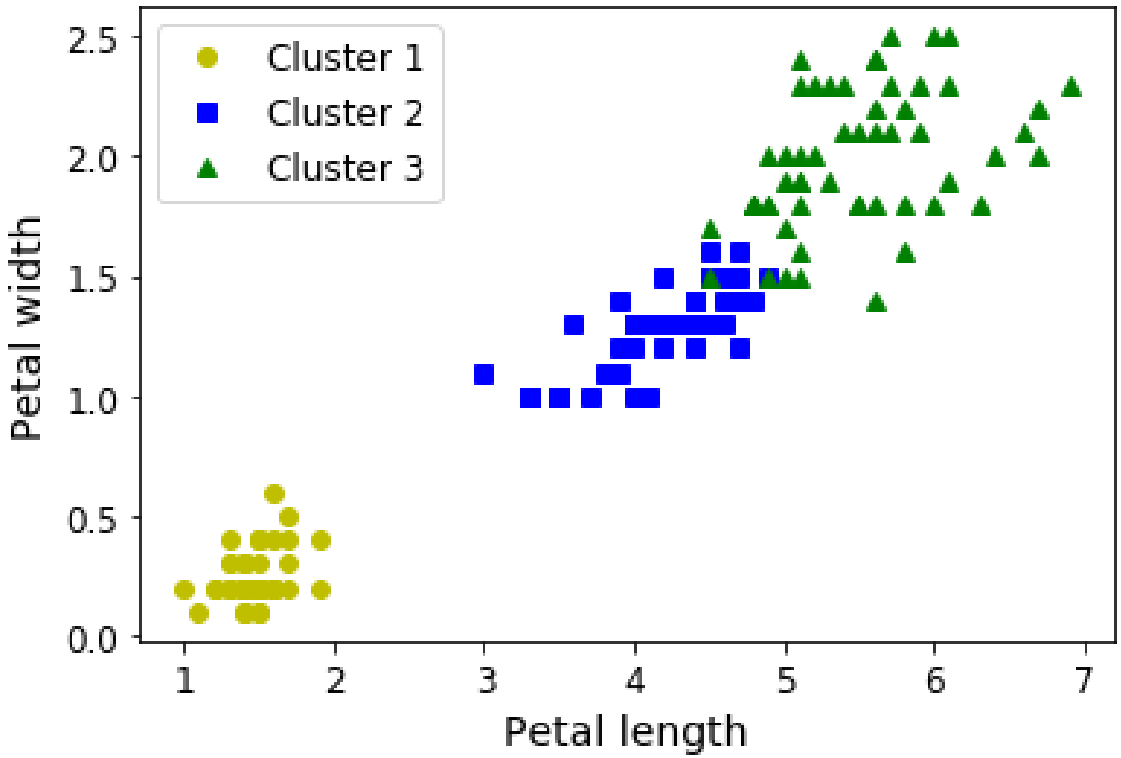

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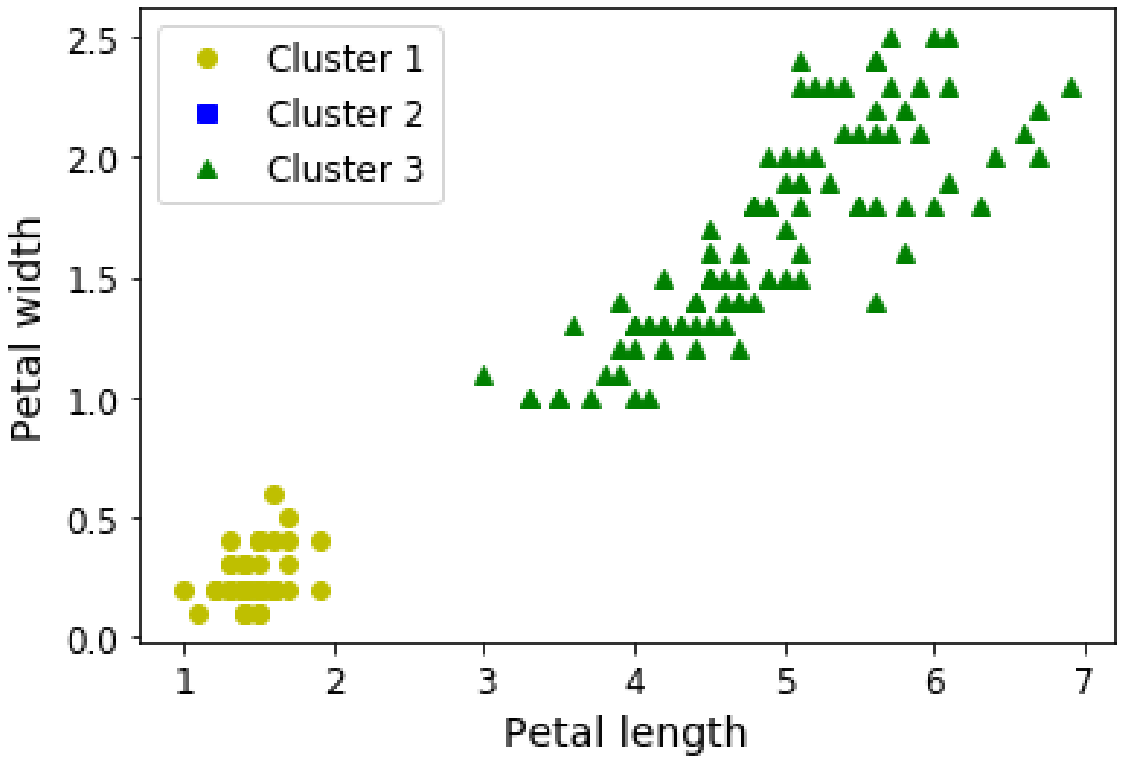
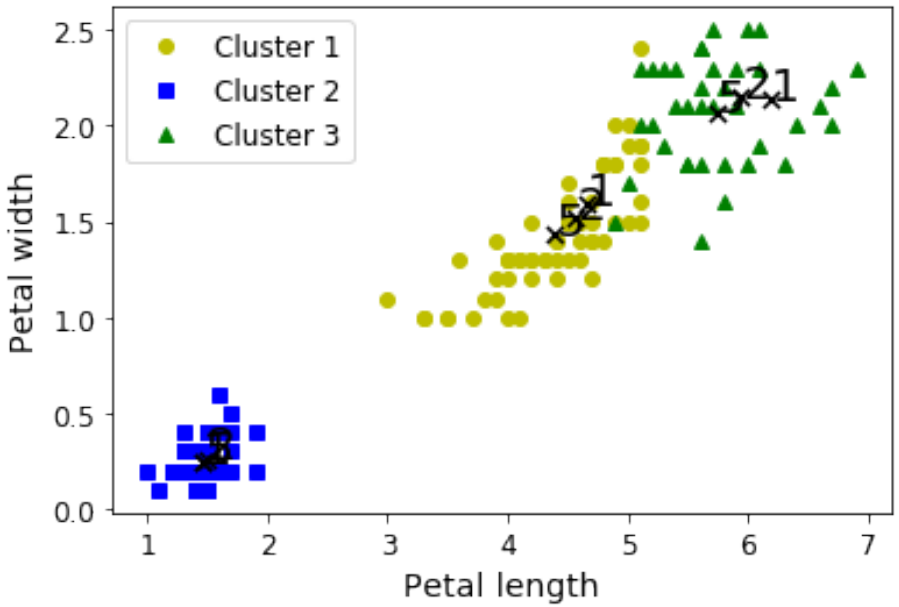


k-means clustering

A special case of GMM. Use an iterative procedure

- first placing the centroids randomly
- data points are assigned to their nearest centroid
- Then label the instances, update the centroids, and repeat



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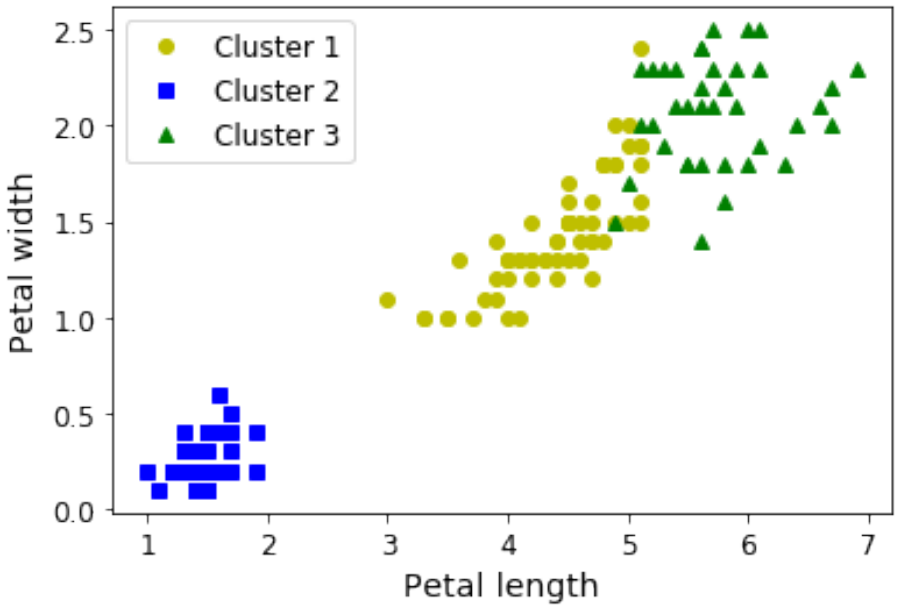
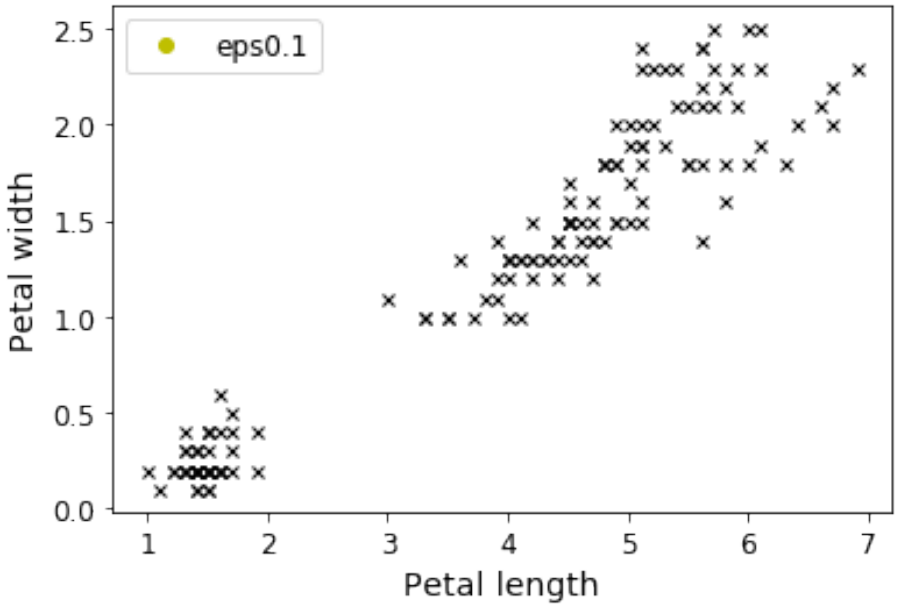


DBSCAN

Density based algorithm relying on two parameters (eps and min_samples)

- Counts number of points with a small distance ϵ
- If the number of neighbors > min_samples, it is a core instance.
- All points in the neighborhood of a core instance belong to the same cluster.
- Anything that is not a core instance and does not have one in its neighborhood is noise.



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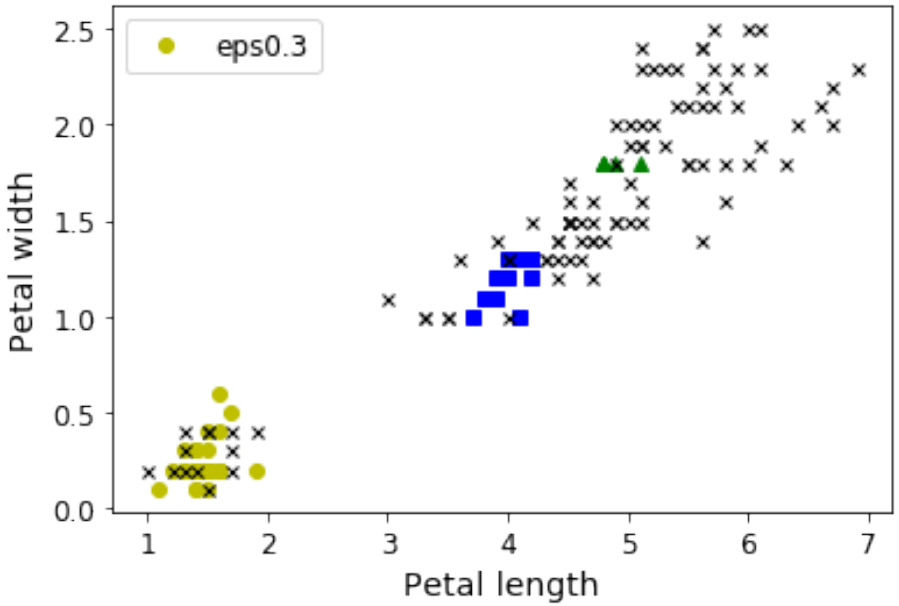

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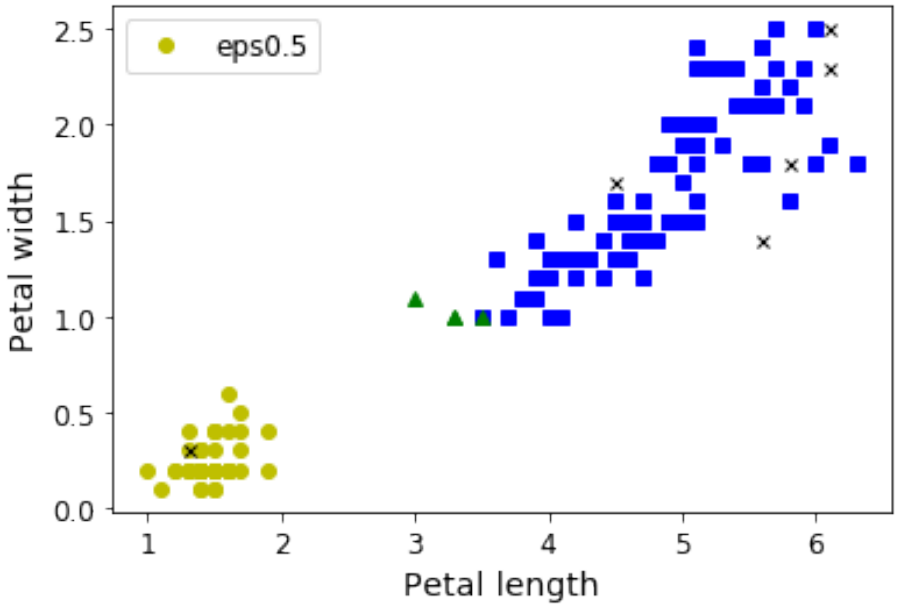
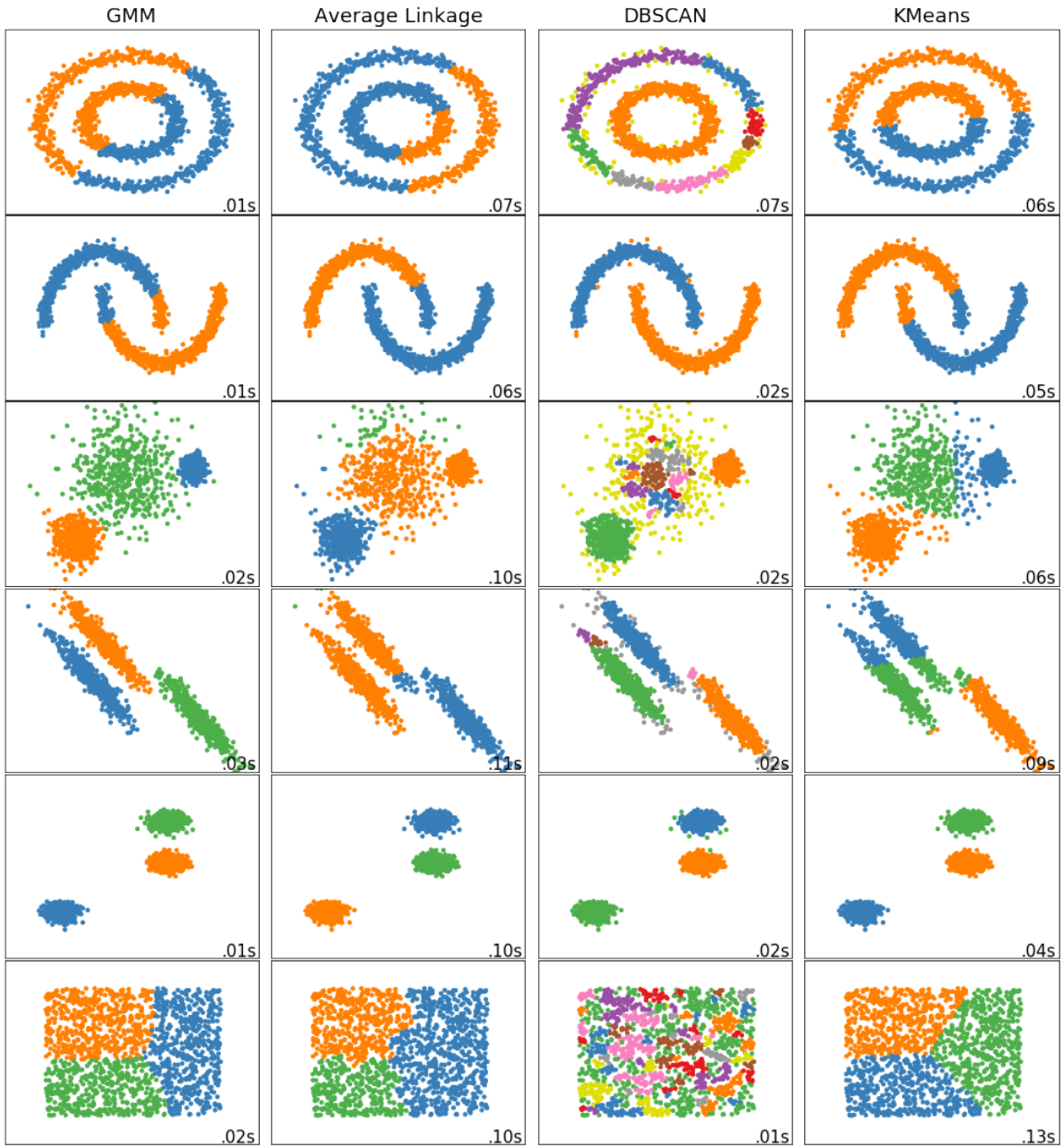


A comparison between clustering algorithms



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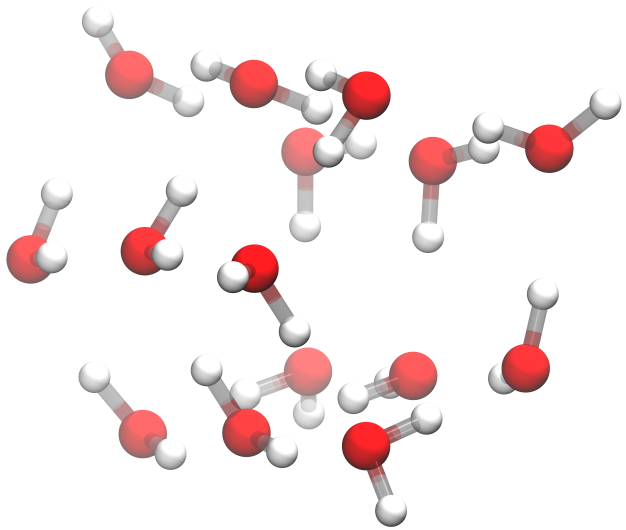
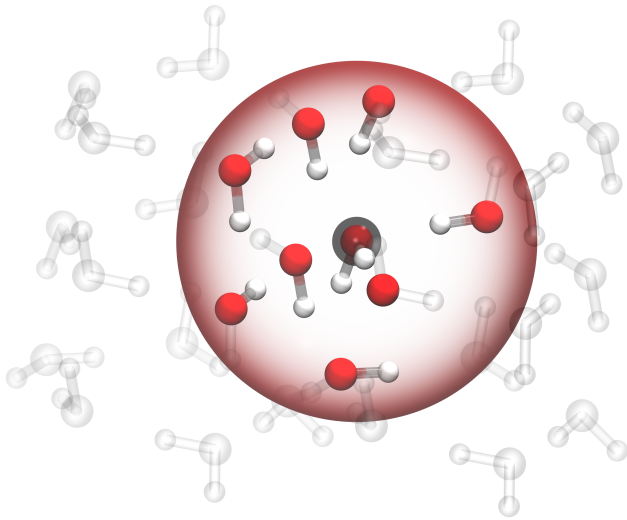
Representing atomistic environments



A



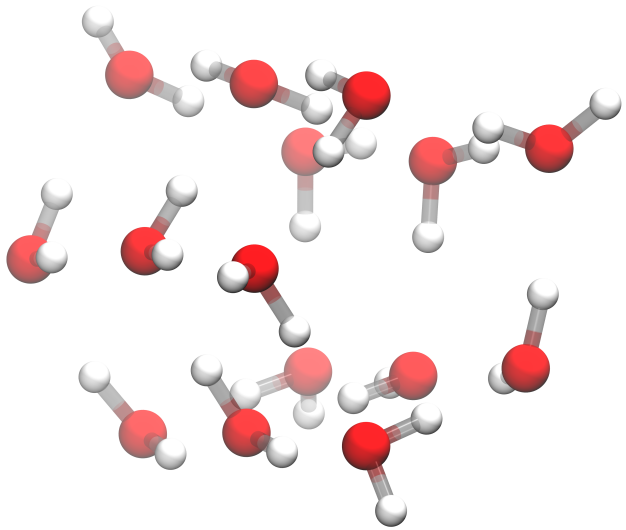
$\mathcal{X}_i$

The first step is to divide the system into a set of atomic environments.
So the task becomes representing atomic environments.

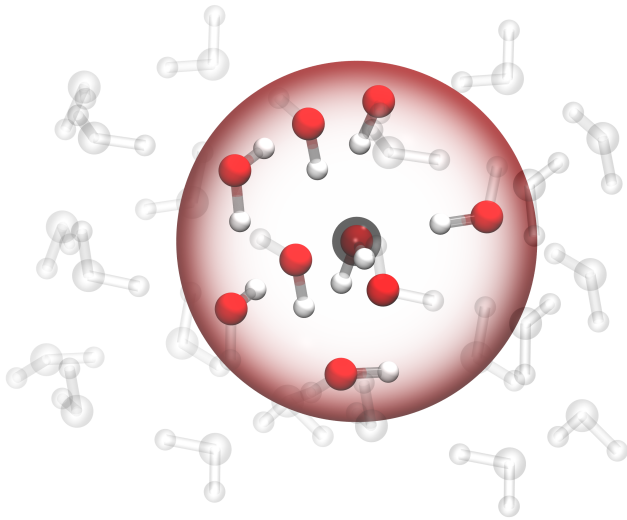
Popular representations (Invariant with respect to translation, rotation and permutation.):

- Smooth overlap of atomic positions (SOAP) [Bartók, Kondor & Csányi PRB 2013]
- Behler-Parrinello symmetry functions [Behler & Parrinello PRL 2008]

Representing atomistic environments



$$\Phi \leftarrow \{\Psi(\mathcal{X}_i)\}$$



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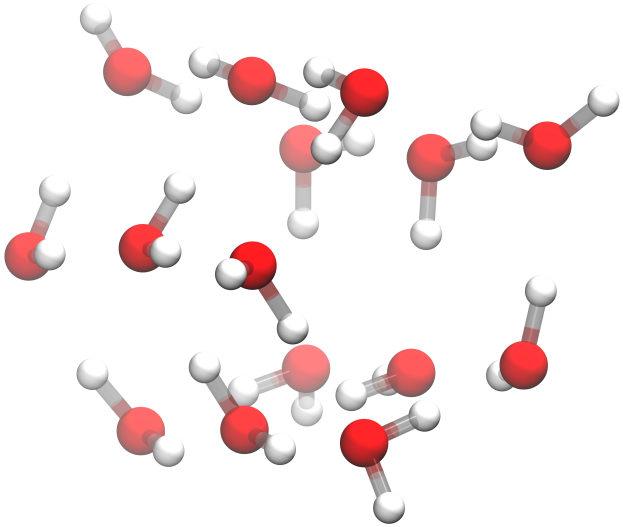

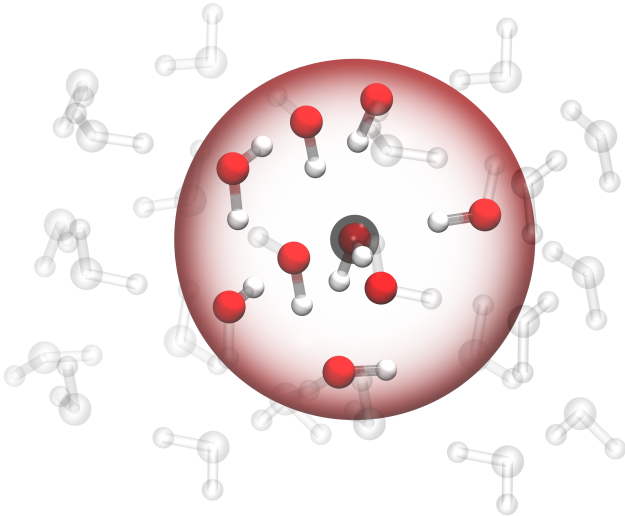

$$O(A) = F(\Phi(A))$$

$$O_i = f(\Psi(\mathcal{X}_i))$$

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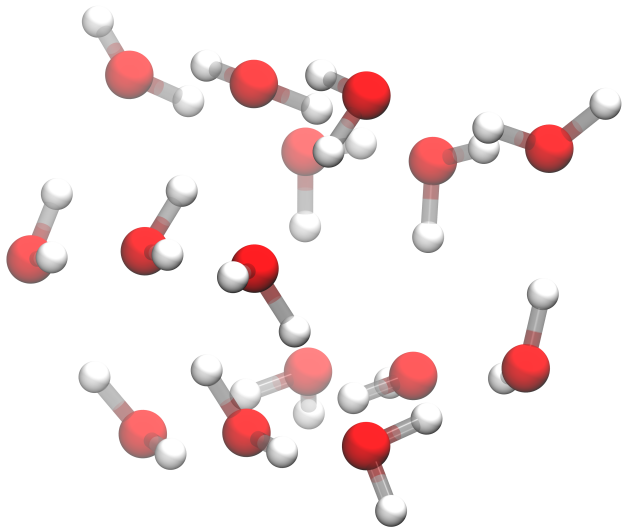

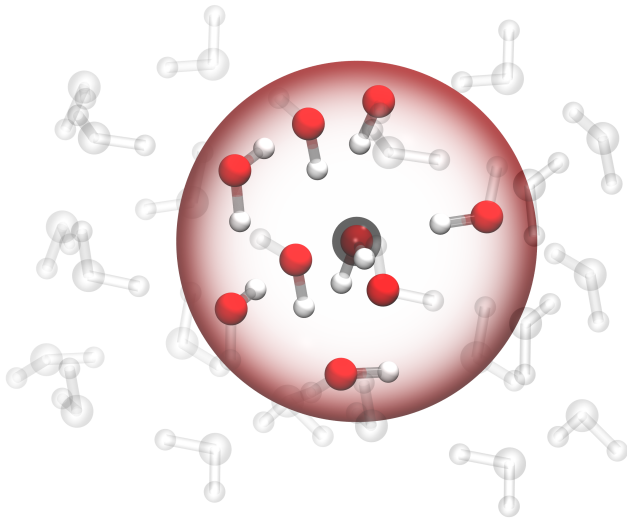

$$E(A) = \sum E_i$$

$$E_i = e(\Psi(\mathcal{X}_i))$$

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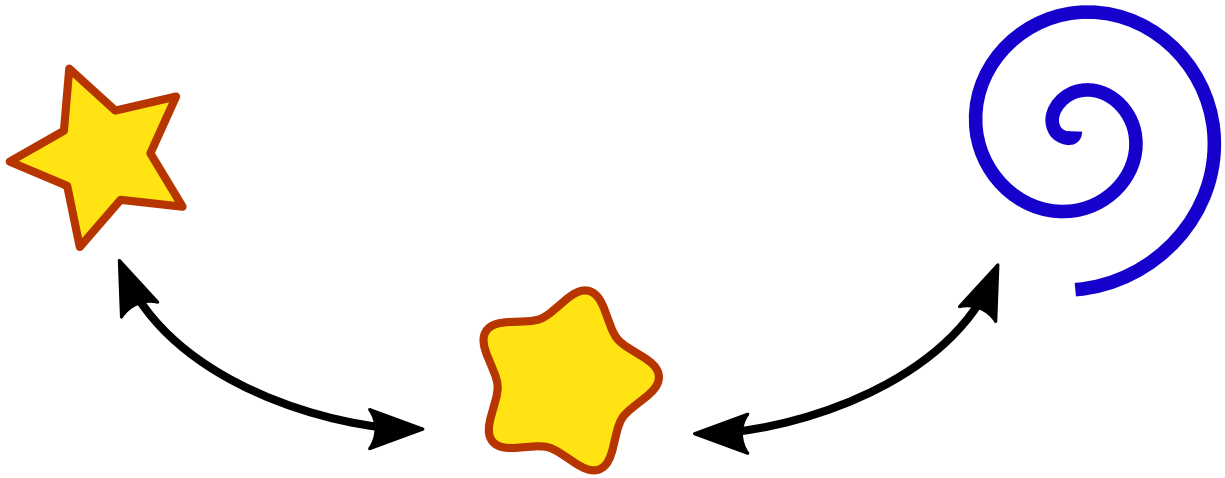
Representing atomic environments

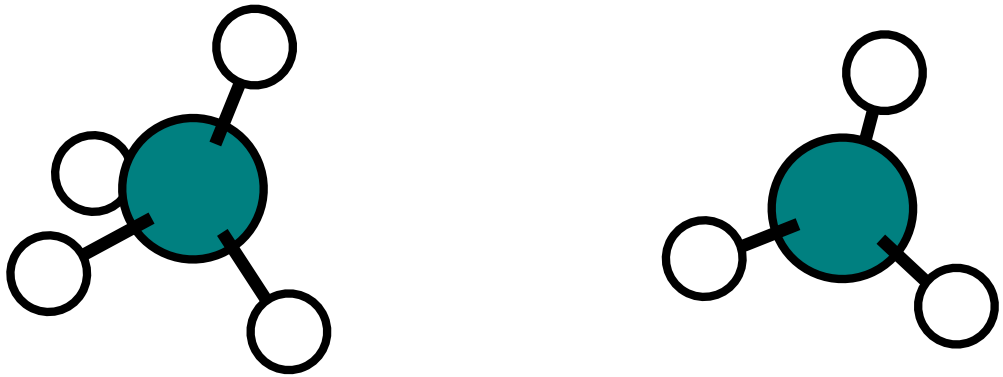
[Bartók, Kondor & Csányi PRB 2013]



$$K(\mathcal{X}, \mathcal{X}') \approx 1 \qquad K(\mathcal{X}, \mathcal{X}') \approx 0$$
$$D(\mathcal{X}, \mathcal{X}') \approx 0 \qquad D(\mathcal{X}, \mathcal{X}') \gg 0$$

Representing atomic environments

[Bartók, Kondor & Csányi PRB 2013]



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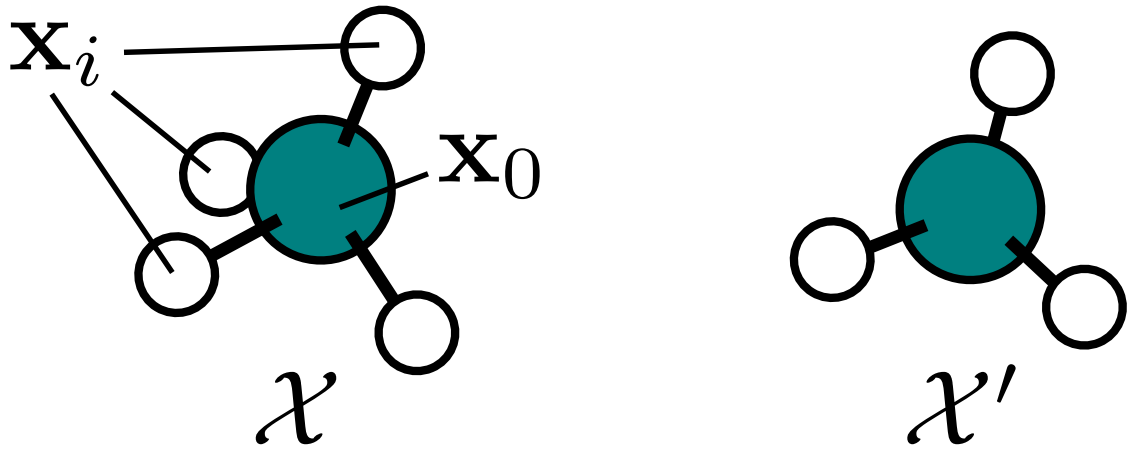
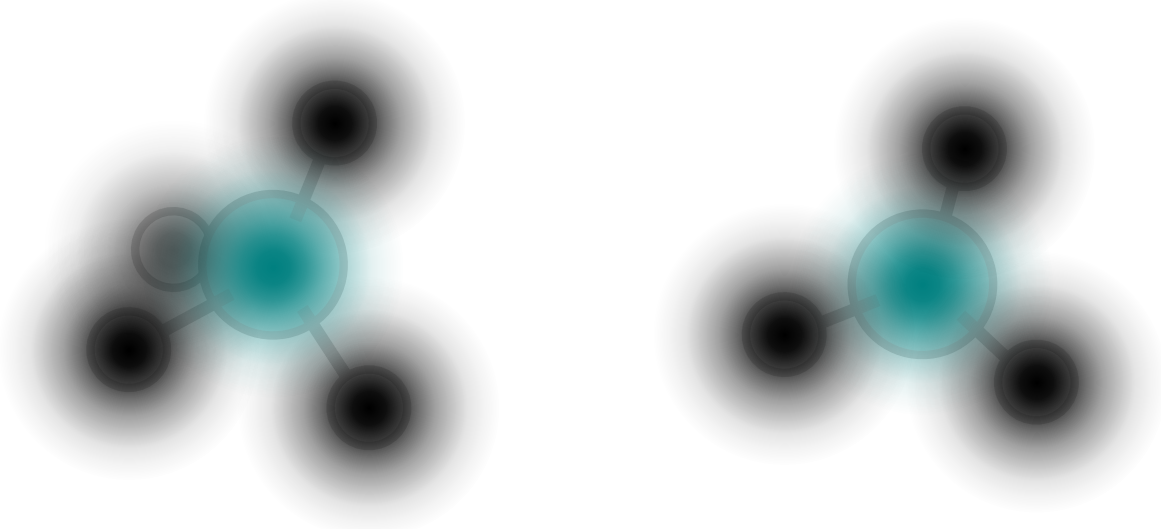


$$\{\mathbf{x}_i - \mathbf{x}_0\} \leftrightarrow \mathcal{X}$$

Representing atomic environments

[Bartók, Kondor & Csányi PRB 2013]



$$\rho_\alpha(\mathbf{x}) = \sum_{i \in \alpha} g(\mathbf{x} - \mathbf{x}_i)$$

Representing atomic environments

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$$k(\mathcal{X}, \mathcal{X}') = \int \rho(\mathbf{x})\rho'(\mathbf{x})$$

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$$k(\mathcal{X}, \mathcal{X}') = \int \mathrm{d}\hat{R} \left| \int \rho(\mathbf{x}) \rho'(\hat{R}\mathbf{x}) \right|^2$$

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Representing atomic environments

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$$\kappa(\mathcal{X}, \mathcal{X}') = \int \mathrm{d}\hat{R} |\rho(\mathbf{x})\rho'(\hat{R}\mathbf{x})|^2$$

$$\rho(\mathbf{x}) = \sum_{nlm} c_{nlm} g_n(|r|) Y_{lm}(\hat{r})$$

$$k_{nn'l}(\mathcal{X}) = \pi \sqrt{\frac{8}{2l+1}} \sum_m (c_{nlm})^* c_{n'lm}$$

The list of vector $\{k_{nn'l}(\mathcal{X})\}$ is the descriptor of the atomic environment $\mathcal{X}$.

Similarity measurement between structures

- The kernel matrix $\{K\}$ records the similarity measurement for each pair of structures in the data set.
- The kernel function $K(A, B)$ for structure A and B is

$$K(A, B) = \Phi(A)^{\mathsf{T}} \Phi(B) = \sum_{i=1}^{M} \phi_i(A) \phi_i(B)$$

- Global features are constructed from local features by taking the average:

$$\Phi(A) = \frac{1}{N_A} \sum_{n=1}^{N_A} \Psi(\mathcal{X}_n^A)$$

- We use SOAP vectors as local features. [Bartók et al. PRB 2013]
  We use DScribe Python libray [Himanen et al. arxiv 2019]

$$k_{nn'l}(\mathcal{X}) = \pi \sqrt{\frac{8}{2l+1}} \sum_m (c_{nlm})^* c_{n'lm}$$

Visualizing and processing the data set

- Build two-dimensional map using dimensionality reduction
  - (kernel) PCA, Multidimensional scaling (MDS), Isometric mapping (ISOMAP), locally linear embedding (LLE)
- Sparsity the train set
  - farthest point sampling, CUR decomposition
- Clustering
  - Gaussian mixture model (GMM), K-means, DBSCAN....
- Regression
  - ridge regression, neural networks

Questions?

Thank you for your attention!