Speeding Up Kernel Methods, and Intro to Unsupervised Learning

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Introduction to Machine Learning (CS771A)

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Recap: Nonlinear Mappings

- Idea: Use a nonlinear mapping $\phi : \mathbb{R}^D \to \mathbb{R}^M$ to map original data to a high-dim space, e.g.,

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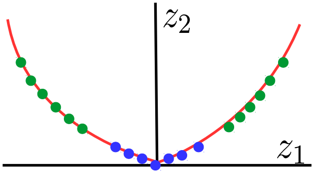

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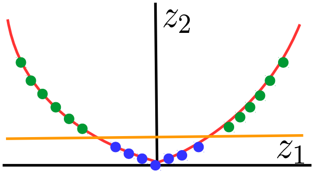

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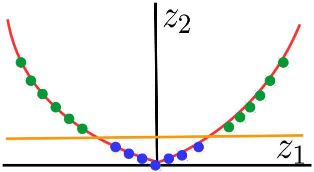

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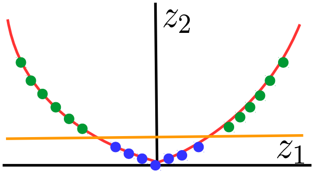

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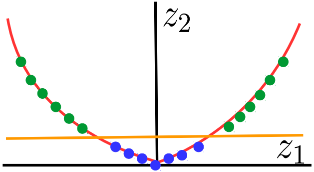

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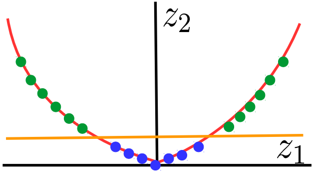

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- Many ML algos only have data appearing as inner products. Can kernelize such algos

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- Again, remember that when using kernels, we don't have to compute ϕ explicitly

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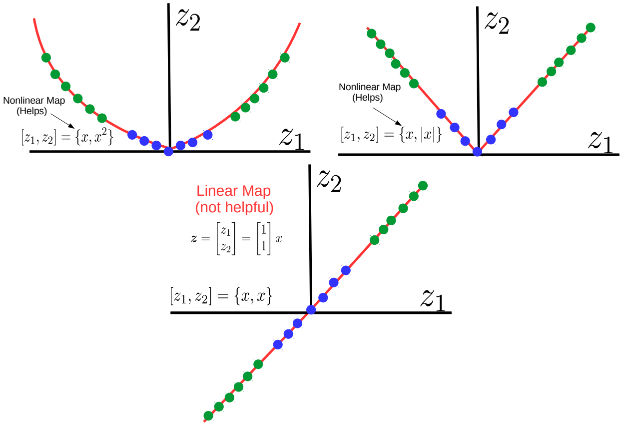
- Not every high-dim mapping is helpful. The mapping ϕ must be nonlinear



Kernel Methods can be Slow

Training phase can be slow (if N is very large)

$$\text{Soft-Margin SVM:} \quad \max_{\boldsymbol{\alpha} \leq C} \; \mathcal{L}_D(\alpha) = \boldsymbol{\alpha}^\top \mathbf{1} - \frac{1}{2}\boldsymbol{\alpha}^\top \underbrace{\mathbf{G}}_{\text{N x N size}}\boldsymbol{\alpha}$$

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Storing the learned model may be expensive

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \phi(\boldsymbol{x}_n)$$

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$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \underbrace{\phi(\boldsymbol{x}_n)}_{\text{Possibly very high-dimensional}}$$

Testing (prediction) phase can be slow (scales in N or at least the number of support vectors)

$$y = \text{sign}(\boldsymbol{w}^\top \phi(\boldsymbol{x})) = \text{sign}(\sum_{n=1}^{N} \alpha_n y_n \phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{x})) = \text{sign}(\sum_{n=1}^{N} \alpha_n y_n k(\boldsymbol{x}_n, \boldsymbol{x}))$$

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Dual form of Ridge Regression: $\boldsymbol{w} = \mathbf{X}^\top (\mathbf{X}\mathbf{X}^\top + \lambda \mathbf{I}_N)^{-1} \boldsymbol{y} = \mathbf{X}^\top \boldsymbol{\alpha} = \sum_{n=1}^{N} \alpha_n \boldsymbol{x}_n$

Kernelized Ridge Regression: $\boldsymbol{w} = \phi(\mathbf{X})^\top (\mathbf{K} + \lambda \mathbf{I}_N)^{-1} \boldsymbol{y} = \phi(\mathbf{X})^\top \boldsymbol{\alpha} = \sum_{n=1}^{N} \alpha_n \phi(\boldsymbol{x}_n)$

N x N size (also need to invert it)

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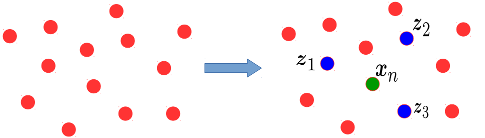
- We will see two popular approaches: Landmarks and Random Features

Using Kernels to "Extract" Good Features: Landmarks

- Suppose we choose a small set of L "landmark" inputs $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L$ in the training data



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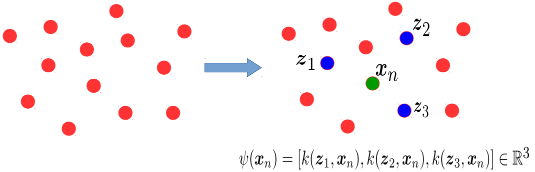

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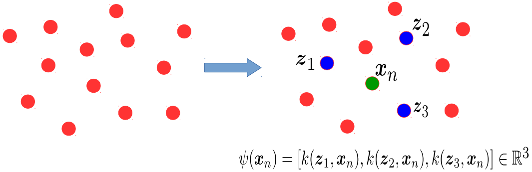

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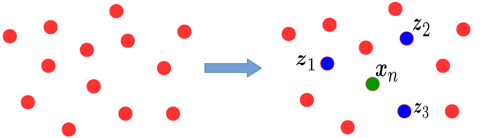

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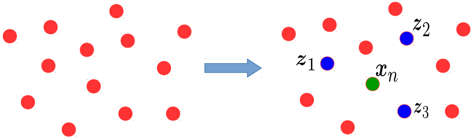

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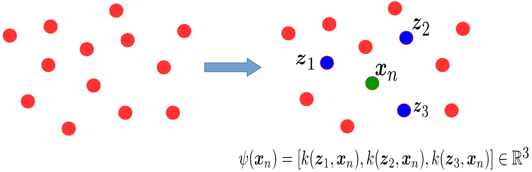
- This will be fast both at training as well as test time if L is small
- No need to kernelize the linear model and work with kernels (but still reap their benefits :-))

Using Kernels to "Extract" Good Features: Landmarks

- Suppose we choose a small set of L "landmark" inputs $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L$ in the training data



- For each input $\boldsymbol{x}_n$, using a kernel k, define an L-dimensional feature vector as follows

$$\psi(\boldsymbol{x}_n) = [k(\boldsymbol{z}_1, \boldsymbol{x}_n), k(\boldsymbol{z}_2, \boldsymbol{x}_n), \ldots, k(\boldsymbol{z}_L, \boldsymbol{x}_n)]$$

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- Note: The landmarks need not be actual inputs. Can even be learned from data.

Using Kernels to “Extract” Good Features: Random Features

- Many kernel functions can be written as[†]

$$k(\boldsymbol{x}_n, \boldsymbol{x}_m) = \phi(\boldsymbol{x}_n)^\top \phi(\boldsymbol{x}_m) = \mathbb{E}_{\boldsymbol{w} \sim p(\boldsymbol{w})}[t_{\boldsymbol{w}}(\boldsymbol{x}_n) t_{\boldsymbol{w}}(\boldsymbol{x}_m)]$$

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- Such techniques exist for several kernels (RBF, polynomial, etc)

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Other Techniques for Speeding Up Kernel Methods

- Reducing the number of support vectors (for SVM based models), For example,
  - Learn the kernelized SV. Identify the support vectors.
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- Similar considerations apply to other kernelizable models too (e.g., SVM)
- If linear model is what you want, still makes sense to look at the relative values of N and D to decide whether to go for the dual (kernelized) formulation of the problem with a linear kernel

Kernel Methods: Some Final Comments

- Kernel methods give us good features to make learning easier
- However, these features are pre-defined (due to the choice of kernel)
- Example: Consider the quadratic kernel applied to input $\boldsymbol{x} = [x_1, x_2]$

$$\phi(\boldsymbol{x}) = [1, \sqrt{2}x_1, x_1^2, \sqrt{2}x_1x_2, x_2, x_2^2, \sqrt{2}x_2] \quad \text{(fixed definition for } \phi\text{)}$$

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- Another alternative is to learn good features from data
- We will revisit this when we talk about deep neural networks

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- Most unsupervised learning algos can also be seen as learning a new representation of data
  - Typically a compressed representation, e.g., clustering can be used to get a one-hot representation

K = 6 clusters

z_n $\boxed{0 \mid 0 \mid 1 \mid 0 \mid 0 \mid 0}$ $\longleftarrow$ x_n belongs to cluster 3

A one-hot (quantized) rep.

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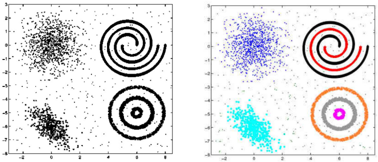

(a) Input data (b) Desired clustering

Picture courtesy: "Data Clustering: 50 Years Beyond K-Means", A.K. Jain (2008)

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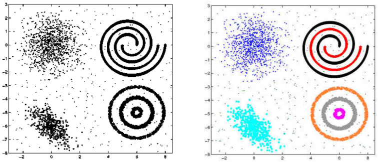

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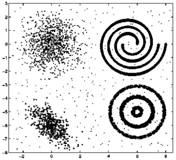

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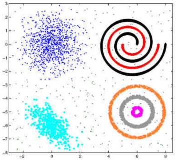

(b) Desired clustering

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- Loosely speaking, it is classification without ground truth labels
- A good clustering is one that achieves:
  - High within-cluster similarity
  - Low inter-cluster similarity

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Picture courtesy: `http://www.guy-sports.com/humor/videos/powerpoint_presentation_dogs.htm`

Clustering: Some Examples

- Document/Image/Webpage Clustering
- Image Segmentation (clustering pixels)

- Clustering web-search results
- Clustering (people) nodes in (social) networks/graphs
- .. and many more..

Picture courtesy: `http://people.cs.uchicago.edu/~pff/segment/`

Types of Clustering

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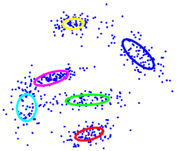

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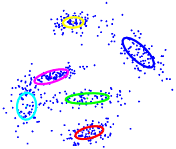
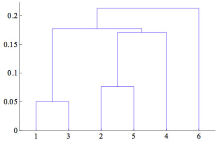
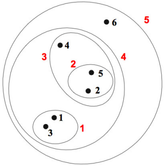


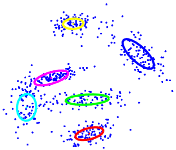
2. **Hierarchical clustering**
   - Partitions can be visualized using a tree structure (a dendrogram)



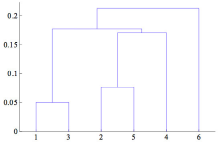


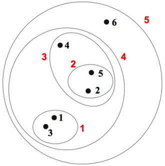
Types of Clustering

1. **Flat or Partitional clustering**
   - Partitions are independent of each other



2. **Hierarchical clustering**
   - Partitions can be visualized using a tree structure (a dendrogram)





   - Possible to view partitions at different levels of granularities by "cutting" the tree at some level

Flat Clustering: K-means algorithm (Lloyd, 1957)

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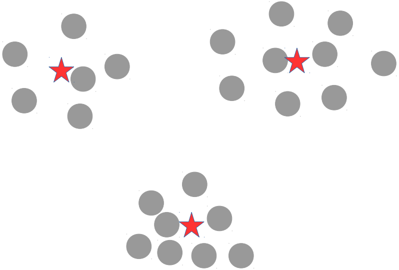
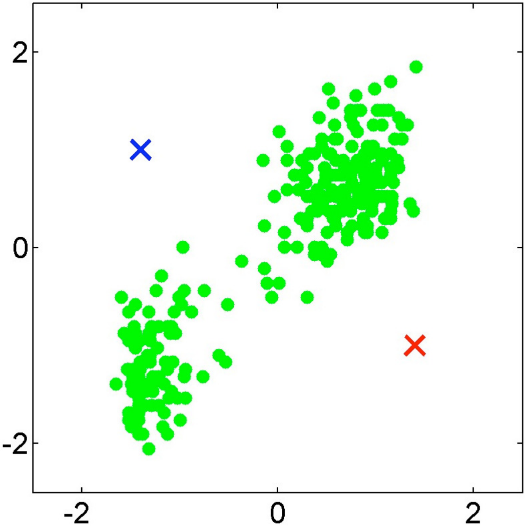
- Stop when cluster means or the "loss" does not change by much

K-means = Prototype Classification (with unknown labels)

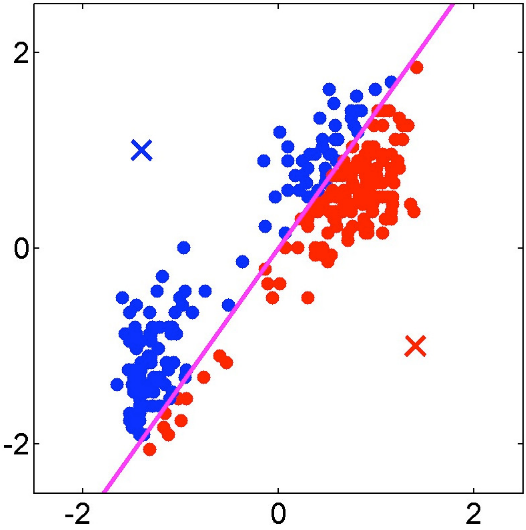


- **Guess the means**
- **Predict the labels**
- **Recompute the means**
- **Repeat**

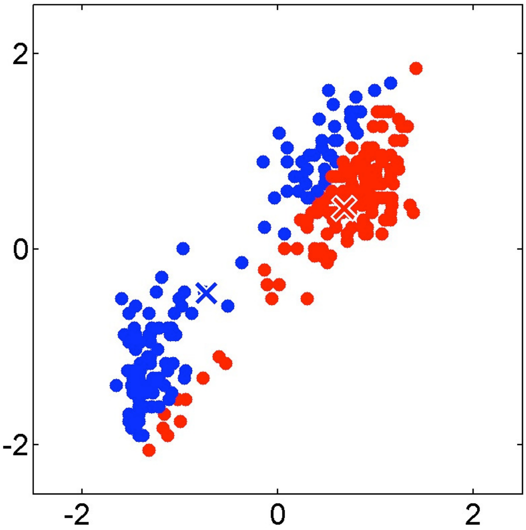
K-means: Initialization (assume $K = 2$)



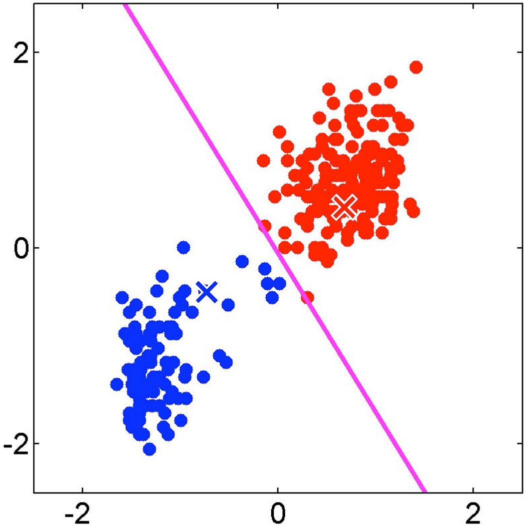
K-means iteration 1: Assigning points



K-means iteration 1: Recomputing the centers



K-means iteration 2: Assigning points



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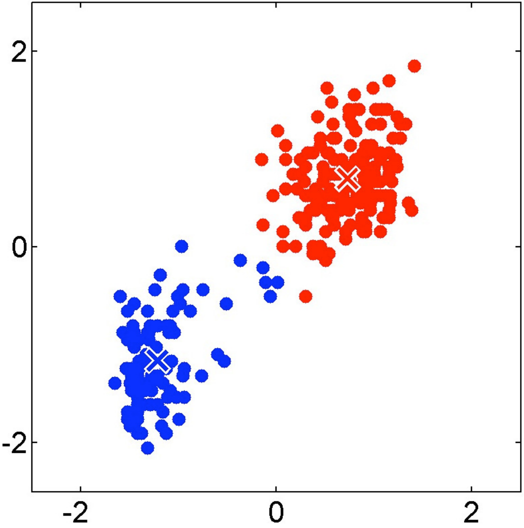
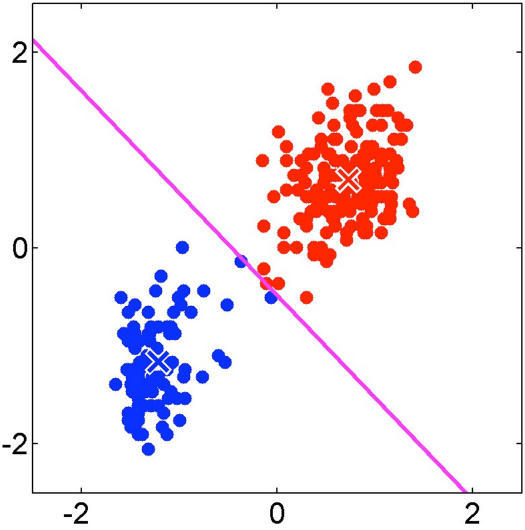


K-means iteration 3: Assigning points



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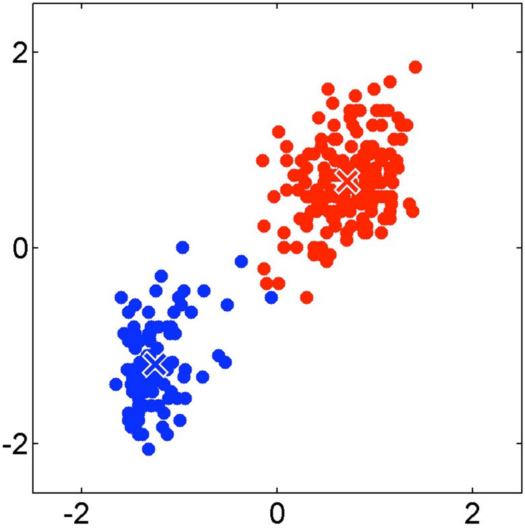
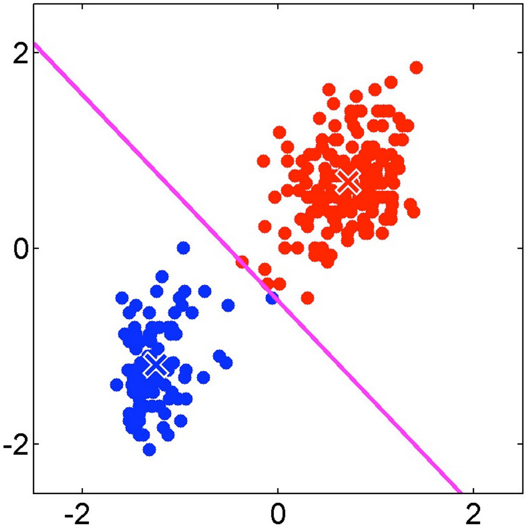
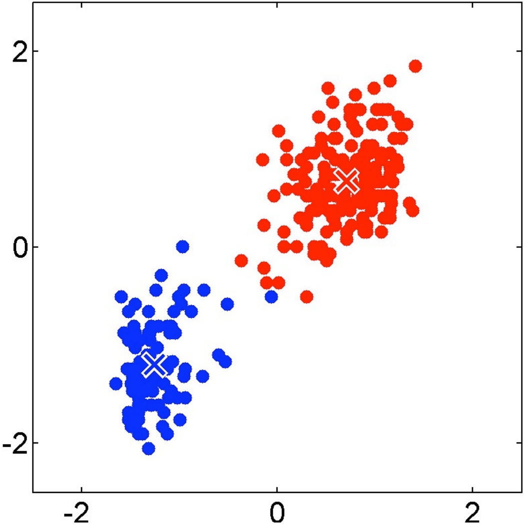


K-means iteration 4: Assigning points



K-means iteration 4: Recomputing the centers



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where $\mathbf{Z}$ is $N \times K$ (row n is $\boldsymbol{z}_n$) and $\boldsymbol{\mu}$ is $K \times D$ (row k is $\boldsymbol{\mu}_k$)

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  - Alternating optimization would give the K-means (Lloyd's) algorithm we saw earlier!

Next Class: Clustering (Contd.)