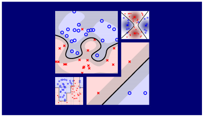
Machine Learning Techniques
(機器學習技法)



Lecture 14: Radial Basis Function Network

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Roadmap

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

Lecture 13: Deep Learning

pre-training with **denoising autoencoder** (**non-linear PCA**) and fine-tuning with **backprop** for NNet with **many layers**

Lecture 14: Radial Basis Function Network

- RBF Network Hypothesis
- RBF Network Learning
- k-Means Algorithm
- k-Means and RBF Network in Action

Gaussian SVM Revisited

$$g_{\text{SVM}}(\mathbf{x}) = \text{sign}\left(\sum_{\text{SV}} \alpha_n y_n \exp\left(-\gamma\|\mathbf{x} - \mathbf{x}_n\|^2\right) + b\right)$$

Gaussian SVM:

achieve large margin in infinite-dimensional space, **remember? :-)**

Gaussian SVM Revisited

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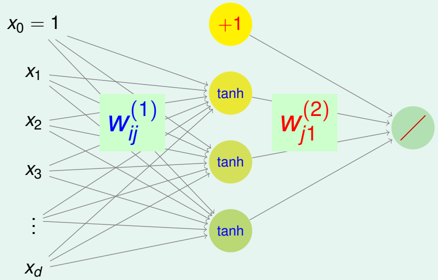
Radial Basis Function (RBF) **Network**: linear aggregation of radial hypotheses

From Neural Network to RBF Network

Neural Network



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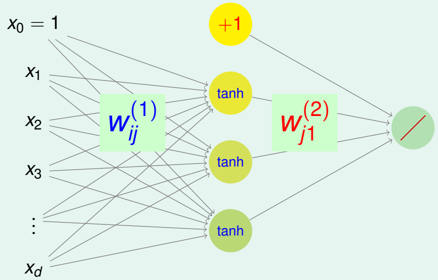

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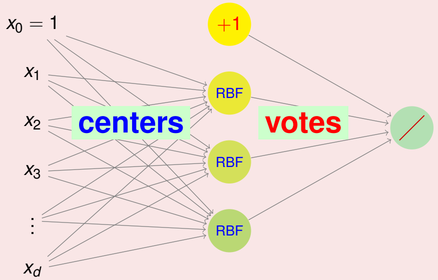

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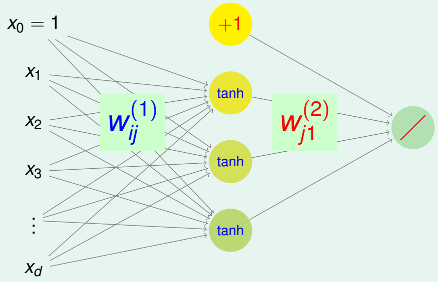

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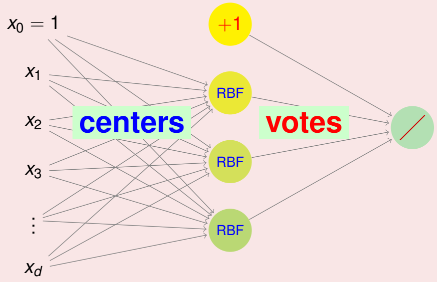

- output layer same: **just linear aggregation**

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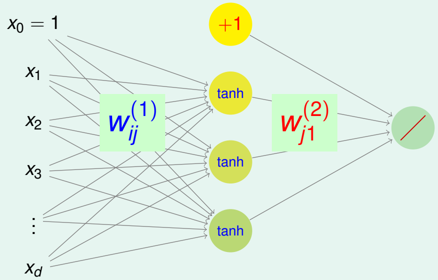

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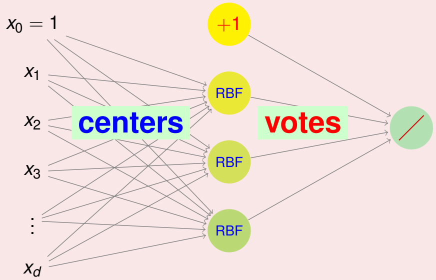

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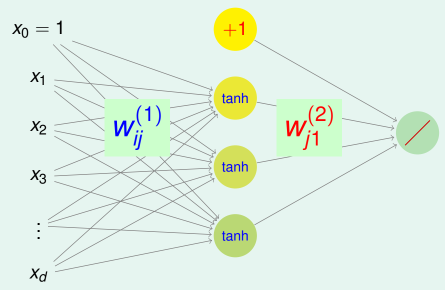

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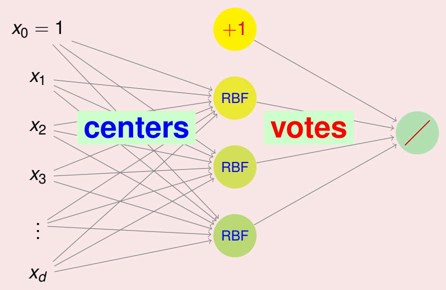

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RBF Network: historically **a type of NNet**

RBF Network Hypothesis

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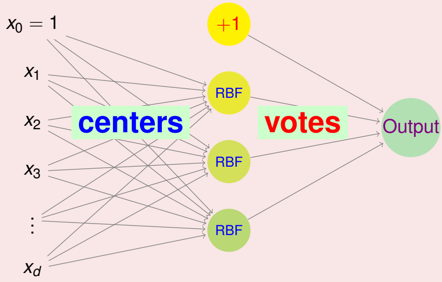

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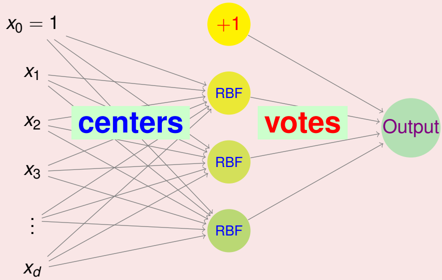

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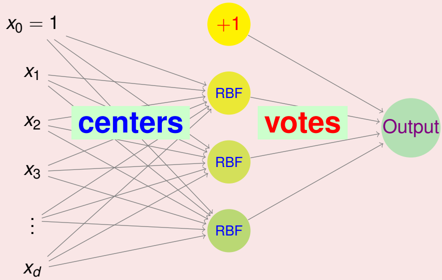

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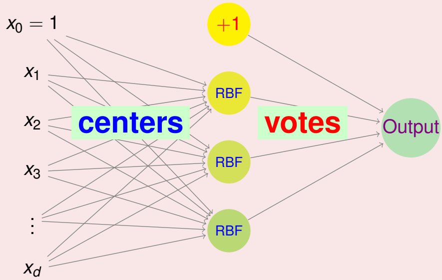

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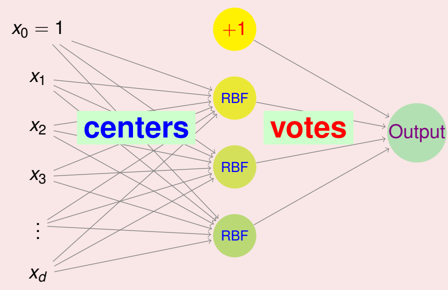

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learning: given RBF and Output,
decide $\boldsymbol{\mu}_m$ and β_m

RBF and Similarity

kernel: similarity via $\mathcal{Z}$-space inner product
—**governed by Mercer's condition, remember? :-)**

$\text{Poly}(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^T \mathbf{x}')^2$

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—often **monotonically non-increasing** to distance

RBF and Similarity

general similarity function between $\mathbf{x}$ and $\mathbf{x}'$:

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RBF Network: distance similarity-to-centers as **feature transform**

Fun Time

Which of the following is not a radial basis function?

1. $\phi(\mathbf{x}, \boldsymbol{\mu}) = \exp(-\gamma\|\mathbf{x} - \boldsymbol{\mu}\|^2)$
2. $\phi(\mathbf{x}, \boldsymbol{\mu}) = -\sqrt{\mathbf{x}^T\mathbf{x} - 2\mathbf{x}^T\boldsymbol{\mu} + \boldsymbol{\mu}^T\boldsymbol{\mu}}$
3. $\phi(\mathbf{x}, \boldsymbol{\mu}) = [\![\mathbf{x} = \boldsymbol{\mu}]\!]$
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Reference Answer: (4)

Note that (3) is an extreme case of (1) (Gaussian) with $\gamma \to \infty$, and (2) contains an $\|\mathbf{x} - \boldsymbol{\mu}\|^2$ somewhere :-).

Full RBF Network

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full RBF Network: **lazy** way to decide $\boldsymbol{\mu}_m$

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k nearest neighbor:
also **lazy** but **very intuitive**

Interpolation by Full RBF Network

full RBF Network for squared error regression:

$$h(\mathbf{x}) = \cancel{\text{Output}}\left(\sum_{m=1}^{N} \beta_m \text{RBF}(\mathbf{x}, \mathbf{x}_m)\right)$$

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- just linear regression on RBF-transformed data

$$\mathbf{z}_n = [\text{RBF}(\mathbf{x}_n, \mathbf{x}_1), \text{RBF}(\mathbf{x}_n, \mathbf{x}_2), \ldots, \text{RBF}(\mathbf{x}_n, \mathbf{x}_N)]$$

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full RBF Network for squared error regression:

$$h(\mathbf{x}) = \cancel{\text{Output}}\left(\sum_{m=1}^{N} \beta_m \text{RBF}(\mathbf{x}, \mathbf{x}_m)\right)$$

- just linear regression on RBF-transformed data

$$\mathbf{z}_n = [\text{RBF}(\mathbf{x}_n, \mathbf{x}_1), \text{RBF}(\mathbf{x}_n, \mathbf{x}_2), \ldots, \text{RBF}(\mathbf{x}_n, \mathbf{x}_N)]$$

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full Gaussian RBF Network for regression: $\boldsymbol{\beta} = \mathrm{Z}^{-1}\mathbf{y}$

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Fewer Centers as Regularization

recall:

$$g_{\text{SVM}}(\mathbf{x}) = \text{sign}\left(\sum_{\text{SV}} \alpha_m y_m \exp\left(-\gamma\|\mathbf{x}-\mathbf{x}_m\|^2\right) + b\right)$$

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remaining question:
how to extract **prototypes**?

Fun Time

If $\mathbf{x}_1 = \mathbf{x}_2$, what happens in the Z matrix of full Gaussian RBF network?

1. the first two rows of the matrix are the same
2. the first two columns of the matrix are different
3. the matrix is invertible
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Reference Answer: (1)

It is easy to see that the first two rows must be the same; so must the first two columns. The two same rows makes the matrix singular; the sub-matrix in (4) contains a constant of $1 = \exp(-0)$ instead of 0.

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goal: with $S_1, \cdots, S_M$ being a partition of $\{\mathbf{x}_n\}$,

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$$\min_{\{S_1,\cdots,S_M;\boldsymbol{\mu}_1,\cdots,\boldsymbol{\mu}_M\}} \sum_{n=1}^{N} \sum_{m=1}^{M} [\![\mathbf{x}_n \in S_m]\!] \|\mathbf{x}_n - \boldsymbol{\mu}_m\|^2$$

- **hard to optimize**: joint combinatorial-numerical optimization
- **two sets** of variables: will optimize alternatingly

if $\boldsymbol{\mu}_1, \cdots, \boldsymbol{\mu}_M$ **fixed**, for each $\mathbf{x}_n$

- $[\![\mathbf{x}_n \in S_m]\!]$: choose one and only one subset
- $\|\mathbf{x}_n - \boldsymbol{\mu}_m\|^2$: distance to each prototype

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Prototype Optimization

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optimal prototype $\boldsymbol{\mu}_m =$ of $\mathbf{x}_n$ within S_m

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k-Means Algorithm

use k **prototypes** instead of M historically

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2. **alternating optimization** of E_{in}: repeatedly
   1. optimize $S_1, S_2, \ldots, S_k$:
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until **converge**

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k-Means: the most popular **clustering** algorithm through **alternating minimization**

RBF Network Using *k*-Means

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1. run *k*-Means with $k = M$ to get $\{\boldsymbol{\mu}_m\}$

RBF Network Using k-Means

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2. construct transform $\boldsymbol{\Phi}(\mathbf{x})$ from RBF (say, Gaussian) at $\boldsymbol{\mu}_m$

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RBF Network: a simple (**old-fashioned**) model

Fun Time

For k-Means, consider examples $\mathbf{x}_n \in \mathbb{R}^2$ such that all $x_{n,1}$ and $x_{n,2}$ are non-zero. When fixing two prototypes $\boldsymbol{\mu}_1 = [1, 1]$ and $\boldsymbol{\mu}_2 = [-1, 1]$, which of the following set is the optimal S_1?

1. $\{\mathbf{x}_n \colon x_{n,1} > 0\}$
2. $\{\mathbf{x}_n \colon x_{n,1} < 0\}$
3. $\{\mathbf{x}_n \colon x_{n,2} > 0\}$
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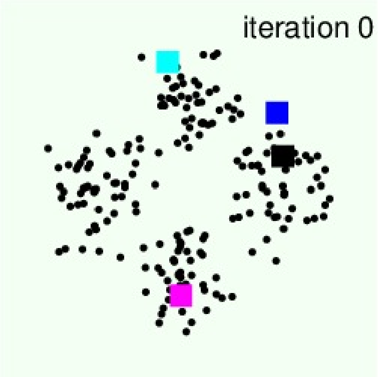
Reference Answer: 1

Note that S_1 contains examples that are closer to $\boldsymbol{\mu}_1$ than $\boldsymbol{\mu}_2$.

Beauty of *k*-Means

$k = 4$



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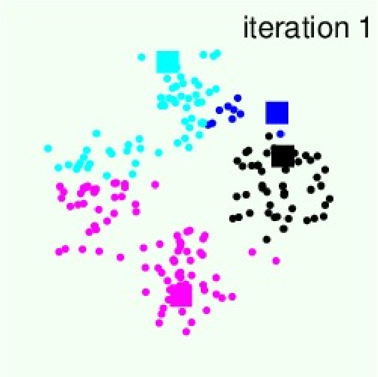

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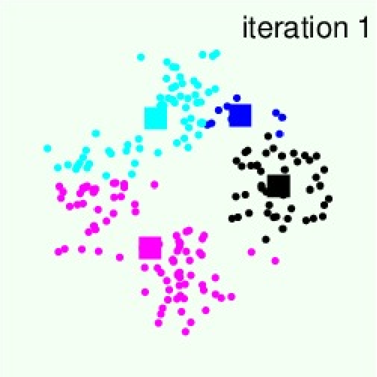

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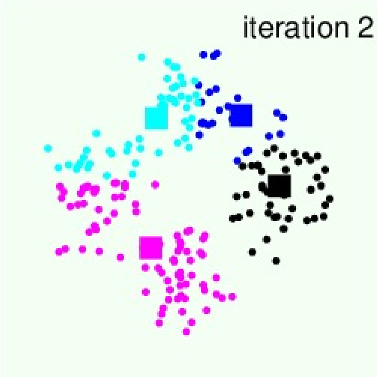

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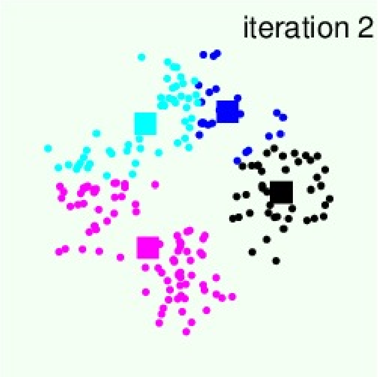

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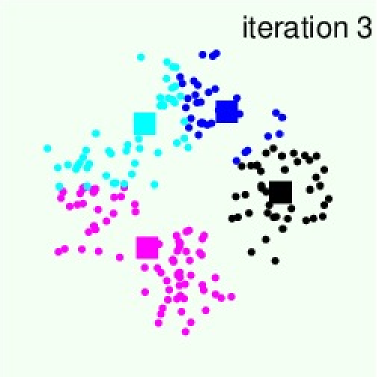

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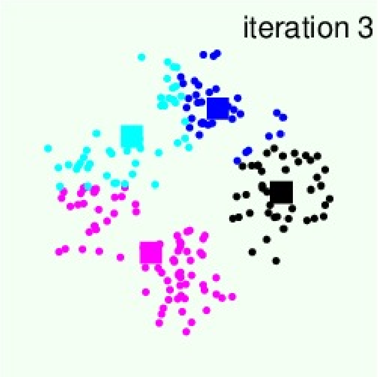

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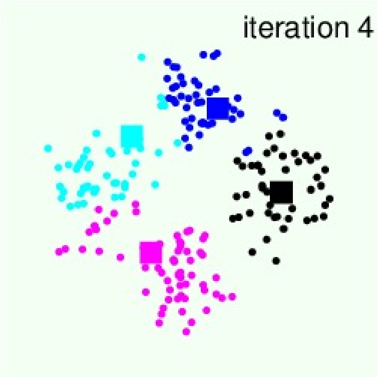

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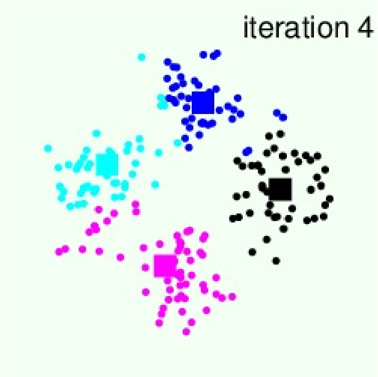

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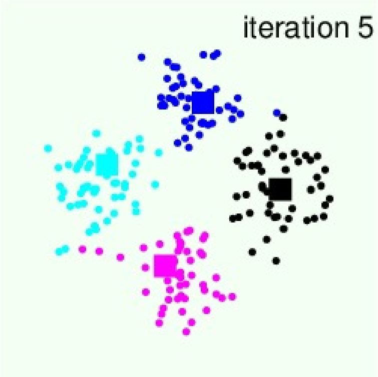

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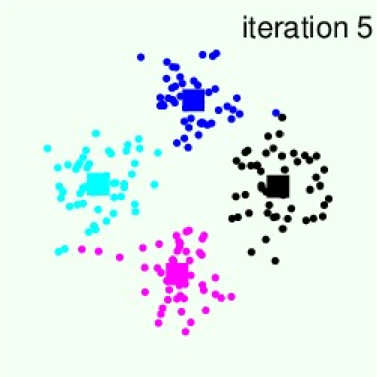

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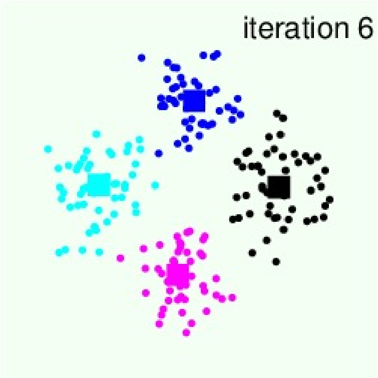
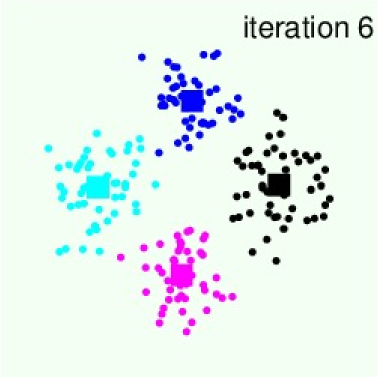


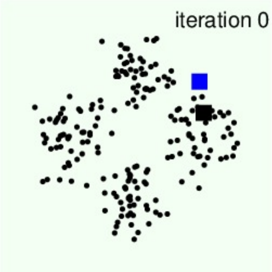
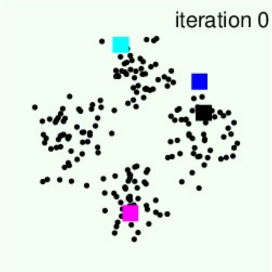
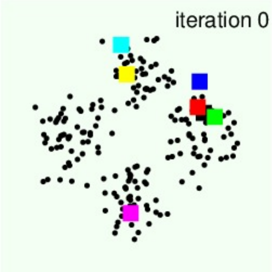
Beauty of *k*-Means

$k = 4$

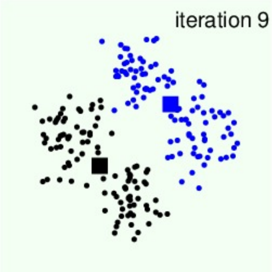
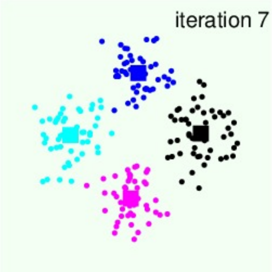
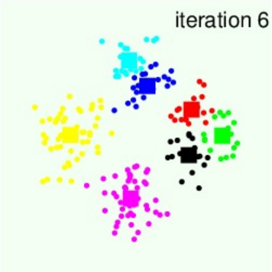


usually works well
with **proper *k* and initialization**

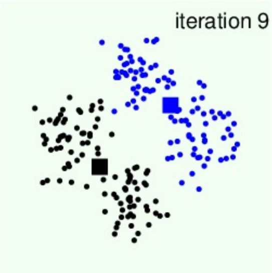
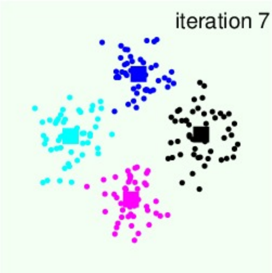
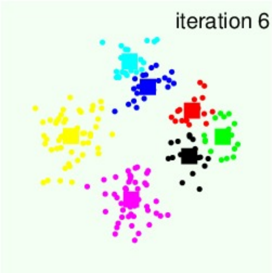
Difficulty of *k*-Means

$k = 2$	$k = 4$	$k = 7$
		

Difficulty of *k*-Means

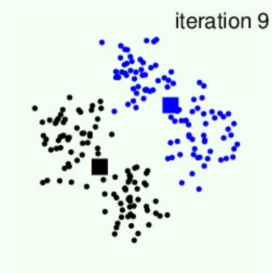
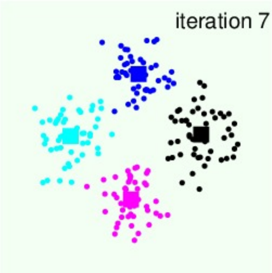
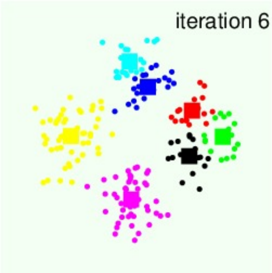
$k = 2$	$k = 4$	$k = 7$
		

Difficulty of *k*-Means

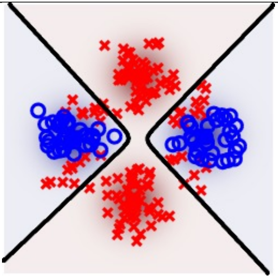
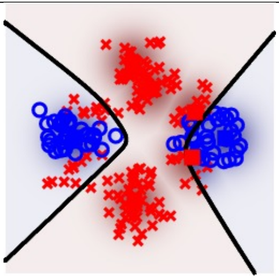
$k = 2$	$k = 4$	$k = 7$
		

'sensitive' to *k* and initialization

RBF Network Using *k*-Means

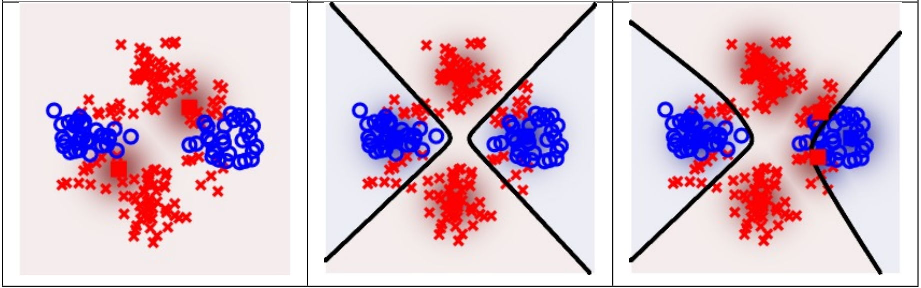
$k = 2$	$k = 4$	$k = 7$
		

RBF Network Using k-Means

$k = 2$	$k = 4$	$k = 7$
		

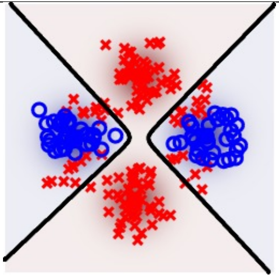
RBF Network Using k-Means

$k = 2$	$k = 4$	$k = 7$

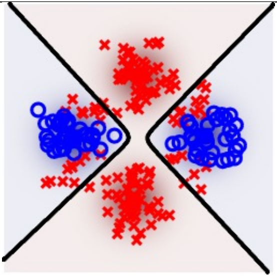
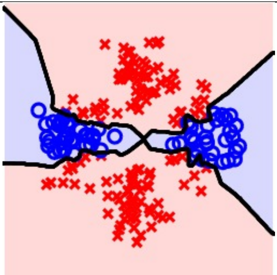


reasonable performance
with **proper centers**

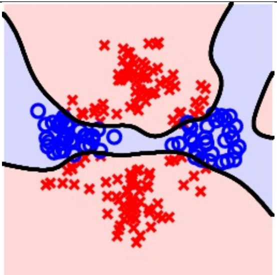
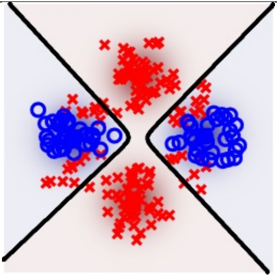
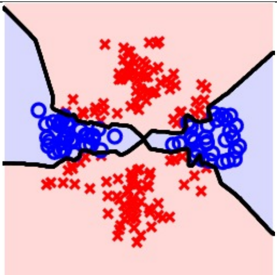
Full RBF Network

$k = N$ $\lambda = 0.001$	$k = 4$	nearest neighbor
		

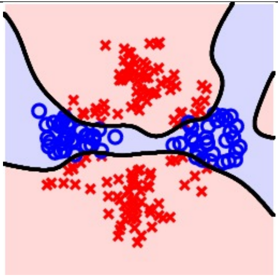
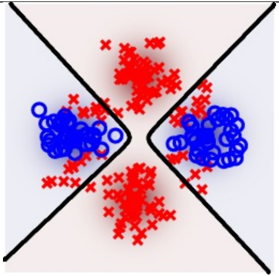
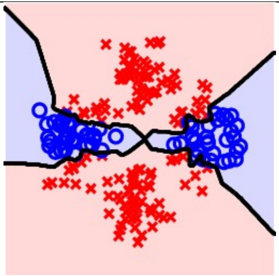
Full RBF Network

$k = N$ $\lambda = 0.001$	$k = 4$	nearest neighbor
		

Full RBF Network

$k = N$ $\lambda = 0.001$	$k = 4$	nearest neighbor
		

Full RBF Network

$k = N$ $\lambda = 0.001$	$k = 4$	nearest neighbor
		

full RBF Network: generally less useful

Fun Time

When coupled with ridge linear regression, which of the following RBF Network is ‘most regularized’?

1. small M and small λ
2. small M and large λ
3. large M and small λ
4. large M and large λ

Fun Time

When coupled with ridge linear regression, which of the following RBF Network is 'most regularized'?

1. small M and small λ
2. small M and large λ
3. large M and small λ
4. large M and large λ

Reference Answer: ②

small M: fewer weights and more regularized;
large λ: shorter β more and more regularized.

Summary

1. Embedding Numerous Features: Kernel Models
2. Combining Predictive Features: Aggregation Models
3. Distilling Implicit Features: Extraction Models

Lecture 14: Radial Basis Function Network

- RBF Network Hypothesis
  prototypes instead of neurons as transform
- RBF Network Learning
  linear aggregation of prototype 'hypotheses'
- *k*-Means Algorithm
  clustering with alternating optimization
- *k*-Means and RBF Network in Action
  proper choice of # prototypes important

- **next: extracting features from abstract data**