Learning From Data
Lecture 18
Radial Basis Functions

Non-Parametric RBF
Parametric RBF
k-RBF-Network

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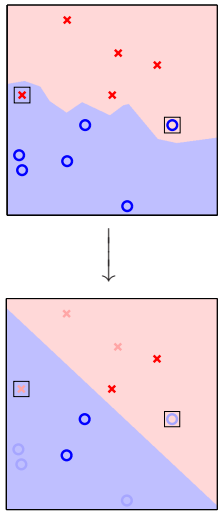
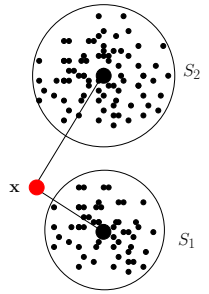
CSCI 4100/6100

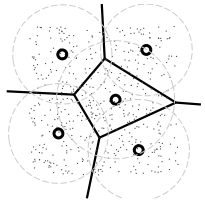
RECAP: Data Condensation and Nearest Neighbor Search

Training Set Consistent





Branch and bound for finding nearest neighbors.



Lloyd's algorithm for finding a good clustering.

Radial Basis Functions (RBF)

k-Nearest Neighbor: Only considers k-nearest neighbors.
each neighbor has equal weight

What about using *all* data to compute $g(\mathbf{x})$?

RBF: Use all data.
data further away from $\mathbf{x}$ have less weight.

Weighting the Data Points: α_n

Test point $\mathbf{x}$.

α_n: the weight of $\mathbf{x}_n$ in $g(\mathbf{x})$.

$$\alpha_n(\mathbf{x}) = \phi\left(\frac{\|\,\mathbf{x}-\mathbf{x}_n\,\|}{r}\right)$$

Weighting the Data Points: α_n

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$$\alpha_n(\mathbf{x}) = \phi\left(\frac{\|\mathbf{x}-\mathbf{x}_n\|}{r}\right)$$

weighting depends on the distance $\|\mathbf{x}-\mathbf{x}_n\|$

Weighting the Data Points: α_n

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. . . relative to a *scale parameter* r

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kernel ϕ determines how the weighting decreases with distance

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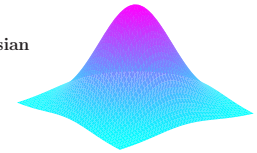
kernel ϕ determines how the weighting decreases with distance

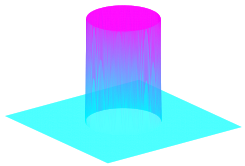
Most popular kernel: Gaussian

$$\phi(z) = e^{-\frac{1}{2}z^2}.$$



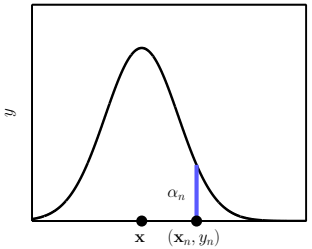
Window kernel, mimics k-NN,

$$\phi(z) = \begin{cases} 1 & z \leq 1, \\ 0 & z > 1, \end{cases}$$



Nonparametric RBF – Regression

$$\alpha_n(\mathbf{x}) = \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right)$$

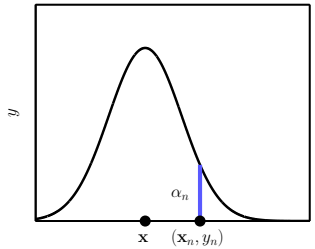


$$g(\mathbf{x}) = \sum_{n=1}^{N}\left(\frac{\alpha_n(\mathbf{x})}{\sum_{m=1}^{N}\alpha_m(\mathbf{x})}\right)\cdot y_n$$

Weighted average of target values

Nonparametric RBF – Classification

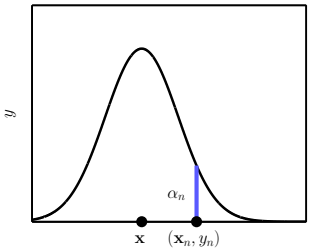
$$\alpha_n(\mathbf{x}) = \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right)$$



$$g(\mathbf{x}) = \text{sign}\left(\sum_{n=1}^{N}\left(\frac{\alpha_n(\mathbf{x})}{\sum_{m=1}^{N}\alpha_m(\mathbf{x})}\right)\cdot y_n\right)$$

Nonparametric RBF – Logistic Regression

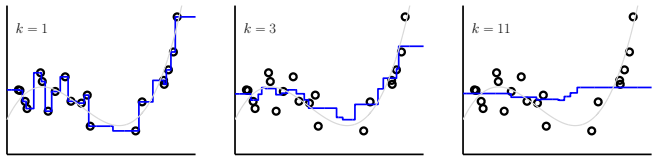
$$\alpha_n(\mathbf{x}) = \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right)$$



$$g(\mathbf{x}) = \sum_{n=1}^{N}\left(\frac{\alpha_n(\mathbf{x})}{\sum_{m=1}^{N}\alpha_m(\mathbf{x})}\right)\cdot [\![y_n = +1]\!]$$

Choice of Scale r

Nearest Neighbor



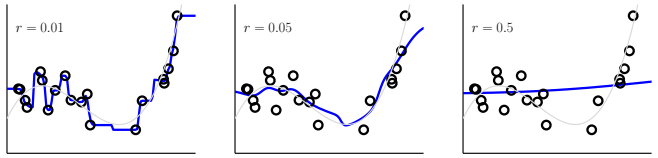
Choosing k:

$k = 3$

$k = \sqrt{N}$

CV

Nonparametric RBF



Choosing r:

$r \sim \frac{1}{\sqrt[3]{N}}$

CV

overfitting underfitting

Highlights of Nonparametric RBF

1. Simple ('smooth' version of k-NN rule).
2. No training.
3. Near optimal E_{out}.
4. Easy to justify classification to customer.

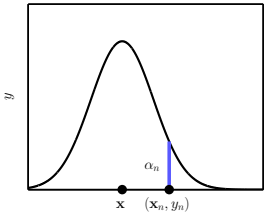
} A **good!** method

5. Can do classification, multi-class, regression, logistic regression.
6. **Computationally demanding**.

Scaled Bumps on Each Data Point

$$g(\mathbf{x}) = \sum_{n=1}^{N} \left(\frac{\alpha_n(\mathbf{x})}{\sum_{m=1}^{N} \alpha_m(\mathbf{x})} \right) \cdot y_n$$

Weighted average of y_n



Scaled Bumps on Each Data Point

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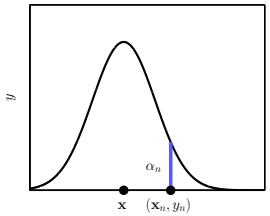
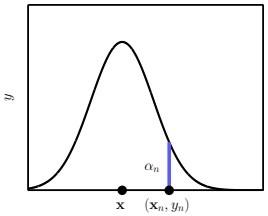


$$g(\mathbf{x}) = \sum_{n=1}^{N} \left(\frac{y_n}{\sum_{m=1}^{N} \alpha_m(\mathbf{x})} \right) \cdot \phi\left(\frac{\| \mathbf{x} - \mathbf{x}_n \|}{r} \right)$$

Scaled Bumps on Each Data Point

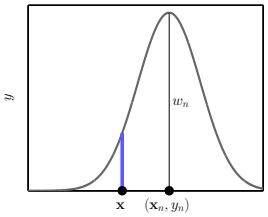
$$g(\mathbf{x}) = \sum_{n=1}^{N} \left(\frac{\alpha_n(\mathbf{x})}{\sum_{m=1}^{N} \alpha_m(\mathbf{x})} \right) \cdot y_n$$

Weighted average of y_n



$$g(\mathbf{x}) = \sum_{n=1}^{N} \left(\frac{y_n}{\sum_{m=1}^{N} \alpha_m(\mathbf{x})} \right) \cdot \phi\left(\frac{\| \mathbf{x} - \mathbf{x}_n \|}{r} \right)$$

$$= \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\| \mathbf{x} - \mathbf{x}_n \|}{r} \right)$$



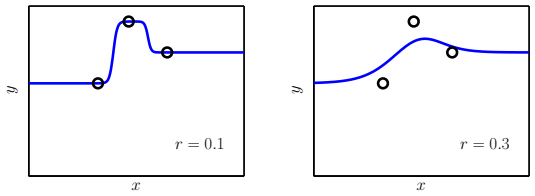
Sum of bumps at $\mathbf{x}_n$ scaled by $w_n(\mathbf{x})$

Nonparametric RBF: $w_n(\mathbf{x})$

Nonparametric RBF

$$g(\mathbf{x}) = \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right)$$

Only need to specify r.

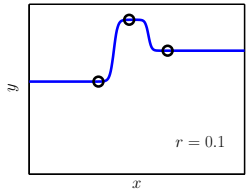


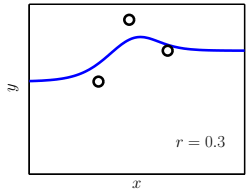
Parametric RBF, w_n – A Linear Model

Nonparametric RBF

$$g(\mathbf{x}) = \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right)$$

Only need to specify r.





Parametric RBF

$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \cdot \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right)$$

Fix r; need to determine the parameters w_n.
— fit the data.

Parametric RBF – A Linear Model

Nonparametric RBF

$$g(\mathbf{x}) = \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right)$$

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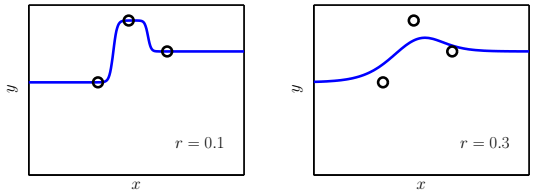

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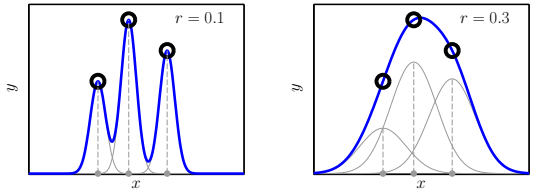
Fix r; need to determine the parameters w_n.
— fit the data.
— overfit the data?



RBF-Nonlinear Transform Depends on Data

$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \cdot \phi\left(\frac{\|\mathbf{x} - \mathbf{x}_n\|}{r}\right) = \mathbf{w}^{\mathrm{T}}\mathbf{z}$$

$$\mathbf{z} = \mathbf{\Phi}(\mathbf{x}) = \begin{bmatrix} \phi_1(\mathbf{x}) \\ \phi_2(\mathbf{x}) \\ \vdots \\ \phi_N(\mathbf{x}) \end{bmatrix}, \quad \phi_n(\mathbf{x}) = \phi\left(\tfrac{\|\mathbf{x}-\mathbf{x}_n\|}{r}\right). \qquad \mathrm{Z} = \begin{bmatrix} — & \mathbf{z}_1^{\mathrm{T}} & — \\ — & \mathbf{z}_2^{\mathrm{T}} & — \\ & \vdots & \\ — & \mathbf{z}_N^{\mathrm{T}} & — \end{bmatrix} = \begin{bmatrix} — & \mathbf{\Phi}(\mathbf{x}_1)^{\mathrm{T}} & — \\ — & \mathbf{\Phi}(\mathbf{x}_2)^{\mathrm{T}} & — \\ & \vdots & \\ — & \mathbf{\Phi}(\mathbf{x}_N)^{\mathrm{T}} & — \end{bmatrix}$$

RBF-Nonlinear Transform Depends on Data

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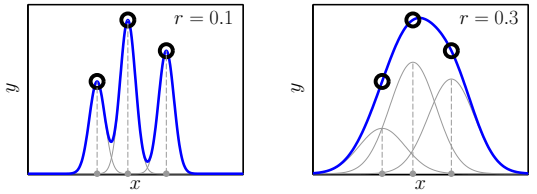
Fit the data $(h(\mathbf{x}_n) = y_n)$:

$$\mathbf{w} = \mathrm{Z}^{\dagger}\mathbf{y} = (\mathrm{Z}^{\mathrm{T}}\mathrm{Z})^{-1}\mathrm{Z}^{\mathrm{T}}\mathbf{y}$$



Reducing the Number of Bumps: Nonparametric

$$g(\mathbf{x}) = \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\|\,\mathbf{x}-\mathbf{x}_n\,\|}{r}\right)$$

Reducing the Number of Bumps: Parametric

$$g(\mathbf{x}) = \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\|\,\mathbf{x}-\mathbf{x}_n\,\|}{r}\right)$$

$$\downarrow$$

$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \cdot \phi\left(\frac{\|\,\mathbf{x}-\mathbf{x}_n\,\|}{r}\right)$$

Reducing the Number of Bumps: k-RBF-Network

$$g(\mathbf{x}) = \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\|\,\mathbf{x}-\mathbf{x}_n\,\|}{r}\right)$$

$$\downarrow$$

$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \cdot \phi\left(\frac{\|\,\mathbf{x}-\mathbf{x}_n\,\|}{r}\right)$$

$$\downarrow$$

$$h(\mathbf{x}) \;=\; w_0 + \sum_{j=1}^{k} w_j \cdot \phi\left(\frac{\|\,\mathbf{x}-\boldsymbol{\mu}_j\,\|}{r}\right) \qquad \text{(nonlinear in } \mu_j\text{)}$$

$$= \mathbf{w}^{\mathrm{T}}\mathbf{\Phi}(\mathbf{x})$$

$\mathbf{\Phi}(\mathbf{x})^{\mathrm{T}} = [1, \Phi_1(\mathbf{x}), \ldots, \Phi_k(\mathbf{x})]$, where $\Phi_j(\mathbf{x}) = \Phi\left(\frac{\|\mathbf{x}-\boldsymbol{\mu}_j\|}{r}\right)$.

Reducing the Number of Bumps: k-RBF-Network

$$g(\mathbf{x}) = \sum_{n=1}^{N} w_n(\mathbf{x}) \cdot \phi\left(\frac{\|\mathbf{x}-\mathbf{x}_n\|}{r}\right)$$

$$\downarrow$$

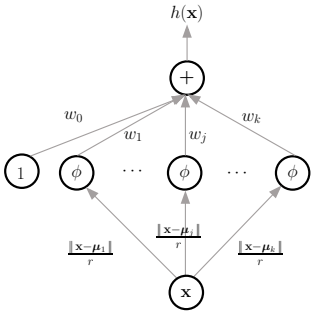
$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \cdot \phi\left(\frac{\|\mathbf{x}-\mathbf{x}_n\|}{r}\right)$$

$$\downarrow$$

nonlinear in μ_j

$$h(\mathbf{x}) = w_0 + \sum_{j=1}^{k} w_j \cdot \phi\left(\frac{\|\mathbf{x}-\boldsymbol{\mu}_j\|}{r}\right)$$

$$= \mathbf{w}^{\mathrm{T}}\boldsymbol{\Phi}(\mathbf{x})$$



$\boldsymbol{\Phi}(\mathbf{x})^{\mathrm{T}} = [1, \Phi_1(\mathbf{x}), \ldots, \Phi_k(\mathbf{x})]$, where $\Phi_j(\mathbf{x}) = \Phi\left(\frac{\|\mathbf{x}-\boldsymbol{\mu}_j\|}{r}\right)$.

Fitting the Data

Before: bumps were centered on $\mathbf{x}_n$ — no choice

Now: we may choose the bump centers $\boldsymbol{\mu}_j$

- Choose them to 'cover' the data
- As the centers of k 'clusters'

Given the bump centers, **we have a linear model to determine the** w_j

- That's 'easy', we know how to do that.

Fitting the Data

Fitting the RBF-network to the data (given k, r):

1: Use the inputs X to determine k centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k$.

2: Compute the $N \times (k+1)$ feature matrix Z

$$\mathrm{Z} = \begin{bmatrix} — & \mathbf{z}_1^{\mathrm{T}} & — \\ — & \mathbf{z}_2^{\mathrm{T}} & — \\ & \vdots & \\ — & \mathbf{z}_N^{\mathrm{T}} & — \end{bmatrix} = \begin{bmatrix} — & \boldsymbol{\Phi}(\mathbf{x}_1)^{\mathrm{T}} & — \\ — & \boldsymbol{\Phi}(\mathbf{x}_2)^{\mathrm{T}} & — \\ & \vdots & \\ — & \boldsymbol{\Phi}(\mathbf{x}_N)^{\mathrm{T}} & — \end{bmatrix}, \text{ where } \boldsymbol{\Phi}(\mathbf{x}) = \begin{bmatrix} 1 \\ \phi_1(\mathbf{x}) \\ \vdots \\ \phi_k(\mathbf{x}) \end{bmatrix}, \ \phi_j(\mathbf{x}) = \phi\left(\frac{\|\mathbf{x}-\boldsymbol{\mu}_j\|}{r}\right)$$

Each row of Z is the RBF-feature corresponding to $\mathbf{x}_n$ (with dummy bias coordinate 1).

3: Fit the *linear* model $\mathrm{Z}\mathbf{w}$ to $\mathbf{y}$ to determine the weights $\mathbf{w}^*$.

classification: PLA, pocket, linear programming,....
regression: pseudoinverse.
logistic regression: gradient descent on cross entropy error.

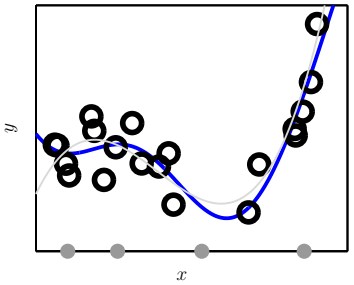
Choose r using CV, or (a heuristic):

$$r \sim \frac{\text{radius of data}}{k^{1/d}}$$

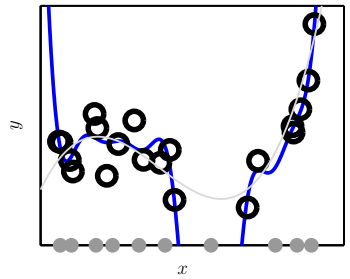
(so your clusters 'cover' the data)

Our Example

$k = 4,\ r = \frac{1}{k}$



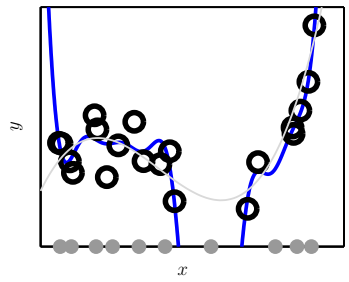
$k = 10,\ r = \frac{1}{k}$



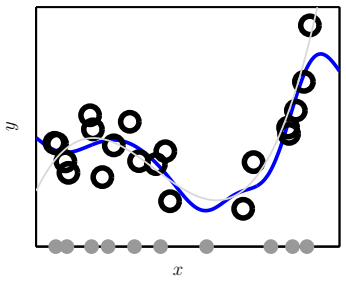
$$\mathbf{w} = (\mathrm{Z}^{\mathrm{T}}\mathrm{Z})^{-1}\mathrm{Z}^{\mathrm{T}}\mathbf{y}$$

Use Regularization to Fight Overfitting

$k = 10,\ r = \frac{1}{k}$



$k = 10,\ r = \frac{1}{k}$, regularized



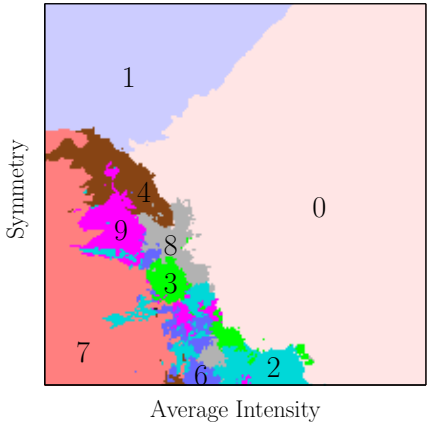
$$\mathbf{w} = (\mathrm{Z}^{\mathrm{T}}\mathrm{Z} + \lambda \mathrm{I})^{-1}\mathrm{Z}^{\mathrm{T}}\mathbf{y}$$

Reflecting on the k-RBF-Network

1. We derived it as a 'soft' generalization of k-NN rule.
   - Can also be derived from regularization theory.
   - Can also be derived from noisy interpolation theory.
2. Can use nonparametric or parametric versions.
3. Given centers, 'easy' to learn the weights using techniques from linear models.
   - A linear model with an adaptable nonlinear transform.
4. We used uniform bumps – can have different shapes Σ_j.
5. **NEXT:** How to better choose the centers: unsupervised learning.

A Peek at Unsupervised Learning

21-NN rule, 10 Classes



10 Clustering of Data