

# 第4章：非参数方法

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# 上次课主要内容回顾

- 特征维数与过拟合
  - 增加特征带来更多判别信息
  - 克服过拟合的方法?
- 期望最大法(EM)
  - 对数似然度对缺失数据的期望
  - EM for Gaussian mixture
- 隐马尔可夫模型(HMM)
  - Three basic problems
  - Viterbi Algorithm (DP)
  - Extensions

# 提 纲

- 第4章 非参数方法
  - 密度估计
  - Parzen窗方法
  - K近邻估计
  - 最近邻规则
  - 距离度量
  - Reduced Coulomb Energy Network
  - Approximation by Series Expansion

# 密度估计

- 概率和密度

- 概率：特征空间中一定区域内样本的比率

$$P = \int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}'$$

- 假设局部区域（体积为 $V$ ，样本数 $k$ ）内等概率密度

$$\int_{\mathcal{R}} p(\mathbf{x}') d\mathbf{x}' \simeq p(\mathbf{x})V \quad p(\mathbf{x}) \simeq \frac{k/n}{V}$$

- 如何决定局部区域的大小：随样本数 $n$ 变化

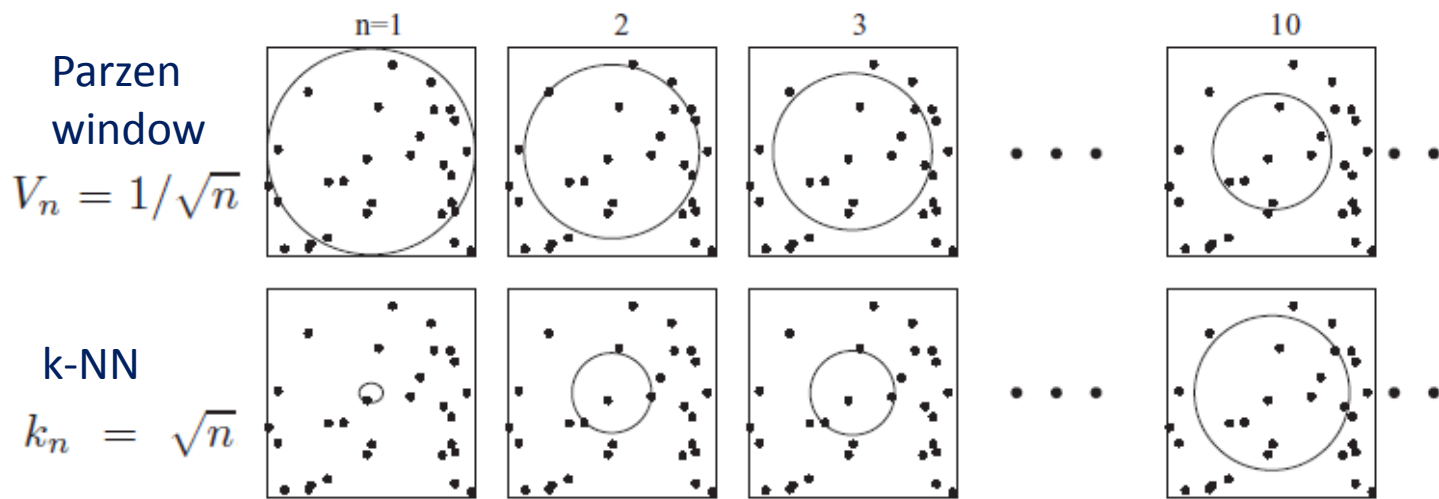
- $p_n(\mathbf{x})$ 收敛到 $p(\mathbf{x})$ 的条件  $\lim_{n \rightarrow \infty} V_n = 0$

$$\lim_{n \rightarrow \infty} k_n = \infty$$

$$\lim_{n \rightarrow \infty} k_n/n = 0$$

# • 非参数概率密度估计

- Parzen window: 固定局部区域体积 $V$ ,  $k$ 变化
- k-nearest neighbor: 固定局部样本数 $k$ ,  $V$ 变化



(这里 $n$ 不一定指样本数)

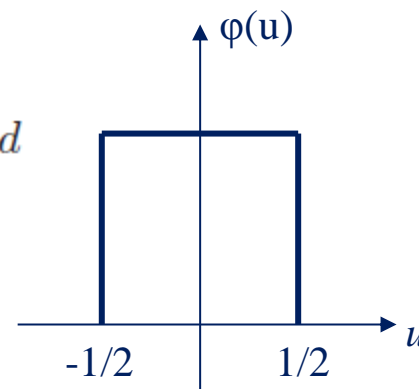
# Parzen Window

- 窗函数： hypercube

$$\varphi(\mathbf{u}) = \begin{cases} 1 & |u_j| \leq 1/2 \quad j = 1, \dots, d \\ 0 & \text{otherwise.} \end{cases}$$

- 满足条件

$$\varphi(\mathbf{x}) \geq 0 \quad \int \varphi(\mathbf{u}) d\mathbf{u} = 1$$



- 以x为中心、体积为  $V_n = h_n^d$  的局部区域内样本数

$$k_n = \sum_{i=1}^n \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right)$$

- 概率密度估计  $k_n/nV_n$

$$p_n(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{V_n} \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right)$$

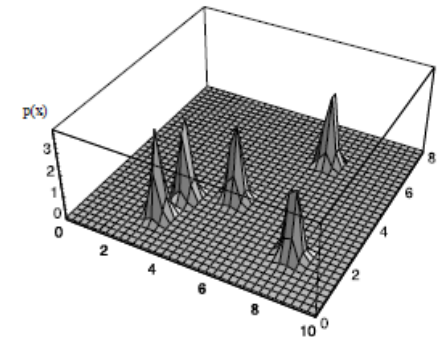
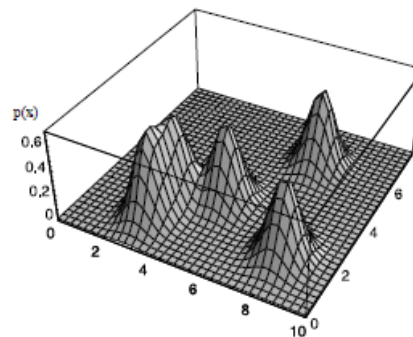
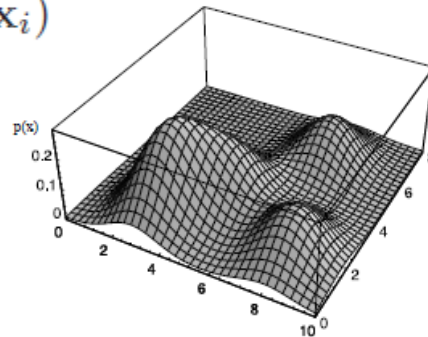
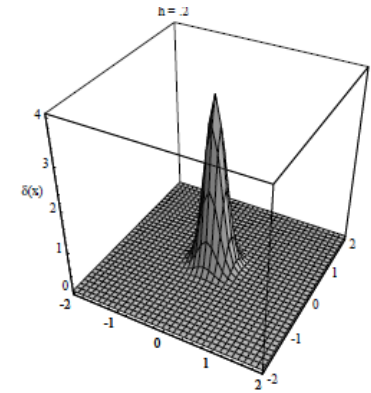
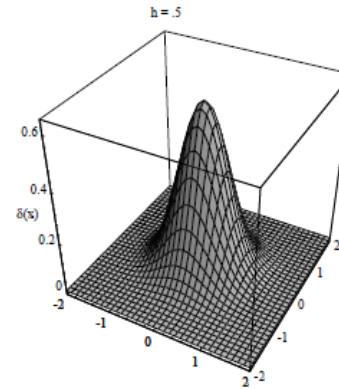
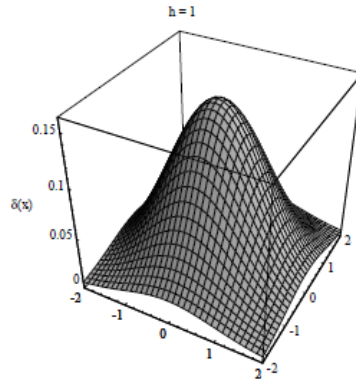
- 推广：满足密度函数要求的窗函数，如高斯函数

$$\varphi(\mathbf{x}) \geq 0 \quad \int \varphi(\mathbf{u}) d\mathbf{u} = 1$$

# Gaussian window, variable width ( $h=1, 0.5, 0.2$ )

$$\delta_n(\mathbf{x}) = \frac{1}{V_n} \varphi\left(\frac{\mathbf{x}}{h_n}\right)$$

$$p_n(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \delta_n(\mathbf{x} - \mathbf{x}_i)$$



Large  $h$ : low variability, under fitting  
Small  $h$ : high variability, overfitting

- Parzen窗密度估计的收敛性
  - $p_n(\mathbf{x})$ 的期望是 $p(\mathbf{x})$ 的平滑（卷积）
    - Samples  $\mathbf{x}_1, \dots, \mathbf{x}_n$  are i.i.d from  $p(\mathbf{x})$

$$\begin{aligned}\bar{p}_n(\mathbf{x}) &= \mathcal{E}[p_n(\mathbf{x})] \\ &= \frac{1}{n} \sum_{i=1}^n \mathcal{E} \left[ \frac{1}{V_n} \varphi \left( \frac{\mathbf{x} - \mathbf{x}_i}{h_n} \right) \right] \\ &= \int \frac{1}{V_n} \varphi \left( \frac{\mathbf{x} - \mathbf{v}}{h_n} \right) p(\mathbf{v}) d\mathbf{v} \\ &= \int \delta_n(\mathbf{x} - \mathbf{v}) p(\mathbf{v}) d\mathbf{v}.\end{aligned}$$

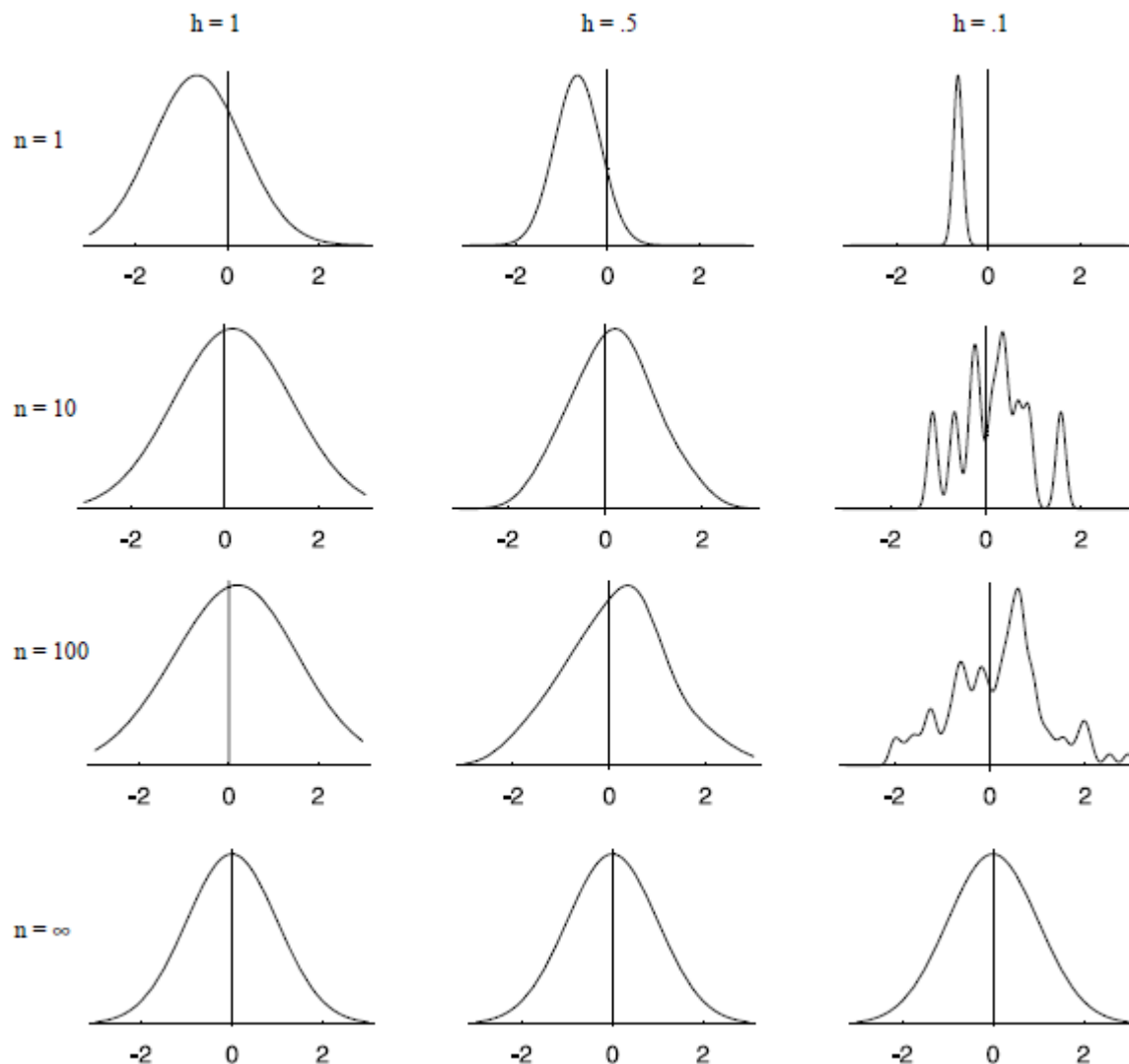
$$\text{When } n \rightarrow \infty \quad \lim_{n \rightarrow \infty} V_n = 0 \quad \lim_{n \rightarrow \infty} nV_n = \infty$$

$$\bar{p}_n(\mathbf{x}) \rightarrow p(\mathbf{x})$$



- 示例：高斯窗函数  $\varphi(u) = \frac{1}{\sqrt{2\pi}} e^{-u^2/2}$

$$p_n(x) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h_n} \varphi\left(\frac{x - x_i}{h_n}\right) \quad \underline{h_n = h_1 / \sqrt{n}}$$



True  $p(x)$ :  
Gaussian

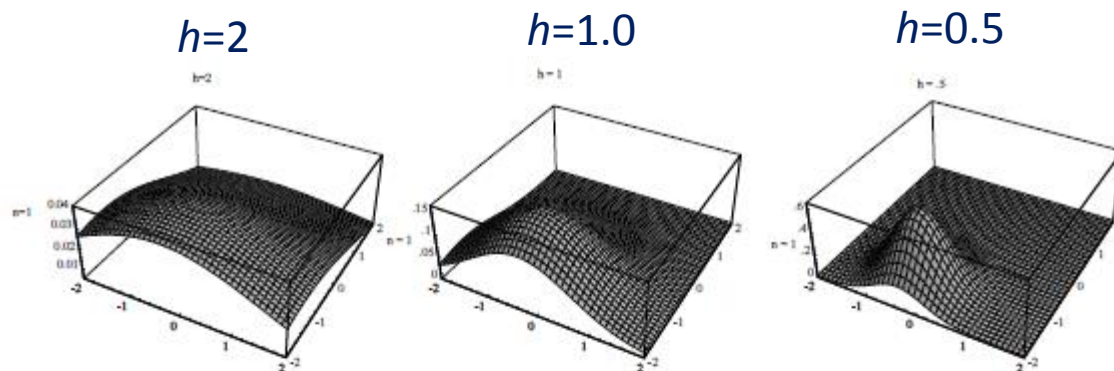


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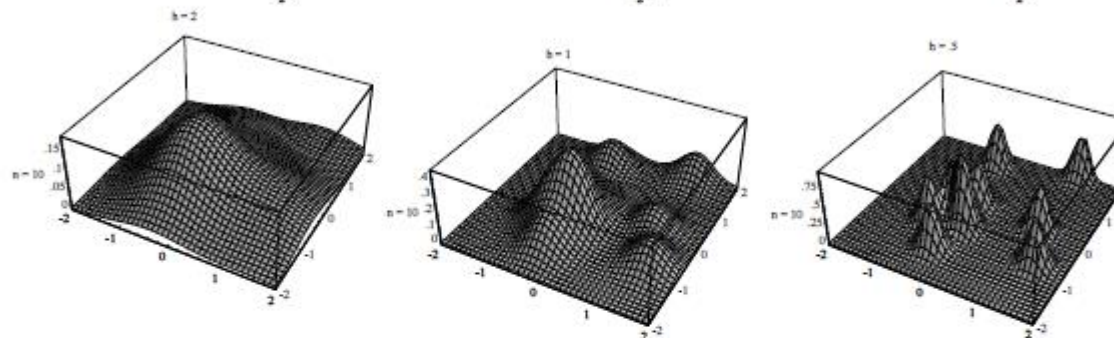
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# 2D case

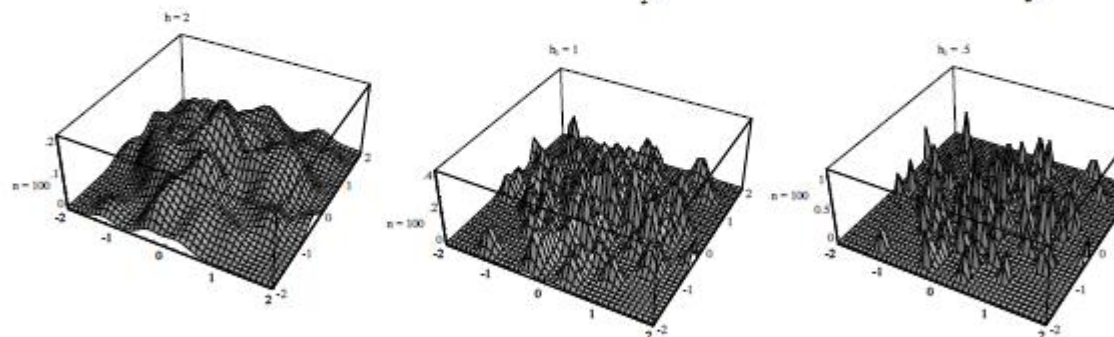
$n=1$



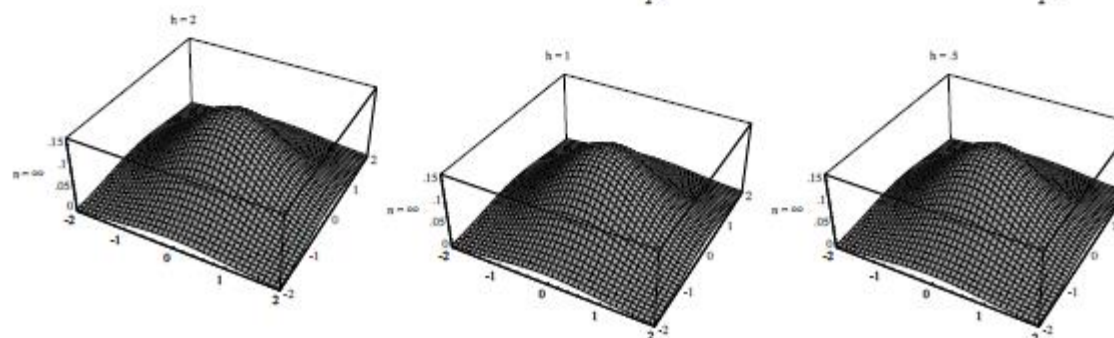
$n=10$



$n=100$

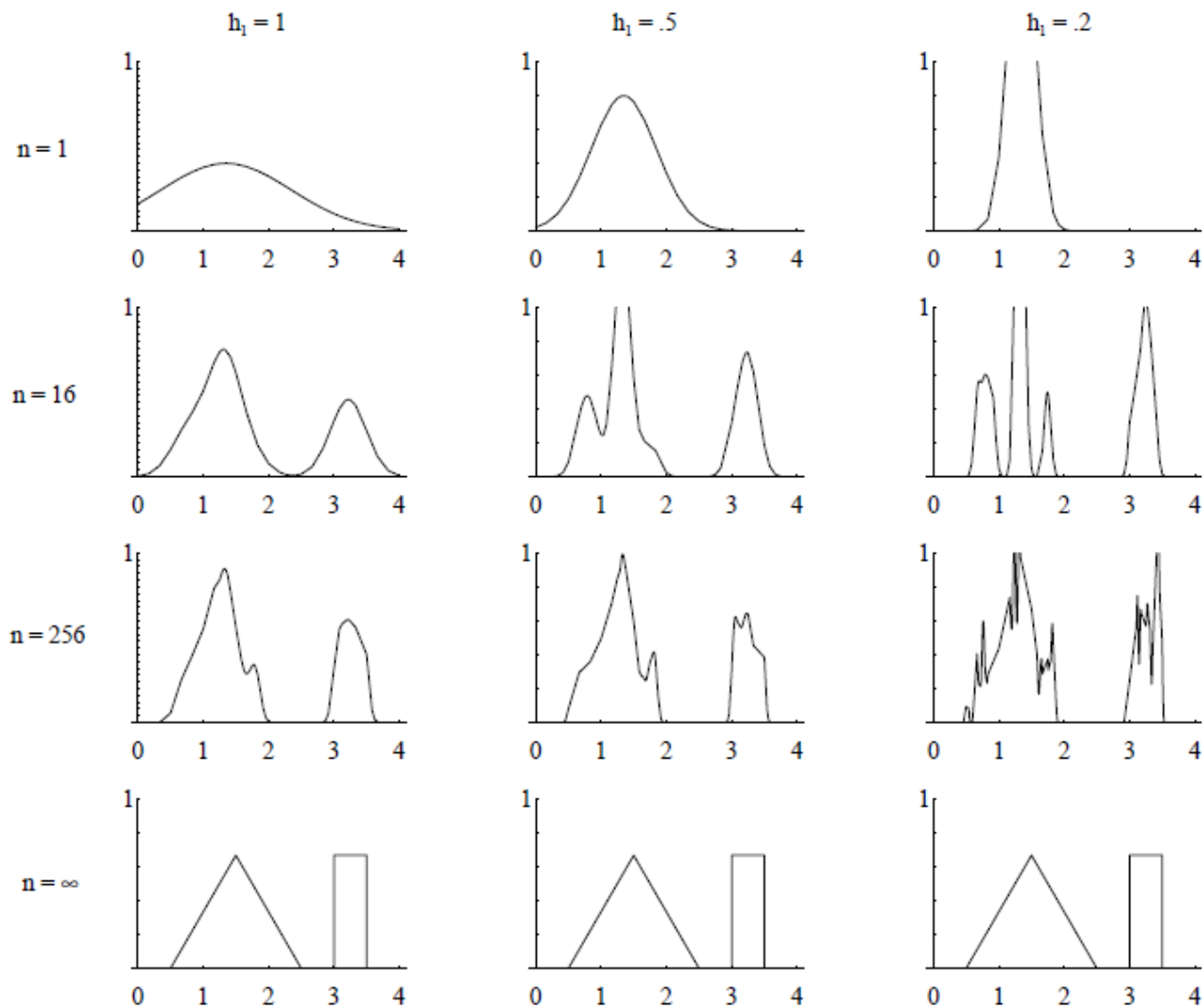


$n=\infty$



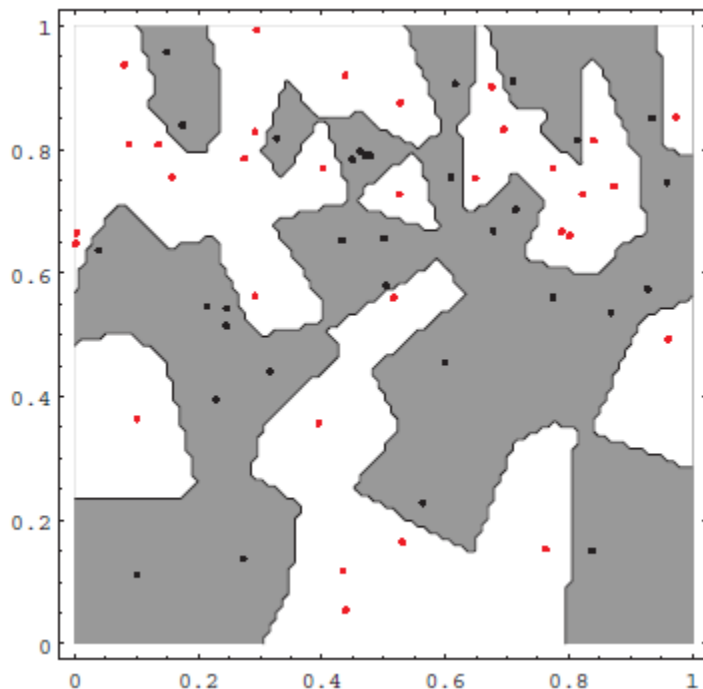
True  $p(x)$ :  
Gaussian

- Bimodal distribution

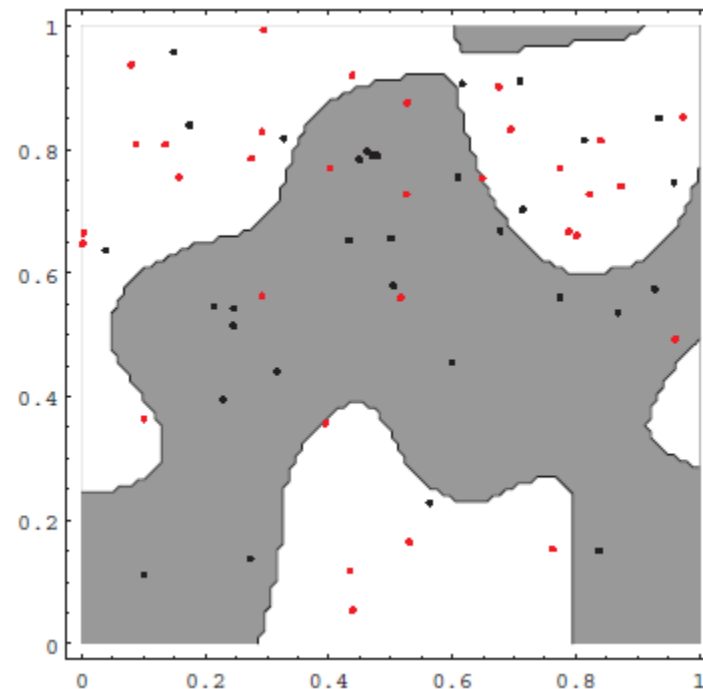


- 分类的例子  $\max_i p(\mathbf{x} | \omega_i) P(\omega_i)$

Small  $h$



Large  $h$



Decision  
regions

上部和下部密度区别大，适合不同的 $h$ 值  
(考虑Generalization)

- 窗宽 $h_n$ 选择经验

- 一般原则： $n$ 越大或密度越大， $h_n$ 越小

- 随 $n$ 变化： $V_n = V_1/\sqrt{n}$

- 随 $x$ 变化： $h(\mathbf{x}), h(\mathbf{x}_i)$

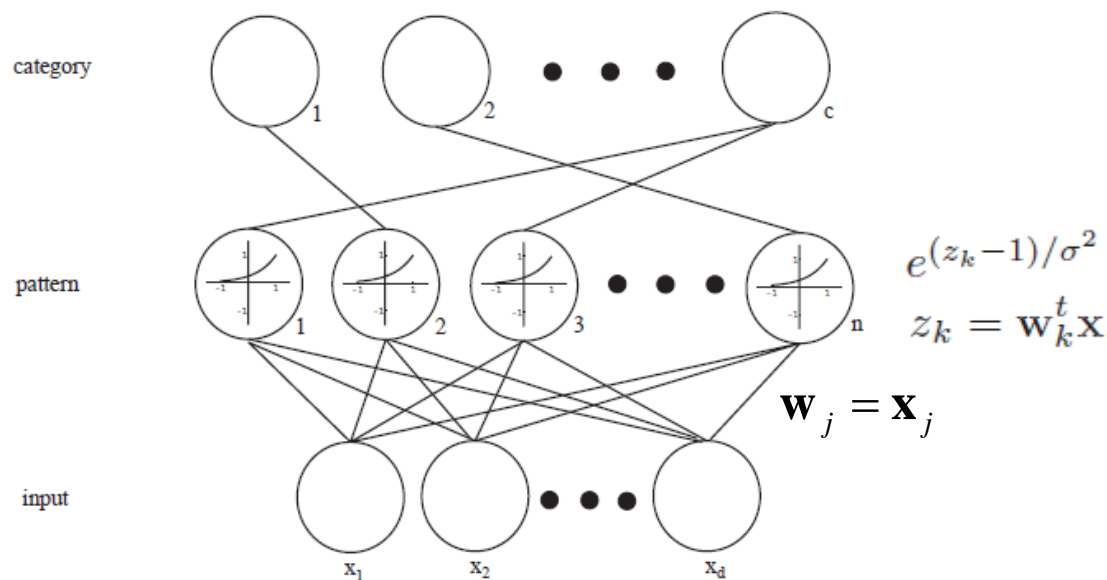
- $\mathbf{x}$ 测试样本， $\mathbf{x}_i$ 训练样本

- 比如：根据k-NN的距离估计局部密度， $h$ 与局部密度成反比

- 交叉验证(cross validation)

- 比如选择 $V_1$ ：设多个候选值，对每个值的效果进行交叉验证

- Probabilistic Neural Network (PNN)
  - 输出每个类别的概率密度
  - 隐节点: pattern unit, 对应Parzen窗函数
  - Normalized pattern:  $\mathbf{x} \leftarrow \mathbf{x} / \|\mathbf{x}\|$



Why  $e^{(z_k-1)/\sigma^2}$

$$\varphi\left(\frac{\mathbf{X}_k - \mathbf{W}_k}{h_n}\right) \propto \overbrace{e^{-(\mathbf{x} - \mathbf{w}_k)^t(\mathbf{x} - \mathbf{w}_k)/2\sigma^2}}^{\text{desired Gaussian}}$$

$$= e^{-(\mathbf{x}^t\mathbf{x} + \mathbf{w}_k^t\mathbf{w}_k - 2\mathbf{x}^t\mathbf{w}_k)/2\sigma^2} = e^{(z_k-1)/\sigma^2}$$



# k近邻估计

- 概率密度估计

- 固定局部区域样本数 $k$ , 体积 $V$ 变化

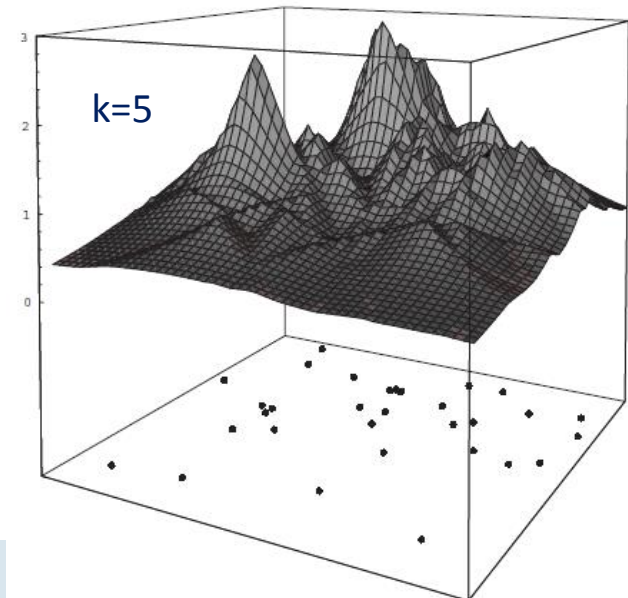
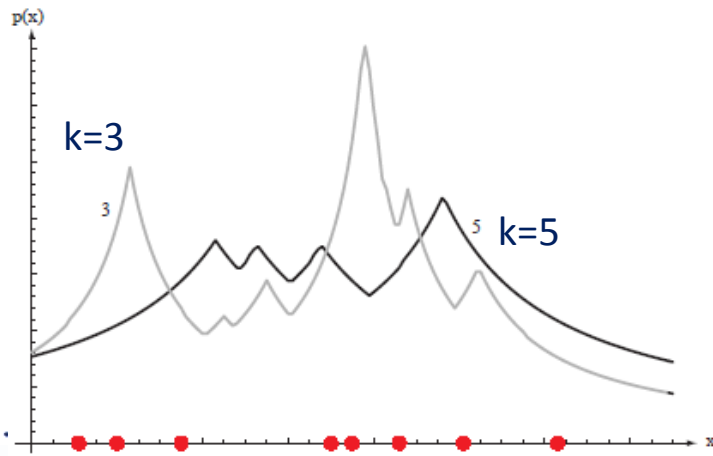
$$p_n(\mathbf{x}) = \frac{k_n/n}{V_n}$$

- 收敛到 $p(\mathbf{x})$ 条件

$$\lim_{n \rightarrow \infty} k_n = \infty \text{ and } \lim_{n \rightarrow \infty} k_n/n = 0$$

- 一种选择:  $k_n = \sqrt{n}$   $V_n \simeq 1/(\sqrt{n}p(\mathbf{x}))$

- 1D, 2D的例子

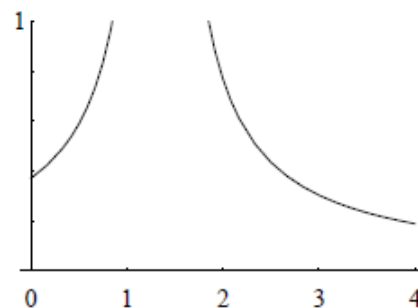
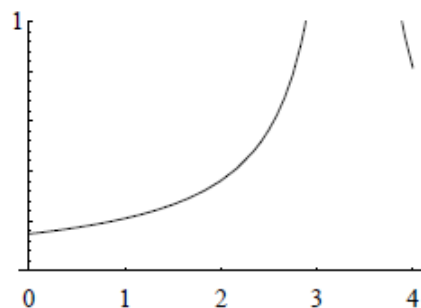


# More 1D examples

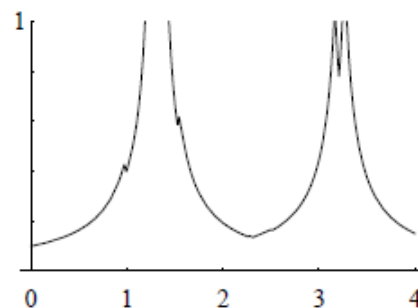
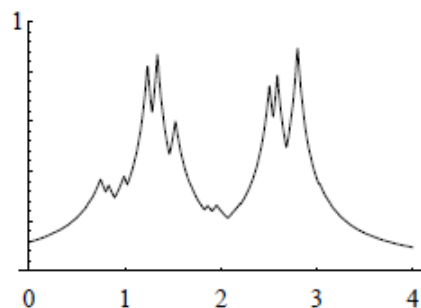
$$k_n = \sqrt{n}$$

$$p_n(x) = \frac{\sqrt{n}/n}{2|x - x_{kNN}|}$$

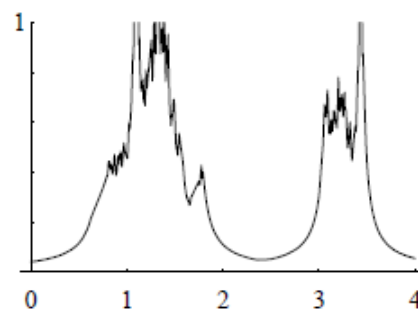
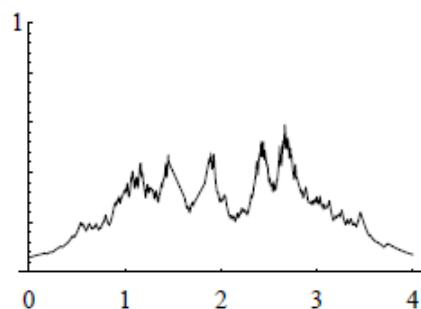
$n = 1$   
 $k_n = 1$



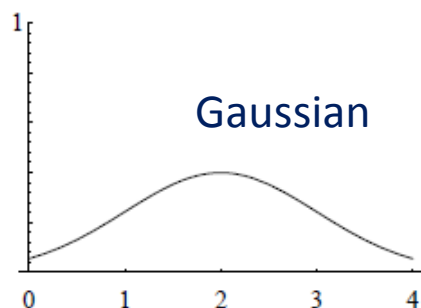
$n = 16$   
 $k_n = 4$



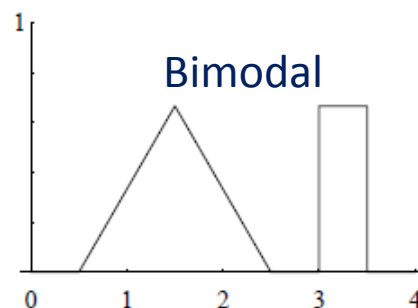
$n = 256$   
 $k_n = 16$



$n = \infty$   
 $k_n = \infty$



Gaussian



Bimodal

True  $p(x)$



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- K-NN分类：后验概率

- $k_i$  NNs from class  $i$        $k = \sum_{i=1}^c k_i$

$$p_n(\mathbf{x}, \omega_i) = \frac{k_i/n}{V}$$

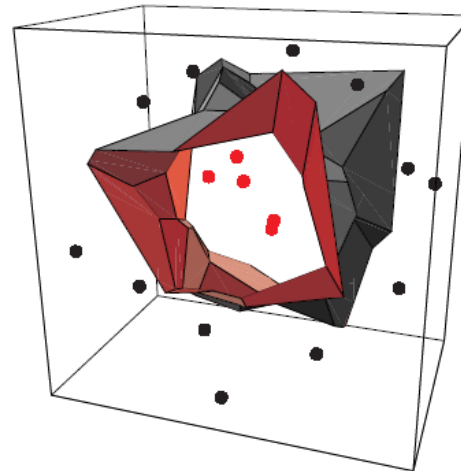
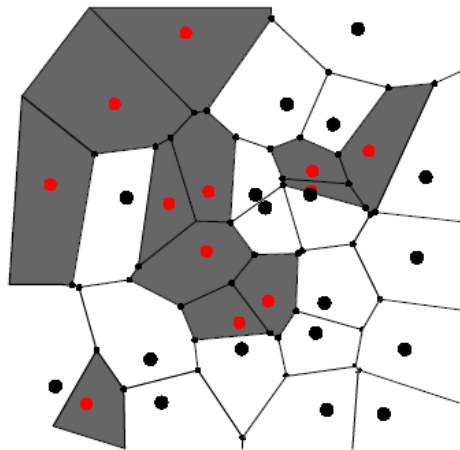
$$P_n(\omega_i|\mathbf{x}) = \frac{p_n(\mathbf{x}, \omega_i)}{\sum_{j=1}^c p_n(\mathbf{x}, \omega_j)} = \frac{k_i}{k}$$

- 分类错误率：当  $\lim_{n \rightarrow \infty} k_n = \infty$  and  $\lim_{n \rightarrow \infty} k_n/n = 0$   
趋近贝叶斯错误率

K-NN分类规则里没有概率密度，但要注意，该规则是从非参数概率密度估计和贝叶斯决策过来的

# 最近邻规则

- Nearest Neighbor (1-NN) Rule
  - Among labeled data  $\mathcal{D}^n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$   $\mathbf{x}'$  is the NN of  $\mathbf{x}$
  - Assume  $P(\omega|\mathbf{x}') \simeq P(\omega_i|\mathbf{x})$
  - Classification: MAP
$$\omega_m = \arg \max_i P(\omega_i | \mathbf{x}) = \omega(\mathbf{x}')$$
  - Decision regions: Voronoi tessellation



# 最近邻规则的错误率

$$P(e) = \int P(e|\mathbf{x})p(\mathbf{x}) d\mathbf{x}$$

$$P(e|\mathbf{x}) = \int \underline{P(e|\mathbf{x}, \mathbf{x}')}p(\mathbf{x}'|\mathbf{x}) d\mathbf{x}' \quad \mathbf{x}': \text{NN of } \mathbf{x}$$

- 当 $n \rightarrow \infty$ ,  $p(\mathbf{x}'|\mathbf{x})$  趋近以 $\mathbf{x}$  为中心的delta函数
- 对 $P(e|\mathbf{x}, \mathbf{x}')$ , 假设  $\mathbf{x}$  和  $\mathbf{x}'_j$  (最近训练样本, 与 $\mathbf{x}$  独立)的类别标号分别为  $\theta$  和  $\theta'_j$

$$P(\theta, \theta'_j|\mathbf{x}, \mathbf{x}'_j) = P(\theta|\mathbf{x})P(\theta'_j|\mathbf{x}'_j)$$

$$P_n(e|\mathbf{x}, \mathbf{x}'_j) = 1 - \sum_{i=1}^c P(\theta = \omega_i, \theta' = \omega_i|\mathbf{x}, \mathbf{x}'_j) = 1 - \sum_{i=1}^c P(\omega_i|\mathbf{x})P(\omega_i|\mathbf{x}'_j)$$

$$\lim_{n \rightarrow \infty} P_n(e|\mathbf{x}) = \int \left[ 1 - \sum_{i=1}^c P(\omega_i|\mathbf{x})P(\omega_i|\mathbf{x}') \right] \underline{\delta(\mathbf{x}' - \mathbf{x})} d\mathbf{x}' = 1 - \sum_{i=1}^c P^2(\omega_i|\mathbf{x})$$



- 最近邻规则的错误率

- Asymptotic error rate  $\lim_{n \rightarrow \infty} P_n(e|\mathbf{x}) = 1 - \sum_{i=1}^c P^2(\omega_i|\mathbf{x})$

$$\begin{aligned}
 P &= \lim_{n \rightarrow \infty} P_n(e) \\
 &= \lim_{n \rightarrow \infty} \int P_n(e|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} \\
 &= \int \left[ 1 - \sum_{i=1}^c P^2(\omega_i|\mathbf{x}) \right] p(\mathbf{x}) d\mathbf{x}
 \end{aligned}$$

- Error bound of 1-NN rule

$$\begin{aligned}
 \sum_{i=1}^c P^2(\omega_i|\mathbf{x}) &= P^2(\omega_m|\mathbf{x}) + \boxed{\sum_{i \neq m} P^2(\omega_i|\mathbf{x})} \quad \text{Minimized when } P_i \text{ (} i \neq m \text{) are equal} \\
 P(\omega_i|\mathbf{x}) &= \begin{cases} \frac{P^*(e|\mathbf{x})}{c-1} & i \neq m \\ 1 - P^*(e|\mathbf{x}) & i = m \end{cases} \quad P^*(e|\mathbf{x}) = 1 - P(\omega_m|\mathbf{x}) \text{ (Bayes error)} \\
 \sum_{i=1}^c P^2(\omega_i|\mathbf{x}) &\geq (1 - P^*(e|\mathbf{x}))^2 + \frac{P^{*2}(e|\mathbf{x})}{c-1}
 \end{aligned}$$

- Error bound of 1-NN rule

$$\sum_{i=1}^c P^2(\omega_i|\mathbf{x}) \geq (1 - P^*(e|\mathbf{x}))^2 + \frac{P^{*2}(e|\mathbf{x})}{c-1}$$

$$1 - \sum_{i=1}^c P^2(\omega_i|\mathbf{x}) \leq 2P^*(e|\mathbf{x}) - \frac{c}{c-1}P^{*2}(e|\mathbf{x})$$

- Error rate

$$P = \int \left[ 1 - \sum_{i=1}^c P^2(\omega_i|\mathbf{x}) \right] p(\mathbf{x}) d\mathbf{x} \rightarrow P \leq 2P^*$$

$$\begin{aligned} \text{Var}[P^*(e|\mathbf{x})] &= \int [P^*(e|\mathbf{x}) - P^*]^2 p(\mathbf{x}) d\mathbf{x} \\ &= \int P^{*2}(e|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} - P^{*2} \geq 0 \rightarrow \int P^{*2}(e|\mathbf{x}) p(\mathbf{x}) d\mathbf{x} \geq P^{*2} \end{aligned}$$

- Error bound

$$P^* \leq P \leq P^* \left( 2 - \frac{c}{c-1} P^* \right)$$

证明这个bound比较费劲，一般来说记住结论即可。  
证明过程中有些思想很有启发，比如 $P(e|\mathbf{x}, \mathbf{x}')$ 假设

# Break

# K近邻的快速计算

- 分类的计算复杂度  $O(dn)$
- 近邻搜索的三种策略
  - Partial distance
  - Prestructuring
  - Editing (pruning, condensing)

Partial square distance ( $r < d$ )

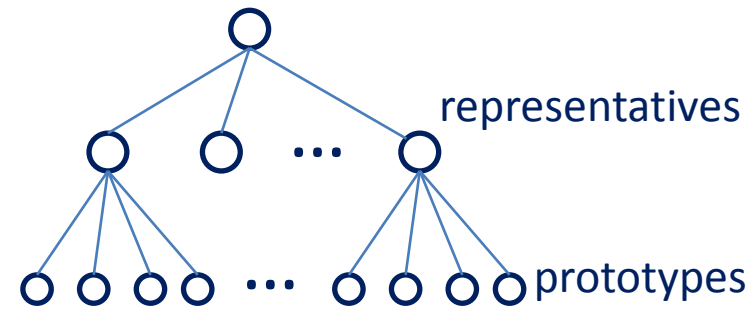
$$D_r^2(\mathbf{a}, \mathbf{b}) = \sum_{i=1}^r (a_i - b_i)^2$$

Full distance to the current closest prototype  $D^2(\mathbf{x}, \mathbf{x}')$

Terminate computing if the partial square distance is greater than  $D^2(\mathbf{x}, \mathbf{x}')$

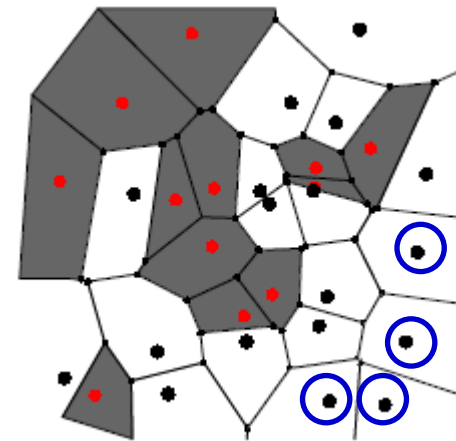
## – Prestructuring

- Search tree, prototypes are linked to the nodes, each labeled with a representative prototype
  - E.g. Constructed by clustering
- 1-NN搜索：先找出到 $x$ 的最近代表点，然后计算与最近代表点连接原型的距离，找出最近原型
- 可结合partial distance
- 为保证找到最近原型，应从多个代表点的原型中搜索



## – Editing

- Remove prototypes that are surrounded by samples (Voronoi neighbors) of same class



有更多近邻搜索的快速算法，如branch-and-bound, k-d tree等（在此省略）



# 距离度量

- 距离度量(metric)的性质

non-negativity:  $D(a, b) \geq 0$

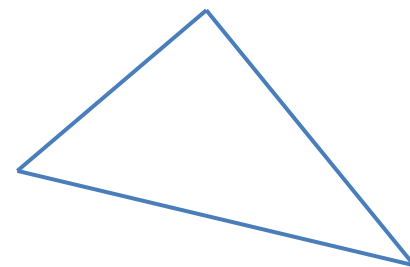
reflexivity:  $D(a, b) = 0$  if and only if  $a = b$

symmetry:  $D(a, b) = D(b, a)$

triangle inequality:  $D(a, b) + D(b, c) \geq D(a, c)$

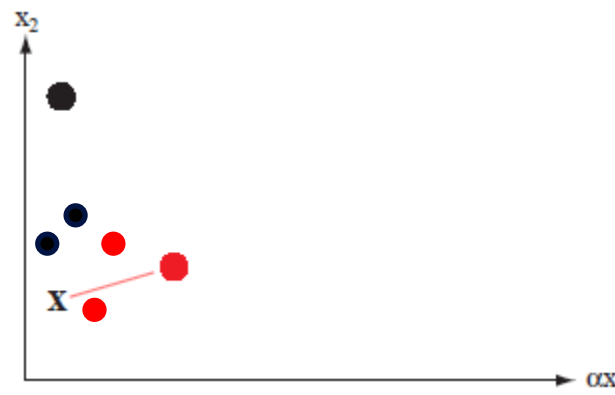
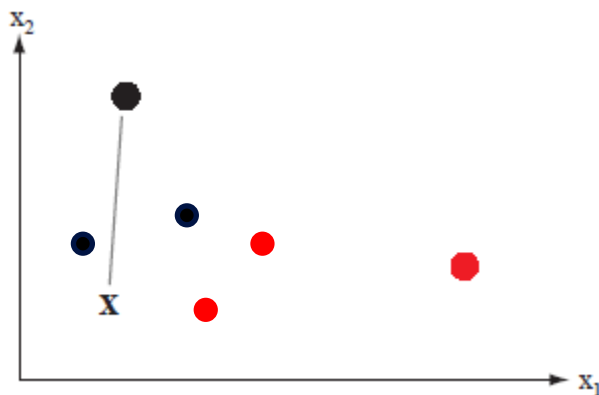
- Metric影响分类性能

– 比如, 当特征变尺度



Euclidean metric

$$D(a, b) = \left( \sum_{k=1}^d (a_k - b_k)^2 \right)^{1/2}$$



- 几种Metric

- Minkowski ( $L_k$  norm)

$$L_k(\mathbf{a}, \mathbf{b}) = \left( \sum_{i=1}^d |a_i - b_i|^k \right)^{1/k}$$

- Manhattan (city block distance):  $k=1$
- Tanimoto metric (for binary features)

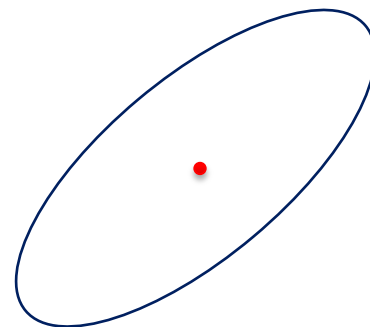
$$D_{Tanimoto}(\mathcal{S}_1, \mathcal{S}_2) = \frac{n_1 + n_2 - 2n_{12}}{n_1 + n_2 - n_{12}}$$

- Metric Learning

- Parameters in metric optimized in learning (e.g., empirical risk minimization)

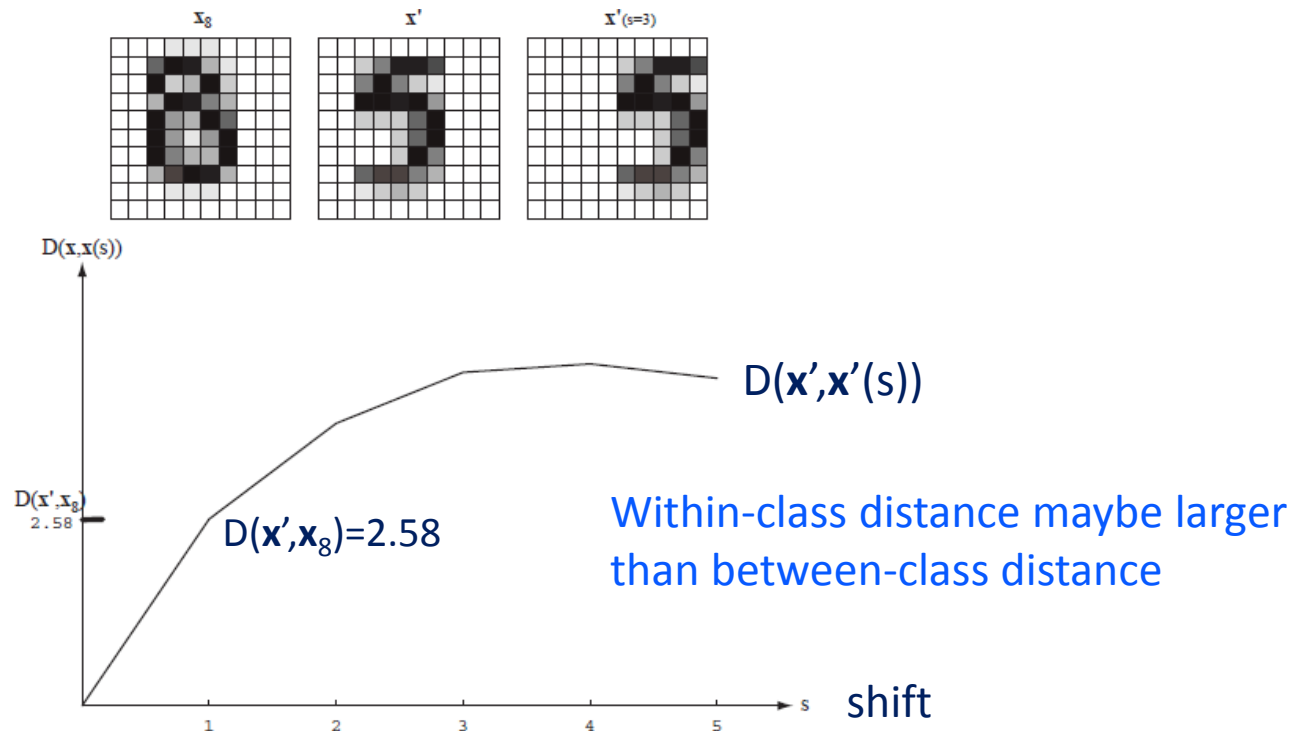
$$D_{\mathbf{w}}(\mathbf{a}, \mathbf{b}) = \sum_{i=1}^d w_i (a_i - b_i)^2$$

$$D_{\Sigma}(\mathbf{a}, \mathbf{b}) = (\mathbf{a} - \mathbf{b})^t \Sigma^{-1} (\mathbf{a} - \mathbf{b})$$



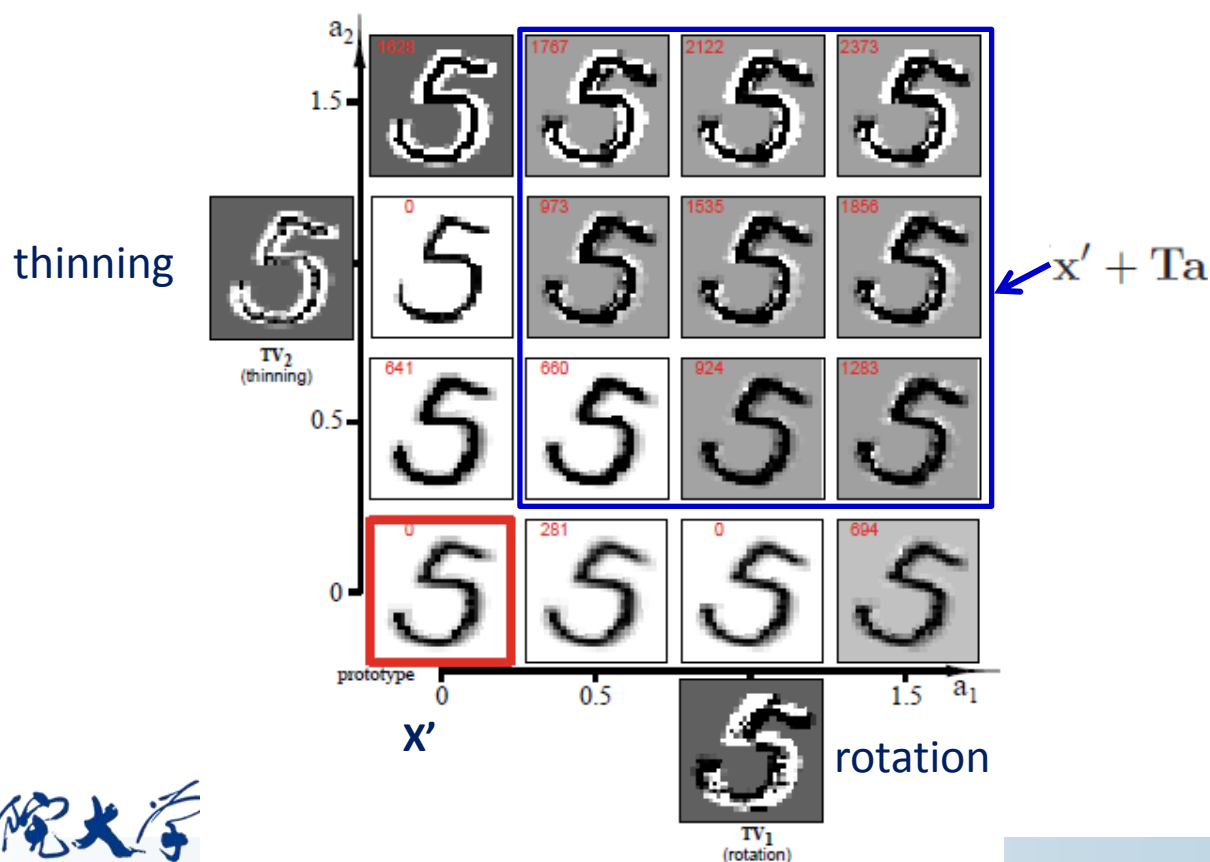
# Tangent Distance

- Image Shape Transformation
  - Shift (translation), rotation, scaling, distortion
  - Distance sensitive to transformation



# • Tangent distance

- Search for optimal parameters for a combination of transformations for a prototype to minimize the distance to test sample
- Parameterized transformation:  $\mathcal{F}_i(\mathbf{x}'; \alpha_i)$
- Tangent vectors:  $\mathbf{TV}_i = \mathcal{F}_i(\mathbf{x}'; \alpha_i) - \mathbf{x}'$     近似梯度方向
- Linear combination in the space spanned by TVs:  $\mathbf{x}' + \mathbf{T}\mathbf{a}$



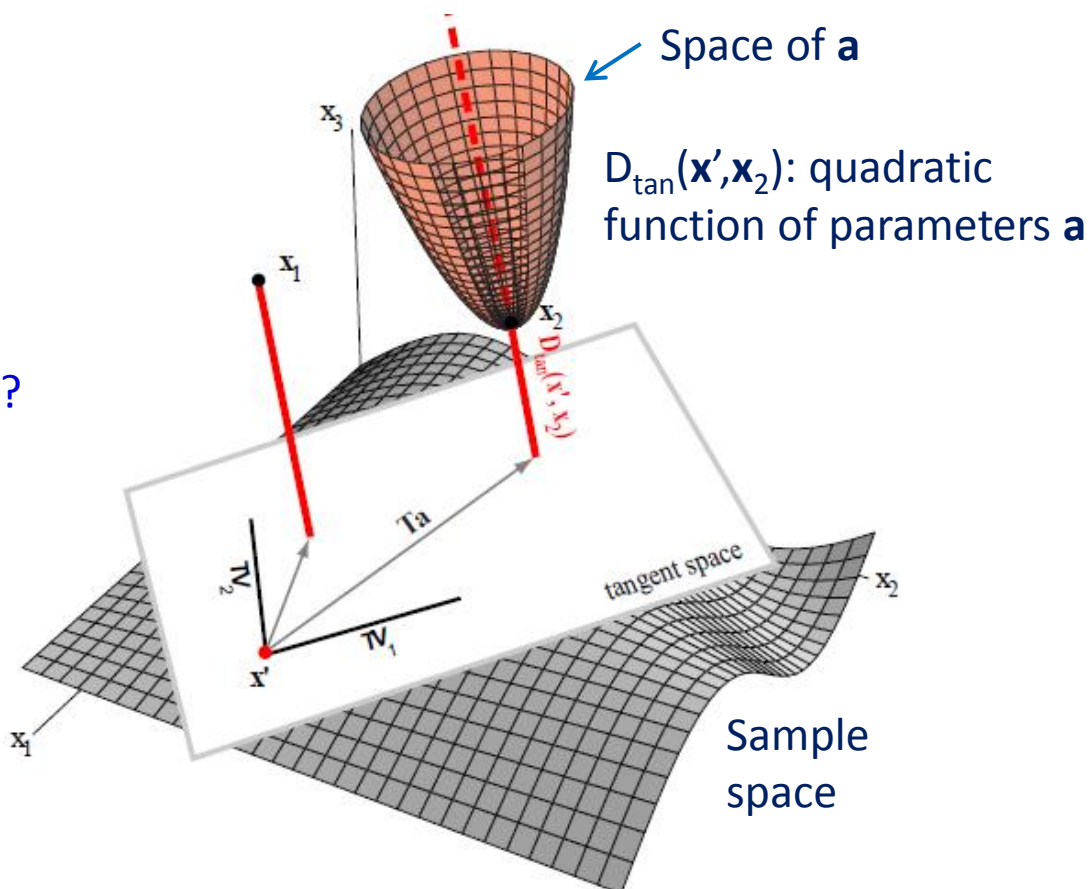
- Tangent distance

- Euclidean distance to tangent space

$$D_{tan}(\mathbf{x}', \mathbf{x}) = \min_{\mathbf{a}} [\|\mathbf{x}' + \mathbf{T}\mathbf{a} - \mathbf{x}\|] \quad \text{点到超平面的最近距离}$$

- Optimization: gradient search w.r.t  $\mathbf{a}$

为什么叫  
tangent space?



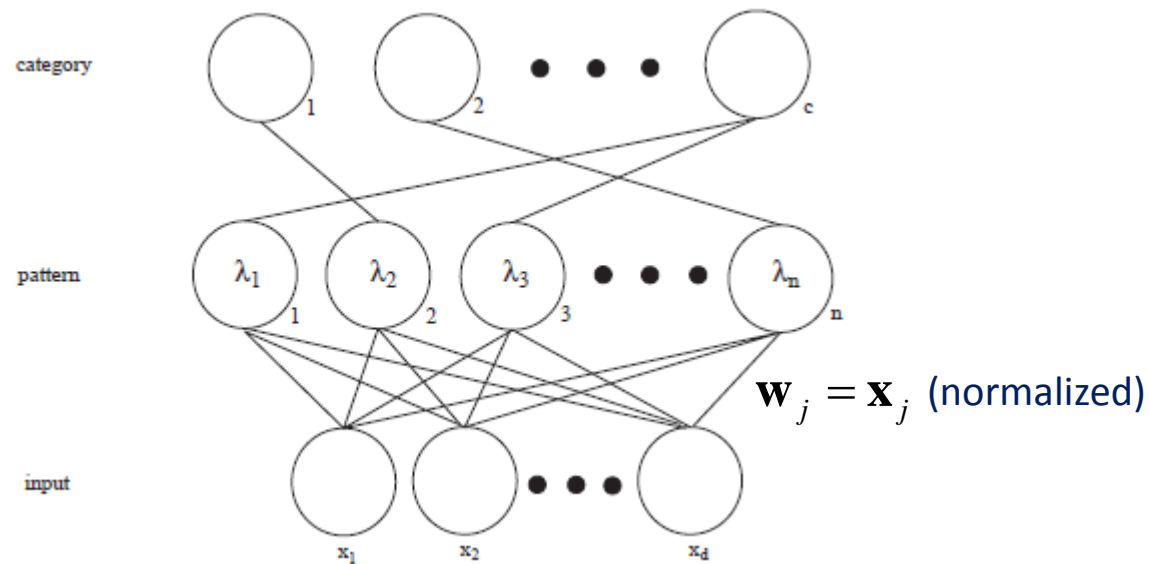
# Reduced Coulomb Energy Network

- RCE Network

- Hidden node (corresponding to a training sample): hypersphere with **radius** according to the distance to nearest point of different class

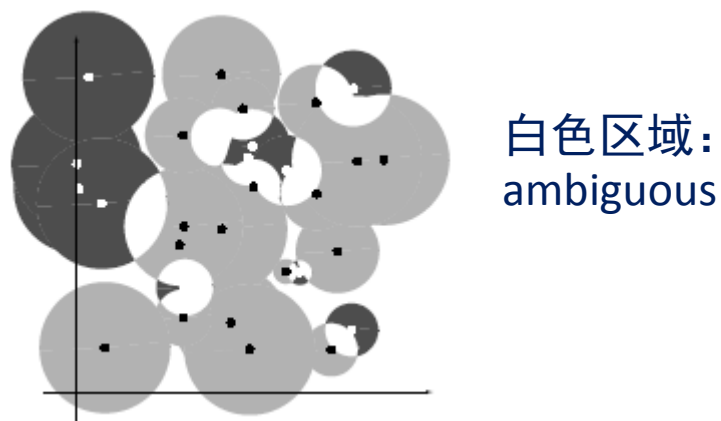
$\epsilon = \text{small param}, \lambda_m = \text{max radius}$

$$\lambda_j \leftarrow \min_{\mathbf{x} \notin \omega_i} [\min D(\mathbf{x}, \mathbf{x}') - \epsilon, \lambda_m]$$



- RCE分类规则

- 找出包含 $x$ 的隐节点（超球体），如果这些节点的类别标号一致，则分类到这个类别
  - 没有节点包含 $x$ ，或者类别不一致（不同类别超球体重叠）的情况，则拒识



RCE Network: 与非参数方法(Parzen window, k-NN)的关系  
与Probabilistic neural network的关系

# Approximation by Series Expansion

- Parzen窗密度估计：计算量大
- 窗函数用序列展开

$$\varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right) = \sum_{j=1}^m a_j \psi_j(\mathbf{x}) \chi_j(\mathbf{x}_i)$$

$$\sum_{i=1}^n \varphi\left(\frac{\mathbf{x} - \mathbf{x}_i}{h_n}\right) = \sum_{j=1}^m a_j \psi_j(\mathbf{x}) \sum_{i=1}^n \chi_j(\mathbf{x}_i)$$

$$p_n(\mathbf{x}) = \sum_{j=1}^m b_j \psi_j(\mathbf{x}) \quad b_j = \frac{a_j}{nV_n} \sum_{i=1}^n \chi_j(\mathbf{x}_i)$$

–  $b_j$ 可离线计算， $p_n(\mathbf{x})$ 只需 $m$ 次计算( $m < n$ )



- 高斯窗函数的Taylor展开

$$\sqrt{\pi} \varphi(u) = e^{-u^2} \simeq \sum_{j=0}^{m-1} (-1)^j \frac{u^{2j}}{j!}$$

$$\begin{aligned} m=2 \quad \sqrt{\pi} \varphi\left(\frac{x-x_i}{h}\right) &\simeq 1 - \left(\frac{x-x_i}{h}\right)^2 \\ &= 1 + \frac{2}{h^2} x x_i - \frac{1}{h^2} x^2 - \frac{1}{h^2} x_i^2 \end{aligned}$$

$$\sqrt{\pi} p_n(x) = \frac{1}{nh} \sum_{i=1}^n \sqrt{\pi} \varphi\left(\frac{x-x_i}{h}\right) \simeq b_0 + b_1 x + b_2 x^2$$

$$b_0 = \frac{1}{h} - \frac{1}{h^3} \frac{1}{n} \sum_{i=1}^n x_i^2 \quad b_1 = \frac{2}{h^3} \frac{1}{n} \sum_{i=1}^n x_i \quad b_2 = -\frac{1}{h^3}$$

只有当 $\max|x-x_i|<h$ 时，展开的近似误差较小，然而这要求 $h$ 比较大  
当 $h$ 较小，使用更多的展开项（ $m$ 比较大）

这个方法实用价值不大，因为密度估计有误差，而从分类的角度，有很多分类器可以代替。但是思路值得借鉴。

# 总结

- 非参数法的基本思想
  - 没有给定概率密度函数形式
  - 基于概率和密度的原始定义，以训练样本的局部分布近似 $x$ 的局部密度
- Parzen window
- K-nearest neighbor (k-NN)
  - 1-nearest neighbor (1-NN), Error bound
  - 快速搜索
- 距离度量
  - Tangent distance
- Series expansion

# 统计模式识别的作用和地位

- 贝叶斯决策
  - MAP, 最小风险决策
  - 贝叶斯分类器：理想情况（样本无穷多、概率密度准确估计）下最优
- Parametric/Non-parametric统计分类器
  - 训练样本较少时比较competitive
- 概率密度估计
  - 概率密度模型：生成模型，可用于判别outlier ( $p(\mathbf{x}) < t$ )
  - 信息论方法的基础，如熵、互信息等
  - K-NN: local density, local accuracy of classifier
- 特征空间分析
  - 假设空间相邻的样本类别也相同(流形假设, Manifold assumption)
  - 基于特征空间划分的分类器设计，如tree classifier
  - 基于特征空间的分类器性能分析，如神经网络的决策面/决策区域
- 与其他分类方法的关系
  - 判别模型(SVM, 神经网络等)：近似后验概率，或输出可近似转换为后验概率
  - 基于距离/相似度的分类器：可从特征空间分析
  - 结构PR问题转换为统计PR: Dissimilarity embedding

# 下次课 (向世明老师)