Kernel Methods

CSci 5525: Machine Learning

Instructor: Arindam Banerjee

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- The final prediction function

$$f(\mathbf{x}) = \sum_{i:\alpha_i>0} \alpha_i y_i \langle \Phi(\mathbf{x}_i), \Phi(\mathbf{x}) \rangle + b = \sum_{i:\alpha_i>0} \alpha_i y_i k(\mathbf{x}_i, \mathbf{x}) + b$$



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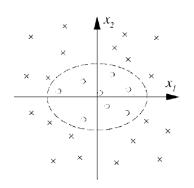
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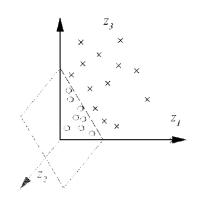
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- How to choose a kernel for a given application?



Example





$$z_1 = x_1^2$$
, $z_2 = \sqrt{2}x_1x_2$, $z_3 = x_2^2$

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- Satisfies Cauchy-Schwartz inequality



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From the representer theorem

$$\mathbf{w} = \sum_{i} \alpha_{i} \Phi(\mathbf{x}_{i}) \quad \Rightarrow \quad \log \left(\frac{P(1|\mathbf{x})}{P(0|\mathbf{x})} \right) = \sum_{i} \alpha_{i} k(\mathbf{x}_{i}, \mathbf{x}) + w_{0}$$



- The kernel trick can be applied elsewhere
 - Several problems are in "dot product" form
 - Extensions to non-vector data types using kernels
- Kernel Logistic Regression (KLR)
 - Log-odds is linear in high-dimensional representation

$$\log\left(\frac{P(1|\mathbf{x})}{P(0|\mathbf{x})}\right) = \langle \mathbf{w}, \Phi(\mathbf{x}) \rangle + w_0$$

The regularized KLR minimizes

$$L = \lambda \|\mathbf{w}\|^2 - \sum_i \log P(y_i|\mathbf{x}_i)$$

• From the representer theorem

$$\mathbf{w} = \sum_{i} \alpha_{i} \Phi(\mathbf{x}_{i}) \quad \Rightarrow \quad \log \left(\frac{P(1|\mathbf{x})}{P(0|\mathbf{x})} \right) = \sum_{i} \alpha_{i} k(\mathbf{x}_{i}, \mathbf{x}) + w_{0}$$

• An efficient algorithm can be designed to learn $\alpha_1, \ldots, \alpha_n$



Kernel Fisher Discriminant

Recall Fisher's Linear Discriminant

$$J(\mathbf{w}) = \frac{\mathbf{w}^T S_B \mathbf{w}}{\mathbf{w}^T S_W \mathbf{w}}$$

$$S_B = (m_2 - m_1)(m_2 - m_1)^T$$

$$S_W = \sum_{k=1,2} \sum_{i \in C_k} (\mathbf{x}_i - m_k)(\mathbf{x}_i - m_k)^T$$

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• Represent w in terms of mapped training points:

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_{i} \phi(\mathbf{x}_{i})$$
$$\langle \mathbf{w}, \phi(\mathbf{x}) \rangle = \sum_{i=1}^{n} \alpha_{i} K(\mathbf{x}_{i}, x)$$



Kernel Fisher Discriminant (Contd.)

The corresponding Rayleigh coefficient

$$J(\alpha) = \frac{(\alpha^T \mu)^2}{\alpha^T N \alpha} = \frac{\alpha^T M \alpha}{\alpha^T N \alpha}$$

where

$$\mu = \mu_2 - \mu_1$$

$$M = \mu \mu^T$$

$$\mu_k = \frac{1}{|C_k|} K \mathbf{1}_k$$

$$N = KK^T - \sum_{k=1,2} |C_k| \mu_k \mu_k^T$$