Statistical Methods in Artificial Intelligence
CSE471 - Monsoon 2015 : Lecture 18

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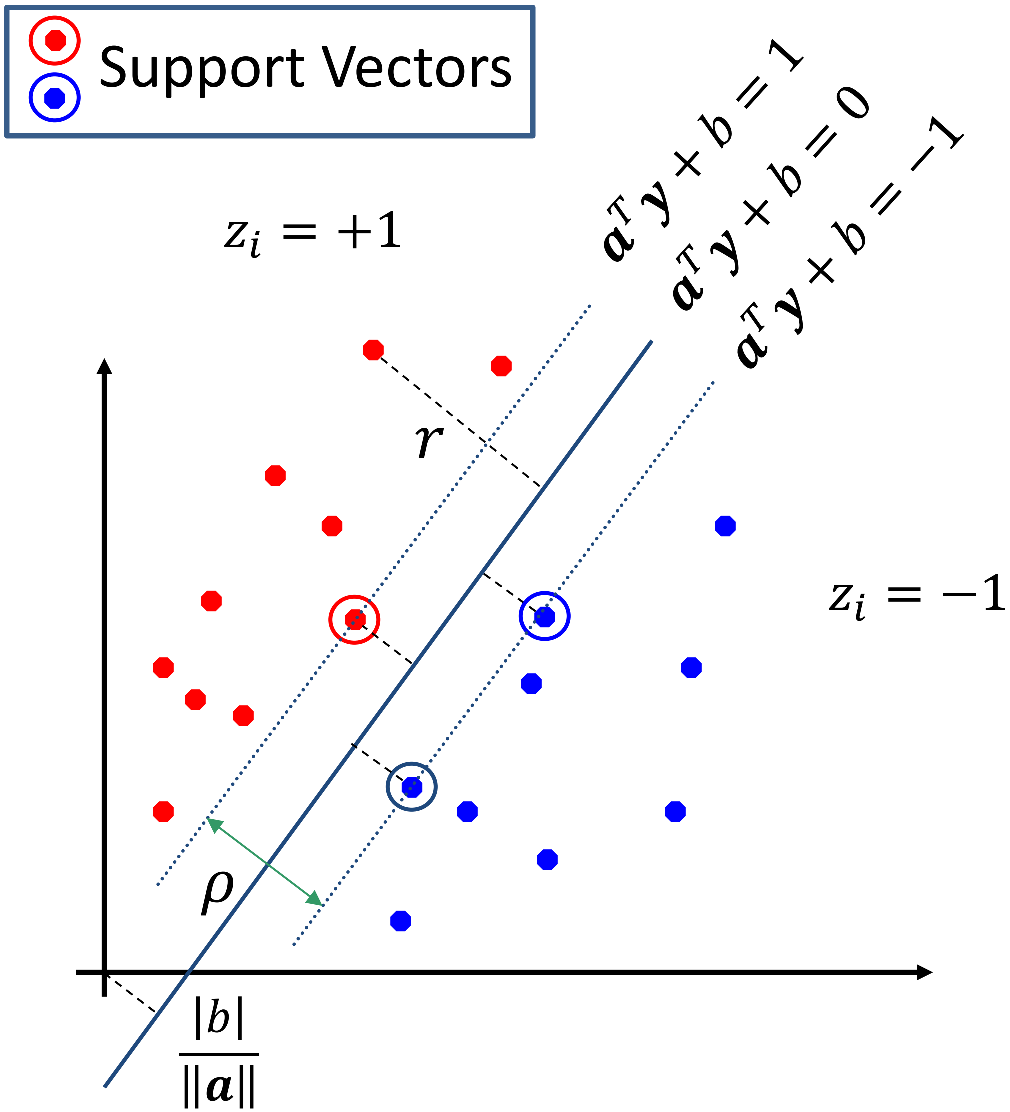
Lecture Plan

- Revision from Previous Lecture
- SVM Example
- Kernel Methods
  - Kernel PCA (KPCA)
  - Kernel LDA (KLDA)
- Data Clustering (Next Class)

Maximum Margin Classification



$$r = \frac{\boldsymbol{a}^T\boldsymbol{y}_i + b}{\|\boldsymbol{a}\|}$$

$$r_0 = \frac{b}{\|\boldsymbol{a}\|}$$

$$z_i(\boldsymbol{a}^T\boldsymbol{y}_i + b) \geq 1$$

$$\rho = \frac{2}{\|\boldsymbol{a}\|}$$

Let $|b| \|\boldsymbol{a}\| = constant$

Linear Support Vector Machine

- Dual Formulation:

$$\arg\min_{\boldsymbol{a},b}\max_{\alpha_1,\ldots,\alpha_n}\left\{\frac{1}{2}\boldsymbol{a}^T\boldsymbol{a}-\sum_{i=1}^{n}\alpha_i(z_i(\boldsymbol{a}^T\boldsymbol{y}_i+b)-1)\right\}$$

such that $z_i(\boldsymbol{a}^T\boldsymbol{y}_i+b)\geq 1$ and $\alpha_i\geq 0 \quad \forall i\in\{1,\ldots,n\}$

Or,

$$\arg\max_{\alpha_1,\ldots,\alpha_n}\sum_{k=1}^{n}\alpha_k-\sum_{k=1,j=1}^{n}\alpha_k\alpha_j z_k z_j \boldsymbol{y}_k{}^T\boldsymbol{y}_j$$

such that $\sum_{k=1}^{n}\alpha_k z_k=0$ and $\alpha_k\geq 0 \quad \forall k\in\{1,\ldots,n\}$

Linear Support Vector Machine

- Given a solution $\alpha_1, \dots, \alpha_n$ to the dual problem, solution to the primal is:

$$\boldsymbol{a} = \sum_{j=1}^{n} \alpha_j z_j \boldsymbol{y}_j \text{ and } b_k = z_k - \sum_{j=1}^{n} \alpha_j z_j \boldsymbol{y}_j{}^T \boldsymbol{y}_k \text{ for } \forall \alpha_k > 0$$

$$b = mean([b_1, \dots, b_k, \dots, b_m])$$

- Each non-zero α_k indicates that corresponding $\boldsymbol{y}_k$ is a support vector.

- The classifying function is:

$$f(\boldsymbol{y}) = \sum_{j=1}^{n} \alpha_j z_j \boxed{\boldsymbol{y}_j{}^T \boldsymbol{y}} + b$$

Transductive SVM

$$\arg \min_{z_{n+1},\ldots,z_m} \arg \min_{\boldsymbol{a},\xi,\eta,b} \left(\frac{1}{2} \boldsymbol{a}^T \boldsymbol{a} + C \sum_{i=1}^{n} \xi_i + D \sum_{i=n+1}^{m} \eta_i \right)$$

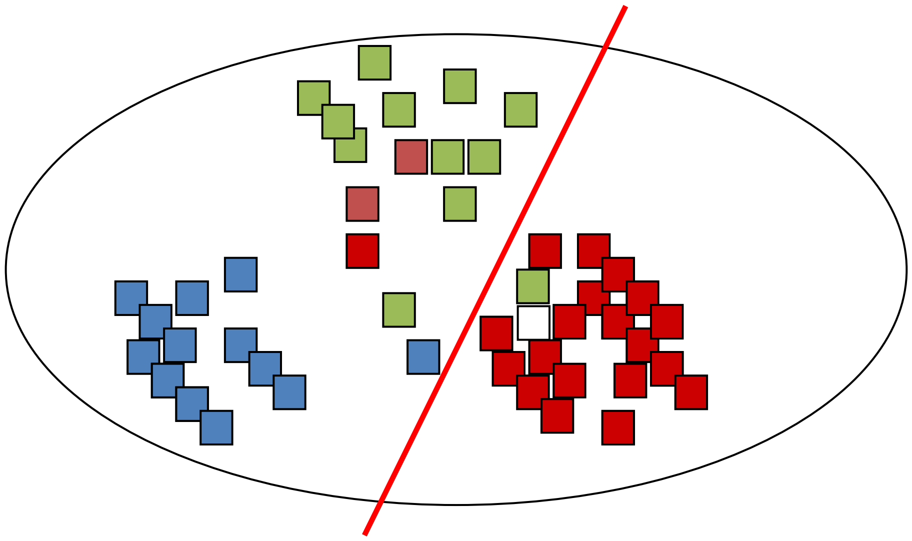
such that $z_i(\boldsymbol{a}^T \boldsymbol{y}_i + b) \geq 1 - \xi_i$ & $\xi_i \geq 0 \quad \forall i \in \{1, \ldots, n\}$,

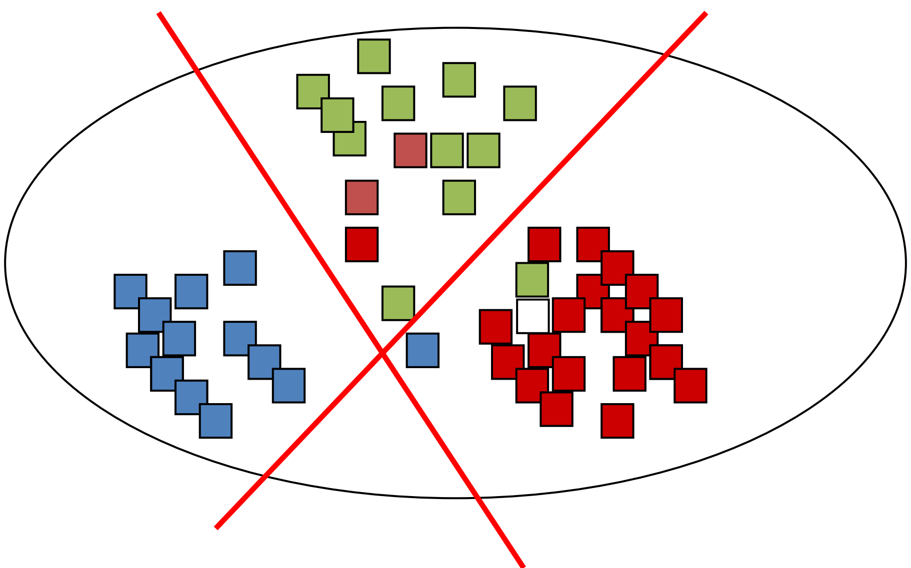
$z_i(\boldsymbol{a}^T \boldsymbol{y}_i + b) \geq 1 - \eta_i$ & $\eta_i \geq 0 \quad \forall i \in \{n+1, \ldots, m\}$,

- Do Iteratively:
- Step 1: fix $z_{n+1}, \ldots, z_m$, learn weight vector $\boldsymbol{a}$
- Step 2: fix weight vector $\boldsymbol{a}$, try to predict $z_{n+1}, \ldots, z_m$

Multi-category SVM

- SVM is a binary classifier.
- Two natural multi-class extensions are:
  - One Class v/s All : Learns C classifiers
  - One Class v/s One Class : Learns C*(C-1) Classifiers





Non-linear SVM

- Non-linear SVM

$$\arg\max_{\alpha_1,\dots,\alpha_n} \sum_{k=1}^{n} \alpha_k - \sum_{k=1,j=1}^{n} \alpha_k \alpha_j z_k z_j \varphi(\boldsymbol{y}_k)^T \varphi(\boldsymbol{y}_j)$$

$$\arg\max_{\alpha_1,\dots,\alpha_n} \sum_{k=1}^{n} \alpha_k - \sum_{k=1,j=1}^{n} \alpha_k \alpha_j z_k z_j K(k, j)$$

$$f(\boldsymbol{y}) = \sum_{j=1}^{n} \alpha_j z_j\, \varphi(\boldsymbol{y}_j)^T\, \varphi(\boldsymbol{y}) \ + b$$

Kernelization

- Commonly used Kernel functions are:
  - Linear Kernel

$$K(k,j) = \boldsymbol{y}_k{}^T \boldsymbol{y}_j$$

  - Polynomial Kernel

$$K(k,j) = (1 + \boldsymbol{y}_k{}^T \boldsymbol{y}_j)^p$$

  - Gaussian /Radial Basis Function (RBF) Kernel

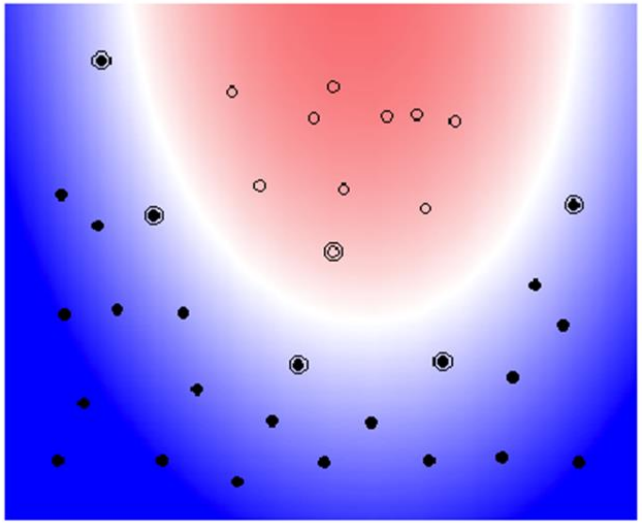
$$K(k,j) = \exp\left(-\frac{\left\|\boldsymbol{y}_k - \boldsymbol{y}_j\right\|^2}{2\sigma^2}\right)$$

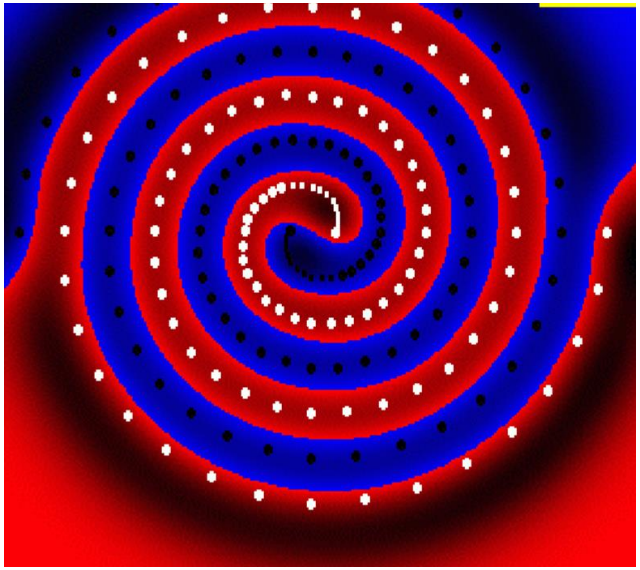
  - Sigmoid Kernel

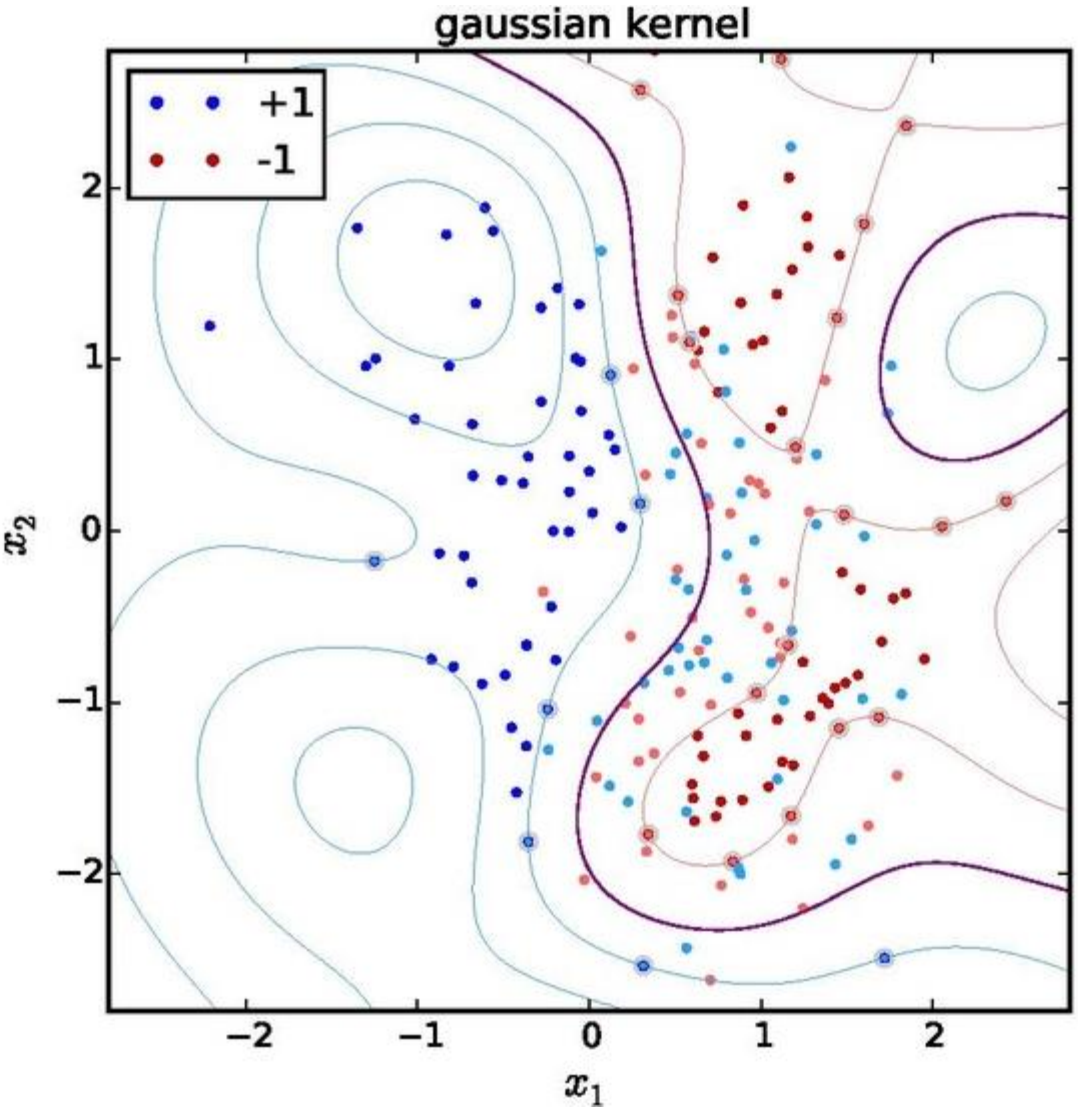
$$K(k,j) = \tanh(\beta_0 \boldsymbol{y}_k{}^T \boldsymbol{y}_j + \beta_1)$$

Kernel SVM

plot by Bell SVM applet







Kernel Trick

- Kernels can be defined on general types of data and many classical algorithms can naturally work with general, non-vectorial, data-types !

- Since the kernelization requires only the dot product matrix, one can avoid defining an explicit mapping function φ.

- For example, kernels on strings, trees and graphs which exploits sequence or topology of the underlying data domain for computing (normalized) similarity which can be represented as dot product.

Properties of Kernels

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= c k_1(\mathbf{x}, \mathbf{x}') && (6.13)\\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x}) k_1(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') && (6.14)\\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15)\\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') k_2(\mathbf{x}, \mathbf{x}') && (6.18)\\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}')\right) && (6.19)\\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}} \mathbf{A} \mathbf{x}' && (6.20)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.21)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.22)
\end{aligned}
$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

SVM Example

- Using the data points, compute the kernel matrix and write the dual formulation.

$$G = \begin{pmatrix} 9 & 1 & 1 \\ 1 & 9 & 9 \\ 1 & 9 & 25 \end{pmatrix}$$

$$\text{Maximize:} \quad \alpha_1 + \alpha_2 + \alpha_3 - \frac{1}{2}\left(9\alpha_1^2 - 2\alpha_1\alpha_2 - 2\alpha_1\alpha_3 + 9\alpha_2^2 + 18\alpha_2\alpha_3 + 25\alpha_3^2\right)$$

$$\text{subject to:} \quad \alpha_1 \geq 0,\ \alpha_2 \geq 0,\ \alpha_3 \geq 0, \quad -\alpha_1 + \alpha_2 + \alpha_3 = 0$$

- Solve for Lagrangian multipliers by setting the partial derivatives of the criterion function to zero and substitutions using the constraints.

$$\alpha_1 = 1/8, \quad \alpha_2 = 1/8, \quad \alpha_3 = 0$$

- Compute the intercept of the boundary hyperplane for each support vector and take the mean as the final value.

$$b_k = -1 - (1 * (-1) * 9 + 1 * 1 * 1)/8 = -1 - (-9 + 8/8)/8 = 0$$

Principal Component Analysis (PCA)

- k -dimensional representation: Let $\mathbf{x} = \mathbf{m} + \sum_{i=1}^{k} a_i \mathbf{e}_i$

$$\mathbf{v}_1, \dots, \mathbf{v}_k = arg \max_{\mathbf{e}_1, \dots, \mathbf{e}_k} J_k = \sum_{i=1}^{n} \left\| \left(\mathbf{m} + \sum_{j=1}^{k} a_j \mathbf{e}_j \right) - \mathbf{x}_i \right\|^2, \qquad \text{for } k \ll d$$

where, $\mathbf{S} = \sum_{i=1}^{n} (\mathbf{x}_i - \mathbf{m})(\mathbf{x}_i - \mathbf{m})^{\boldsymbol{T}} = \sum_{i=1}^{n} \widetilde{\mathbf{x}}_i \, \widetilde{\mathbf{x}}_i^{\boldsymbol{T}}$

$$\mathbf{S}\mathbf{v}_i = \lambda_i \mathbf{v}_i \,, \qquad \mathbf{v}_i \perp \mathbf{v}_j \,, \|\mathbf{v}_i\| = 1 \; \forall \; i, j \; \in \{1, \dots, k\}$$

$$\sum_{i=1}^{n} \widetilde{\mathbf{x}}_i \, \widetilde{\mathbf{x}}_i^{\boldsymbol{T}} \, \mathbf{v}_j = \lambda_j \mathbf{v}_j \Rightarrow \boxed{\mathbf{v}_j = \frac{1}{\lambda_j} \sum_{i=1}^{n} \widetilde{\mathbf{x}}_i \, \widetilde{\mathbf{x}}_i^{\boldsymbol{T}} \, \mathbf{v}_j = \sum_{i=1}^{n} \alpha_i \widetilde{\mathbf{x}}_i}$$

Kernel PCA

- Let $\boldsymbol{y}_i = \varphi(\mathbf{x}_i)$ be the centered non-linear projection (mapping) of the data such that $\sum_{i=1}^{n} \varphi(\mathbf{x}_i) = 0$.
- Then $C = \sum_{i=1}^{n} \varphi(\mathbf{x}_i)\varphi(\mathbf{x}_i)^T$ will be the scatter matrix of the *centered mapping*.
- Let $\mathbf{w}_i$ be the eigenvector of the C matrix:

$C\mathbf{w} = \lambda\mathbf{w}$ and $\mathbf{w} = \sum_{k=1}^{n} \alpha_k \varphi(\mathbf{x}_k)$

- Combining these equations:

$$\sum_{i=1}^{n} \varphi(\mathbf{x}_i)\varphi(\mathbf{x}_i)^T \sum_{k=1}^{n} \alpha_k \varphi(\mathbf{x}_k) = \lambda \sum_{k=1}^{n} \alpha_k \varphi(\mathbf{x}_k)$$

Kernel PCA

$$\sum_{k=1}^{n}\sum_{i=1}^{n}\varphi(\mathbf{x}_i)\varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_k)\alpha_k = \lambda\sum_{k=1}^{n}\alpha_k\,\varphi(\mathbf{x}_k)$$

$$\sum_{k=1}^{n}\sum_{i=1}^{n}\varphi(\mathbf{x}_l)^T\varphi(\mathbf{x}_i)\varphi(\mathbf{x}_i)^T\varphi(\mathbf{x}_k)\alpha_k = \lambda\sum_{k=1}^{n}\alpha_k\,\varphi(\mathbf{x}_l)^T\varphi(\mathbf{x}_k) \quad \forall l = 1{:}\,n$$

$$K^2\boldsymbol{\alpha} = \lambda K\boldsymbol{\alpha} \;\Rightarrow K\boldsymbol{\alpha} = \lambda\boldsymbol{\alpha}$$

$$\|\mathbf{w}\| = \mathbf{w}^{\boldsymbol{T}}\mathbf{w} \; = \textstyle\sum_{k=1}^{n}\alpha_k\,\varphi(\mathbf{x}_k)^{\boldsymbol{T}}\sum_{k=1}^{n}\alpha_k\,\varphi(\mathbf{x}_k) = \boldsymbol{\alpha}^T K\boldsymbol{\alpha} = 1$$

$$\boldsymbol{\alpha}^T\boldsymbol{\alpha} = {}^{1}\!/_{\lambda}$$

- For centered mapping:

$$\widetilde{K} = (I - \mathbf{1}\mathbf{1}^T/n)K(I - \mathbf{1}\mathbf{1}^T/n), \qquad \sum_{k=1}^{n}\varphi(\mathbf{x}_k) = 0$$

Kernel PCA

- Compute $n \times n$ Gram Matrix K using any kernel function.
- Compute eigen-(values/vectors) or K as $\lambda_j, \boldsymbol{\alpha}^j\ \forall j = 1{:}\,m$
- Normalize the eigenvectors: $\boldsymbol{\alpha}^j = \boldsymbol{\alpha}^j / \lambda_j$ such that eigenvector of C matrix is: $\mathbf{w}^l = \sum_{k=1}^{n} \alpha^l{}_k\, \varphi(\mathbf{x}_k)$
- Project any data point $\varphi(\mathbf{x})$ onto $\mathbf{w}^l$ as:

$$\varphi(\mathbf{x})^T \mathbf{w}^l = \varphi(\mathbf{x})^T \sum_{k=1}^{n} \alpha^l{}_k\, \varphi(\mathbf{x}_k) = \sum_{k=1}^{n} \alpha^l{}_k\, K(\mathbf{x}_k, \mathbf{x})$$

Scholkopf, Smola, Muller, “Nonlinear component analysis as a kernel eigenvalue problem,” Technical report #44, Max Plank Institute, 1996.

Fisher's LDA

$$\text{inter-class: } |\tilde{m}_1 - \tilde{m}_2| = |w^{\mathrm{T}}(m_1 - m_2)|$$

$$\text{intra-class: } \tilde{s}_i^2 = \sum_{y \in Y_i} (y - \tilde{m}_i)^2$$

$$\text{want to maximize: } J(w) = \frac{|\tilde{m}_1 - \tilde{m}_2|^2}{\tilde{s}_1^2 + \tilde{s}_2^2}$$

$$y, \tilde{m}_1, \tilde{m}_2 : \left[\quad\right]_{1}^{1} \qquad (w^{\mathrm{T}}x - w^{\mathrm{T}}m_i) : \left[\quad\right]_{1}^{1}$$

$$x, w, m_1, m_2 : \left[\quad\right]_{1}^{\mathrm{D}} \qquad S_{\mathrm{B}}, S_{\mathrm{w}} : \left[\quad\right]_{\mathrm{D}}^{\mathrm{D}}$$

$$\tilde{s}_i^2 = \sum_{x \in D_i} (w^{\mathrm{T}}x - w^{\mathrm{T}}m_i)(w^{\mathrm{T}}x - w^{\mathrm{T}}m_i)^{\mathrm{T}} = \sum_{x \in D_i} w^{\mathrm{T}}(x - m_i)(x - m_i)^{\mathrm{T}} w = w^{\mathrm{T}} S_i w$$

$$\tilde{s}_1^2 + \tilde{s}_2^2 = w^{\mathrm{T}} S_1 w + w^{\mathrm{T}} S_2 w = w^{\mathrm{T}} S_{\mathrm{w}} w$$

$$|\tilde{m}_1 - \tilde{m}_2|^2 = (w^{\mathrm{T}}m_1 - w^{\mathrm{T}}m_2)^2 = w^{\mathrm{T}}(m_1 - m_2)(m_1 - m_2)^{\mathrm{T}} w = w^{\mathrm{T}} S_{\mathrm{B}} w$$

$$\text{want to maximize: } J(w) = \frac{w^{\mathrm{T}} S_{\mathrm{B}} w}{w^{\mathrm{T}} S_{\mathrm{w}} w}$$

$$S_{\mathrm{B}} w = \lambda S_{\mathrm{w}} w$$

Kernel LDA

- Let, $\mathbf{m}_i^\phi = \frac{1}{l_i}\sum_{j=1}^{l_i}\phi(\mathbf{x}_j^i).$ $\mathbf{S}_B^\phi = (\mathbf{m}_2^\phi - \mathbf{m}_1^\phi)(\mathbf{m}_2^\phi - \mathbf{m}_1^\phi)^{\mathrm{T}}$

$$\mathbf{w} = \sum_{i=1}^{l}\alpha_i\phi(\mathbf{x}_i).$$

$$\mathbf{S}_W^\phi = \sum_{i=1,2}\sum_{n=1}^{l_i}(\phi(\mathbf{x}_n^i) - \mathbf{m}_i^\phi)(\phi(\mathbf{x}_n^i) - \mathbf{m}_i^\phi)^{\mathrm{T}},$$

- We can write the criterion function as: $J(\mathbf{w}) = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_B^\phi\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_W^\phi\mathbf{w}},$

- This can further be rewritten as: $J(\alpha) = \frac{\alpha^{\mathrm{T}}\mathbf{M}\alpha}{\alpha^{\mathrm{T}}\mathbf{N}\alpha}$,

where,

$$\mathbf{M} = (\mathbf{M}_2 - \mathbf{M}_1)(\mathbf{M}_2 - \mathbf{M}_1)^{\mathrm{T}}$$

$$(\mathbf{M}_i)_j = \frac{1}{l_i}\sum_{k=1}^{l_i}k(\mathbf{x}_j, \mathbf{x}_k^i).$$

$$\mathbf{N} = \sum_{j=1,2}\mathbf{K}_j(\mathbf{I} - \mathbf{1}_{l_j})\mathbf{K}_j^{\mathrm{T}},$$

Kernel LDA

- After setting analytical derivative of criterion function $J(\alpha)$ to 0:

$$(\alpha^{\mathrm{T}}\mathbf{M}\alpha)\mathbf{N}\alpha = (\alpha^{\mathrm{T}}\mathbf{N}\alpha)\mathbf{M}\alpha.$$

$$\alpha = \mathbf{N}^{-1}(\mathbf{M}_2 - \mathbf{M}_1).$$

$$\mathbf{N}_\epsilon = \mathbf{N} + \epsilon\mathbf{I}.$$

- Given solution vector α, we can project a data point to lower dimensional discriminating space as:

$$y(\mathbf{x}) = (\mathbf{w} \cdot \phi(\mathbf{x})) = \sum_{i=1}^{l} \alpha_i k(\mathbf{x}_i, \mathbf{x}).$$

https://en.wikipedia.org/wiki/Kernel_Fisher_discriminant_analysis

Self Study

- Multiple Kernel Learning
  - Seeking optimal parameters for combining multiple kernels
    - https://en.wikipedia.org/wiki/Multiple_kernel_learning

- Non-linear Dimensionality Reduction
  - Higher dimensional data sampled from lower dimensional manifold
    - https://en.wikipedia.org/wiki/Nonlinear_dimensionality_reduction

Mid Term 2 Syllabus

- What all is covered in the class & tutorial.
- Chapter 2 (Normal Density, DF, Mahalanobis Distance)
  - ❖ 2.1—2.3, 2.5, 2.6, 2.8.3
- Chapter 3 (Parameter Estimation, BPE, MLE, PCA, LDA)
  - ❖ 3.1, 3.2, 3.3, 3.4, 3.5, 3.5.1, 3.7, 3.8
- Chapter 5 (SVM, Kernel SVM, Kernel definition/trick/properties)
  - ❖ 5.11, 5.12,
- Do refer to related public material from books/online resources.