Notes on Kernel Fisher Discriminant

23rd October 2002

Basic idea: Map patterns into Hilbert space and then compute Fisher discriminant. For a two class problem, the Fisher discriminant maximizes

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

where

$$S_B = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^T$$

and

$$S_W = S_{W_1} + S_{W_2} = \sum_{i \in C_1} (\mathbf{x}_i - \mathbf{m}_1)(\mathbf{x}_i - \mathbf{m}_1)^T + \sum_{j \in C_2} (\mathbf{x}_j - \mathbf{m}_2)(\mathbf{x}_j - \mathbf{m}_2)^T$$

with $\mathbf{m}_1 = \frac{1}{N_1} \sum_{i \in C_1} \mathbf{x}_i$ and $\mathbf{m}_2 = \frac{1}{N_2} \sum_{j \in C_2} \mathbf{x}_j$. An easier way of writing S_{W_1} and S_{W_2} which will be useful later on is

$$S_{W_1} = \sum_{i \in C_1} (\mathbf{x}_i - \mathbf{m}_1)(\mathbf{x}_i - \mathbf{m}_1)^T = \sum_{i \in C_1} (\mathbf{x}_i \mathbf{x}_i^T - \mathbf{m}_1 \mathbf{m}_1^T) \tag{1}$$

with a similar expression for S_{W_2}. When we first map the patterns into a higher dimensional space, $\mathbf{x}_i$ becomes $\Phi(\mathbf{x}_i)$. We now consider solutions for $\mathbf{w}$ of the form $\mathbf{w} = \sum_{r=1}^{N} \alpha_r \Phi(\mathbf{x}_r)$. After using this expression for $\mathbf{w}$,

$$\mathbf{w}^T \mathbf{m}_1 = \sum_{r=1}^{N} \alpha_r \Phi(\mathbf{x}_r) \cdot \frac{1}{N_1} \sum_{i \in C_1} \Phi(\mathbf{x}_i) = \sum_{r=1}^{N} \alpha_r \sum_{i \in C_1} \frac{k(\mathbf{x}_r, \mathbf{x}_i)}{N_1} = \alpha^T M_1$$

where $(M_1)_r \stackrel{def}{=} \frac{\sum_{l \in C_1} k(\mathbf{x}_r, \mathbf{x}_l)}{N_1}$. Using this definition, we may write

$$\mathbf{w}^T S_B \mathbf{w} = \alpha^T (M_2 - M_1)(M_2 - M_1)^T \alpha. \tag{2}$$

Now

$$\mathbf{w}^T \Phi(\mathbf{x}) = \sum_{r=1}^{N} \alpha_r \Phi(\mathbf{x}_r) \cdot \Phi(\mathbf{x}) = \sum_{r=1}^{N} \alpha_r k(\mathbf{x}_r, \mathbf{x})$$

and using (1), we can write

$$\begin{aligned}
\mathbf{w}^T S_{W_1}\mathbf{w} &= \sum_{i\in C_1} \mathbf{w}^T\left[\Phi(\mathbf{x}_i)\Phi^T(\mathbf{x}_i) - \mathbf{m}_1\mathbf{m}_1^T\right]\mathbf{w} \\
&= \sum_{i\in C_1}\left[\mathbf{w}^T\Phi(\mathbf{x}_i)\Phi^T(\mathbf{x}_i)\mathbf{w} - \mathbf{w}^T\mathbf{m}_1\mathbf{m}_1^T\mathbf{w}\right] \\
&= \sum_{i\in C_1}\left[\sum_{r=1}^N \alpha_r k(\mathbf{x}_r,\mathbf{x}_i)\sum_{s=1}^N \alpha_s k(\mathbf{x}_s,\mathbf{x}_i) - \sum_{r=1}^N \alpha_r \sum_{l\in C_1}\frac{k(\mathbf{x}_r,\mathbf{x}_l)}{N_1}\sum_{s=1}^N \alpha_s\sum_{l\in C_1}\frac{k(\mathbf{x}_s,\mathbf{x}_l)}{N_1}\right]
\end{aligned}$$

This can be simplified to yield

$$\begin{aligned}
\mathbf{w}^T S_{W_1}\mathbf{w} &= \sum_{r=1}^N \alpha_r \sum_{s=1}^N \alpha_s \sum_{i\in C_1}\left[k(\mathbf{x}_r,\mathbf{x}_i)k(\mathbf{x}_s,\mathbf{x}_i) - \frac{\sum_{l=1}^{N_1} k(\mathbf{x}_r,\mathbf{x}_l)}{N_1}\frac{\sum_{l=1}^{N_1} k(\mathbf{x}_s,\mathbf{x}_l)}{N_1}\right] \\
&= \alpha^T[K_1K_1^T - N_1M_1M_1^T]\alpha \qquad (3)
\end{aligned}$$

where $(K_1)_{ri} = k(\mathbf{x}_r,\mathbf{x}_i)$, $i \in C_1$. K_1 is an $N \times N_1$ matrix. Similarly, $(K_2)_{rj} = k(\mathbf{x}_r,\mathbf{x}_j)$, $j \in C_2$. K_2 is a $N \times N_2$ matrix. With these expansions in place, we may write

$$\mathbf{w}^T S_B \mathbf{w} = \alpha^T M \alpha$$

where $M = (M_2 - M_1)(M_2 - M_1)^T$ and

$$\mathbf{w}^T S_W \mathbf{w} = \alpha^T K \alpha$$

where $K = K_1K_1^T - N_1M_1M_1^T + K_2K_2^T - N_2M_2M_2^T$. The maximization problem becomes

$$J_W(\alpha) = \max_\alpha \frac{\alpha^T M\alpha}{\alpha^T K\alpha} \qquad (4)$$

with the solution

$$\hat{\alpha} \propto K^{-1}(M_2 - M_1).$$

Having found a solution for α, you can project all the patterns onto a single dimension which is $y = \mathbf{w}^T\Phi(\mathbf{x}) = \sum_{r=1}^N \alpha_r k(\mathbf{x}_r,\mathbf{x})$.