Linear Discriminants

CSci 5525: Machine Learning

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Discriminant Functions

One of the simplest representation for a 2-class problem

$$f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

- Class assignment based on sign(f(x))
 - If $f(\mathbf{x}) \geq 0$, sign $(f(\mathbf{x})) = +1$, then $\mathbf{x} \in C_1$, otherwise $\mathbf{x} \in C_2$
- **w** is orthogonal to the decision boundary $f(\mathbf{x}) = w_0$
- With $\tilde{\mathbf{w}} = (\mathbf{w}, w_0)$ and $\tilde{\mathbf{x}} = (\mathbf{x}, 1)$, we have

$$f(\mathbf{x}) = \tilde{\mathbf{w}}^T \tilde{\mathbf{x}}$$

• At times, we will ignore the offset term w_0 w.l.o.g. (without loss of generality)



Least Squares for Classification

- Consider a training dataset $\{\mathbf{x}_n, \mathbf{y}_n\}_{n=1}^N$ for a K-class problem
 - \mathbf{y}_n encodes the class membership, say $\mathbf{y}_n^T = (0, 1, 0, 0)$
 - $Y: N \times K$ matrix with rows $\mathbf{y}_{\underline{n}}^T$
 - $X : N \times D$ matrix with rows \mathbf{x}_n^T
 - $W: D \times K$ matrix with columns \mathbf{w}_k
 - Goal:

$$\mathbf{w}_k^T \mathbf{x}_n = \mathbf{x}_n^T \mathbf{w}_k = X_{n,:} \mathbf{w}_k \approx Y_{nk}$$

ullet The sum-of-squares error to be minimized over W is

$$E(W) = \frac{1}{2} \sum_{k=1}^{K} \sum_{n=1}^{N} \|Y_{nk} - X_{n,:} \mathbf{w}_{k}\|^{2} = \frac{1}{2} \operatorname{Tr} \left\{ (Y - XW)^{T} (Y - XW) \right\}$$



Least Squares for Classification (Contd.)

ullet The sum-of-squares error to be minimized over W is

$$E(W) = \frac{1}{2} \sum_{k=1}^{K} \sum_{n=1}^{N} \|Y_{nk} - X_{n,i} \mathbf{w}_{k}\|^{2} = \frac{1}{2} \operatorname{Tr} \left\{ (Y - XW)^{T} (Y - XW) \right\}$$

The problem has a closed form solution

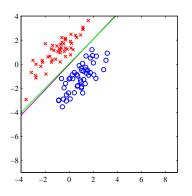
$$W = (X^T X)^{-1} X^T Y = X^{\dagger} Y$$

- ullet Solving each problem separately: $oldsymbol{w}_k = X^\dagger oldsymbol{y}_k$
- The discriminant function has the following form

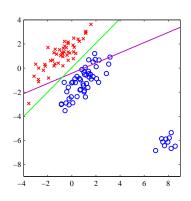
$$f(\mathbf{x}) = W^T \mathbf{x} = Y^T (X^{\dagger})^T \mathbf{x}$$



Least Squares is Noise Sensitive

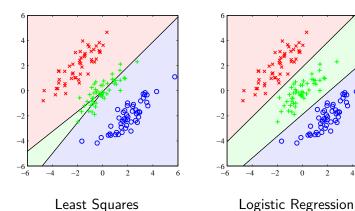


Least Squares vs Logistic



Least Squares with noise

Least Squares for Multiclass Problems



Classification by Projection

- Classify after dimensionality reduction
 - Project D dimensional data x to 1 dimensions: w^Tx
 - Make sure class separation is maximized
- If $\mathbf{m}_1, \mathbf{m}_2$ are the means of the two classes

$$\max_{\|\boldsymbol{w}\|^2=1} \ \boldsymbol{w}^T \big(\boldsymbol{m}_2 - \boldsymbol{m}_1\big)$$

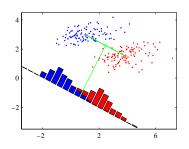
Performing the optimization (using 'Langrange multipliers')

$$\mathbf{w} \propto (\mathbf{m}_2 - \mathbf{m}_1)$$

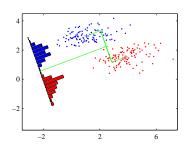
May be problematic if data has non-diagonal covariance



Classification by Projection (Contd.)



Classification by Projection



Fisher's Linear Discriminant

Fisher's Linear Discriminant

Desirable to have low within class variance

$$\sigma_k^2 = \sum_{\mathbf{x}_n \in C_k} \| w^T (\mathbf{x}_n - \mathbf{m}_k) \|^2$$

Between-class and within-class covariance matrices

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

$$S_W = \sum_{\mathbf{x}_n \in C_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^T + \sum_{\mathbf{x}_n \in C_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^T$$

 Fisher's criterion: Ratio of between-class and within-class variance

$$J(\mathbf{w}) = \frac{\|\mathbf{w}^T (\mathbf{m}_2 - \mathbf{m}_1)\|^2}{\sigma_1^2 + \sigma_2^2} = \frac{\mathbf{w}^T S_B \mathbf{w}}{\mathbf{w}^T S_W \mathbf{w}}$$



Fisher's Linear Discriminant (Contd.)

Fisher's criterion is

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

A 'direct calculation' gives

$$\mathbf{w} \propto S_w^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

- A linear discriminant can be constructed using w
 - Construct the projected version of the data $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$
 - Choose a threshold w_0 to form linear discriminant $f(\mathbf{x}) \geq w_0$
- Extension to multiclass: Project to (K-1) dimensions
- Need to train a classifier in the low dimensional representation

