On the Equivalence of Kernel Fisher Discriminant Analysis and Kernel Quadratic Programming Feature Selection

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Outline

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Feature Selection and Extraction Methods (I)

- Increasing size and dimensionality of real-world datasets.

Linear Feature Selection and Extraction Methods

- Fast and simple.
- Do not handle nonlinear relationships in the data.
- Principal Component Analysis (PCA).
- Canonical Correlation Analysis (CCA).
- Fisher Discriminant Analysis (FDA).
- ...

Feature Selection and Extraction Methods (II)

Kernelized Feature Selection and Extraction Methods

- Capture nonlinear dependences in the data.
- Maps the data from an original space to a *feature space* $\mathcal{F}$ via a (nonlinear) mapping $\Phi : \mathbb{R}^d \longrightarrow \mathcal{F}$.
- The dot-product in the feature space $\mathcal{F}$ is defined by a Mercer kernel $K : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$.
- Reformulation of traditional linear methods using only dot-products of training samples $\Rightarrow$ nonlinear method in the input space.
  - Kernel Principal Component Analysis (KPCA).
  - Kernel Canonical Correlation Analysis (KCCA).
  - Kernel Fisher Discriminant Analysis (KFDA).
  - ...

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Kernel Fisher Discriminant Analysis (KFDA) (I)

Notation

- $\mathcal{X}_1 = \{x_1^1, \dots, x_{l_1}^1\}$ and $\mathcal{X}_2 = \{x_1^2, \dots, x_{l_2}^2\}$ samples from two different classes ($x_i \in \mathbb{R}^d$).
- $\mathcal{X} = \mathcal{X}_1 \cup \mathcal{X}_2$.
- $y \in \{-1, 1\}^l$ be the target vector.
- Mapping function to the kernel space: $\Phi : \mathbb{R}^d \longrightarrow \mathcal{F}$.
- Mercer Kernel: $K(x, y) =< \Phi(x), \Phi(y) >$.

Kernel Fisher Discriminant Analysis (KFDA) (II)

- Mapping the data nonlinearly into the feature space $\mathcal{F}$ and computing Fisher's linear discriminant there.

KFDA Objective Function

$$\max_{w \in \mathcal{F}} J(w) = \max_{w \in \mathcal{F}} \frac{w^T S_B^\Phi w}{w^T S_W^\Phi w}$$

$\mathcal{F}$ Mean Vector

$m_i^\Phi = \frac{1}{l_i} \sum_{j=1}^{l_i} \Phi(x_j^i)$

$\mathcal{F}$ Between Scatter Matrix

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

$\mathcal{F}$ Within Scatter Matrix

$S_W^\Phi = \sum_{i=1,2} \sum_{x \in \chi_i} (\Phi(x) - m_i^\Phi)(\Phi(x) - m_i^\Phi)^T$

Kernel Fisher Discriminant Analysis (KFDA) (III)

- $\Phi(x)$ is not known in general.
- Finding a solution in $\mathcal{F} \Rightarrow$ reformulate it in terms of only dot products of the input patterns.

KFDA Objective Function

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

Reproducing Kernels

$w = \sum_{i=1}^{l} \alpha_i \Phi(x_i)$

Kernelized Between Scatter Matrix

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

$(M_i)_j = \frac{1}{l_i} \sum_{k=1}^{l_i} K(x_j, x_k^i)$

Kernelized Within Scatter Matrix

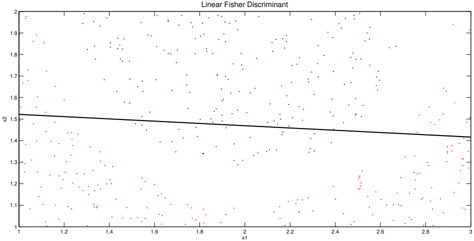
$N = \sum_{j=1,2} K_j (I - 1_{l_j}) K_j^T$

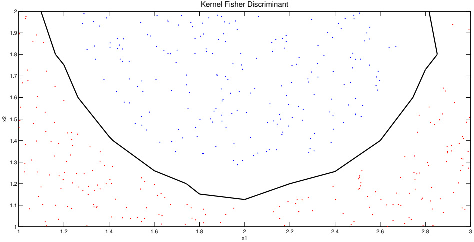
Kernel Fisher Discriminant Analysis (KFDA) (IV)

Kernel Fisher Coefficients (α^*_{KFD})

- $\alpha^*_{\text{KFD}} \equiv$ the leading eigenvector of $N^{-1}M$.
- $\alpha^*_{\text{KFD}} = N^{-1}(M_2 - M_1)$.
  - Ill-posed problem: N matrix not positive.
  - Some kind of regularization in needed ($\|\alpha\|^2$, $\|w\|^2$, ...).
  - Used regularization: $N_\mu = N + \mu_N I$.

Kernel Fisher Discriminant Analysis (KFDA) (V)





Outline

Quadratic Programming Feature Selection (QPFS)

- Select those features which provide a good tradeoff between relevance maximization and redundancy minimization for the classification task.

QPFS Objective Function

$$
\begin{aligned}
\min_{x} \quad & \tfrac{1}{2}x^T Q x - F^T x \\
\text{s.t.} \quad & x_i \geq 0 \qquad \forall i = 1 \dots M \\
& \|x\|_1 = 1.
\end{aligned}
$$

- **Q**: similarity among variables (redundancy).
- **F**: how correlated each feature is with the target class (relevance).
- Components of solution vector $\mathbf{x}^*$: weight of each feature.

Kernel QPFS (KQPFS) (I)

- For some kernels, it is not possible to give a weight to each feature in the kernel space due to its potential infinite dimension.
- QPFS objective function can be adapted to find an optimal direction w to project the data into the kernel space $\mathcal{F}$.
- KQPFS represents a **feature extraction** method.

KQPFS Objective Function

$$\min_{w} \frac{1}{2} w^T Q^{\Phi} w - \left(F^{\Phi}\right)^T w$$

Kernel QPFS (KQPFS) (II)

Similarity Measures

- QPFS: Correlation and Mutual Information.
  - The mapping function Φ is usually *implicit*.
  - The dimension of the kernel space $\mathcal{F}$ may be infinite.
  - Basis set in the kernel space is needed.
- KQPFS: **Covariance** $\Rightarrow$ KQPFS formulation does not require an explicit basis in the kernel space.

Kernel QPFS (KQPFS) (III)

KQPFS Redundacy-Relevance Matrices

$$
\begin{aligned}
Q^{\Phi} &= \sum_{x\in\mathcal{X}} \left(\Phi(x) - m^{\Phi}\right)\left(\Phi(x) - m^{\Phi}\right)^{T} \\
F^{\Phi} &= \sum_{x\in\mathcal{X}} (y_x - m^{y})\left(\Phi(x) - m^{\Phi}\right) \\
m^{\Phi} &= \frac{1}{l}\sum_{x\in\mathcal{X}} \Phi(x) \\
m^{y} &= \frac{1}{l}\sum_{i=1}^{l} y_i \; .
\end{aligned}
$$

Kernel QPFS (KQPFS) (IV)

- Theory of Reproducing Kernels: $w = \sum_{i=1}^{l} \alpha_i \Phi(x_i)$.
- $Q_K = K(I - 1_l) K$.
- $F_K = K(I - 1_l) y$.

KQPFS Objective Function

$$\min_{\alpha} G(\alpha) = \min_{\alpha} \frac{1}{2}\alpha^T Q_K \alpha - F_K^T \alpha$$

Kernel QPFS Coefficients

- $\nabla_\alpha G(\alpha) = 0 \Rightarrow Q_K \cdot \alpha = F_K$.
  - matrix Q_K is always singular.
  - Again, some kind of regularization in needed ($\|\alpha\|^2$, $\|w\|^2$, ...).
  - Used regularization: $Q_\mu = Q_K + \mu_Q I$.

Kernel QPFS (KQPFS) (V)

Regularized KQPFS Objective Function

$$G_\mu(\alpha) = \frac{1}{2}\alpha^T \left(Q_K + \mu_Q I\right) \alpha - F_K^T \alpha$$

Regularized Kernel QPFS Coefficients (α^*_{KQPFS})

$$\alpha^*_{\text{KQPFS}} = \left(Q_K + \mu_Q I\right)^{-1} F_K$$

- α^*_{KQPFS}: minimizes the covariance among features in the kernel space + maximizes the covariance of each feature in the kernel space with the target class.
- α^*_{KQPFS} only depends on the kernel matrix K and the class labels y.

Outline

Kernel Fisher Discriminant Analysis as Quadratic Programming Problem (I)

Proposition Mika et al.

KFD is equivalent to the quadratic programming problem:

$$\begin{aligned} \min_{\alpha} \quad & \alpha^T N\alpha + CP(\alpha) \\ \text{s.t.} \quad & \alpha^T (M_1 - M_2) = 2 \end{aligned} \tag{1}$$

Regularization: $N_\mu = N + \mu_N I$

- $C = \mu_N$.
- $P(\alpha) = \|\alpha\|^2$.

Kernel Fisher Discriminant Analysis as Quadratic Programming Problem (II)

Proposition Mika et al.

For given $C \in \mathbb{R}$, any optimal solution α to the optimization problem (1) is also optimal for

$$\begin{array}{ll} \min_{\alpha,b,\xi} & \|\xi\|^2 + \mu_N \|\alpha\|^2 \\ \text{s.t.} & K\alpha + \overrightarrow{1} b = y + \xi \\ & \overrightarrow{1}_i^T \xi = 0 \ \text{ for } i = 1,2 \end{array}$$

and vice versa

Proposition

Given $\mu_N \in \mathbb{R}$ and let $\mu_N = \mu_Q$, any optimal solution (α^*, b^*, ξ^*) to the optimization problem (2) is also optimal for the Regularized KQPFS and vice versa.

Proof (I)

- It is straightforward to show that the following proof is also valid for other regularization functions.

1. Working out ξ in (3):

$$\xi\,(\alpha, b) = K\alpha + \overrightarrow{1}b - y$$

$$\min_{\alpha,b,\xi} \quad \|\xi\|^2 + \mu_N\|\alpha\|^2 \tag{2}$$

$$\text{s.t.} \quad K\alpha + \overrightarrow{1}b = y + \xi \tag{3}$$

$$\overrightarrow{1}_i^T\xi = 0 \;\text{ for } i = 1, 2 \tag{4}$$

Proof (I)

- It is straightforward to show that the following proof is also valid for other regularization functions.

$$
\begin{array}{lll}
\min\limits_{\alpha,b,\xi} & \|\xi\|^2 + \mu_N \|\alpha\|^2 & (2) \\
\text{s.t.} & K\alpha + \overrightarrow{1} b = y + \xi & (3) \\
 & \overrightarrow{1}_i^T \xi = 0 \;\; \text{for } i = 1,2 & (4)
\end{array}
$$

1. Working out ξ in (3):

$$\xi\,(\alpha, b) = K\alpha + \overrightarrow{1} b - y$$

2. Optimization problem (2):

$$
\begin{array}{ll}
\min\limits_{\alpha,b} & \{\alpha^T KK\alpha - lb^2 - 2y^T K\alpha + \\
 & +y^T y + \mu_N \|\alpha\|^2\} \\
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Proof (I)

- It is straightforward to show that the following proof is also valid for other regularization functions.

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3. b depends on α as (4):

$$b(\alpha) = -\frac{1}{l} 1_l K\alpha + 1_l y$$

Proof(II)

- It is straightforward to show that the following proof is also valid for other regularization functions.

$$\min_{\alpha,b,\xi} \quad \|\xi\|^2 + \mu_N \|\alpha\|^2 \tag{5}$$

$$\text{s.t.} \quad K\alpha + \vec{1}\, b = y + \xi \tag{6}$$

$$\vec{1}_i^T \xi = 0 \ \text{ for } i = 1, 2 \tag{7}$$

4. Substituting $b(\alpha)$ we have an optimization problem with no constraints:

$$\begin{aligned} \min_\alpha \quad & \{\alpha^T K \left(I - 1_l\right) K\alpha \\ & -2y^T \left(I - 1_l\right) K\alpha + \\ & + \frac{\mu_N}{2} \|\alpha\|^2 + D\} \end{aligned} \tag{8}$$

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5. Minimum value of Equation (8) is the same as those of the regularized KQPFS when $\mu_N = \mu_Q$.

$$G_\mu(\alpha) = \frac{1}{2}\alpha^T (Q_K + \mu_Q I)\alpha - F_K^T \alpha$$

Outline

Complexity

Standard KFDA

$$O(l^3) + 2l(l_1^2 + l_2^2) + 5l^2 + l_1^2 + l_2^2 + 7l$$

- Depends on the prior distributions of classes.

KQPFS

$$O(l^3) + 2l^3 + 4l^2$$

- Independent of the prior distributions of classes.

When is KQPFS faster than KFDA?

$$(l_1^2 + l_2^2)(2l + 1) + 5l^2 + 7l \gg 2l^3 + 4l^2$$

- Prior distributions of the class labels are highly unbalanced.

Outline

Empirical Equivalence

- Thirteen artificial and real world datasets were considered from the Rätsch benchmark repository.
- *Optimal* parameter values are known (Rätsch benchmark repository).
  - Width of the Gaussian kernel σ: $K(x, y) = e^{\frac{\|x-y\|^2}{\sigma}}$.
  - Regularization parameter μ_N.
  - $\mu_Q = \mu_N$.

For every training set

$$\cos\left(\alpha^*_{\text{KFD}}\ ,\ \alpha^*_{\text{KQPFS}}\right) = 1 \Longrightarrow \cos\left(w^*_{\text{KFD}}\ ,\ w^*_{\text{KQPFS}}\right) = 1$$

Computational Cost

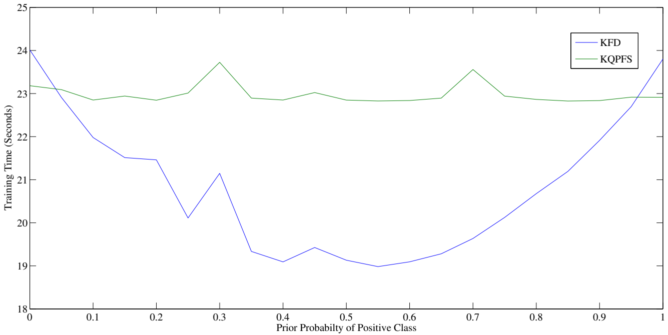

Figure: Abalone. Training time in seconds for the KFD and KQPFS algorithms.

Outline

Conclusions

- **Reformulation** of the Quadratic Programming Feature Selection (QPFS) method in a kernel space (KQPFS).
- **Proof** of the equivalence between KQPFS direction and KFD direction.
  - **New interpretation** of the KFD vector: direction which minimizes the covariance among features and maximizes the covariance of each feature with the target class in the kernel space.
  - **New solution** for KFD disregarding the explicitly dependence on the kernelized between and within scatter matrices.
  - **More efficient computation** of the Kernel Fisher direction when the classes are highly unbalanced.

Thank you!