Adaptive Discriminant Analysis by Minimum Squared Errors

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Stanford, June 2006

Adaptive Dimension Reduction for Clustered Data

- Linear Discriminant Analysis (LDA) and its Generalizations for undersampled problems, LDA/GSVD
- Extension to kernel-based nonlinear method KDA/GSVD
- Relationship to Classifier design by MSE
- Adaptive feature subspace tracking method
- Test results: Facial recognition, efficient cross-validation by downdating, etc.

Clustered Data: Facial Recognition

The 1st sample

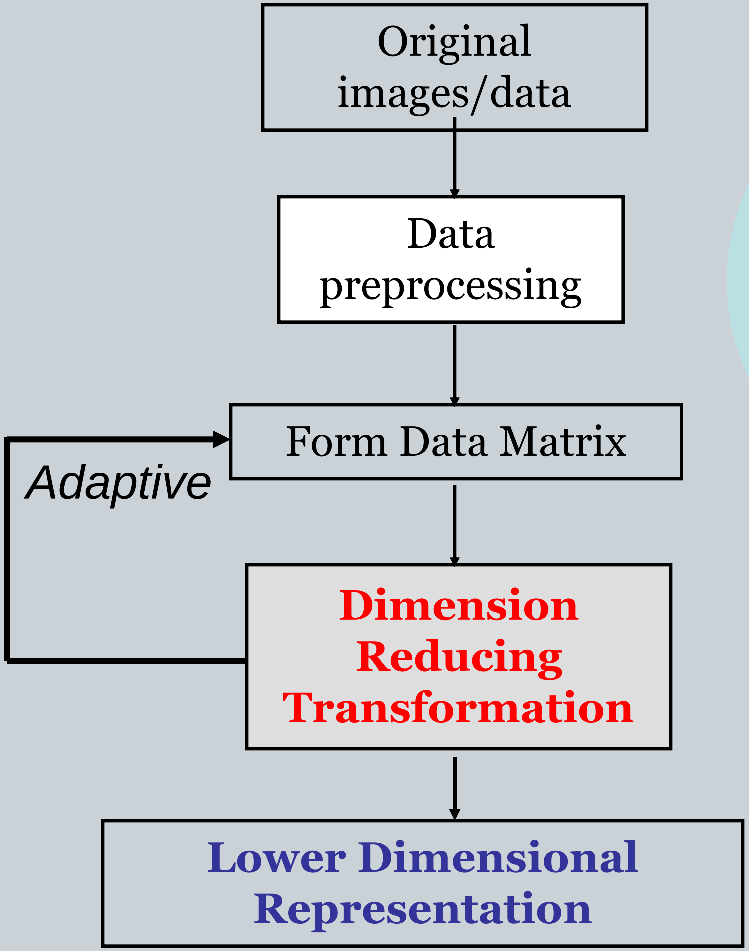
The 35th sample

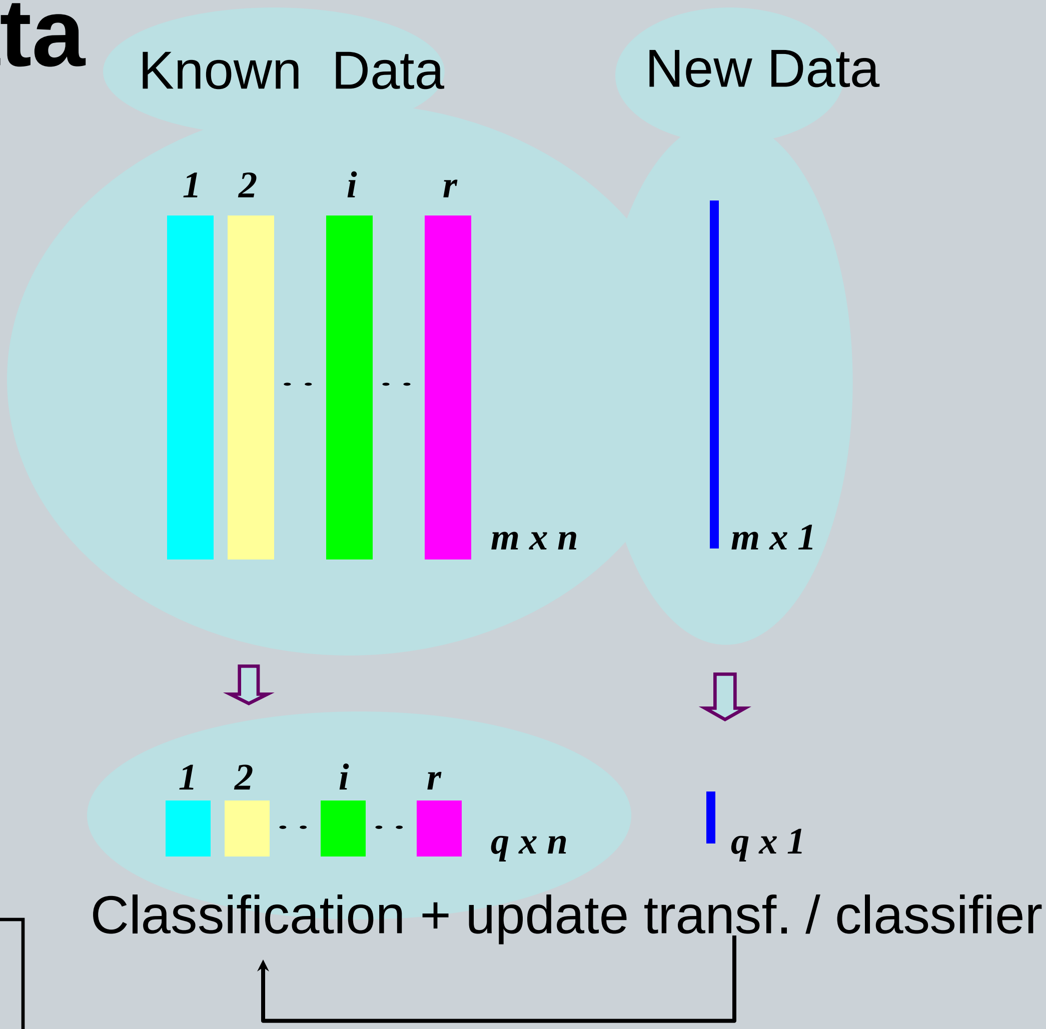
AT&T (ORL) Face Database

- 400 frontal images = 40 person x 10 images each, variations in pose, facial expression
- image size :92 x 112
- Severely Undersampled:

10304 x 400

Adaptive Dimension Reduction of Clustered Data





Want: *Adaptive Dimension Reducing Transformation* *that can be effectively applied* ***across many application areas***

Measure for Cluster Quality

$A = [a_1 \ldots a_n]$: mxn, clustered data
N_i = items in class i, $|N_i| = n_i$, total r classes
c_i = average of data items in class i, *centroid*
c = global average, *global centroid*

(1) Within-class scatter matrix

$$S_w = \sum_{1 \le i \le r} \sum_{j \in N_i} (a_j - c_i)(a_j - c_i)^T$$

(2) Between-class scatter matrix

$$S_b = \sum_{1 \le i \le r} \sum_{j \in N_i} (c_i - c)(c_i - c)^T$$

(3) Total scatter matrix

$$S_t = \sum_{1 \le i \le n} (a_i - c)(a_i - c)^T$$

NOTE: $S_w + S_b = S_t$

Trace of Scatter Matrix

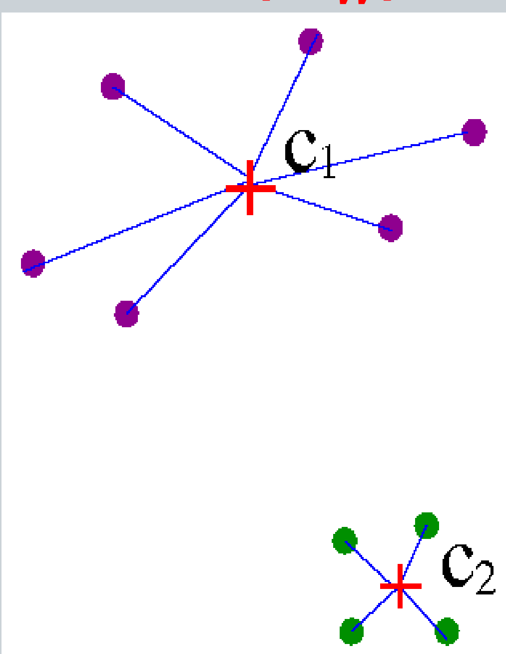
$$trace\,(S_w) = \sum_{1\le i\le r} \sum_{j\in N_i} \|a_j - c_i\|_2^2$$

$$trace\,(S_b) = \sum_{1\le i\le r} \sum_{j\in N_i} \|c_i - c\|_2^2$$

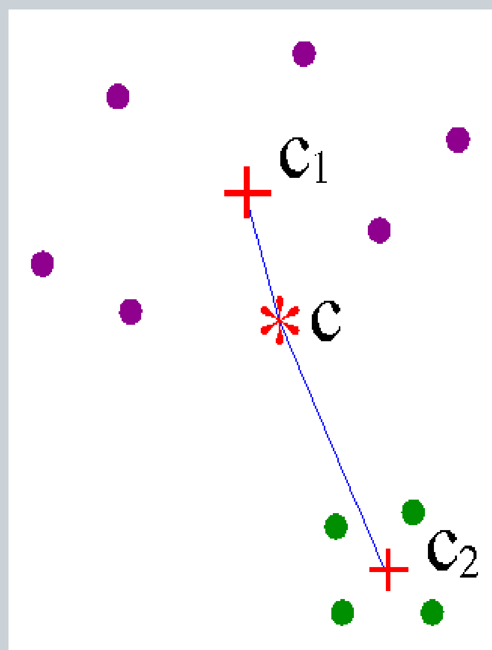
$$trace\,(S_t) = \sum_{1\le i\le r} \sum_{j\in N_i} \|a_j - c\|_2^2$$

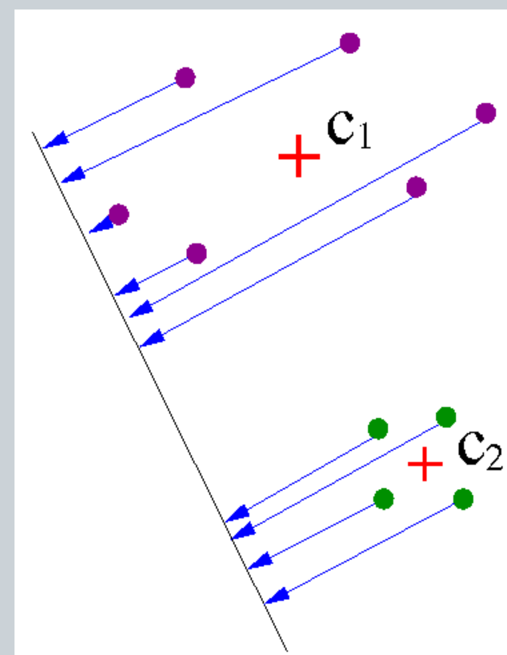
Dimension Reducing Transformation

trace (S_w)



trace (S_b)





Optimal Dimension Reducing Transformation

$$y : mx1 \xrightarrow{G^T : qxm} G^T y : qx1, \quad q << m$$

High quality clusters have

small trace(S_w) **&** ***large trace(S_b)***

Want: G

s.t. ***min trace($G^T S_w G$)*** **&** ***max trace($G^T S_b G$)***

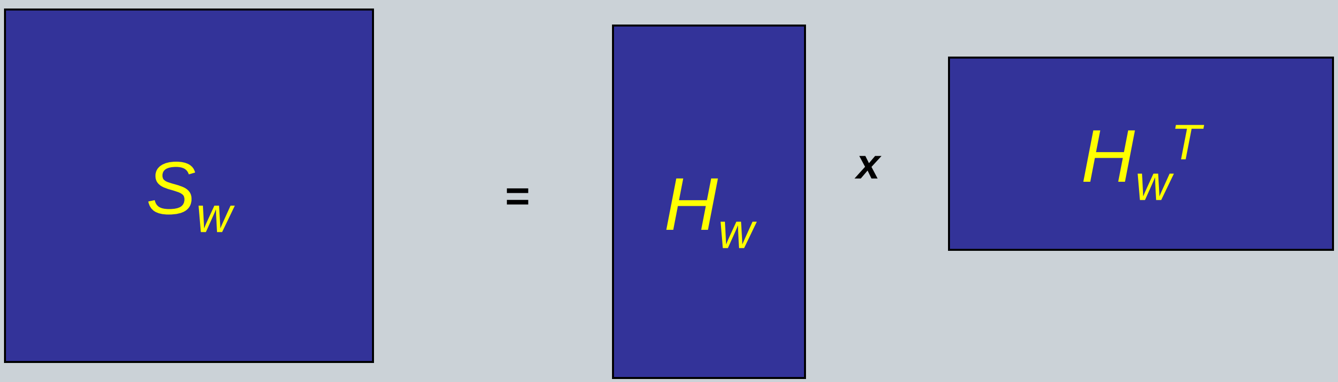
- **max trace (($G^T S_w G$)$^{-1}$ ($G^T S_b G$))** → **LDA** ***(Fisher 36, Rao 48)***
- **max trace ($G^T S_b G$)** → **Orthogonal Centroid** ***(Park et al. 03)*** $G^TG=I$
- **max trace ($G^T (S_w+S_b) G$)** → **PCA** ***(Hotelling 33)*** $G^TG=I$
- **max trace ($G^T A A^T G$)** → **LSI** ***(Deerwester et al. 90)*** $G^TG=I$

Classical LDA

(Fisher '36, Rao '48)

max trace $((G^T S_w G)^{-1} (G^T S_b G))$

- G : leading (r-1) e.vectors of $S_w^{-1} S_b$
  Fails when m>n (undersampled), S_w *singular*



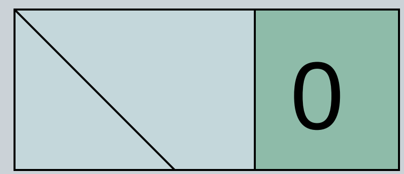
- $S_w = H_w H_w^T$, $H_w = [a_1 - c_1, a_2 - c_1, \ldots, a_n - c_r]$: $m \times n$
- $S_b = H_b H_b^T$, $H_b = [1/\sqrt{n_1}(c_1 - c), \ldots, 1/\sqrt{n_r}(c_r - c)]$: $m \times r$

LDA based on GSVD (LDA/GSVD)

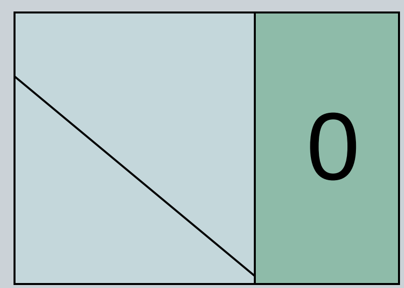
(Howland, Jeon, Park, SIMAX03, Howland and Park, IEEE TPAMI 04)

- Works regardless of singularity of *scatter matrices*
- $S_w^{-1} S_b x = / \ x \rightarrow S_b x = / \ S_w x \rightarrow \ {}^2 H_b H_b^T x = g^2 H_w H_w^T x$
- G comes from leading (r-1) generalized singular vectors of H_b^T and H_w^T

$$U^T H_b^T X = (S_b \ \ 0) =$$



$$V^T H_w^T X = (S_w \ \ 0) =$$



$X^T H_b H_b^T X = X^T S_b X$ and $X^T H_w H_w^T X = X^T S_w X$

Classical LDA is a special case of LDA/GSVD

Generalized SVD

(Paige and Saunders '81)

$$S_b x = / \, S_w x \rightarrow \quad {}^2 H_b H_b^T x = g^2 H_w H_w^T x$$

$$X^T S_b X = \begin{bmatrix} I & & & \\ & D_b & & \\ & & 0 & \\ & & & 0 \end{bmatrix} \qquad X^T S_w X = \begin{bmatrix} 0 & & & \\ & D_w & & \\ & & I & \\ & & & 0 \end{bmatrix}$$

Want ***G*** s.t. ***max trace*** $(G^T S_b G)$ and ***min trace*** $(G^T S_w G)$

X = [X1 X2 X3 X4]	g	δ	x_i belongs to
X_1	1	0	$null(S_b)^c \cap null(S_w)$
X_2	$1 > \beta > 0$	$0 < \delta < 1$	$null(S_b)^c \cap null(S_w)^c$
X_3	0	1	$null(S_b) \cap null(S_w)^c$
X_4	any	any	$null(S_b) \cap null(S_w)$

Generalization of LDA for Undersampled Problems

- **Regularized LDA** *(Friedman '89, Zhao et al. '99 …)*
- **LDA/GSVD** : Solution $G = [\ X_1 \ \ X_2\ ]$ *(Howland, Jeon, Park '03)*
- Solutions based on $Null(S_w)$ and $Range(S_b)$…

(Chen et al. '00, Yu & Yang '01, Park & Park '03 …)

- **Two-stage methods**:

  - Face Recognition: PCA + LDA *(Swets & Weng '96, Zhao et al. 99)*
  - Information Retrieval: LSI + LDA *(Torkkola '01)*
  - Mathematical Equivalence: *(Howland and Park '03)*

PCA+ LDA/GSVD = LDA/GSVD

LSI +LDA/GSVD = LDA/GSVD

More efficient = QRD + LDA/GSVD

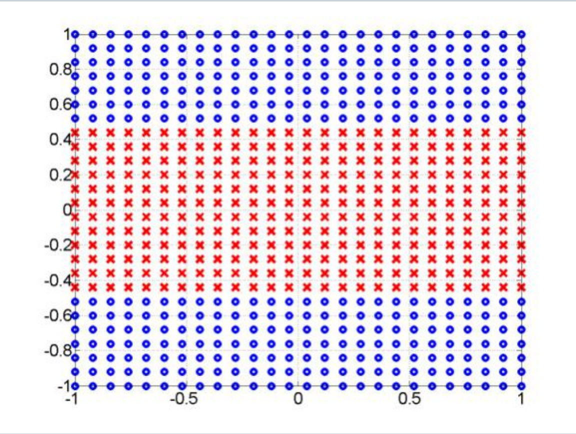
Nonlinear Dimension Reduction by Kernel Functions

Ex. Feature mapping F

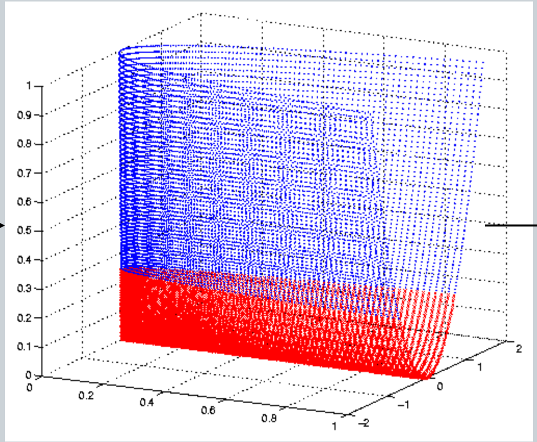
$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \longrightarrow F(x) = \begin{bmatrix} x_1^2 \\ \sqrt{2}\, x_1 x_2 \\ x_2^2 \end{bmatrix},$$

$$k(x, y) = \langle F(x), F(y) \rangle = \langle x, y \rangle^2$$

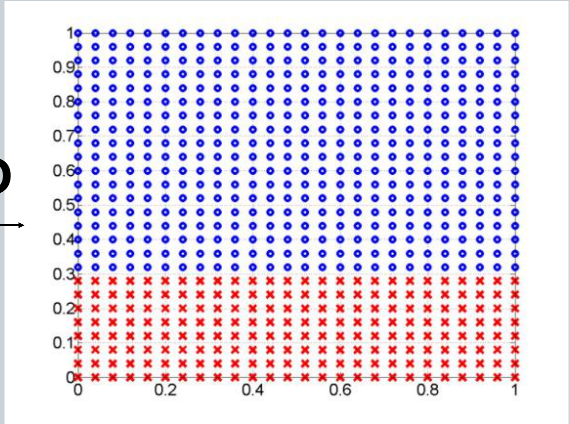
(a polynomial kernel function)



F



2D



Nonlinear Dimension Reduction by Kernel Functions

If $k(x,y)$ satisfies Mercer's condition, then there is a mapping F to an inner product space,

$$k(x,y) = < F(x), F(y) >$$

$$A \xrightarrow{F} F(A)$$

$$< x, y > \qquad k(x,y) = < F(x), F(y) >$$

Mercer's Condition for $A=[a_1, \cdots ,a_n]$:

kernel matrix $K = [\, k(a_i, a_j)\,]_{1 \le i,\, j \le n}$

is **positive semi-definite**.

Ex) RBF Kernel Function: $k(a_i, a_j) = \exp(-s \|a_i - a_j\|^2)$

Nonlinear Discriminant Analysis based on Kernel Functions (KDA/GSVD)

(C. Park and H. Park, SIMAX 04)

Assume a feature mapping: $f : a: mx1 \rightarrow f(a): px1$, m<<p

and apply LDA/GSVD to S_w and S_b in feature space

G : leading (r-1) generalized singular vectors of (H_w^f , H_b^f)

$$S_w^f = H_w^f \times H_w^{f\,T}$$

- $S_w^f = H_w^f H_w^{fT}$, $H_w^f = [a_1^f - c_1^f, a_2^f - c_1^f, \ldots, a_n^f - c_r^f]$: pxn
- $S_b^f = H_b^f H_b^{f\,T}$, $H_b^f = [\, a_1(c_1^f - c^f), \ldots, a_r (c_r^f - c^f)]$: pxr

- *f unknown but problem can be formulated to utilize kernel fcn.*

Classifier by MSE and Dimension Reduction by LDA/GSVD

(Binary Case) *(Duda et al. 01, C. Park and H. Park 04)*

- **MSE**

$$f(a) = a^T w + b$$

$$= \begin{cases} n/n_1 & \text{if } a \in \text{class } 1 \\ -n/n_2 & \text{if } a \in \text{class } 2 \end{cases}$$

$$\min \left\| \begin{bmatrix} 1 & a_1^T \\ \vdots & \\ 1 & a_n^T \end{bmatrix} \begin{bmatrix} b \\ w \end{bmatrix} - \begin{bmatrix} n/n_1 \\ \vdots \\ -n/n_2 \\ \vdots \end{bmatrix} \right\|_2 \longrightarrow$$

- **LDA/GSVD**

$$d^2 S_b x = g^2 S_w x$$

$$\downarrow$$

$$\boxed{\begin{aligned} & w^T a + b \\ & = w^T (a-c) \\ & = a\, x^T (a-c) \end{aligned}}$$

* *Extended to* ***(non)linear multi-class relationship***

(C. Park and H. Park , SIMAX, 05)

Relationship between Kernelized MSE and KDA/GSVD

(Binary Case) *(Billings and Lee 02, C. Park and H. Park 05)*

- **MSE**

$$f(a) = f(a)^T w + b$$

$$= \begin{cases} n/n_1 & \text{if } a \in \text{class } 1 \\ -n/n_2 & \text{if } a \in \text{class } 2 \end{cases}$$

$$\min \left\| \begin{bmatrix} 1 & f(a_1)^T \\ \vdots & \\ 1 & f(a_n)^T \end{bmatrix} \begin{bmatrix} b \\ w \end{bmatrix} - \begin{bmatrix} n/n_1 \\ \vdots \\ -n/n_2 \\ \vdots \end{bmatrix} \right\|_2 \longrightarrow$$

$$= \min \left\| \begin{bmatrix} e & f(A)^T \end{bmatrix} \begin{bmatrix} b \\ w \end{bmatrix} - y \right\|_2$$

- **LDA/GSVD**

$$d^2 S_b^f x = g^2 S_w^f x$$

$$\downarrow$$

$$\boxed{\begin{aligned} & w^T f(a) + b \\ & = w^T (f(a) - c^f) \\ & = a\, x^T (f(a) - c^f) \end{aligned}}$$

However, f is not known.

Formulation of Kernelized MSE

f is unknown but nonlinearization is possible using kernel functions and the fact that $w = f(A)\, z$ for some z

$$\min \left\| \begin{bmatrix} e & f(A)^T \end{bmatrix} \begin{bmatrix} b \\ w \end{bmatrix} - y \right\|_2 = \min \left\| \begin{bmatrix} e, & f(A)^T f(A) \end{bmatrix} \begin{bmatrix} b \\ z \end{bmatrix} - y \right\|_2$$

$$= \min \left\| \begin{bmatrix} e & K \end{bmatrix} \begin{bmatrix} b \\ z \end{bmatrix} - y \right\|_2$$

- Let $G = [\, e \quad K]$: nx(n+1)
- K : symmetric positive semidefinite
- Solution related to KDA/GSVD is $\begin{bmatrix} b \\ z \end{bmatrix} = G^+ y$
- If rank(G) = n, then G^+ can be obtained from QRD of G^T

  Let $G^T = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$, then $G^+ = G^T (GG^T)^{-1} = Q \begin{bmatrix} R^{-T} \\ 0 \end{bmatrix}$

Adaptive KDA by Regularized MSE (KDA/RMSE)

Replace
$$\min \left\| \begin{bmatrix} e & K \end{bmatrix} \begin{bmatrix} b \\ z \end{bmatrix} - y \right\|_2$$

by
$$\min \left\| \begin{bmatrix} e & K + / \; I \end{bmatrix} \begin{bmatrix} b \\ z \end{bmatrix} - y \right\|_2$$

- $G_/ = [\, e \quad K + / \; I \,]$: nx(n+1), rank($G_/$) = n for l > 0
- Solution can be obtained by QRD of $G_/{}^T$
- Updated and downdated sol. can be obtained by QRD updating/downdating.
- At least an order of magnitude faster than GSVD updates.

Adaptive Kernel MSE

(Kim, Drake, and Park '05)

- Kernel MSE

$$G_{/} = [e \quad K + / \; I\,] = \begin{bmatrix} 1 & k_{1,1} + / & \dots & k_{1,n} \\ \vdots & \vdots & & \vdots \\ 1 & k_{n,1} & \dots & k_{n,n} + / \end{bmatrix}$$

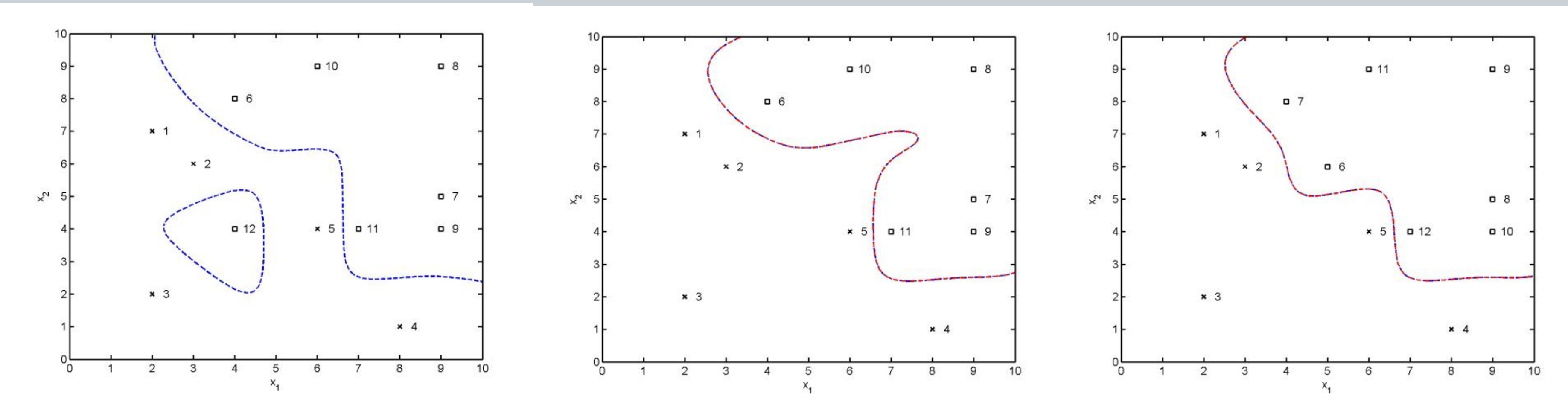
Appending a data point ***a'*** *: apply QRD updating twice*

$$G_{/}{}^{‘} = \left[\begin{array}{c|c|ccc} 1 & k_{a',a'} + / & k_{a',1} & \dots & k_{a',n} \\ \hline 1 & k_{1,a'} & & & \\ \vdots & \vdots & & K + / \; I & \\ 1 & k_{n,a'} & & & \end{array}\right]$$

Removing a data point $\boldsymbol{a_k}$ *: apply QRD downdating twice*

$$G_{/}{}^{‘} = \left[\begin{array}{ccc|cc|cc} 1 & k_{1,1} + / & \dots & k_{1,k-1} & k_{1,k+1} & \dots & k_{1,n} \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ \hline 1 & k_{k-1,1} & \dots & k_{k-1,k-1} + / & k_{k-1,k+1} & \dots & k_{k-1,n} \\ 1 & k_{k+1,1} & \dots & k_{k+1,k-1} & k_{k+1,k+1} + / & \dots & k_{k+1,n} \\ \hline \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 1 & k_{n,1} & \dots & k_{n,k-1} & k_{n,k+1} & \dots & k_{n,n} + / \end{array}\right]$$

New Decision Boundaries after Deletion and Addition of Data Points



- New decision boundaries after deleting the 12th point and inserting (5,6)
- Dash-dotted contour : a decision boundary of the adaptive KDA/RMSE
- Dashed contour : a decision boundary obtained by computing sol. from scratch by the RMSE.

$$K(\mathbf{a}_1, \mathbf{a}_2) = \exp(-\gamma \|\mathbf{a}_1 - \mathbf{a}_2\|^2)$$

Comparison Between KDA and KDA/RMSE

Method	Thyroid	Diabetes	Heart	Titanic
KDA	3.9 +- 2.0	26.3 +- 2.2	16.1 +- 3.5	24.1 +- 2.7
KDA(75%) + adaptive KDA(25%)	3.9 +- 2.0	26.3 +- 2.2	16.1 +- 3.5	24.1 +- 2.7

Average and standard deviation of test set classification errors in % for 100 partitions

Face Recognition Training Dataset (AT&T)

- 10 persons x 5 images/person = 50 images total
- Each image: 46x56
- Five-fold CV using KDA
  SVD of $G = (e \;\; K)$: 40x41 is computed for each fold

  $K(a_1, a_2) = \exp(-\gamma \|a_1 - a_2\|^2)$

  $Err_{min} = 4.0\%$
- Five-fold CV using KDA/RMSE

  QRD of $G_\lambda = (e \;\; K+\lambda I)$: 50x51, and block downdate.

  $Err_{min} = 2.0\%$

Face Recognition Testing

1. Cross validation on training dataset

$$Err_{cv} = 2.0\%$$

2. Classification of test dataset using optimal parameters obtained from CV.

Updated Face Recognition Training Dataset

Target:
1st image

Efficient Computing

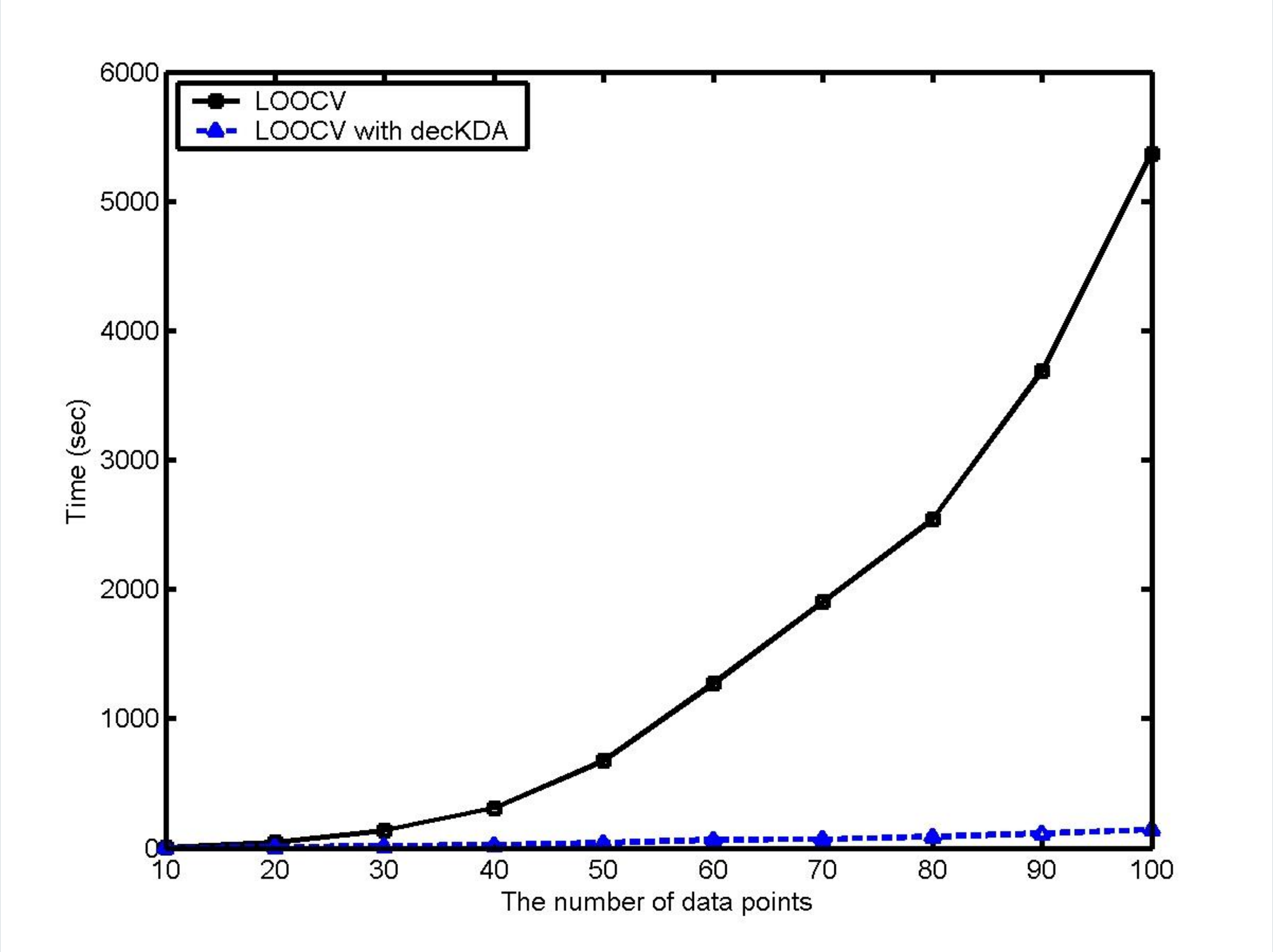
1. Removed an old image by decKDA
2. Appended a new image by incKDA

Result:

$$Err_{cv} = 2.0\%$$

$$Err_{tst} = 0.0\%$$

Computation time for leave-one-out cross validation (LOOCV): 2001 KDD cup drug design data, 8000 features



Solid black line : computation time of ordinary LOOCV

Dashed blue line : computation time of LOOCV using decKDA/RMSE

Summary / Future Research

Effective Algorithm for Adaptive Disc. Analysis

- Utilized the relationship between LDA/GSVD and MSE
- Replaced SVD up/down-dating by QRD up/down-dating
- Applicable to a wide range of problems (Facial recognition, text classification, faster cross validation algorithms …)

Current and Future Research

* Development of recursive feature tracking system
  based on recursive KDA/RMSE / parallel implementation
* Utilization of other efficient methods such as
  complete orthogonal decomposition
* Establish **Mathematical Relationships** among
  Dimension Reduction, Classifier Design, Data Reduction, …

Thank you !