

Discriminant Analysis

Fisherfaces

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Some references

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Diverse Ensemble Evolution: Curriculum based Data-Model Marriage

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Knowledge Distillation by On-the-Fly Native Ensemble

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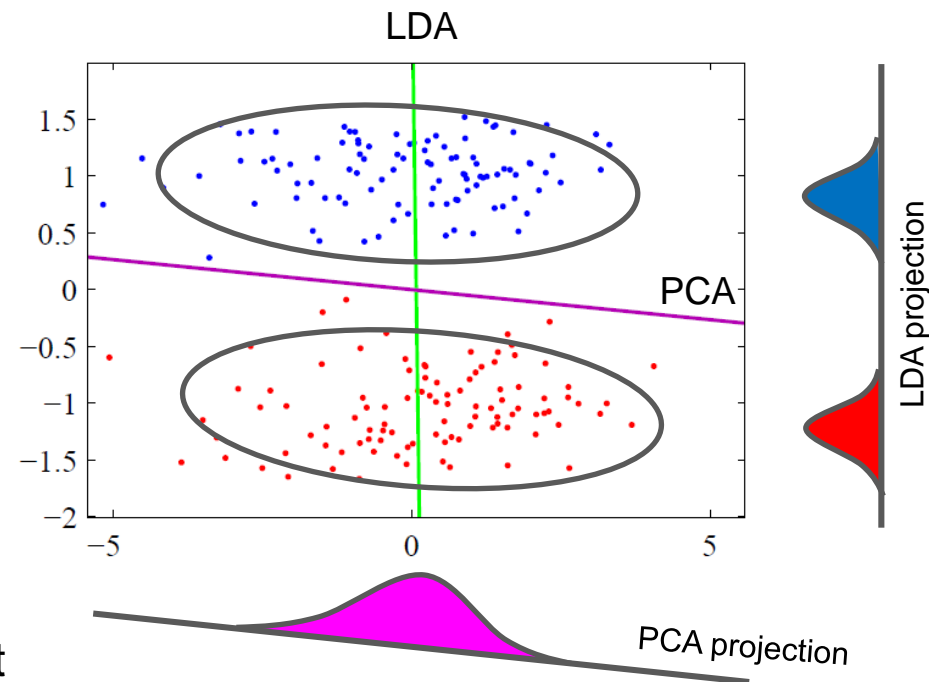
Using Large Ensembles of Control Variates for Variational Inference

Tomas Geffner · Justin Domke

Motivation

Projection that best separates the data in a least-squares sense:

- PCA finds components that are useful for representing data.
- Pooling (or projecting) data may discard essential information for discriminating between data in different classes.
- PCA finds the direction for maximum data variance (unsupervised/generative).
- LDA (Linear Discriminant Analysis) or MDA (Multiple Discriminant Analysis) finds the direction that optimally separates data of different classes (supervised/discriminative).



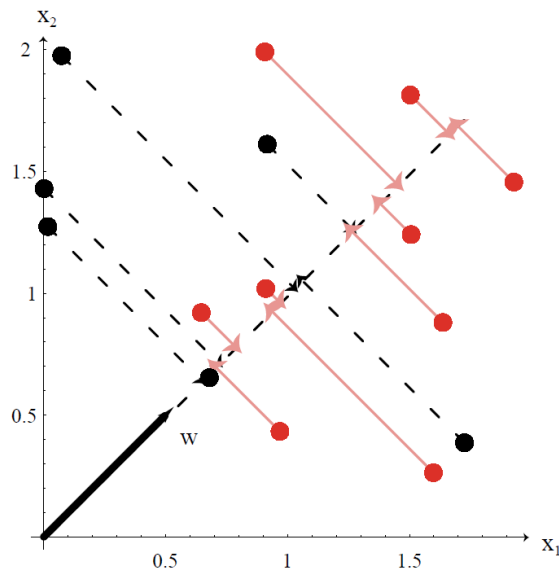
Fisher Linear Discriminant (FLD)

- We first consider **2-class problem** i.e. binary-classification.
- Data are projected from D dimensions onto a line, i.e. one-dimensional subspace.
- Given a set of N D -dimensional samples $\mathbf{x}_1, \dots, \mathbf{x}_N$,
where N_1 samples belong to the class c_1 and N_2 to the class c_2 .
- We wish to form a linear combination of the components of \mathbf{x} as
 $y = \mathbf{w}^T \mathbf{x}$
and a corresponding set of N samples y_1, \dots, y_N .

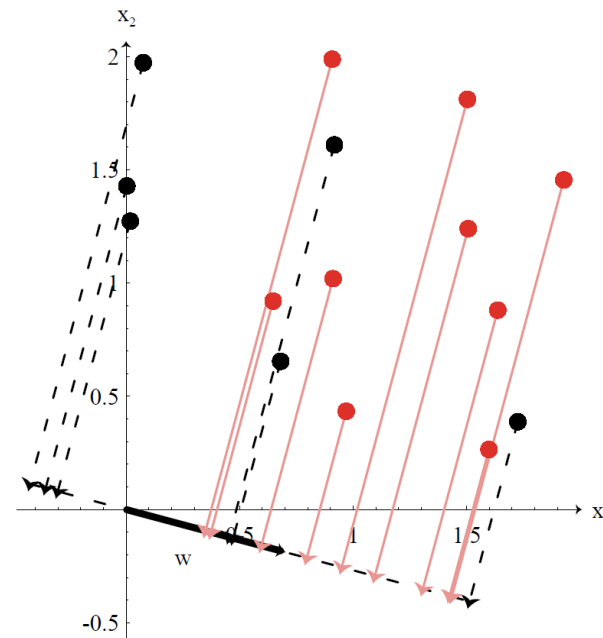
FLD: two-dimensional example

- Projection of same set of two-class samples onto two different lines in the direction marked w .

Classes mixed



Better separation



Finding best direction \mathbf{w}

- **Class mean** in D-dimensional space:

$$\mathbf{m}_i = \frac{1}{N_i} \sum_{\mathbf{x} \in c_i} \mathbf{x}$$

- Class mean of projected points:

$$\tilde{\mathbf{m}}_i = \frac{1}{N_i} \sum_{y \in c_i} y = \frac{1}{N_i} \sum_{\mathbf{x} \in c_i} \mathbf{w}^T \mathbf{x} = \mathbf{w}^T \mathbf{m}_i$$

- Distance between projected class means is

$$|\tilde{\mathbf{m}}_1 - \tilde{\mathbf{m}}_2| = |\mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)|$$

Criterion for Fisher Linear Discriminant

- Define the scatter of the projected samples as

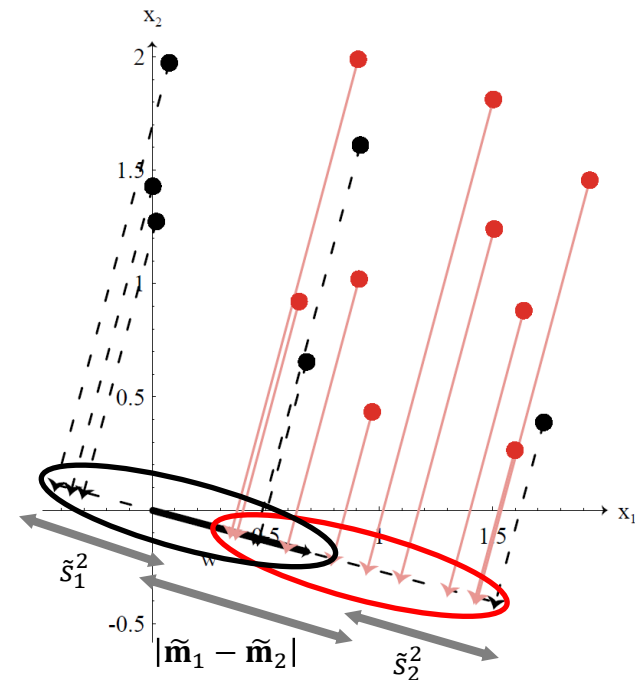
$$\tilde{s}_i^2 = \sum_{y \in \mathcal{C}_i} (\mathbf{y} - \tilde{\mathbf{m}}_i)^2$$

- Thus $(1/N)(\tilde{s}_1^2 + \tilde{s}_2^2)$ is the variance of the pooled (or projected) data.
- **Total within-class scatter** is $\tilde{s}_1^2 + \tilde{s}_2^2$.

- Find that linear function $\mathbf{w}^T \mathbf{x}$ for which

$$J(\mathbf{w}) = \frac{|\tilde{\mathbf{m}}_1 - \tilde{\mathbf{m}}_2|^2}{\tilde{s}_1^2 + \tilde{s}_2^2}$$

is maximum and independent of $\|\mathbf{w}\|$.



Scatter matrices

- To obtain $J(\cdot)$ as an explicit function of \mathbf{w} , we define scatter matrices \mathbf{S}_i and \mathbf{S}_W

$$\mathbf{S}_i = \sum_{\mathbf{x} \in c_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^T$$

And Within-class scatter matrix $\mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2$.

- We can then write

$$\begin{aligned} \tilde{s}_i^2 &= \sum_{\mathbf{x} \in c_i} (\mathbf{w}^T \mathbf{x} - \mathbf{w}^T \mathbf{m}_i)^2 \\ &= \sum_{\mathbf{x} \in c_i} \mathbf{w}^T (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^T \mathbf{w} \\ &= \mathbf{w}^T \mathbf{S}_i \mathbf{w} \end{aligned}$$

Therefore, $\tilde{s}_1^2 + \tilde{s}_2^2 = \mathbf{w}^T (\mathbf{S}_1 + \mathbf{S}_2) \mathbf{w} = \mathbf{w}^T \mathbf{S}_W \mathbf{w}$

- The within-class scatter matrix $\mathbf{S}_W \in \mathbb{R}^{D \times D}$ is symmetric and positive semidefinite, and is nonsingular if $N > D$.

Scatter matrices

- Similarly, the separation of the projected class means is

$$\begin{aligned} |\tilde{\mathbf{m}}_1 - \tilde{\mathbf{m}}_2|^2 &= (\mathbf{w}^T \mathbf{m}_1 - \mathbf{w}^T \mathbf{m}_2)^2 \\ &= \mathbf{w}^T (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T \mathbf{w} \\ &= \mathbf{w}^T \mathbf{S}_B \mathbf{w} \end{aligned}$$

Where Between-class scatter matrix $\mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T$.

- The between-class scatter matrix \mathbf{S}_B is also symmetric and positive semidefinite.
- Its rank is at most one, since it is the outer product of two vectors.

Criterion function in terms of scatter matrices and optimisation

- The criterion function is written as

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

- This is well known the generalised Rayleigh quotient.
- Maximizing the ratio is equivalent to maximizing the numerator while keeping the denominator constant, i.e.

$$\max_{\mathbf{w}} \mathbf{w}^T \mathbf{S}_B \mathbf{w} \quad \text{subject to} \quad \mathbf{w}^T \mathbf{S}_W \mathbf{w} = k$$

- This can be accomplished using Lagrange multipliers as

$$L = \mathbf{w}^T \mathbf{S}_B \mathbf{w} + \lambda(k - \mathbf{w}^T \mathbf{S}_W \mathbf{w})$$

maximize L with respect to both \mathbf{w} and λ .

Optimisation for Fisher Discriminant

- Setting the gradient of

$$L = \mathbf{w}^T (\mathbf{S}_B - \lambda \mathbf{S}_W) \mathbf{w} + \lambda k$$

with respect to \mathbf{w} to zero, we get

$$2(\mathbf{S}_B - \lambda \mathbf{S}_W) \mathbf{w} = 0$$

then

$$\mathbf{S}_B \mathbf{w} = \lambda \mathbf{S}_W \mathbf{w}$$

- This is a generalized eigenvalue problem.
- The solution is easy, when \mathbf{S}_W is *nonsingular*.

$$\mathbf{S}_W^{-1} \mathbf{S}_B \mathbf{w} = \lambda \mathbf{w}$$

where \mathbf{w} and λ are the eigenvector and eigenvalue of $\mathbf{S}_W^{-1} \mathbf{S}_B$.

Multiple Discriminant Analysis

- Generalization of Fisher's Linear Discriminant, for multiple c classes, involves M discriminant functions \mathbf{w}_i , $i = 1, \dots, M$.
- Projection is from a D -dimensional space to a M -dimensional subspace.
- The Within-class and Between-class scatter matrices are defined as

$$\mathbf{S}_W = \sum_{i=1}^c \mathbf{S}_i$$

where $\mathbf{S}_i = \sum_{\mathbf{x} \in C_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^T$,

$$\mathbf{S}_B = \sum_{i=1}^c (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T.$$

- The desired projections are found as generalised eigenvectors:

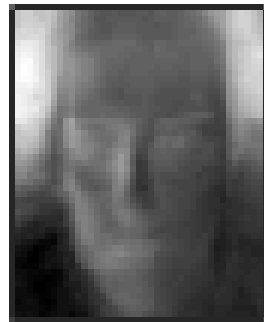
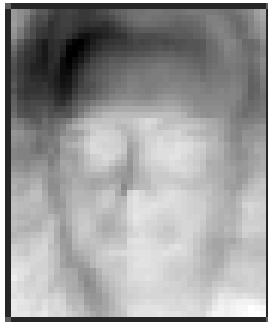
$$\mathbf{S}_B \mathbf{w}_i = \lambda_i \mathbf{S}_W \mathbf{w}_i, \quad i = 1, \dots, M$$

for eigenvalues λ_i .

- If \mathbf{S}_W has full rank, the solutions are generalized eigenvectors of $\mathbf{S}_W^{-1} \mathbf{S}_B$ with largest M eigenvalues.

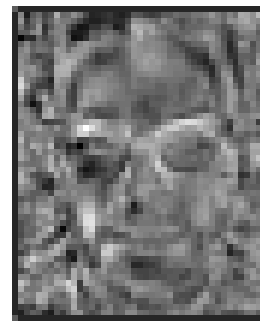
Fisherfaces

Eigenfaces



VS

Fisherfaces



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Recognition using class specific linear projection

- Let us consider N sample images $\{\mathbf{x}_n\}$, $n = 1, \dots, N$ and $\mathbf{x}_n \in \mathbb{R}^D$ in an D -dimensional image space, and assume that each image belongs to one of c classes $\{c_i\}$, $i = 1, \dots, c$.
- We consider a linear transformation mapping the D -dimensional image space into an M -dimensional feature space, where $M < D$.
- The feature vectors $\mathbf{y}_n \in \mathbb{R}^M$ are defined by the following linear transformation:

$$\mathbf{y}_n = \mathbf{W}^T \mathbf{x}_n$$

where $\mathbf{W} \in \mathbb{R}^{D \times M}$ is a matrix with orthonormal columns.

Eigenfaces

- The total scatter matrix \mathbf{S}_T (or the covariance matrix) is defined as

$$\mathbf{S}_T = \sum_n (\mathbf{x}_n - \mathbf{m})(\mathbf{x}_n - \mathbf{m})^T$$

where $\mathbf{m} \in \mathbb{R}^D$ is the mean of all samples.

Recognition using class specific linear projection

- After applying the linear transformation \mathbf{W}^T , the scatter matrix of the feature vectors $\mathbf{y}_n \in \mathbb{R}^M$, $n = 1, \dots, N$, is $\mathbf{W}^T \mathbf{S}_T \mathbf{W}$
- In PCA, the projection \mathbf{W}_{opt} is chosen to maximize the determinant of the total scatter matrix of the projected samples, i.e.,

$$\mathbf{W}_{\text{opt}} = \arg \max_{\mathbf{W}} |\mathbf{W}^T \mathbf{S}_T \mathbf{W}| = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_M]$$

where \mathbf{w}_i , $i = 1, \dots, M$ is the set of D -dimensional eigenvectors of \mathbf{S}_T corresponding to the M largest eigenvalues.

- A drawback of this approach is that both the between-class and within-class scatter are maximized, since $\mathbf{S}_T = \mathbf{S}_B + \mathbf{S}_W$.

Recognition using class specific linear projection

Fisherfaces

- Since the learning set is class-labelled, we use this information to build a more discriminative method for reducing the feature space dimensionality.
- Using class specific linear methods for dimensionality reduction and NN classifiers in the reduced feature space, we may get better recognition rates than with the Eigenface method.
- FLD is a class specific method that selects \mathbf{W} in such a way that the ratio of the between-class scatter and the within-class scatter is maximized.
- Let the between-class scatter matrix be defined as

$$\mathbf{S}_B = \sum_{i=1}^c (\mathbf{m}_i - \mathbf{m})(\mathbf{m}_i - \mathbf{m})^T,$$

the within-class scatter matrix be defined as

$$\mathbf{S}_W = \sum_{i=1}^c \sum_{\mathbf{x} \in c_i} (\mathbf{x} - \mathbf{m}_i)(\mathbf{x} - \mathbf{m}_i)^T$$

where \mathbf{m}_i is the mean image of class c_i , and N_i is the number of samples in class c_i .

Fisherfaces

- If \mathbf{S}_W is nonsingular, the optimal projection \mathbf{W}_{opt} is chosen as the matrix with orthonormal columns which maximizes the ratio of the determinant of the between-class scatter matrix to the determinant of the within-class scatter matrix of the projected samples, i.e.,

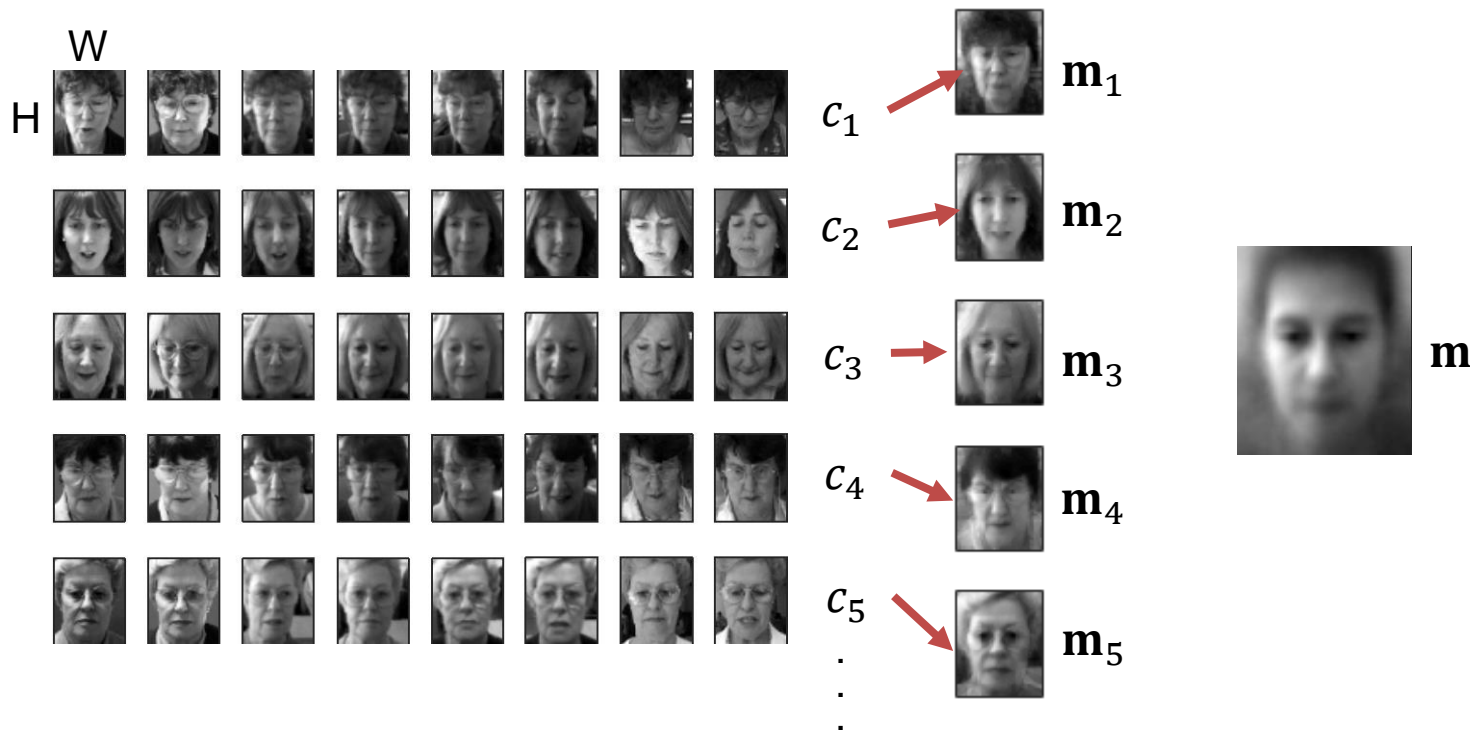
$$\mathbf{W}_{\text{opt}} = \arg \max_{\mathbf{W}} \frac{|\mathbf{W}^T \mathbf{S}_B \mathbf{W}|}{|\mathbf{W}^T \mathbf{S}_W \mathbf{W}|} = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_M]$$

where \mathbf{w}_i is the set of generalized eigenvectors of \mathbf{S}_B and \mathbf{S}_W corresponding to the M largest eigenvalues:

$$\mathbf{S}_B \mathbf{w}_i = \lambda_i \mathbf{S}_W \mathbf{w}_i, \quad i = 1, \dots, M$$

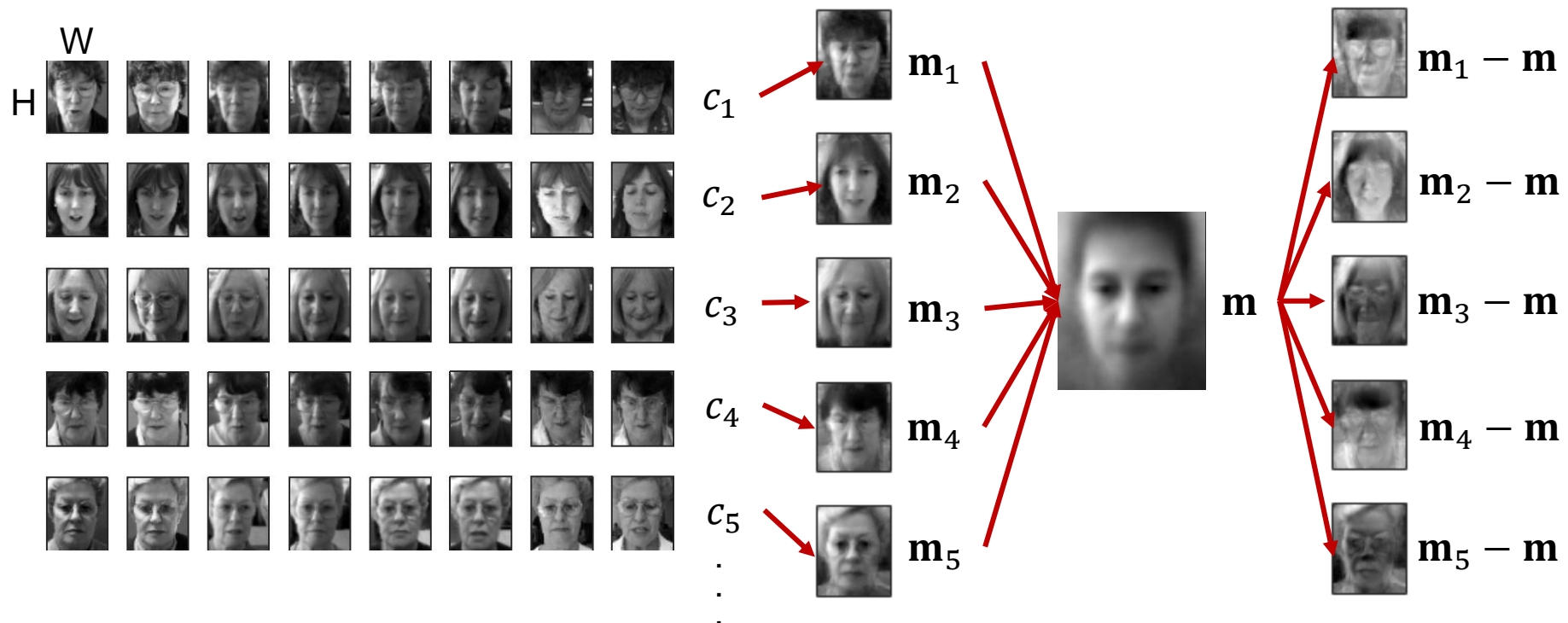
Procedures: Fisherfaces

- Collect training images \mathbf{x}_n of c classes ($c=26$, $N=208$, $D=2576$)
- Compute the class means \mathbf{m}_i , $i = 1, \dots, c$, and the global mean \mathbf{m}



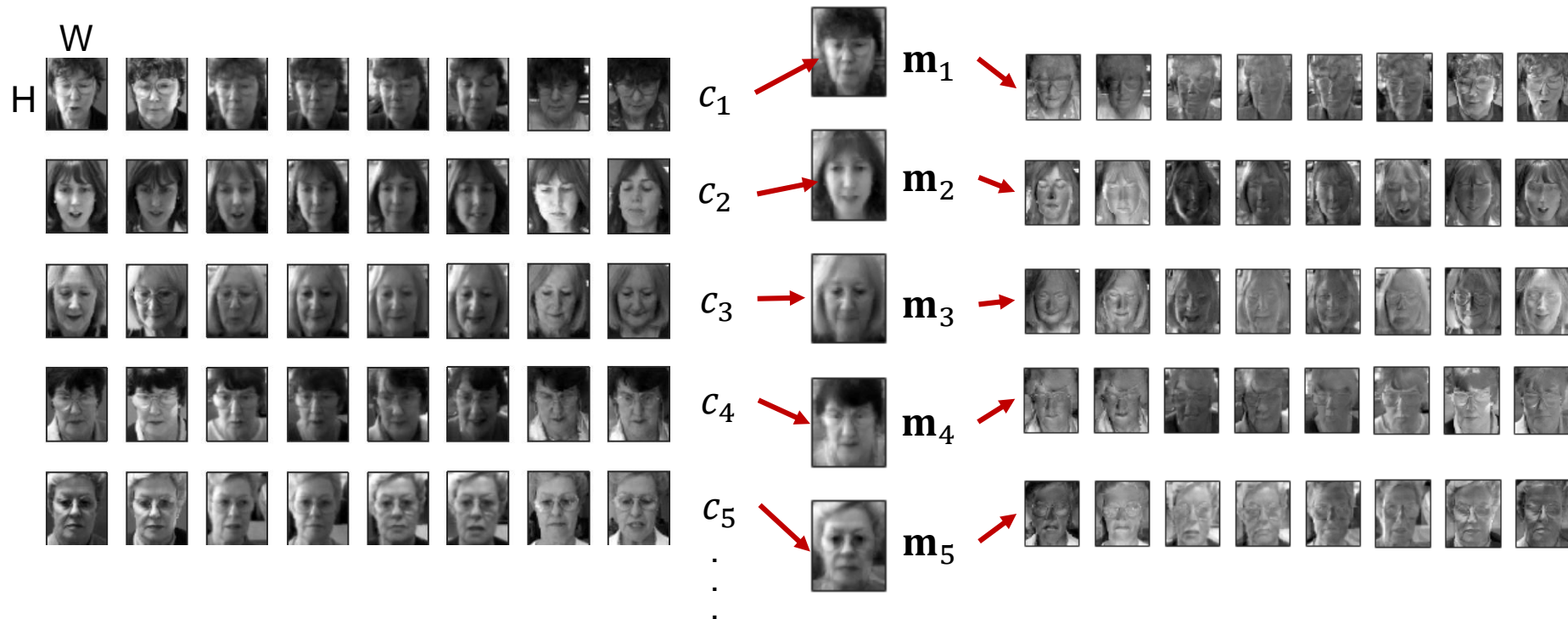
Procedures: Fisherfaces

- Compute $\mathbf{m}_i - \mathbf{m}$, and \mathbf{S}_B , where $\text{rank}(\mathbf{S}_B) = c - 1$.



Procedures: Fisherfaces

- Compute $\mathbf{x} - \mathbf{m}_i$, and \mathbf{S}_W , where $\text{rank}(\mathbf{S}_W)$ is $N - c$.



Fisherfaces

- Given the generalized eigenvalue/vector problem of \mathbf{S}_B and \mathbf{S}_W :

$$\mathbf{S}_B \mathbf{w}_i = \lambda_i \mathbf{S}_W \mathbf{w}_i, \quad i = 1, \dots, M$$

- Note that there are at most $c - 1$ nonzero generalized eigenvalues i.e. the rank of \mathbf{S}_B , and so an upper bound on M is $c - 1$.
- The within-class scatter matrix $\mathbf{S}_W \in \mathbb{R}^{D \times D}$ is often singular, since the rank of \mathbf{S}_W is at most $N - c$, and, in general, N is smaller than D .

Fisherfaces

- In order to overcome the singular \mathbf{S}_W , we propose an alternative to the criterion.
- This method, which we call Fisherfaces, avoids the problem by projecting the image set to a lower dimensional space.
- We use PCA to reduce the dimension of the feature space M_{pca} ($\leq N-c$), and then apply the standard FLD to reduce the dimension to M_{lda} ($\leq c-1$).
- Formally, \mathbf{W}_{opt} is given by

$$\mathbf{W}_{opt}^T = \mathbf{W}_{lda}^T \mathbf{W}_{pca}^T$$

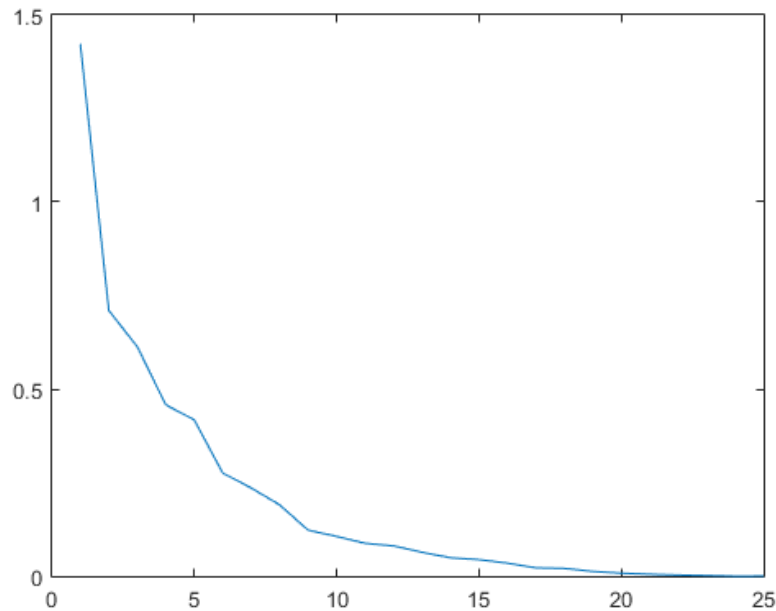
$$\mathbf{W}_{pca} = \arg \max_{\mathbf{W}} |\mathbf{W}^T \mathbf{S}_T \mathbf{W}|$$

$$\mathbf{W}_{lda} = \arg \max_{\mathbf{W}} \frac{|\mathbf{W}^T \mathbf{W}_{pca}^T \mathbf{S}_B \mathbf{W}_{pca} \mathbf{W}|}{|\mathbf{W}^T \mathbf{W}_{pca}^T \mathbf{S}_W \mathbf{W}_{pca} \mathbf{W}|}$$

- There are other ways of reducing the withinclass scatter while preserving between-class scatter e.g. Direct LDA, Null LDA, etc.

Procedures: Fisherfaces

- $\text{rank}(\mathbf{S}_W) = 182 (=N - c)$, $\text{rank}(\mathbf{S}_B) = 25 (=c - 1)$
- Perform PCA to get \mathbf{W}_{pca} ($M_{\text{pca}}=25$), and compute $\mathbf{W}_{\text{pca}}^T \mathbf{S}_B \mathbf{W}_{\text{pca}}$ and $\mathbf{W}_{\text{pca}}^T \mathbf{S}_W \mathbf{W}_{\text{pca}}$.
- Get the generalized eigenvectors of $(\mathbf{W}_{\text{pca}}^T \mathbf{S}_W \mathbf{W}_{\text{pca}})^{-1} (\mathbf{W}_{\text{pca}}^T \mathbf{S}_B \mathbf{W}_{\text{pca}})$ with largest M_{lda} eigenvalues.

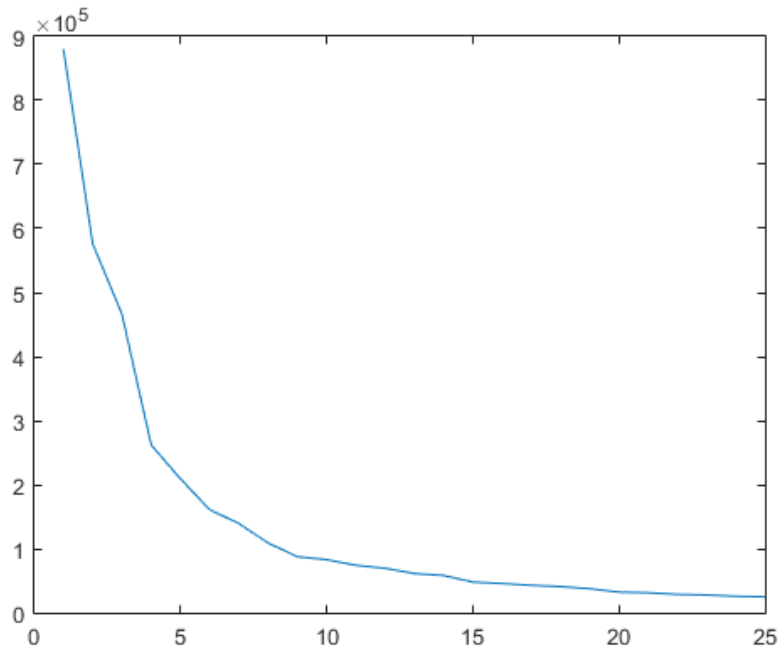


Generalized eigenvalues



Top 25 generalized eigenvectors

Comparison to Eigenfaces



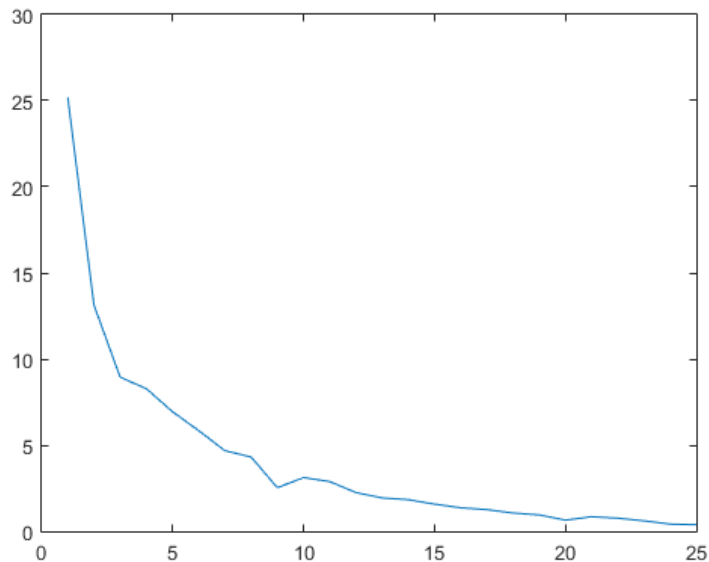
Eigenvalues



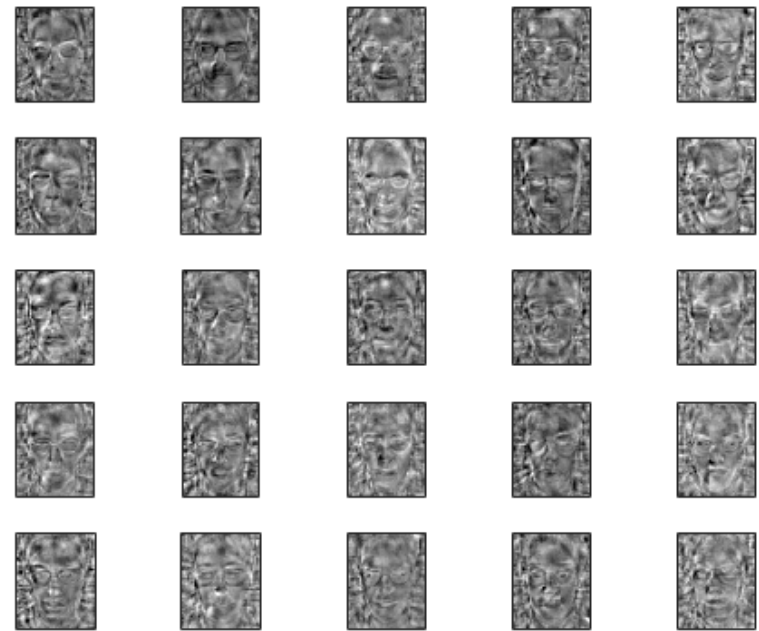
Top 25 eigenvectors

Procedures: Fisherfaces

- $\text{rank}(\mathbf{S}_W) = 182 (=N - c)$, $\text{rank}(\mathbf{S}_B) = 25 (=c - 1)$
- Perform PCA to get \mathbf{W}_{pca} ($M_{\text{pca}}=150$), and compute $\mathbf{W}_{\text{pca}}^T \mathbf{S}_B \mathbf{W}_{\text{pca}}$ and $\mathbf{W}_{\text{pca}}^T \mathbf{S}_W \mathbf{W}_{\text{pca}}$.
- Get the generalized eigenvectors of $(\mathbf{W}_{\text{pca}}^T \mathbf{S}_W \mathbf{W}_{\text{pca}})^{-1} (\mathbf{W}_{\text{pca}}^T \mathbf{S}_B \mathbf{W}_{\text{pca}})$ with largest M_{lda} eigenvalues.

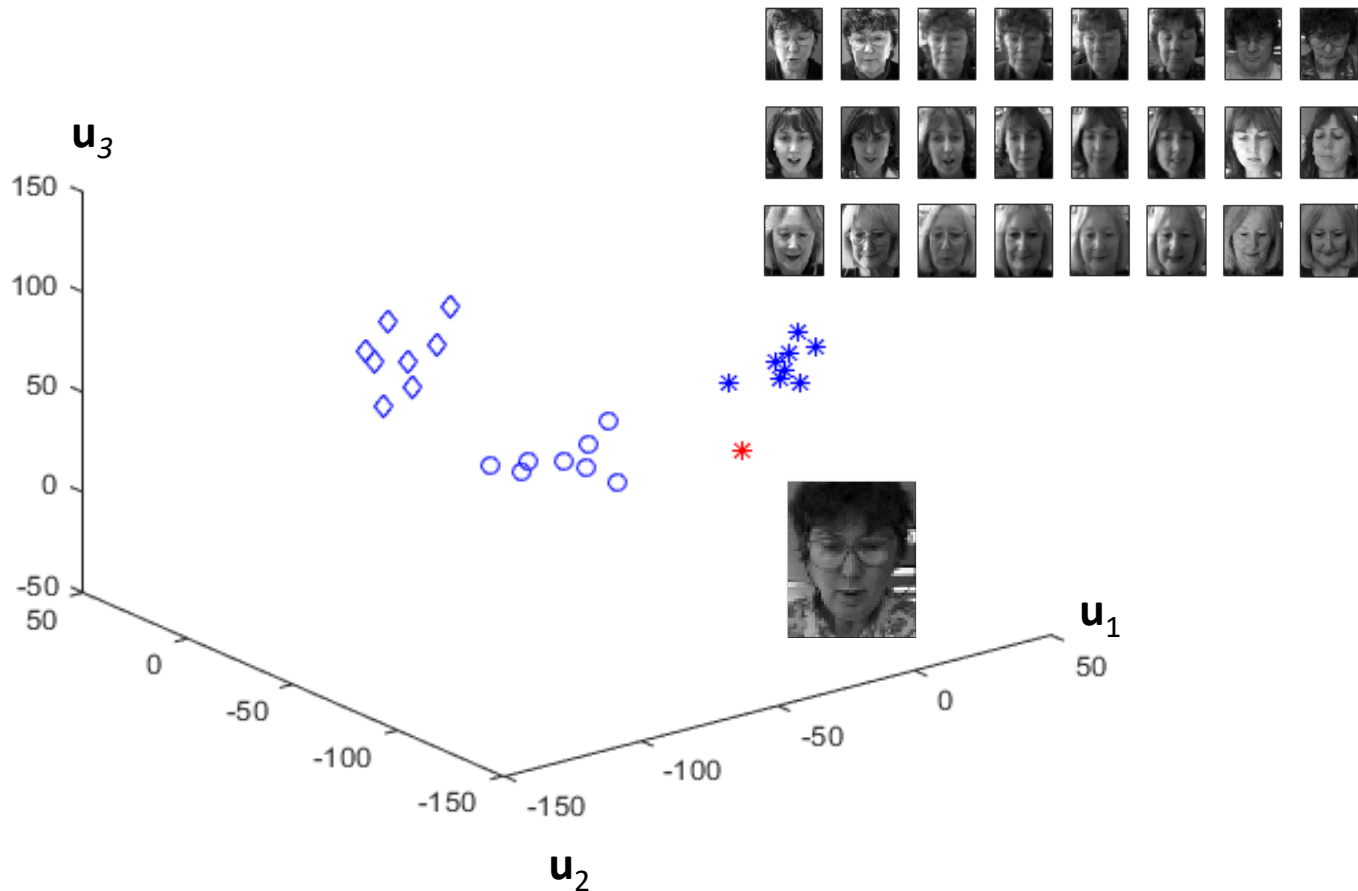


Generalized eigenvalues



Top 25 generalized eigenvectors

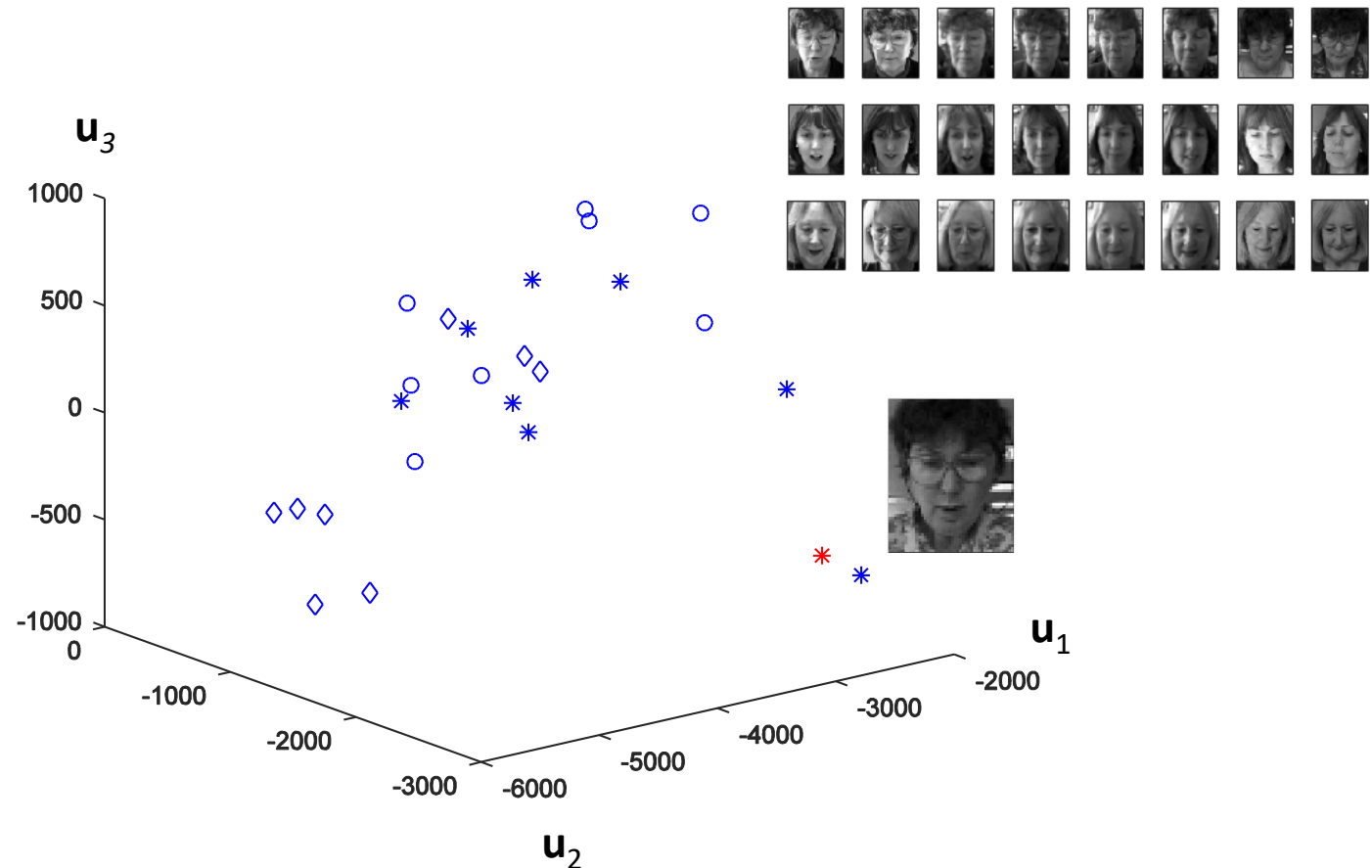
Procedures: Fisherfaces



Face images in 3-dimensional fisher-subspace

24 training images of 3 different face classes (star, diamond, circle, “in blue”) are projected. A query image projection is “in red”.

Comparison to Eigenfaces



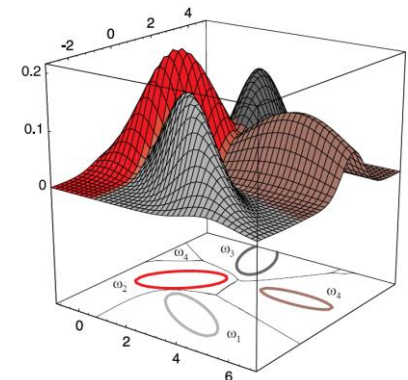
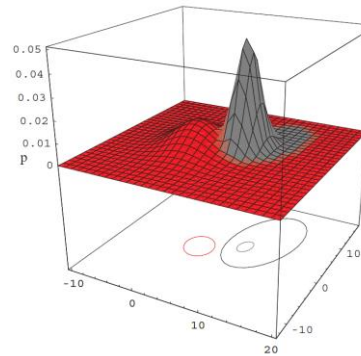
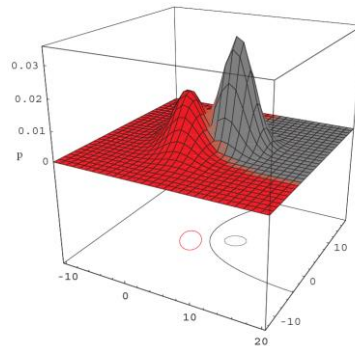
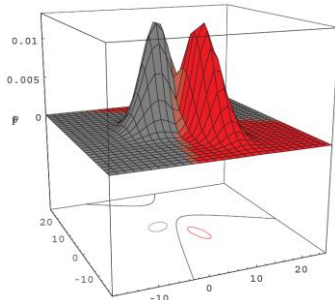
Face images in 3-dimensional eigen-subspace

24 training images of 3 different face classes (star, diamond, circle, “in blue”) are projected. A query image projection is “in red”.

Relation to optimal bayesian decision theory

Bayes Decision Theory

- Fundamental statistical approach to pattern classification
- Quantifies trade-offs between classification using probabilities and costs of decisions
- Assumes all relevant probabilities are known
- Σ_i (data covariance matrix of class i) = arbitrary
 - Arbitrary Gaussian distributions lead to Bayes decision boundaries that are general hyperquadrics

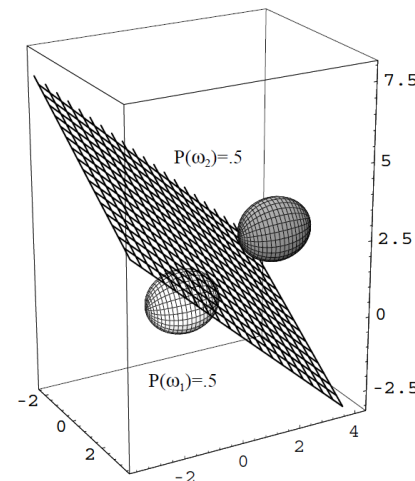
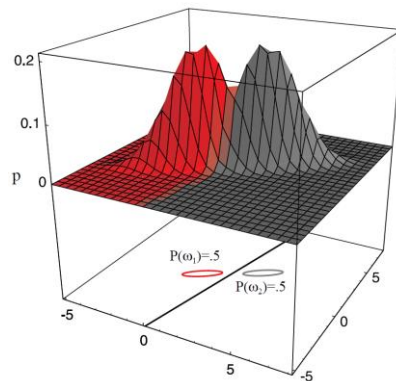


Relation to optimal bayesian decision theory

- $\Sigma_i = \Sigma$
 - For a classification problem with Gaussian classes of equal covariance $\Sigma_i = \Sigma$, the Bayes decision boundaries (or the discriminant function) is the plane of normal

$$\mathbf{w} = \Sigma^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$$

- The hyperplane is generally not orthogonal to the line between the means.



Relation to optimal bayesian decision theory

- If $\Sigma_1 = \Sigma_2$, this is also the FLD solution.
- In FLD, $\mathbf{S}_W = \mathbf{S}_1 + \mathbf{S}_2$, $\mathbf{w} = \mathbf{S}_W^{-1}(\mathbf{m}_1 - \mathbf{m}_2)$
- This gives some interpretations of FLD/LDA
 - It is optimal if and only if the classes are Gaussian and have equal covariance.
 - The extension from two-classes to multiple classes in LDA is ad-hoc.

T-K Kim, PhD dissertation: Discriminant Analysis of Patterns in Images, Image Ensembles, and Videos, Univ. of Cambridge, 2008.