中国科学院大学人工智能学院硕士课《模式识别》

特征提取与特征选择

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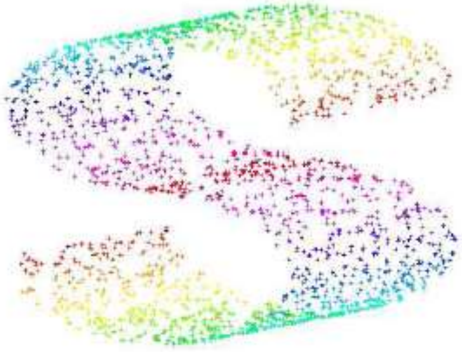
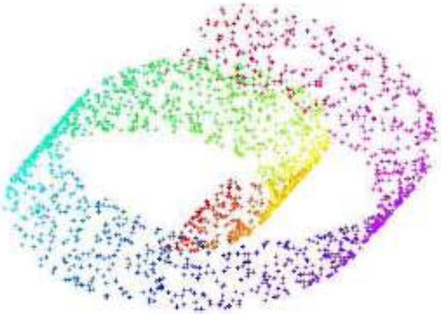
Nonlinear Extensions

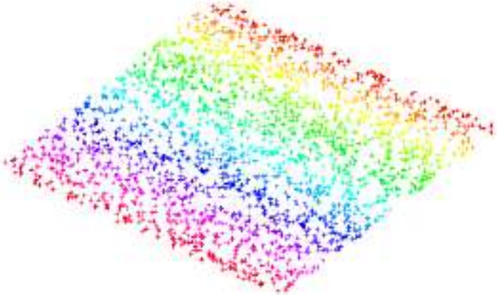
Nonlinear Extensions

- Given: Low-dim. surface embedded **nonlinearly** in high-dim. space
  - Such a structure is called a **Manifold**



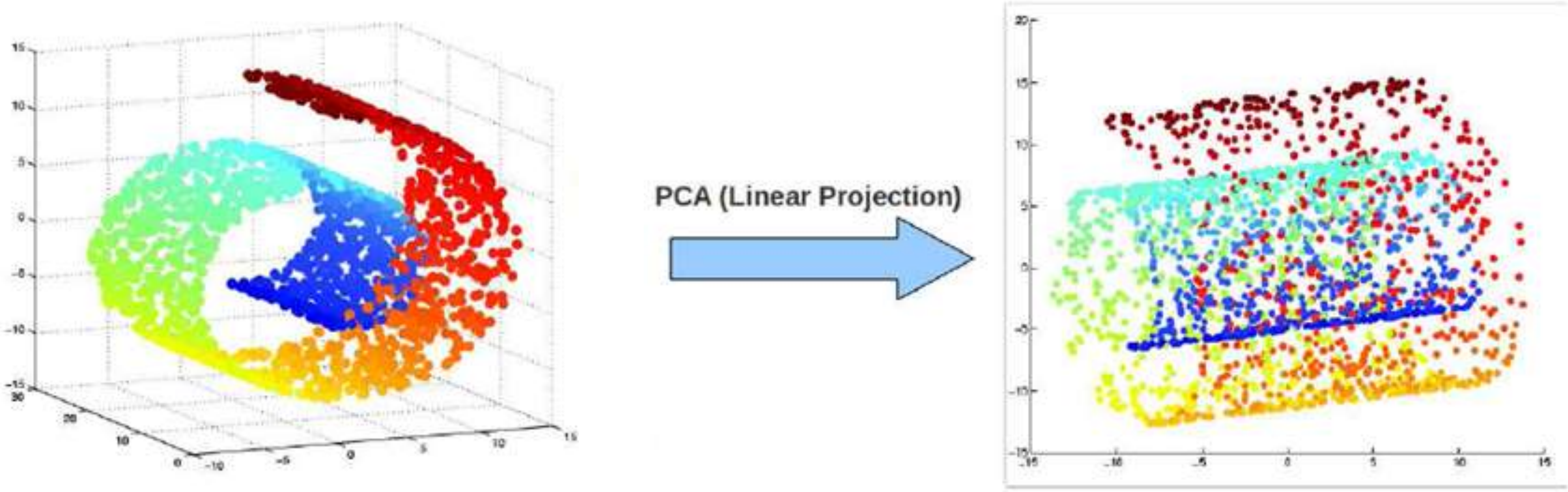


- Goal: Recover the low-dimensional surface



Nonlinear Extensions

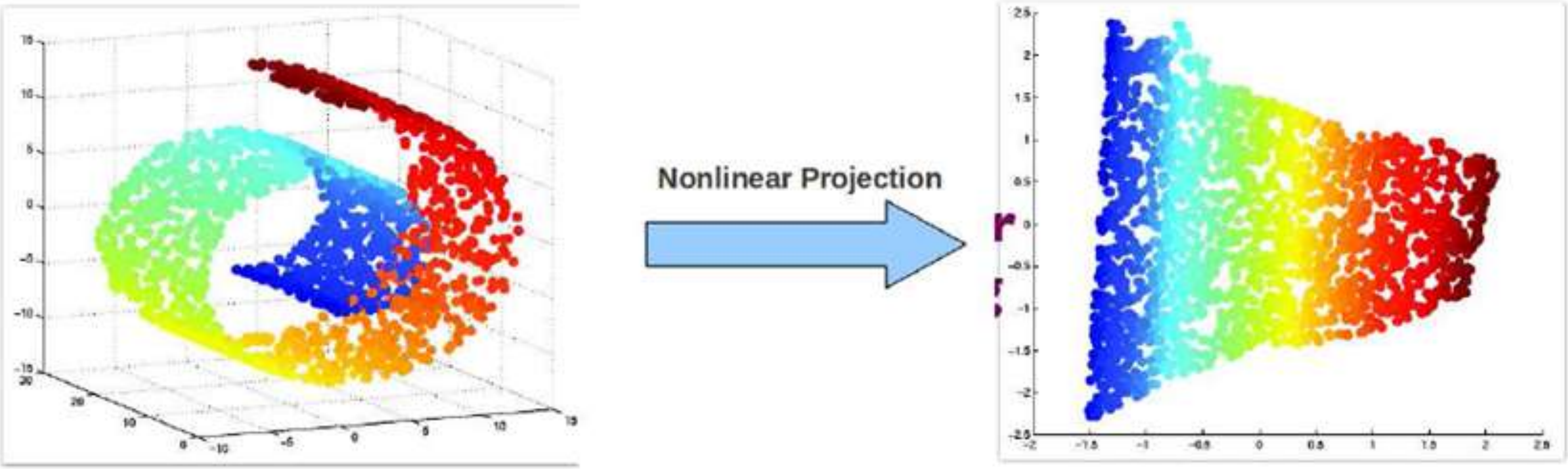
- Consider the swiss-roll dataset (points lying close to a manifold)



- Linear projection methods (e.g., PCA) can't capture intrinsic nonlinearities

Nonlinear Extensions

- We want to do nonlinear projections
- Different criteria could be used for such projections
- Most nonlinear methods try to preserve the neighborhood information
  - Locally linear structures (locally linear ⇒ globally nonlinear)
  - Pairwise distances (along the nonlinear manifold)
- Roughly translates to "unrolling" the manifold



Nonlinear Projection

Nonlinear Extensions

Two ways of doing it:

- Nonlinearize a linear dimensionality reduction method. E.g.:
    - **Kernel PCA (nonlinear PCA)**
- Using manifold based methods. E.g.:
    - **Locally Linear Embedding (LLE)**
    - **Isomap**
    - Maximum Variance Unfolding
    - Laplacian Eigenmaps
    - And several others (Hessian LLE, Hessian Eigenmaps, etc.)

Kernel PCA

- Given N observations $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, $\forall \mathbf{x}_n \in \mathbb{R}^D$, define the $D \times D$ covariance matrix (assuming centered data $\sum_n \mathbf{x}_n = \mathbf{0}$)

$$\mathbf{S} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^\top$$

- Linear PCA: Compute eigenvectors $\mathbf{u}_i$ satisfying: $\mathbf{S}\mathbf{u}_i = \lambda_i \mathbf{u}_i \; \forall i = 1, \ldots, D$
- Consider a nonlinear transformation $\phi(\mathbf{x})$ of $\mathbf{x}$ into an M dimensional space
- $M \times M$ covariance matrix **in this space** (assume centered data $\sum_n \phi(\mathbf{x}_n) = \mathbf{0}$)

$$\mathbf{C} = \frac{1}{N} \sum_{n=1}^{N} \phi(\mathbf{x}_n) \phi(\mathbf{x}_n)^\top$$

- Kernel PCA: Compute eigenvectors $\mathbf{v}_i$ satisfying: $\mathbf{C}\mathbf{v}_i = \lambda_i \mathbf{v}_i \; \forall i = 1, \ldots, M$
- Ideally, we would like to do this without having to compute the $\phi(\mathbf{x}_n)$'s

Kernel PCA

- Kernel PCA: Compute eigenvectors $\mathbf{v}_i$ satisfying: $\mathbf{C}\mathbf{v}_i = \lambda_i \mathbf{v}_i$
- Plugging in the expression for $\mathbf{C}$, we have the eigenvector equation:

$$\frac{1}{N}\sum_{n=1}^{N} \phi(\mathbf{x}_n)\{\phi(\mathbf{x}_n)^\top \mathbf{v}_i\} = \lambda_i \mathbf{v}_i$$

- Using the above, we can write $\mathbf{v}_i$ as: $\boxed{\mathbf{v}_i = \sum_{n=1}^{N} a_{in}\phi(\mathbf{x}_n)}$
- Plugging this back in the eigenvector equation:

$$\frac{1}{N}\sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^\top \sum_{m=1}^{N} a_{im}\phi(\mathbf{x}_m) = \lambda_i \sum_{n=1}^{N} a_{in}\phi(\mathbf{x}_n)$$

- Pre-multiplying both sides by $\phi(\mathbf{x}_l)^\top$ and re-arranging

$$\frac{1}{N}\sum_{n=1}^{N} \phi(\mathbf{x}_l)^\top \phi(\mathbf{x}_n) \sum_{m=1}^{N} a_{im}\phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m) = \lambda_i \sum_{n=1}^{N} a_{in}\phi(\mathbf{x}_l)^\top \phi(\mathbf{x}_n)$$

Kernel PCA

- Using $\phi(\mathbf{x}_n)^\top \phi(\mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m)$, the eigenvector equation becomes:

$$\frac{1}{N} \sum_{n=1}^{N} k(\mathbf{x}_l, \mathbf{x}_n) \sum_{m=1}^{N} a_{im} k(\mathbf{x}_n, \mathbf{x}_m) = \lambda_i \sum_{n=1}^{N} a_{in} k(\mathbf{x}_l, \mathbf{x}_n)$$

- Define $\mathbf{K}$ as the $N \times N$ **kernel matrix** with $K_{nm} = k(\mathbf{x}_n, \mathbf{x}_m)$
  - $\mathbf{K}$ is the similarity of two examples $\mathbf{x}_n$ and $\mathbf{x}_m$ in the ϕ space
  - ϕ is implicitly defined by kernel function k (which can be, e.g., RBF kernel)
- Define $\mathbf{a}_i$ as the $N \times 1$ vector with elements a_{in}
- Using $\mathbf{K}$ and $\mathbf{a}_i$, the eigenvector equation becomes:

$$\mathbf{K}^2 \mathbf{a}_i = \lambda_i N \mathbf{K} \mathbf{a}_i \quad \Rightarrow \quad \boxed{\mathbf{K}\mathbf{a}_i = \lambda_i N \mathbf{a}_i}$$

- This corresponds to the original Kernel PCA eigenvalue problem $\mathbf{C}\mathbf{v}_i = \lambda_i \mathbf{v}_i$
- For a projection to $K < D$ dimensions, top K eigenvectors of $\mathbf{K}$ are used

$$\boxed{\mathbf{v}_i = \sum_{n=1}^{N} a_{in} \phi(\mathbf{x}_n)}$$

Kernel PCA: Centering Data

- In PCA, we centered the data before computing the covariance matrix

- For kernel PCA, we need to do the same

$$\tilde{\phi}(\mathbf{x}_n) = \phi(\mathbf{x}_n) - \frac{1}{N}\sum_{l=1}^{N}\phi(\mathbf{x}_l)$$

- How does it affect the kernel matrix $\mathbf{K}$ which is eigen-decomposed?

$$\begin{aligned}
\tilde{K}_{nm} &= \tilde{\phi}(\mathbf{x}_n)^\top\tilde{\phi}(\mathbf{x}_m) \\
&= \phi(\mathbf{x}_n)^\top\phi(\mathbf{x}_m) - \frac{1}{N}\sum_{l=1}^{N}\phi(\mathbf{x}_n)^\top\phi(\mathbf{x}_l) - \frac{1}{N}\sum_{l=1}^{N}\phi(\mathbf{x}_l)^\top\phi(\mathbf{x}_m) + \frac{1}{N^2}\sum_{j=1}^{N}\sum_{l=1}^{N}\phi(\mathbf{x}_j)^\top\phi(\mathbf{x}_l) \\
&= k(\mathbf{x}_n, \mathbf{x}_m) - \frac{1}{N}\sum_{l=1}^{N}k(\mathbf{x}_n, \mathbf{x}_l) - \frac{1}{N}\sum_{l=1}^{N}k(\mathbf{x}_l, \mathbf{x}_m) + \frac{1}{N^2}\sum_{j=1}^{N}\sum_{l=1}^{N}k(\mathbf{x}_l, \mathbf{x}_l)
\end{aligned}$$

- In matrix notation, the centered $\boxed{\tilde{\mathbf{K}} = \mathbf{K} - \mathbf{1}_N\mathbf{K} - \mathbf{K}\mathbf{1}_N + \mathbf{1}_N\mathbf{K}\mathbf{1}_N}$
- $\mathbf{1}_N$ is the $N \times N$ matrix with every element $= 1/N$

- Eigen-decomposition is then done for the centered kernel matrix $\tilde{\mathbf{K}}$

Kernel PCA: The Projection

- Suppose $\{\mathbf{a}_1, \ldots, \mathbf{a}_K\}$ are the top K eigenvectors of kernel matrix $\tilde{\mathbf{K}}$

- The K-dimensional KPCA projection $\mathbf{z} = [z_1, \ldots, z_K]$ of a point $\mathbf{x}$:

$$z_i = \phi(\mathbf{x})^\top \mathbf{v}_i$$

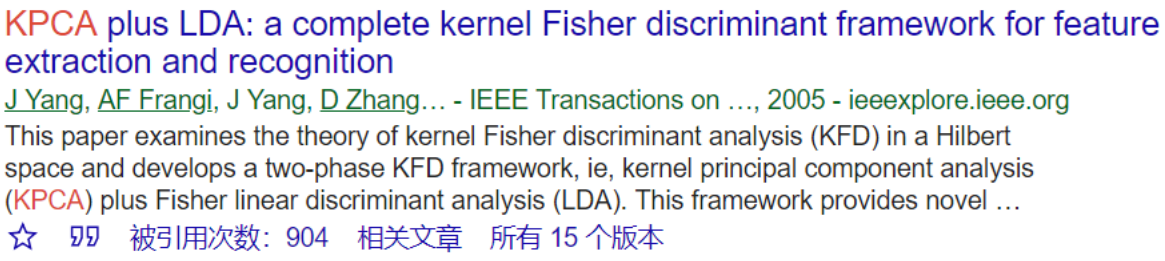
- Recall the definition of $\mathbf{v}_i$

$$\boxed{\mathbf{v}_i = \sum_{n=1}^{N} a_{in} \phi(\mathbf{x}_n)}$$

- Thus

$$\boxed{z_i = \phi(\mathbf{x})^\top \mathbf{v}_i = \sum_{n=1}^{N} a_{in} k(\mathbf{x}, \mathbf{x}_n)}$$

Kernel Subspace Learning



KPCA plus LDA: a complete kernel Fisher discriminant framework for feature extraction and recognition

J Yang, AF Frangi, J Yang, D Zhang… - IEEE Transactions on …, 2005 - ieeexplore.ieee.org

This paper examines the theory of kernel Fisher discriminant analysis (KFD) in a Hilbert space and develops a two-phase KFD framework, ie, kernel principal component analysis (KPCA) plus Fisher linear discriminant analysis (LDA). This framework provides novel …

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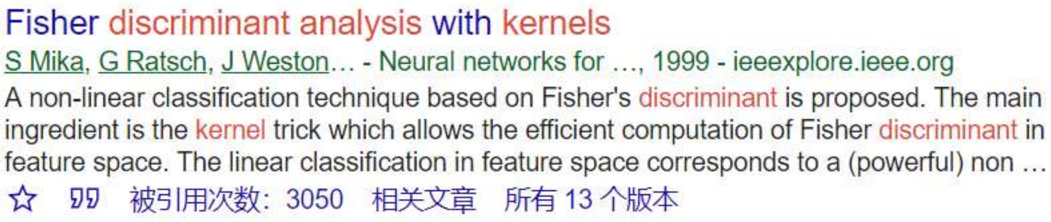
Kernel PCA



Fisher discriminant analysis with kernels

S Mika, G Ratsch, J Weston… - Neural networks for …, 1999 - ieeexplore.ieee.org

A non-linear classification technique based on Fisher's discriminant is proposed. The main ingredient is the kernel trick which allows the efficient computation of Fisher discriminant in feature space. The linear classification in feature space corresponds to a (powerful) non …

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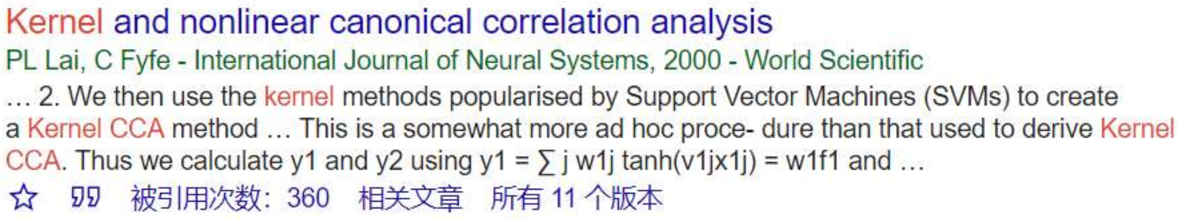
Kernel LDA



Kernel and nonlinear canonical correlation analysis

PL Lai, C Fyfe - International Journal of Neural Systems, 2000 - World Scientific

… 2. We then use the kernel methods popularised by Support Vector Machines (SVMs) to create a Kernel CCA method … This is a somewhat more ad hoc proce- dure than that used to derive Kernel CCA. Thus we calculate y1 and y2 using y1 = ∑ j w1j tanh(v1jx1j) = w1f1 and …

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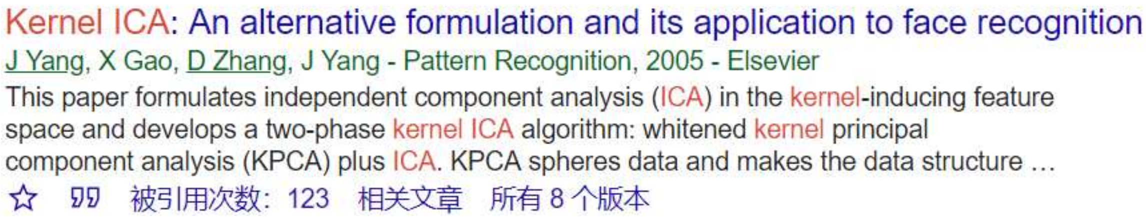
Kernel CCA



Kernel ICA: An alternative formulation and its application to face recognition

J Yang, X Gao, D Zhang, J Yang - Pattern Recognition, 2005 - Elsevier

This paper formulates independent component analysis (ICA) in the kernel-inducing feature space and develops a two-phase kernel ICA algorithm: whitened kernel principal component analysis (KPCA) plus ICA. KPCA spheres data and makes the data structure …

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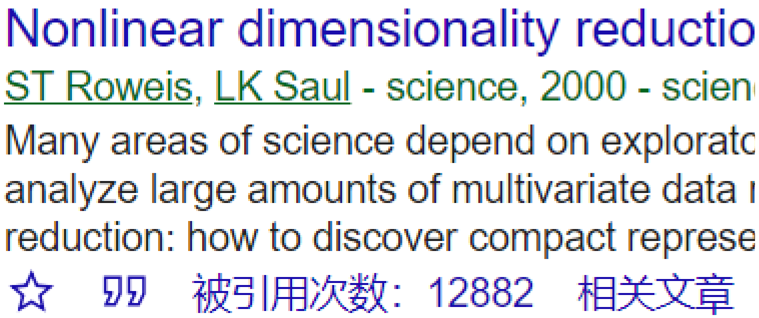
Kernel ICA

Manifold Learning

- **Locally Linear Embedding (LLE)**
- **Isomap**
- Maximum Variance Unfolding
- Laplacian Eigenmaps
- And several others (Hessian LLE, Hessian Eigenmaps, etc.)

Locally Linear Embedding (LLE)



Nonlinear dimensionality reductio

ST Roweis, LK Saul - science, 2000 - scien

Many areas of science depend on exploratc analyze large amounts of multivariate data r reduction: how to discover compact represe

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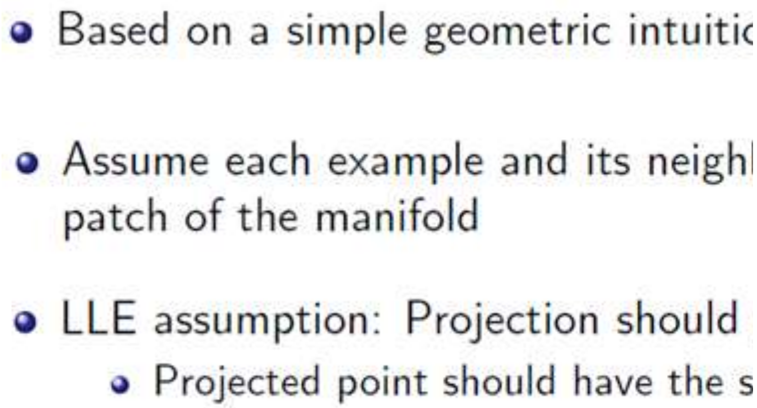
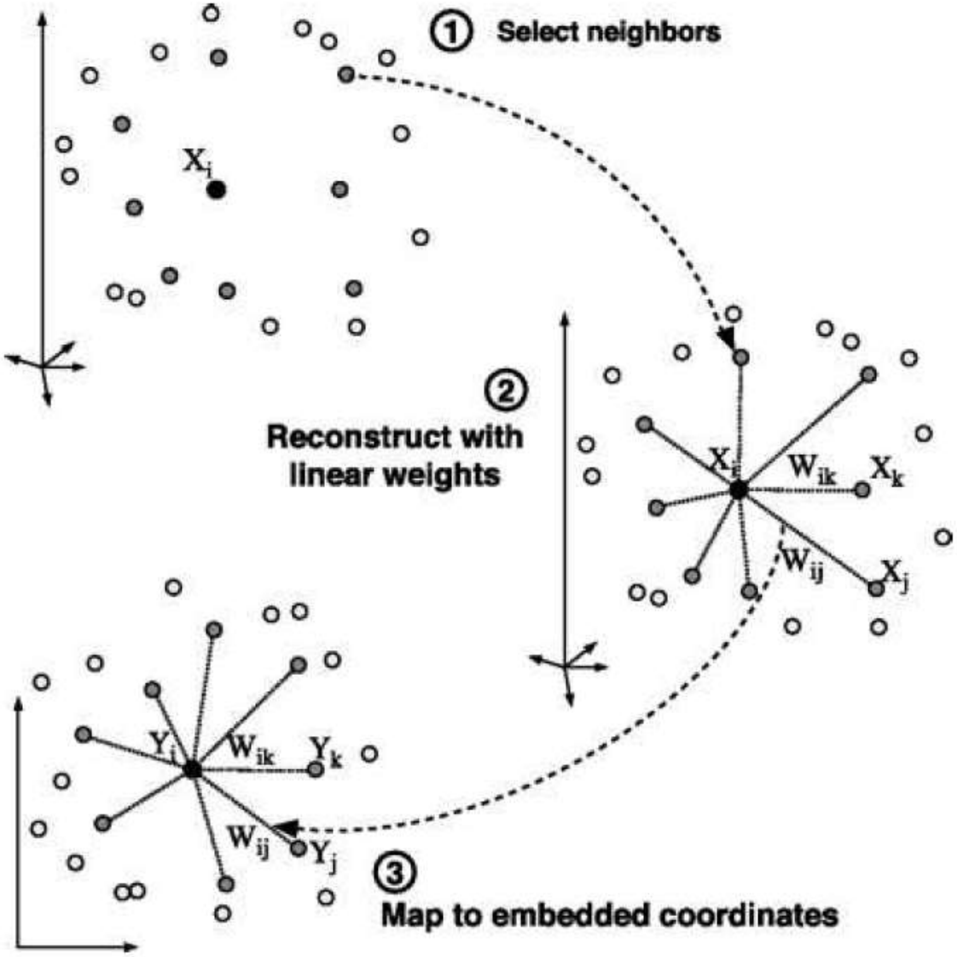


- Based on a simple geometric intuitic
- Assume each example and its neighl patch of the manifold
- LLE assumption: Projection should
  - Projected point should have the s



Locally Linear Embedding (LLE)

- Given D dim. data $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, compute K dim. projections $\{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$

- For each example $\mathbf{x}_i$, find its L nearest neighbors

- Assume $\mathbf{x}_i$ to be a weighted linear combination of the L nearest neighbors

$$\mathbf{x}_i \approx \sum_{j \in \mathcal{N}} W_{ij} \mathbf{x}_j \qquad \text{(so the data is assumed locally linear)}$$

- Find the weights by solving the following least-squares problem:

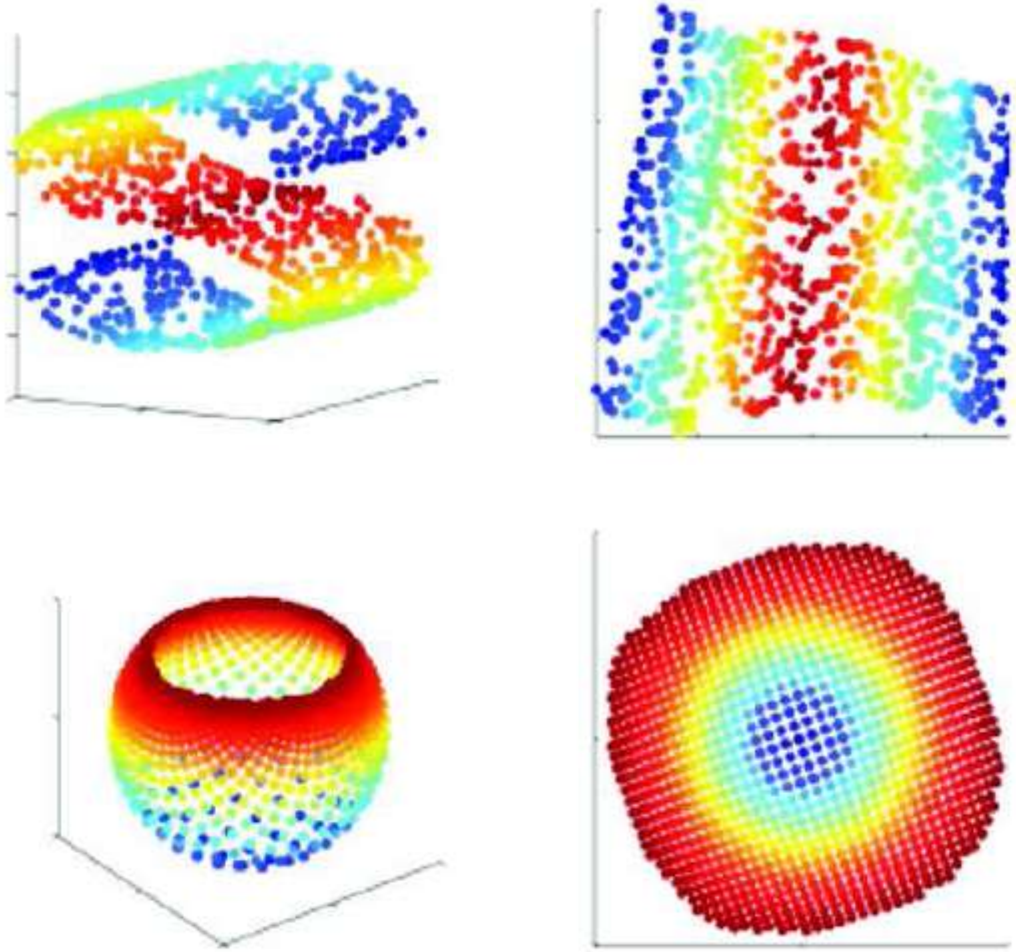
$$\boxed{W = \arg\min_{W} \sum_{i=1}^{N} ||\mathbf{x}_i - \sum_{j \in \mathcal{N}_i} W_{ij} \mathbf{x}_j||^2} \qquad s.t. \forall i \quad \sum_{j} W_{ij} = 1$$

- $\mathcal{N}_i$ are the L nearest neighbors of $\mathbf{x}_i$ (note: should choose $L \geq K + 1$)

- Use W to compute low dim. projections $\mathbf{Z} = \{\mathbf{z}_1, \ldots, \mathbf{z}_N\}$ by solving:

$$\boxed{\mathbf{Z} = \arg\min_{\mathbf{Z}} \sum_{i=1}^{N} ||\mathbf{z}_i - \sum_{j \in \mathcal{N}} W_{ij} \mathbf{z}_j||^2} \qquad s.t. \forall i \quad \sum_{i=1}^{N} \mathbf{z}_i = 0, \quad \frac{1}{N} \mathbf{Z}\mathbf{Z}^\top = \mathbf{I}$$

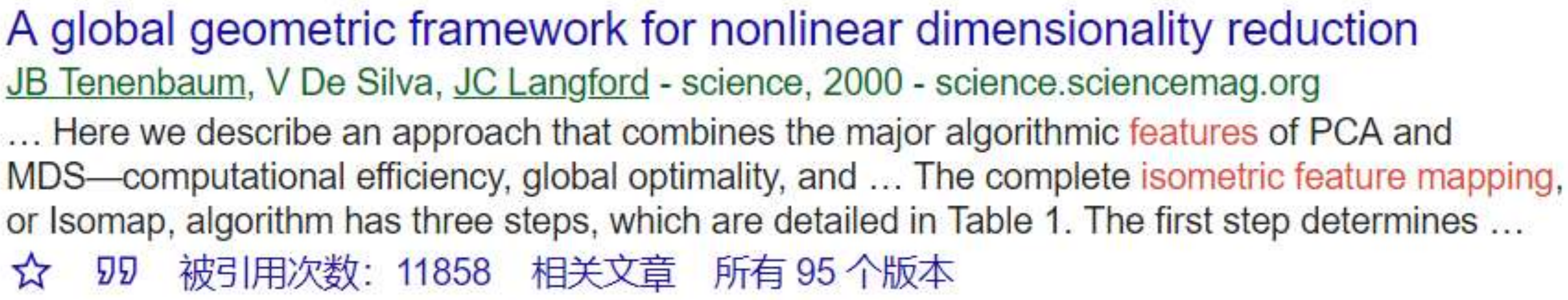
LLE: Examples



✓ *Nonlinear dimension reduction*

✓ *Out-of-sample problem*

Isometric Feature Mapping (ISOMAP)



A global geometric framework for nonlinear dimensionality reduction

JB Tenenbaum, V De Silva, JC Langford - science, 2000 - science.sciencemag.org

… Here we describe an approach that combines the major algorithmic features of PCA and MDS—computational efficiency, global optimality, and … The complete isometric feature mapping, or Isomap, algorithm has three steps, which are detailed in Table 1. The first step determines …

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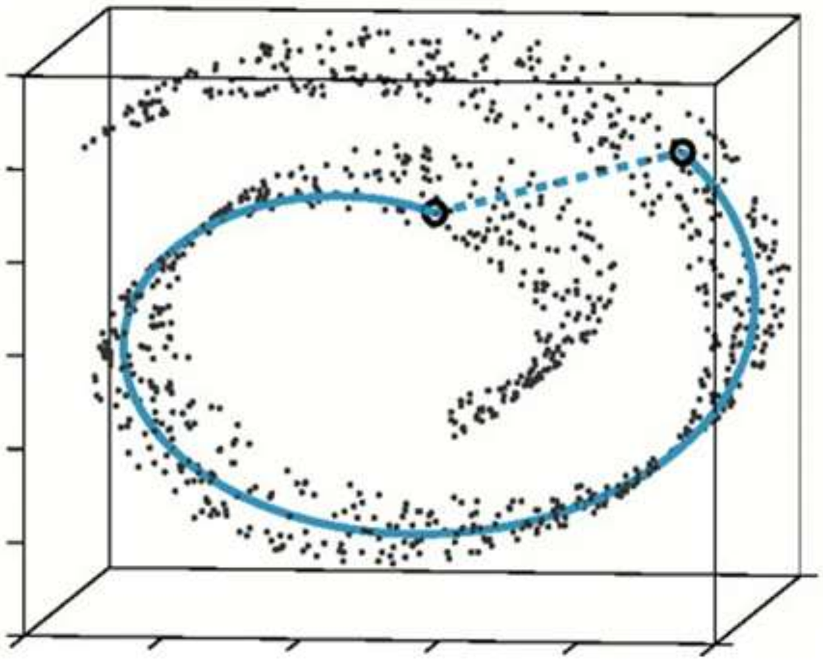
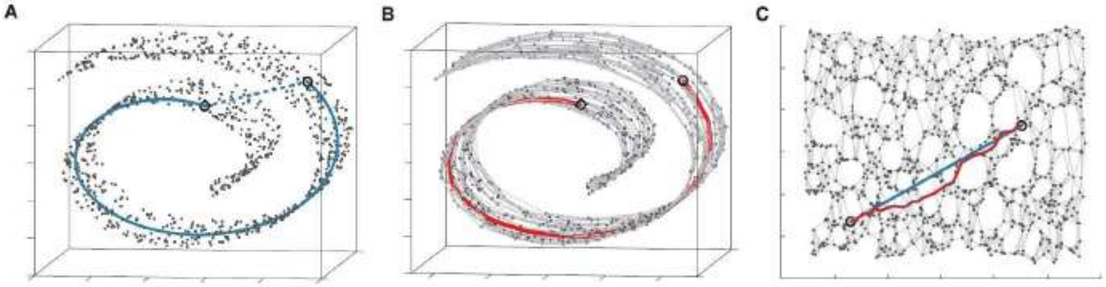


Isometric Feature Mapping (ISOMAP)

A graph based algorithm based on constructing a matrix of geodesic distances

- Identify the L nearest neighbors for each data point (just like LLE)
- Connect each point to all its neighbors (an edge for each neighbor)
- Assign weight to each edge based on the Euclidean distance
- Estimate the geodesic distance d_{ij} between any two data points i and j
  - Approximated by the sum of arc lengths along the shortest path between i and j in the graph (can be computed using Djikstras algorithm)
- Construct the $N \times N$ distance matrix $\mathbf{D} = \{d_{ij}^2\}$



Isometric Feature Mapping (ISOMAP)

- Use the distance matrix **D** to construct the Gram Matrix

$$\boxed{\mathbf{G} = -\frac{1}{2}\mathbf{HDH}}$$

where **G** is $N \times N$ and

$$\mathbf{H} = \mathbf{I} - \frac{1}{N}\mathbf{1}\mathbf{1}^\top$$

I is $N \times N$ identity matrix, **1** is $N \times 1$ vector of 1s

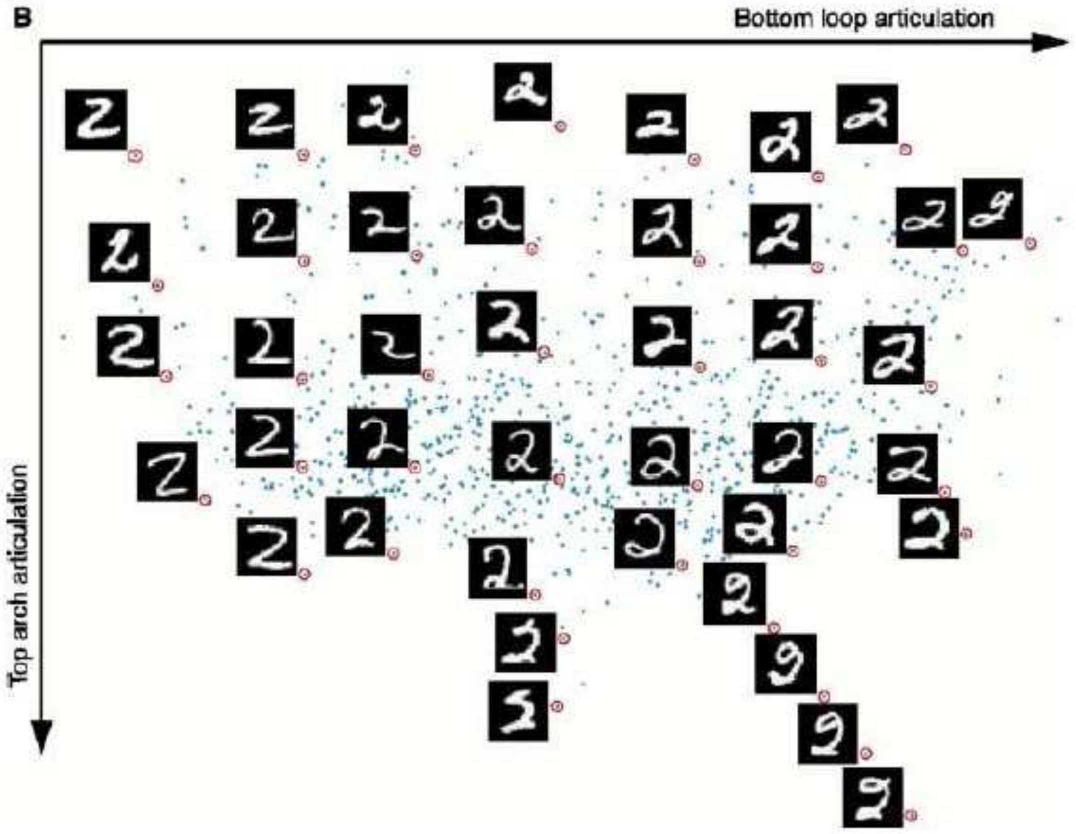
- Do an eigen decomposition of **G**
- Let the eigenvectors be $\{\mathbf{v}_1, \ldots, \mathbf{v}_N\}$ with eigenvalues $\{\lambda_1, \ldots, \lambda_N\}$
  - Each eigenvector $\mathbf{v}_i$ is N-dimensional: $\mathbf{v}_i = [v_{1i}, v_{2i}, \ldots, v_{Ni}]$
- Take the top K eigenvalue/eigenvectors
- The K dimensional embedding $\mathbf{z}_i = [z_{i1}, z_{i2}, \ldots, z_{iK}]$ of a point $\mathbf{x}_i$:

$$\boxed{z_{ik} = \sqrt{\lambda_k}\, v_{ki}}$$

Out-of-sample problem

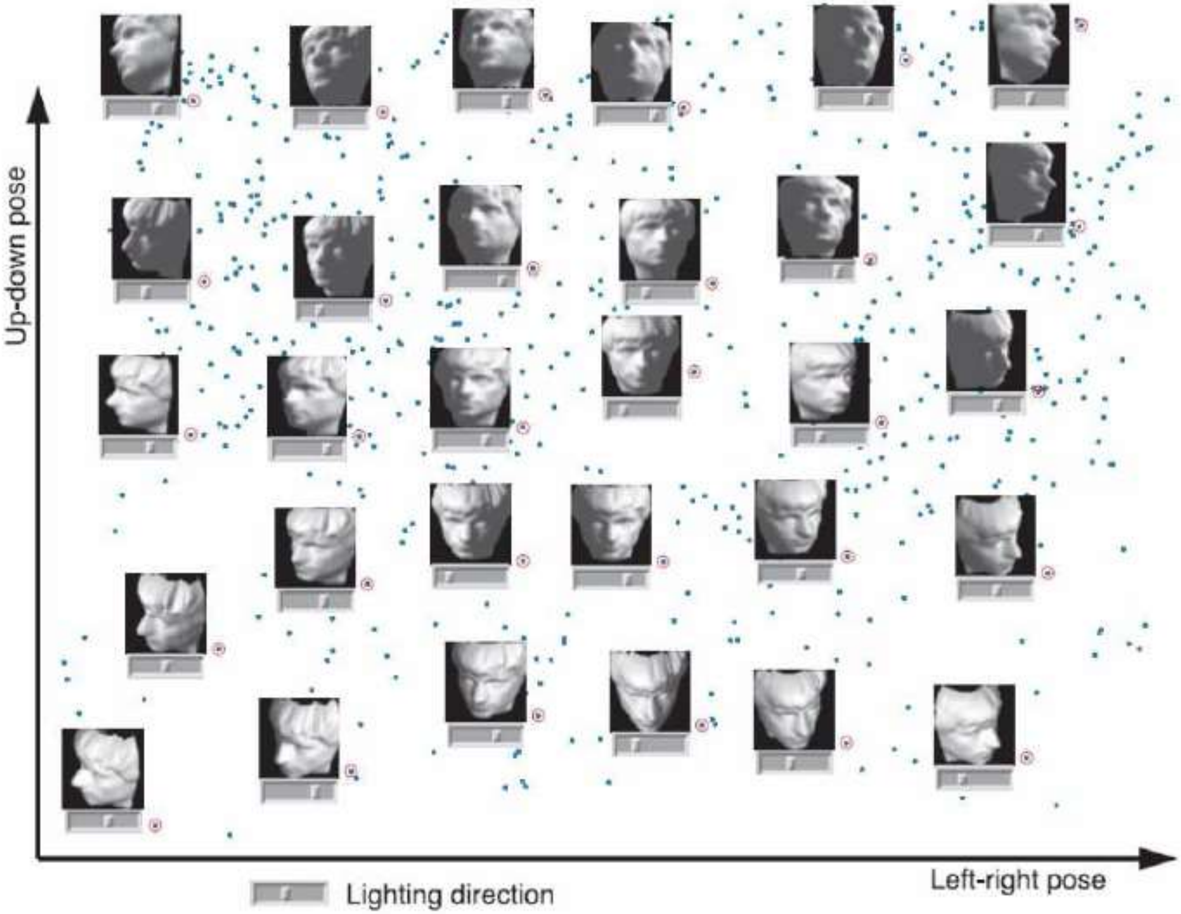
ISOMAP: Example

Digit images projected down to 2 dimensions



ISOMAP: Example

Face images with varying poses



LPP: Locality Preserving Projection

- **Out-of-sample problem:**
  - LLE and ISOMAP are computationally intensive
  - **The embedding is only defined on actual data points**.
- Solution:
  - LPP is a **linear method that approximates nonlinear methods** (specifically, the Laplacian Eigenmap.)
  - LPP is a linear approximation to nonlinear methods, which takes locality into account

$$S_{ij} = \begin{cases} \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/t), & \|\mathbf{x}_i - \mathbf{x}_j\|^2 < \varepsilon \\ 0 & \text{otherwise} \end{cases}$$

$$\min \sum_{ij} (y_i - y_j)^2 S_{ij}$$

$$S_{ij} = \begin{cases} \exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/t), & \text{if } \mathbf{x}_i \text{ is among } k \text{ nearest neighbors of } \mathbf{x}_j \\ & \text{or } \mathbf{x}_j \text{ is among } k \text{ nearest neighbors of } \mathbf{x}_i \\ 0 & \text{otherwise,} \end{cases}$$

LPP: Locality Preserving Projection

$$\frac{1}{2}\sum_{ij}(y_i - y_j)^2 S_{ij}$$

$$= \frac{1}{2}\sum_{ij}(\boxed{\mathbf{w}^T\mathbf{x}_i} - \boxed{\mathbf{w}^T\mathbf{x}_j})^2 S_{ij}$$

$$= \sum_{ij}\mathbf{w}^T\mathbf{x}_i S_{ij}\mathbf{x}_i^T\mathbf{w} - \sum_{ij}\mathbf{w}^T\mathbf{x}_i S_{ij}\mathbf{x}_j^T\mathbf{w}$$

$$= \sum_i \mathbf{w}^T\mathbf{x}_i D_{ii}\mathbf{x}_i^T\mathbf{w} - \mathbf{w}^T XSX^T\mathbf{w}$$

$$= \mathbf{w}^T XDX^T\mathbf{w} - \mathbf{w}^T XSX^T\mathbf{w}$$

$$= \mathbf{w}^T X(D-S)X^T\mathbf{w}$$

$$= \boxed{\mathbf{w}^T XLX^T\mathbf{w}}$$

The matrix D provides a natural measure on data points → a measure importance of the ith image

So a constraint can be imposed

$$\mathbf{y}^T D\mathbf{y} = 1$$

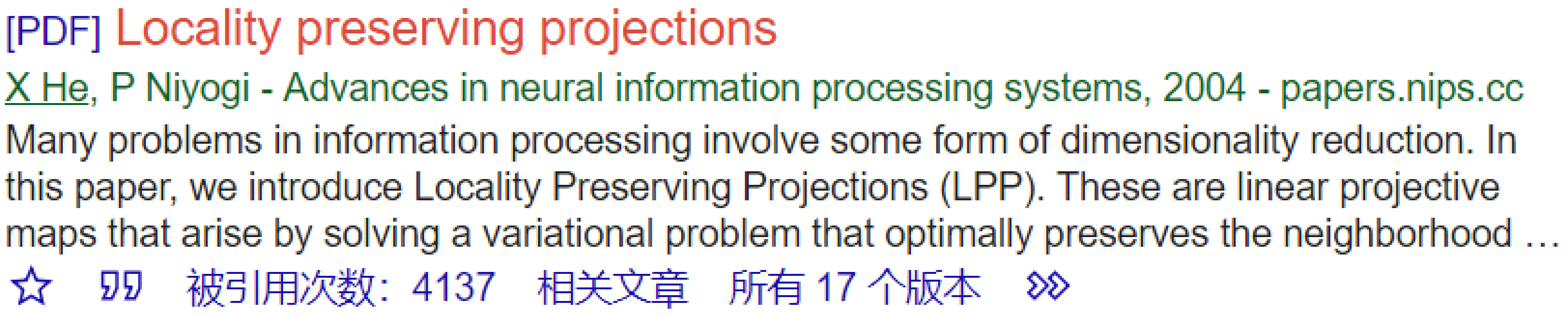
$$\Rightarrow \mathbf{w}^T XDX^T\mathbf{w} = 1$$

Thus the optimization problem is:

$$\underset{\substack{\mathbf{w} \\ \mathbf{w}^T XDX^T\mathbf{w}=1}}{\arg\min} \quad \mathbf{w}^T XLX^T\mathbf{w}$$

- The solution is the Generalized Eigenvalue problem.
- The solution is also called Laplacianfaces.

Face Recognition



[PDF] Locality preserving projections

X He, P Niyogi - Advances in neural information processing systems, 2004 - papers.nips.cc

Many problems in information processing involve some form of dimensionality reduction. In this paper, we introduce Locality Preserving Projections (LPP). These are linear projective maps that arise by solving a variational problem that optimally preserves the neighborhood …

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Eigenface (PCA) – preserves global structure of image space (unsupervised)

Fischerface (LDA) – preserves discriminating information (supervised)

Laplacianface (LPP) – preserves local structure of image space (unsupervised)

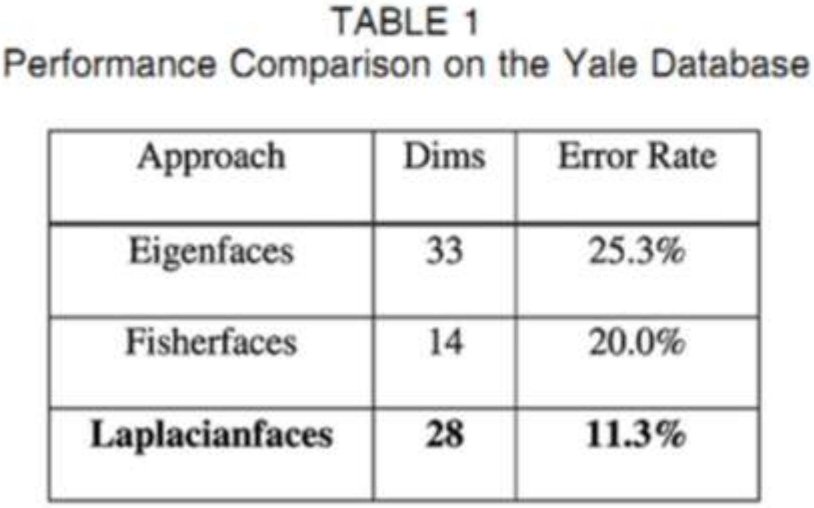


TABLE 1
Performance Comparison on the Yale Database

Approach	Dims	Error Rate
Eigenfaces	33	25.3%
Fisherfaces	14	20.0%
Laplacianfaces	**28**	**11.3%**

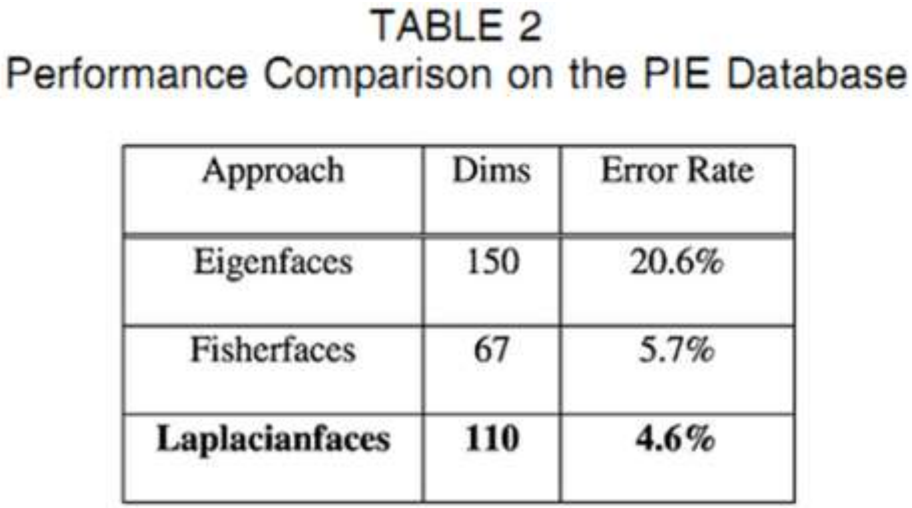


TABLE 2
Performance Comparison on the PIE Database

Approach	Dims	Error Rate
Eigenfaces	150	20.6%
Fisherfaces	67	5.7%
Laplacianfaces	**110**	**4.6%**

特征选择
Feature Selection

降维 vs 特征选择

- Dimensionality reduction
  - All original features are used
  - The transformed features are linear combinations of the original features
- Feature selection
  - Only a subset of the original features are selected

- Continuous versus discrete

Feature Selection

- Definitions of subset optimality

- Perspectives of feature selection
  - Subset search and feature ranking
  - Feature/subset evaluation measures
  - Models: filter vs. wrapper
  - Results validation and evaluation

An Example for Optimal Subset

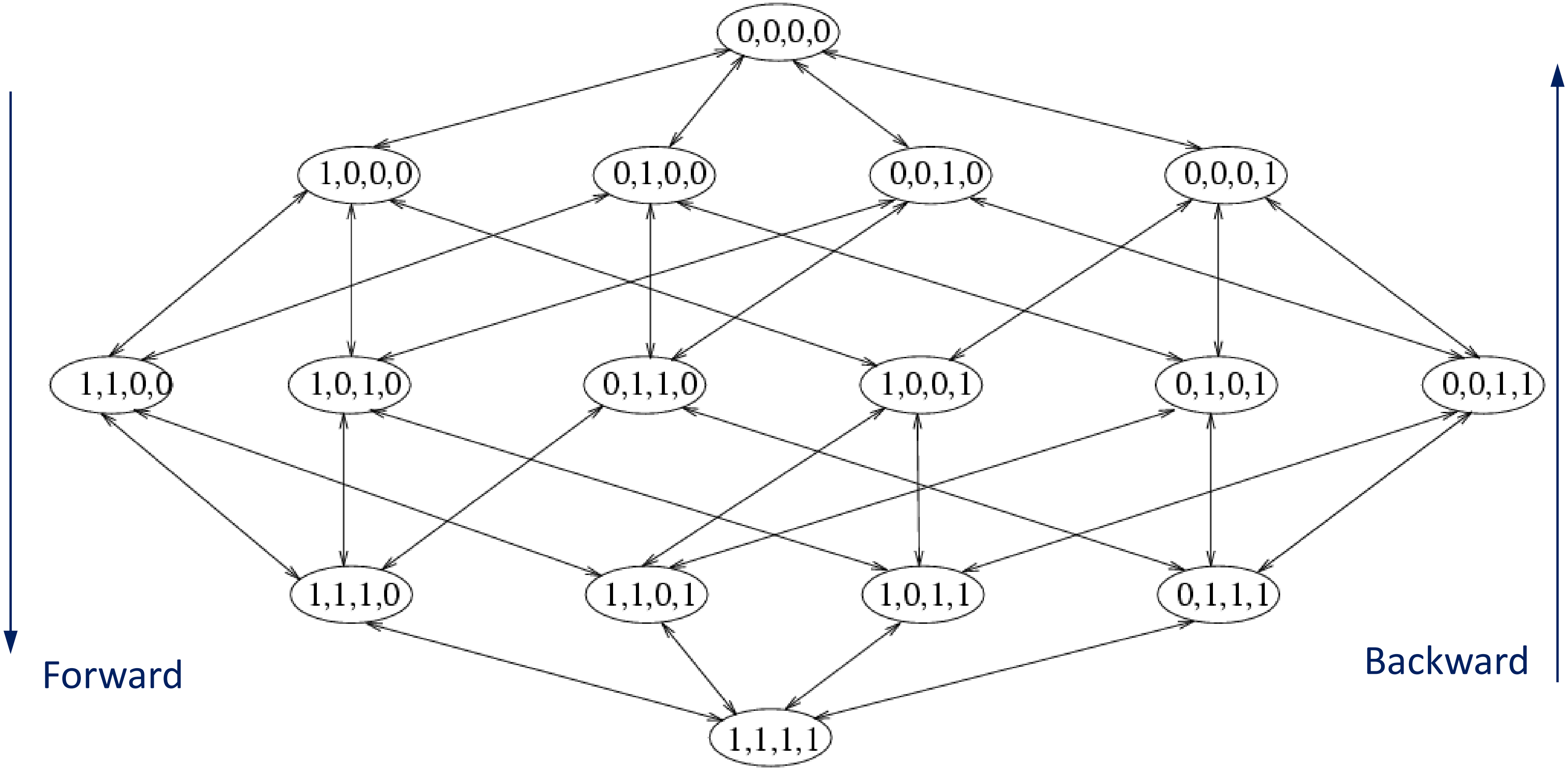
F_1	F_2	F_3	F_4	F_5	C
0	0	1	0	1	0
0	1	0	0	1	1
1	0	1	0	1	1
1	1	0	0	1	1
0	0	1	1	0	0
0	1	0	1	0	1
1	0	1	1	0	1
1	1	0	1	0	1

- Data set (whole set)
  - Five Boolean features
  - $C = F_1 \vee F_2$
  - $F_3 = \neg F_2$, $F_5 = \neg F_4$
  - Optimal subset:

    $\{F_1, F_2\}$ or $\{F_1, F_3\}$
- Combinatorial nature of searching for an optimal subset

Subset Search Problem

- An example of search space (*Kohavi & John 1997*)



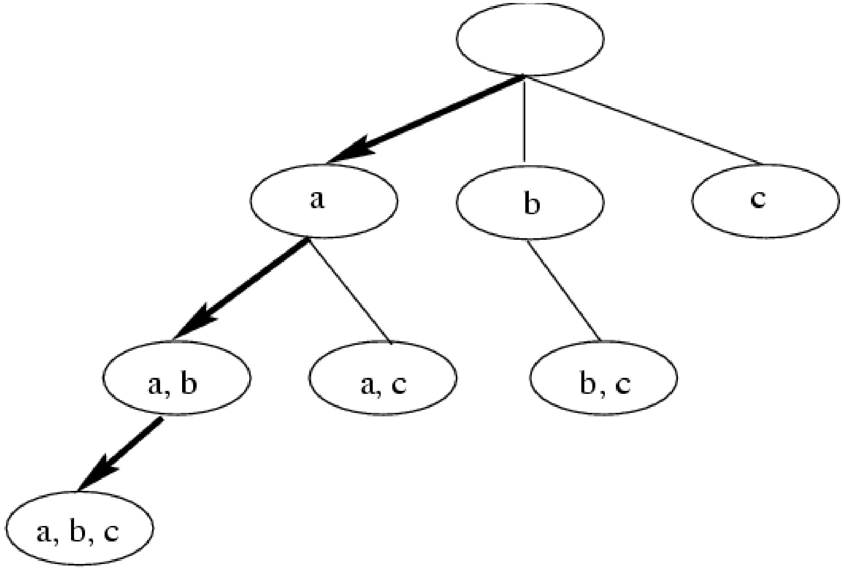
Forward

Backward

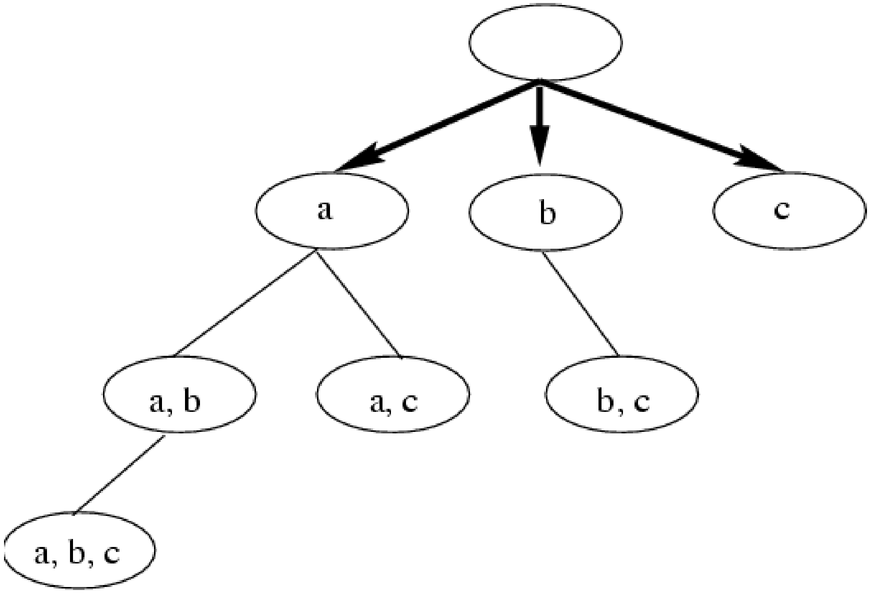
Different Aspects of Search

- Search starting points
  - Empty set
  - Full set
  - Random point
- Search directions
  - Sequential forward selection
  - Sequential backward elimination
  - Bidirectional generation
  - Random generation
- Search Strategies
  - Exhaustive/complete search
  - Heuristic search
  - Nondeterministic search

Illustration of Search Strategies



Depth-first search

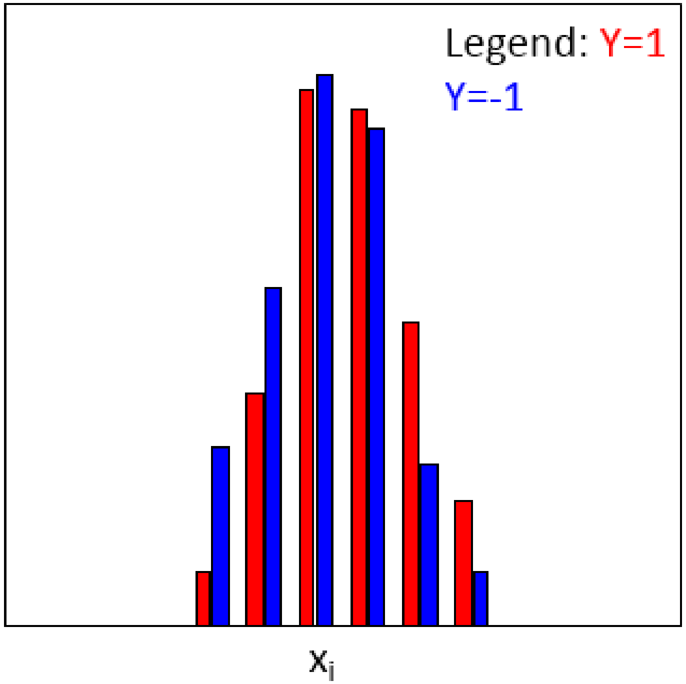


Breadth-first search

Feature Ranking

- Weighting and ranking individual features
- Selecting top-ranked ones for feature selection
- Advantages
  - Efficient: $O(N)$ in terms of dimensionality N
  - Easy to implement
- Disadvantages
  - Hard to determine the threshold
  - Unable to consider correlation between features

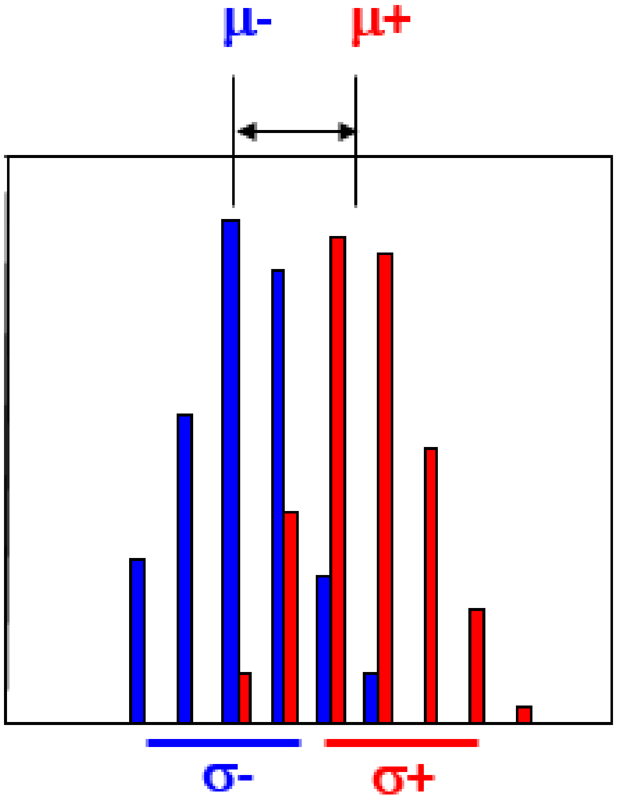
Individual Feature Measures



$P(X_i, Y) = P(X_i)\ P(Y)$

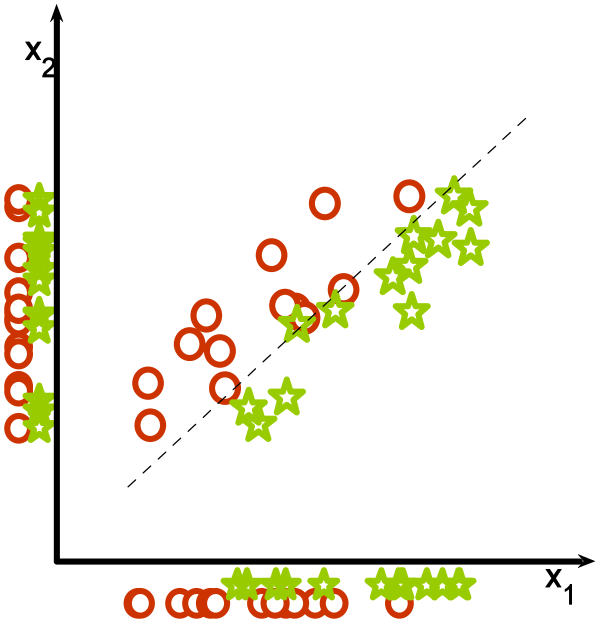
$P(X_i \mid Y) = P(X_i)$

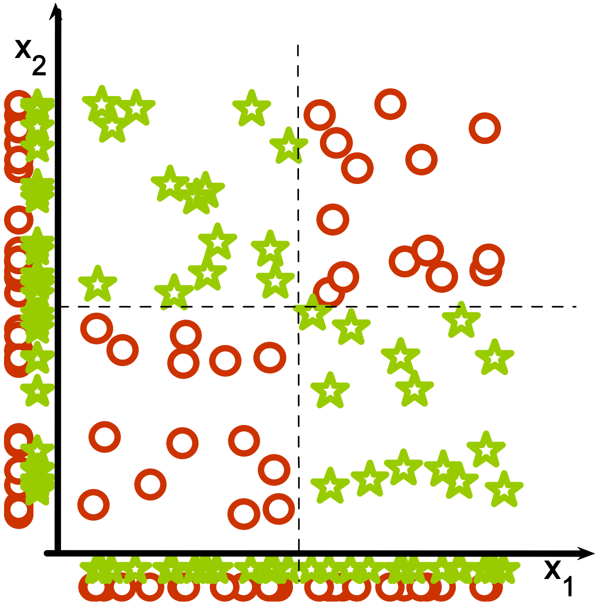
$P(X_i \mid Y=1) = P(X_i \mid Y=-1)$



$$FDR = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2}$$

Univariate Selection May Fail

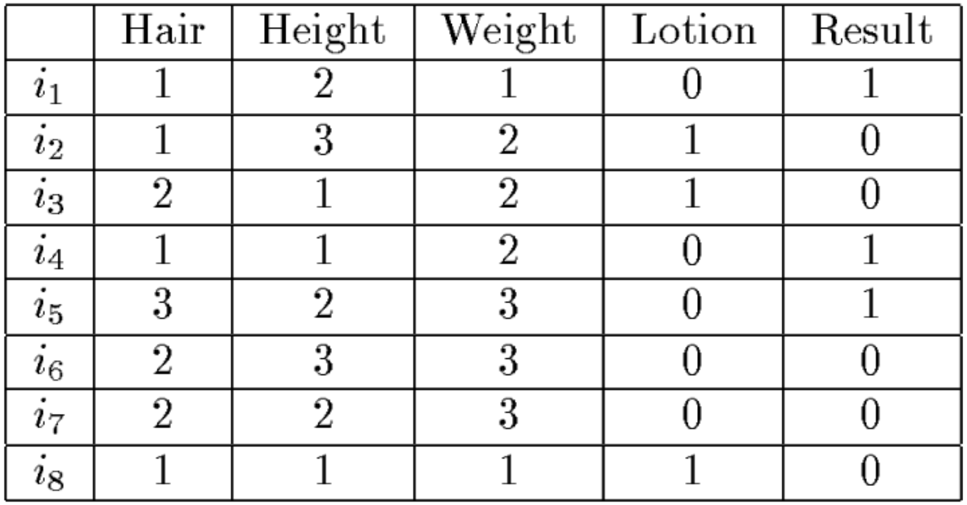




Evaluation Measures

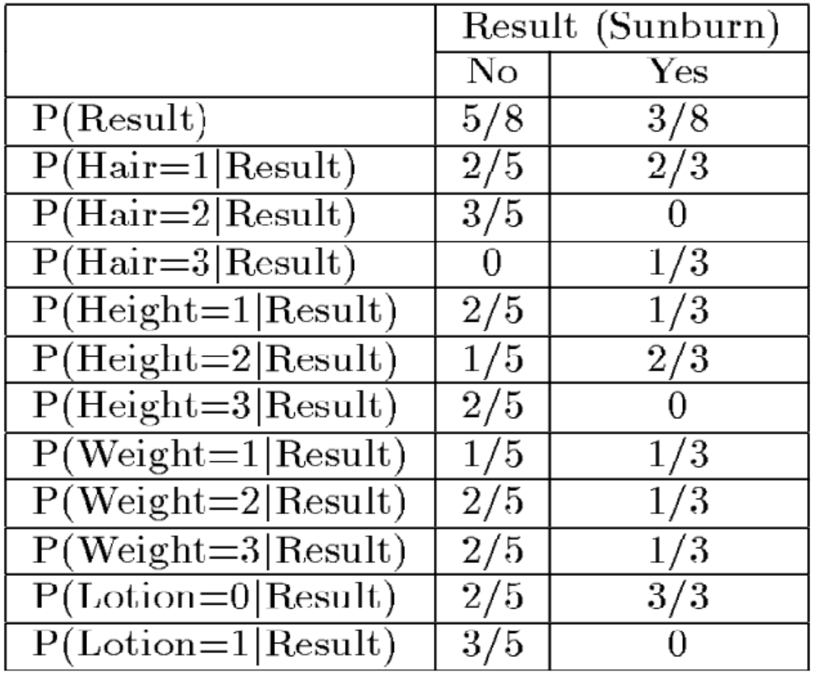
- The goodness of a feature/feature subset is dependent on measures
- Various measures
  - Information measures (Yu & Liu 2004, Jebara & Jaakkola 2000)
  - Distance measures (Robnik & Kononenko 03, Pudil & Novovicov 98)
  - Dependence measures (Hall 2000, Modrzejewski 1993)
  - Consistency measures (Almuallim & Dietterich 94, Dash & Liu 03)
  - Accuracy measures (Dash & Liu 2000, Kohavi&John 1997)

Illustrative Data set



	Hair	Height	Weight	Lotion	Result
i_1	1	2	1	0	1
i_2	1	3	2	1	0
i_3	2	1	2	1	0
i_4	1	1	2	0	1
i_5	3	2	3	0	1
i_6	2	3	3	0	0
i_7	2	2	3	0	0
i_8	1	1	1	1	0

Sunburn data



	Result (Sunburn)	
	No	Yes
P(Result)	5/8	3/8
P(Hair=1|Result)	2/5	2/3
P(Hair=2|Result)	3/5	0
P(Hair=3|Result)	0	1/3
P(Height=1|Result)	2/5	1/3
P(Height=2|Result)	1/5	2/3
P(Height=3|Result)	2/5	0
P(Weight=1|Result)	1/5	1/3
P(Weight=2|Result)	2/5	1/3
P(Weight=3|Result)	2/5	1/3
P(Lotion=0|Result)	2/5	3/3
P(Lotion=1|Result)	3/5	0

Priors and class conditional probabilities

Information Measures

- Entropy of variable X

$$H(X) = -\sum_i P(x_i) \log_2(P(x_i))$$

- Entropy of X after observing Y

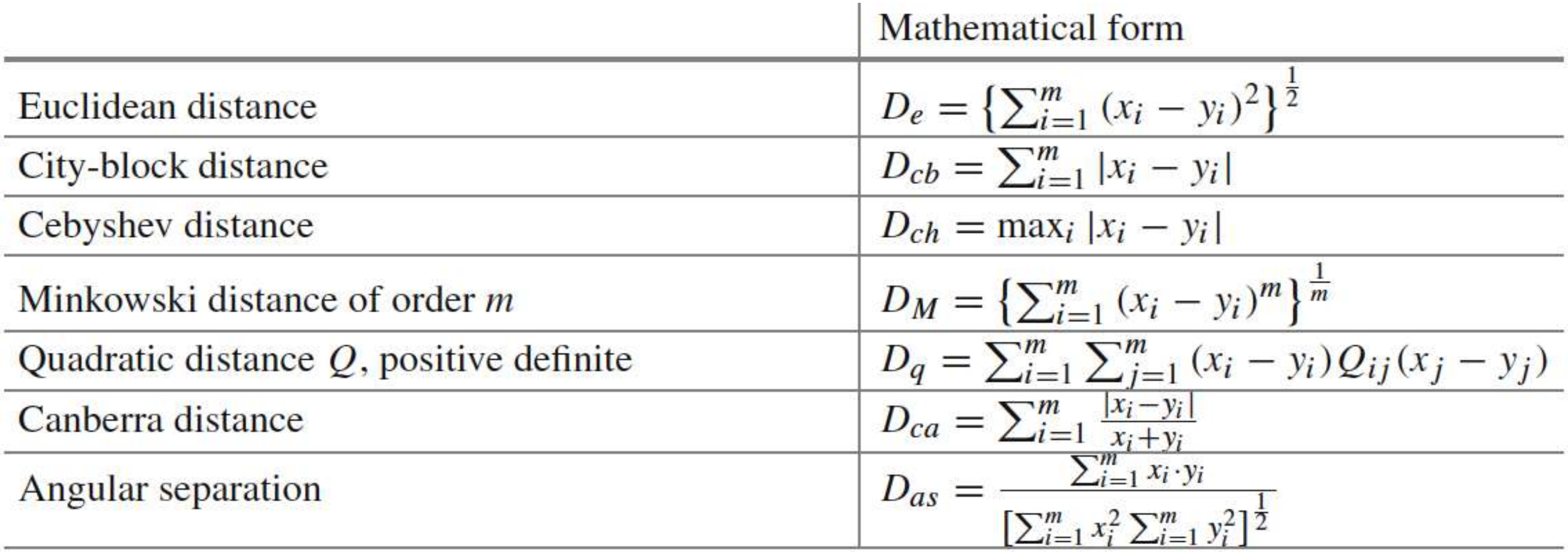
$$H(X|Y) = -\sum_j P(y_j) \sum_i P(x_i|y_j) \log_2(P(x_i|y_j))$$

- Information Gain

$$IG(X|Y) = H(X) - H(X|Y)$$

Distance Measures

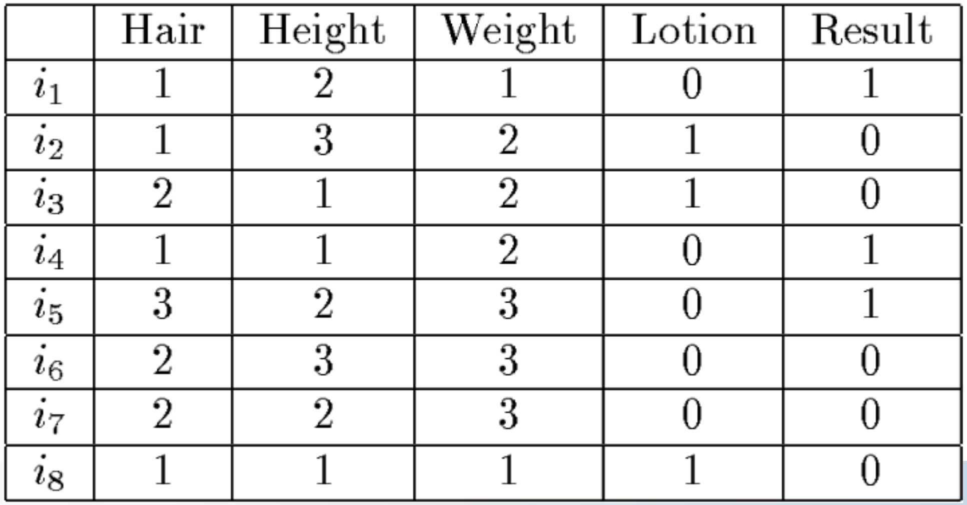
- Distance Measures.
  - Measures of separability, discrimination or divergence measures. The most typical is derived from distance between the class conditional density functions.



	Mathematical form
Euclidean distance	$D_e = \{\sum_{i=1}^{m} (x_i - y_i)^2\}^{\frac{1}{2}}$
City-block distance	$D_{cb} = \sum_{i=1}^{m} \lvert x_i - y_i \rvert$
Cebyshev distance	$D_{ch} = \max_i \lvert x_i - y_i \rvert$
Minkowski distance of order *m*	$D_M = \{\sum_{i=1}^{m} (x_i - y_i)^m\}^{\frac{1}{m}}$
Quadratic distance *Q*, positive definite	$D_q = \sum_{i=1}^{m} \sum_{j=1}^{m} (x_i - y_i) Q_{ij} (x_j - y_j)$
Canberra distance	$D_{ca} = \sum_{i=1}^{m} \frac{\lvert x_i - y_i \rvert}{x_i + y_i}$
Angular separation	$D_{as} = \frac{\sum_{i=1}^{m} x_i \cdot y_i}{[\sum_{i=1}^{m} x_i^2 \sum_{i=1}^{m} y_i^2]^{\frac{1}{2}}}$

Consistency Measures

- Consistency measures
  - Trying to find a minimum number of features that separate classes as consistently as the full set can
  - They aim to achieve **P(C|FullSet) = P(C|SubSet)**.
  - An inconsistency is defined as two instances having the same feature values but different classes
    - E.g., one inconsistency is found between instances i4 and i8 if we just look at the first two columns of the data table



	Hair	Height	Weight	Lotion	Result
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i_3	2	1	2	1	0
i_4	1	1	2	0	1
i_5	3	2	3	0	1
i_6	2	3	3	0	0
i_7	2	2	3	0	0
i_8	1	1	1	1	0

Dependence Measures

– Dependence Measures.

- known as measures of association or correlation.
- Its main goal is to quantify how strongly two variables are correlated or present some association with each other, in such way that knowing the value of one of them, we can derive the value for the other.
- *Pearson correlation* coefficient:

$$\rho(X, Y) = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\left[\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2\right]^{\frac{1}{2}}}$$

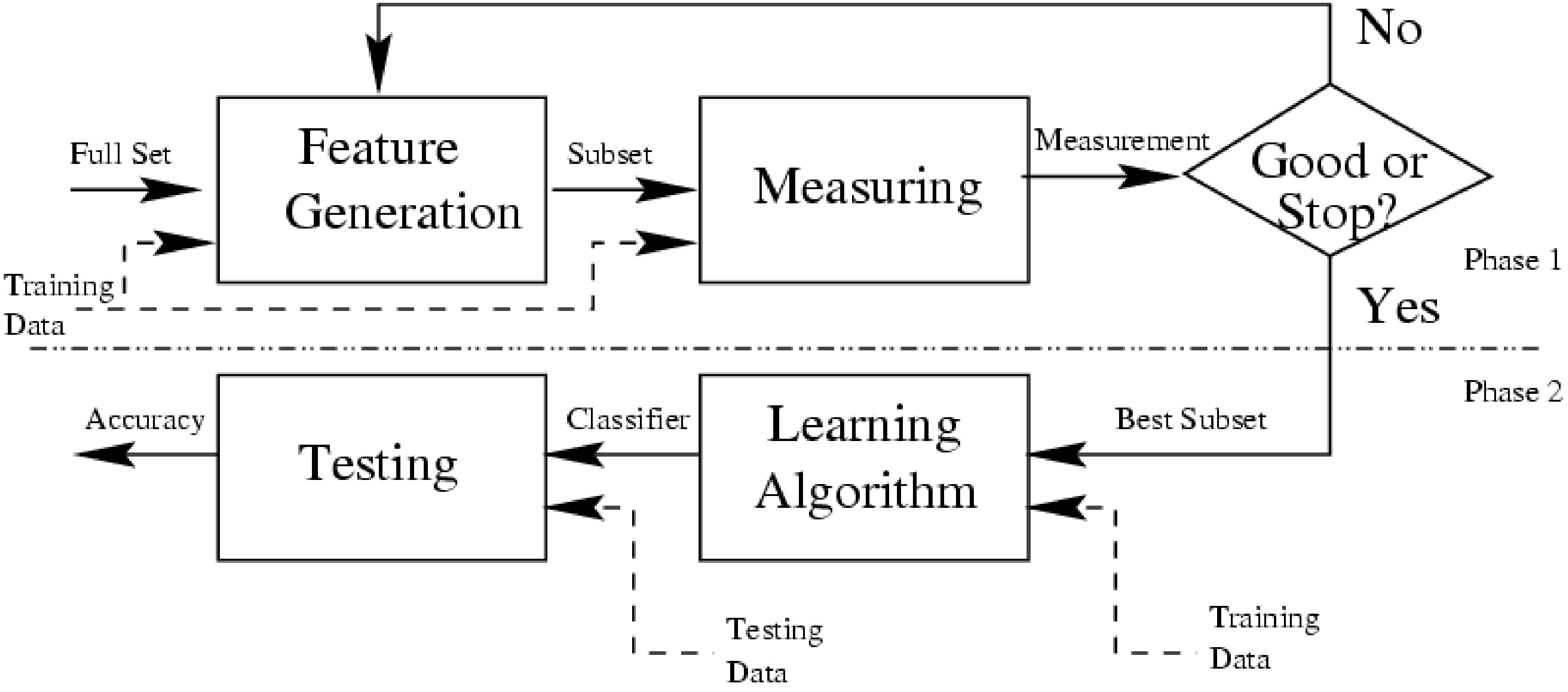
Accuracy Measures

- Using classification accuracy of a classifier as an evaluation measure
- Factors constraining the choice of measures
  - Classifier being used
  - The speed of building the classifier
- Compared with previous measures
  - Directly aimed to improve accuracy
  - Biased toward the classifier being used
  - More time consuming

Models of Feature Selection

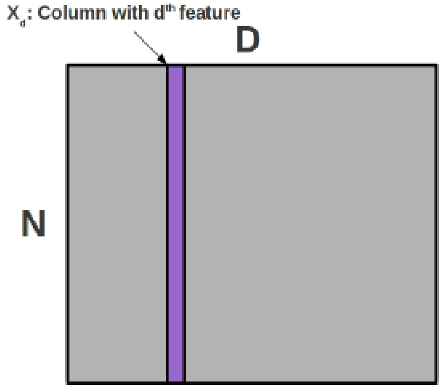
- Filter model
  - Separating feature selection from classifier learning
  - Relying on general characteristics of data (*information, distance*, *dependence*, *consistency*)
  - No bias toward any learning algorithm, fast
- Wrapper model
  - Relying on a predetermined classification algorithm
  - Using predictive accuracy as goodness measure
  - High accuracy, computationally expensive
- Embedded model
  - Feature selected during learning process

Filter Model



Filter Feature Selection

- Uses heuristics but is much faster than wrapper methods



- **Correlation Critera:** Rank features in order of their correlation with the labels

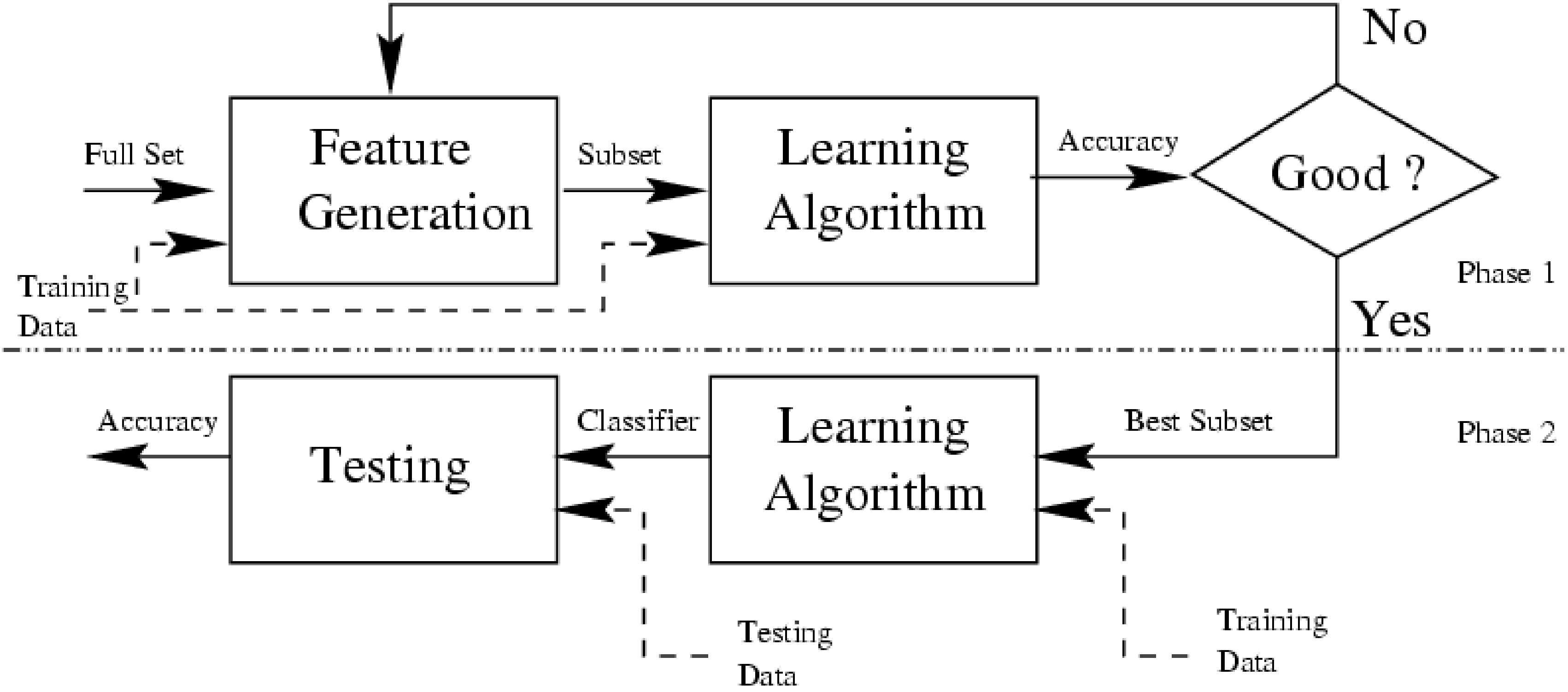
$$R(X_d, Y) = \frac{cov(X_d, Y)}{\sqrt{var(X_d)var(Y)}}$$

- **Mutual Information Criteria:**

$$MI(X_d, Y) = \sum_{X_d \in \{0,1\}} \sum_{Y \in \{-1,+1\}} P(X_d, Y) \frac{\log P(X_d, Y)}{P(X_d)P(Y)}$$

  - High mutual information mean high relevance of that feature

Wrapper Model



Wrapper Feature Selection

- **Forward Search**
  - Let $\mathcal{F} = \{\}$
  - While not selected desired number of features
  - For each unused feature f:
    - Estimate model's error on feature set $\mathcal{F} \bigcup f$ (using cross-validation)
  - Add f with lowest error to $\mathcal{F}$

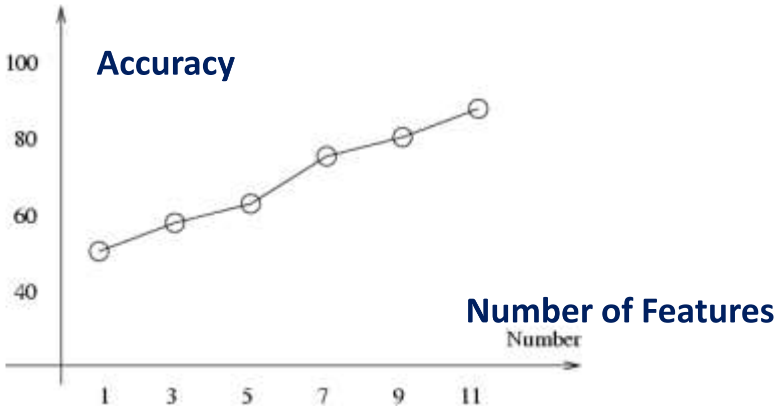
- **Backward Search**
  - Let $\mathcal{F} = \{\text{all features}\}$
  - While not reduced to desired number of features
  - For each feature $f \in \mathcal{F}$:
    - Estimate model's error on feature set $\mathcal{F} \backslash f$ (using cross-validation)
  - Remove f with lowest error from $\mathcal{F}$

How to Validate Selection Results

- Direct evaluation (if we know *a priori* …)
  - Often suitable for artificial data sets
  - Based on prior knowledge about data

- Indirect evaluation (if we don't know …)
  - Often suitable for real-world data sets
  - Based on
    - number of features selected
    - performance on selected features (e.g., predictive accuracy, goodness of resulting clusters)
    - interpretability, speed

Methods for Result Evaluation



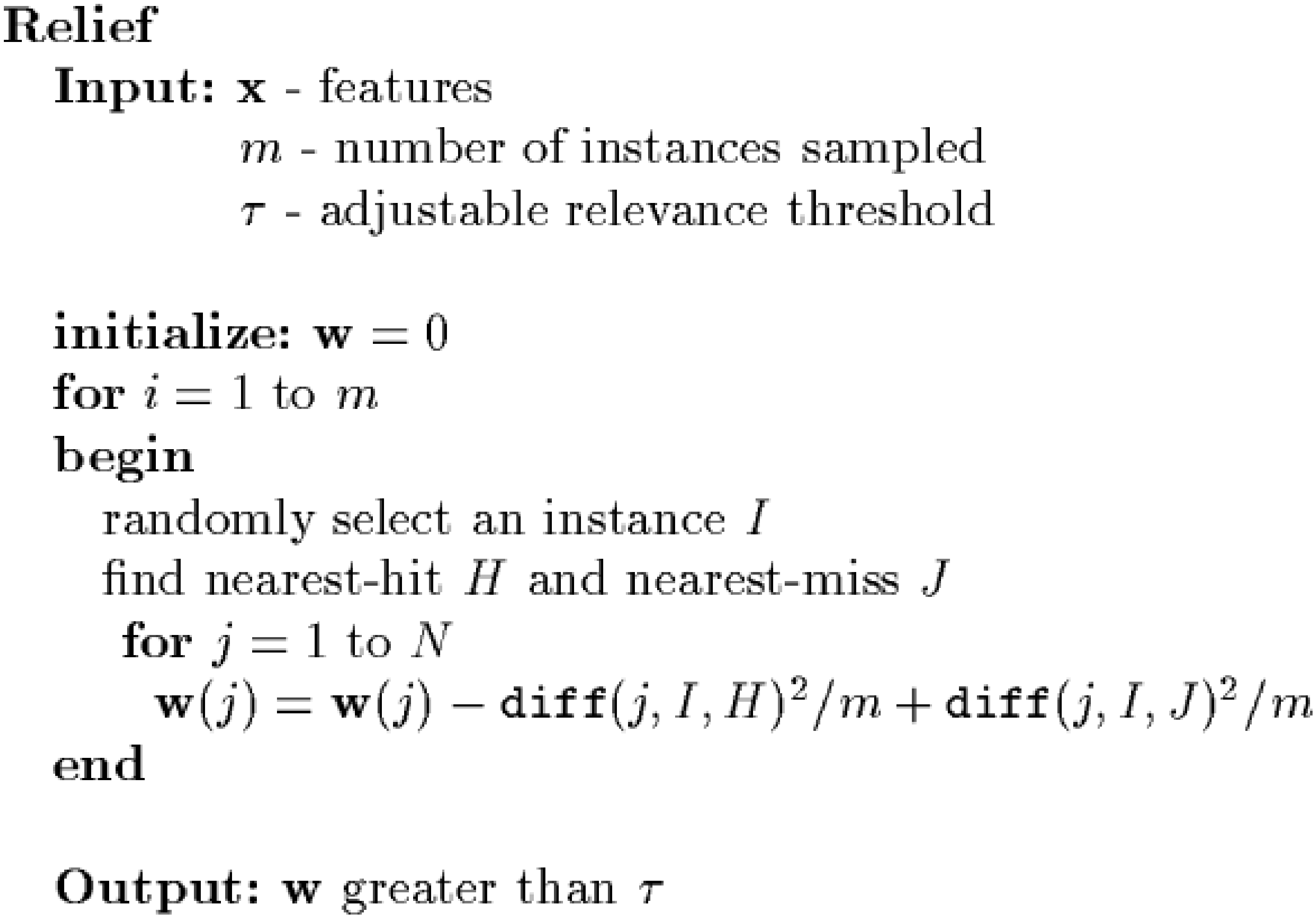
- Learning curves
  - For results in the form of a ranked list of features
- Before-and-after comparison
  - For results in the form of a minimum subset
- Comparison using different classifiers
  - To avoid learning bias of a particular classifier
- Repeating experimental results
  - For non-deterministic results

Representative Algorithms

- Filter algorithms
  - Feature ranking algorithms
    - Example: Relief (*Kira & Rendell 1992*)
  - Subset search algorithms
    - Example: consistency-based algorithms
      - Focus (*Almuallim & Dietterich, 1994*)

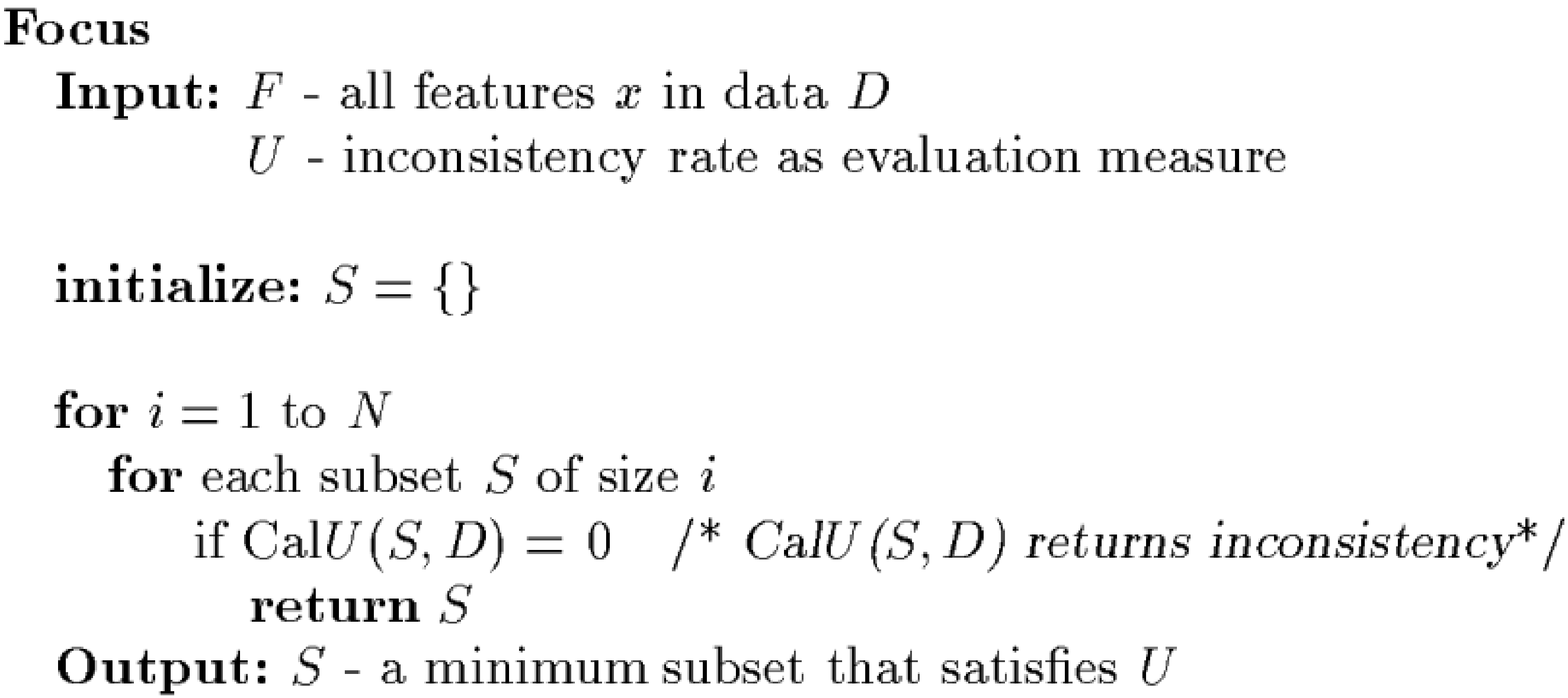
- Wrapper algorithms
  - Feature ranking algorithms
    - Example: SVM
  - Subset search algorithms
    - Example: RFE

Relief Algorithm



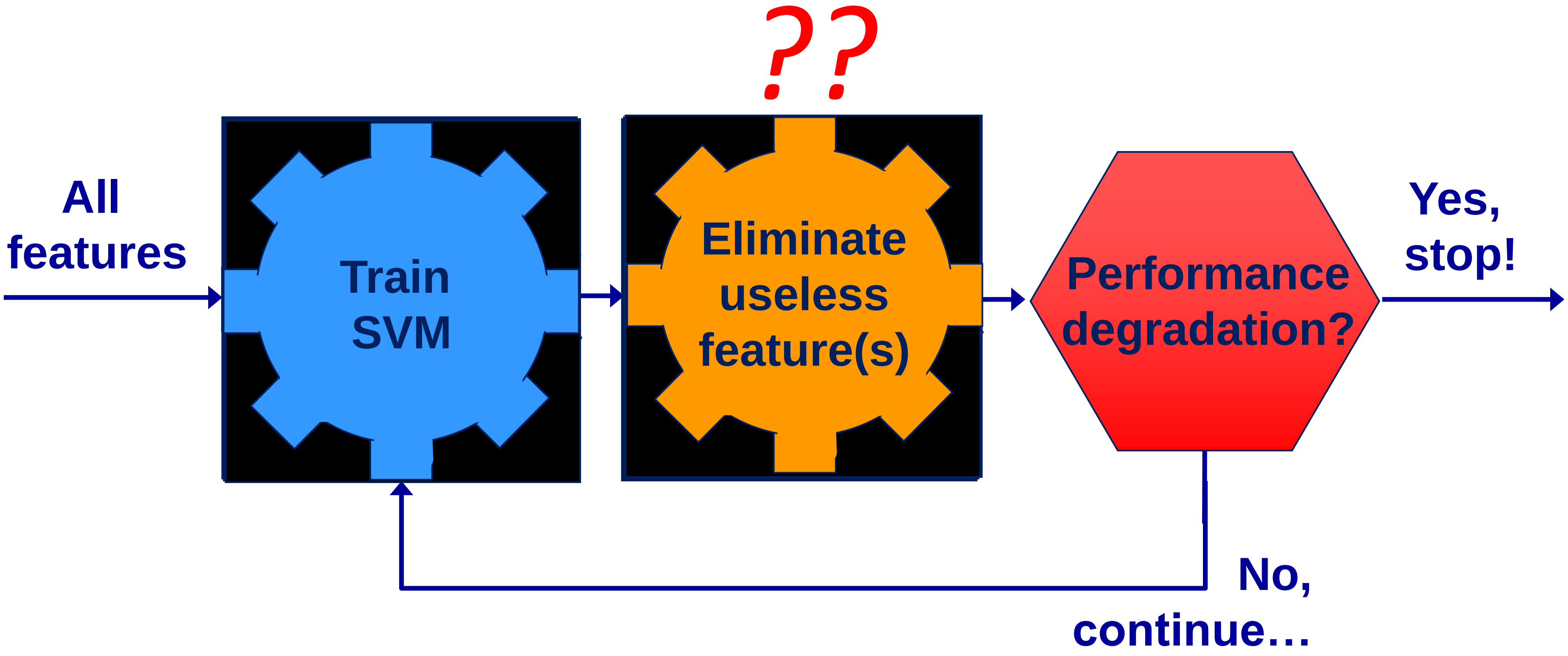
```
Relief
  Input: $\mathbf{x}$ - features
         $m$ - number of instances sampled
         $\tau$ - adjustable relevance threshold

  initialize: $\mathbf{w} = 0$
  for $i = 1$ to $m$
  begin
    randomly select an instance $I$
    find nearest-hit $H$ and nearest-miss $J$
     for $j = 1$ to $N$
      $\mathbf{w}(j) = \mathbf{w}(j) - \texttt{diff}(j, I, H)^2/m + \texttt{diff}(j, I, J)^2/m$
  end

  Output: $\mathbf{w}$ greater than $\tau$
```

Focus Algorithm



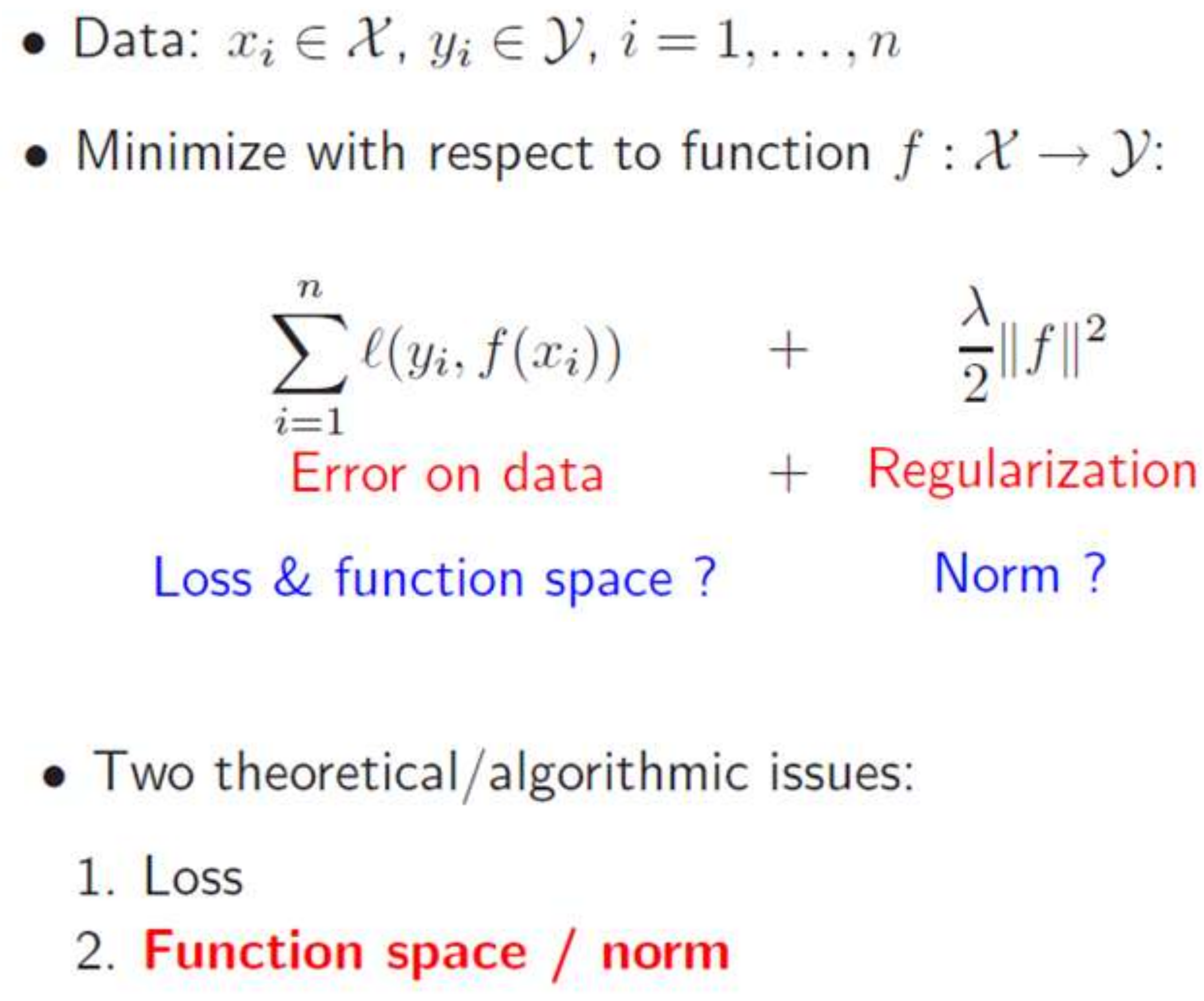
```
Focus
  Input: $F$ - all features $x$ in data $D$
         $U$ - inconsistency rate as evaluation measure

  initialize: $S = \{\}$

  for $i = 1$ to $N$
    for each subset $S$ of size $i$
       if Cal$U(S, D) = 0$    /* $CalU(S, D)$ returns inconsistency*/
          return $S$
  Output: $S$ - a minimum subset that satisfies $U$
```

Embedded Methods (RFE)



Recursive Feature Elimination (RFE) SVM. *Guyon-Weston, 2000. US patent 7,117,188*

Feature Selection via Regularization (Sparse)



- Data: $x_i \in \mathcal{X}$, $y_i \in \mathcal{Y}$, $i = 1, \ldots, n$
- Minimize with respect to function $f : \mathcal{X} \rightarrow \mathcal{Y}$:

$$\sum_{i=1}^{n} \ell(y_i, f(x_i)) \qquad + \qquad \frac{\lambda}{2} \|f\|^2$$

Error on data + Regularization

Loss & function space ? Norm ?

- Two theoretical/algorithmic issues:

1. Loss
2. **Function space / norm**

Ridge Regression and LASSO

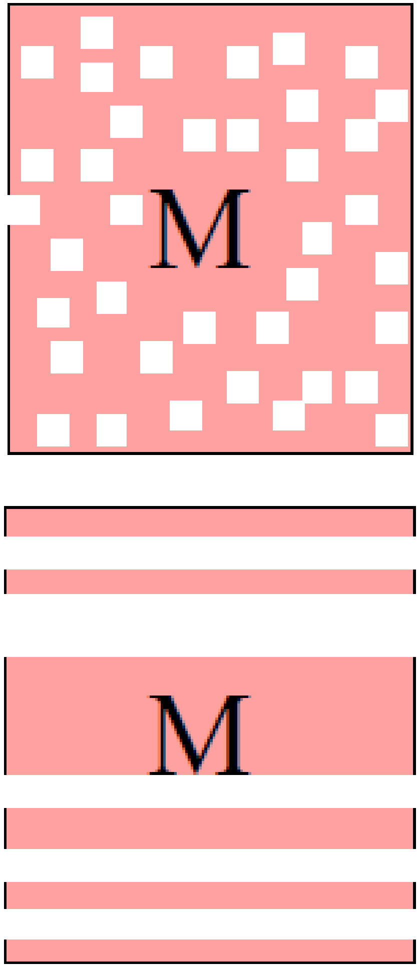
- Compared methods to reach the least-square solution
  - Ridge regression: $\min_{w \in \mathbb{R}^p} \frac{1}{2}\|y - Xw\|_2^2 + \frac{\lambda}{2}\|w\|_2^2$
  - Lasso: $\min_{w \in \mathbb{R}^p} \frac{1}{2}\|y - Xw\|_2^2 + \lambda\|w\|_1$
  - Forward greedy:
    - ∗ Initialization with empty set
    - ∗ Sequentially add the variable that best reduces the square loss
- Each method builds a path of solutions from 0 to ordinary least-squares solution

Group Sparsity (Multi-Class)

$$\min_{\mathbf{W},\mathbf{b}} \sum_{i=1}^{n} \left\| \mathbf{W}^T\mathbf{x}_i + \mathbf{b} - \mathbf{y}_i \right\|_2^2 + \lambda \|\mathbf{W}\|_F^2$$

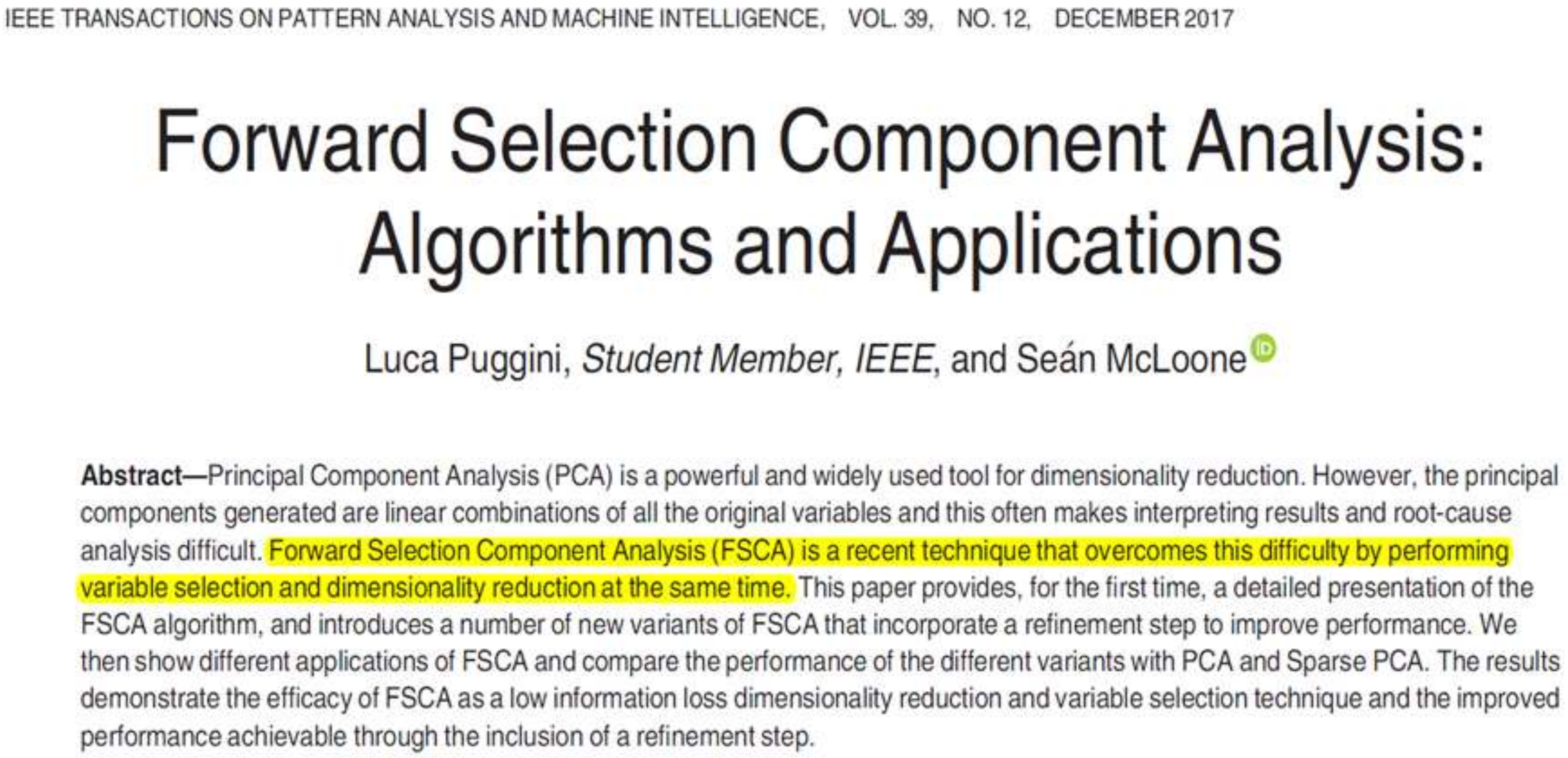
$$\|\mathbf{W}\|_{2,1} = \|\bar{\mathbf{w}}\|_1 = \sum_{i=1}^{m} \sqrt{\sum_{j=1}^{c} W_{ij}^2}.$$

$$\begin{aligned} \min_{\mathbf{W},\mathbf{t},\mathbf{M}} \quad & ||\mathbf{X}\mathbf{W} + \mathbf{e}_n\mathbf{t}^T - \mathbf{Y} - \mathbf{B} \odot \mathbf{M}||_{2,1} + \lambda||\mathbf{W}||_{2,1} \\ \text{s.t.} \quad & \mathbf{M} \geq \mathbf{0} \end{aligned}$$



S. Xiang et al, ***Discriminative Least Squares Regression*** for Multiclass Classification and Feature Selection, IEEE Trans. NNLS, 2012.

Dimension Reduction + Feature Selection



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Forward Selection Component Analysis: Algorithms and Applications

Luca Puggini, *Student Member, IEEE*, and Seán McLoone

Abstract—Principal Component Analysis (PCA) is a powerful and widely used tool for dimensionality reduction. However, the principal components generated are linear combinations of all the original variables and this often makes interpreting results and root-cause analysis difficult. Forward Selection Component Analysis (FSCA) is a recent technique that overcomes this difficulty by performing variable selection and dimensionality reduction at the same time. This paper provides, for the first time, a detailed presentation of the FSCA algorithm, and introduces a number of new variants of FSCA that incorporate a refinement step to improve performance. We then show different applications of FSCA and compare the performance of the different variants with PCA and Sparse PCA. The results demonstrate the efficacy of FSCA as a low information loss dimensionality reduction and variable selection technique and the improved performance achievable through the inclusion of a refinement step.

Discussion

- Dimensionality reduction vs feature selection
- Advantage and disadvantage of manifold learning?
- Which criterion is best?
- What is a good feature representation?
- Can these ideas be extended to deep learning?

Thank You!
Q&A