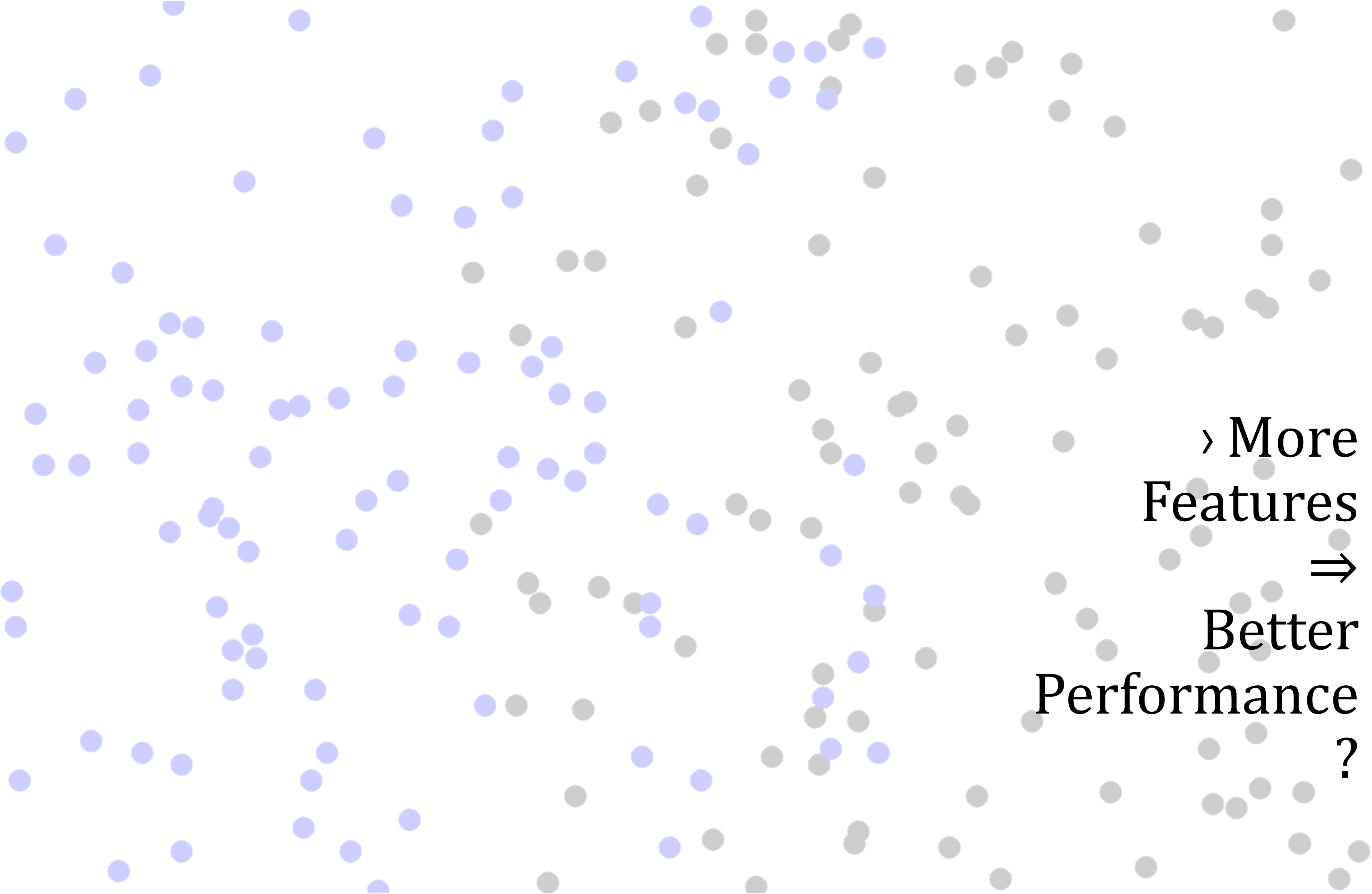


› More Features ⇒ Better Performance ?

Feature Extraction and Selection

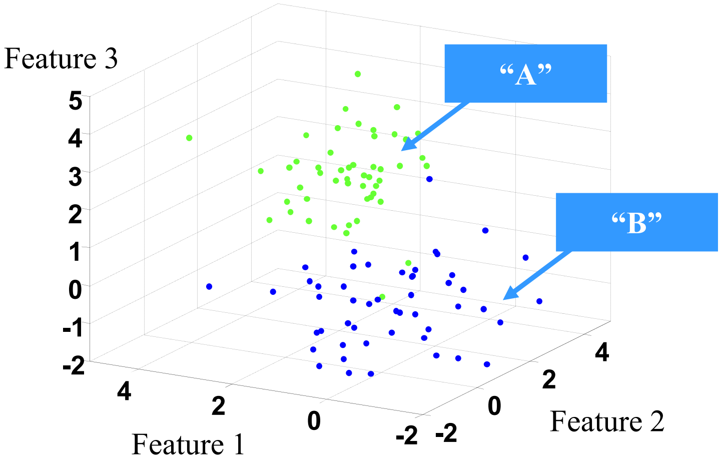
› Marco Loog

Outline

- A bit on high-dimensional spaces
- Some basics of feature extraction
- Some basics of feature selection

Feature Space

- A p-dimensional space, in which each dimension is a feature containing N [labeled] samples [objects]



- Why and how should lower number of features?

Curse of Dimensionality

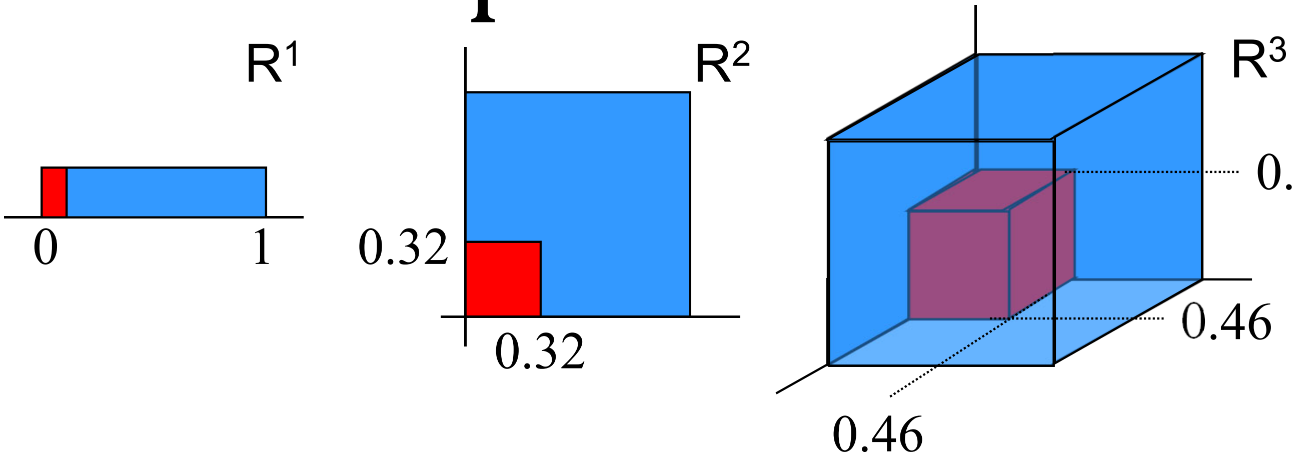
› Problem : too few samples in too many dimensions [the curse of dimensionality]

Let’s discuss histogram-based density estimation
…with increasingly finer binning?

› Anyway : in high-dimensional spaces,
our 2D/3D intuition does not work anymore...

High-Dimensional Spaces

High-Dimensional Spaces

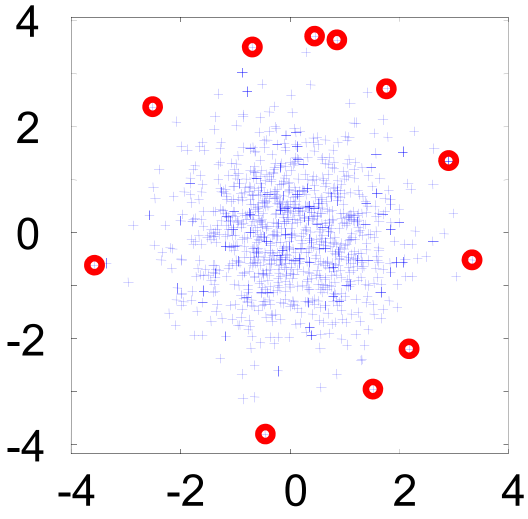


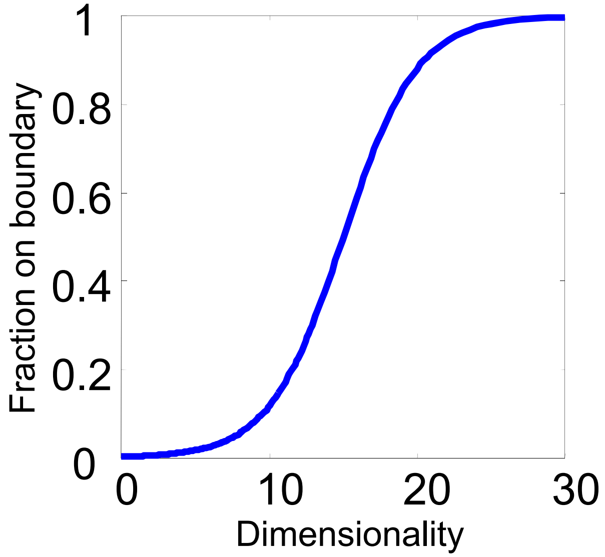
› Example : neighborhood capturing 10% of uniformly distributed data in hypercube

› E.g. in $\mathbb{R}^{20}$sides of $\sqrt[20]{.1} \approx 0.89$

So, not a small block anymore…

High-Dimensional Spaces



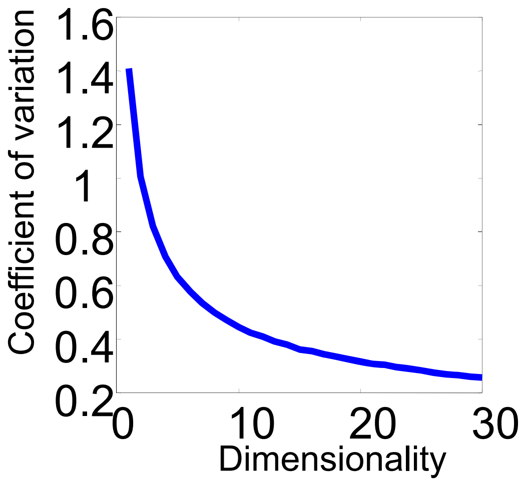


- Example : boundary points
  - 1000 normal samples in 2D then 1% on convex hull
  - 1000 in 20D then 95% on convex hull

High-Dimensional Spaces

› Example : points tend to have equal distances

Consider $\frac{\mathrm{std}(d^2)}{\mathrm{mean}(d^2)}$ for squared distance d^2



For points in $\mathbb{R}^{1000}$ from standard normal, distribution is approximately $N(2000,8000)$

High-Dimensional Spaces

› This means [roughly] for increasing dimensionality

local, distance-based methods suffer most, e.g. NN-methods

global, more restricted models suffer less, e.g. linear models

› So…

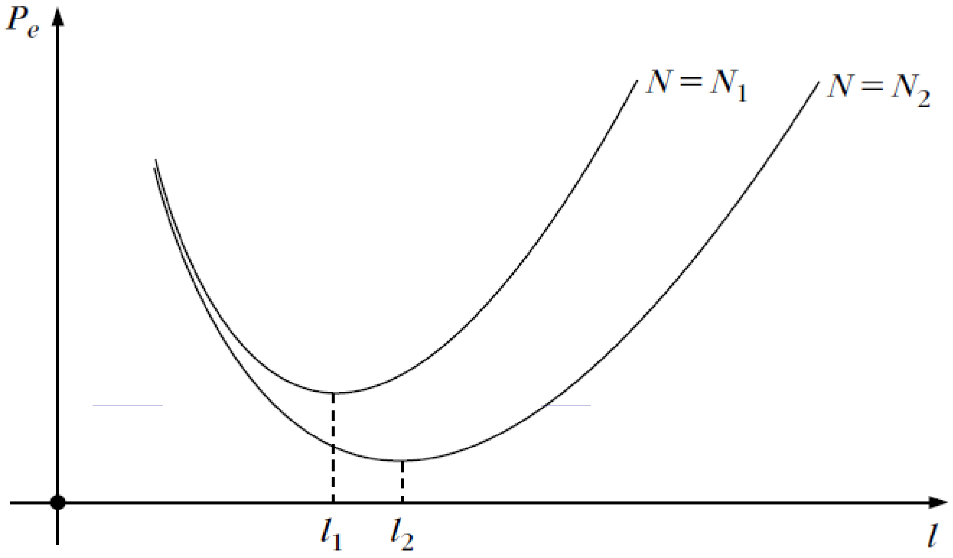
controlling classifier complexity important

p should be kept as low as possible : dimensionality reduction

Dimensionality Reduction by Selection and Extraction

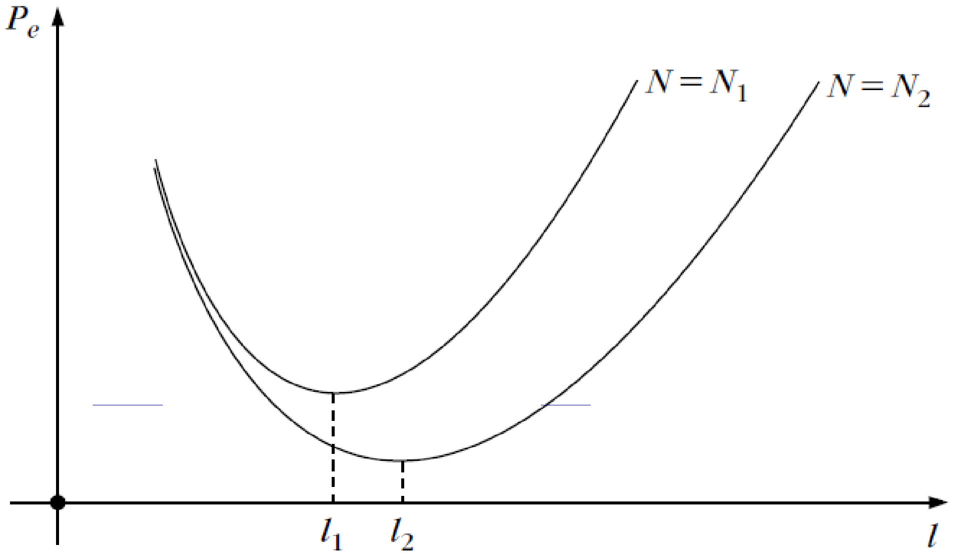
Dimensionality Reduction

- Problem : too few samples in too many dimensions [the curse of dimensionality]



Dimensionality Reduction

- Problem : too few samples in too many dimensions [the curse of dimensionality]
- Solution : drop dimensions / features
  - Feature selection
  - Feature extraction
- Questions :
  - Which dimensions to drop?
  - What feature subset to keep?



Dimensionality Reduction

› Other uses :

Fewer parameters give faster algorithms and parameters are easier to estimate

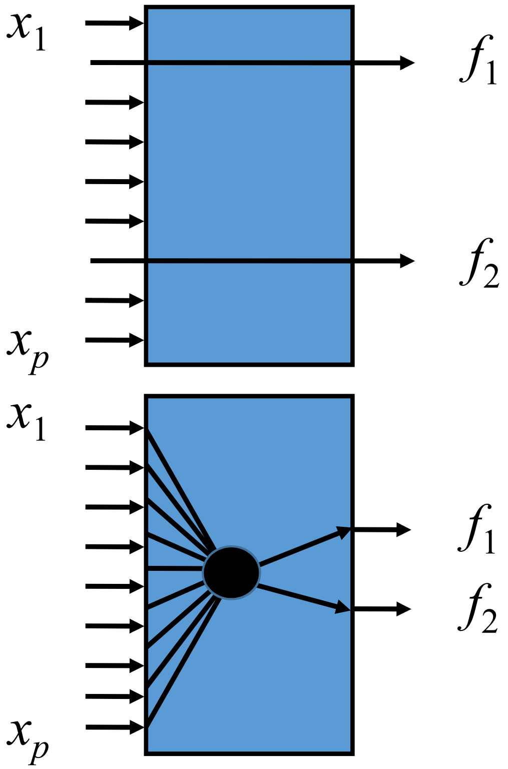
Explaining which measurements are useful and which are not [reducing redundancy]

Visualization of data can be a powerful tool when designing pattern recognition systems

Feature Selection vs Extraction

- Feature selection : select d out of p measurements

- Feature extraction : map p measurements to d measurements



Feature Selection vs Extraction

- Think of selection and extraction as finding a mapping

- We need :
  - Criterion function, e.g. error, class overlap, information loss,…
  - Optimization or “search” algorithm to find mapping for given criterion

Note on Criteria

- The optimal[?] criterion :
  final performance of the entire system
  - Maybe calculated using cross-validation

- Approximate performance predictors
  - Calculate performance of easy-to-use criterion giving indication of how well a more powerful / realistic criterion may perform

Two
Classical
Linear
Feature Extractors

Linear Feature Extraction

› Unsupervised :

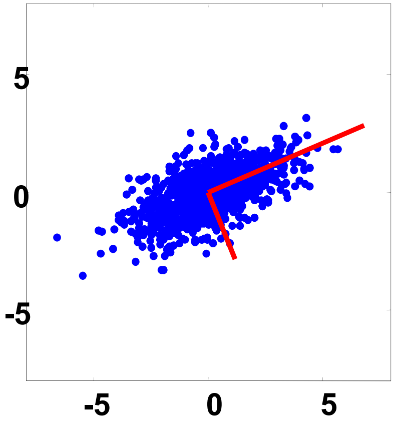
Principal Component Analysis [PCA]

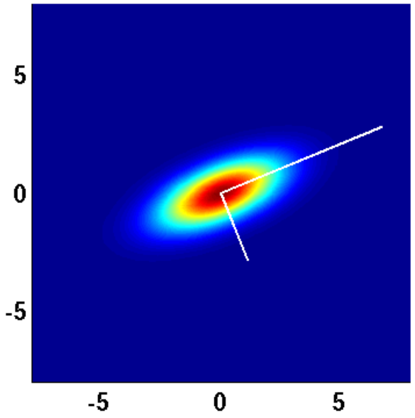
› Supervised :

Linear Discriminant Analysis [LDA]
Fisher mapping [fisherm]

PCA is one of the most widely used feature extraction methods
LDA is its supervised cousin
Similar ideas are at the basis of many “novel” methods

PCA





- Principal component analysis [PCA, 1901] : find directions in data which…
  - Retain as much [total] variance as possible
  - Make projected data uncorrelated
  - Minimize squared reconstruction error

PCA

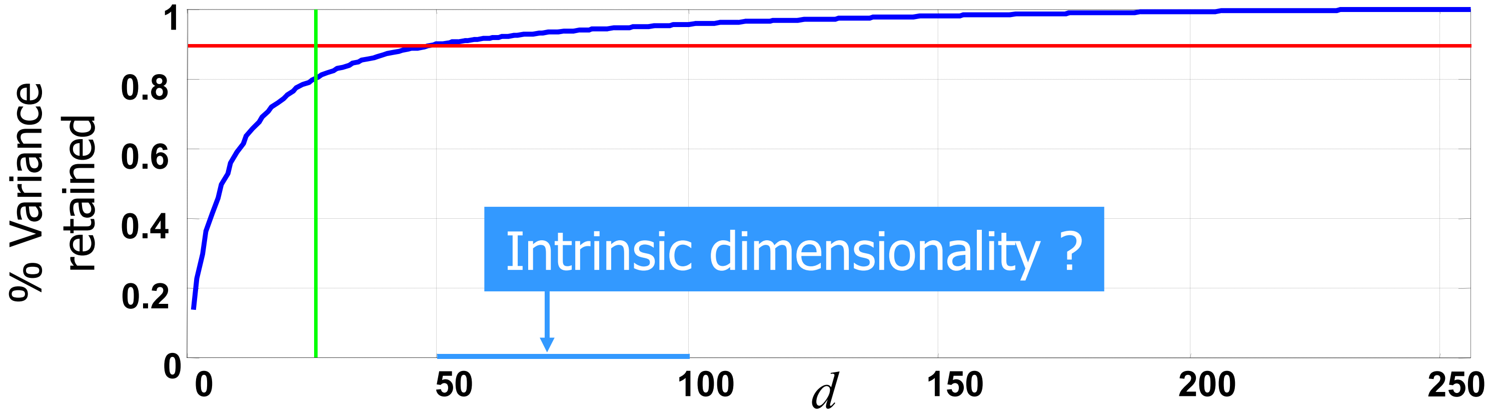
- Let a be a projection vector that reduces to 1D
- Let’s say our data has covariance matrix C
  - What value does $a^T Ca$ equal to?
  - So, what should we maximize?

PCA

- Let a be a projection vector that reduces to 1D
- Let's say our data has covariance matrix C
  - What value does $a^T Ca$ equal to?
  - So, what should we maximize?

- Seems we need an assumption…
  - Assume the constraint $\|a\|^2 = 1$
  - Then solve, for instance, with Lagrangian : $a^T Ca - \lambda(\|a\|^2 - 1)$

PCA Example

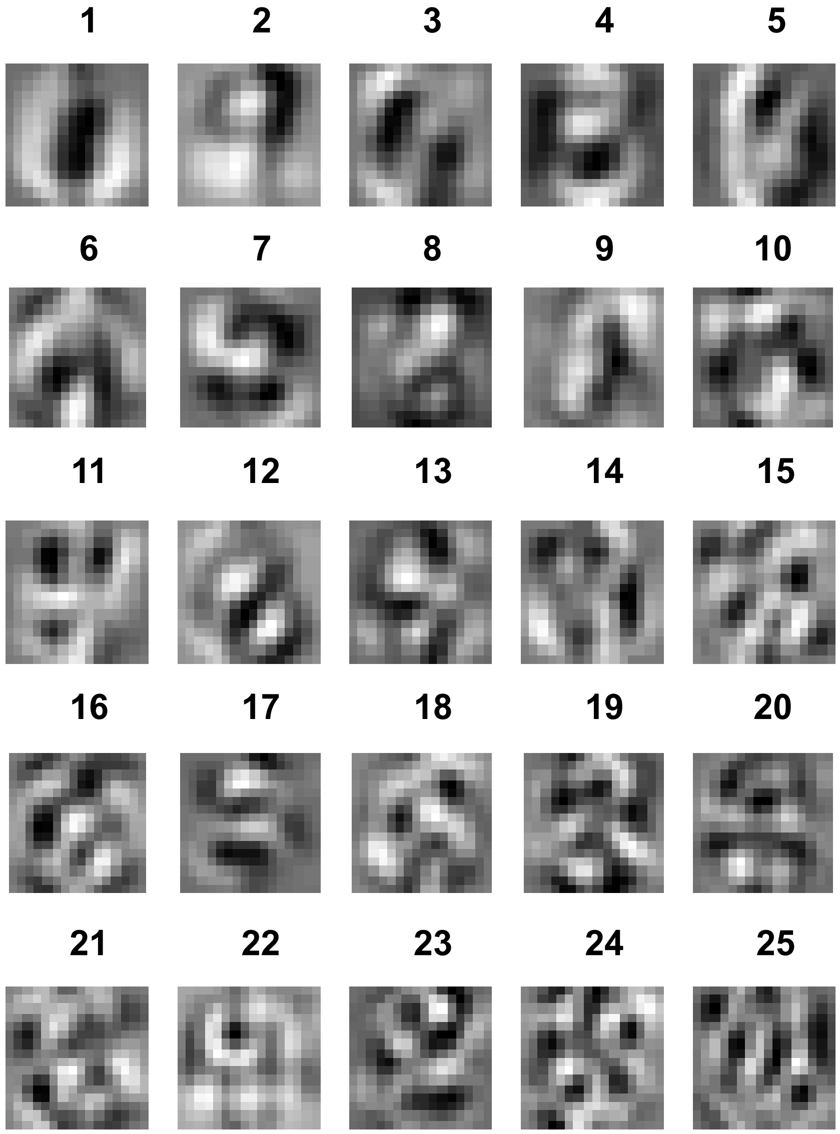


Intrinsic dimensionality ?

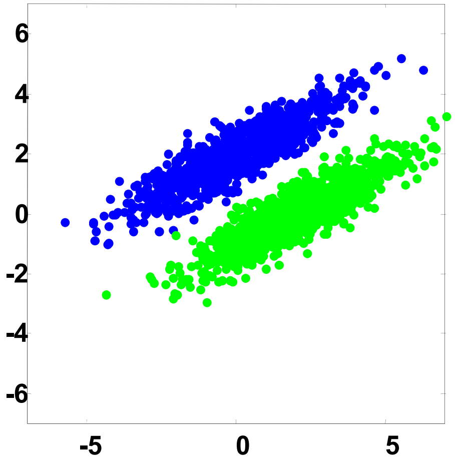
- E.g. NIST digits : 2000 samples, $p = 256$

PCA Example

- › For image data, principal components might[!] also be interpretable…
- › Here : largest occuring variations between digits



Remarks on PCA



- Principal component analysis :

  Global and linear

  May need considerable amount of data to estimate covariance $[C, \Sigma, S_T, \ldots]$ well

- Danger :

  Criterion is not necessarily related to the goal

  E.g. might discard important directions

  [Then again, most classifier also do not optimize error rate directly…]

Supervised Linear Feature Extraction

- If desired output is given, supervised criteria can be used

  One illustration only : Linear Discriminant Analysis [LDA, or in PRTools terms fisherm]

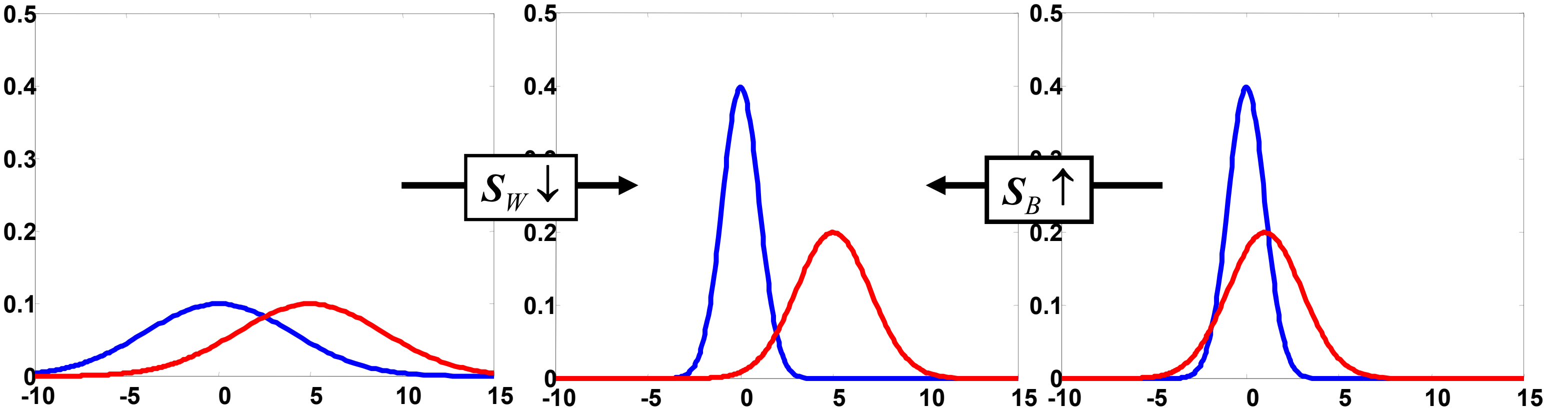
Intermezzo : Scatter Matrices

- $m, S_T = \Sigma$: mean and covariance of all samples
- m_i, Σ_i : mean and covariance of class i

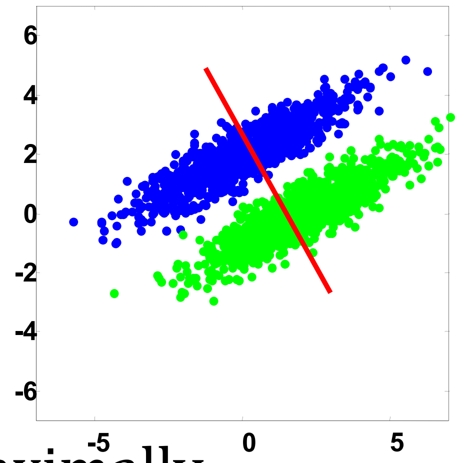
- Total scatter : Σ equals sum of within and between
- Within-scatter : $\boldsymbol{S}_w = \sum_{i=1}^{C} \frac{n_i}{n} \Sigma_i$
- Between-scatter : $\boldsymbol{S}_B = \sum_{i=1}^{C} \frac{n_i}{n} (\boldsymbol{m}_i - \boldsymbol{m})(\boldsymbol{m}_i - \boldsymbol{m})^T$

Intermezzo : Scatter Matrices

- S_T = total scatter, “overall width”
- S_W = “average class width”; the smaller, the better
- S_B = “average distance between class means”; the larger, the better



LDA [or Fisher mapping]



- Reduction to 1D for two classes
  - Find projection vector a such that classes are maximally separated
  - Choose a to maximize Fisher criterion :

$$J_F(a) = \frac{a^T S_B a}{a^T S_W a}$$

- Solution: Eigenanalysis of $S_W^{-1} S_B$

Nonlinear Feature Extraction

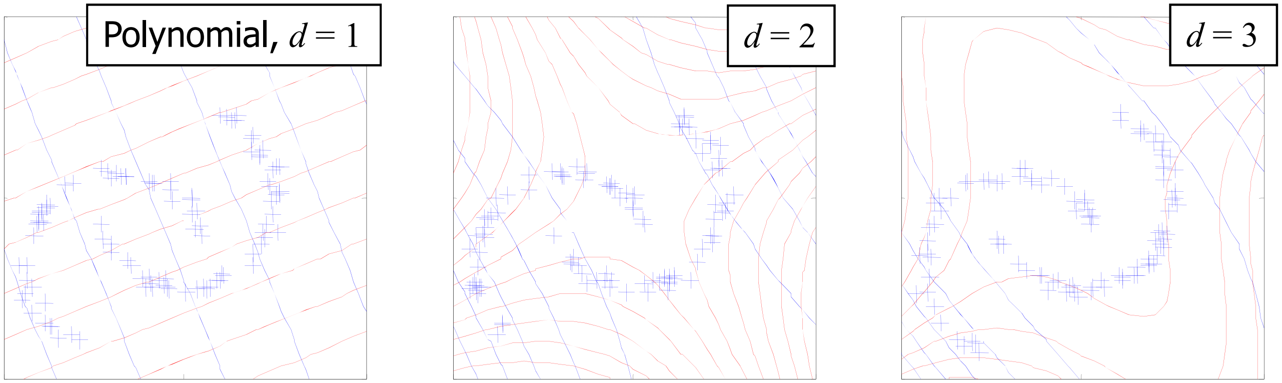
- Large collection of possible mappings…

- Today : only one unsupervised method

  What is *the* way to make linear stuff nonlinear?

- Tomorrow : [the gist of] so-called auto-encoders

KPCA



› Kernelize PCA by relating eigenvectors of $X^T X$ and XX^T [assuming centralized feature vectors]

Summary

- Feature extraction, like selection :
  - Useful for visualization
  - Necessary because of curse of dimensionality

- Feature extraction :
  - Linear vs. nonlinear
  - Supervised vs. unsupervised

- PCA possibly most important method

On to Feature Selection

Feature Selection

- The general idea is to pick a set of good features from the original/initial set of features

Feature Selection

- We need a criterion function

  How do we measure how good a feature subset is?

  E.g. error, class overlap, information loss

- We need a search algorithm

  How do we go through all possible subsets?

  E.g. pick best single feature at each time

- Maybe more than for feature extraction : optimality is sacrificed

Feature Selection

- Which approach to feature selection have we seen?

Criteria

Criteria

- Actual classification performance : “best” possible criterion, but potentially very expensive

- Approximate performance predictors : calculate easy-to-use measure that gives indication of real performance

Probabilistic Criteria

- Probabilistic distance
- Expresses distance between two distributions
  - E.g. Kullback-Leibler divergences and variations
- Often needs estimates of class-conditional densities
  - Potentially difficult
  - Potentially expensive

Scatter Matrices Again…

- $m, S_T = \Sigma$: mean and covariance of all samples
- m_i, Σ_i : mean and covariance of class i

- Total scatter : Σ equals sum of within and between
- Within-scatter : $\boldsymbol{S}_w = \sum_{i=1}^{C} \frac{n_i}{n} \Sigma_i$
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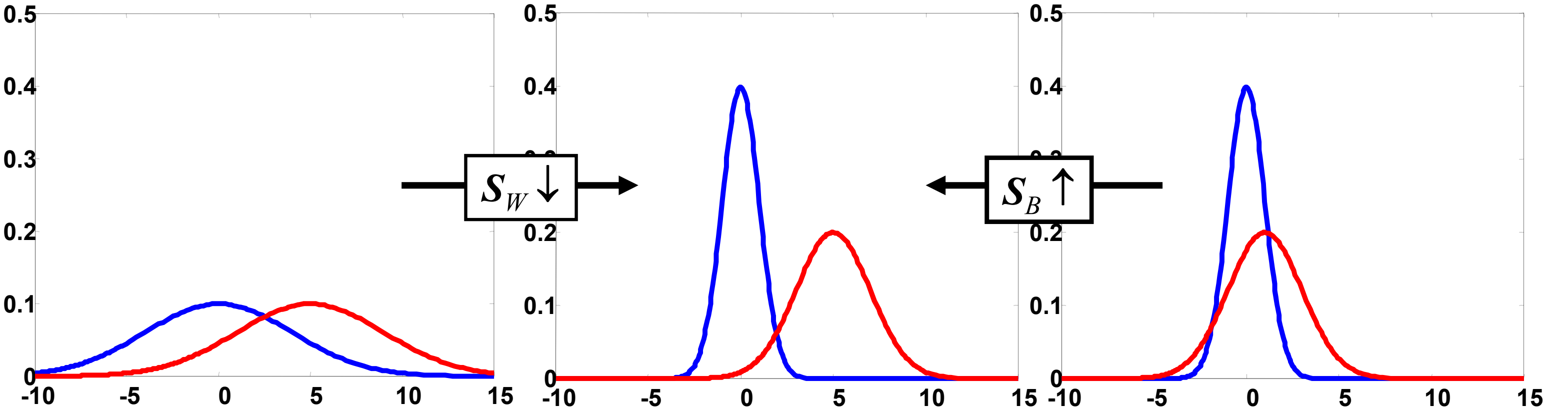
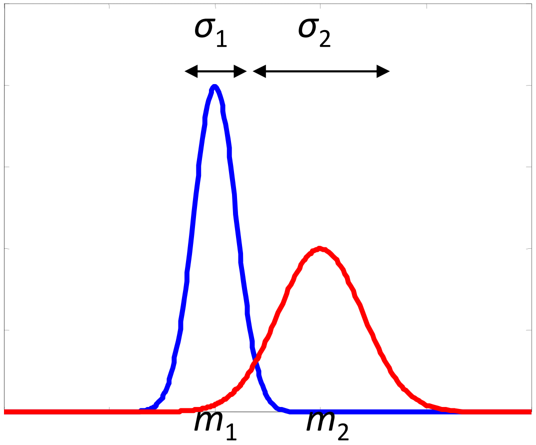


Heuristic Scatter-based Criteria

› Example scatter-based performance indicators

$$J_1 = \text{trace}\ (\boldsymbol{S}_W + \boldsymbol{S}_B) = \text{trace}\ (\boldsymbol{\Sigma}) = \text{trace}(\boldsymbol{S}_T)$$
$$J_2 = \text{trace}\ (\boldsymbol{S}_B\ /\ \boldsymbol{S}_w)$$
$$J_3 = \det\ (\boldsymbol{\Sigma}\ )\ /\ \det\ (\boldsymbol{S}_w)$$
$$J_4 = \text{trace}\ (\boldsymbol{S}_W\ )\ /\ \text{trace}\ (\boldsymbol{S}_B)$$

Yet Another Criterion



- Mahalanobis distance

  $D_M = (m_1 - m_2)^T C^{-1}(m_1 - m_2)$

  Assumes Gaussian distributions with equal covariance matrix C

  In which case, some of the probabilistic distances reduce to this

- Multi-class, e.g. take sum or minimum

  Of course, general solution to extend two-class criteria

- 1D case : Fisher criterion $J_F = \frac{(m_1 - m_2)^2}{\sigma_1^2 + \sigma_2^2}$

Sub-optimality of Criteria

$$D_M = (m_1 - m_2)^T C^{-1}(m_1 - m_2)$$

- Give a 2D problem in which Euclidean distance [this assumes $C = I$] picks up the wrong 1D feature…
- Give a 2D problem in which Mahalanobis distance picks up the wrong 1D feature…

Now, on to Search Algorithms

Now, on to Search Algorithms

- Feature selection : Select a subset of d out of p measurements which optimizes chosen criterion

- Simplest solution : look at all possible subsets

  Any problems there?

Now, on to Search Algorithms

› Feature selection : Select a subset of d out of p measurements which optimizes chosen criterion

› Simplest solution : look at all possible subsets

Any problems there?

› There are $\binom{p}{d} = \frac{p!}{d!(p-d)!}$ subsets

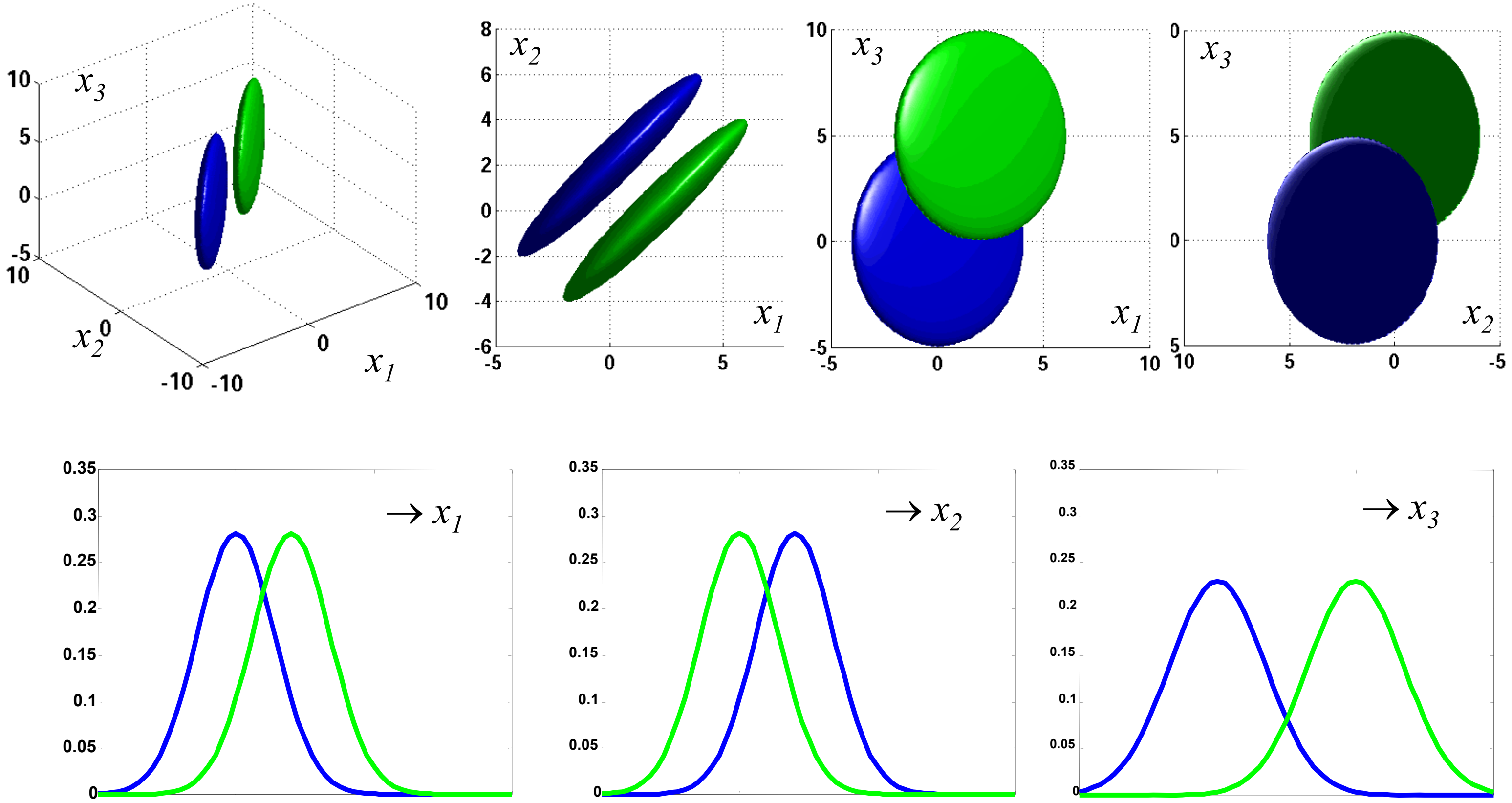
So, like for the criteria, we settle for approximations…

Search Algorithms

- Sub-optimal algorithms : select one feature [or a few features] at a time

- Simplest variation : best individual d
  - But these are not necessarily the best d!

d Best or Best d?



More Sub-Optimal Strategies

- Forward selection

  Start with empty feature set

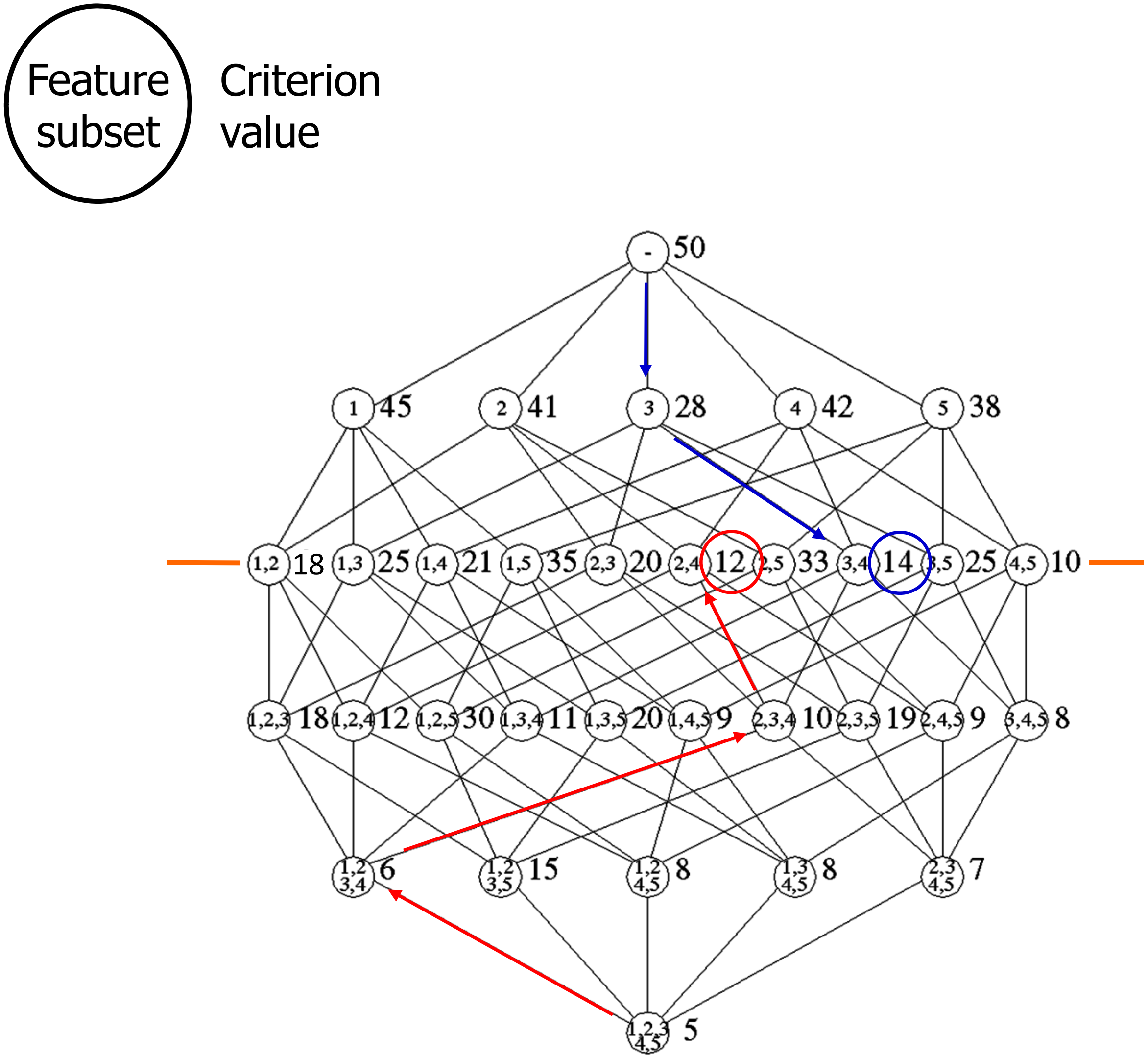
  One at a time, keep adding feature that gives best performance considering entire chosen feature set

More Sub-Optimal Strategies

› Backward selection

Same as forward selection
...but then the other way ‘round

E.g.



- Select $d = 2$ out of $p = 5$ features

More Sub-Optimal Strategies

› Plus-l-take-away-r

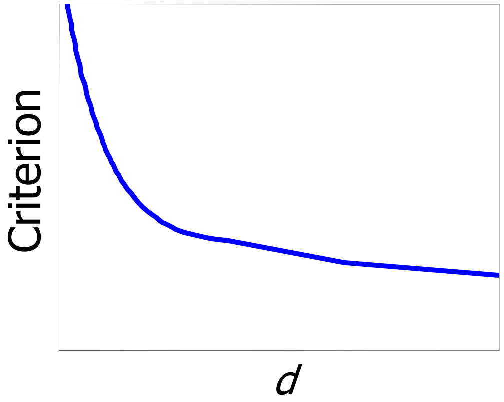
Start with empty set [if $l > r$] or entire set [if $l < r$]

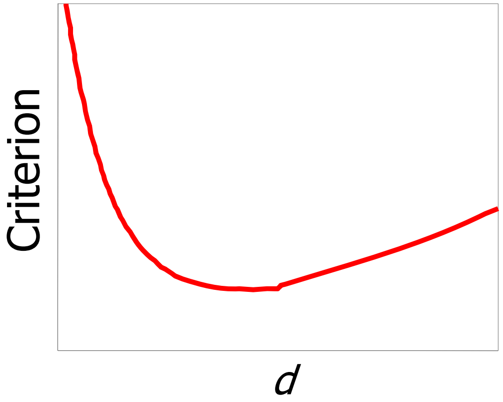
Keep adding best l and removing worst r
[...or vice versa]

Benefit over previous strategies?

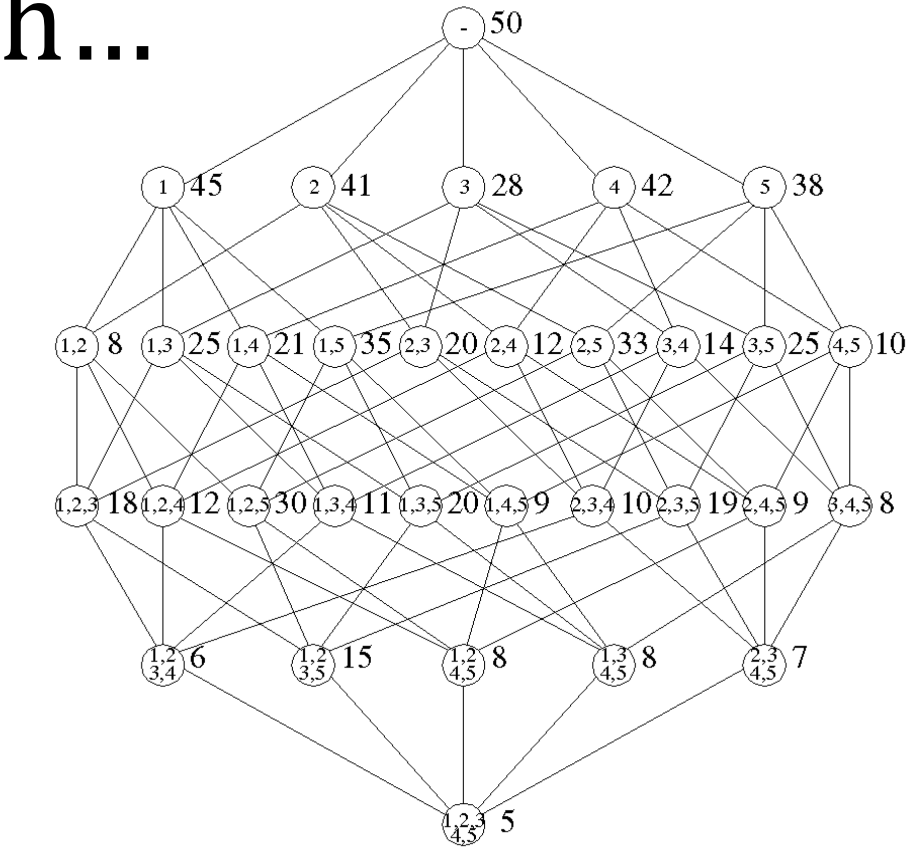
Branch & Bound

- Branch & bound
- Optimal when criterion is monotonic in number of features d



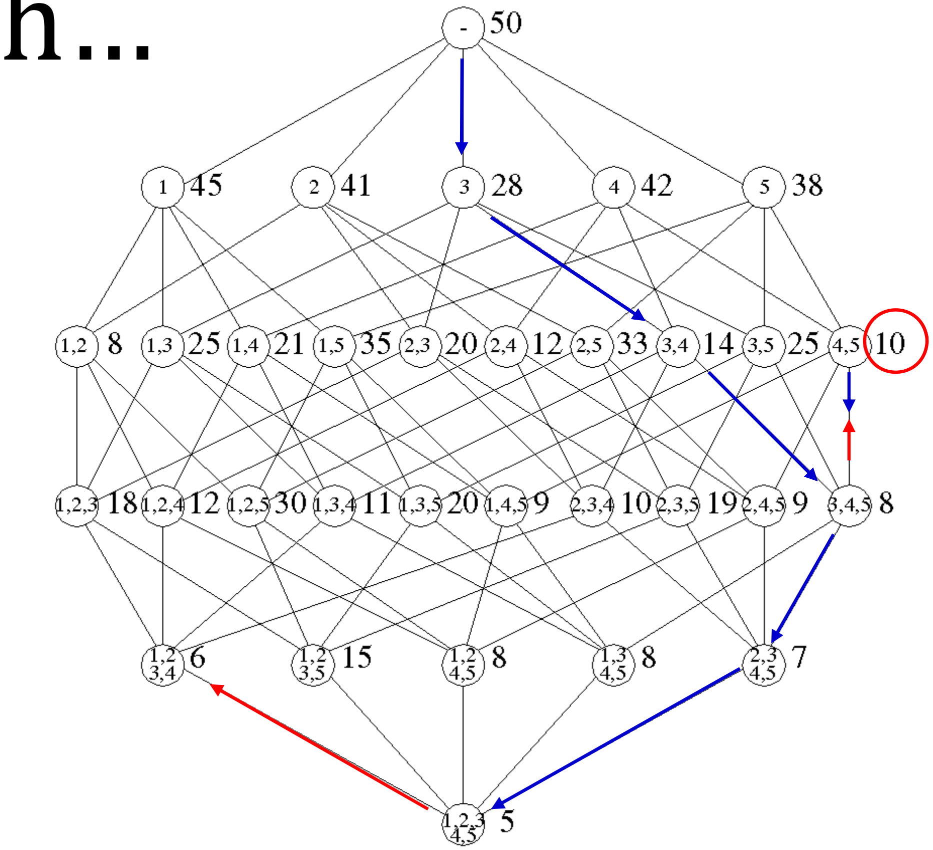


Floating Search…



- › Backtrack if that improves criterion for given # features

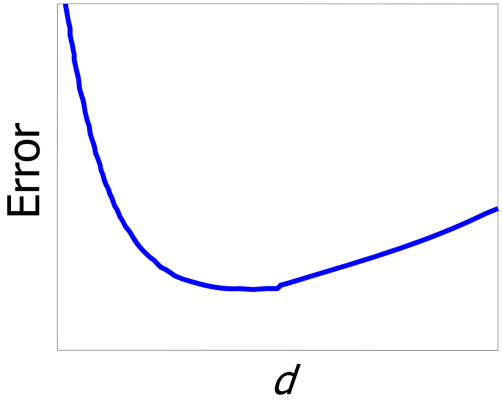
Floating Search…



When Should One Stop?

- Due to estimation problems [e.g. covariance matrix], criterion may have an optimum

- Or we could specify desired number of measurements, say, based on data set size



- Or? Use error rate?

Discussion / Conclusion

- Some unexpected behaviors in higher dimensions
- Considered curse of dimensionality
  - Way to counter it and improve performance : lower dimensionality
- Linear approaches to dimensionality reduction
  - Feature selection and feature extraction
  - Feature extraction can be nonlinear…
- Approaches are approximative / suboptimal
  - But that holds for many classifiers to start with…

› Q?