UVA CS 4774: Machine Learning

Lecture 14: Dimension Reduction

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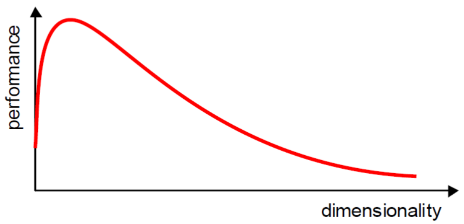
Curse of Dimensionality

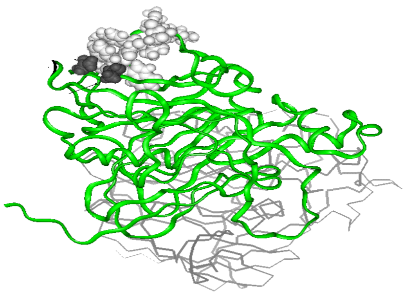
- Increasing the number of features will not always improve classification accuracy.



- In practice, the inclusion of more features might actually lead to worse performance.

- The number of training examples required increases exponentially with dimensionality **p**

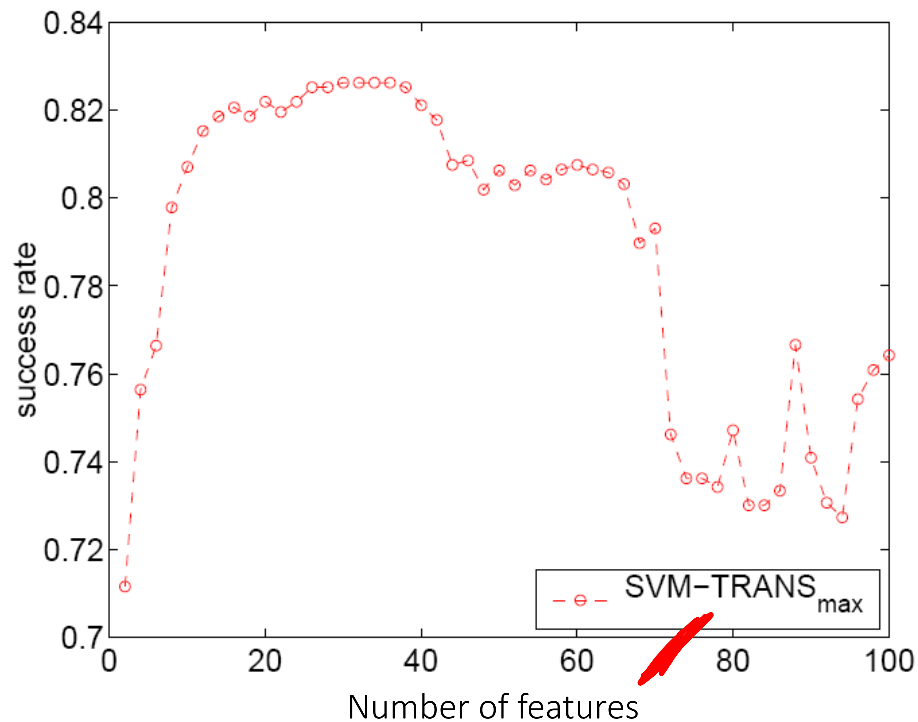
e.g., QSAR: Drug Screening



Binding to Thrombin
(DuPont Pharmaceuticals)

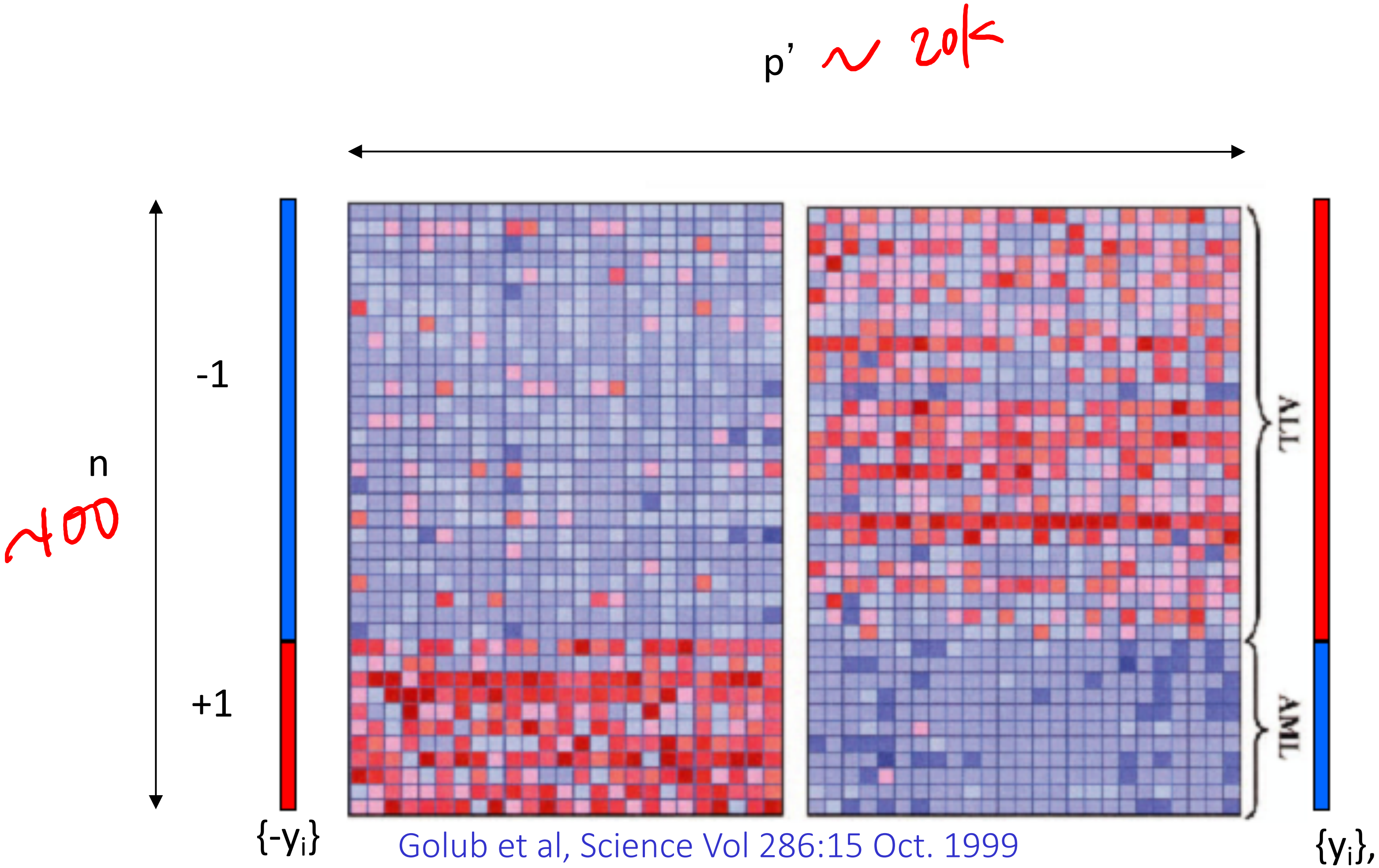
- 2543 compounds tested for their ability to bind to a target site on thrombin, a key receptor in blood clotting; 192 “active” (bind well); the rest “inactive”. Training set (1909 compounds) more depleted in active compounds.

- 139,351 binary features, which describe three-dimensional properties of the molecule.



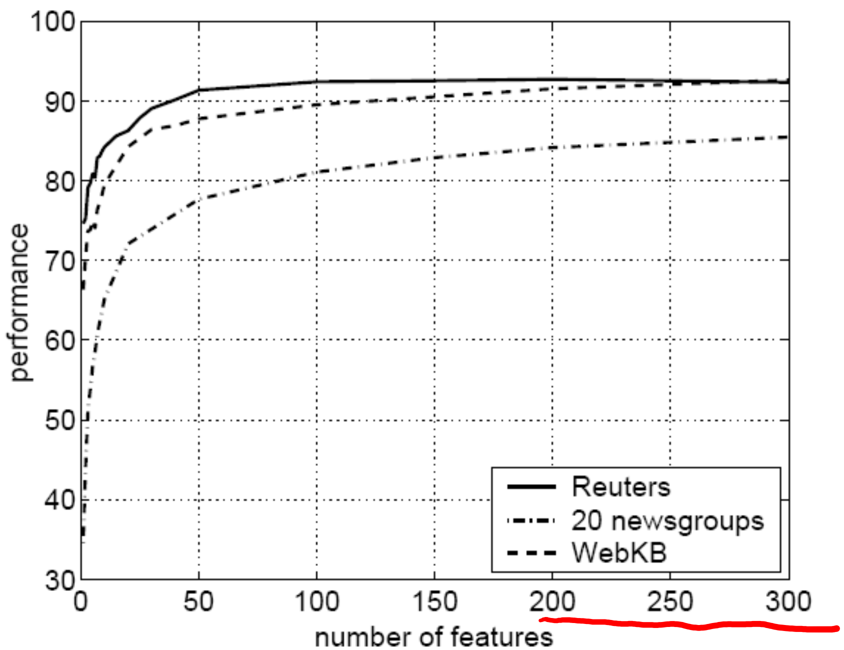
Weston et al, Bioinformatics, 2002

e.g., Leukemia Diagnosis



Golub et al, Science Vol 286:15 Oct. 1999

e.g., Text Categorization with many BOW featuers



Reuters: 21578 news wire, 114 semantic categories.

20 newsgroups: 19997 articles, 20 categories.

WebKB: 8282 web pages, 7 categories.

Bag-of-words: >100,000 features.

Bekkerman et al, JMLR, 2003

e.g., Movie Reviews and Revenues: An Experiment in Text Regression, Proceedings of HLT '10 (1.7k n / >3k features)

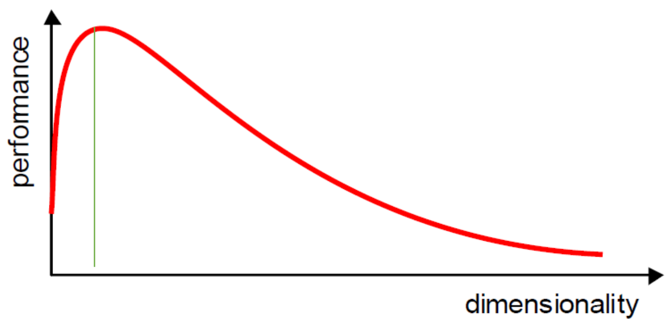
IV. Features	
I	Lexical n-grams (1,2,3)
II	Part-of-speech n-grams (1,2,3)
III	Dependency relations (nsubj,advmod,...)
Meta	U.S. origin, running time, budget (log), # of opening screens, genre, MPAA rating, holiday release (summer, Christmas, Memorial day,...), star power (Oscar winners, high-grossing actors)

e.g. counts of a ngram in the text

$n \approx 1700$ / $p > 30,000$

Dimensionality Reduction

- What is the objective?
  - Choose an optimum set of features of lower dimensionality to improve classification accuracy.



Dimension Reduction ➔ Simpler models

- Because:
  - Simpler to use (lower computational complexity)
  - Easier to train (needs less examples)
  - Less sensitive to noise
  - Easier to explain (more interpretable)
  - Generalizes better (lower variance)

Adapted from Dr. Christoph Eick Slides

Today: Dimensionality Reduction (Two Ways)

Feature extraction: finds a set of new features (i.e., through some mapping f()) from the existing features.

The mapping f() could be linear or non-linear

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix} \xrightarrow{f()} \mathbf{h} = \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_K \end{bmatrix}$$

K<<N

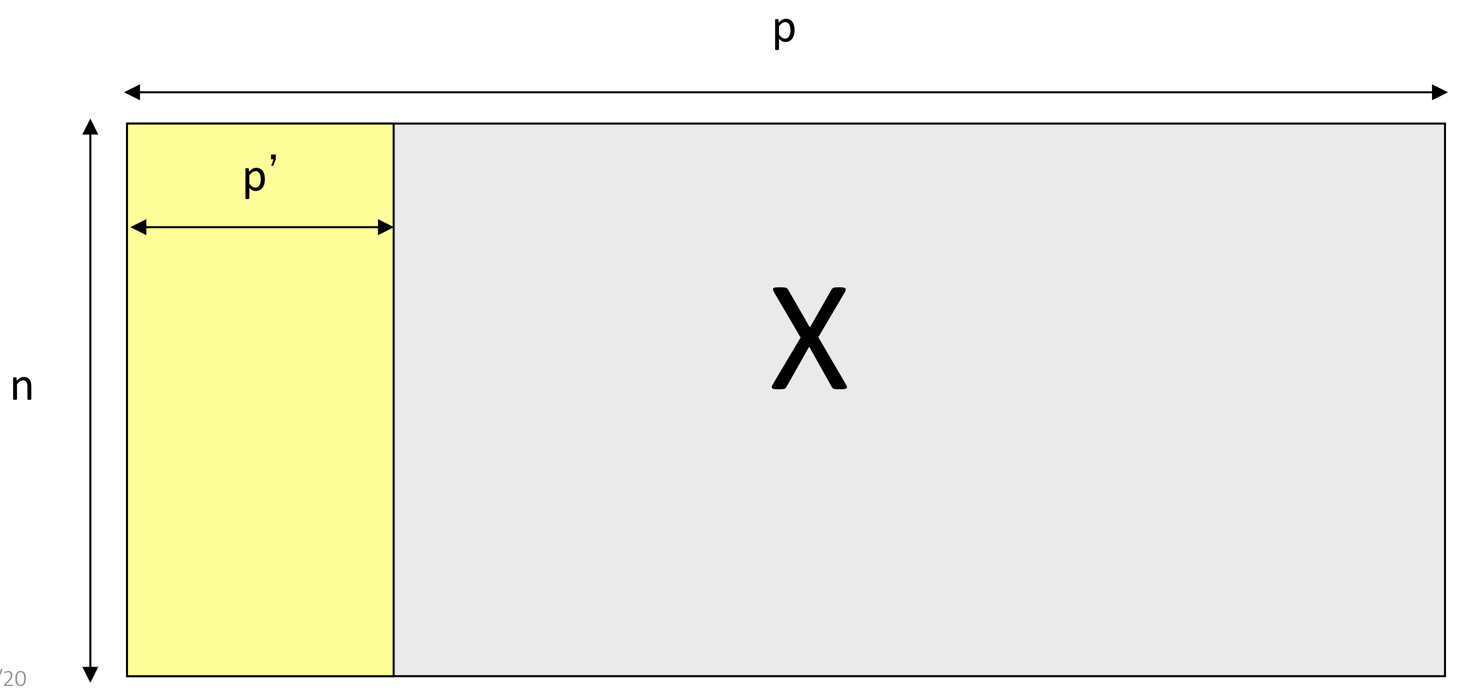
Feature selection: chooses a subset of the original features.

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix} \longrightarrow \mathbf{x}' = \begin{bmatrix} x_{k1} \\ x_{k2} \\ \vdots \\ x_{kK} \end{bmatrix}$$

K<<N

Feature Selection

- Select the most relevant ones to build better, faster, and easier to understand learning models.



From Dr. **Isabelle Guyon**

Summary: Feature Selection

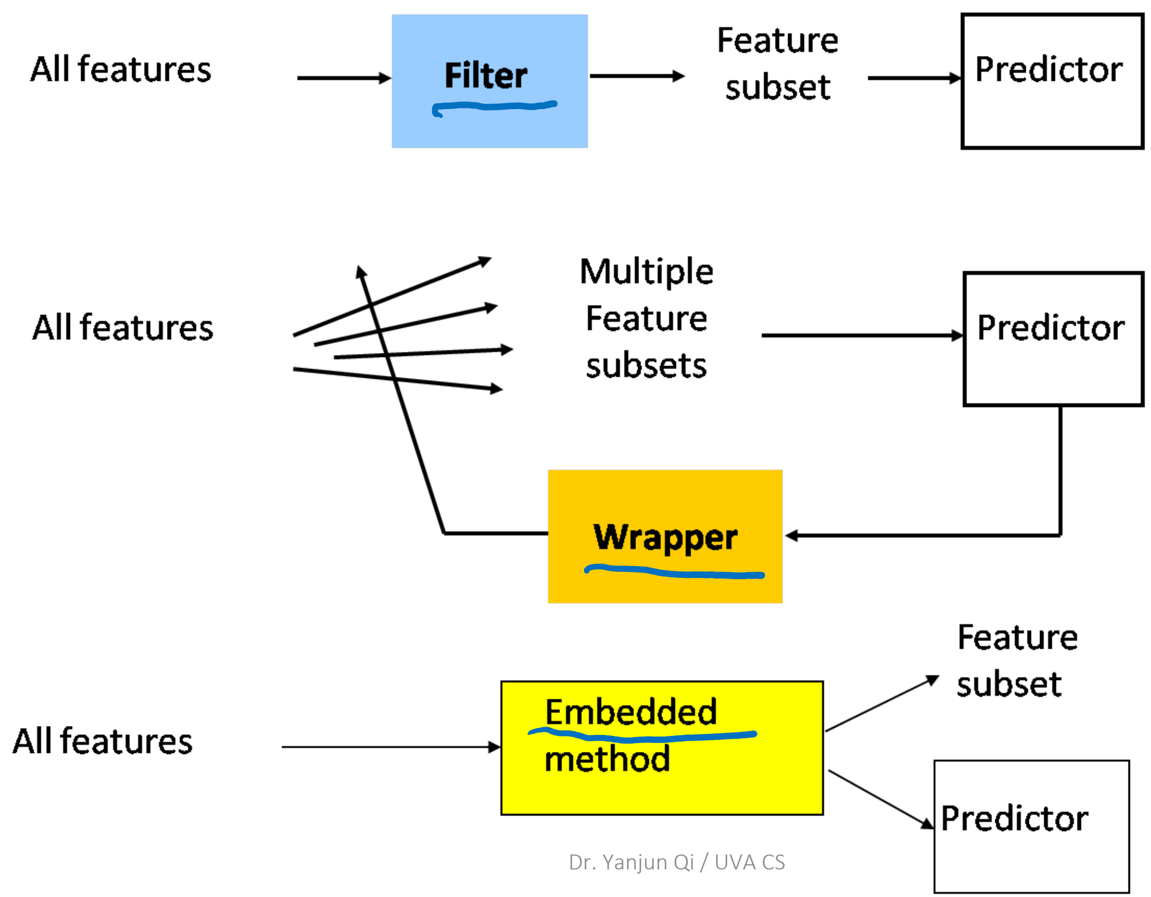
- Filtering approach:
  ranks features or feature subsets independently of the predictor.
  - ...using univariate methods: consider one variable at a time
  - ...using multivariate methods: consider more than one variables at a time

- Wrapper approach:
  uses a predictor to assess (many) features or feature subsets.

- Embedding approach:
  uses a predictor to build a (single) model with a subset of features that are internally selected.

Summary: filters vs. wrappers vs. embedding

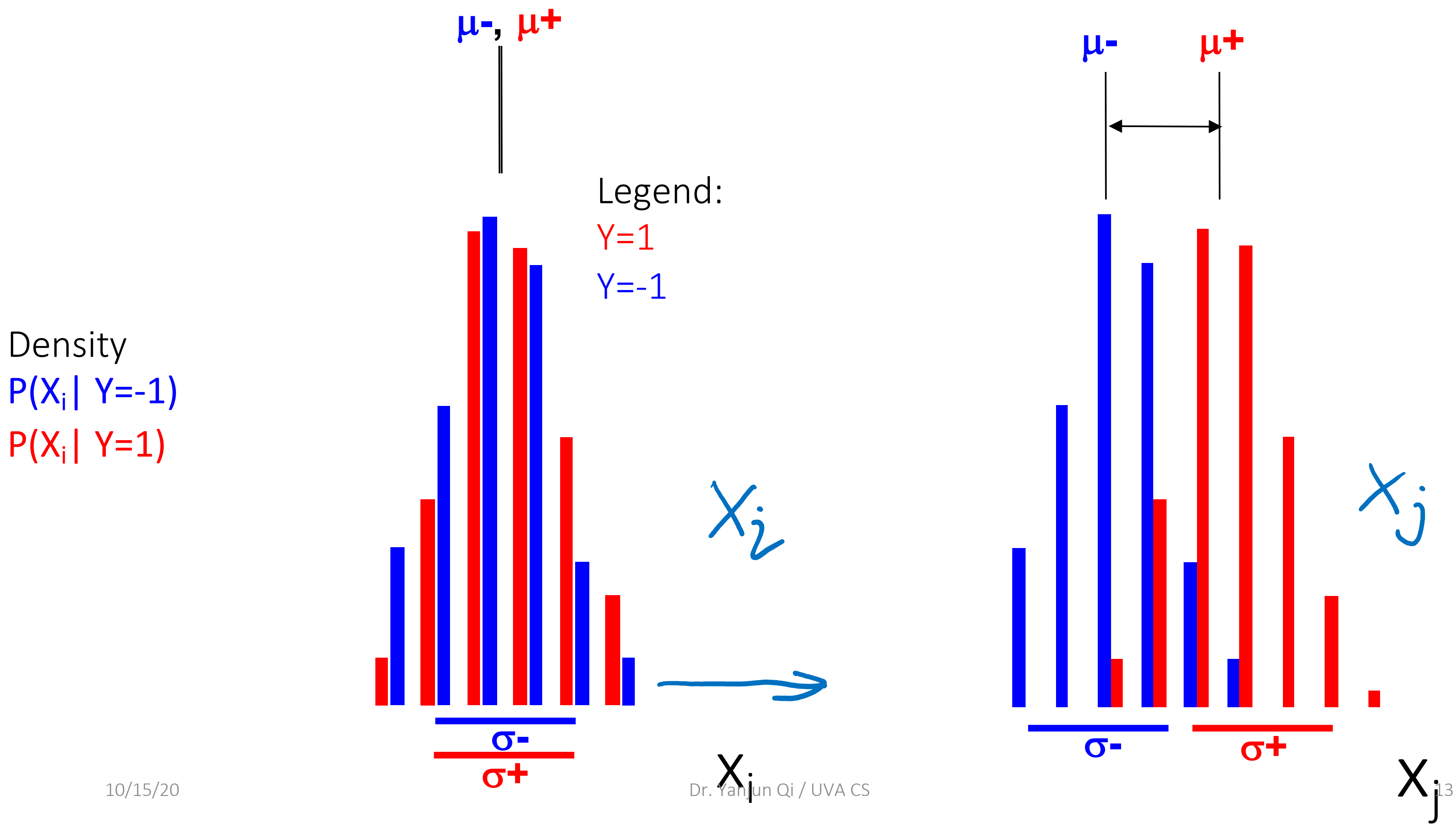
- **Main goal**: rank subsets of useful features



From Dr. **Isabelle Guyon**

(I) Filtering: univariate filtering
e.g. T-test

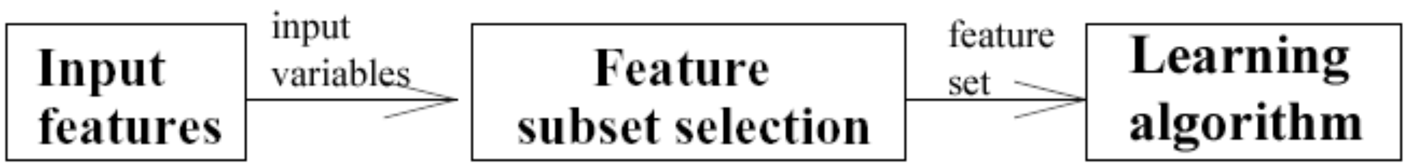
- **Goal:** determine the relevance of a given single feature for two classes of samples.



(I) Filtering : multi-variate: Feature Subset Selection

Filter Methods

- Select subsets of variables as a pre-processing step, independently of the used classifier!!



- E.g. Group correlation
- E.g. Information theoretic filtering methods such as Markov blanket

(I) Filtering : Summary

Filter Methods

- usually fast
- provide generic selection of features, not tuned by given learner (universal)
- this is also often criticised (feature set not optimized for used learner)
- Often used as a preprocessing step for other methods

(I) Filtering : (many choices)

Method		X			Y			Comments
Name	Formula	B	M	C	B	M	C	
Bayesian accuracy	Eq. 3.1	+	s		+	s		Theoretically the golden standard, rescaled Bayesian relevance Eq. 3.2.
Balanced accuracy	Eq. 3.4	+	s		+	s		Average of sensitivity and specificity; used for unbalanced dataset, same as AUC for binary targets.
Bi-normal separation	Eq. 3.5	+	s		+	s		Used in information retrieval.
F-measure	Eq. 3.7	+	s		+	s		Harmonic of recall and precision, popular in information retrieval.
Odds ratio	Eq. 3.6	+	s		+	s		Popular in information retrieval.
Means separation	Eq. 3.10	+	i	+	+			Based on two class means, related to Fisher's criterion.
T-statistics	Eq. 3.11	+	i	+	+			Based also on the means separation.
Pearson correlation	Eq. 3.9	+	i	+	+	i	+	Linear correlation, significance test Eq. 3.12, or a permutation test.
Group correlation	Eq. 3.13	+	i	+	+	i	+	Pearson's coefficient for subset of features.
χ^2	Eq. 3.8	+	s		+	s		Results depend on the number of samples m.
Relief	Eq. 3.15	+	s	+	+	s	+	Family of methods, the formula is for a simplified version ReliefX, captures local correlations and feature interactions.
Separability Split Value	Eq. 3.41	+	s	+	+	s		Decision tree index.
Kolmogorov distance	Eq. 3.16	+	s	+	+	s	+	Difference between joint and product probabilities.
Bayesian measure	Eq. 3.16	+	s	+	+	s	+	Same as Vajda entropy Eq. 3.23 and Gini Eq. 3.39.
Kullback-Leibler divergence	Eq. 3.20	+	s	+	+	s	+	Equivalent to mutual information.
Jeffreys-Matusita distance	Eq. 3.22	+	s	+	+	s	+	Rarely used but worth trying.
Value Difference Metric	Eq. 3.22	+	s		+	s		Used for symbolic data in similarity-based methods, and symbolic feature-feature correlations.
Mutual Information	Eq. 3.29	+	s	+	+	s	+	Equivalent to information gain Eq. 3.30.
Information Gain Ratio	Eq. 3.32	+	s	+	+	s	+	Information gain divided by feature entropy, stable evaluation.
Symmetrical Uncertainty	Eq. 3.35	+	s	+	+	s	+	Low bias for multivalued features.
J-measure	Eq. 3.36	+	s	+	+	s	+	Measures information provided by a logical rule.
Weight of evidence	Eq. 3.37	+	s	+	+	s	+	So far rarely used.
MDL	Eq. 3.38	+	s		+	s		Low bias for multivalued features.

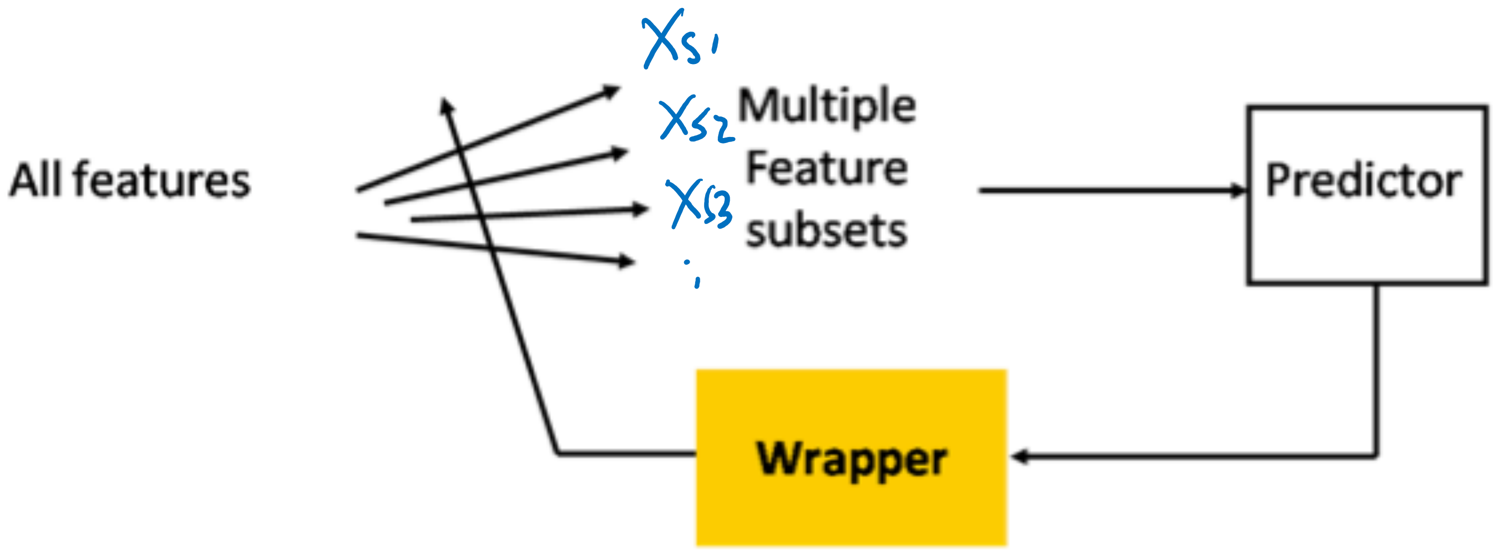
Guyon-Elisseeff, JMLR 2004; Springer 2006

(2) Wrapper

- Wrapper approach:

uses a predictor to assess (many) features or feature subsets.

Wrapper Methods



(2) Wrapper : Feature Subset Selection

Wrapper Methods

- Learner is considered a black-box
- Interface of the black-box is used to score subsets of variables according to the predictive power of the learner when using the subsets.

- Results vary for different learners

(b). Search: even more search strategies for selecting feature subset

$p \longrightarrow 2^p$ feature subsets

- **Forward selection** or **backward elimination.**
- **Beam search:** keep k best path at each step.
- **GSFS:** generalized sequential forward selection – when (n-k) features are left try all subsets of g features. More trainings at each step, but fewer steps.
- **PTA(l,r):** plus l , take away r – at each step, run SFS l times then SBS r times.
- **Floating search**: One step of SFS (resp. SBS), then SBS (resp. SFS) as long as we find better subsets than those of the same size obtained so far.

From Dr. **Isabelle Guyon**

(3) Embedded

- Embedding approach:

  uses a predictor to build a (single) model with a subset of features that are internally selected.

lasso

elastiNet

In practice…

- No method is universally better:
  - wide variety of types of variables, data distributions, learning machines, and objectives.
- Feature selection is not always necessary to achieve good performance.

From Dr. **Isabelle Guyon**

Today: Dimensionality Reduction (Two Ways)

Feature extraction: finds a set of new features (i.e., through some mapping f()) from the existing features.

The mapping f() could be linear or non-linear

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix} \xrightarrow{f()} \mathbf{h} = \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_K \end{bmatrix}$$

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K<<N

Feature Extraction

- Linear combinations are particularly attractive because they are simpler to compute and analytically tractable.

$\rightarrow p \times K$

- Given $x \in R^p$, find an N x K matrix U such that:

$$y = U^T x \in R^K \text{ where } K<P$$

$$R^p \xrightarrow{f(\,)} R^K$$

This is a projection from the N-dimensional space to a K-dimensional space.

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix} \xrightarrow{U^T} \mathbf{h} = \begin{bmatrix} h_1 \\ h_2 \\ \vdots \\ h_K \end{bmatrix}$$

$$f(x) = \underset{K \times P}{U^T} \underset{P \times 1}{x}$$

Feature Extraction (cont'd)

- From a mathematical point of view, finding an optimum mapping $\mathbf{y}=f(\mathbf{x})$ is equivalent to optimizing an **objective** function.

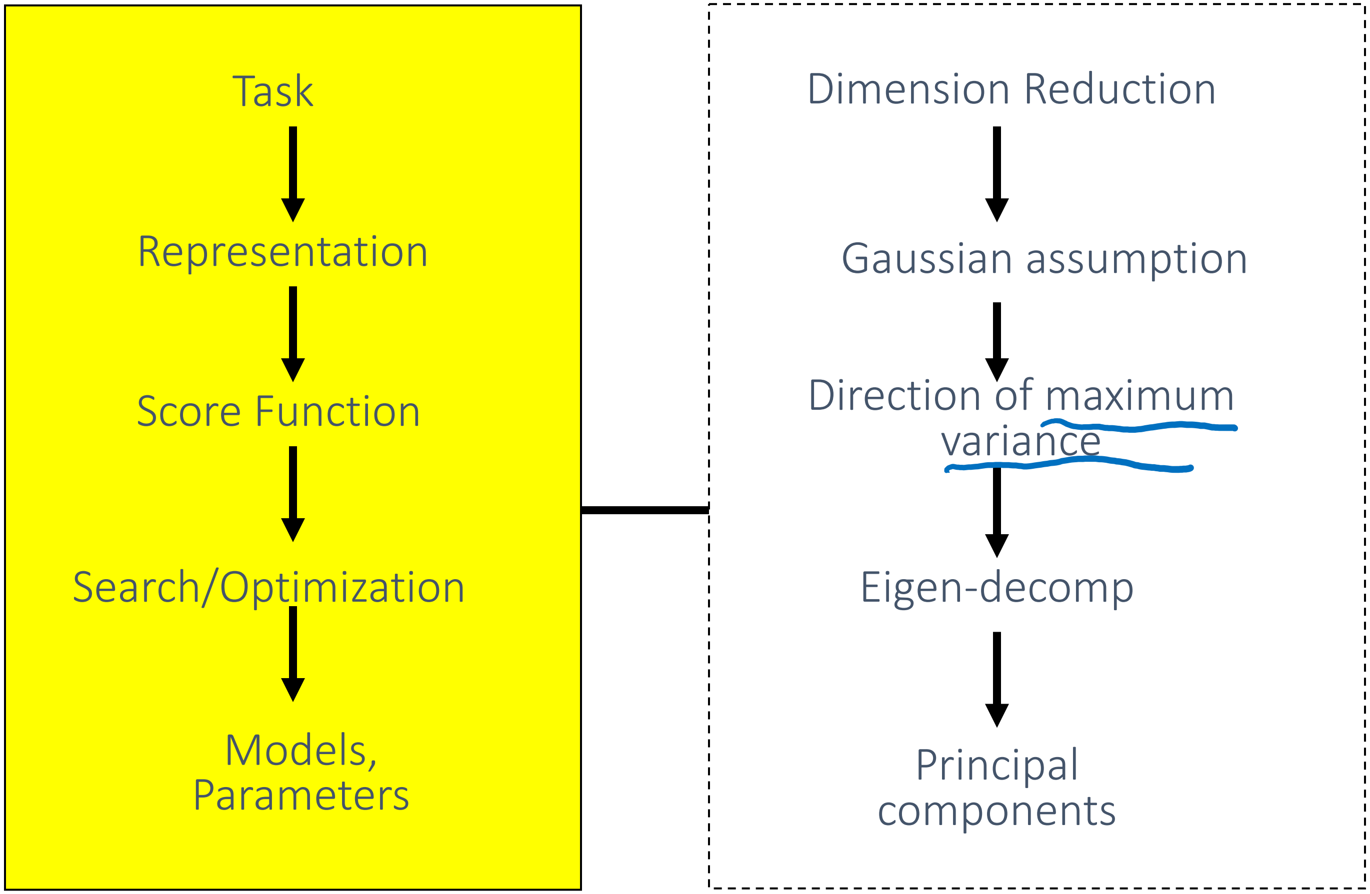
- Different methods use different objective functions, e.g.,
  - Information Loss: The goal is to represent the data as accurately as possible (i.e., no loss of information) in the lower-dimensional space.
  - Discriminatory Information: The goal is to enhance the class-discriminatory information in the lower-dimensional space.

Feature Extraction (cont'd)

- Commonly used linear feature extraction methods:
  - Principal Components Analysis (PCA): Seeks a projection that **preserves** as much **information** in the data as possible.
  - Linear Discriminant Analysis (LDA): Seeks a projection that **best discriminates** the data.

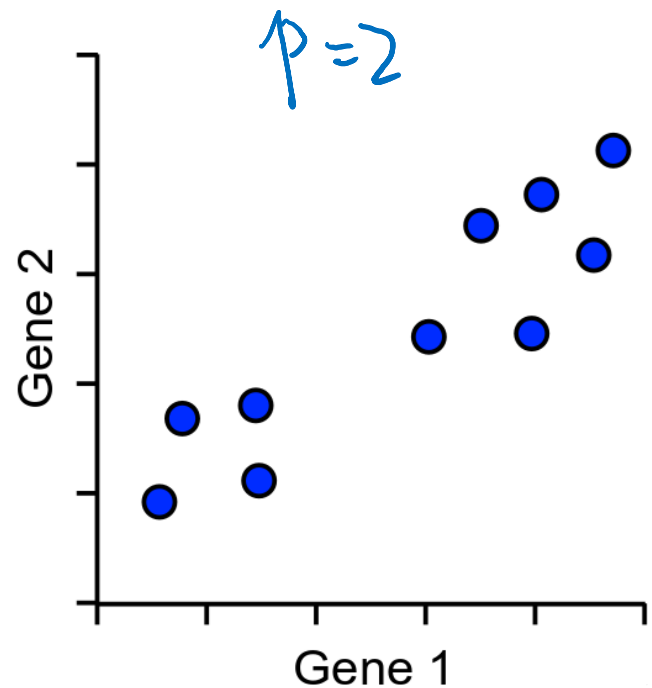
- More methods:
  - Retaining interesting directions (Projection Pursuit),
  - Making features as independent as possible (Independent Component Analysis or ICA),
  - Embedding to lower dimensional manifolds (Isomap, Locally Linear Embedding or LLE).

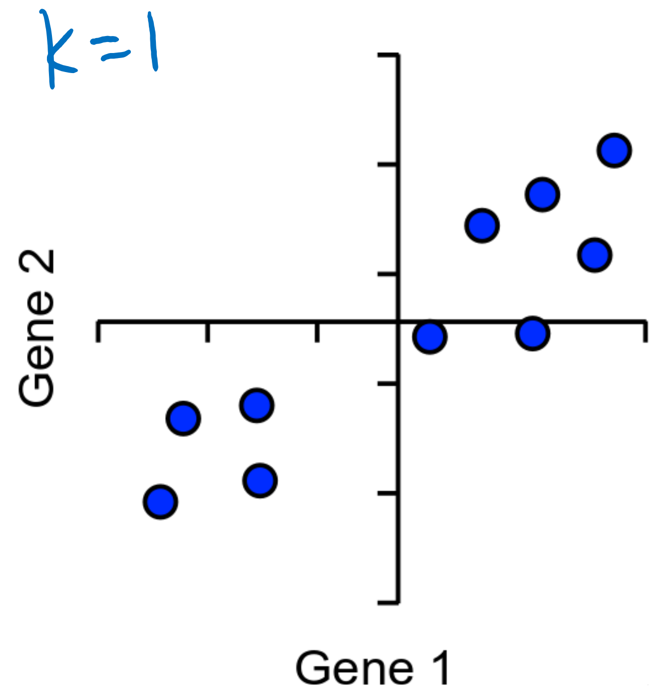
Principal Component Analysis



How does PCA work?

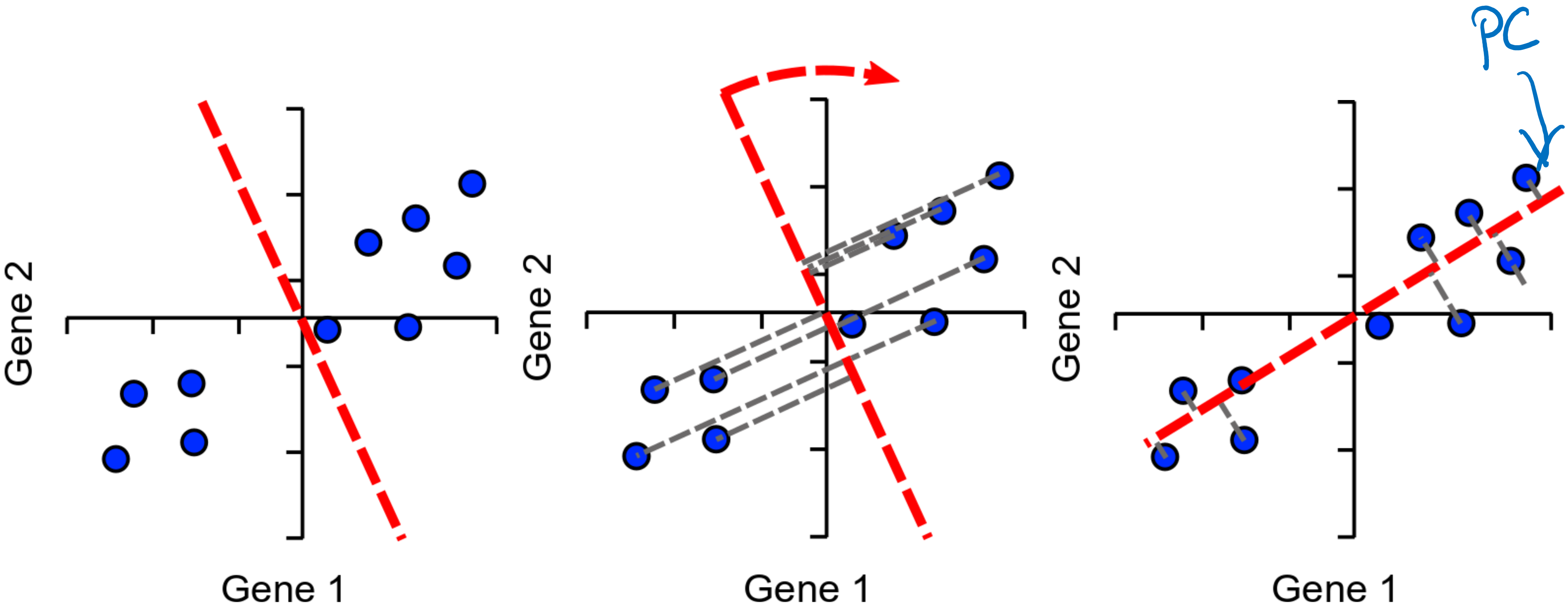
- Principal Components Analysis (PCA): approximating a high-dimensional data set with a lower-dimensional linear subspace





How does PCA work?

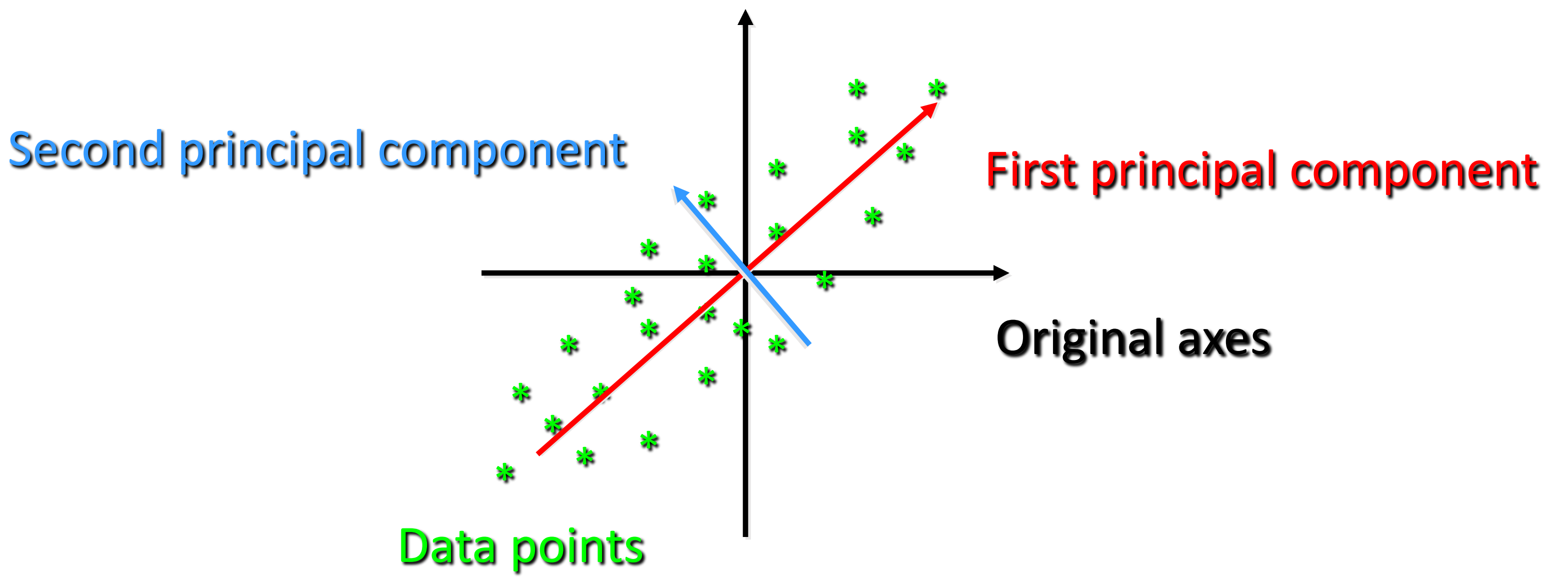
- Find line of best fit, passing through the origin



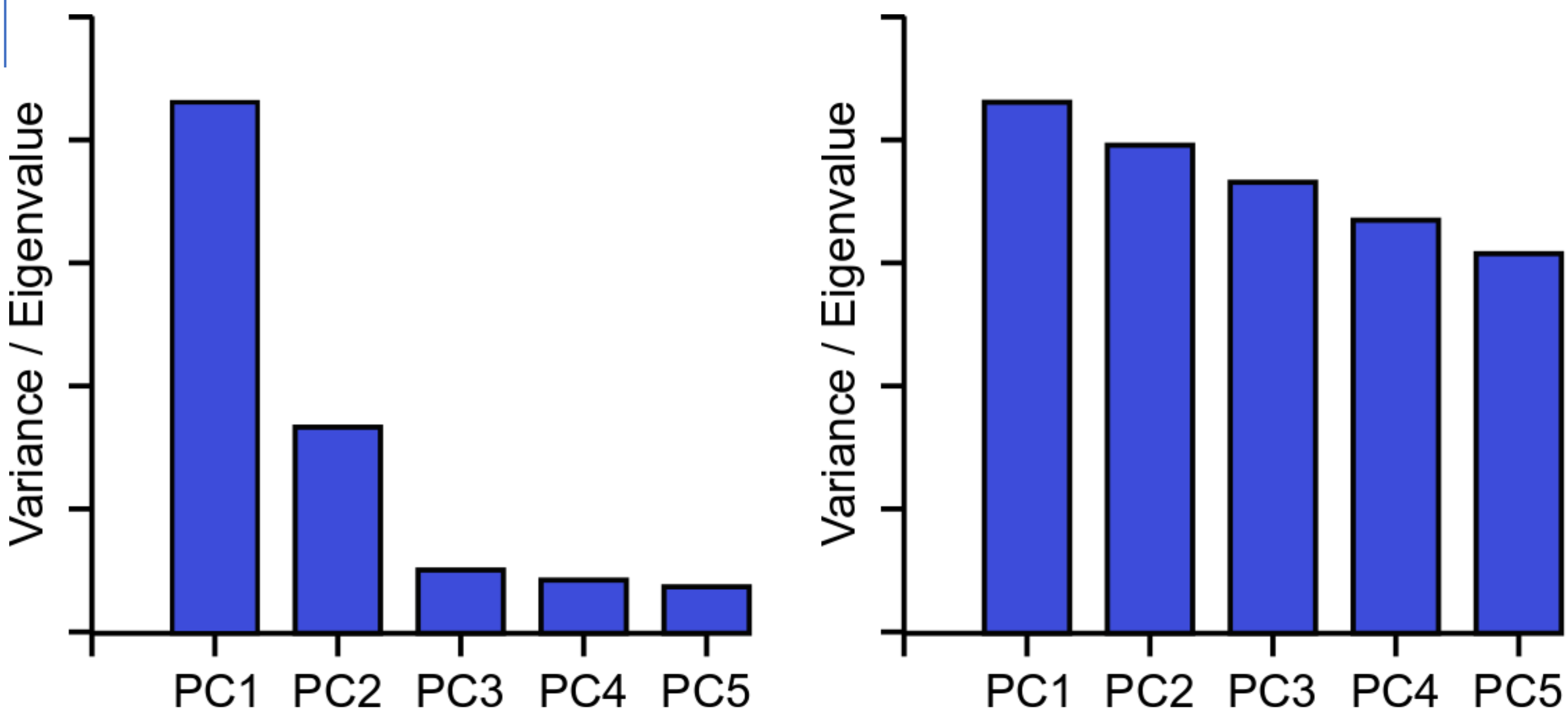
How does PCA work? Explaining Variance

- Each PC always explains some proportion of the total variance in the data. Between them they explain everything
  - PC1 always explains the most
  - PC2 is the next highest etc. etc.

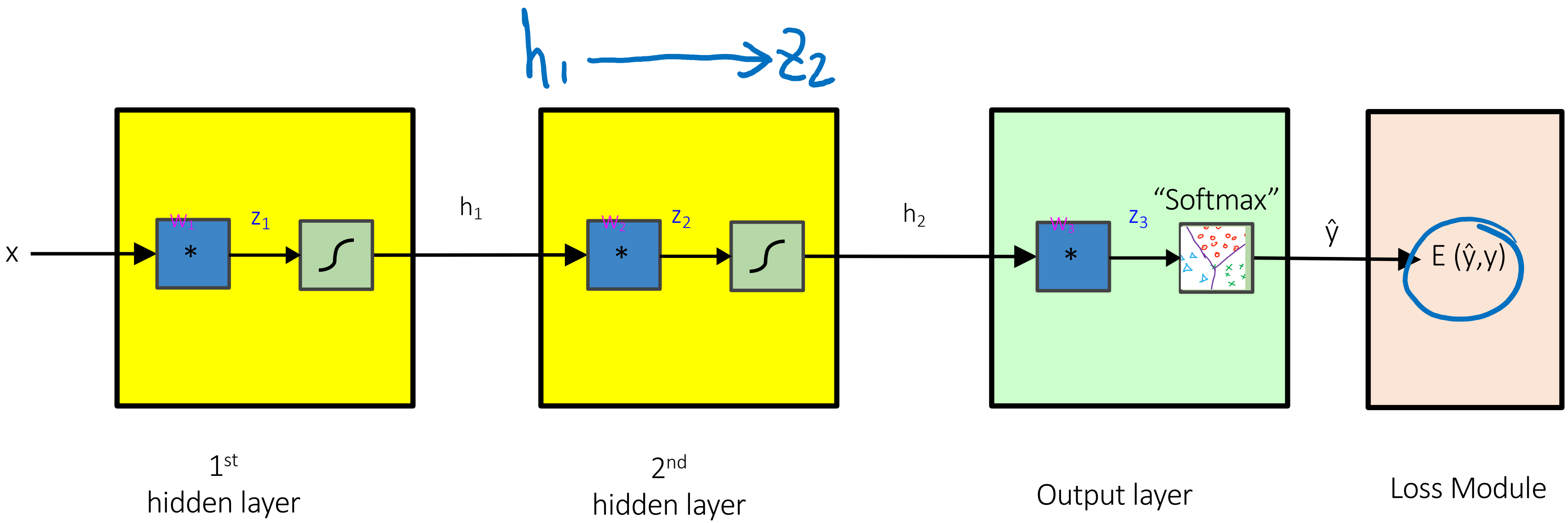
p → PCs



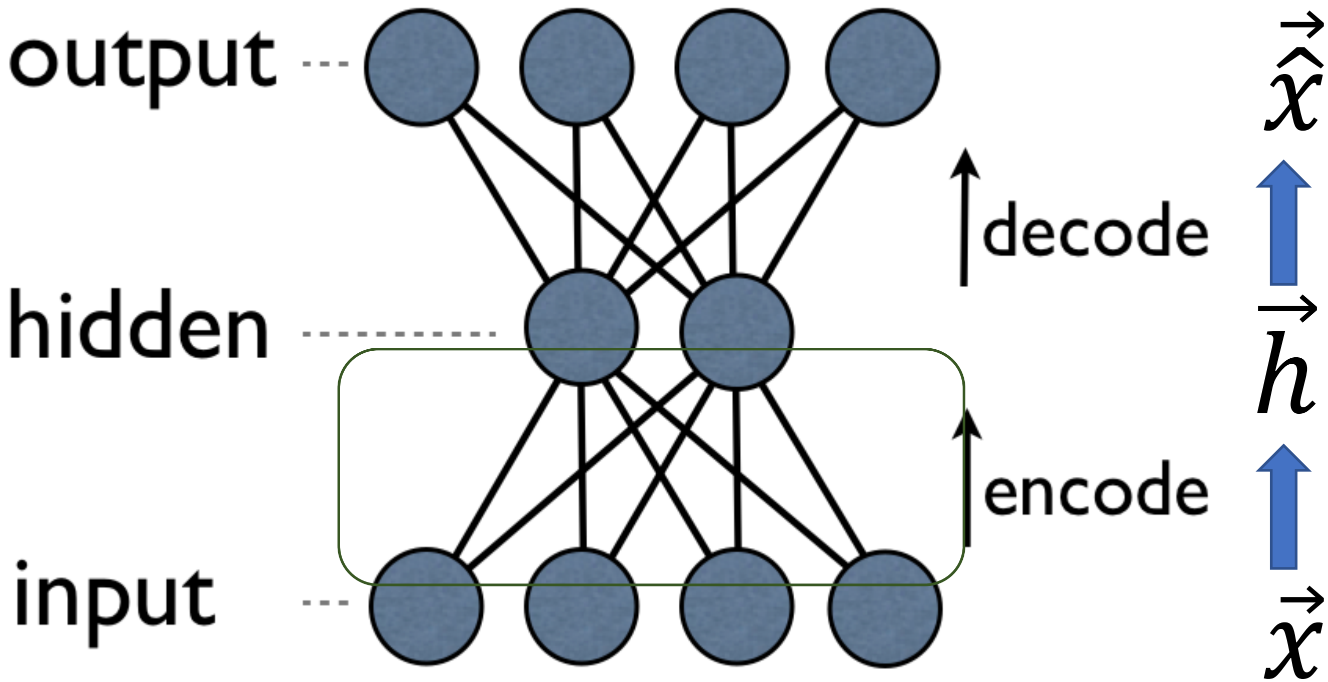
Explaining Variance – Scree Plots



Recap: “Block View”



an auto-encoder-decoder is trained to reproduce the input



Minimize diff

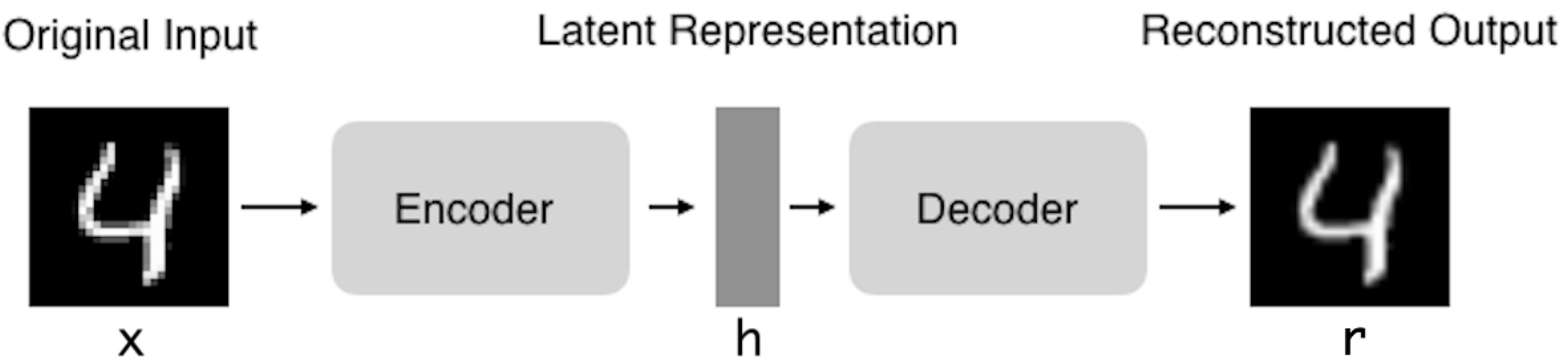
$$|\vec{\hat{x}} - \vec{x}|$$

Reconstruction Loss: force the 'hidden layer' units to become good / reliable feature detectors

https://www.macs.hw.ac.uk/~dwcorne/Teaching/introdl.ppt

Autoencoders: structure

- Encoder: compress input into a latent-space of usually smaller dimension. $h = f(x)$
- Decoder: reconstruct input from the latent space. $r = g(f(x))$ with r as close to x as possible

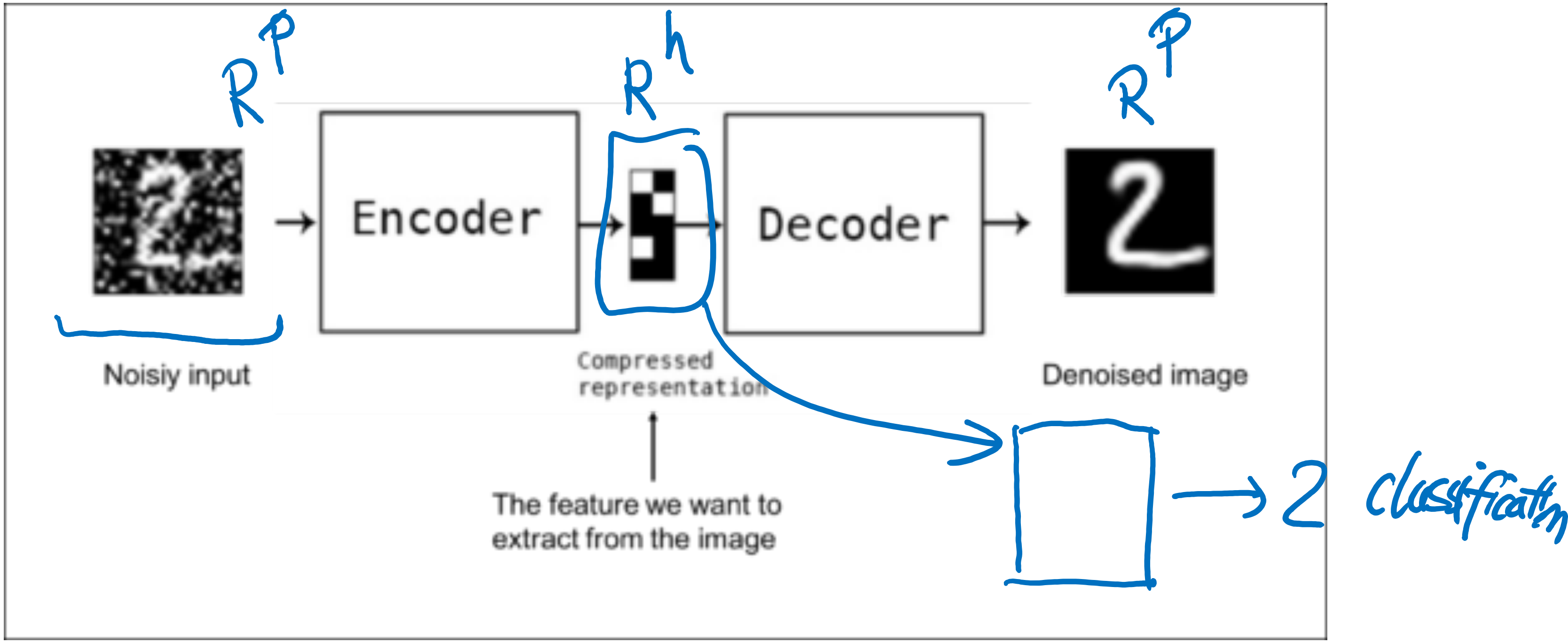


https://towardsdatascience.com/deep-inside-autoencoders-7e41f319999f

Autoencoders: many variations

- Denoising: input clean image + noise and train to reproduce the clean image.

- Neural network autoencoders
  - Can learn nonlinear dependencies
  - Can use convolutional layers
  - Can use transfer learning



https://www.edureka.co/blog/autoencoders-tutorial/

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K<<N

Thank You

UVA CS 4774:
Machine Learning

Lecture 14: Dimension Reduction

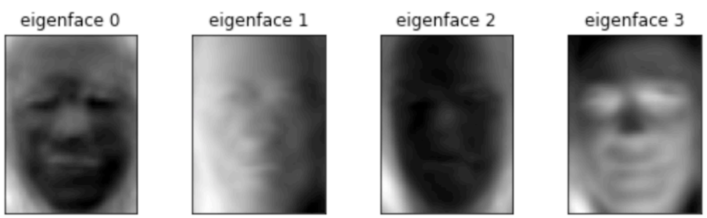
Module IV
Notebook PCA

Dr. Yanjun Qi

University of Virginia
Department of Computer Science

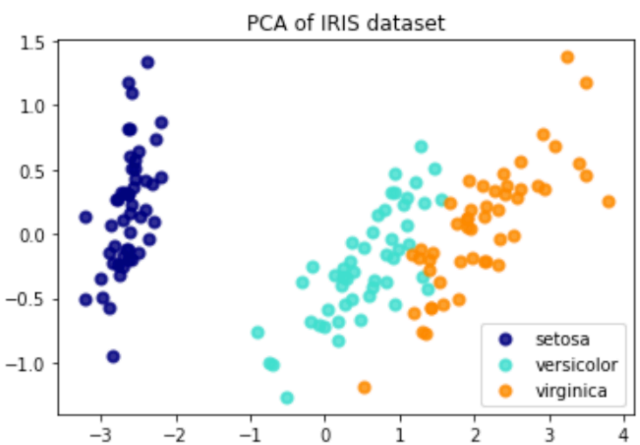
I will run notebook using PCA on face images / Iris

```
# plot the gallery of the most significative eigenfaces

eigenface_titles = ["eigenface %d" % i for i in range(eigenfaces.shape[0])]
plot_gallery(eigenfaces, eigenface_titles, h, w)

plt.show()
```



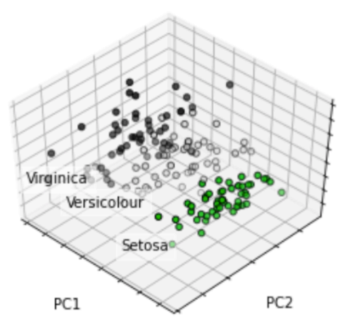
https://drive.google.com/file/d/10zwaPdAYdz9kzCg5Qh03idASiCm9sKUw/view?usp=sharing

```
explained variance ratio (first two components): [0.92461872 0.05306648]
Text(0.5, 1.0, 'PCA of IRIS dataset')
```




```
ax.set_xlabel('PC1')
ax.set_ylabel('PC2')
ax.set_zlabel('PC3')
```

```
explained variance ratio (first two components): [0.92461872 0.05306648 0.01710261]
Text(0.5, 0, 'PC3')
```

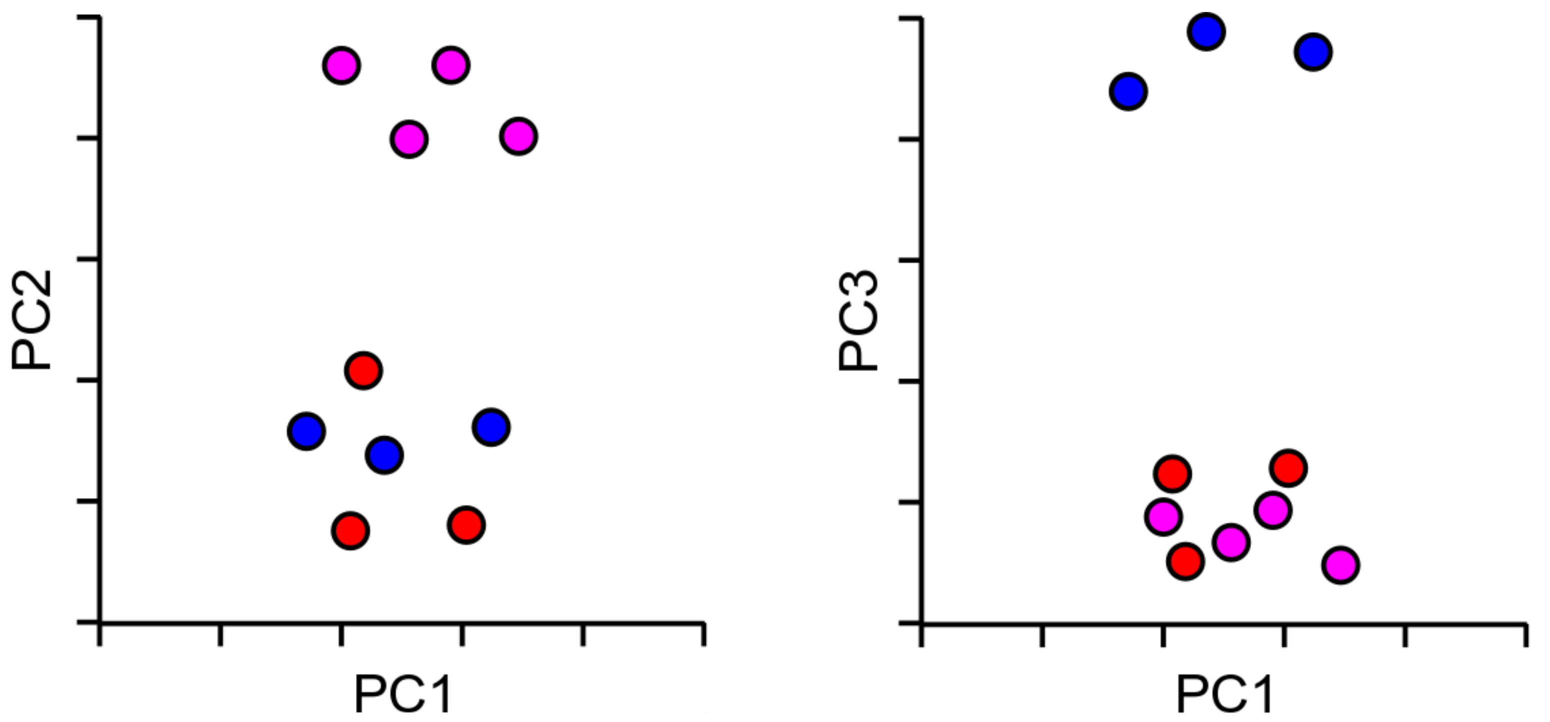


References

- Hastie, Trevor, et al. *The elements of statistical learning*. Vol. 2. No. 1. New York: Springer, 2009.
- Dr. S. Narasimhan's PCA lectures
- Prof. Derek Hoiem's eigenface lecture

So PCA is great then?

- Kind of...

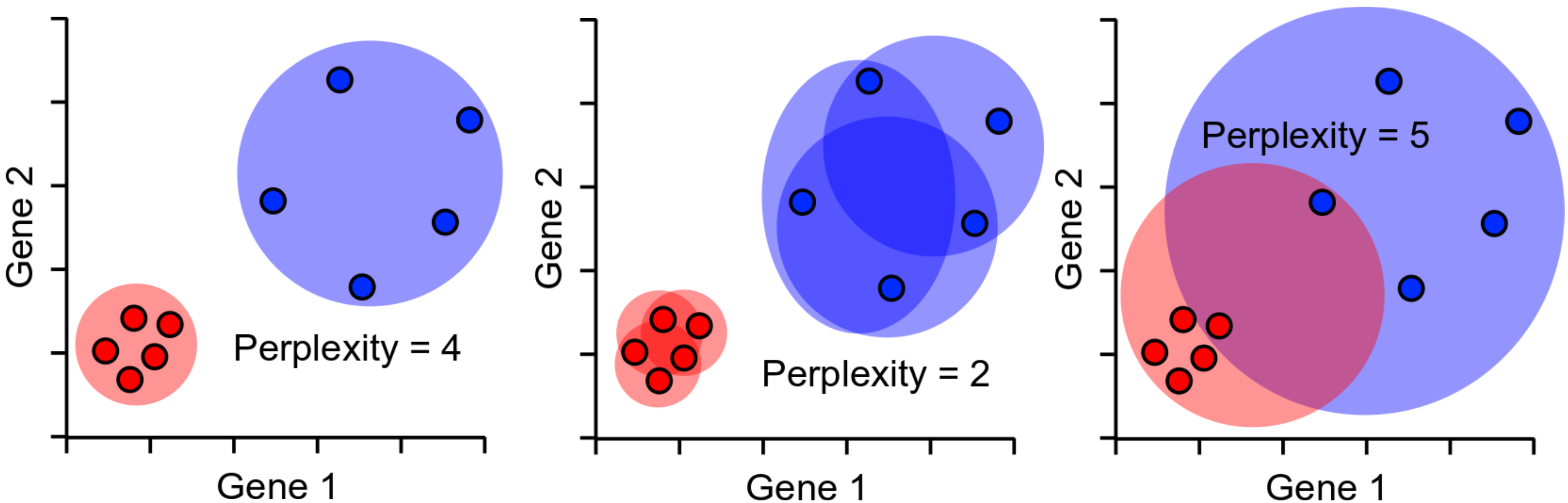


tSNE to the rescue…

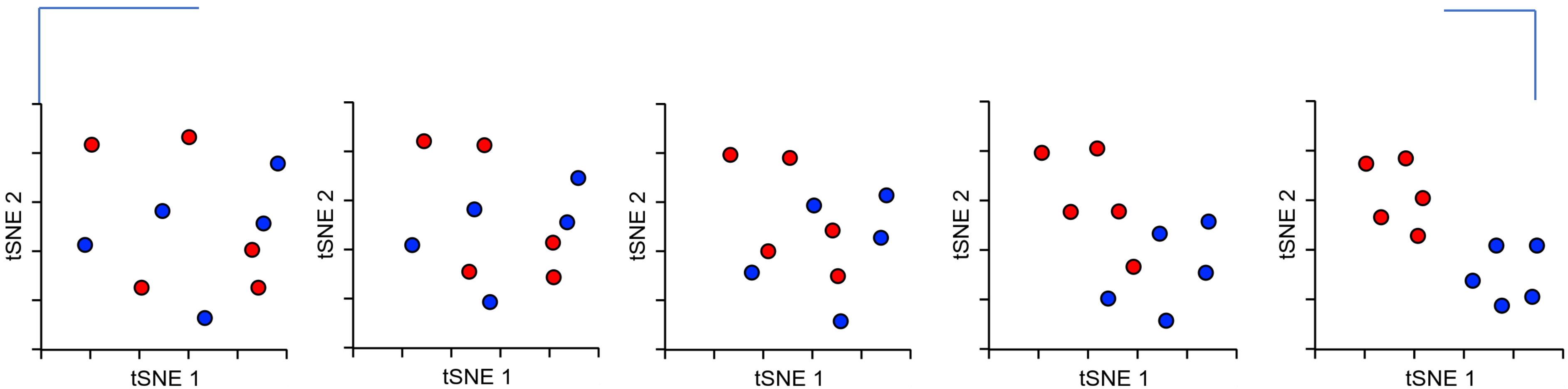
- T-Distributed Stochastic Neighbour Embedding

- Aims to solve the problems of PCA
  - Non-linear scaling to represent changes at different levels
  - Optimal separation in 2-dimensions

Perplexity Robustness



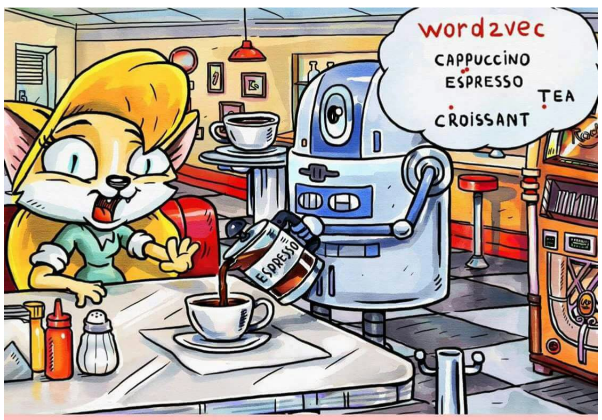
tSNE Projection



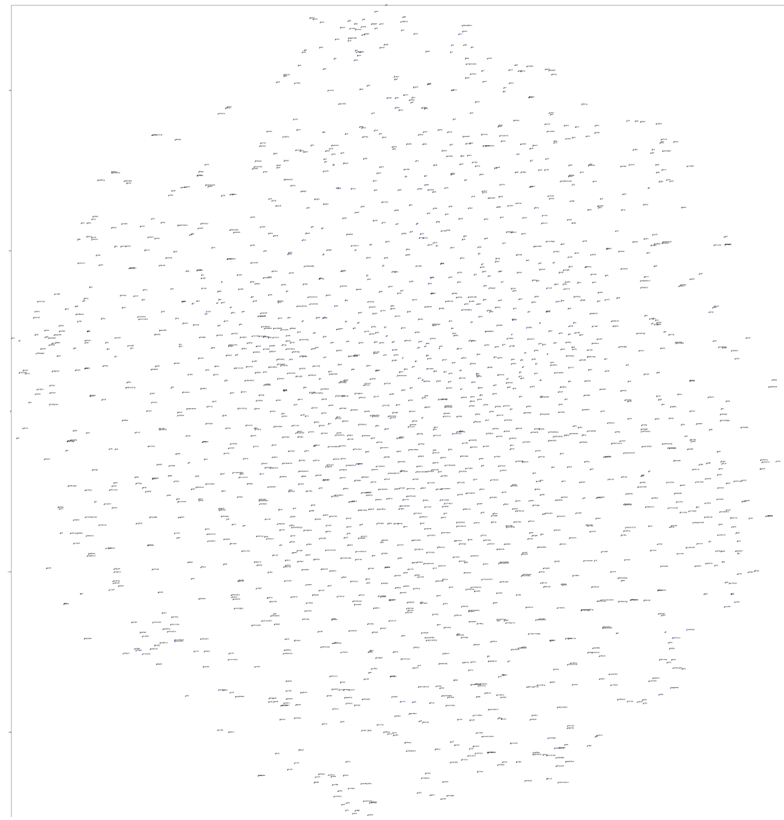
- X and Y don’t mean anything (unlike PCA)
- Distance doesn’t mean anything (unlike PCA)
- Close proximity is highly informative
- Distant proximity isn’t very interesting
- Can’t rationalise distances, or add in more data

Word2vec

- Input: large corpus of text
- Embed words into a high-dim space
  - words with common contexts in the corpus are close in the space



- Espresso? But I ordered a cappuccino!
- Don't worry, the cosine distance between them is so small that they are almost the same thing.



http://nlp.yvespeirsman.be/blog/visualizing-word-embeddings-with-tsne/