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# UVA CS 4774: Machine Learning

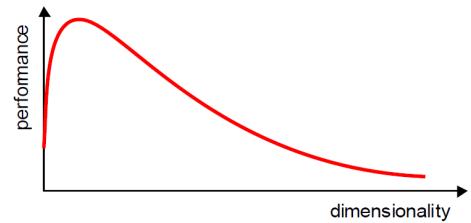
## Lecture 14: Dimension Reduction

Dr. Yanjun Qi

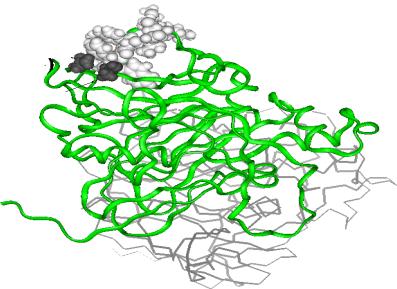
University of Virginia  
Department of Computer Science

# 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

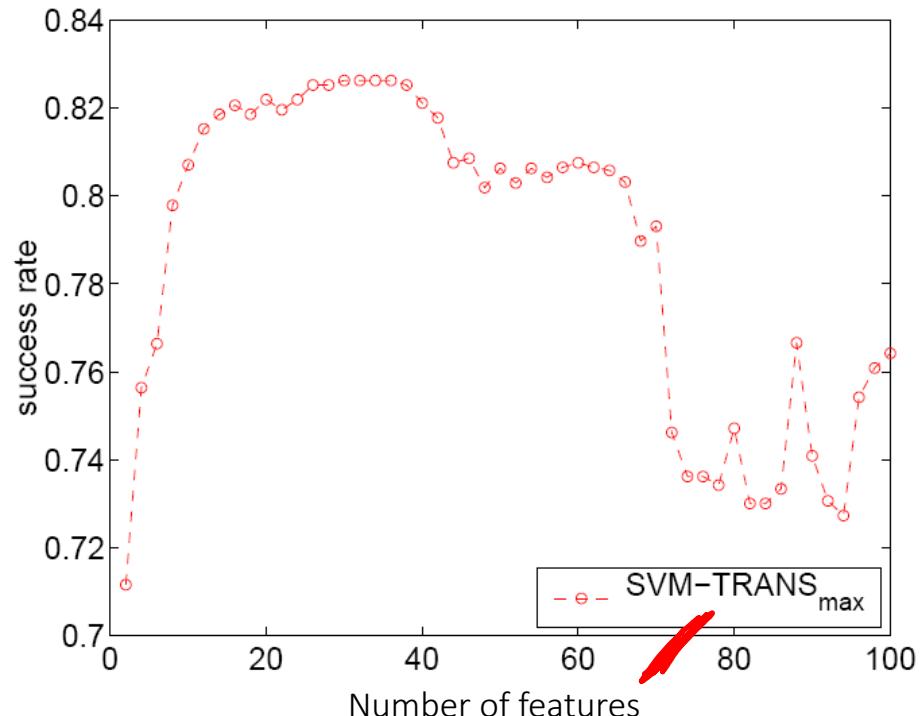


Binding to Thrombin

(DuPont Pharmaceuticals)

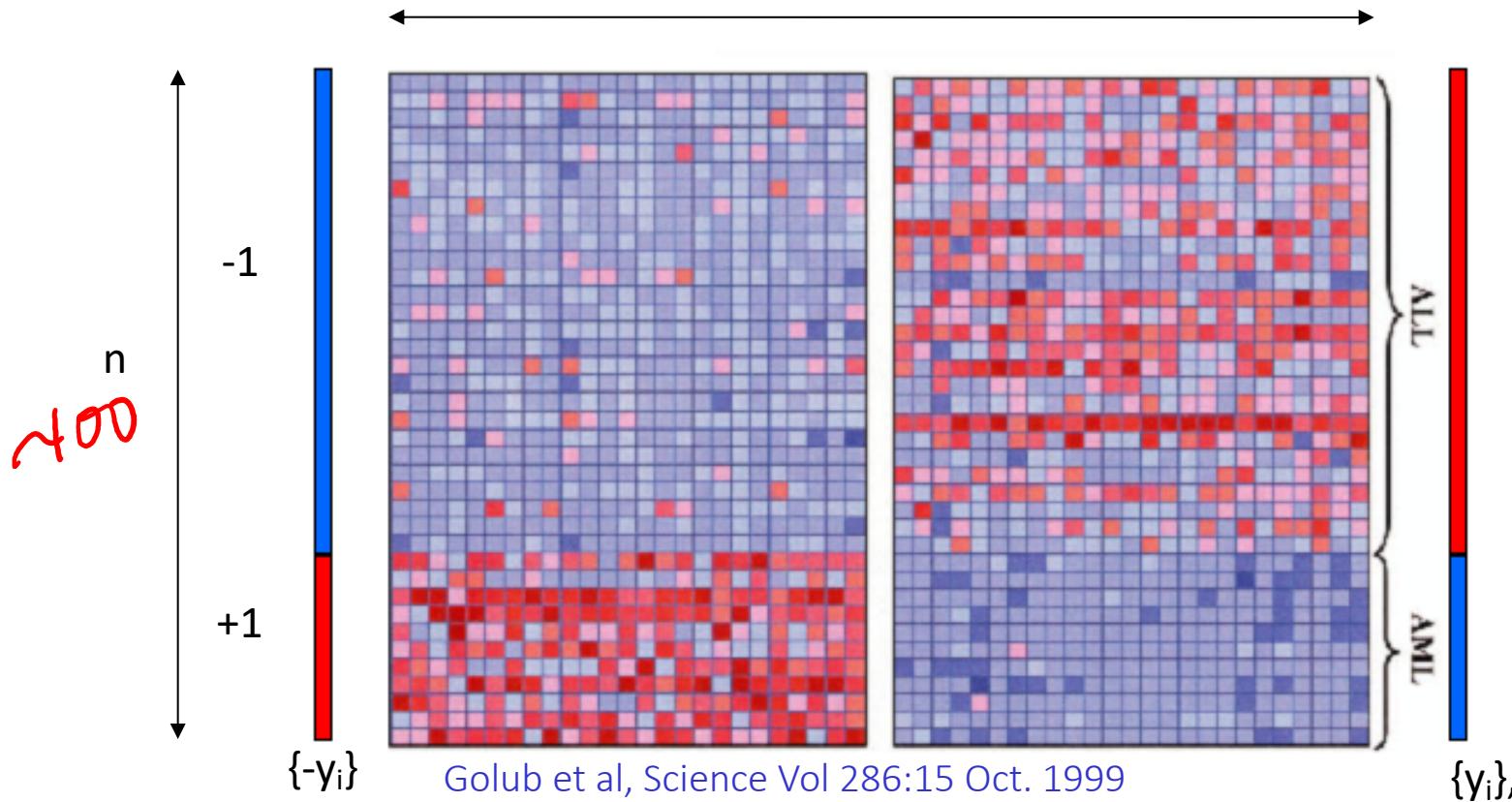
[2543 compounds tested] for their ability to bind to a target site on thrombin, a key receptor in blood clotting; 192 “active” (bind well); the rest “inactive”. Training set (1909 compounds) more depleted in active compounds.

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

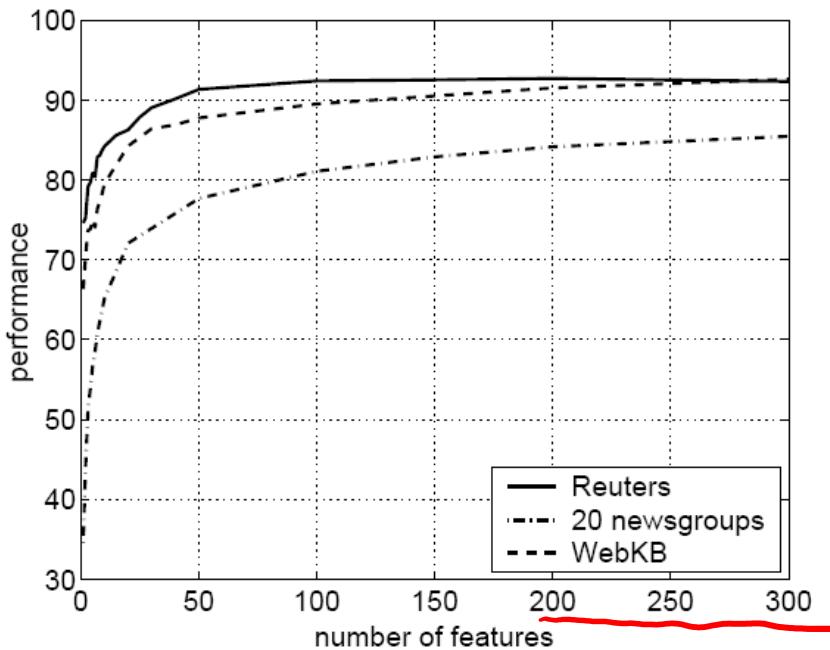


# e.g., Leukemia Diagnosis

$p' \sim 20k$



# e.g., Text Categorization with many BOW features



Reuters: 21578 news wire, 114 semantic categories.

20 newsgroups: [19997] articles, 20 categories.  
n

WebKB: 8282 web pages, 7 categories.

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

[↑P)

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)

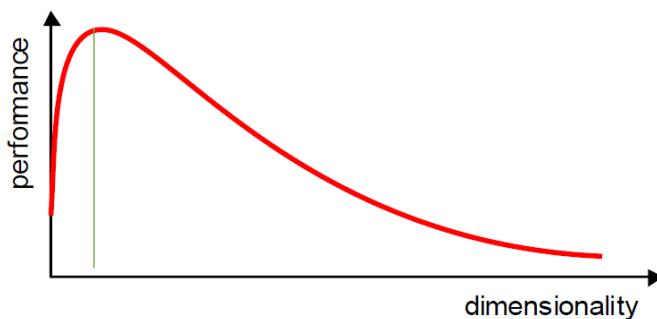
III Dependency relations (nsubj,advmod,...)

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

# 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)

# Today: Dimensionality Reduction (Two Ways)

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

Feature selection: chooses a subset of the **original** features.



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

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

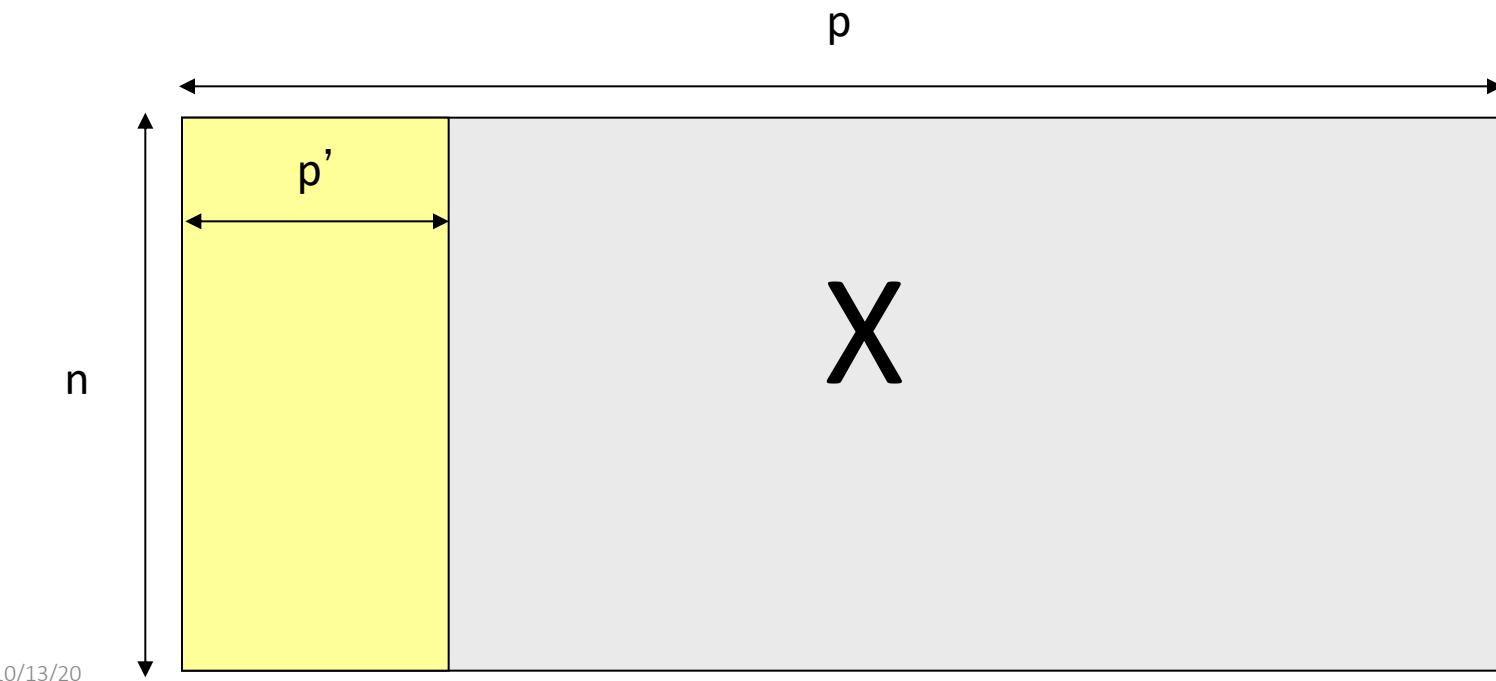
$K \ll N$

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

$K \ll N$

# Feature Selection

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

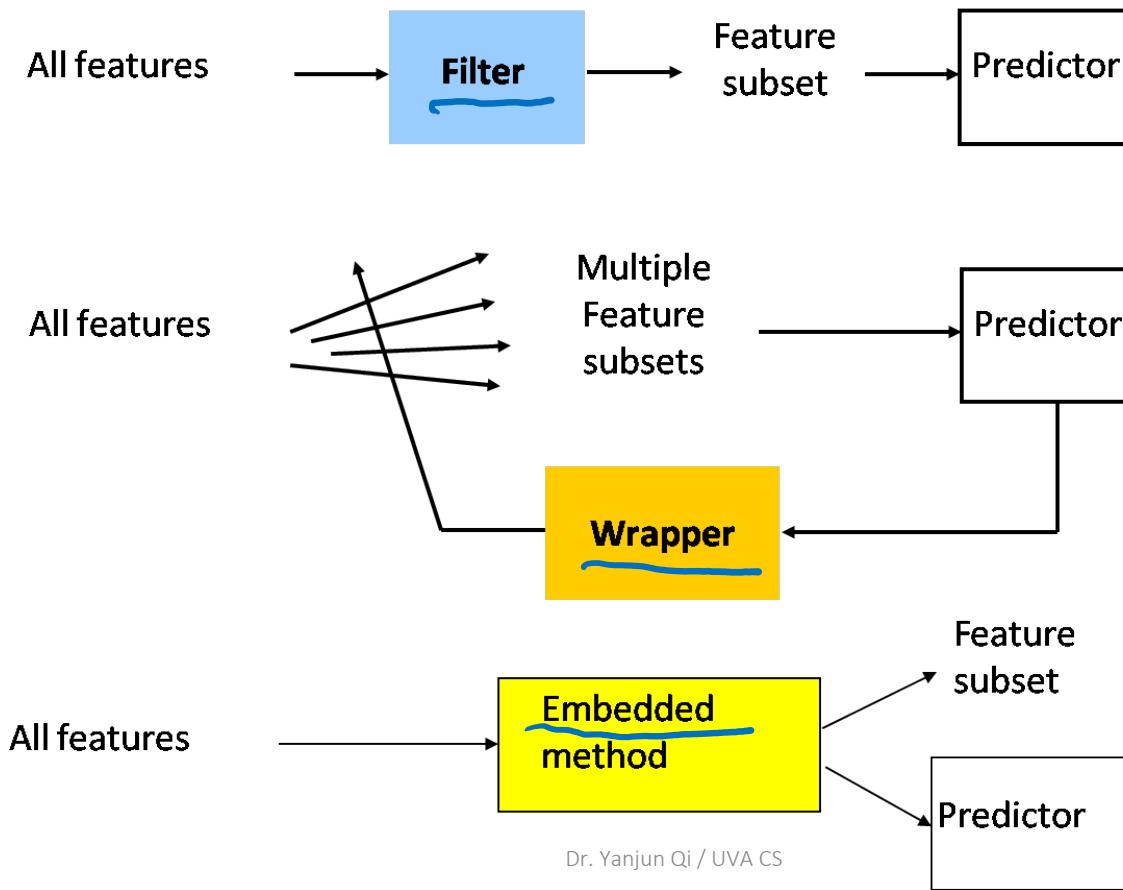


# Summary: Feature Selection

- 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

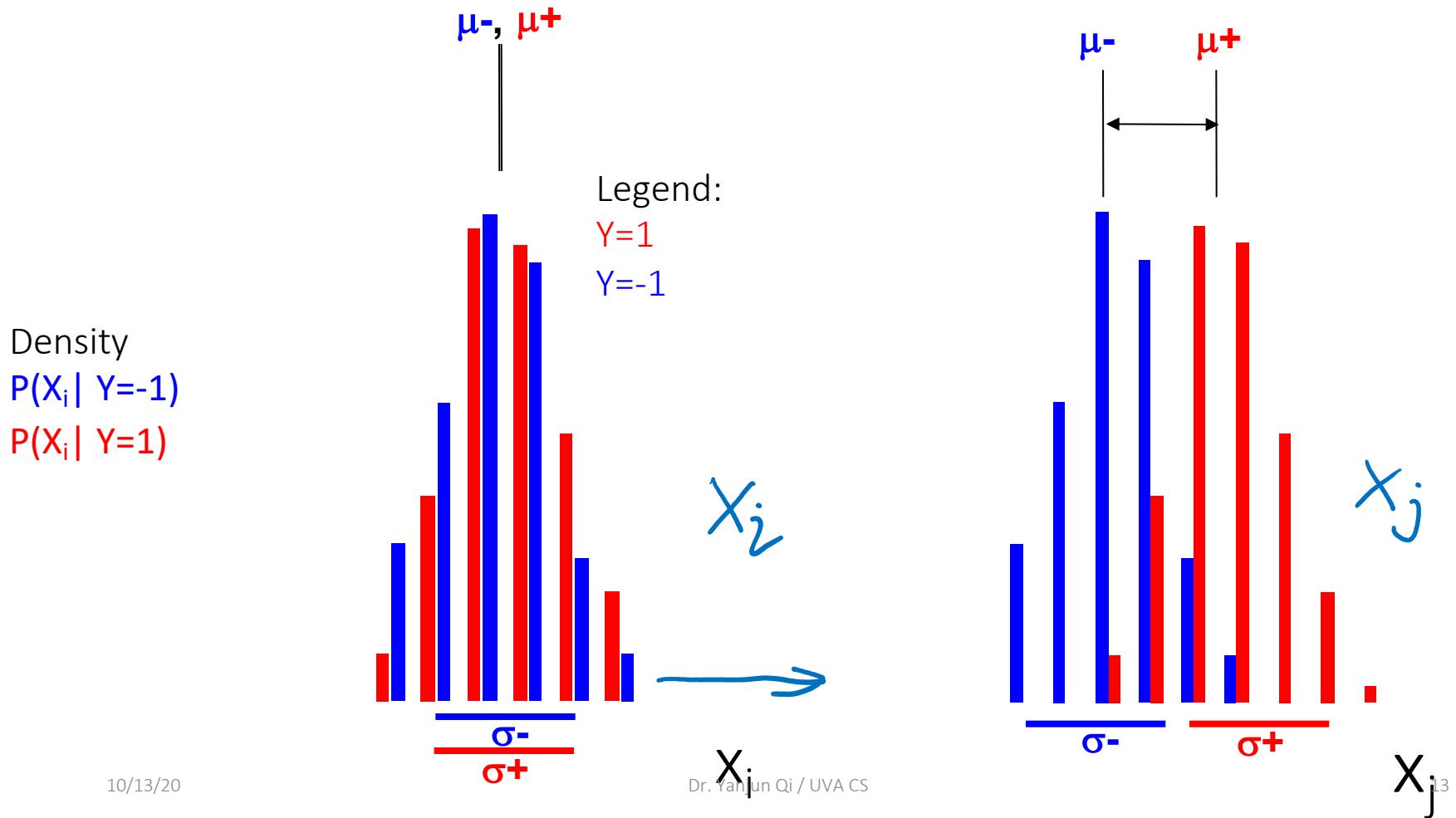
- Main goal: rank subsets of useful features



# (I) Filtering: univariate filtering

e.g. T-test

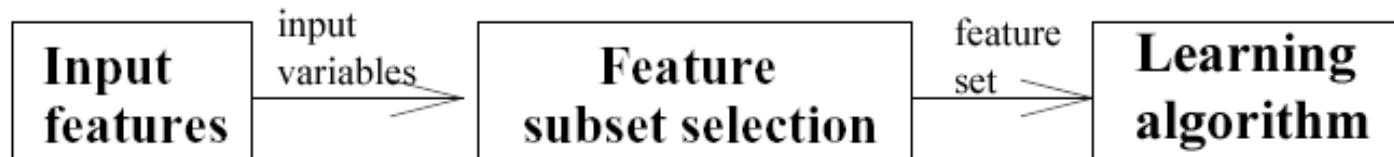
- Goal: determine the relevance of a given single feature for two classes of samples.



# (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

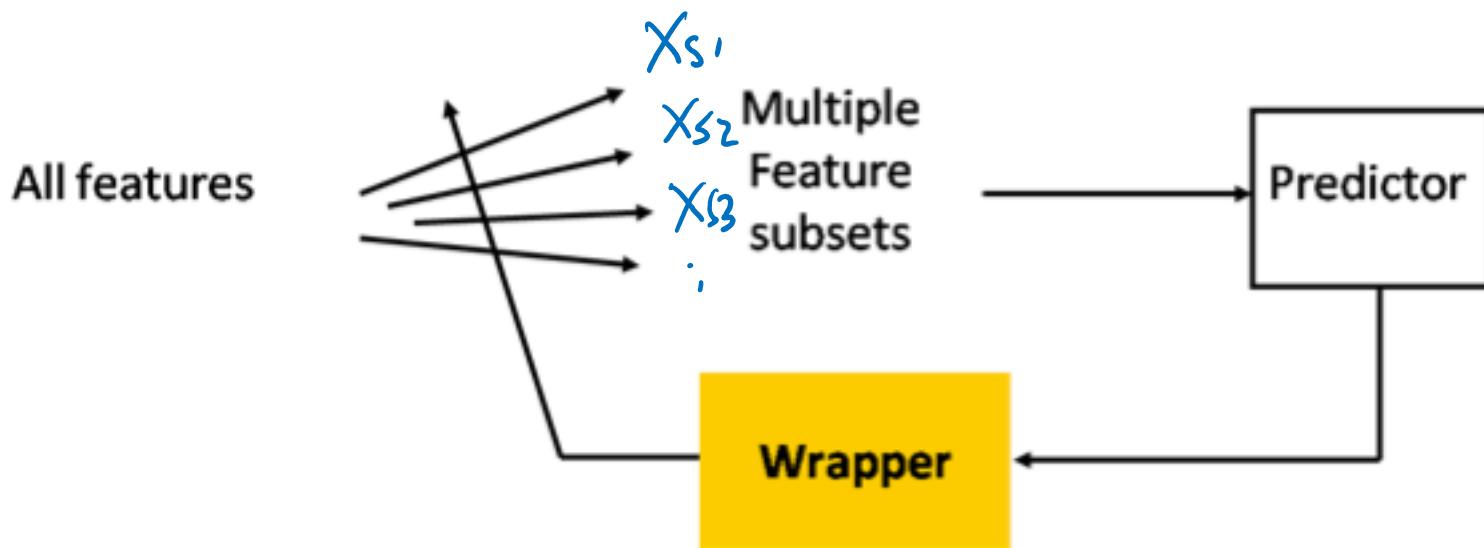
# (I) Filtering : (many choices)

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.
$\chi^2$	✓	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	10/13/20	Eq. 3.37 + s + + s +	So far rarely used.
MDL		Eq. 3.38 + s + s	Dr. Yanjun Qi / UVA CS Low bias for multivalued features.

## (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

$P \rightarrow 2^P$  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.

### (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.

# Today: Dimensionality Reduction (Two Ways)

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



Feature selection: chooses a subset of the **original** features.

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

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

$K \ll N$

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

$K \ll N$

# 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  $N \times K$  matrix  $U$  such that:

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

~~$R^P$~~   
 $R^P \xrightarrow{f(x)} R^K$

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

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

$f(x) = U^T x$   
 $P \times 1$

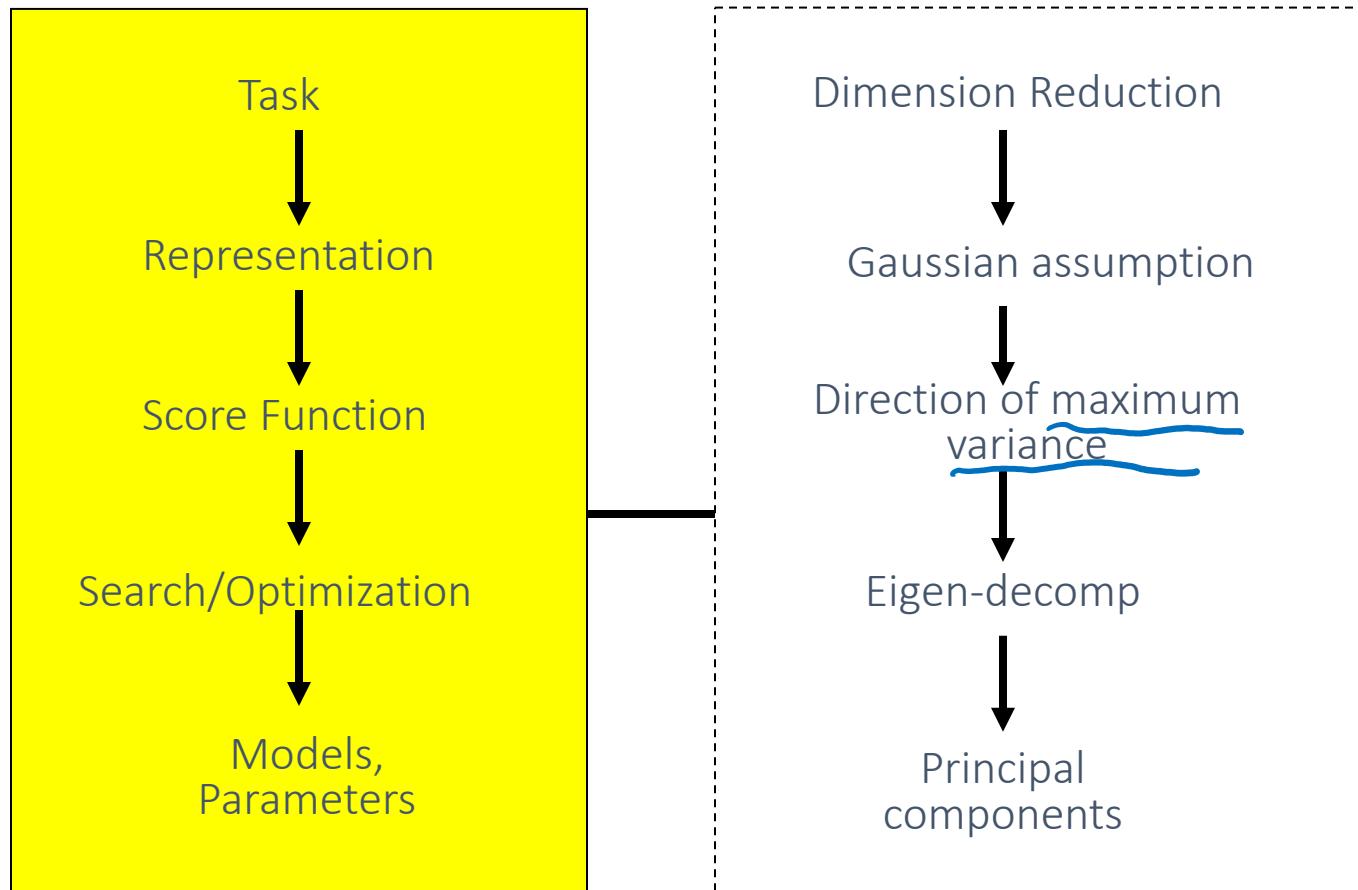
# Feature Extraction (cont'd)

- From a mathematical point of view, finding an **optimum** mapping  $\mathbf{h} = f(\mathbf{x})$  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)

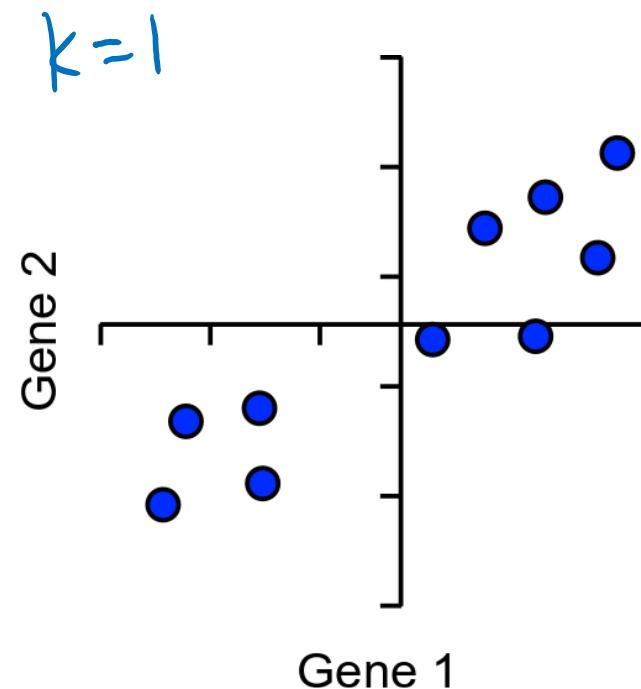
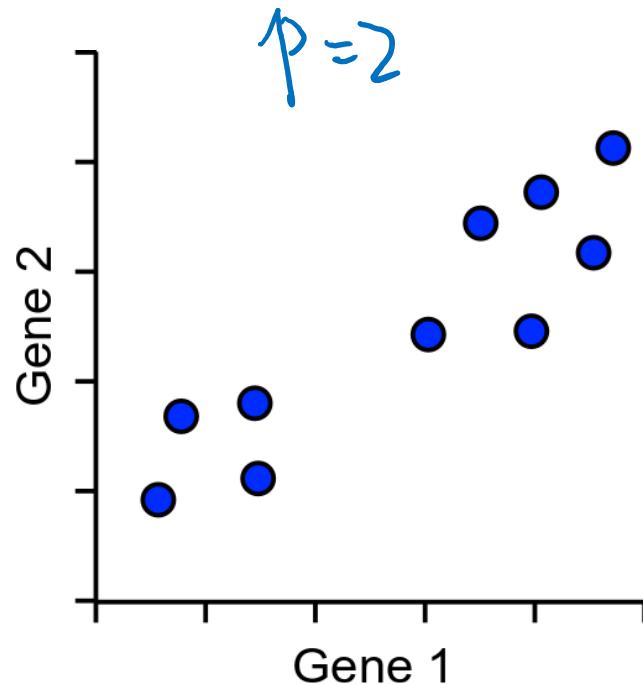
- Commonly used **linear** feature extraction methods:
  - Principal Components Analysis (PCA): Seeks a projection that **preserves** as much **information** in the data as possible.
  - Linear Discriminant Analysis (LDA): Seeks a projection that **best discriminates** the data.
- More methods:
  - Retaining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



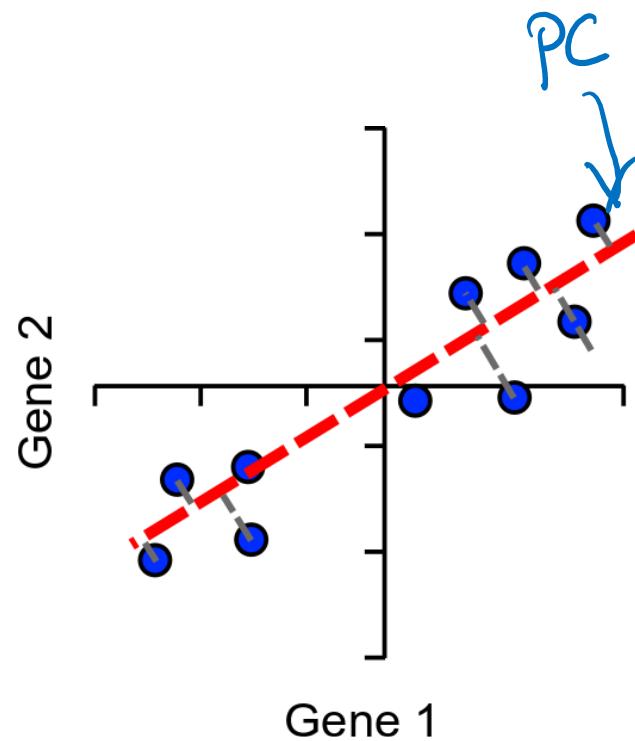
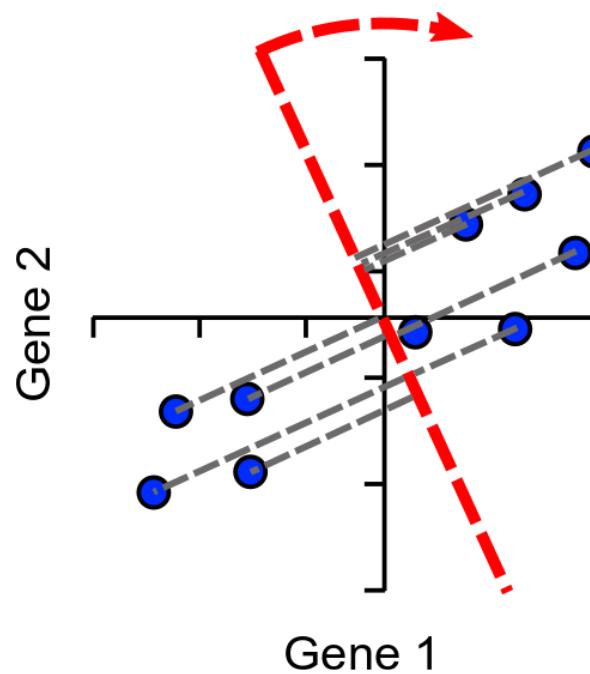
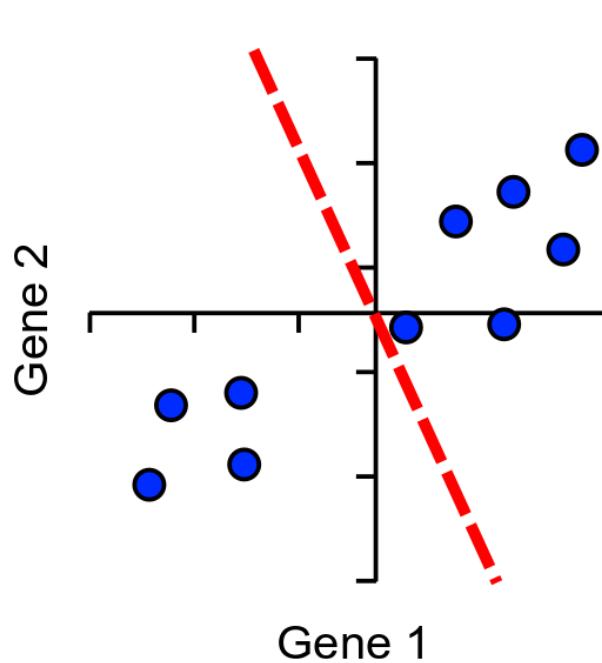
# How does PCA work?

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



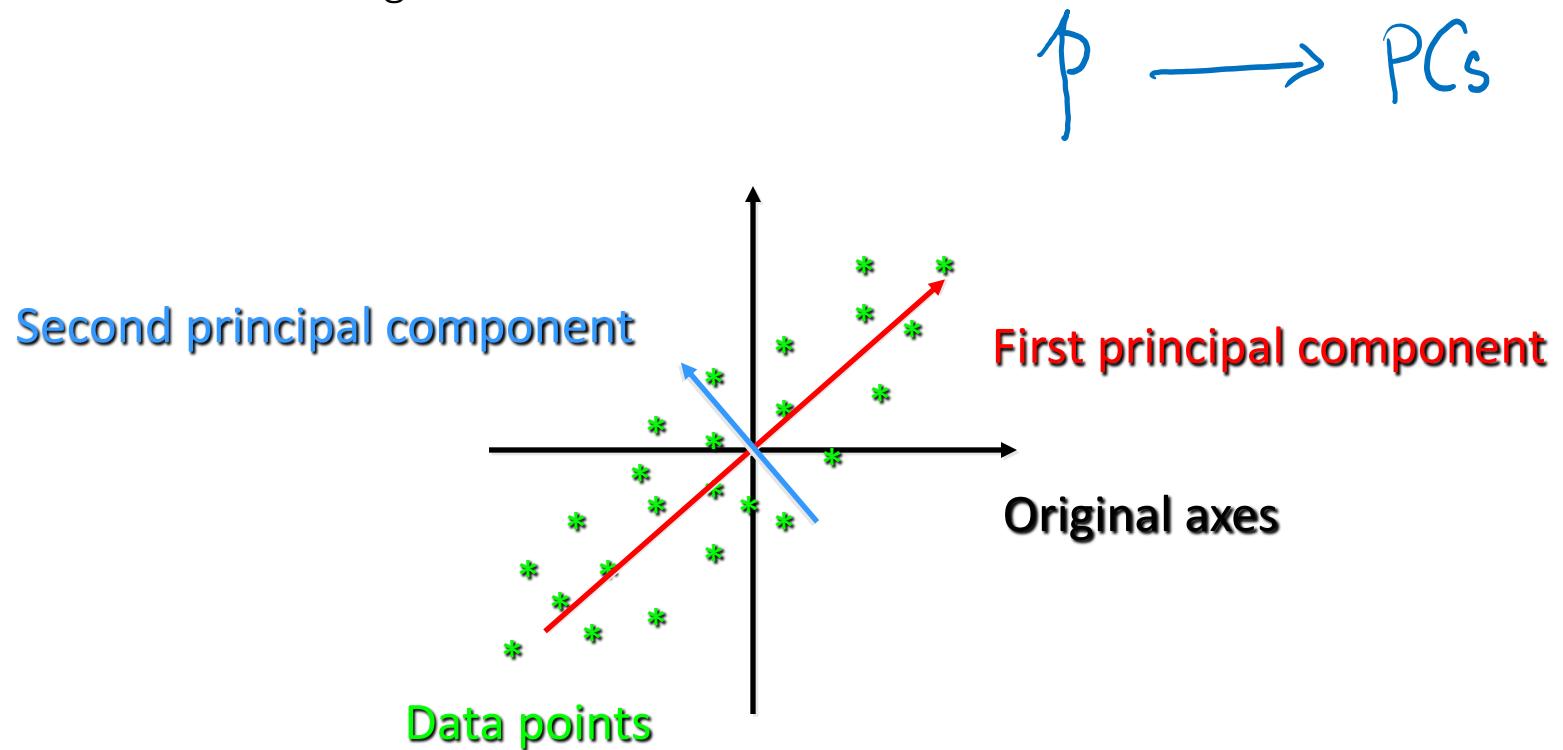
# How does PCA work?

- Find line of best fit, passing through the origin

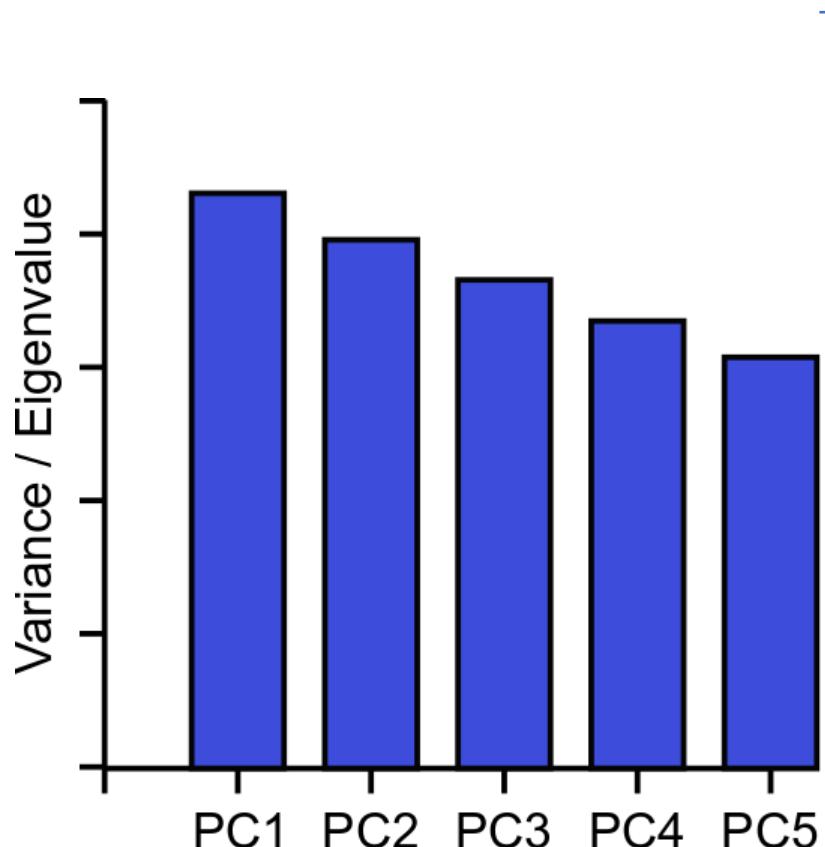
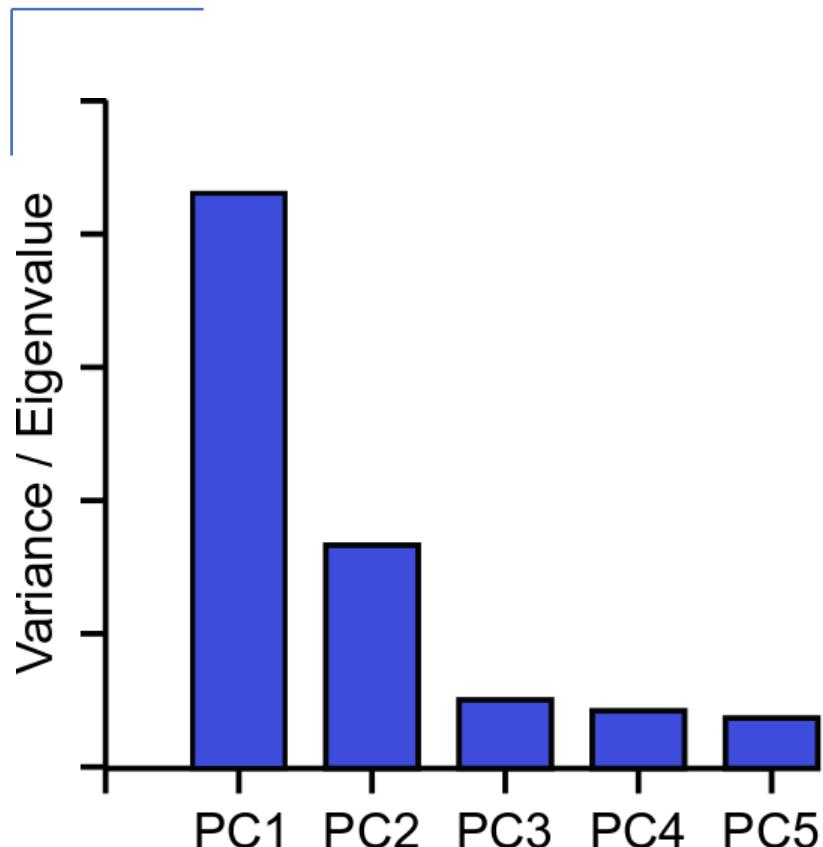


# How does PCA work? Explaining Variance

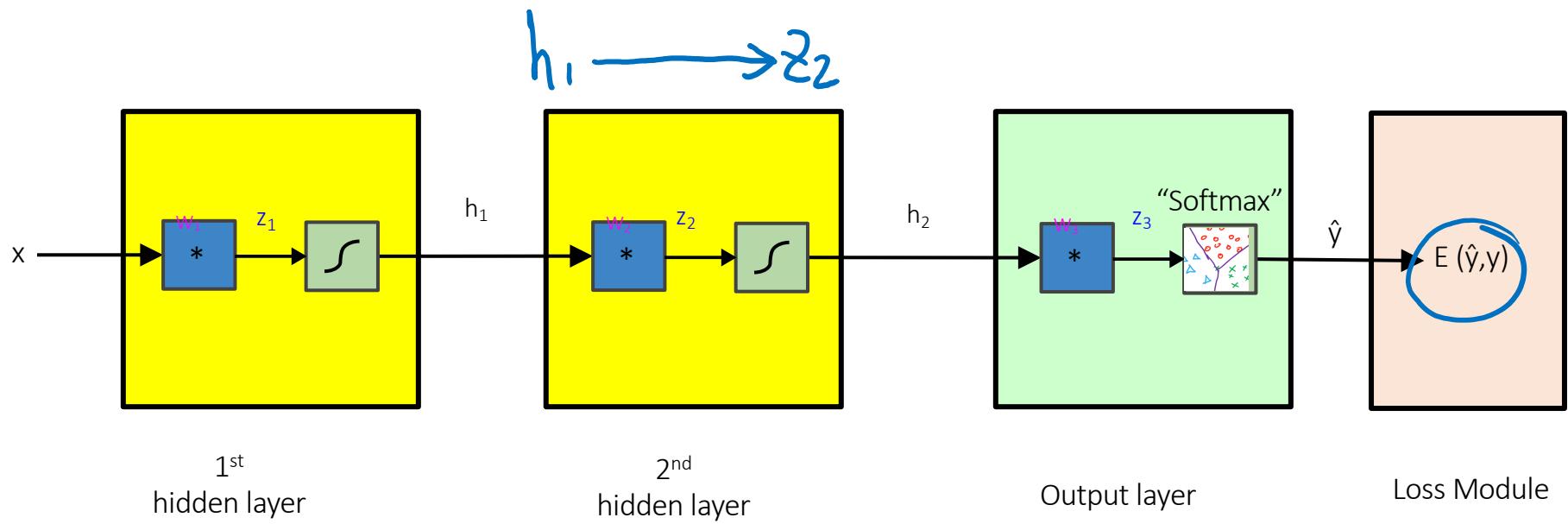
- Each PC always explains some proportion of the total variance in the data. Between them they explain everything
  - PC1 always explains the most
  - PC2 is the next highest etc. etc.



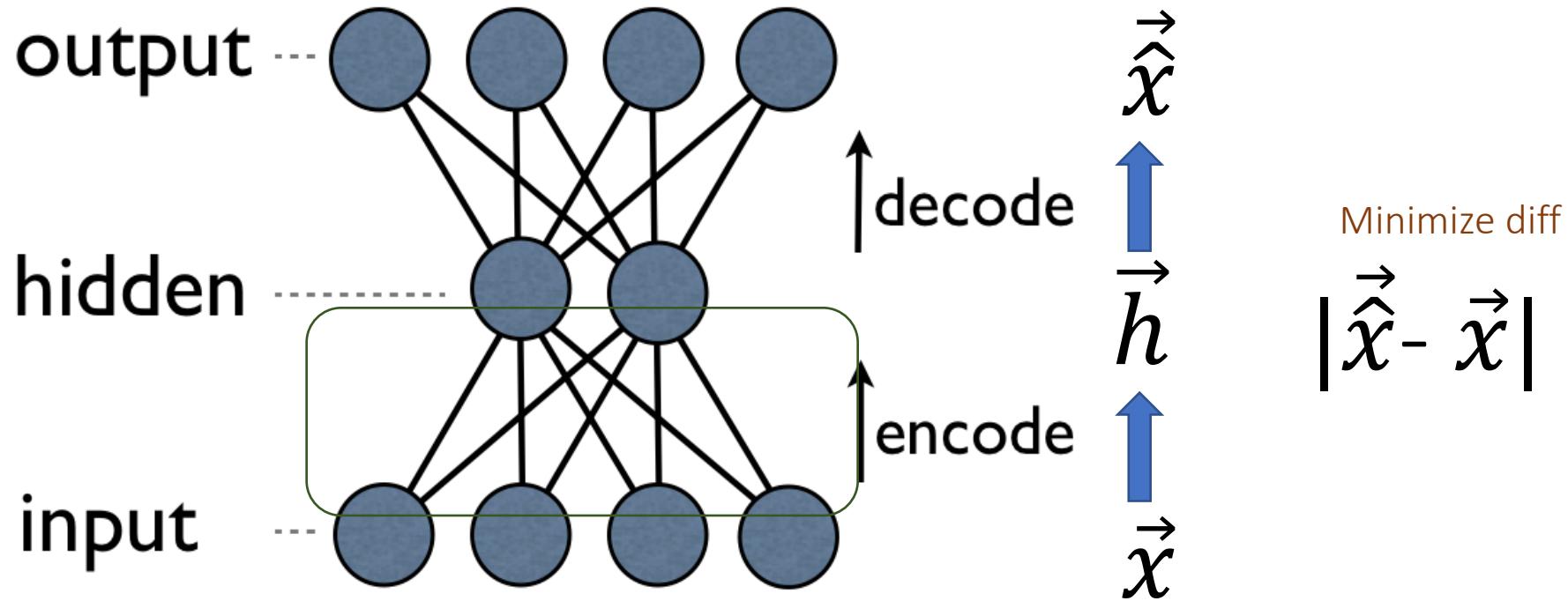
# Explaining Variance – Scree Plots



# Recap: “Block View”



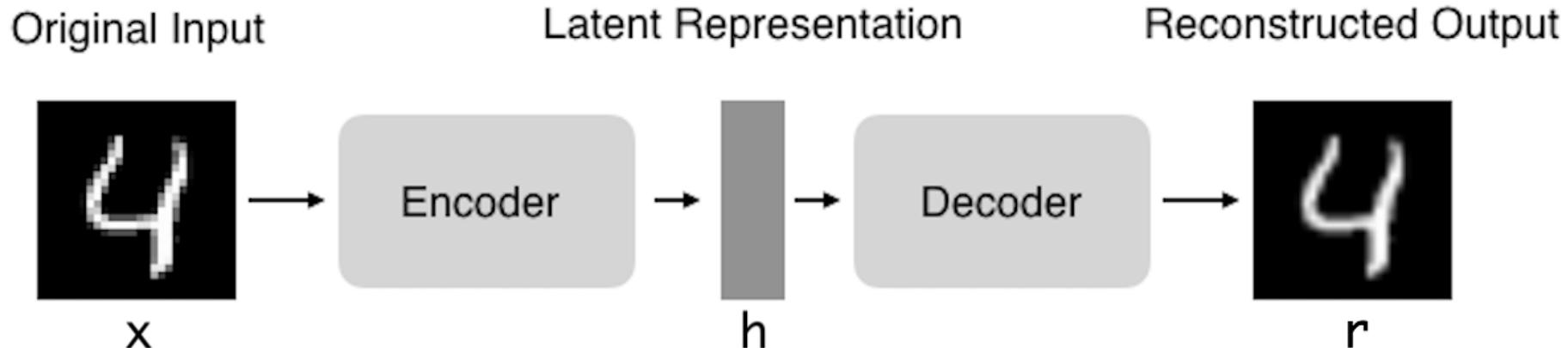
an auto-encoder-decoder is trained to reproduce the input



[Reconstruction Loss] force the ‘hidden layer’ units to become good / reliable feature detectors

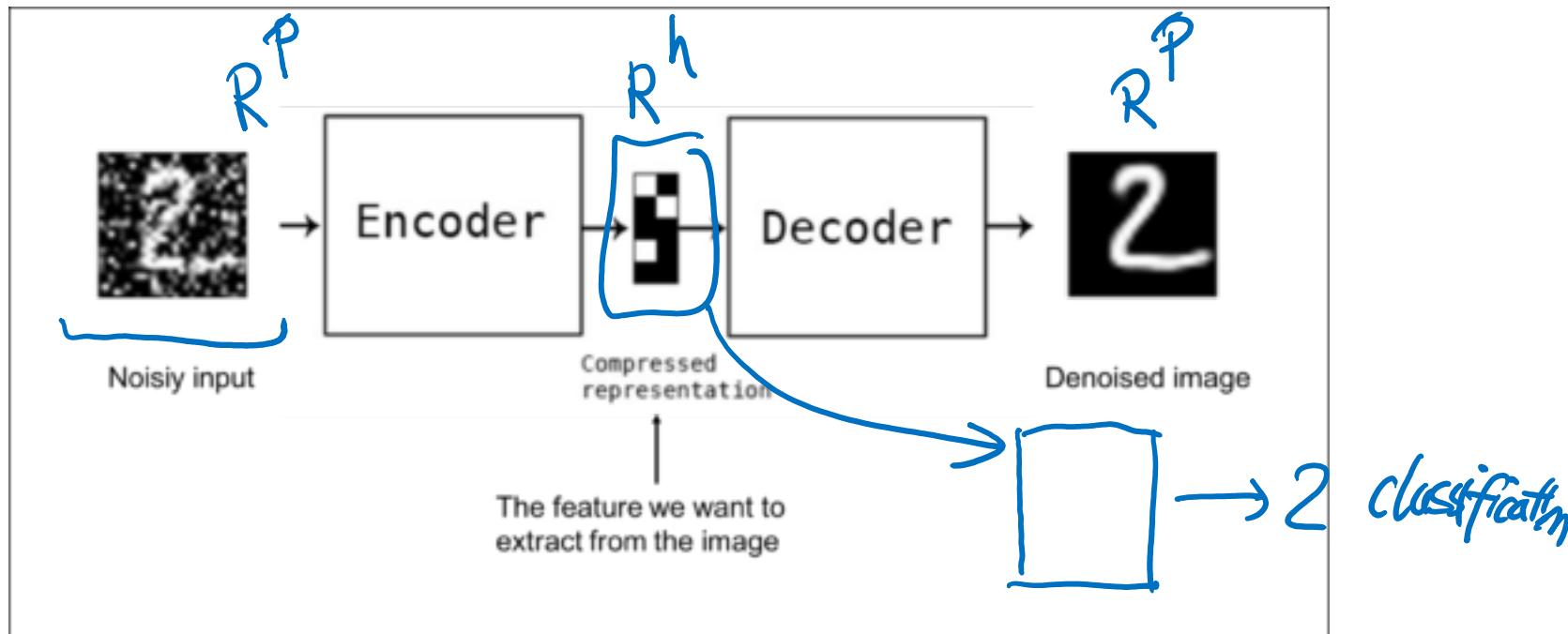
# Autoencoders: structure

- 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



# 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



# Today Recap: Dimensionality Reduction (Two Ways)

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# Thank You



□

# UVA CS 4774: Machine Learning

## Lecture 14: Dimension Reduction

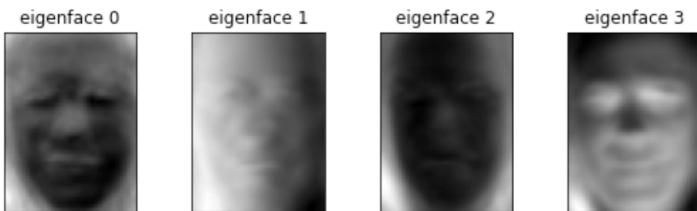
Dr. Yanjun Qi

Module IV  
Notebook PCA

University of Virginia  
Department of Computer Science

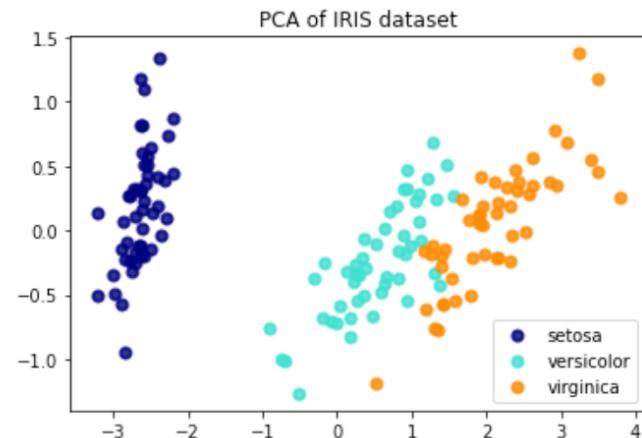
# I will run notebook using PCA on face images / Iris

```
| # 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>

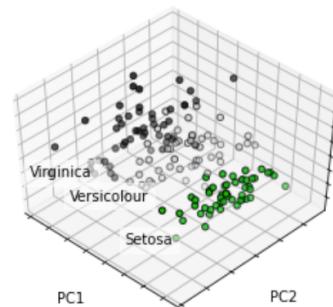
```
explained variance ratio (first two components): [0.92461872 0.05306648]  
Text(0.5, 1.0, 'PCA of IRIS dataset')
```



10/13/20

```
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')
```

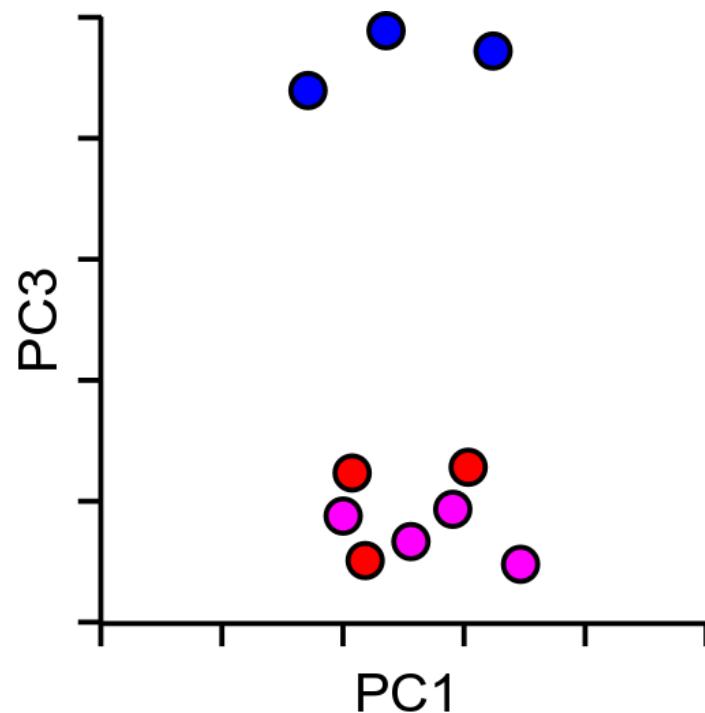
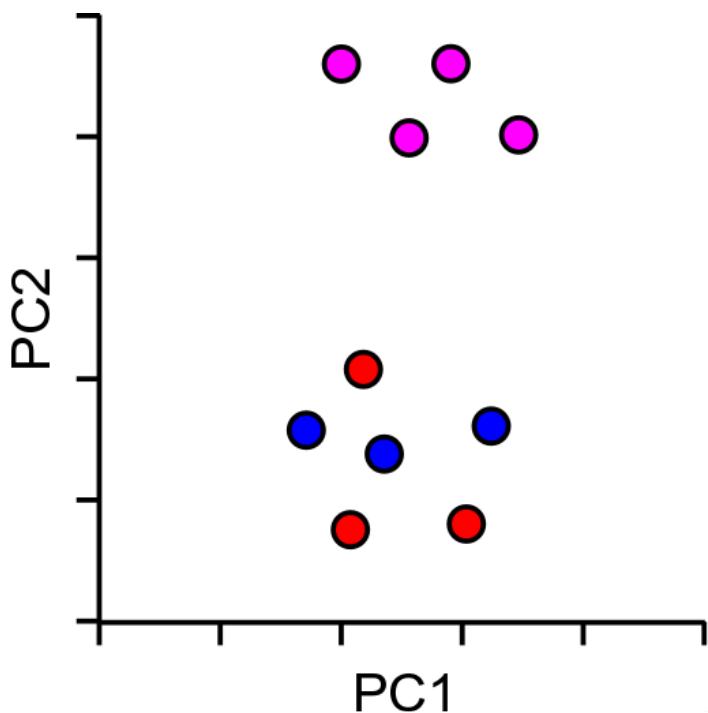


# References

- ❑ 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?

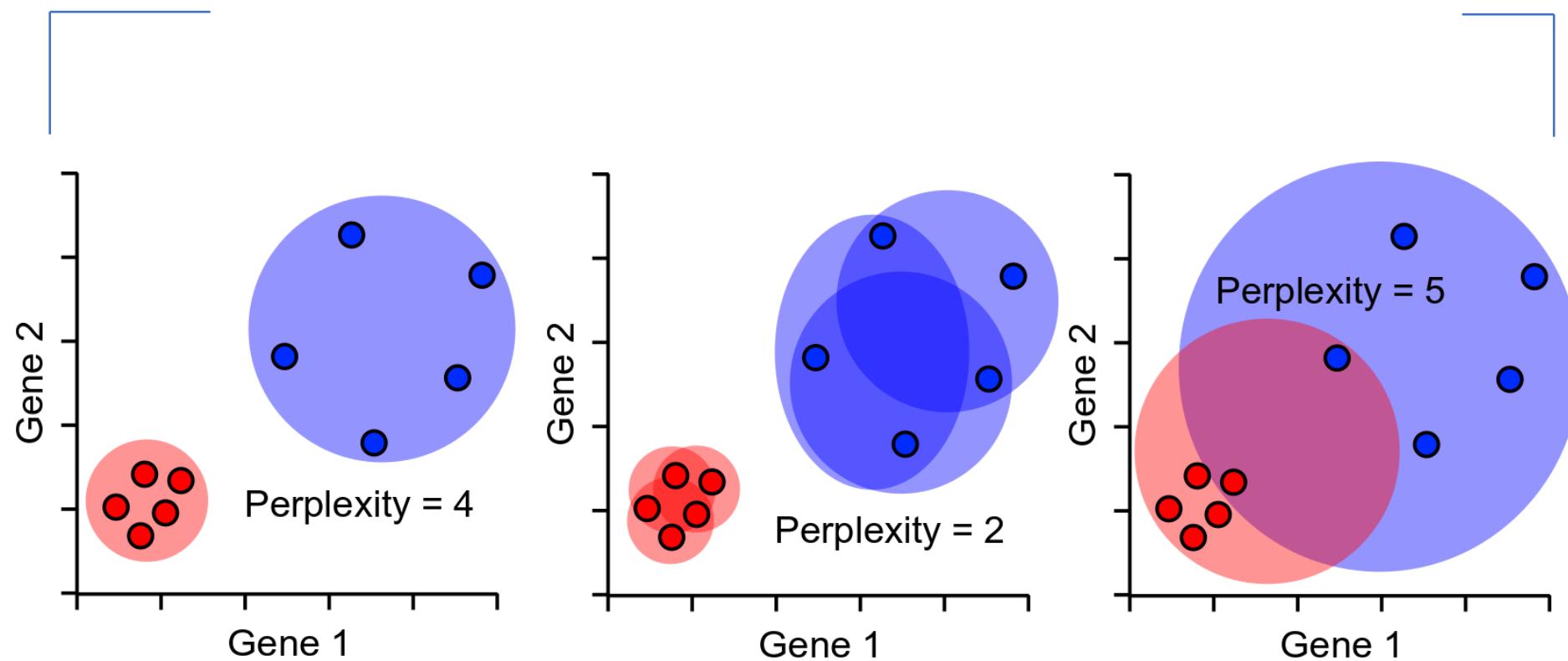
- Kind of...



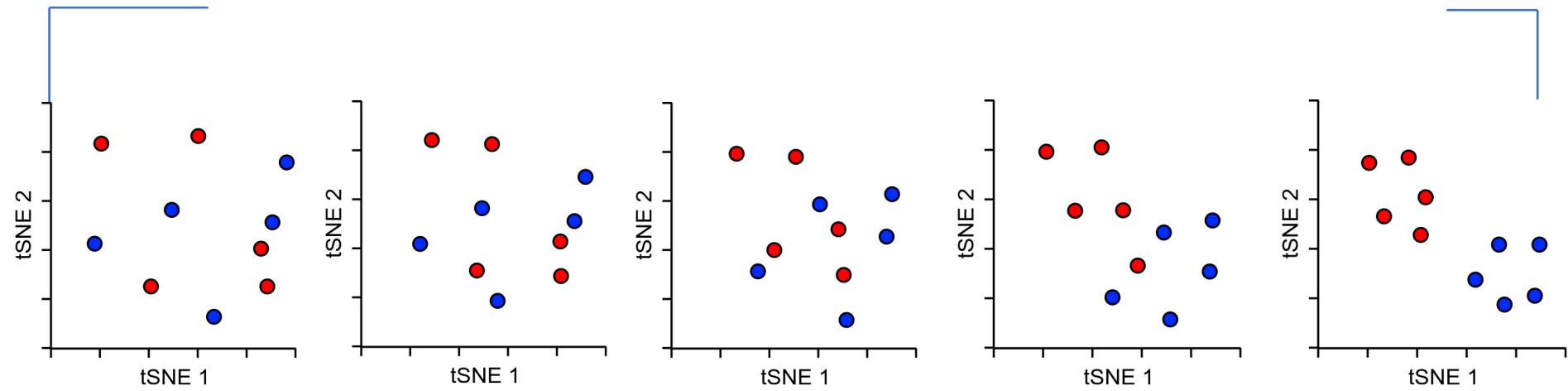
# tSNE to the rescue...

- 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



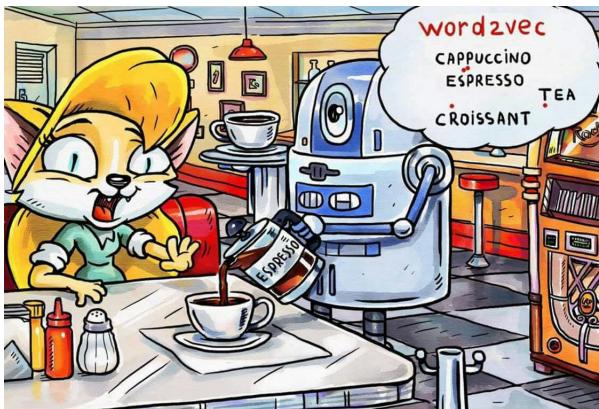
# tSNE Projection



- 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.

