

# **UVA CS 6316/4501**

## **– Fall 2016**

# **Machine Learning**

## **Lecture 22: Review**

Dr. Yanjun Qi

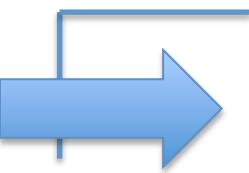
University of Virginia

Department of  
Computer Science

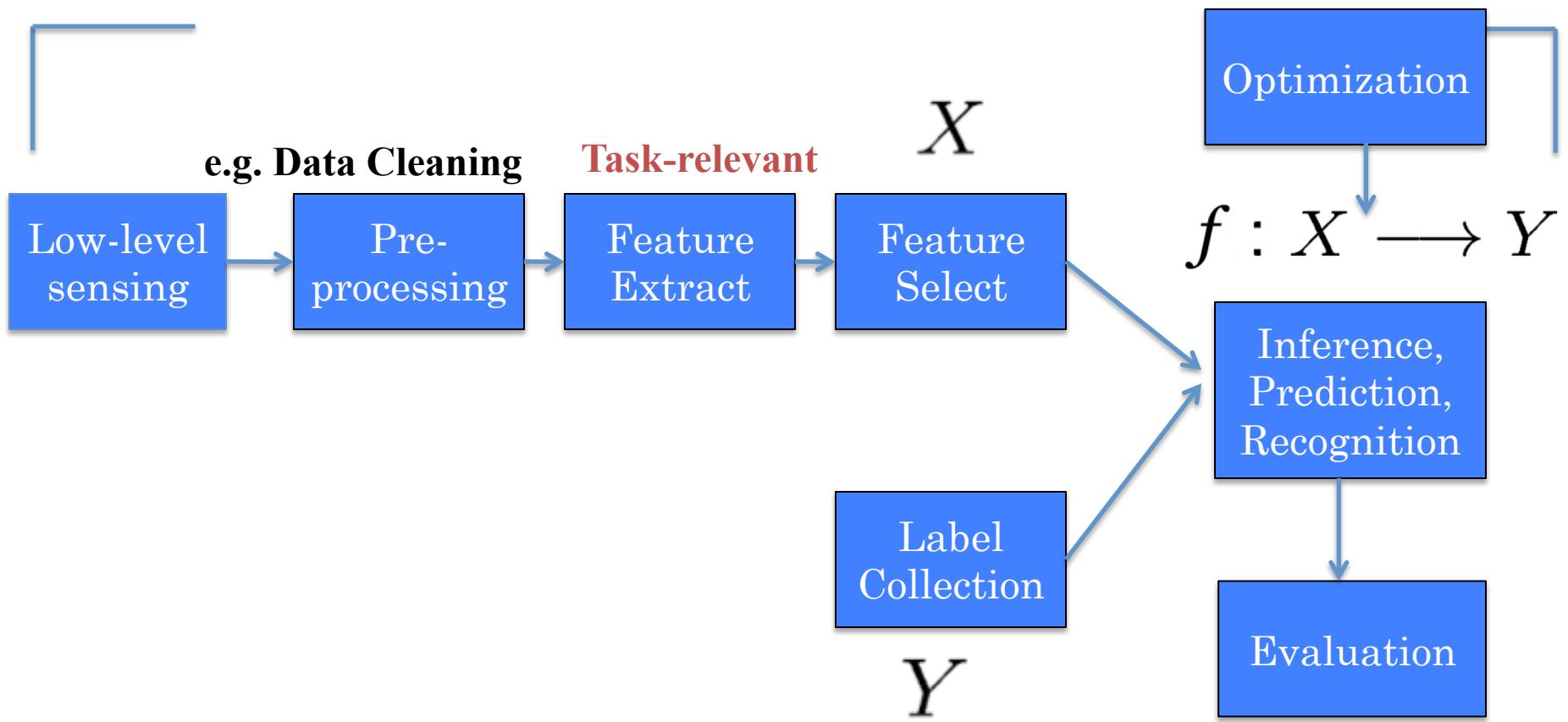
# Announcements: Final Exam

- Closed Note
- Allowing a paper (us letter size) of cheat sheet
- No laptop / No Cell phone / No internet access / No electronic devices
- Recital session this Friday (@OSL120, 4pm-5pm) for HW7
- Covering post-midterm contents (L12-) till today
  - Practice with sample questions in HW7
  - HW7 due next Monday noon
  - Please review course slides carefully

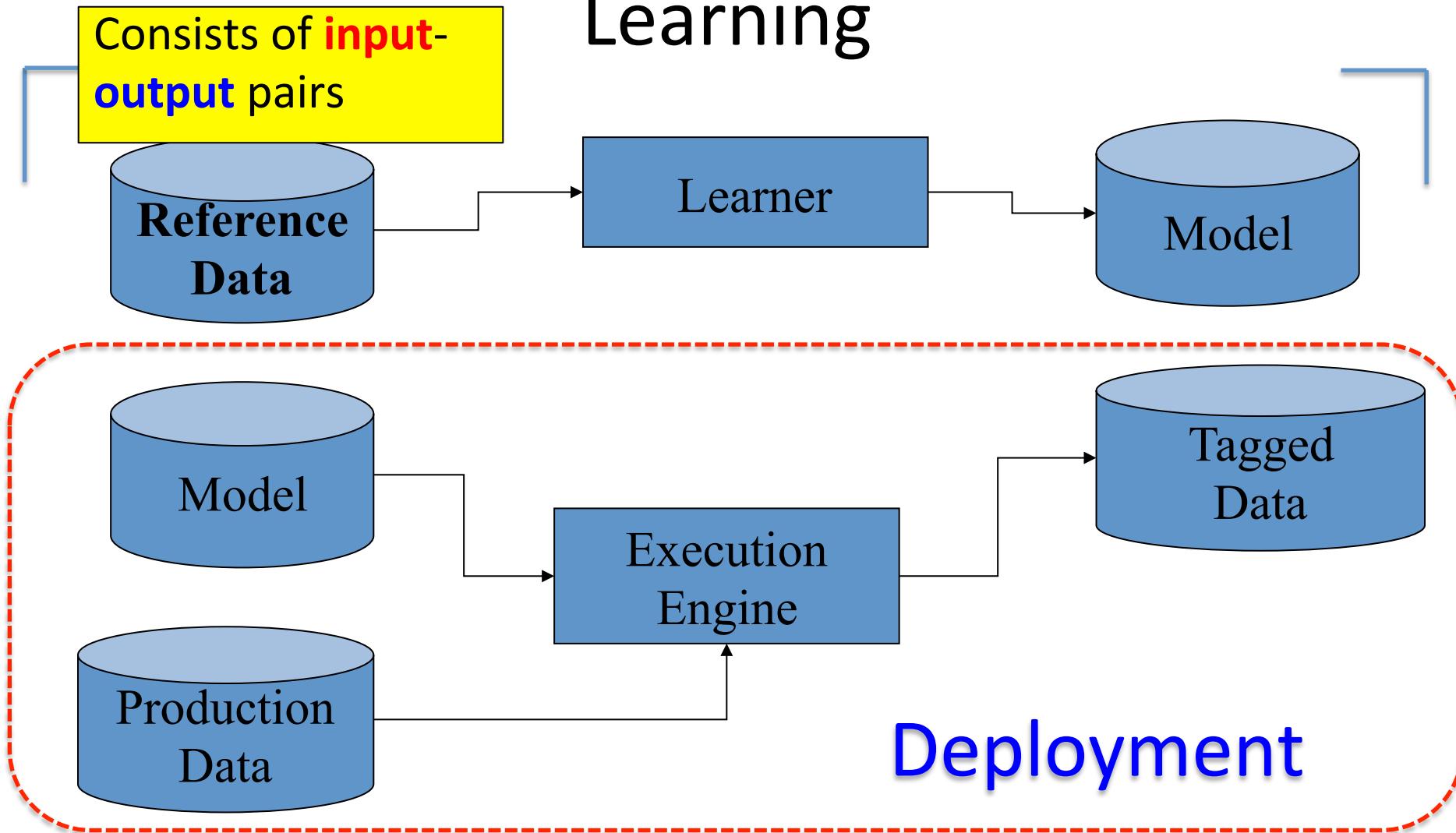
# Today

- 
- ❑ Review of ML methods covered so far
    - ❑ Regression (supervised)
    - ❑ Classification (supervised)
    - ❑ Unsupervised models
    - ❑ Learning theory
  
  - ❑ Review of Assignments covered so far
- 

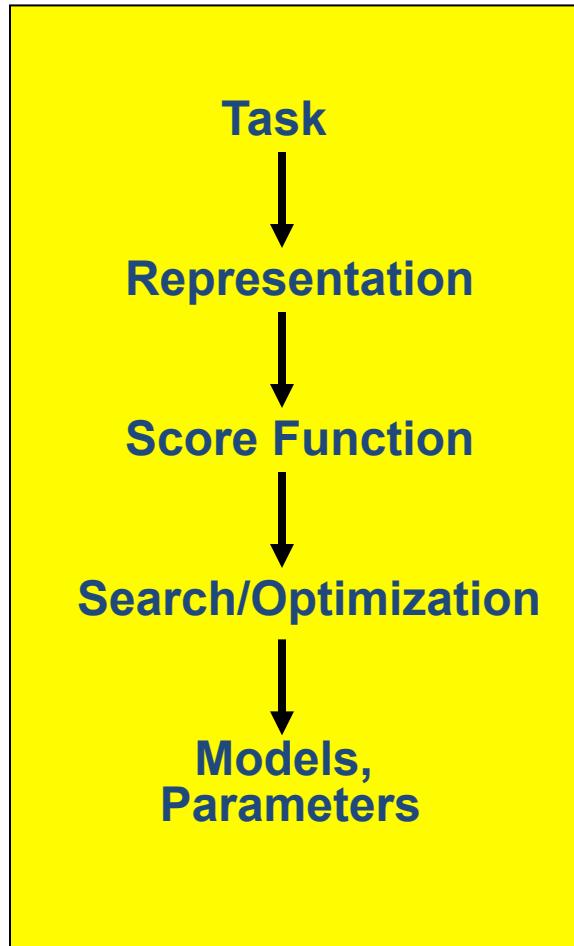
# A Typical Machine Learning Pipeline



# An Operational Model of Machine Learning



# Machine Learning in a Nutshell



ML grew out of  
work in AI

*Optimize a  
performance criterion  
using example data or  
past experience,*

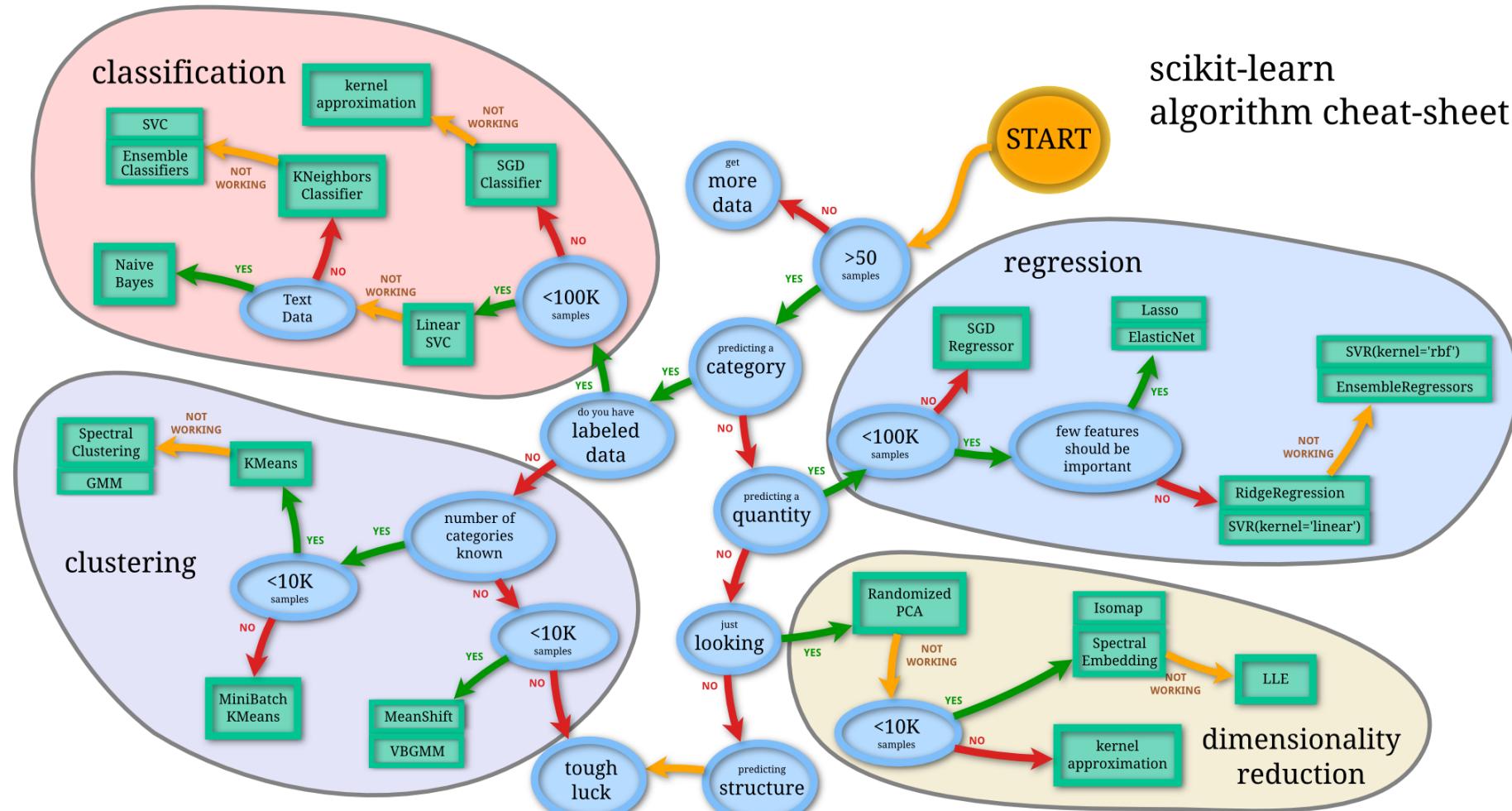
*Aiming to generalize to  
unseen data*

# What we have covered

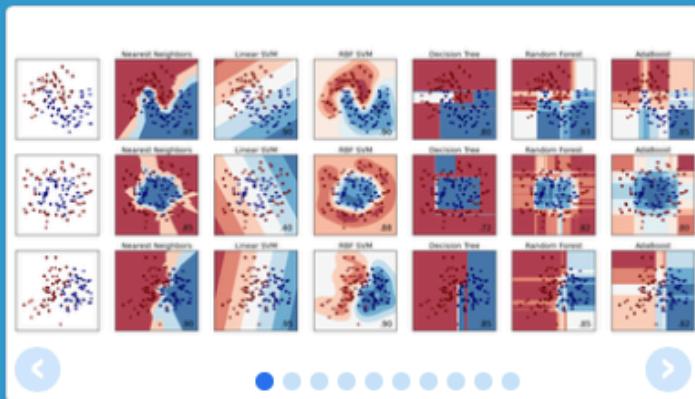
Task	
Representation	
Score Function	
Search/ Optimization	
Models, Parameters	

[http://scikit-learn.org/stable/tutorial/machine\\_learning\\_map/](http://scikit-learn.org/stable/tutorial/machine_learning_map/)

# Scikit-learn algorithm cheat-sheet



<http://scikit-learn.org/stable/>



# scikit-learn

Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

## Classification

Identifying to which set of categories a new observation belongs to.

**Applications:** Spam detection, Image recognition.

**Algorithms:** *SVM, nearest neighbors, random forest, ...*

— Examples

## Regression

Predicting a continuous value for a new example.

**Applications:** Drug response, Stock prices.

**Algorithms:** *SVR, ridge regression, Lasso, ...*

— Examples

## Clustering

Automatic grouping of similar objects into sets.

**Applications:** Customer segmentation, Grouping experiment outcomes

**Algorithms:** *k-Means, spectral clustering, mean-shift, ...*

— Examples

## Dimensionality reduction

Reducing the number of random variables to consider.

**Applications:** Visualization, Increased efficiency

**Algorithms:** *PCA, feature selection, non-negative matrix factorization.*

— Examples

## Model selection

Comparing, validating and choosing parameters and models.

**Goal:** Improved accuracy via parameter tuning

**Modules:** *grid search, cross validation, metrics.*

— Examples

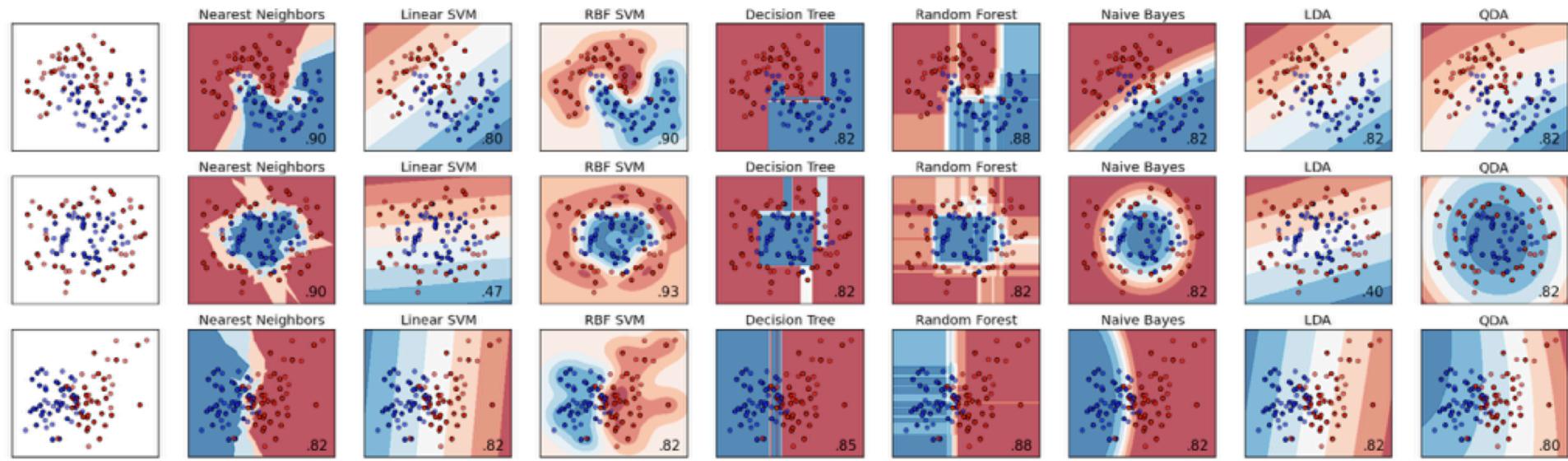
## Preprocessing

Feature extraction and normalization.

**Application:** Transforming input data such as text for use with machine learning algorithms.

**Modules:** *preprocessing, feature extraction.*

— Examples



- ✓ different assumptions on data
- ✓ different scalability profiles at training time
- ✓ different latencies at prediction (test) time
- ✓ different model sizes (embedability in mobile devices)

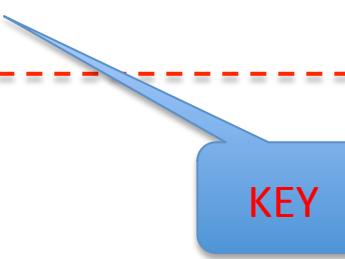
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  - ❑ Learning theory
- ❑ Review of Assignments covered so far

# SUPERVISED LEARNING

$$f : X \longrightarrow Y$$

- Find function to map **input** space  $X$  to **output** space  $Y$
- **Generalisation**: learn function / hypothesis from **past data** in order to “explain”, “predict”, “model” or “control” **new** data examples



KEY

# What we have covered (I)

## ❑ Supervised Regression models

- Linear regression (LR)
- LR with non-linear basis functions
- Locally weighted LR
- LR with Regularizations
- Feature selection \*

	$X_1$	$X_2$	$X_3$	$Y$
$S_1$				
$S_2$				
$S_3$				
$S_4$				
$S_5$				
$S_6$				

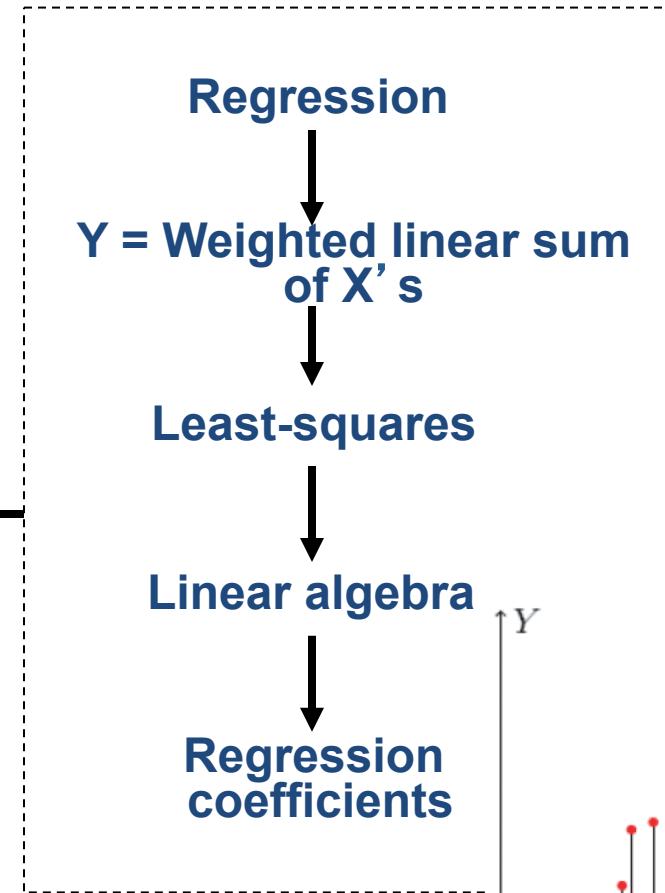
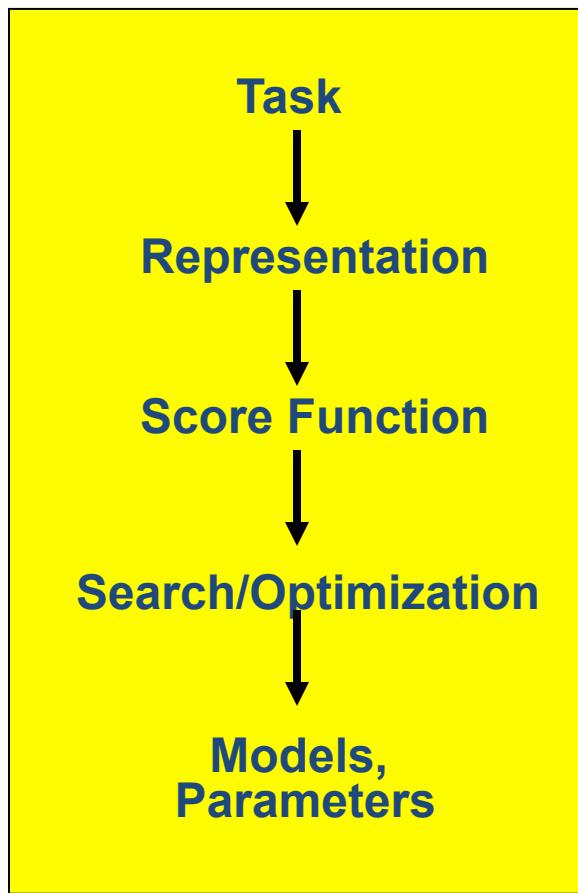
# A Dataset

$$f : \boxed{X} \longrightarrow \boxed{Y}$$

Output Y as  
continuous values

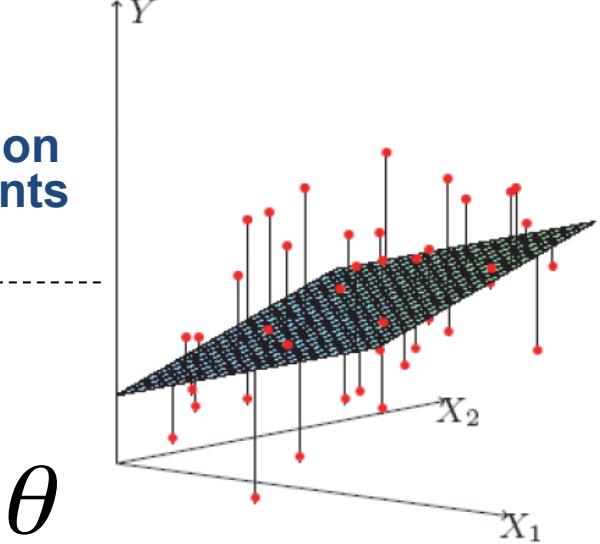
- **Data/points/instances/examples/samples/records:** [ rows ]
- **Features/attributes/dimensions/independent variables/covariates/predictors/regressors:** [ columns, except the last ]
- **Target/outcome/response/label/dependent variable:** special column to be predicted [ last column ]

# (1) Multivariate Linear Regression

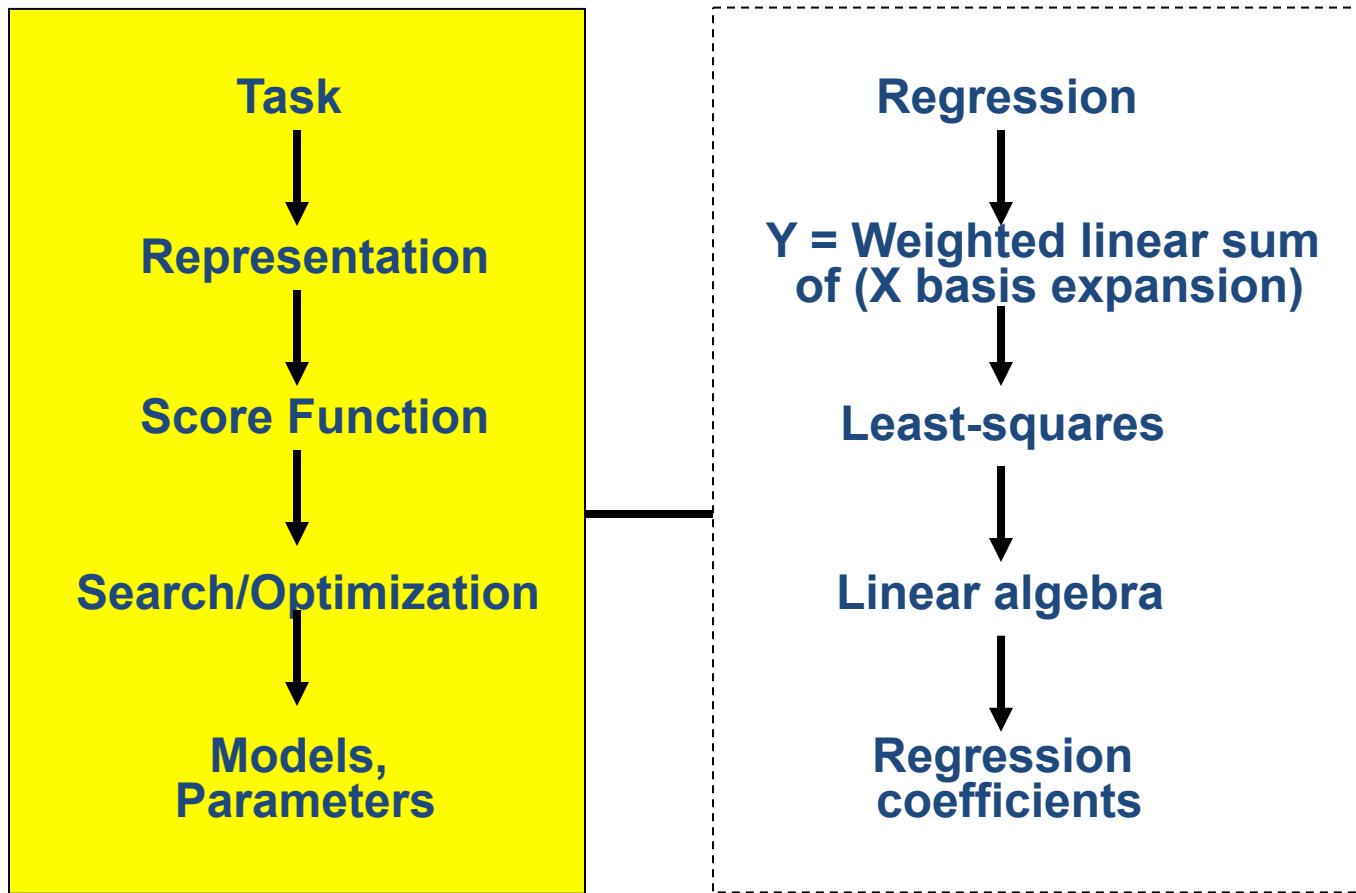


$$\hat{y} = f(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2$$

$$\theta$$

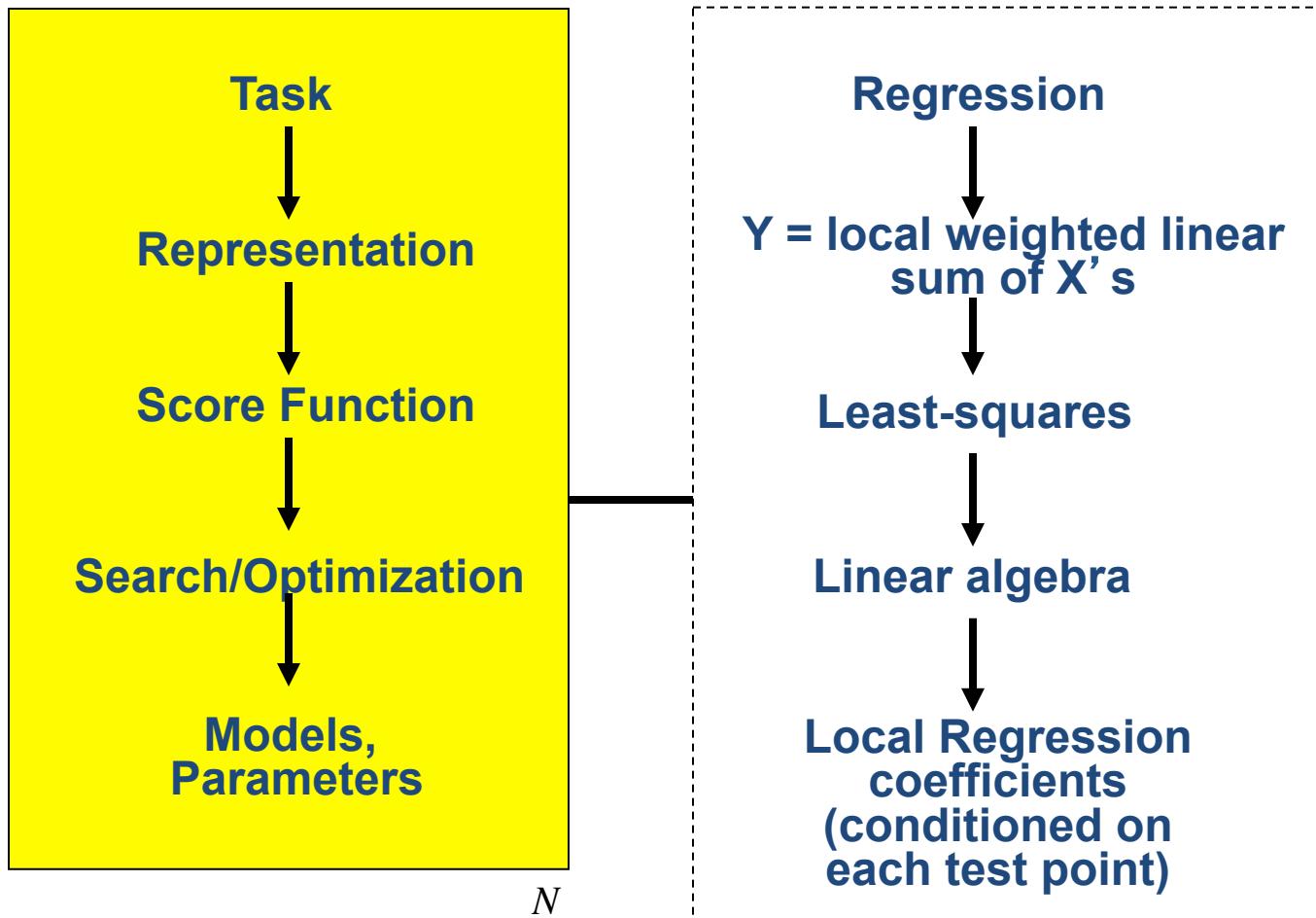


## (2) Multivariate Linear Regression with basis Expansion



$$\hat{y} = \theta_0 + \sum_{j=1}^m \theta_j \varphi_j(x) = \varphi(x)\theta$$

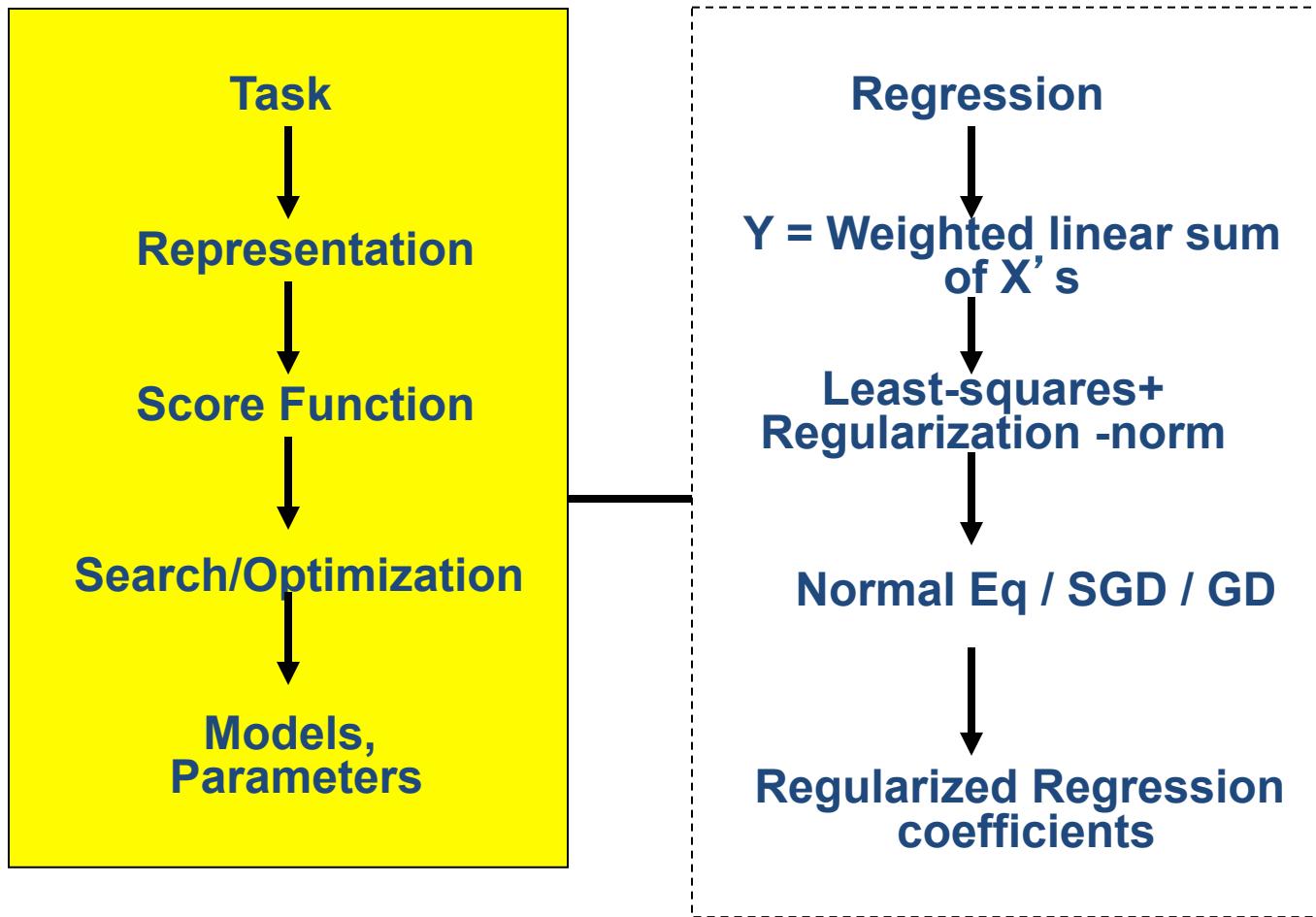
### (3) Locally Weighted / Kernel Regression



$$\min_{\alpha(x_0), \beta(x_0)} \sum_{i=1}^N K_\lambda(x_i, x_0) [y_i - \alpha(x_0) - \beta(x_0)x_i]^2$$

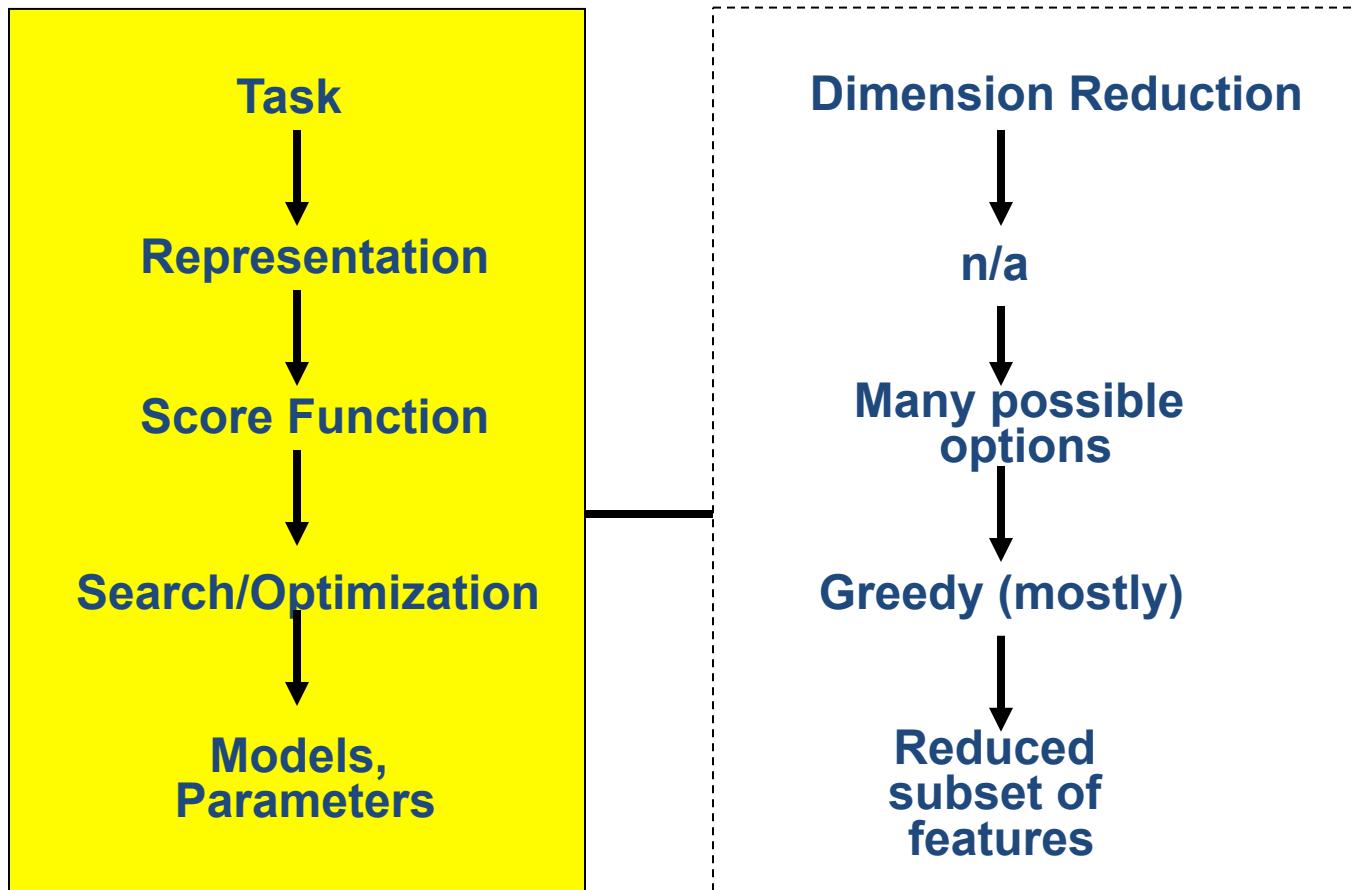
$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0)x_0$$

## (4) Regularized multivariate linear regression



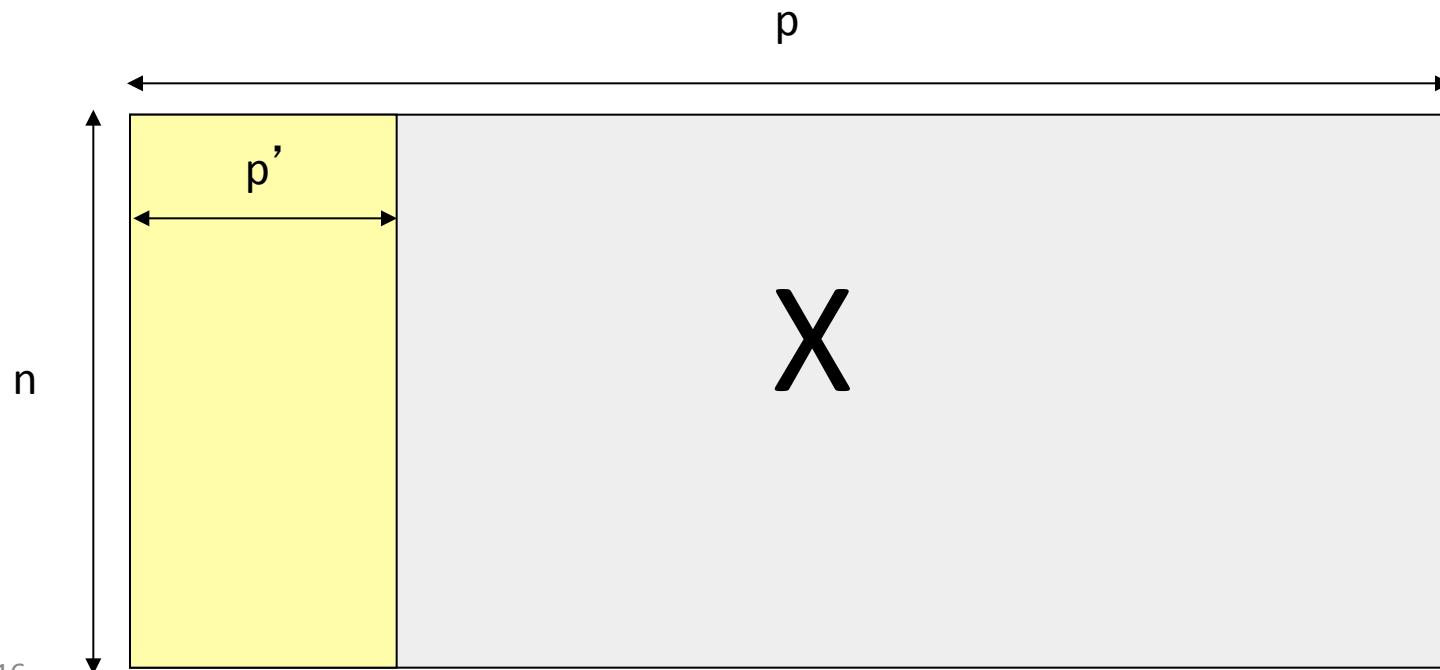
$$\min J(\beta) = \sum_{i=1}^n (Y - \hat{Y})^2 + \lambda \sum_{j=1}^p \beta_j^2$$

## (5) Feature Selection



# (5) Feature Selection

- **Thousands to millions of low level features:** select the most relevant one to build **better, faster, and easier to understand** learning machines.



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- ❑ Review of Assignments covered so far

# What we have covered (II)

## ❑ Supervised Classification models

- Support Vector Machine
- Bayes Classifier
- Logistic Regression
- K-nearest Neighbor
- Random forest / Decision Tree
- Neural Network (e.g. MLP)

# Three major sections for classification

- We can divide the large variety of classification approaches into **roughly three major types**
- 1. Discriminative
  - directly estimate a decision rule/boundary
  - e.g., **logistic regression**, support vector machine, decisionTree
- 2. Generative:
  - build a generative statistical model
  - e.g., **naïve bayes classifier**, Bayesian networks
- 3. Instance based classifiers
  - Use observation directly (no models)
  - e.g. **K nearest neighbors**

X <sub>1</sub>	X <sub>2</sub>	X <sub>3</sub>	C

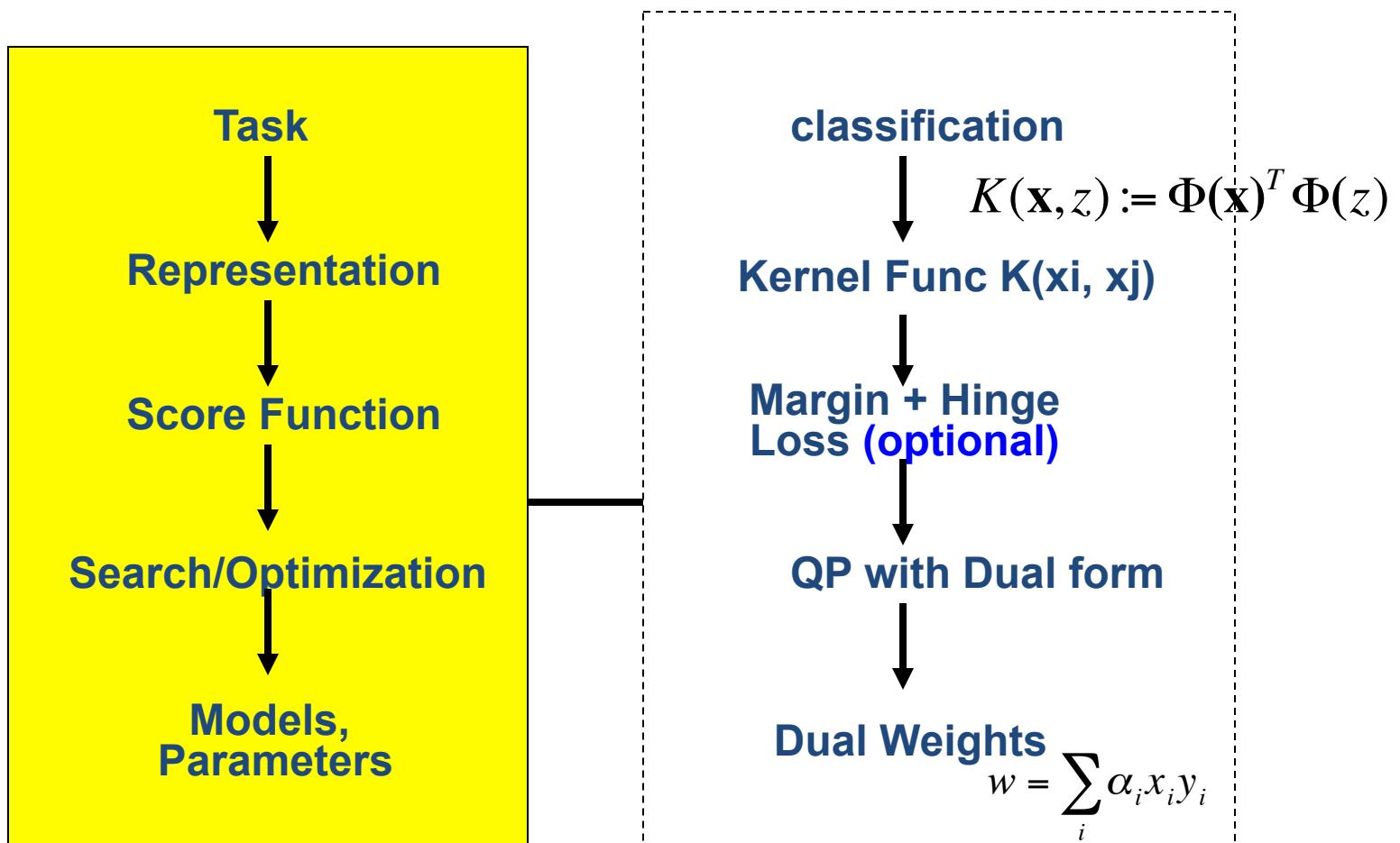
# A Dataset for classification

$$f : [X] \longrightarrow [C]$$

Output as Discrete Class Label  
 $C_1, C_2, \dots, C_L$

- Data/points/instances/examples/samples/records: [ rows ]
- Features/attributes/dimensions/independent variables/covariates/predictors/regressors: [ columns, except the last ]
- Target/outcome/response/label/dependent variable: special column to be predicted [ last column ]

# (1) Support Vector Machine

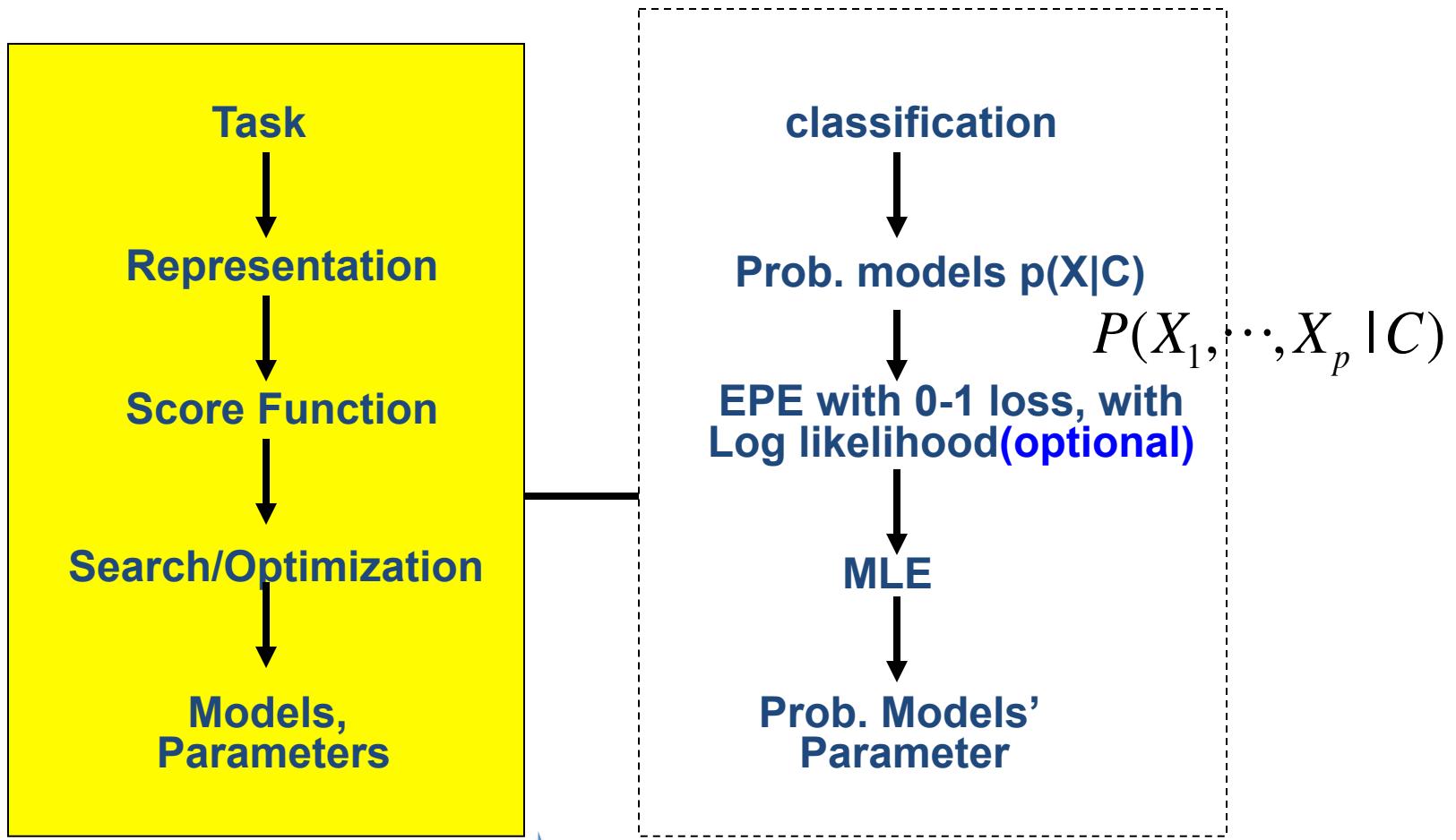


$$\underset{\mathbf{w}, b}{\operatorname{argmin}} \sum_{i=1}^p w_i^2 + C \sum_{i=1}^n \varepsilon_i$$

$$\text{subject to } \forall \mathbf{x}_i \in D_{train} : y_i (\mathbf{x}_i \cdot \mathbf{w} + b) \geq 1 - \varepsilon_i$$

$$\underset{k}{\operatorname{argmax}} P(C_k | X) = \underset{k}{\operatorname{argmax}} P(X, C) = \underset{k}{\operatorname{argmax}} P(X|C)P(C)$$

## (2) Bayes Classifier



Gaussian  
Naïve

Multinomial

$$\hat{P}(X_j | C = c_k) = \frac{1}{\sqrt{2\pi}\sigma_{jk}} \exp\left(-\frac{(X_j - \mu_{jk})^2}{2\sigma_{jk}^2}\right)$$

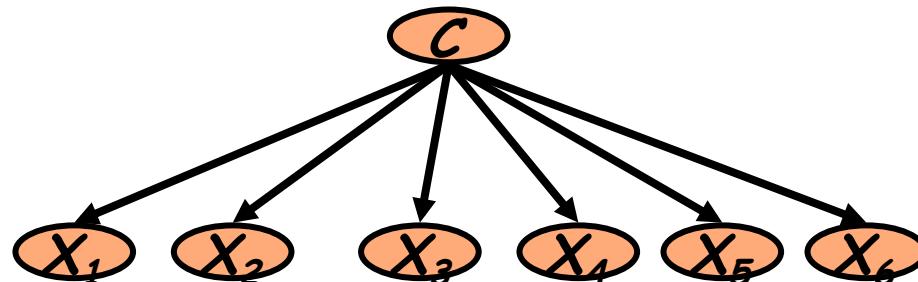
$$P(W_1 = n_1, \dots, W_v = n_v | c_k) = \frac{N!}{n_{1k}! n_{2k}! \dots n_{vk}!} \theta_{1k}^{n_{1k}} \theta_{2k}^{n_{2k}} \dots \theta_{vk}^{n_{vk}}$$

# Naïve Bayes Classifier

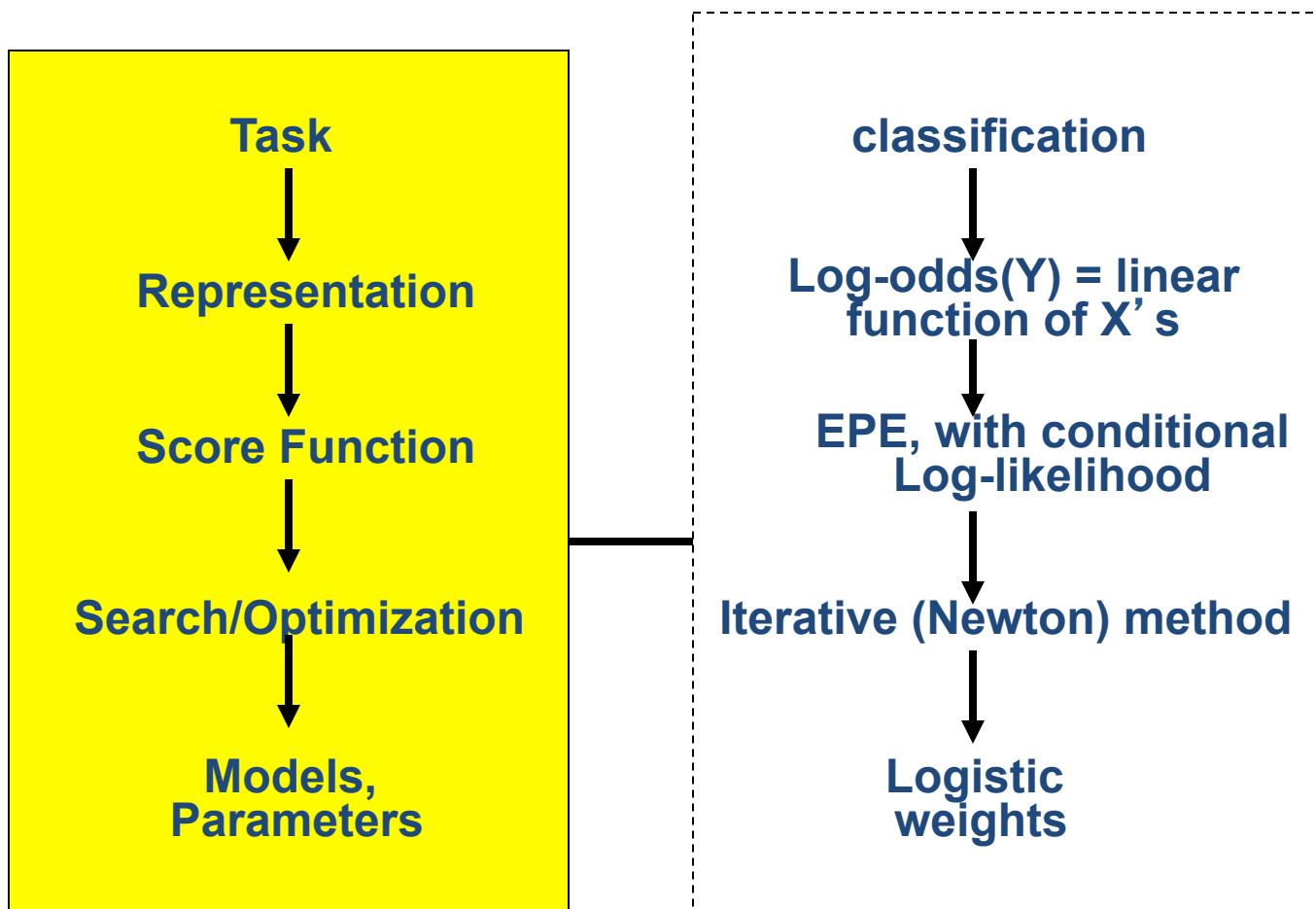
Difficulty: learning the joint probability  $P(X_1, \dots, X_p | C)$

- Naïve Bayes classification
  - Assumption that **all input attributes are conditionally independent!**

$$\begin{aligned}
 P(X_1, X_2, \dots, X_p | C) &= P(X_1 | X_2, \dots, X_p, C)P(X_2, \dots, X_p | C) \\
 &= \underline{P(X_1 | C)} \underline{P(X_2, \dots, X_p | C)} \\
 &= \underline{P(X_1 | C)} \underline{P(X_2 | C)} \cdots \underline{P(X_p | C)}
 \end{aligned}$$



### (3) Logistic Regression



$$P(c=1|x) = \frac{e^{\alpha+\beta x}}{1+e^{\alpha+\beta x}}$$

# Logistic Regression—when?

Logistic regression models are appropriate for target variable coded as 0/1.

We only observe “0” and “1” for the target variable—but we think of the target variable conceptually as a probability that “1” will occur.

This means we use Bernoulli distribution to model the target variable with its Bernoulli parameter  $p=p(y=1 | x)$  predefined.

The main interest → predicting the probability that an event occurs (i.e., the probability that  $p(y=1 | x)$  ).

# Logistic regression models for binary target variable coded 0/1.

e.g.  
Probability of  
disease

$P(C=1|X)$

1.0

0.8

0.6

0.4

0.2

0.0

logistic function

$$P(c = 1|x) = \frac{e^{\alpha + \beta x}}{1 + e^{\alpha + \beta x}}$$

$x$

Logit function

Decision Boundary → equals to zero

$$\ln \left[ \frac{P(c = 1|x)}{P(c = 0|x)} \right] = \ln \left[ \frac{P(c = 1|x)}{1 - P(c = 1|x)} \right] = \alpha + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_p x_p$$

# Discriminative vs. Generative

## Generative approach

- Model the joint distribution  $p(X, C)$  using  
 $p(X | C = c_k)$  and  $p(C = c_k)$

Class prior

## Discriminative approach

- Model the conditional distribution  $p(c | X)$  directly

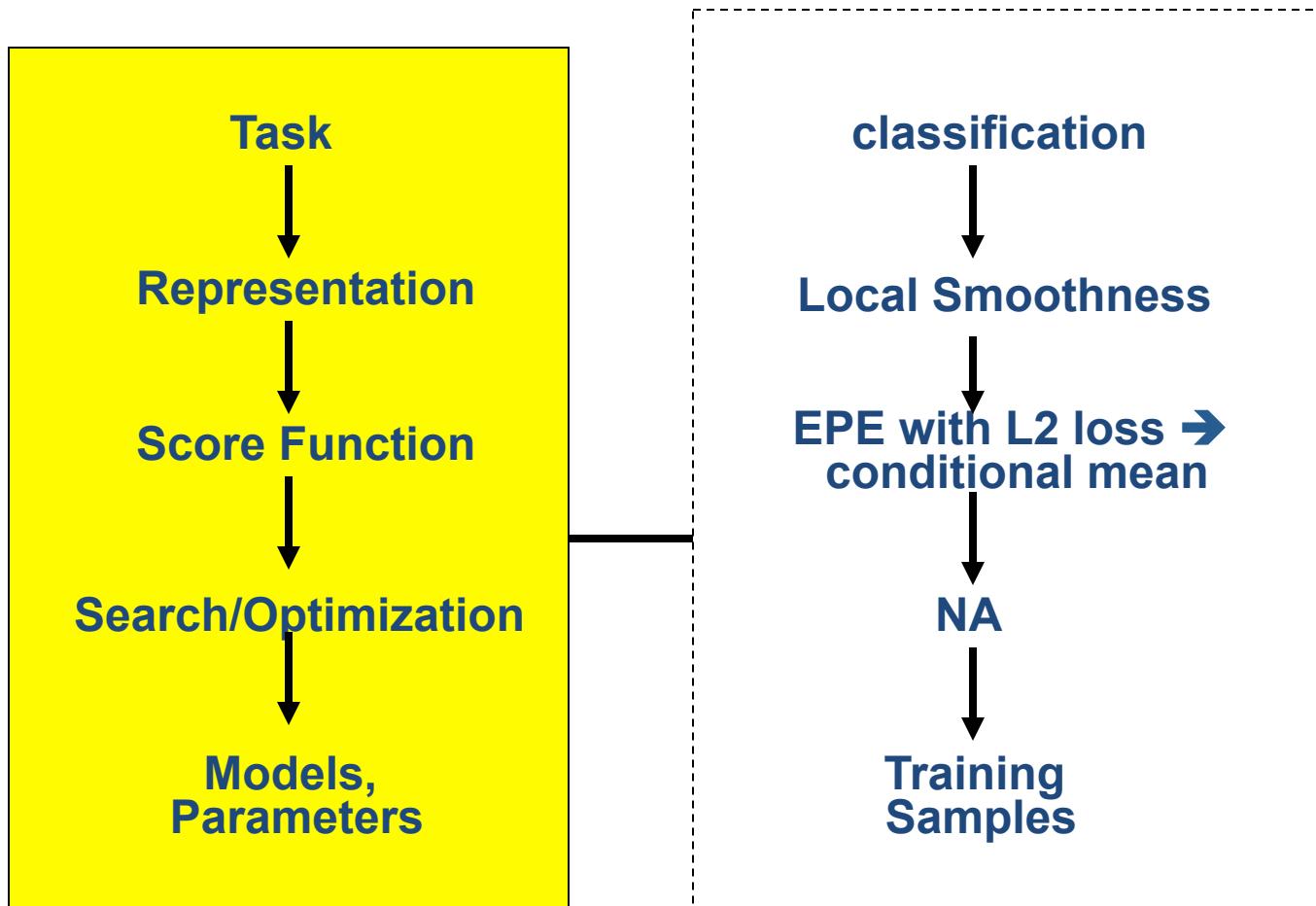
e.g.,

$$\frac{1}{1 + e^{-(\beta_0 + \beta_1 * X)}}$$

# Discriminative vs. Generative

- Empirically, **generative** classifiers approach their asymptotic error faster than discriminative ones
  - Good for small training set
  - Handle missing data well (EM)
- Empirically, **discriminative** classifiers have lower asymptotic error than generative ones
  - Good for larger training set

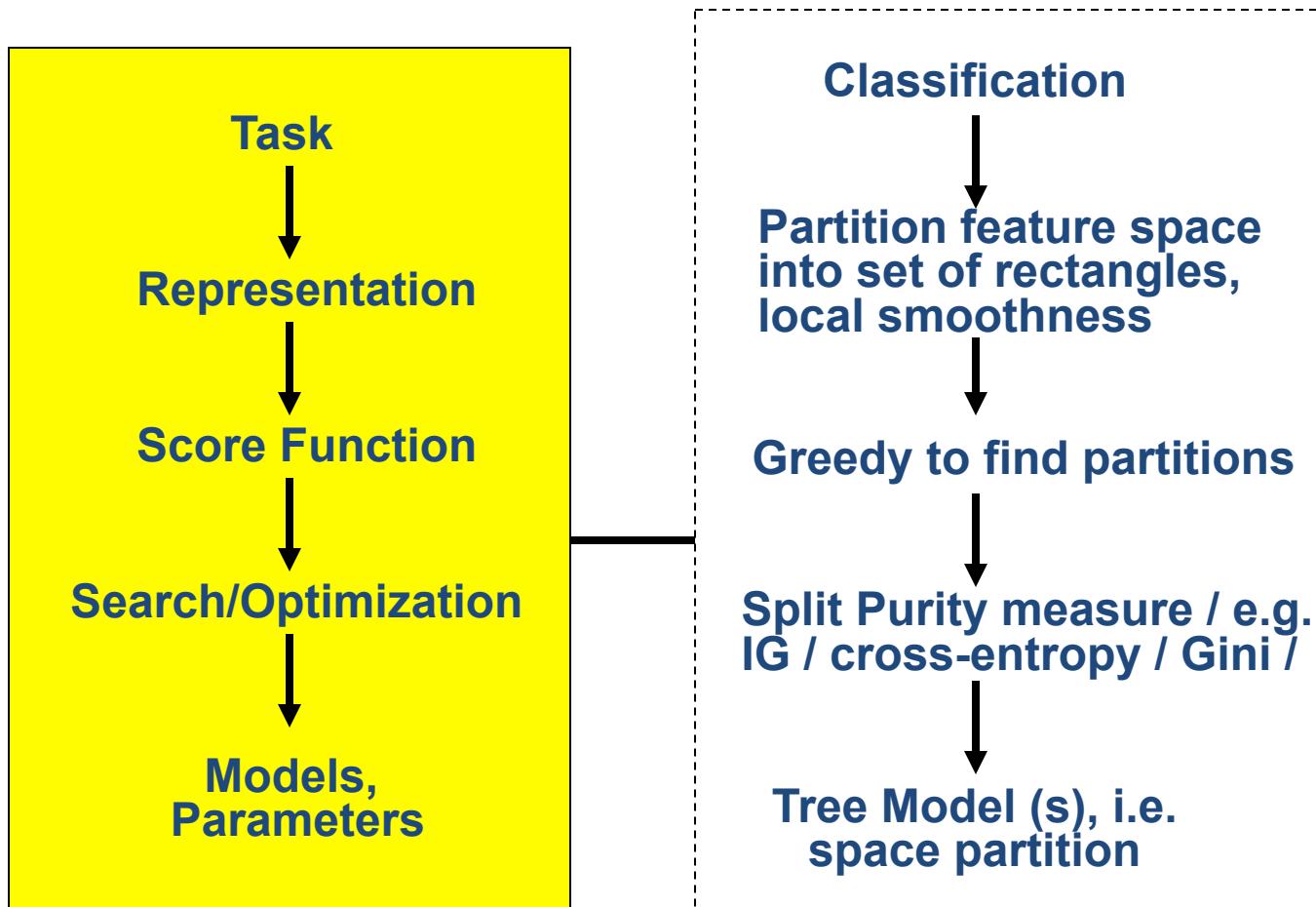
## (4) K-Nearest Neighbor



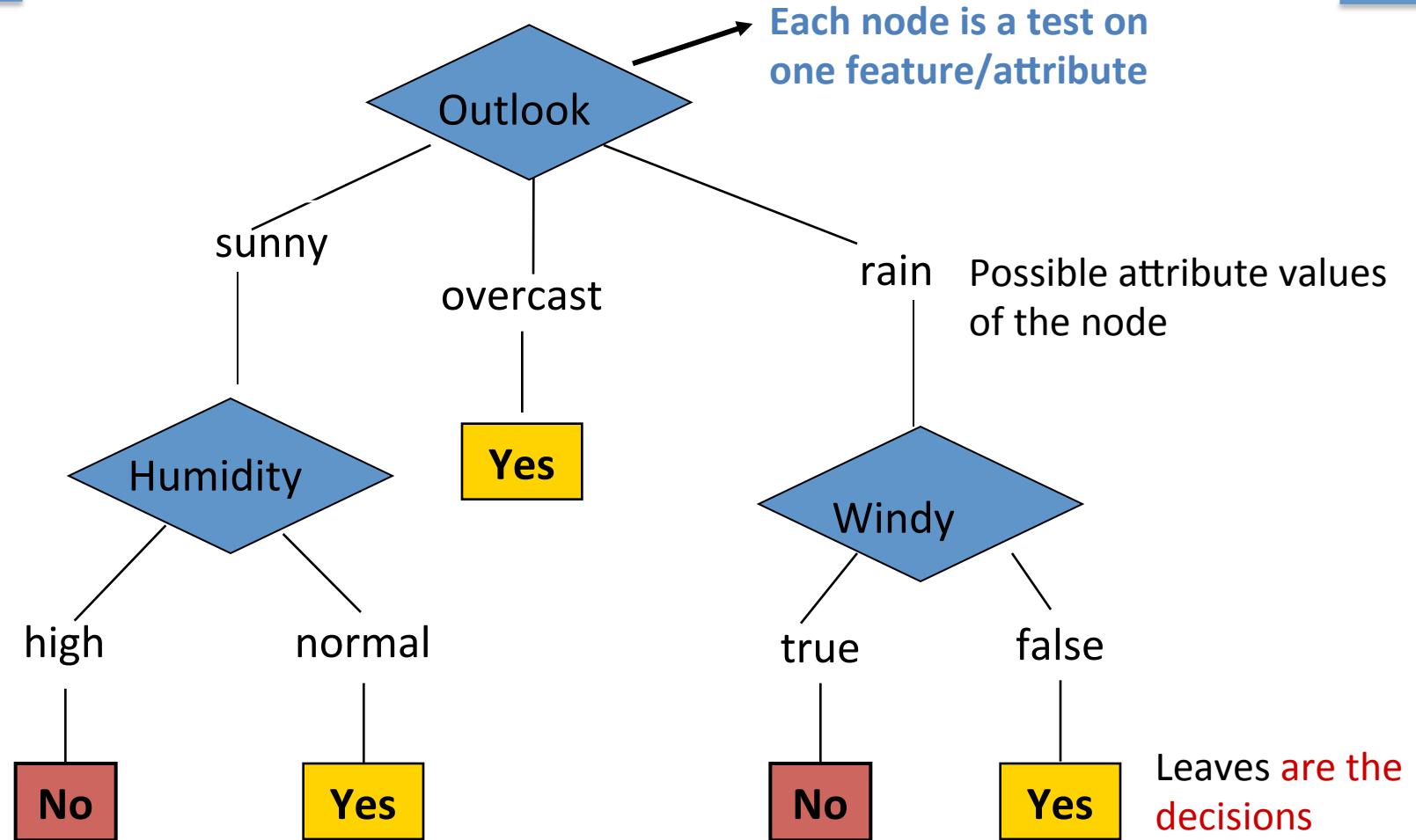
# Nearest neighbor classification

- *k*-Nearest neighbor classifier is a **lazy** learner
  - Does not build model explicitly.
  - Unlike **eager** learners such as decision tree induction and rule-based systems.
  - Classifying unknown samples is relatively expensive.
- *k*-Nearest neighbor classifier is a **local** model, vs. **global** model of linear classifiers.

## (5) Decision Tree / Random Forest



# Anatomy of a decision tree



# Decision trees

- Decision trees represent a disjunction of conjunctions of constraints on the attribute values of instances.

- (Outlook ==overcast)
- OR
- ((Outlook==rain) and (Windy==false))
- OR
- ((Outlook==sunny) and (Humidity=normal))
- => yes play tennis

# Information gain

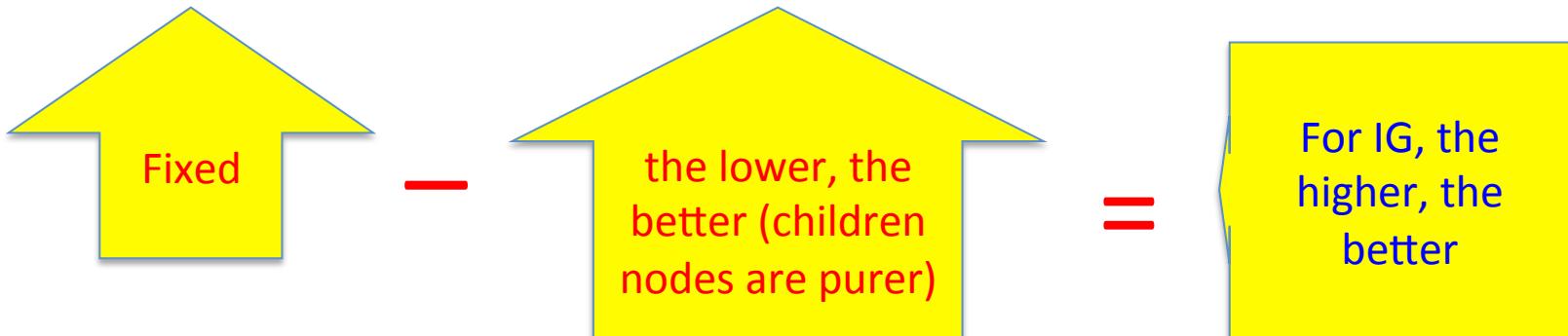
- $IG(X_i, Y) = H(Y) - H(Y|X_i)$

Reduction in uncertainty by knowing a feature  $X_i$

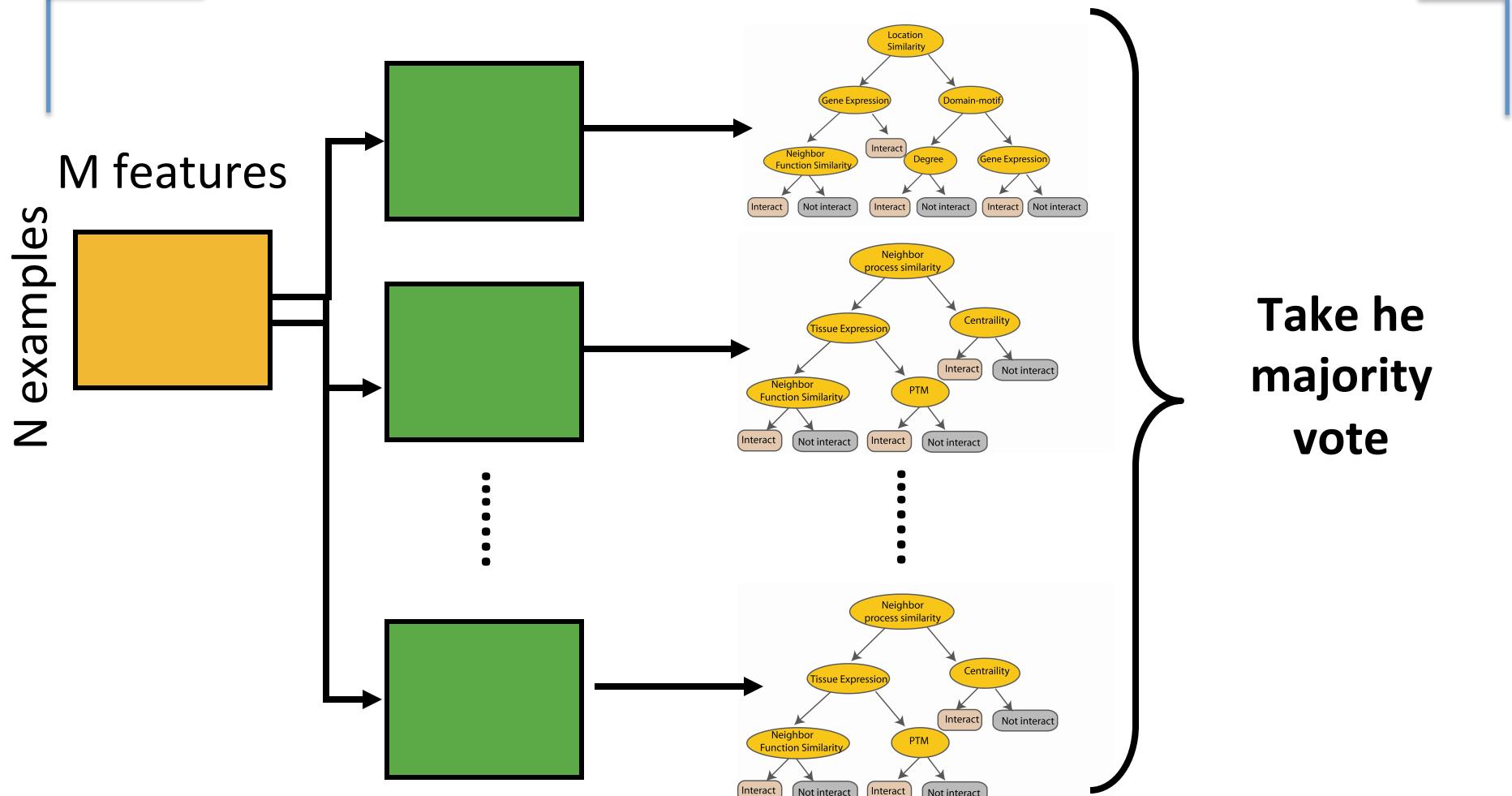
Information gain:

= (information before split) – (information after split)

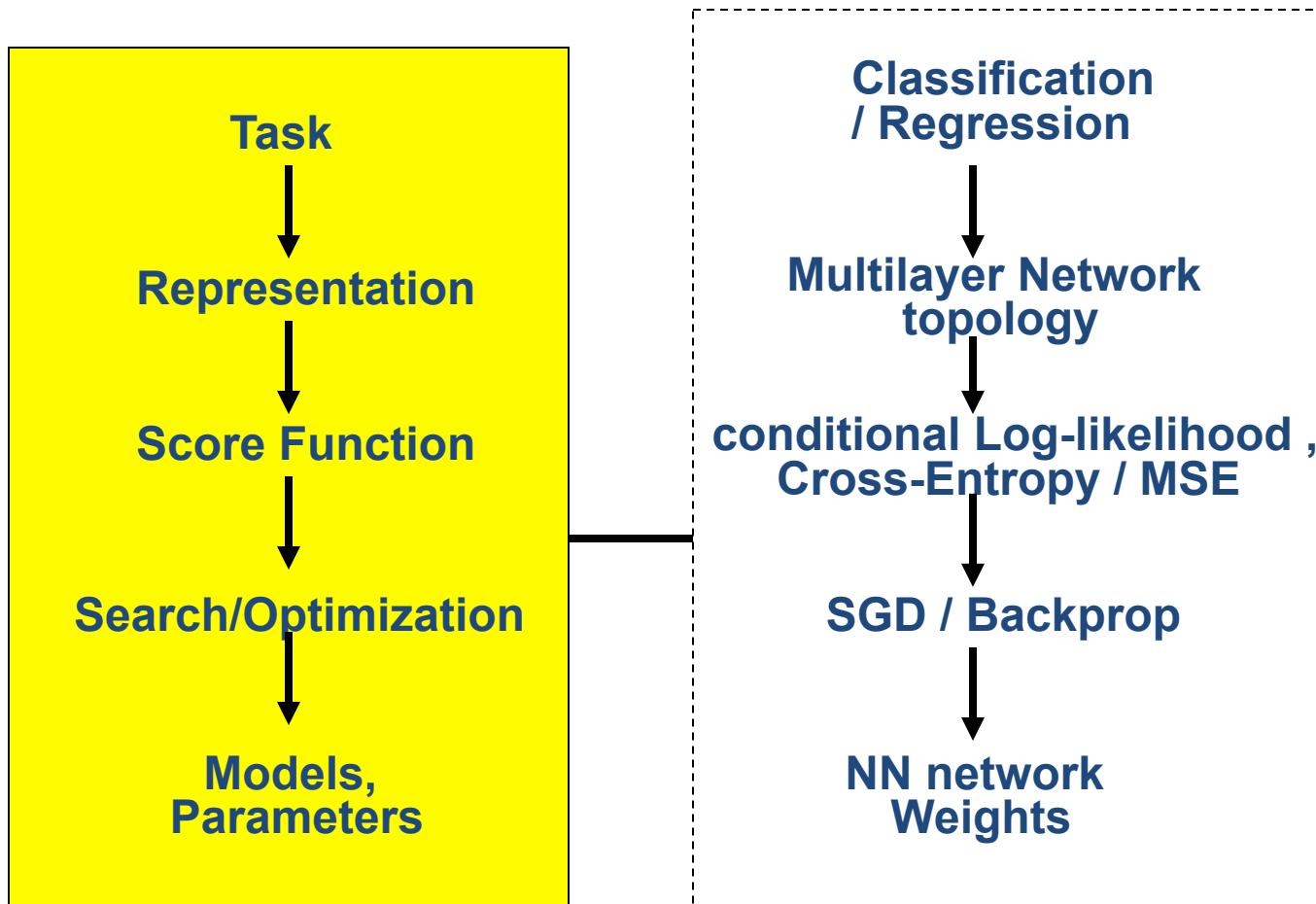
= entropy(parent) – [average entropy(children)]



# Random Forest Classifier



## (6) Neural Network

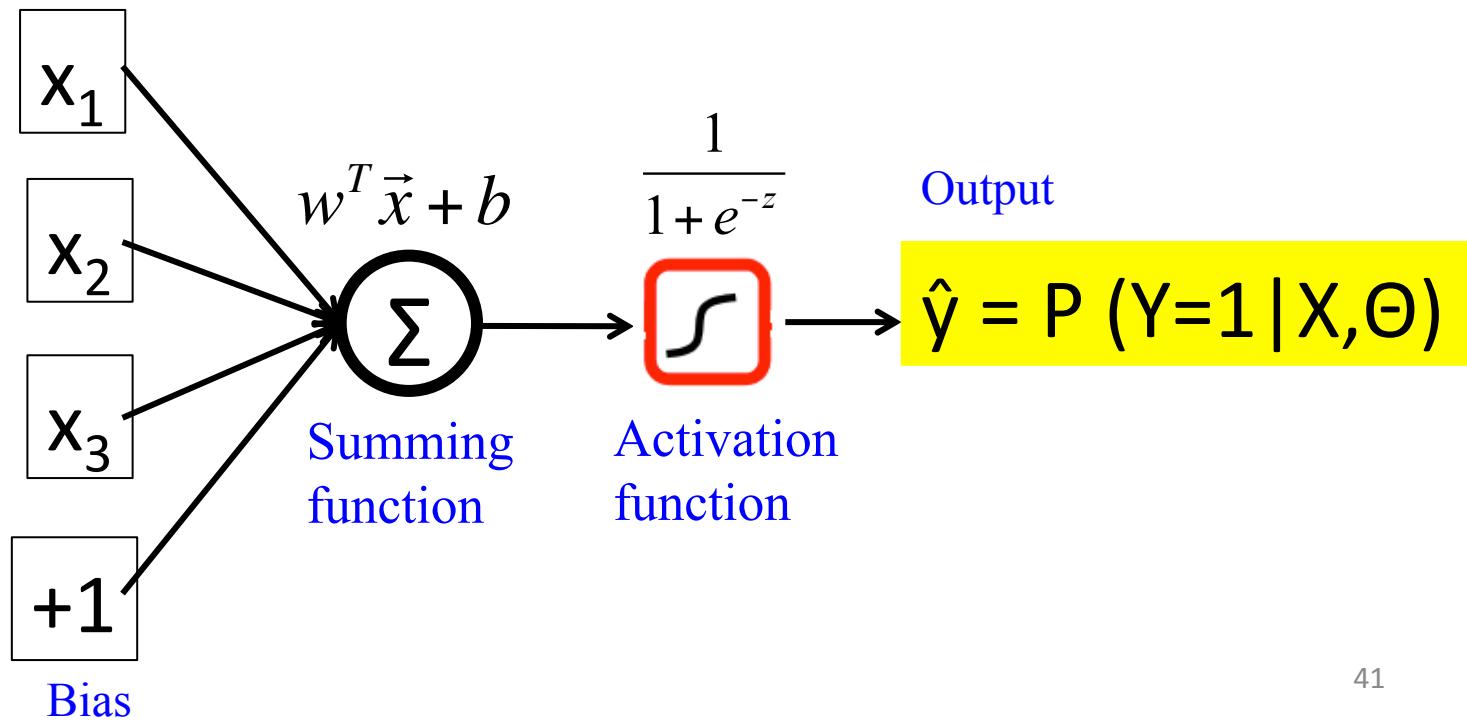


# Logistic regression

Logistic regression could be illustrated as a module

On input  $x$ , it outputs  $\hat{y}$ :

where

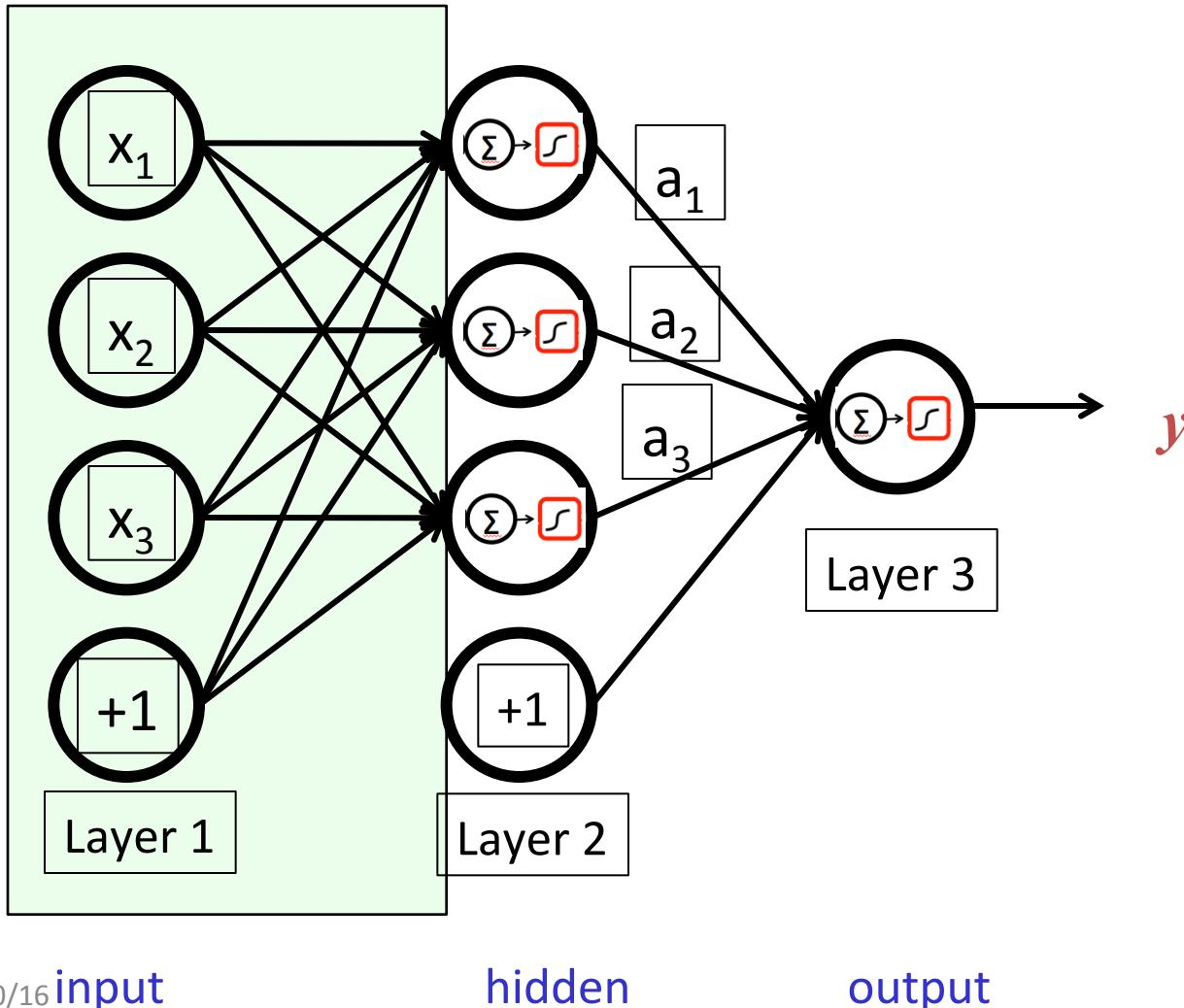


Draw a logistic regression unit as:

11/30/16

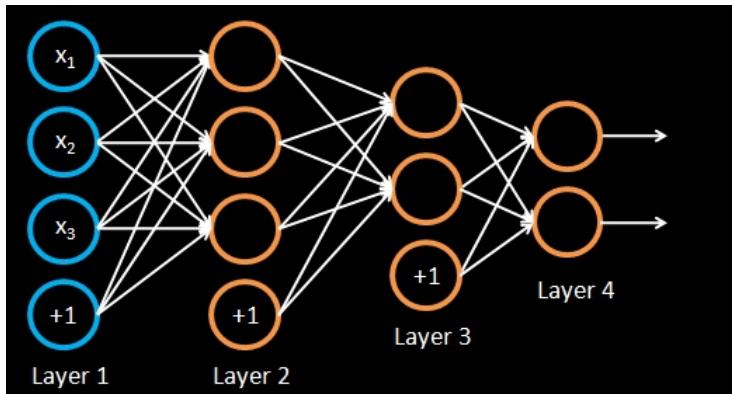
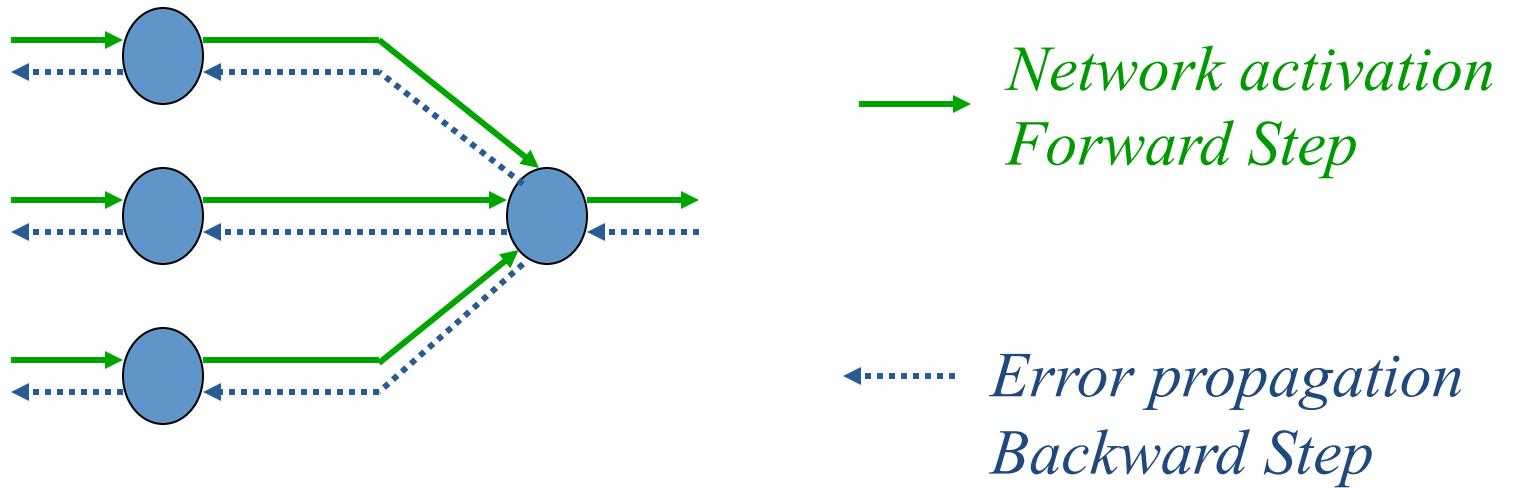
# Multi-Layer Perceptron (MLP)

String a lot of logistic units together. Example: 3 layer network:

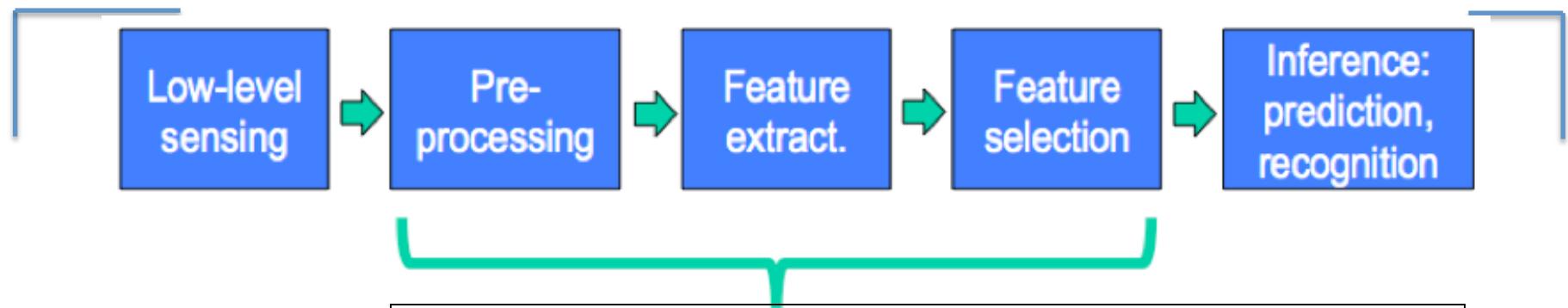


# Backpropagation

- Back-propagation training algorithm

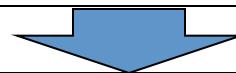


# Deep Learning Way: Learning features / Representation from data



## Feature Engineering

- ✓ Most critical for accuracy
- ✓ Account for most of the computation for testing
- ✓ Most time-consuming in development cycle
- ✓ Often hand-craft and task dependent in practice



## Feature Learning

- ✓ Easily adaptable to new similar tasks
- ✓ Layerwise representation
- ✓ Layer-by-layer unsupervised training
- ✓ Layer-by-layer supervised training

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# What we have covered (III)

## ❑ Unsupervised models

- Dimension Reduction (PCA)
- Hierarchical clustering
- K-means clustering
- GMM/EM clustering

	$X_1$	$X_2$	$X_3$
$s_1$			
$s_2$			
$s_3$			
$s_4$			
$s_5$			
$s_6$			

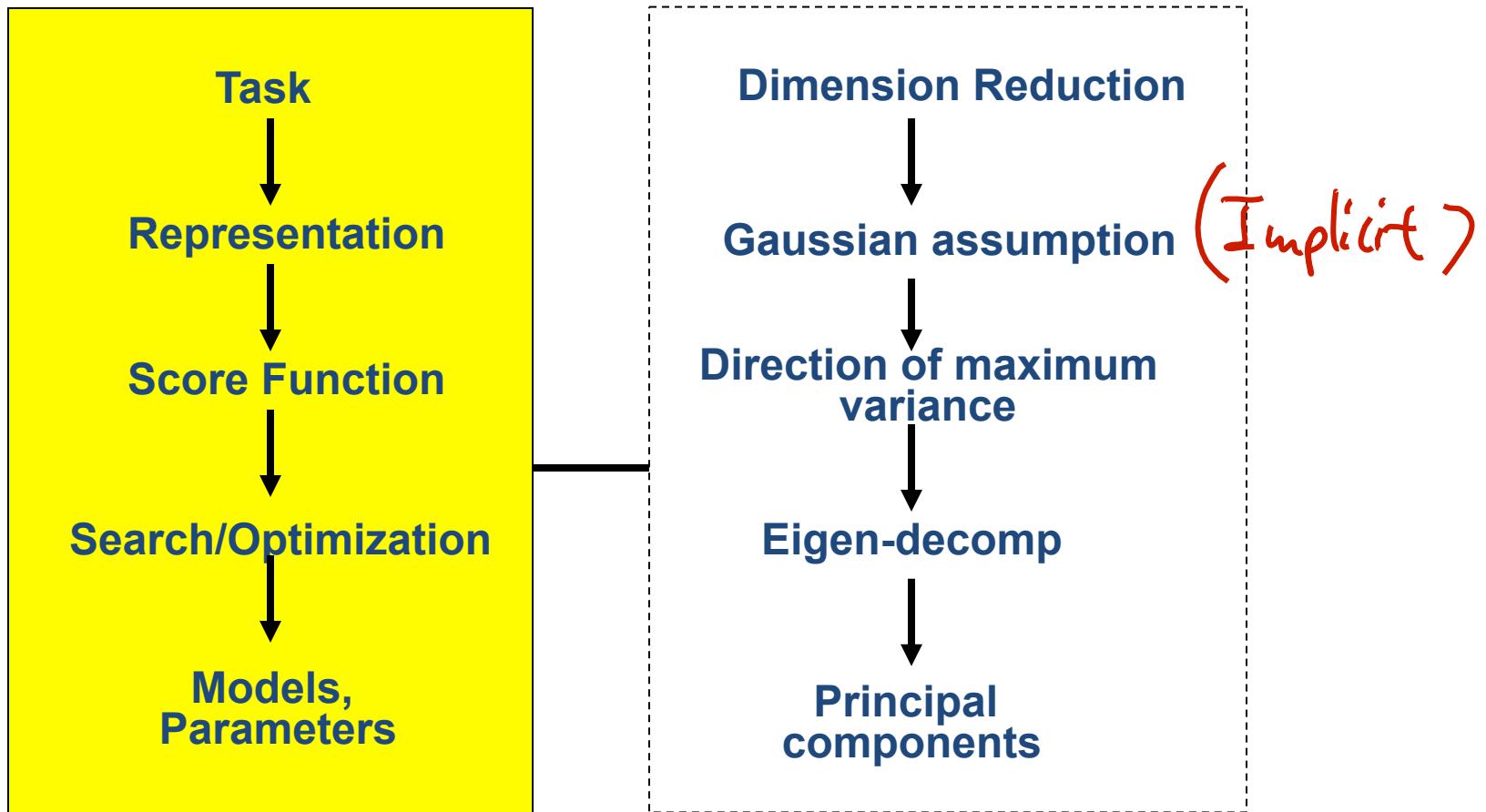
# An unlabeled Dataset X

a data matrix of  $n$  observations on  $p$  variables  $x_1, x_2, \dots, x_p$

**Unsupervised learning** = learning from raw (unlabeled, unannotated, etc) data, as opposed to supervised data where a label of examples is given

- Data/points/instances/examples/samples/records: [rows]
- Features/attributes/dimensions/independent variables/covariates/predictors/regressors: [columns]

# (0) Principal Component Analysis

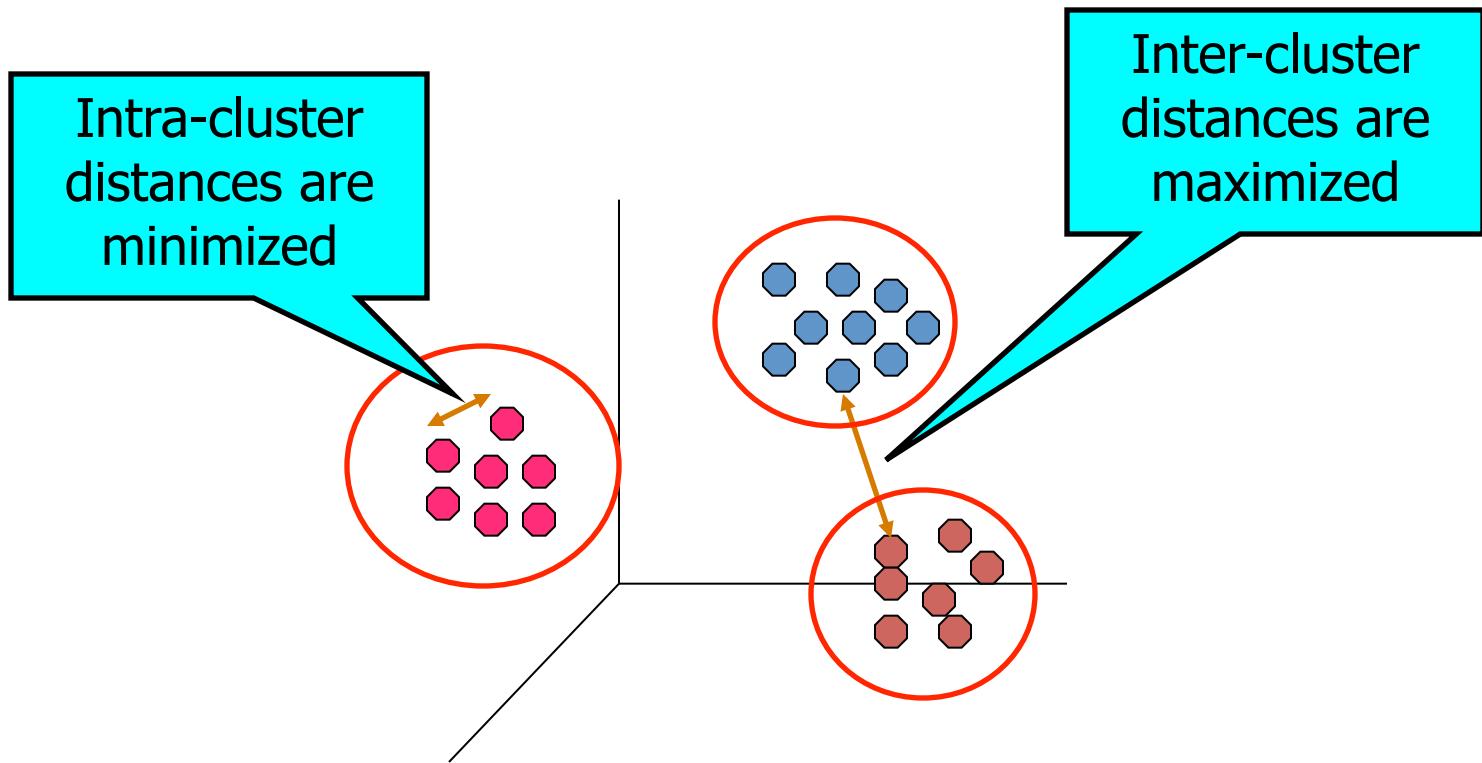


# What we have covered (III)

- ❑ Unsupervised models
  - Dimension Reduction (PCA)
  - Hierarchical clustering
  - K-means clustering
  - GMM/EM clustering

# What is clustering?

- Find groups (clusters) of data points such that data points in a group will be similar (or related) to one another and different from (or unrelated to) the data points in other groups

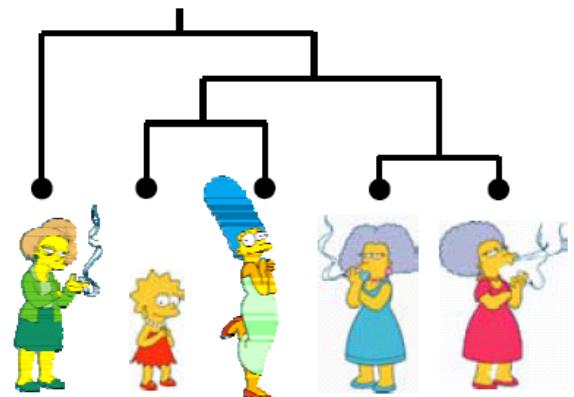
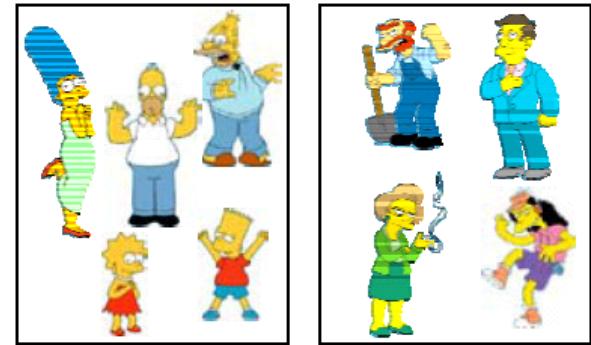


# Issues for clustering

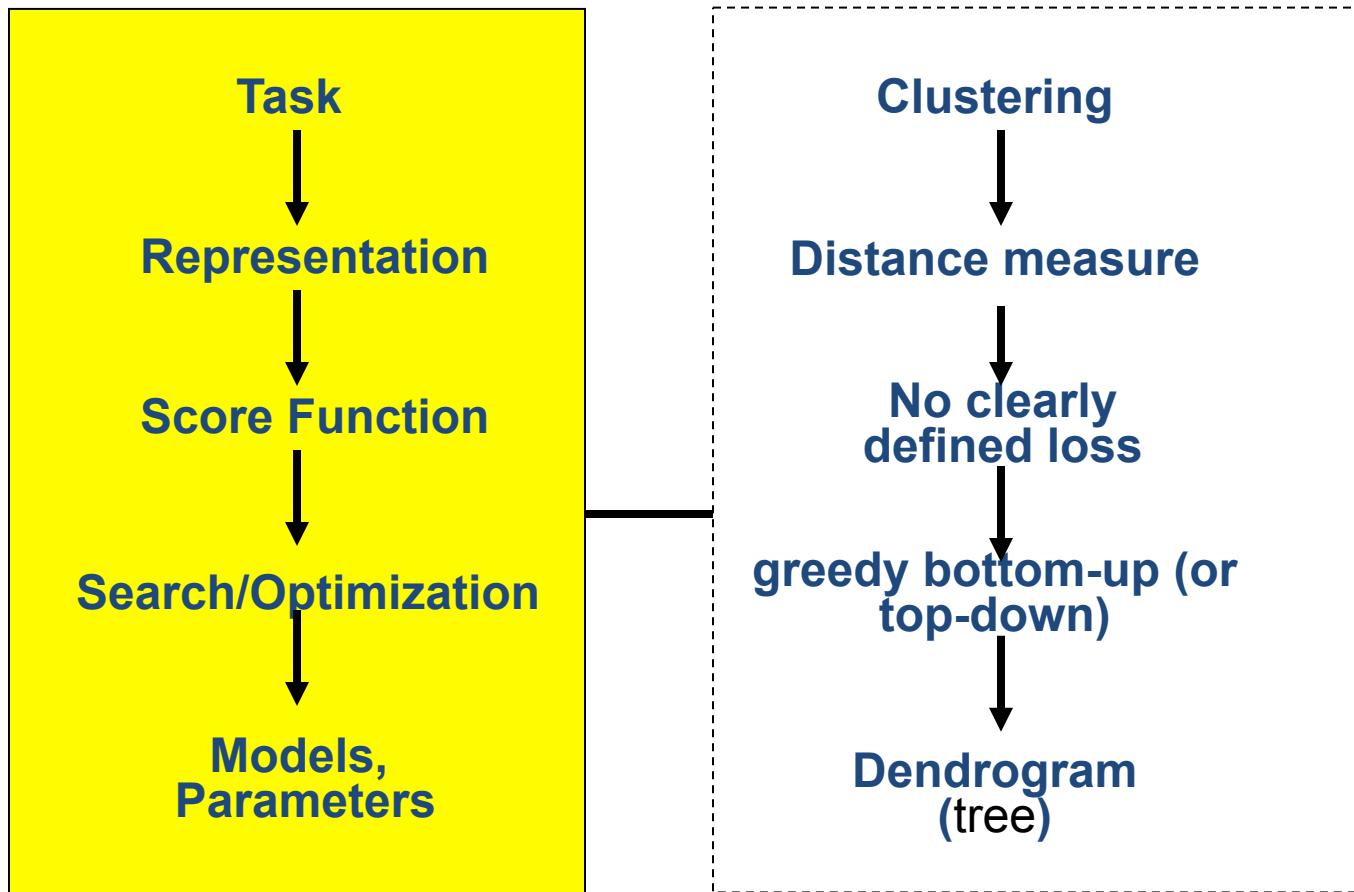
- What is a natural grouping among these objects?
  - Definition of "groupness"
- What makes objects “related”?
  - Definition of "similarity/distance"
- Representation for objects
  - Vector space? Normalization?
- How many clusters?
  - Fixed a priori?
  - Completely data driven?
    - Avoid “trivial” clusters - too large or small
- Clustering Algorithms
  - Partitional algorithms
  - Hierarchical algorithms
- Formal foundation and convergence

# Clustering Algorithms

- Partitional algorithms
  - Usually start with a random (partial) partitioning
  - Refine it iteratively
    - K means clustering
    - Mixture-Model based clustering
- Hierarchical algorithms
  - Bottom-up, agglomerative
  - Top-down, divisive



# (1) Hierarchical Clustering



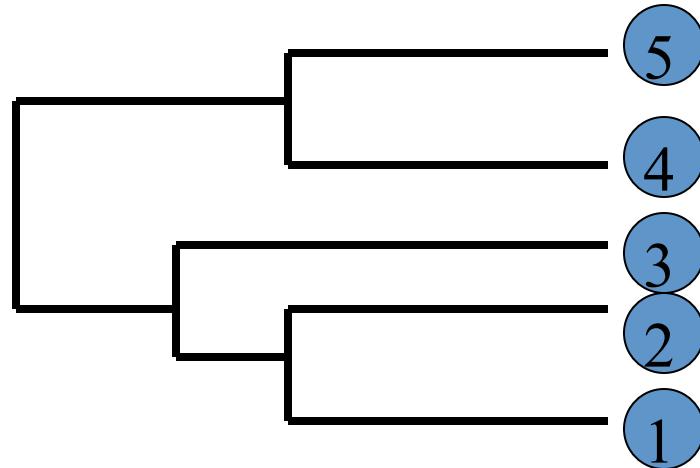
# Example: single link

$$\begin{array}{cc}
 & \begin{matrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 0 \\ 2 & 2 & 0 \\ 3 & 6 & 3 & 0 \\ 4 & 10 & 9 & 7 & 0 \\ 5 & 9 & 8 & 5 & 4 & 0 \end{matrix} \\
 \longrightarrow &
 \end{array}$$

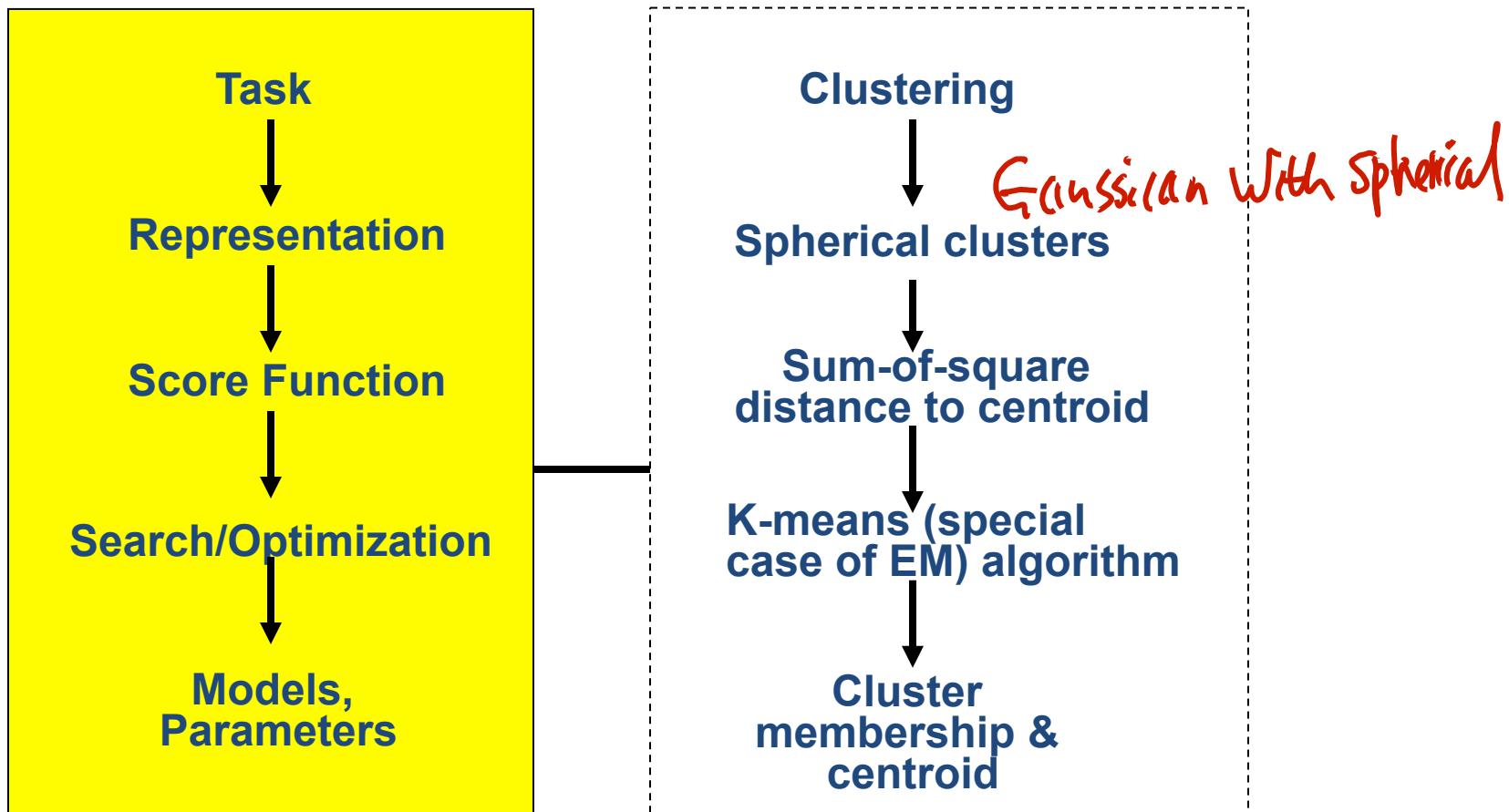
$$\begin{array}{cc}
 & \begin{matrix} (1,2) & 3 & 4 & 5 \\ (1,2) & 0 \\ 3 & 3 & 0 \\ 4 & 9 & 7 & 0 \\ 5 & 8 & 5 & 4 & 0 \end{matrix} \\
 \longrightarrow &
 \end{array}$$

$$\begin{array}{cc}
 & \begin{matrix} (1,2,3) & 4 & 5 \\ (1,2,3) & 0 \\ 4 & 7 & 0 \\ 5 & 5 & 4 & 0 \end{matrix}
 \end{array}$$

$$d_{(1,2,3),(4,5)} = \min\{ d_{(1,2,3),4}, d_{(1,2,3),5} \} = 5$$

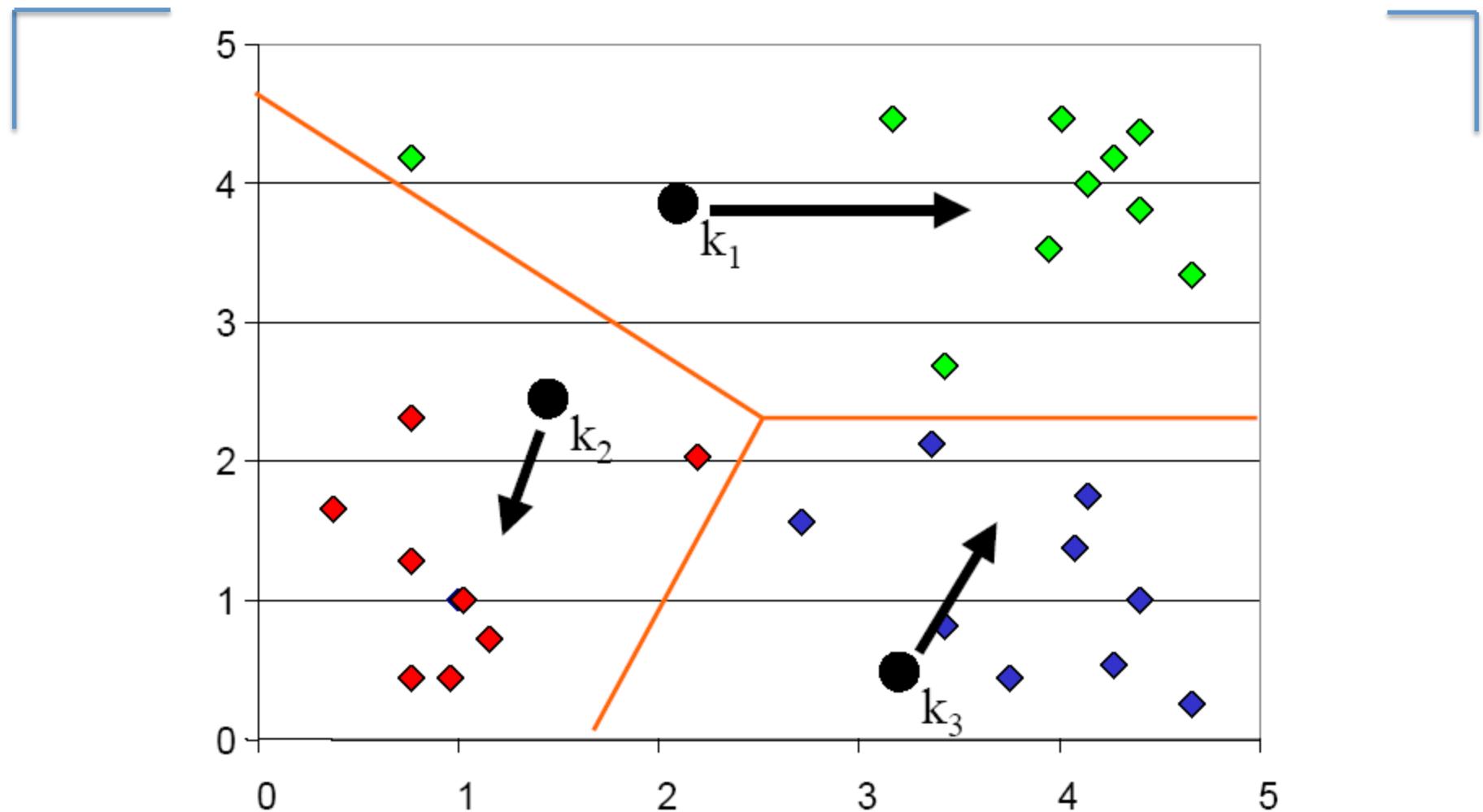


## (2) K-means Clustering



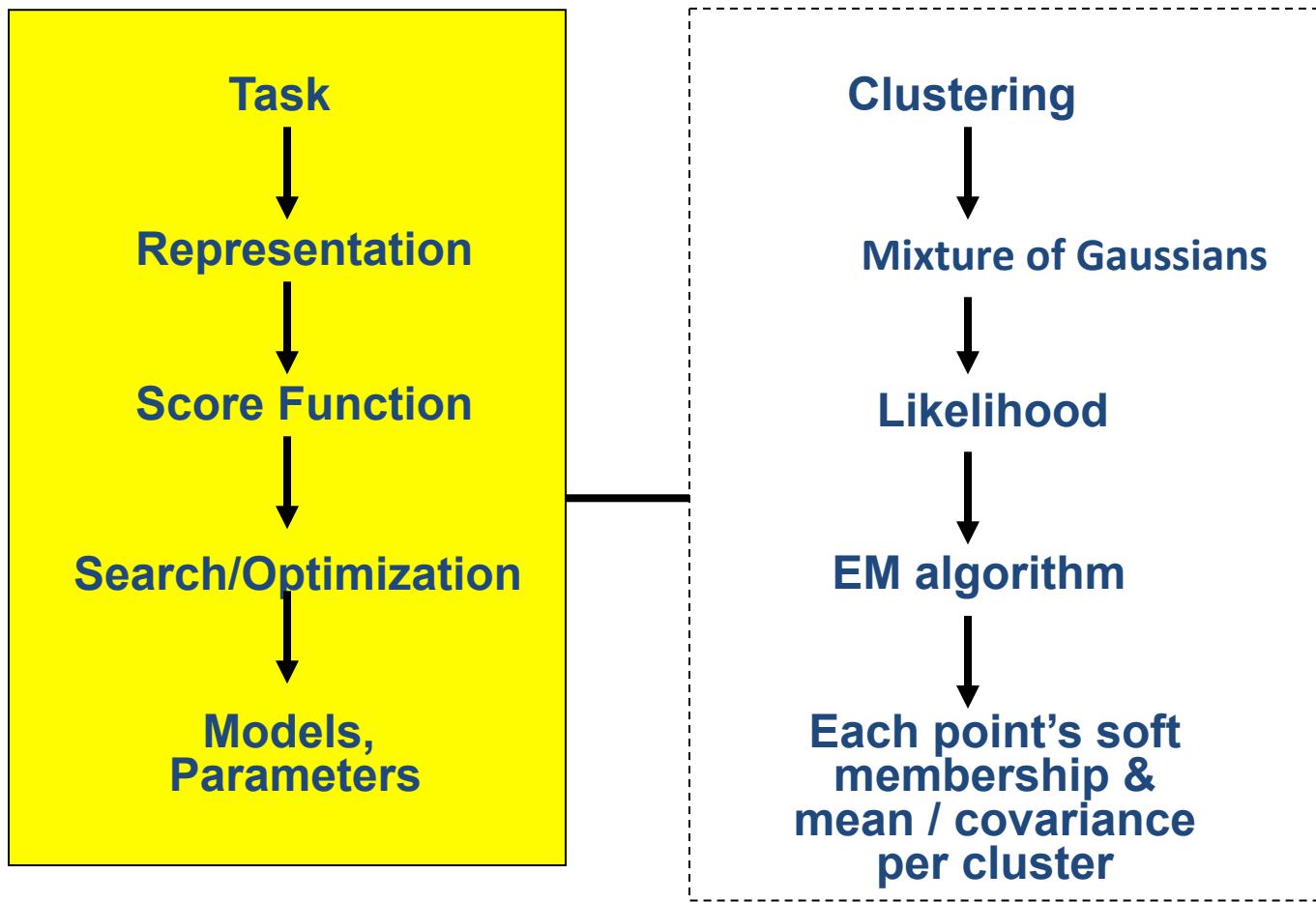
## K-means Clustering: Step 2

- Determine the membership of each data points



### (3) GMM Clustering

Dr. Yanjun Qi / UVA CS 6316 / f16



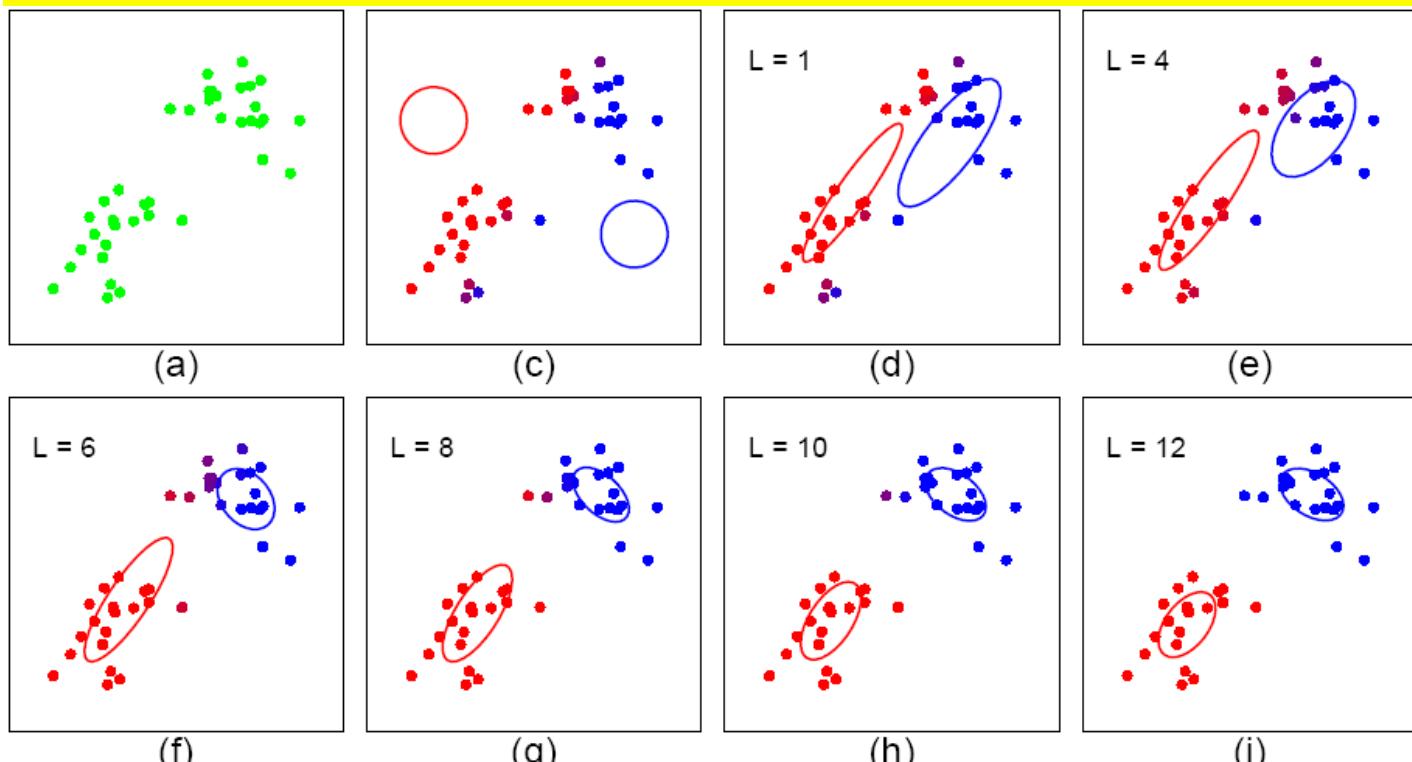
$$\sum_i \log \prod_{i=1}^n p(x = x_i) = \sum_i \log \left[ \sum_{\mu_j} p(\mu = \mu_j) \frac{1}{(2\pi)^{p/2} |\Sigma_j|^{1/2}} e^{-\frac{1}{2} (\vec{x} - \vec{\mu}_j)^T \Sigma_j^{-1} (\vec{x} - \vec{\mu}_j)} \right]$$

# Expectation-Maximization

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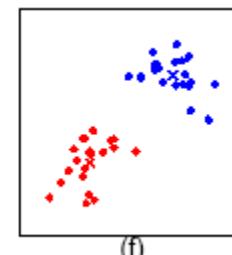
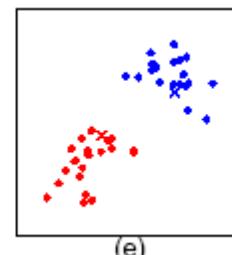
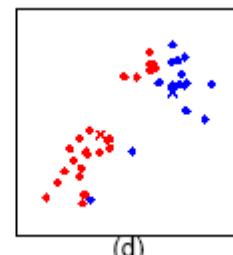
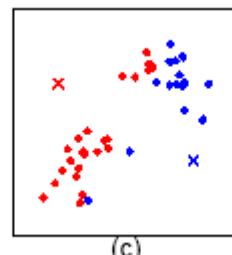
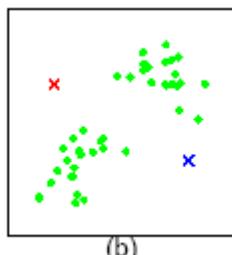
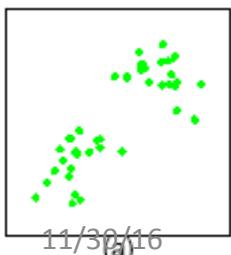
## for training GMM

- Start:
  - "Guess" the centroid  $m_k$  and covariance  $S_k$  of each of the K clusters
- Loop
  - each cluster, revising both the mean (centroid position) and covariance (shape)



# Compare: K-means

- The EM algorithm for mixtures of Gaussians is like a "soft version" of the K-means algorithm.
- In the K-means “E-step” we do hard assignment:
- In the K-means “M-step” we update the means as the weighted sum of the data, but now the weights are 0 or 1:



11/30 (16)

# Today

- ❑ Review of ML methods covered so far
  - ❑ Regression (supervised)
  - ❑ Classification (supervised)
  - ❑ Unsupervised models
  - ❑ Learning theory
  
- ❑ Review of Assignments covered so far

# What we have covered (IV)

- ❑ Learning theory / Model selection
  - K-folds cross validation
  - Expected prediction error
  - Bias and variance tradeoff

# CV-based Model Selection

We're trying to decide which algorithm / hyperparameter to use.

- We train each model and make a table...

$i$	$f_i$	TRAINERR	10-FOLD-CV-ERR	Choice
1	$f_1$			
2	$f_2$			
3	$f_3$			✓
4	$f_4$			
5	$f_5$			
6	$f_6$			

Hyperparameter tuning ....

# Which kind of cross-validation ?

	<b>Downside</b>	<b>Upside</b>
<b>Test-set</b>	Variance: unreliable estimate of future performance	Cheap
<b>Leave-one-out</b>	Expensive. Has some weird behavior	Doesn't waste data
<b>10-fold</b>	Wastes 10% of the data. 10 times more expensive than test set	Only wastes 10%. Only 10 times more expensive instead of R times.
<b>3-fold</b>	Wastier than 10-fold. Expensivier than test set	Slightly better than test-set
<b>R-fold</b> 11/30/16	Identical to Leave-one-out	

# What we have covered (IV)

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  - K-folds cross validation
  - Expected prediction error
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# Statistical Decision Theory

- Random input vector:  $X$
  - Random output variable:  $Y$
  - Joint distribution:  $\Pr(X, Y)$
  - Loss function  $L(Y, f(X))$
  - Expected prediction error (EPE):
    - $\text{EPE}(f) = \mathbb{E}(L(Y, f(X))) = \int L(y, f(x)) \Pr(dx, dy)$   
e.g.  $= \int (y - f(x))^2 \Pr(dx, dy)$
- e.g. Squared error loss (also called L2 loss )

Consider population distribution

# Bias-Variance Trade-off for EPE:

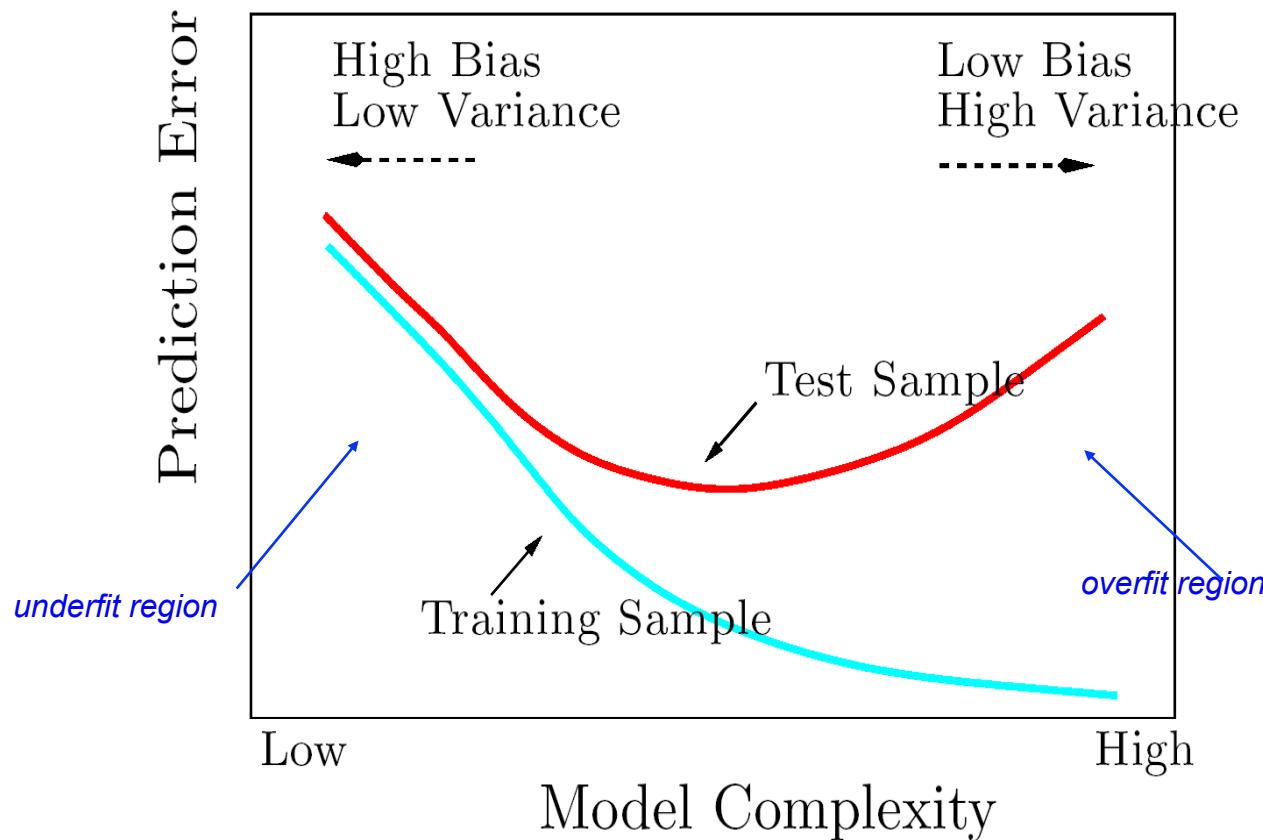
$$\text{EPE} (\cancel{x_0}) = \text{noise}^2 + \text{bias}^2 + \text{variance}$$

Unavoidable  
error

Error due to  
incorrect  
assumptions

Error due to  
variance of training  
samples

# Bias-Variance Tradeoff / Model Selection



# Model “bias” & Model “variance”

- Middle RED:
  - TRUE function

$\theta$   
[middle red]

- Error due to bias:
  - How far off in general from the middle red

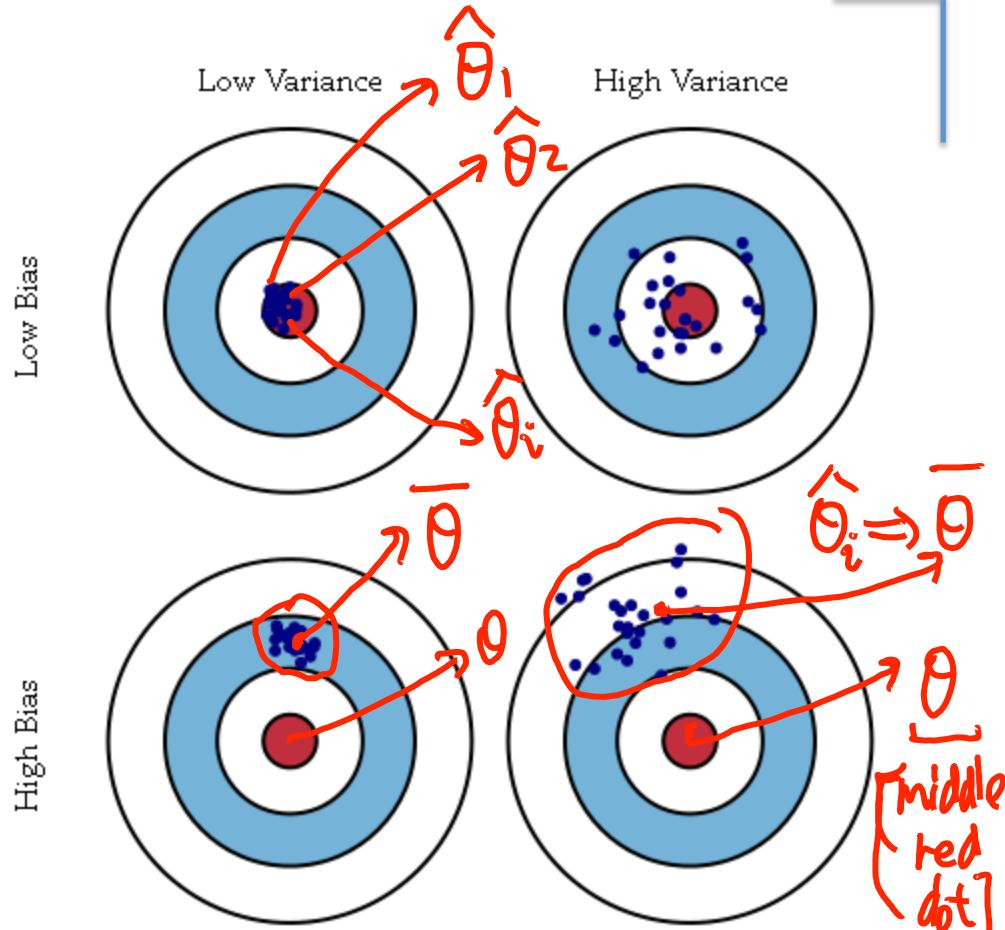
$$E(\theta - \bar{\theta})$$

mean of  $\hat{\theta}$

- Error due to variance:
  - How wildly the blue points spread

$$E((\hat{\theta} - \bar{\theta})^2)$$

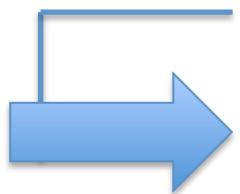
$\{\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3, \dots\}$  Blue dots



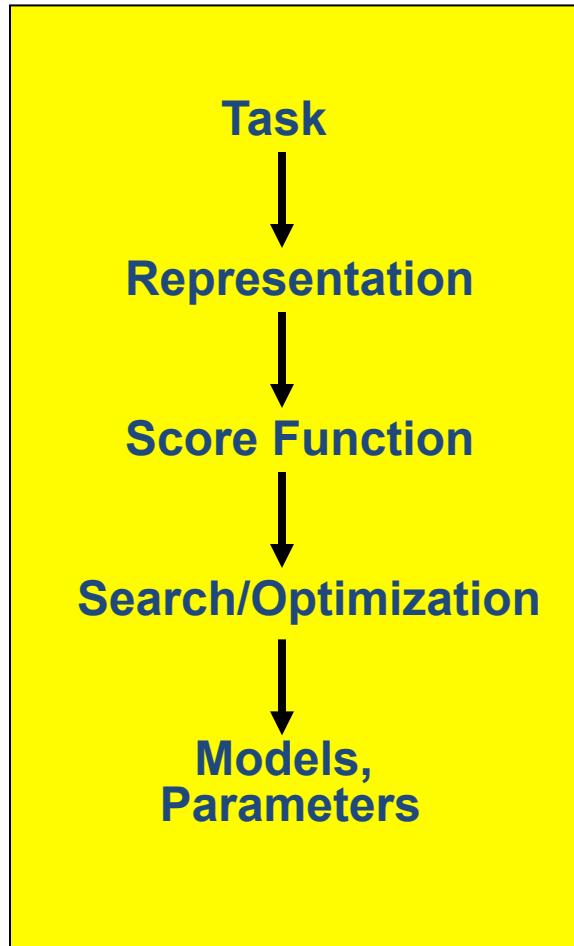
# need to make assumptions that are able to generalize

- Components of generalization error
  - **Bias**: how much the average model over all training sets differ from the true model?
    - Error due to inaccurate assumptions/simplifications made by the model
  - **Variance**: how much models estimated from different training sets differ from each other
- **Underfitting**: model is too “simple” to represent all the relevant class characteristics
  - High bias and low variance
  - **High training error and high test error**
- **Overfitting**: model is too “complex” and fits irrelevant characteristics (noise) in the data
  - Low bias and high variance
  - **Low training error and high test error**

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- 

# Machine Learning in a Nutshell



ML grew out of  
work in AI

*Optimize a  
performance criterion  
using example data or  
past experience,*

*Aiming to generalize to  
unseen data*

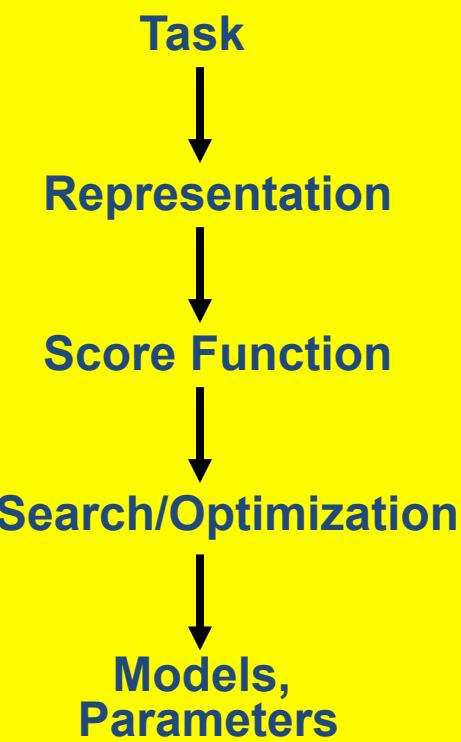
# What we have covered for each component

<b>Task</b>	Regression, classification, clustering, dimen-reduction
<b>Representation</b>	Linear func, nonlinear function (e.g. polynomial expansion), local linear, logistic function (e.g. $p(c x)$ ), tree, multi-layer, prob-density family (e.g. Bernoulli, multinomial, Gaussian, mixture of Gaussians), local func smoothness, kernel matrix, local smoothness, partition of feature space,
<b>Score Function</b>	MSE, Margin, log-likelihood, EPE (e.g. L2 loss for KNN, 0-1 loss for Bayes classifier), cross-entropy, cluster points distance to centers, variance, conditional log-likelihood, complete data-likelihood, regularized loss func (e.g. L1, L2) ,
<b>Search/ Optimization</b>	Normal equation, gradient descent, stochastic GD, Newton, Linear programming, Quadratic programming (quadratic objective with linear constraints), greedy, EM, asyn-SGD, eigenDecomp, backprop
<b>Models, Parameters</b>	Linear weight vector, basis weight vector, local weight vector, dual weights, training samples, tree-dendrogram, multi-layer weights, principle components, member (soft/hard) assignment, cluster centroid, cluster covariance (shape), ...

# Today

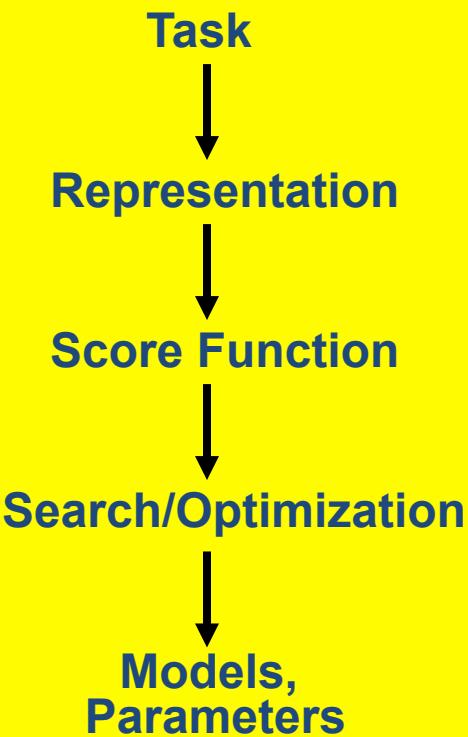
- ❑ Review of ML methods covered so far
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# HW1



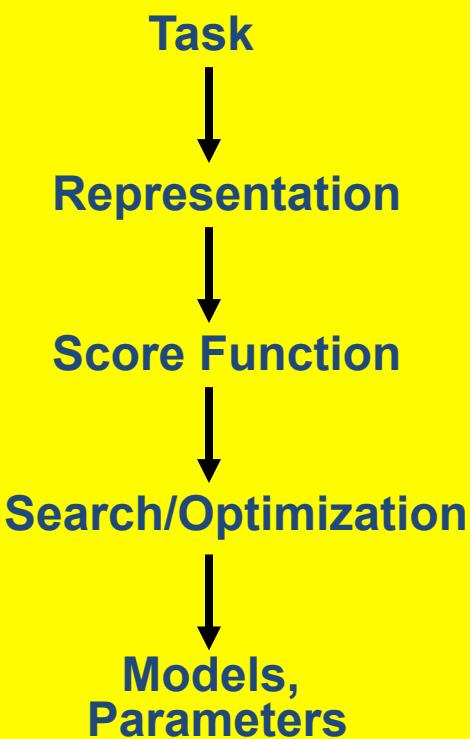
- Q1: Linear algebra review
- Q2: Linear regression + LOOCV
  - Regression
  - Evaluation pipeline
- Q3: Machine learning pipeline practice
  - Basic pipeline
  - GUI Toolbox
  - Evaluation

# HW2



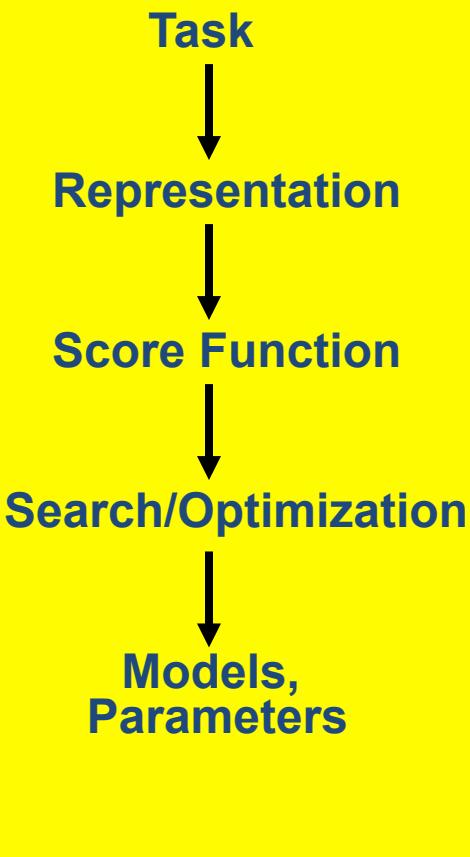
- Q1: Linear regression model fitting
  - Data loading
  - Basic linear regression
  - Three ways to train : Normal equation / SGD / Batch GD
  - Polynomial regression
- Q2: Ridge regression
  - Math derivation of ridge
  - Understand why/how Ridge
  - Model selection of Ridge with K-CV<sup>75</sup>

# HW3



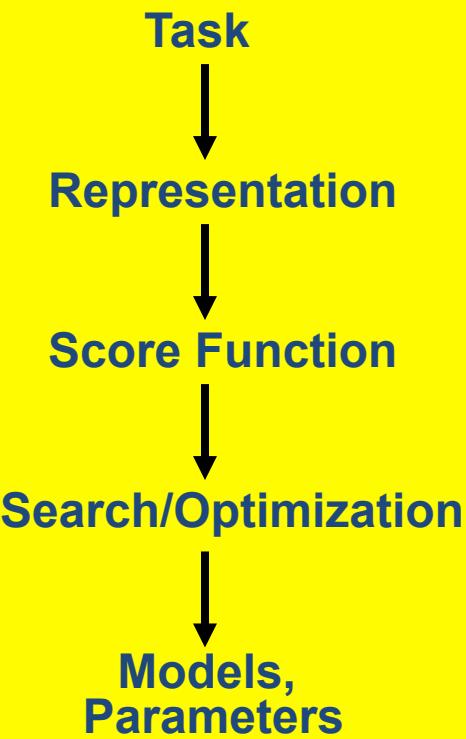
- Q1: Support Vector Machines with Scikit-Learn
  - Data preprocessing
  - How to use SVM package
  - Model selection for SVM
  - Model selection pipeline with train-vali, or train-CV; then test

# HW5



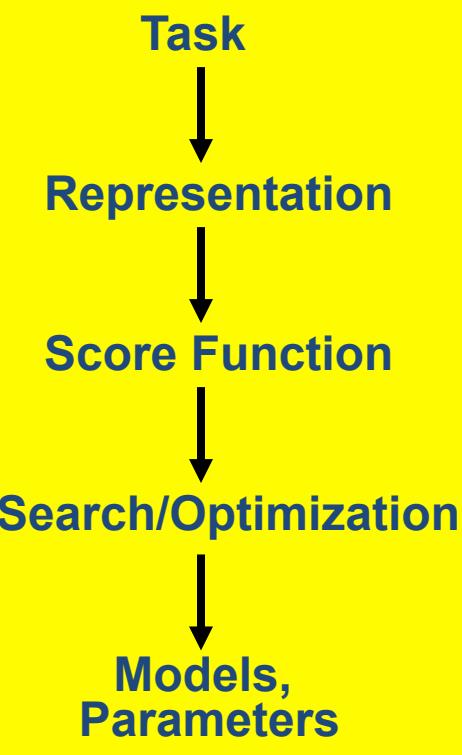
- Q1: Naive Bayes Classifier for Text-base Movie Review Classification
  - Preprocessing of text samples
  - BOW Document Representation
  - Multinomial Naive Bayes Classifier
    - BOW way
    - Language model way
  - Multivariate Bernoulli Naive Bayes Classifier

# HW6



- Q1: Neural Network  
Tensorflow Playground
  - Interactive learning of MLP
  - Feature engineering vs.
  - Feature learning
- Q2: Image Classification
  - Tool using
  - DT / KNN / SVM
  - PCA effect for image classification

# HW6



- Q3: Unsupervised Clustering of audio data and consensus data
  - Data loading
  - K-mean clustering
  - GMM clustering
  - How to find K: knee-finding plot
  - How to measure clustering: purityMetric

# References

- Hastie, Trevor, et al. The elements of statistical learning. Vol. 2. No. 1. New York: Springer, 2009.
- Prof. M.A. Papalaskar's slides
- Prof. Andrew Ng's slides