

UVA CS 6316/4501

– Fall 2016

Machine Learning

Lecture 22: Review

Dr. Yanjun Qi

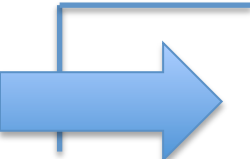
University of Virginia

Department of
Computer Science

Announcements: Final Exam

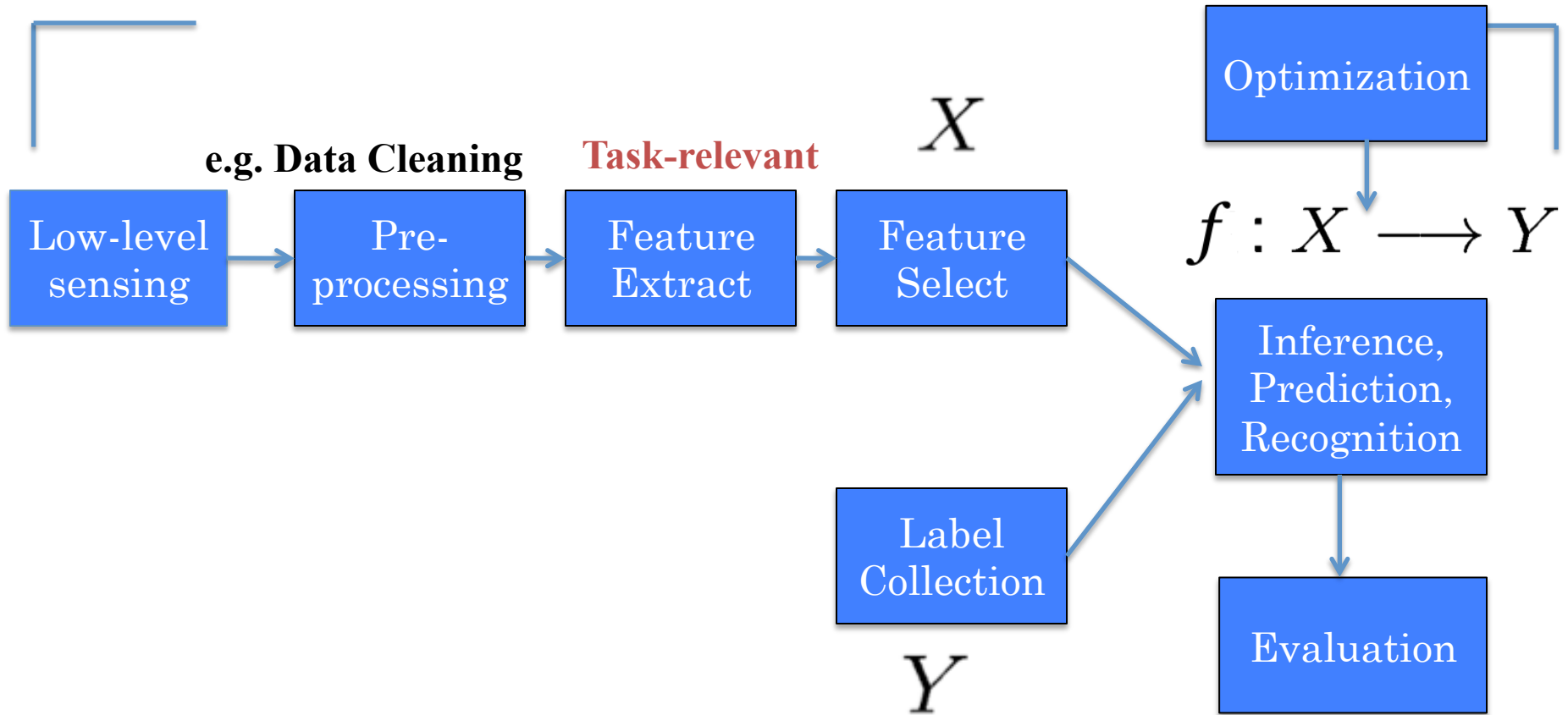
- Closed Note
- Allowing a paper (us letter size) of cheat sheet
- No laptop / No Cell phone / No internet access / No electronic devices
- Recital session this Friday (@OSL120, 4pm-5pm) for HW7
- Covering post-midterm contents (L12-) till today
 - Practice with sample questions in HW7
 - HW7 due next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

Today

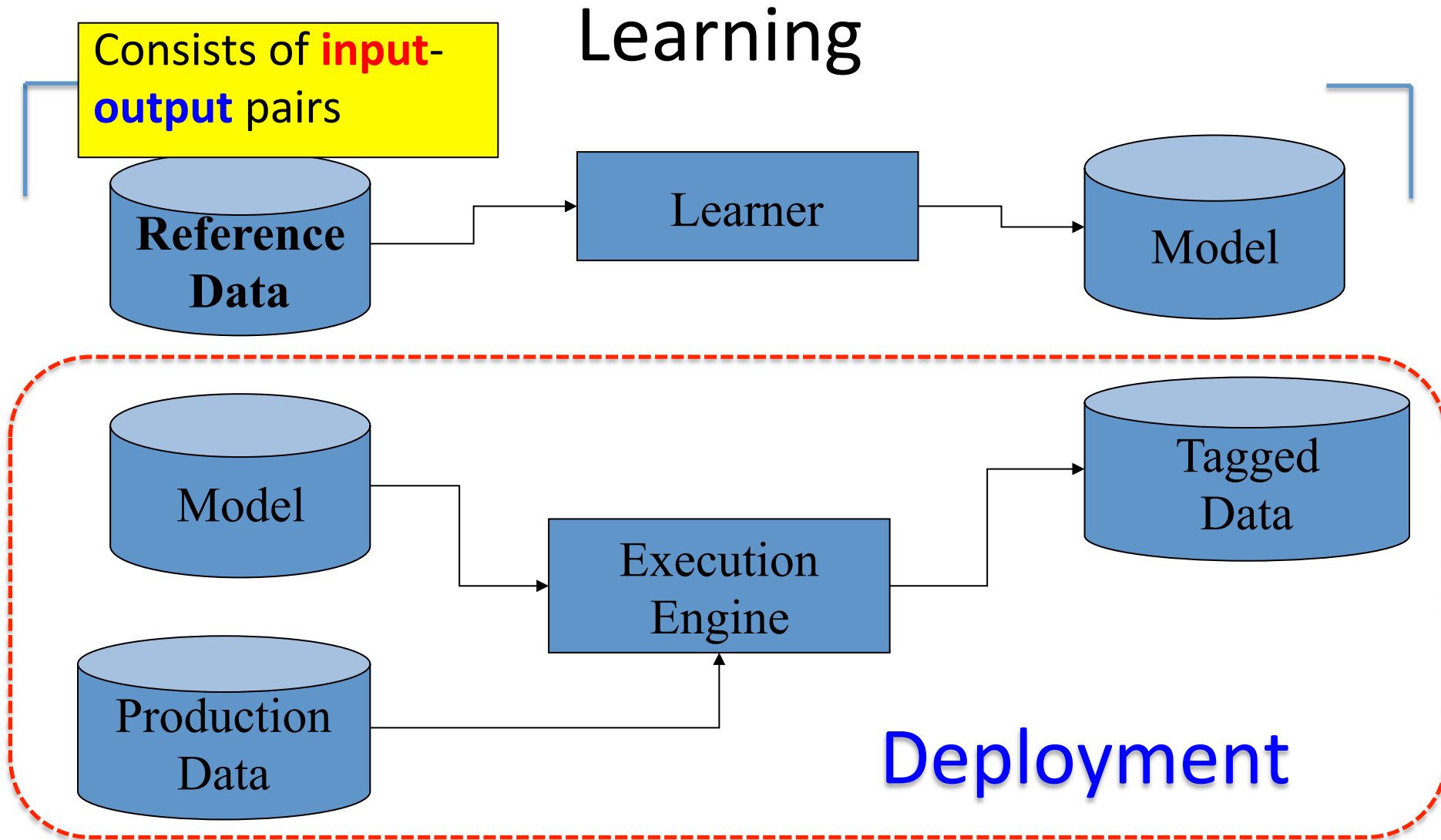
- 
- ❑ Review of ML methods covered so far
 - ❑ Regression (supervised)
 - ❑ Classification (supervised)
 - ❑ Unsupervised models
 - ❑ Learning theory

 - ❑ Review of Assignments covered so far

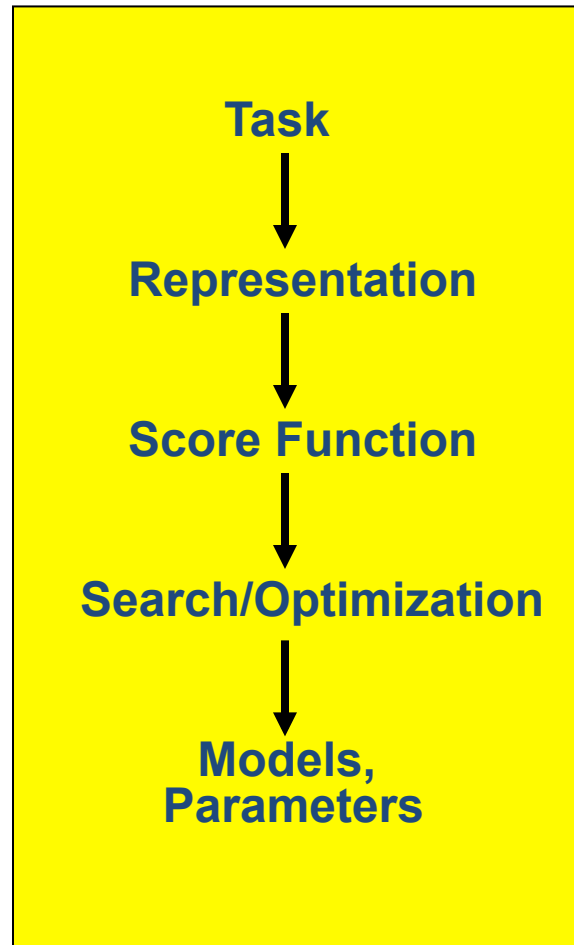
A Typical Machine Learning Pipeline



An **Operational** Model of Machine



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

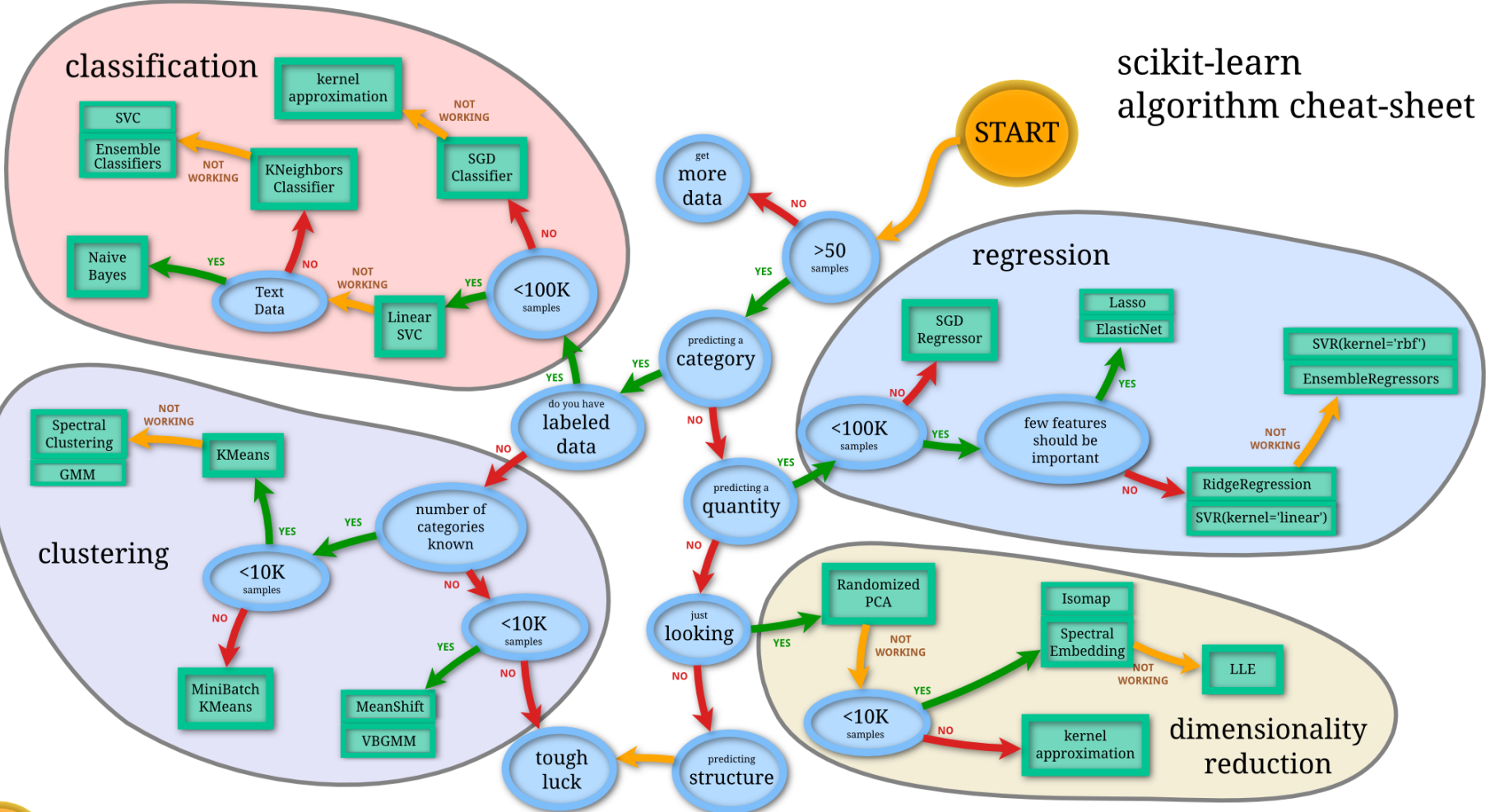
What we have covered

| | |
|---------------------------------|--|
| Task | |
| Representation | |
| Score Function | |
| Search/ Optimization | |
| Models, Parameters | |

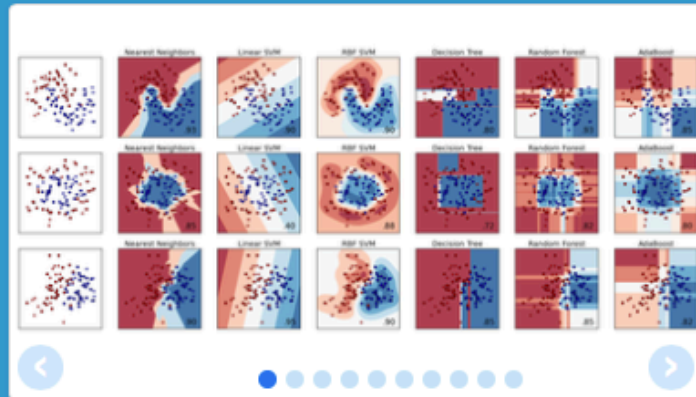
http://scikit-learn.org/stable/tutorial/machine_learning_map/

Scikit-learn algorithm cheat-sheet

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 belong 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

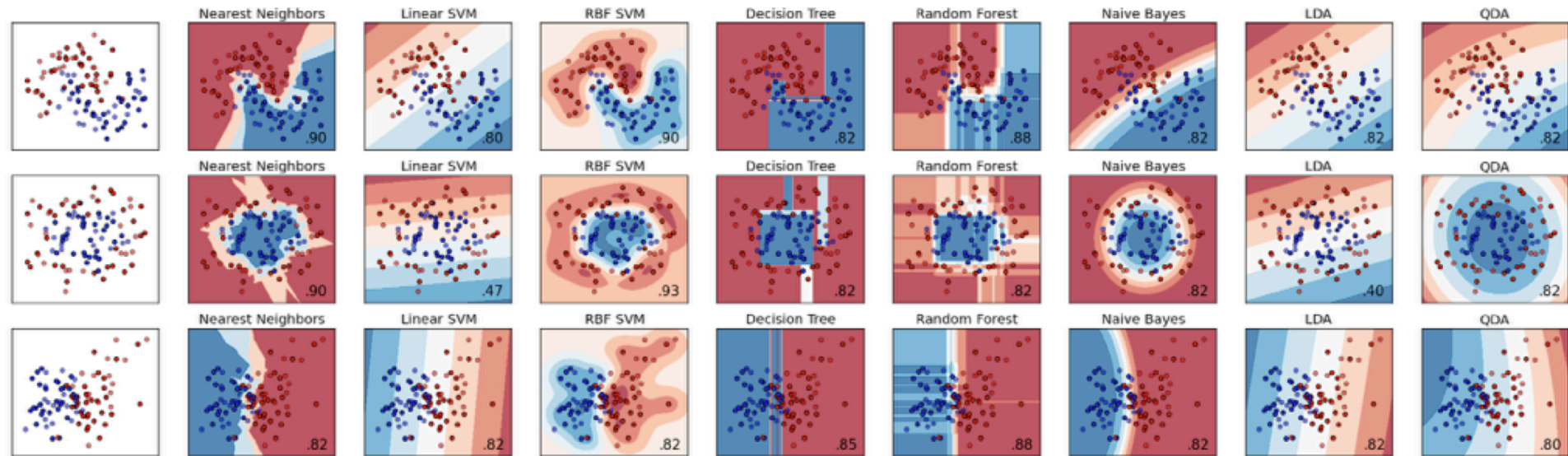
Modules: *grid search, cross validation, metrics.* — Examples

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)

Today



- ❑ Review of ML methods covered so far

- ❑ Regression (supervised)

- ❑ Classification (supervised)

- ❑ Unsupervised models

- ❑ 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 | | | | |

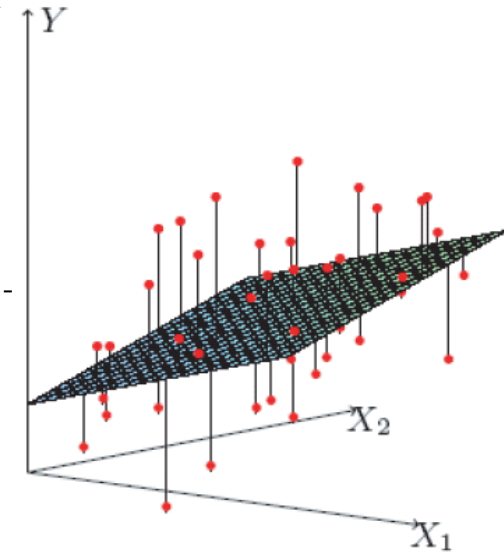
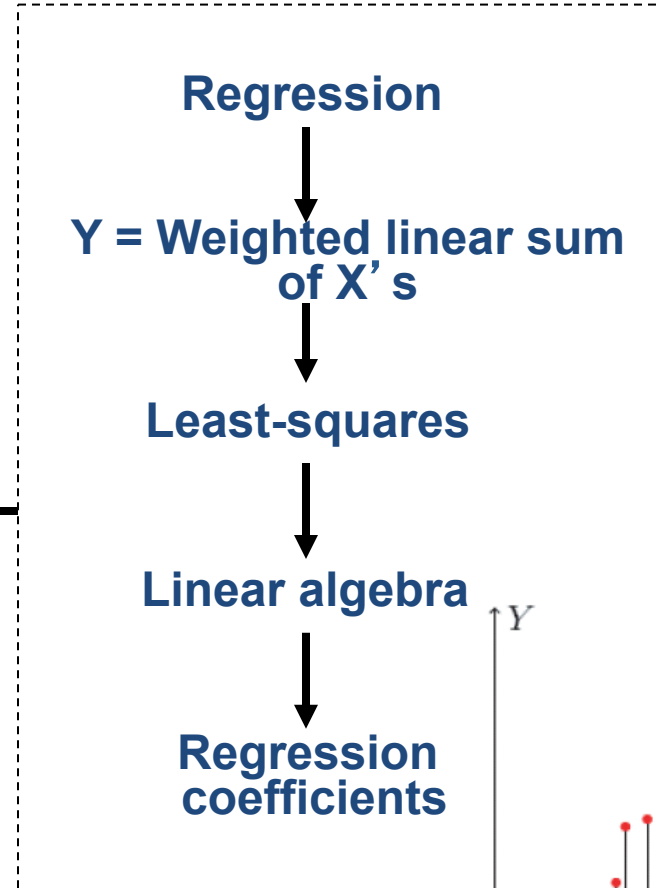
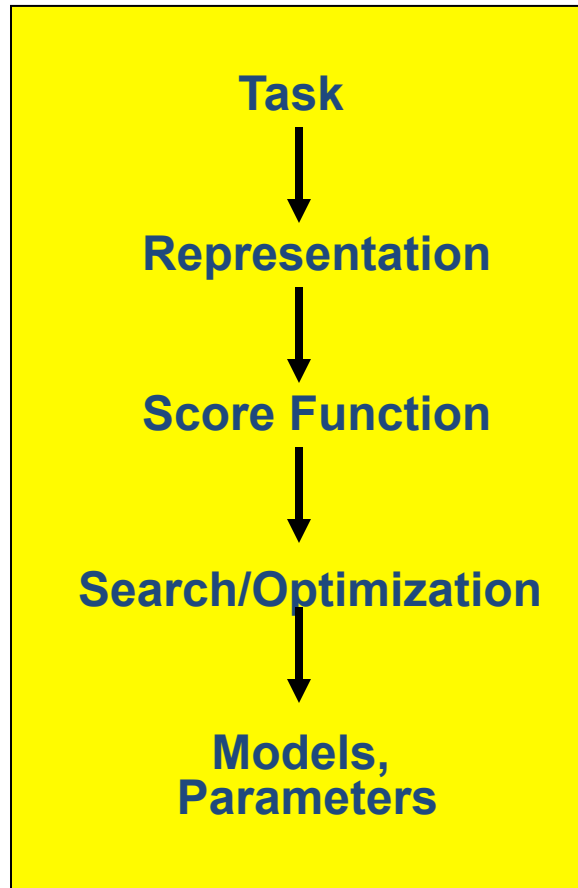
A Dataset

$$f : X \longrightarrow Y$$

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]

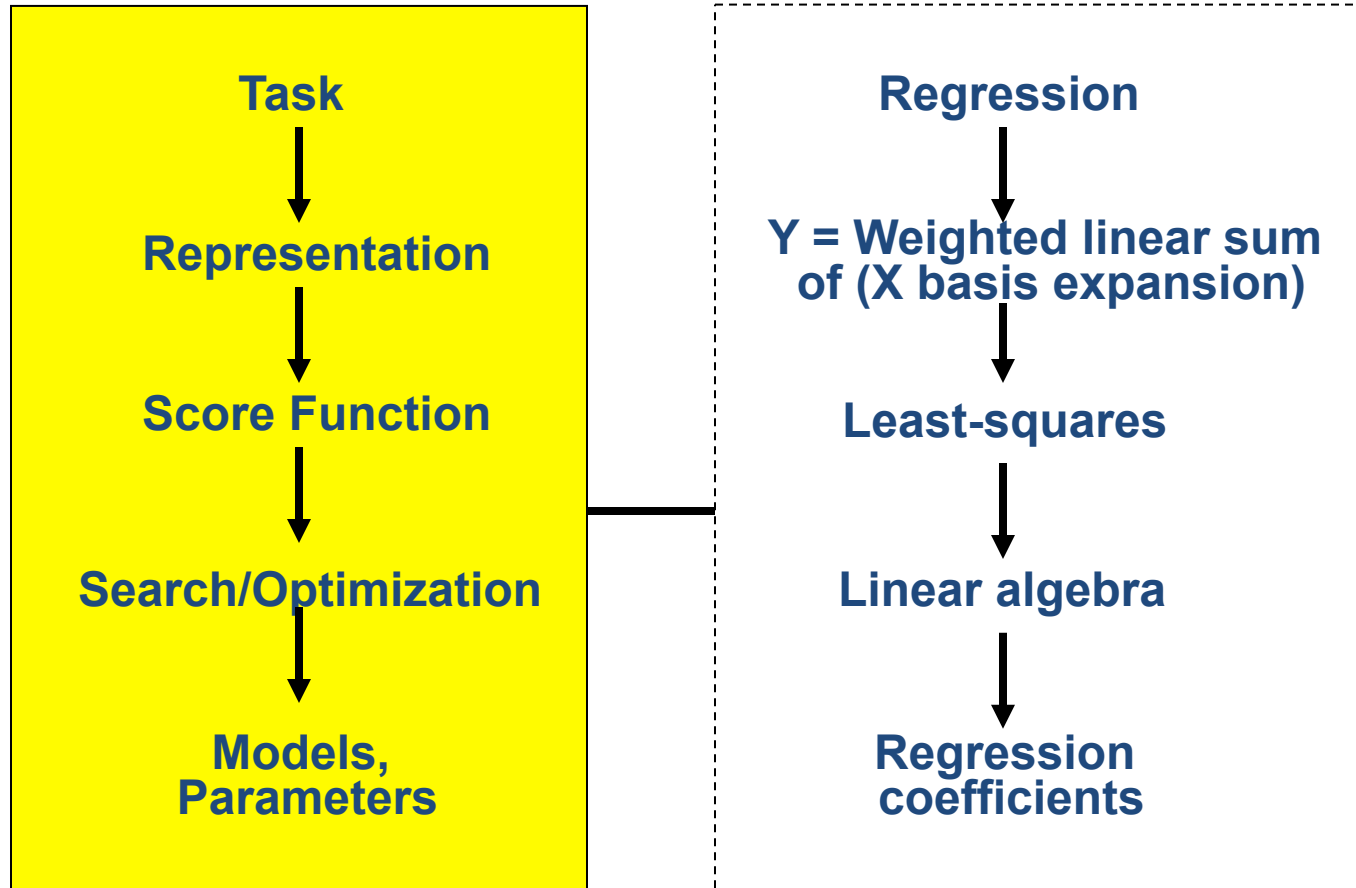
(1) Multivariate Linear Regression



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

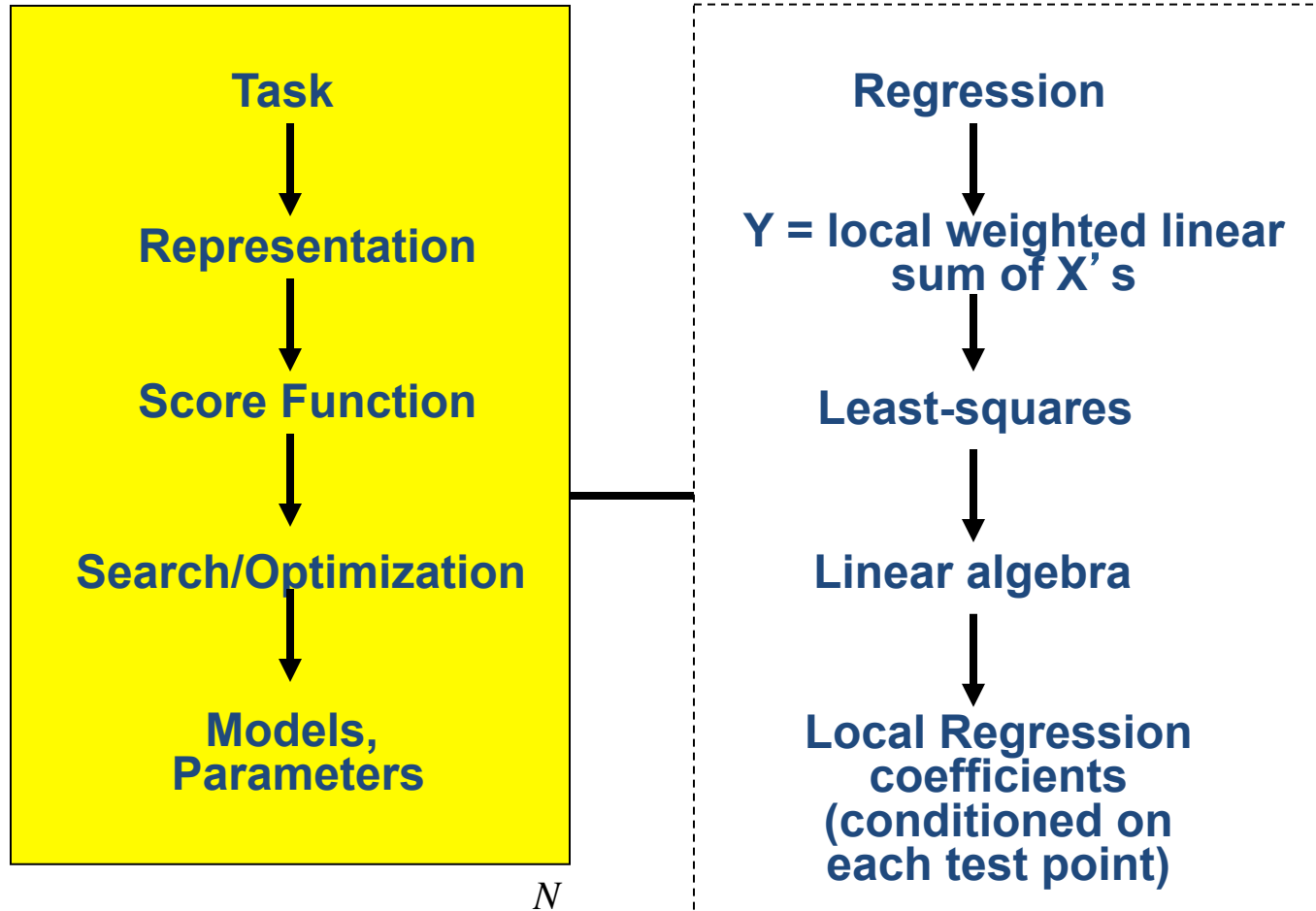

 θ

(2) Multivariate Linear Regression with basis Expansion



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

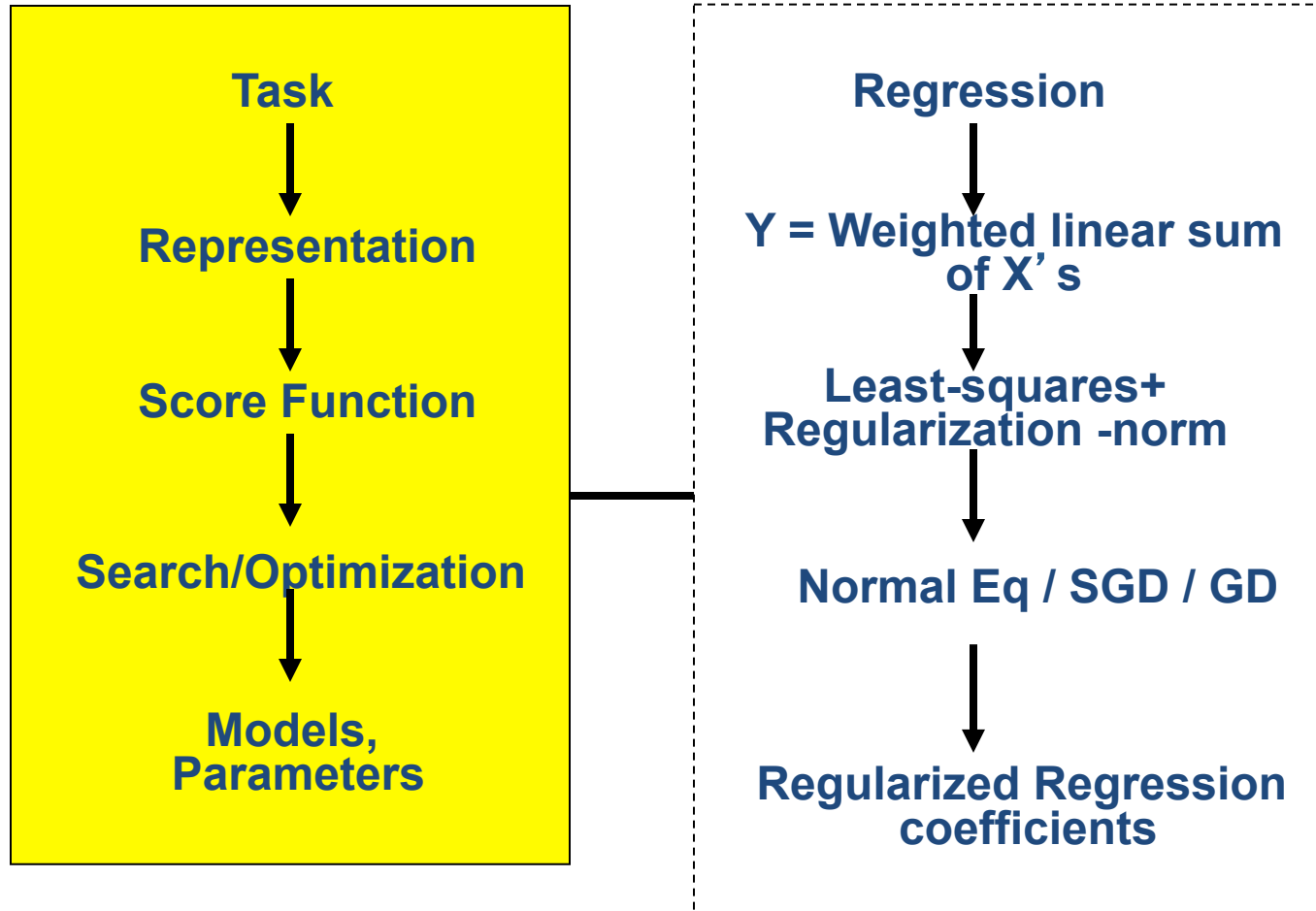
(3) Locally Weighted / Kernel Regression



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

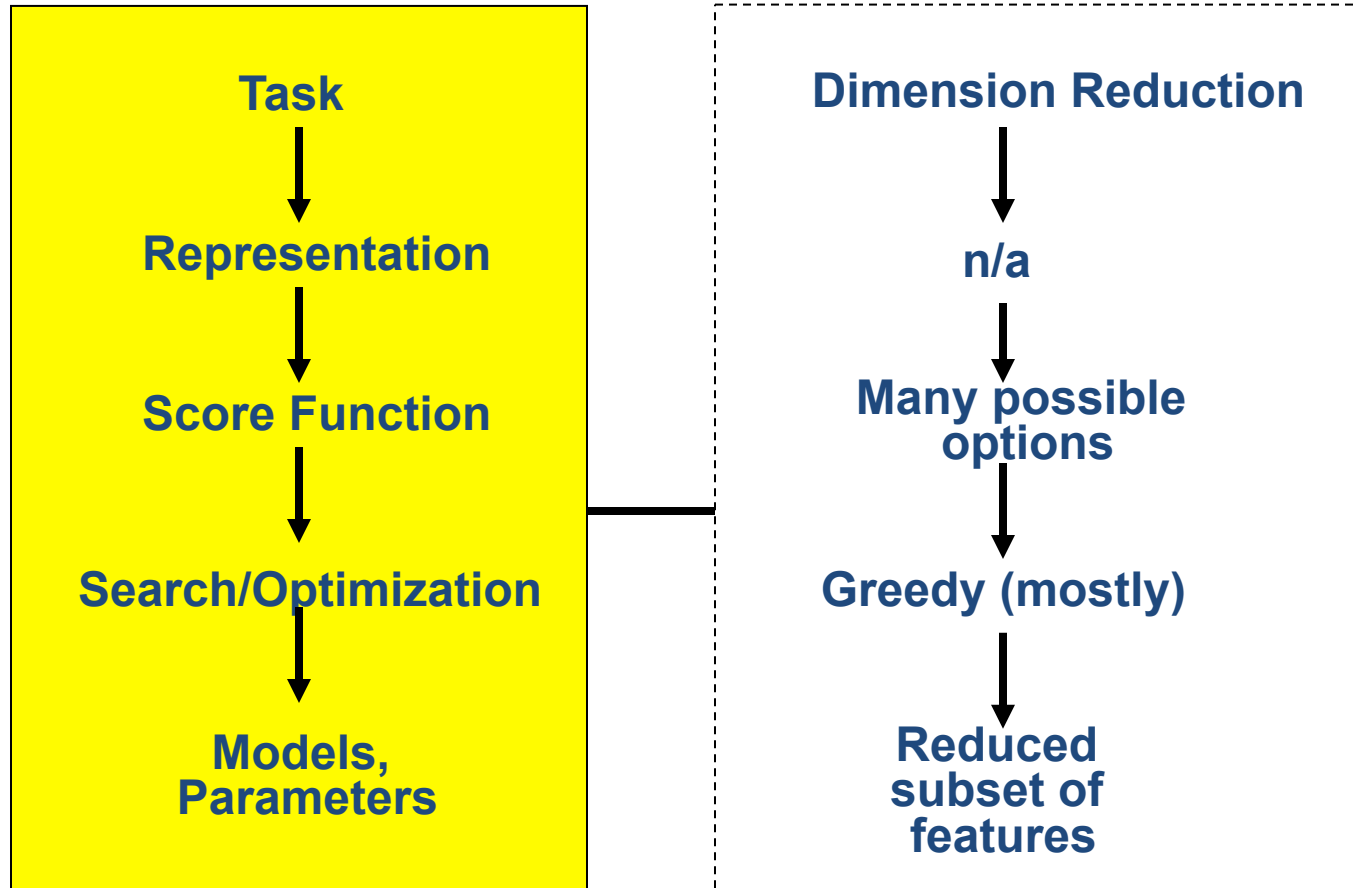
$$\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0)x_0$$

(4) Regularized multivariate linear regression



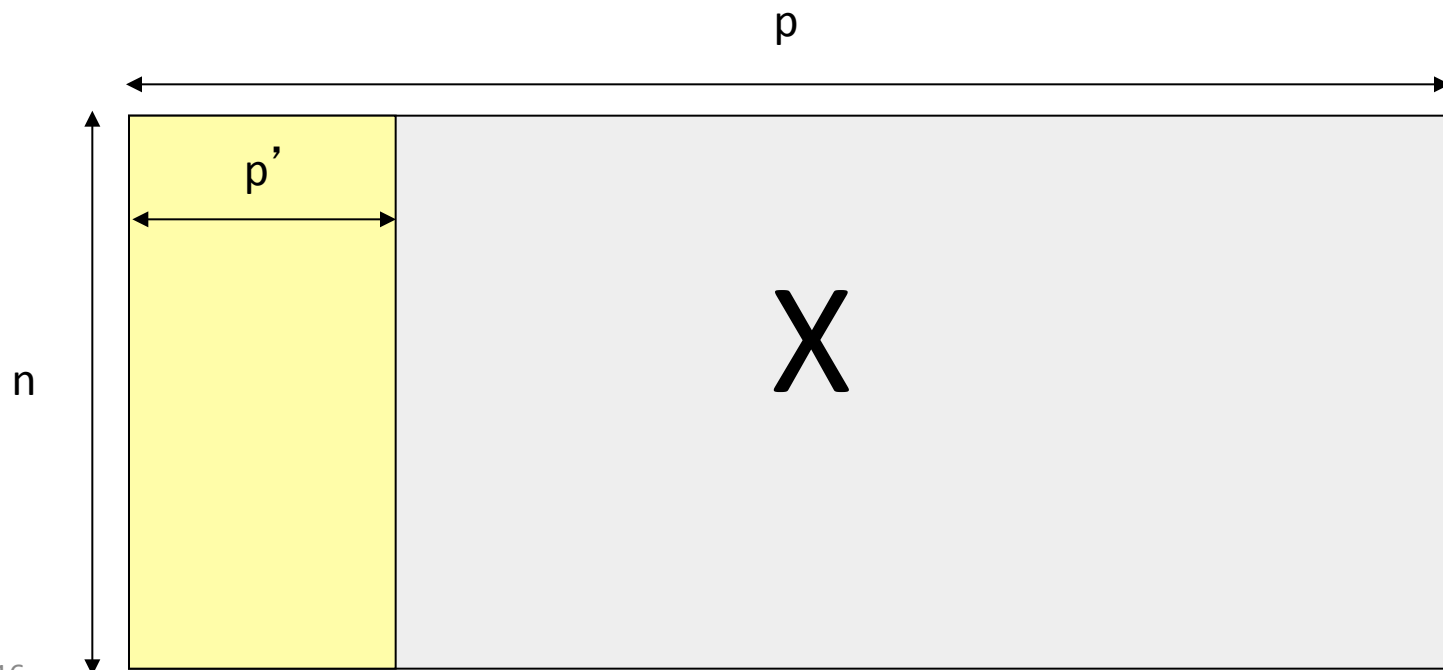
$$\min J(\beta) = \sum_{i=1}^n \left(Y - \hat{Y} \right)^2 + \lambda \sum_{j=1}^p \beta_j^2$$

(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.



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 (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_1 | X_2 | X_3 | C |
|-------|-------|-------|-----|
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |

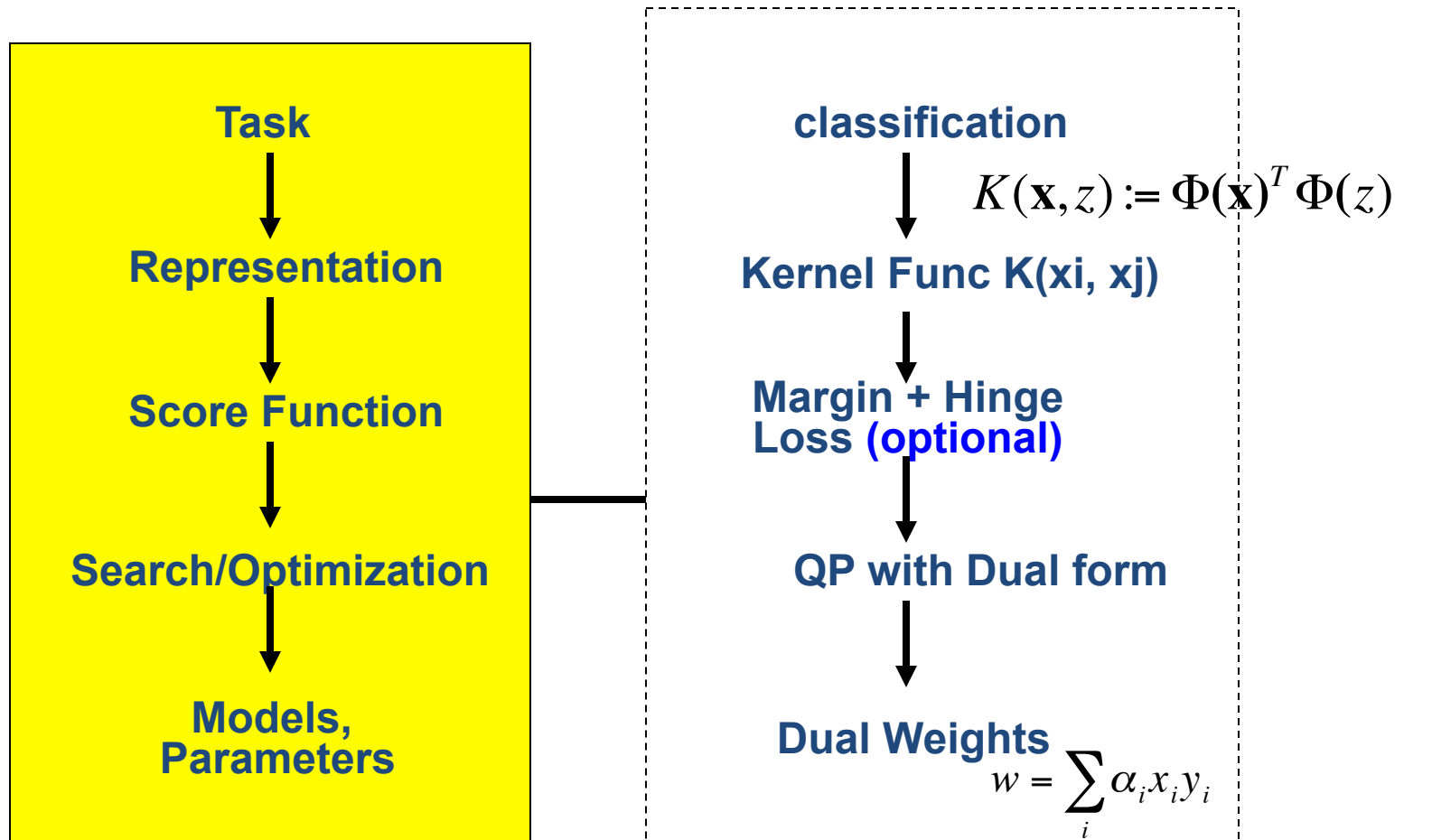
A Dataset for classification

$$f : X \longrightarrow C$$

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

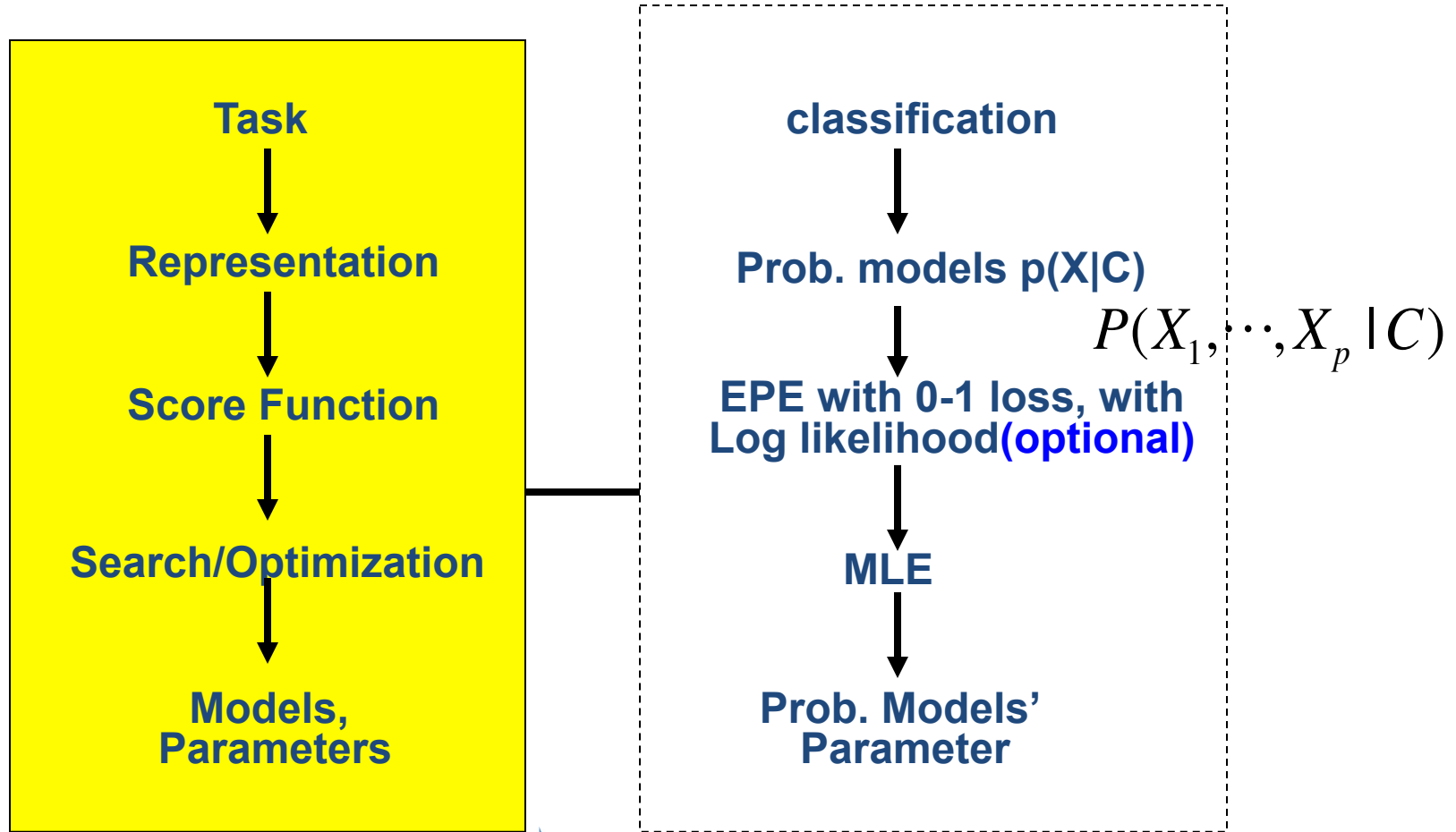


$$\operatorname{argmin}_{\mathbf{w}, b} \sum_{i=1}^p w_i^2 + C \sum_{i=1}^n \varepsilon_i$$

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

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

(2) Bayes Classifier



$$P(X_1, \dots, X_p | C)$$

EPE with 0-1 loss, with Log likelihood(optional)

MLE

Prob. Models' Parameter

Bernoulli Naïve

$$p(W_i = true | c_k) = p_{i,k}$$

Gaussian Naïve

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

Multinomial

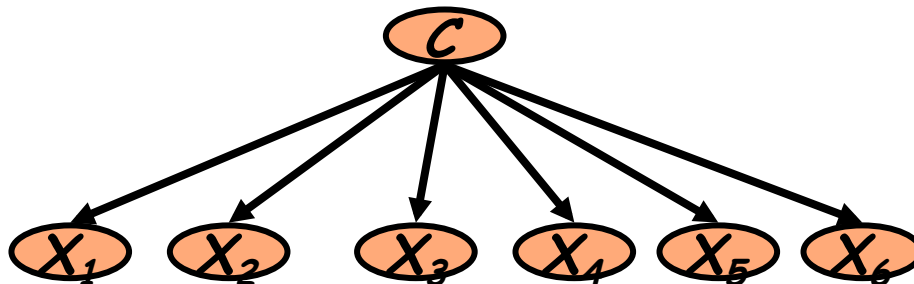
$$P(W_1 = n_1, \dots, W_v = n_v | c_k) = \frac{N!}{n_{1k}! n_{2k}! \dots n_{vk}!} \theta_{1k}^{n_{1k}} \theta_{2k}^{n_{2k}} \dots \theta_{vk}^{n_{vk}}$$

Naïve Bayes Classifier

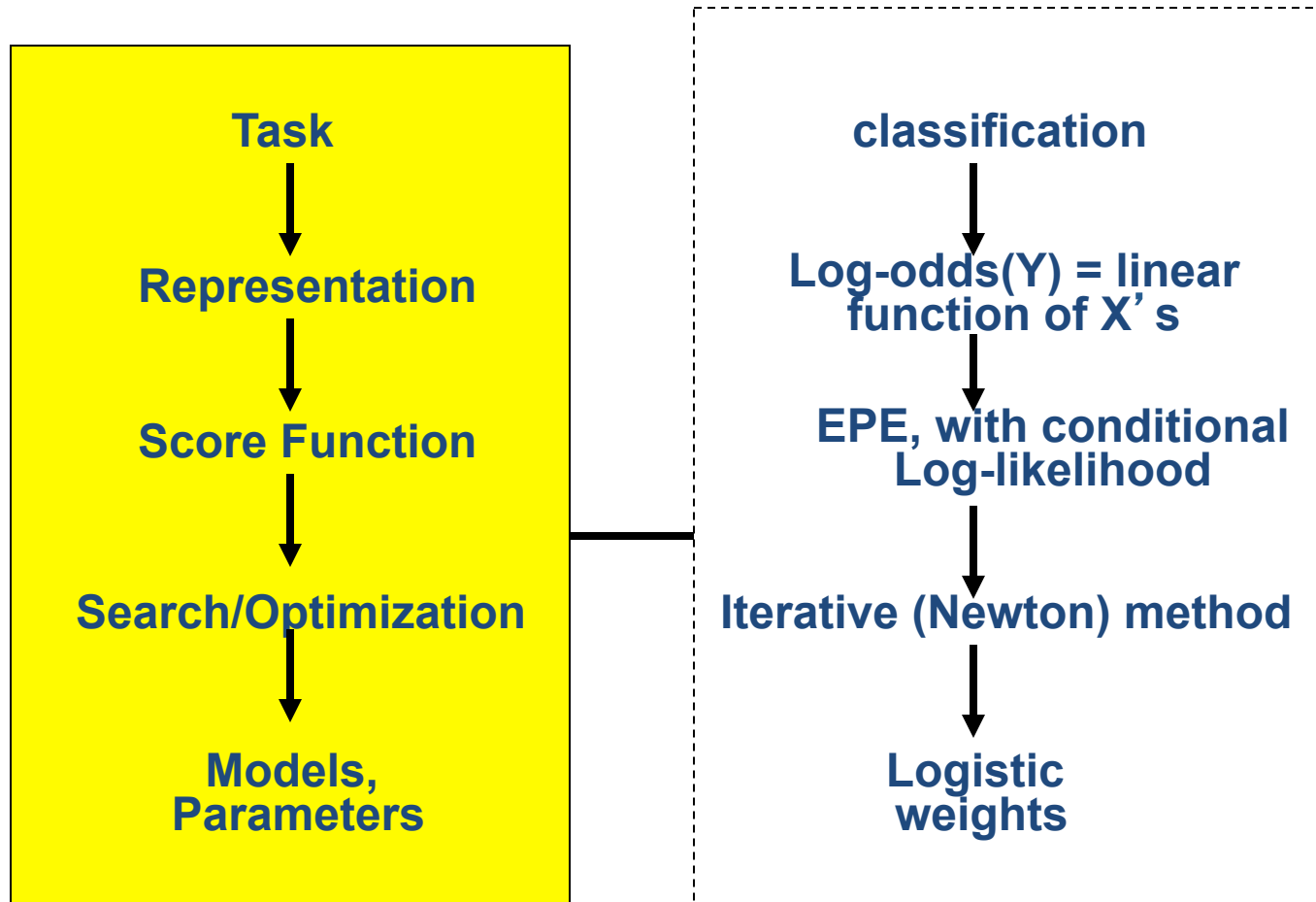
Difficulty: learning the joint probability $P(X_1, \dots, X_p | C)$

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

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



(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.

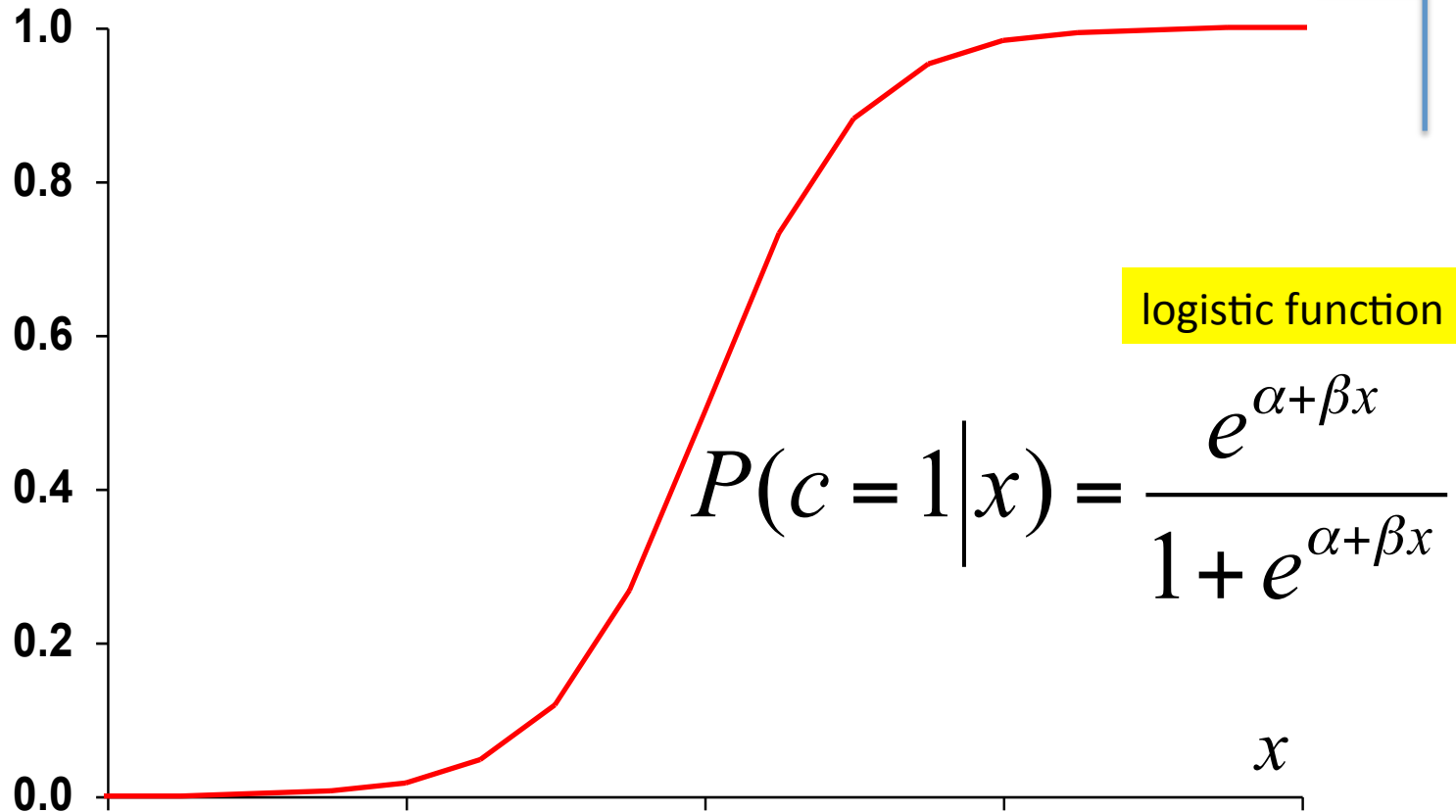
The main interest → predicting the probability that an event occurs (i.e., the probability that $p(y=1 | x)$).

Discriminative

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

e.g.
Probability of
disease

$P(C=1|X)$



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

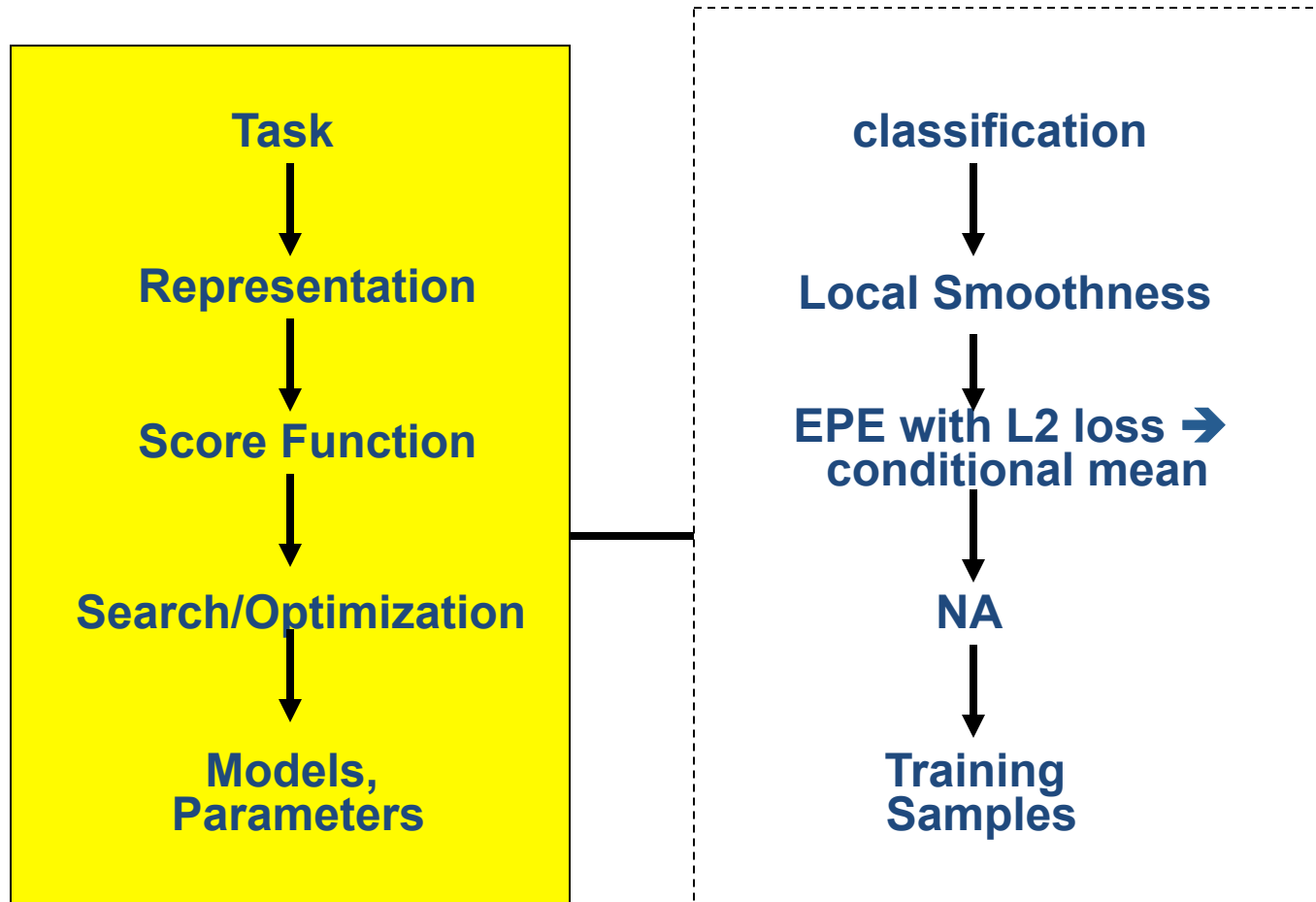
e.g.,

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


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

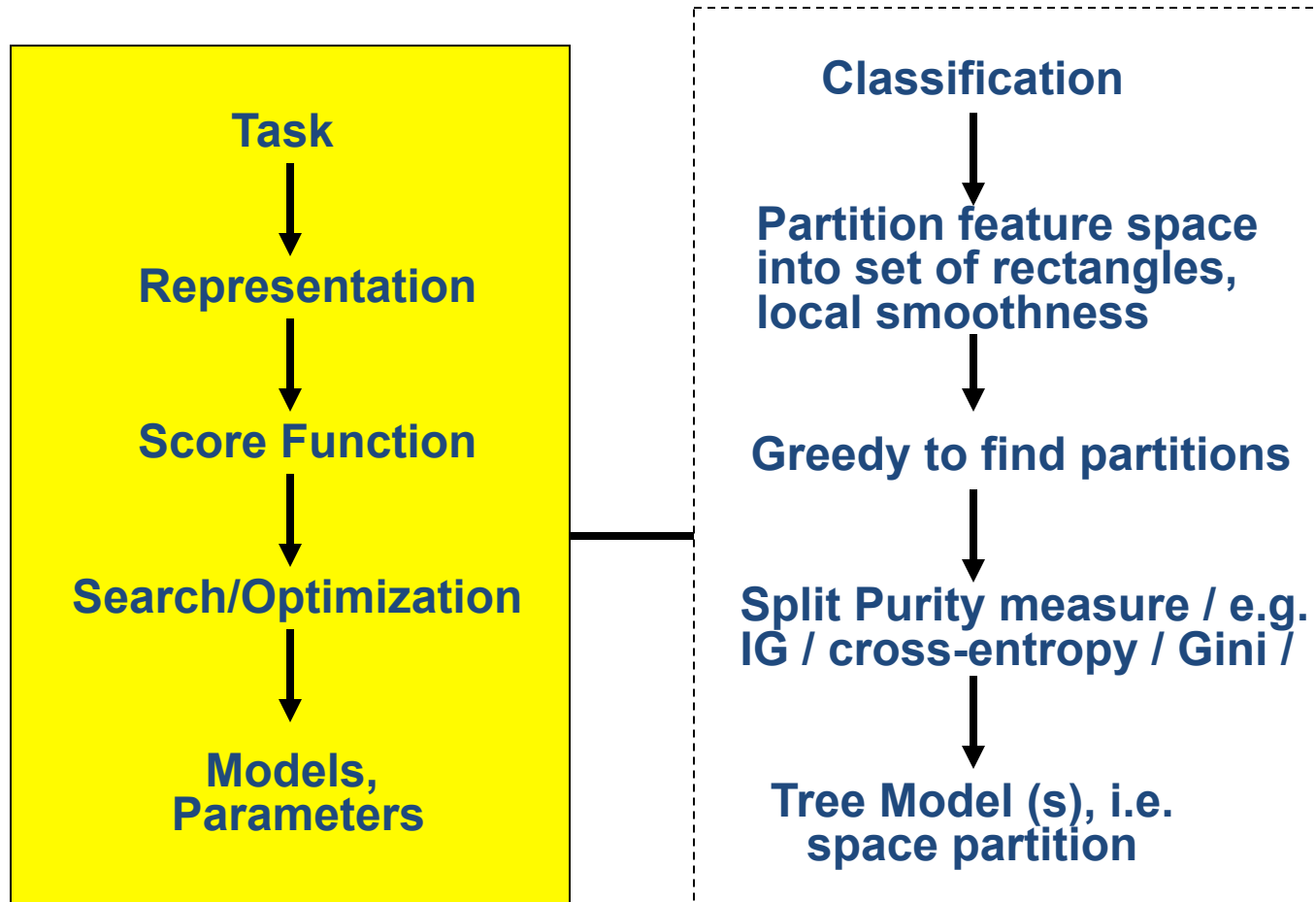
(4) K-Nearest Neighbor



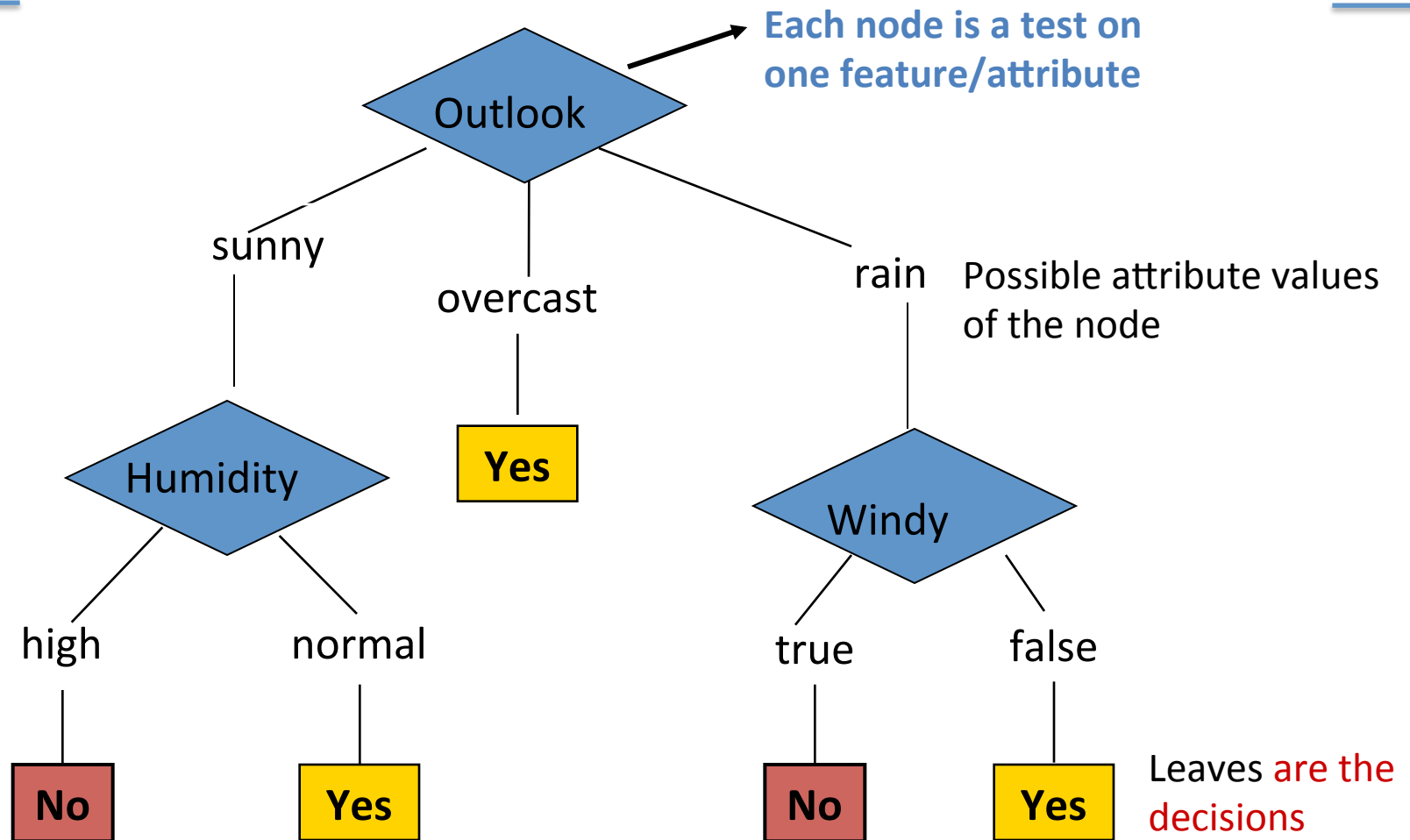
Nearest neighbor classification

- 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

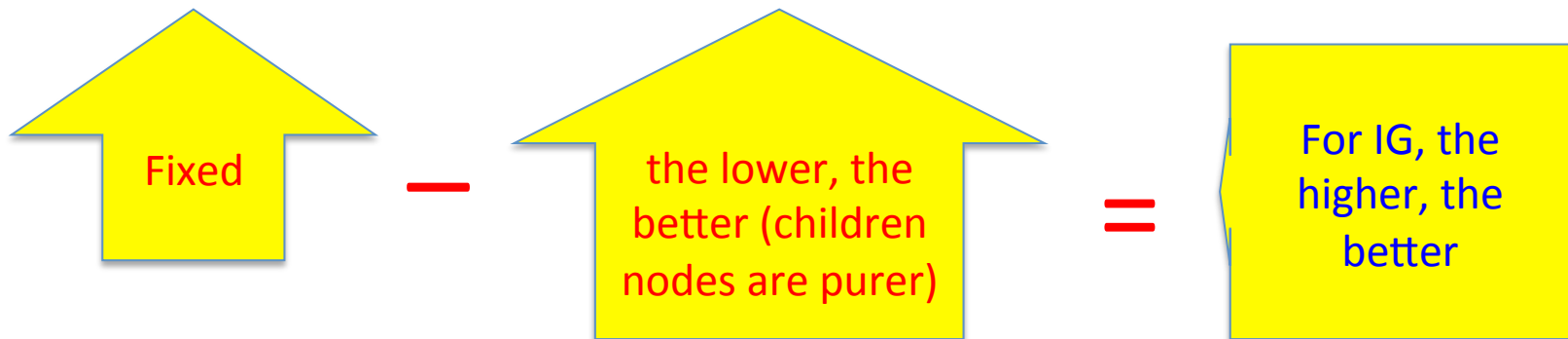
- $IG(X_i, Y) = H(Y) - H(Y | X_i)$

Reduction in uncertainty by knowing a feature X_i

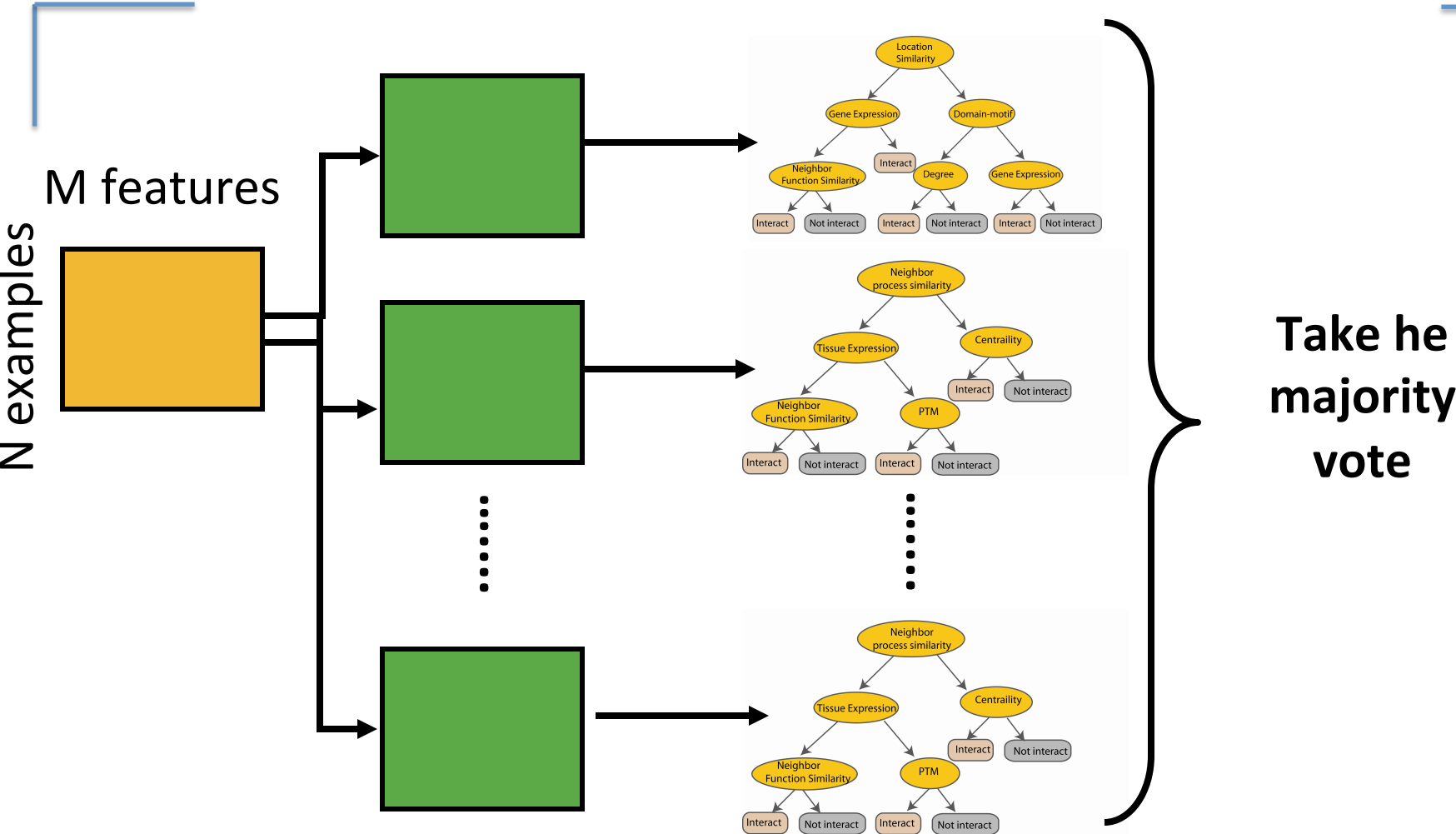
Information gain:

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

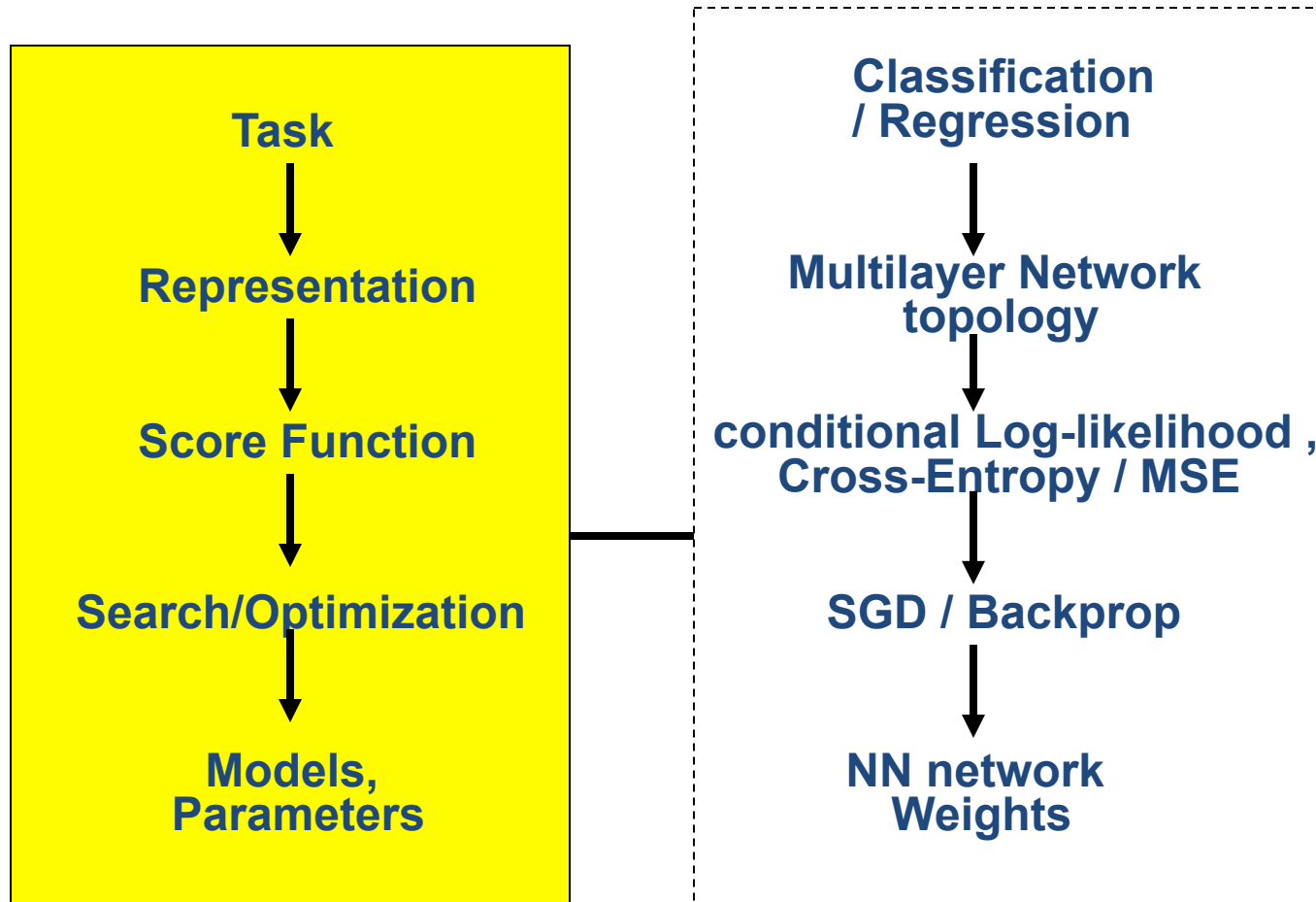
= entropy(parent) – [average entropy(children)]



Random Forest Classifier



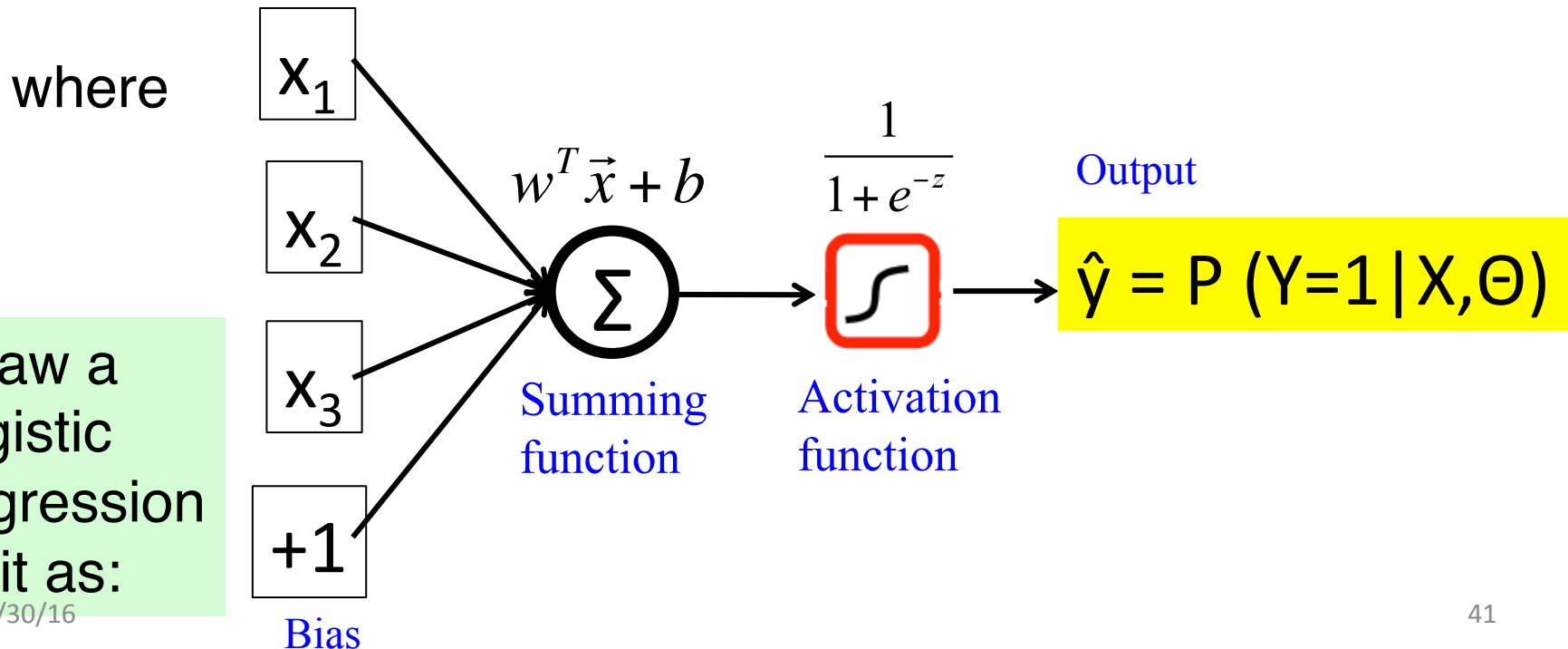
(6) Neural Network



Logistic regression

Logistic regression could be illustrated as a module

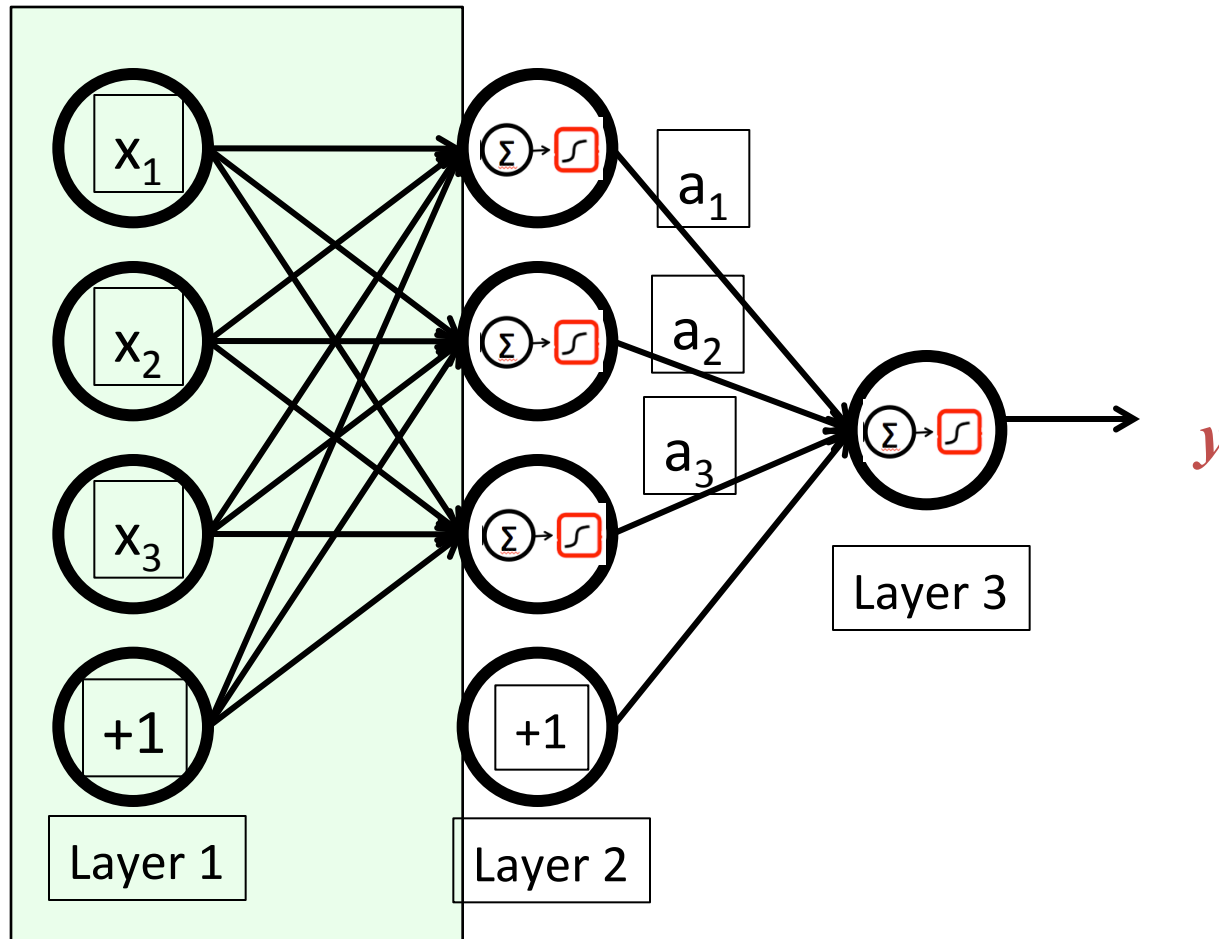
On input x , it outputs \hat{y} :



Draw a logistic regression unit as:

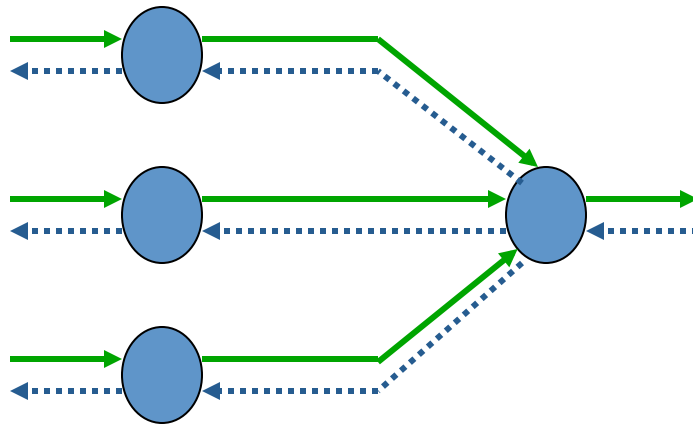
Multi-Layer Perceptron (MLP)

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



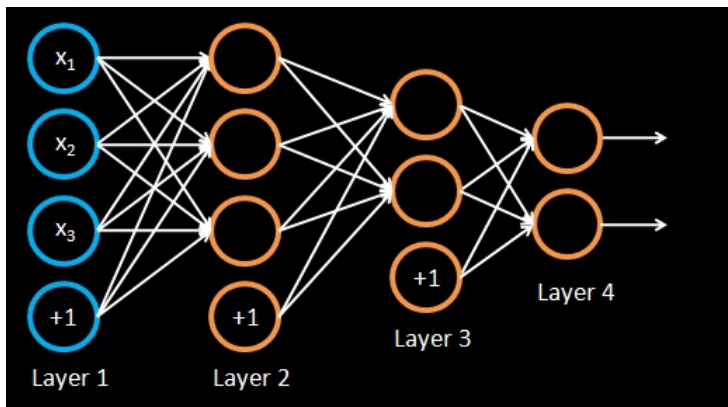
Backpropagation

- Back-propagation training algorithm

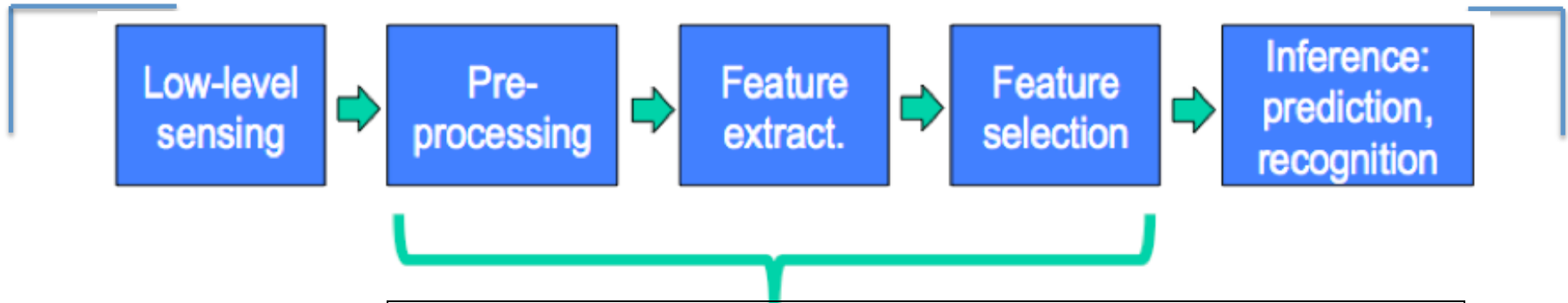


→ *Network activation
Forward Step*

←····· *Error propagation
Backward Step*



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

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 (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 | | | |

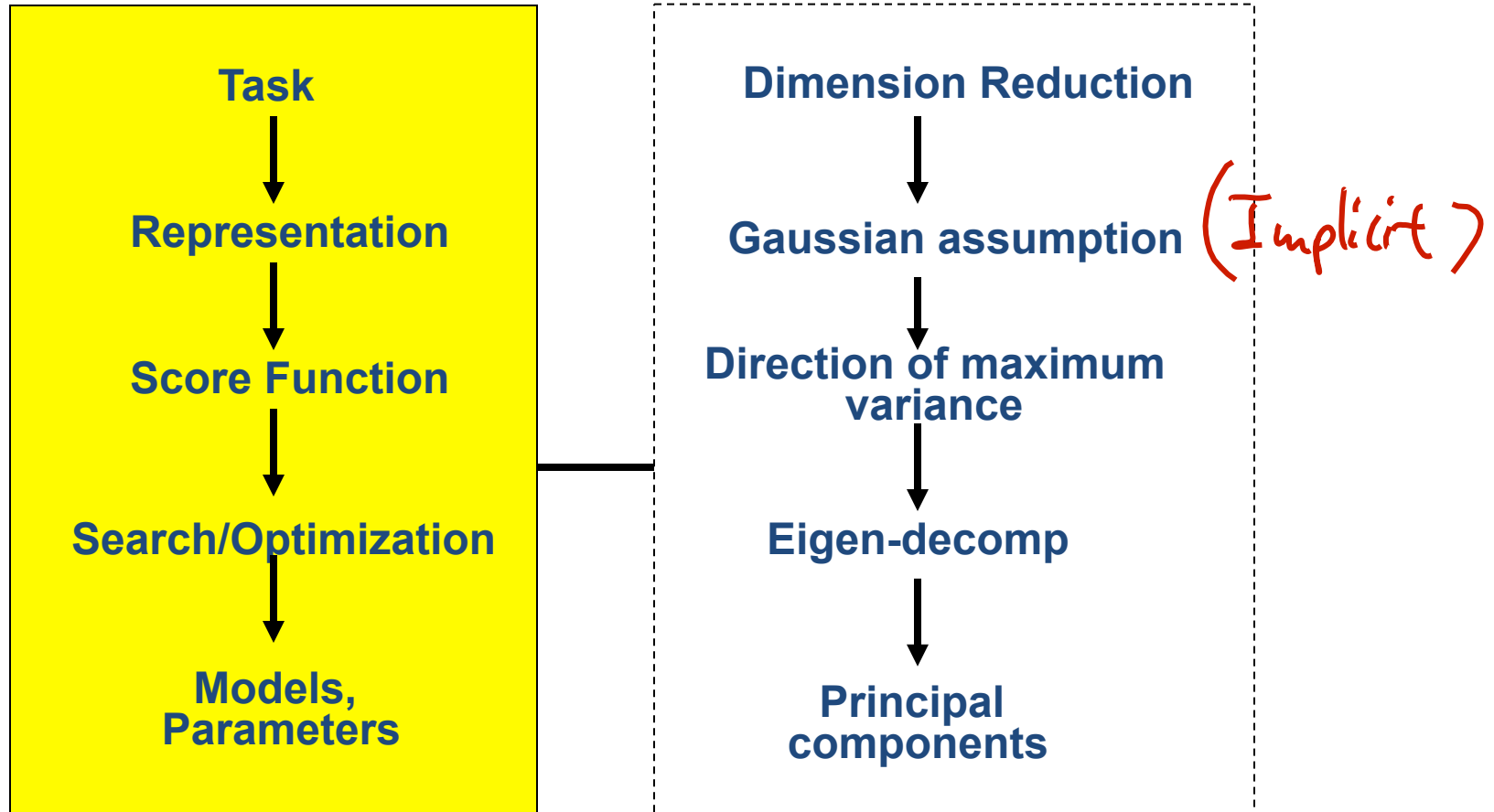
An unlabeled Dataset X

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

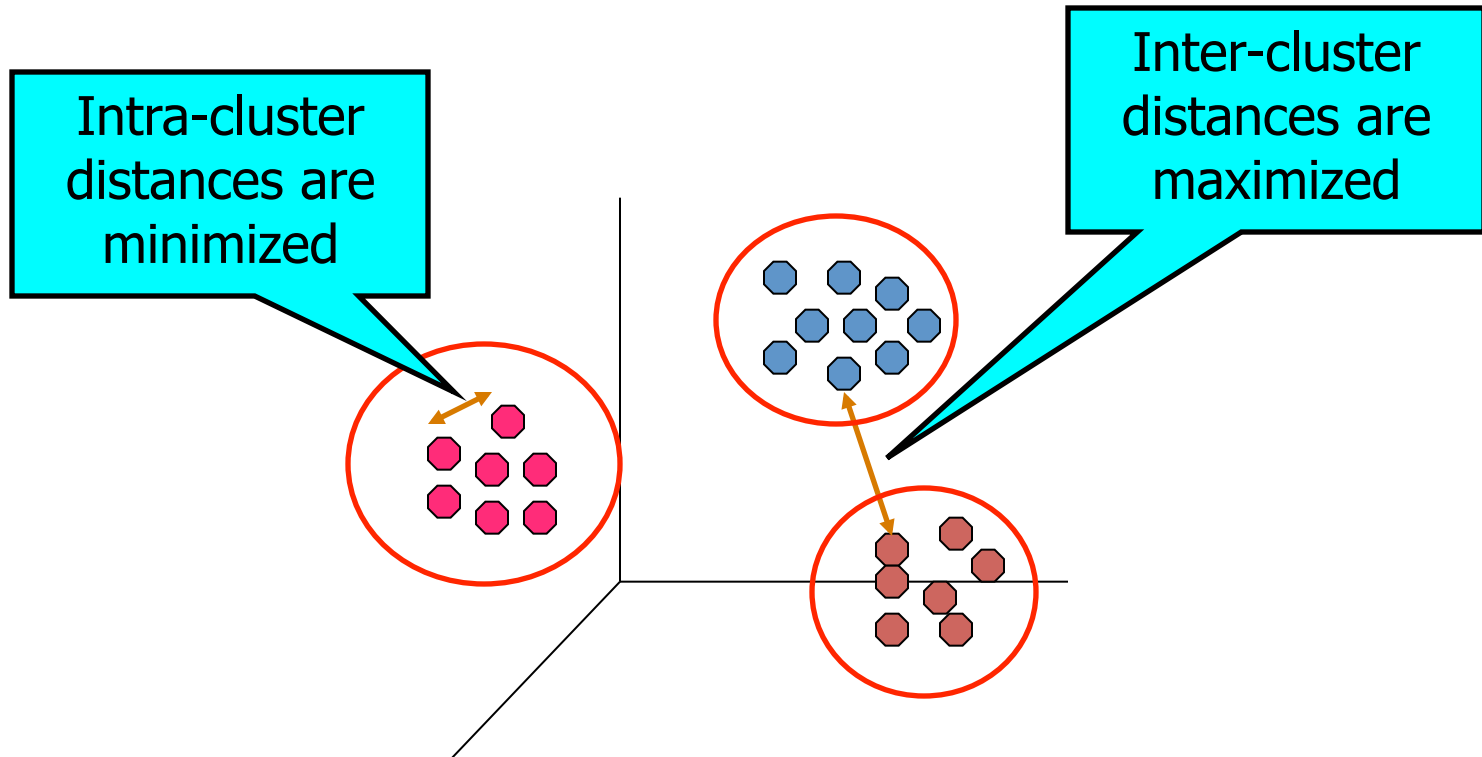


What we have covered (III)

- 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



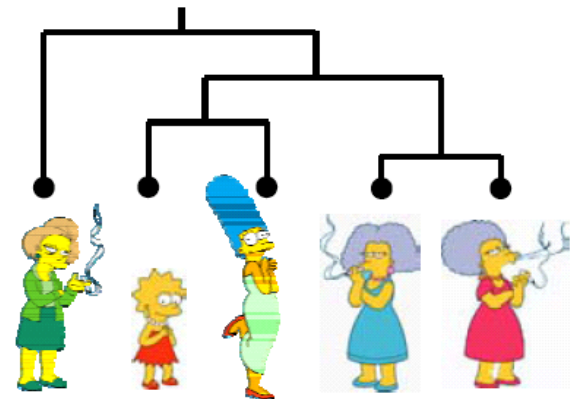
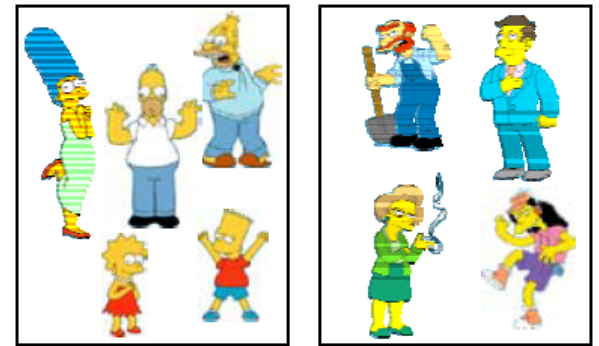
Issues for clustering

- 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

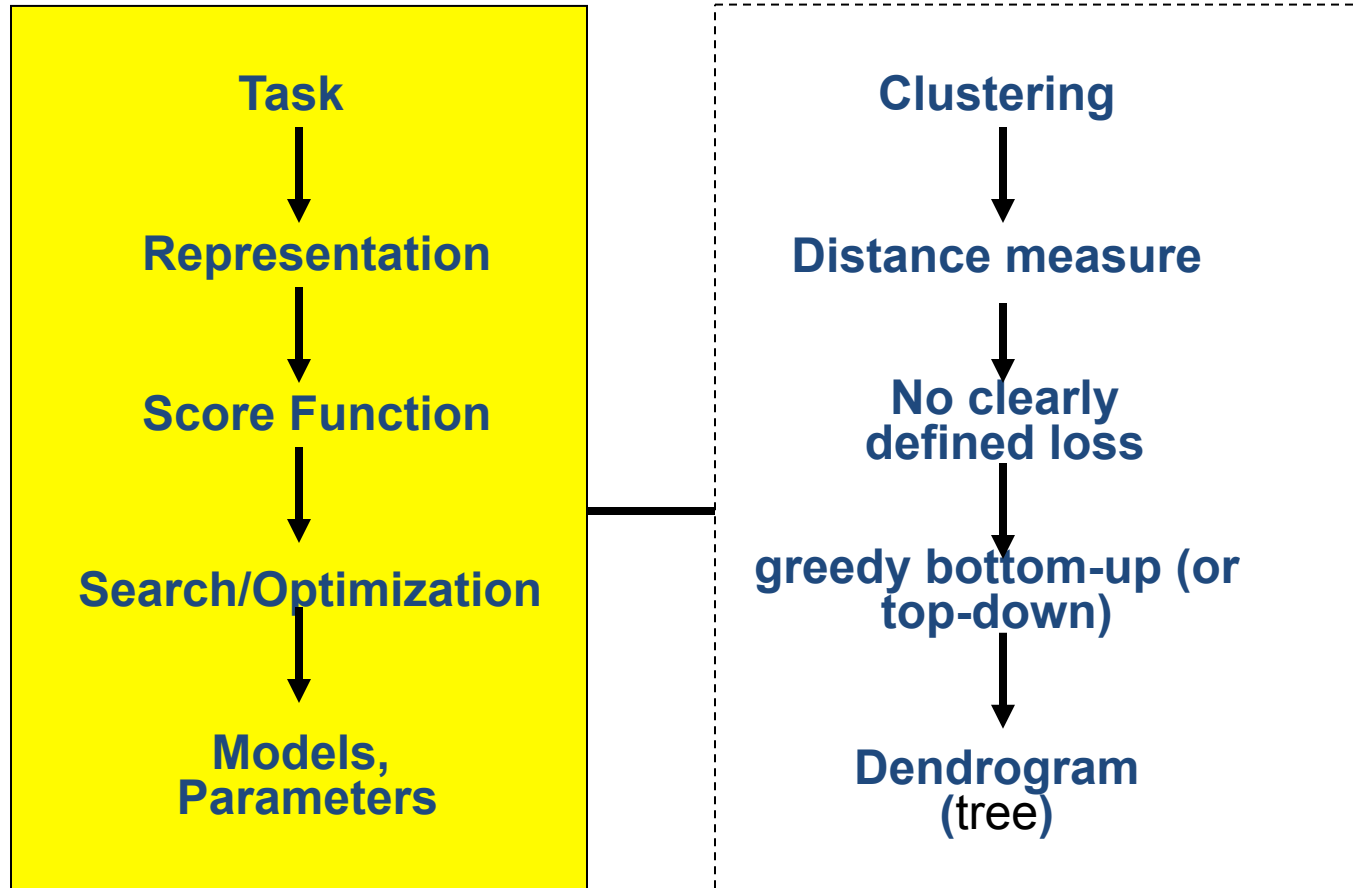
Clustering Algorithms

- Partitional algorithms
 - Usually start with a random (partial) partitioning
 - Refine it iteratively
 - K means clustering
 - Mixture-Model based clustering

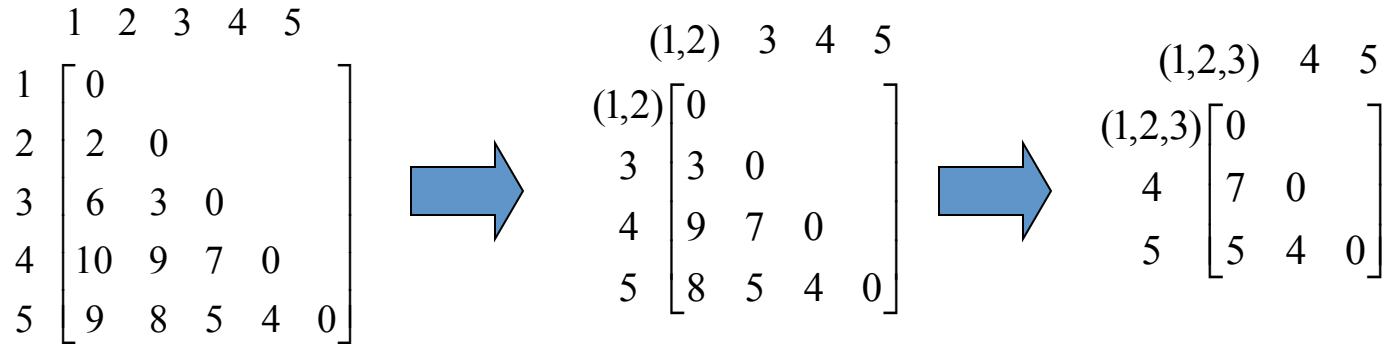
- Hierarchical algorithms
 - Bottom-up, agglomerative
 - Top-down, divisive



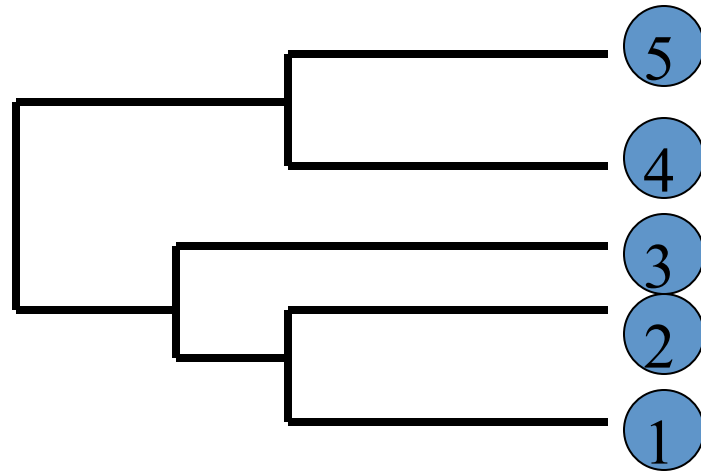
(1) Hierarchical Clustering



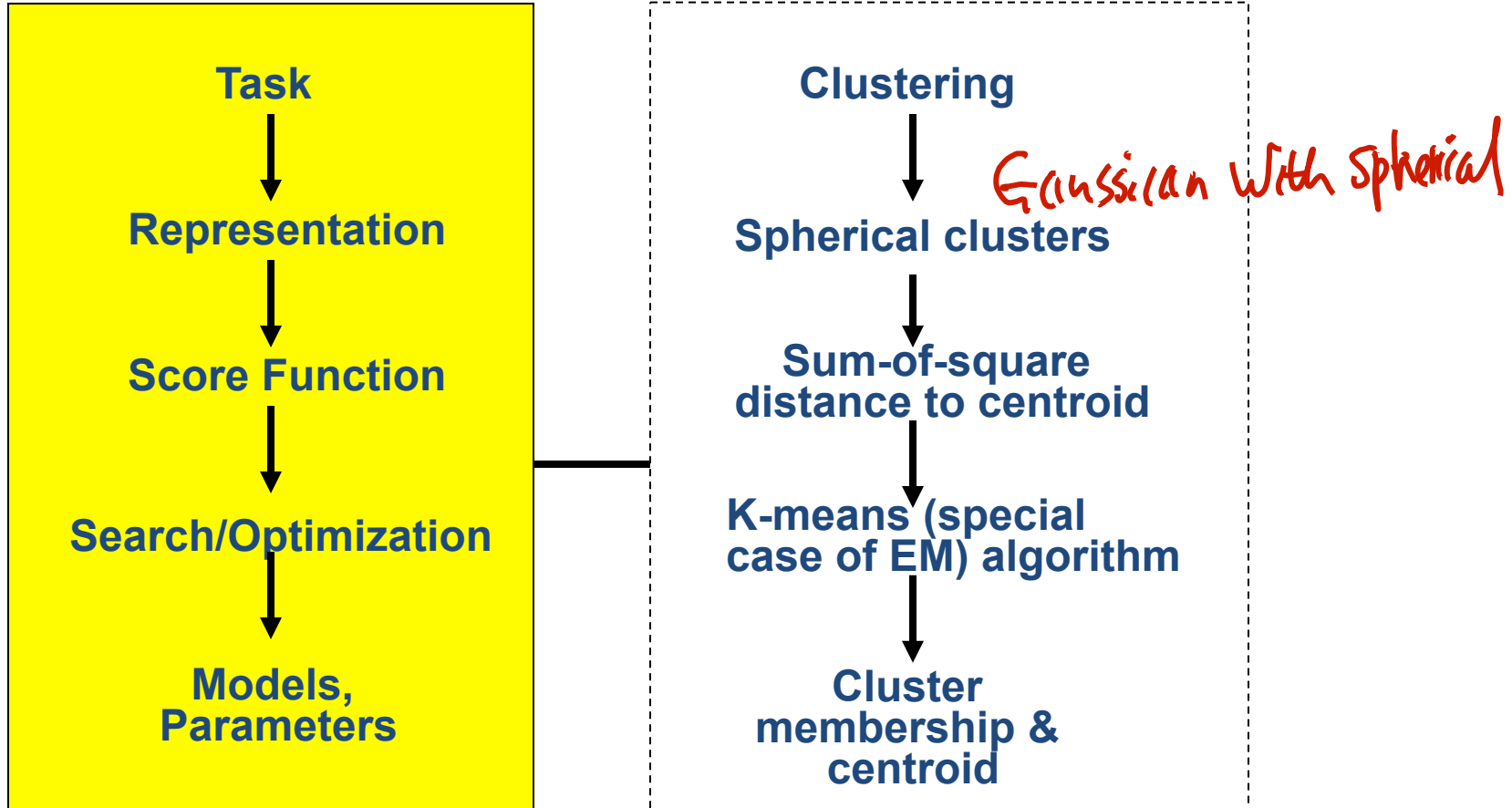
Example: single link



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

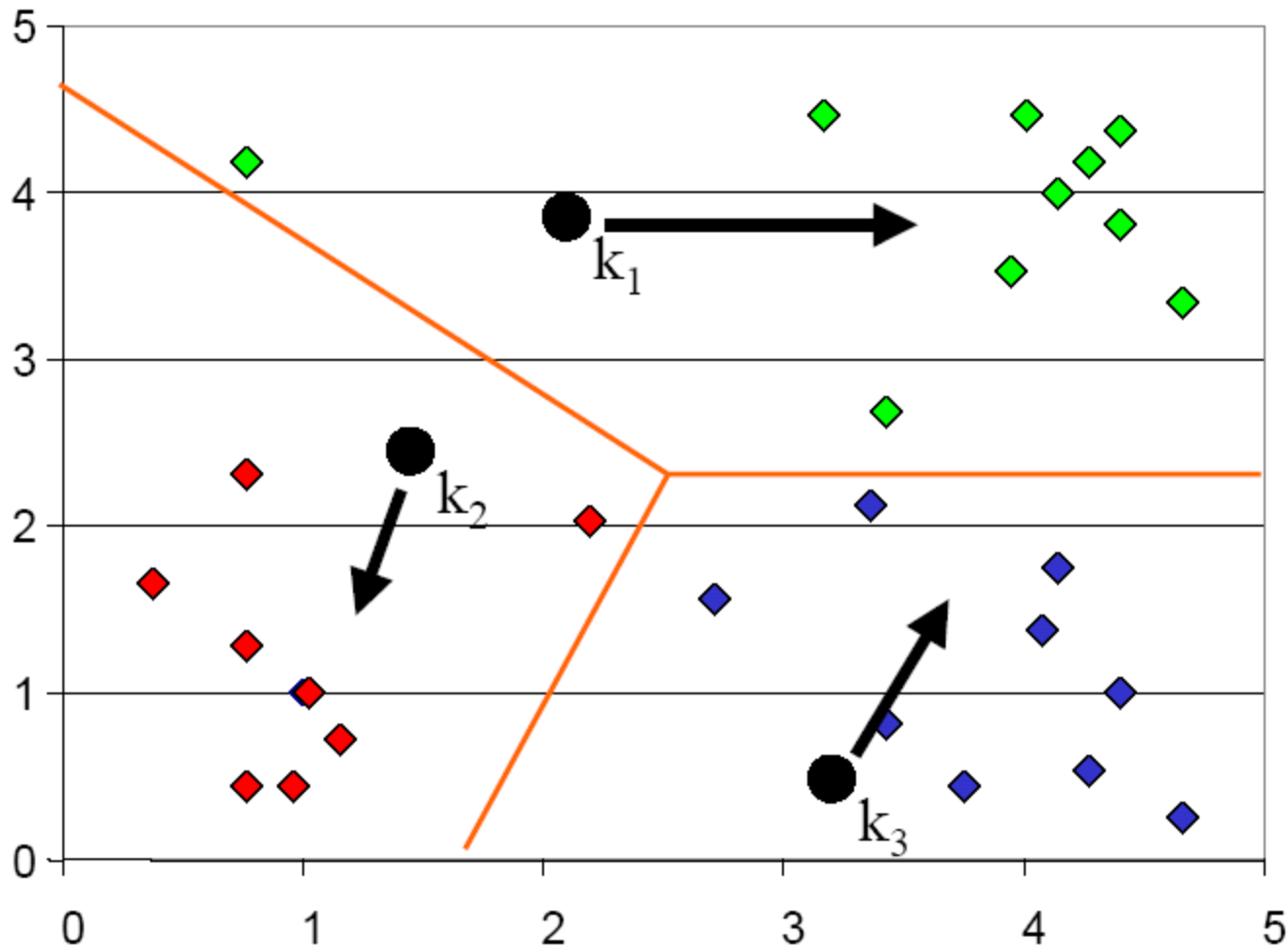


(2) K-means Clustering

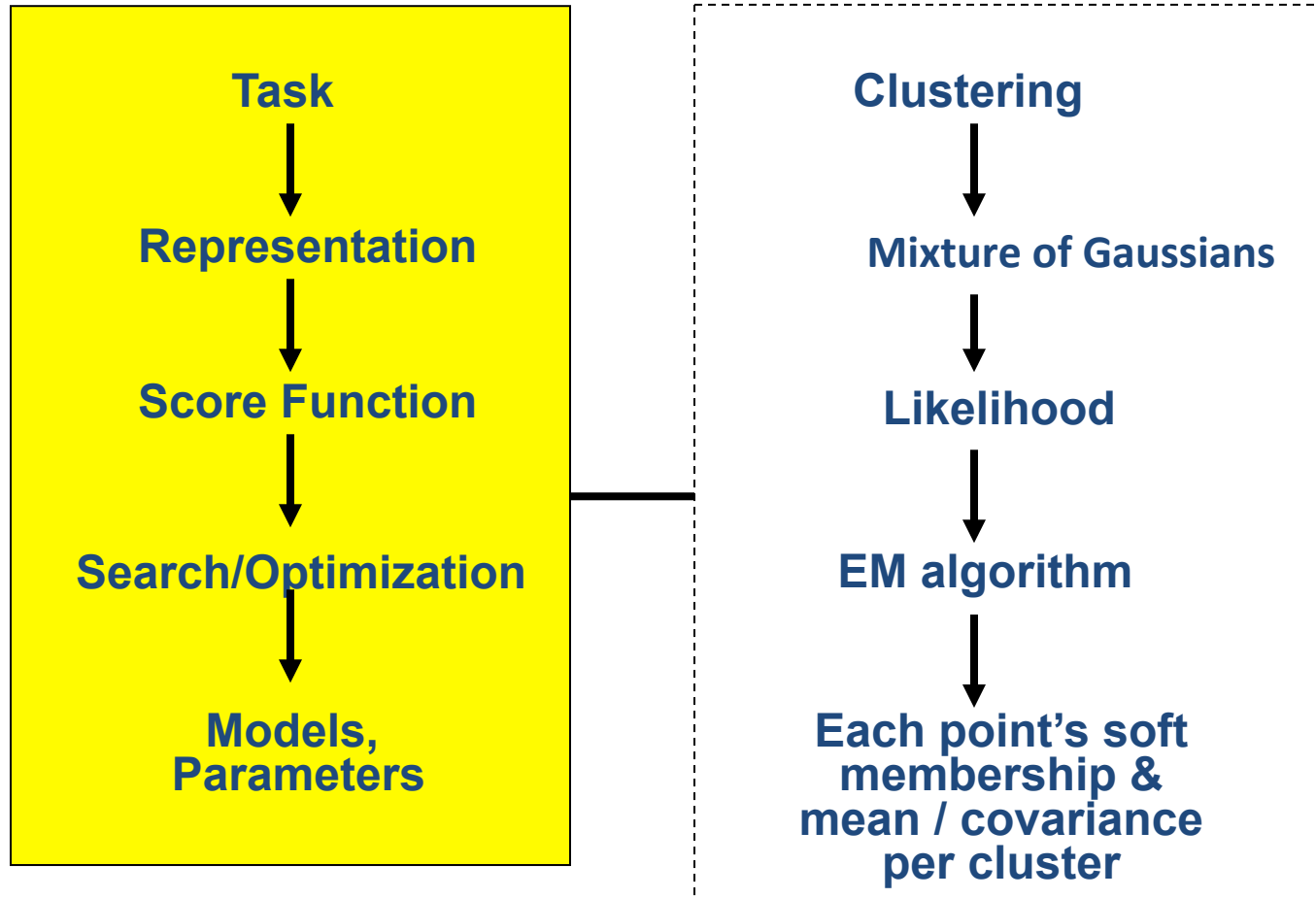


K-means Clustering: Step 2

- Determine the membership of each data points



(3) GMM Clustering



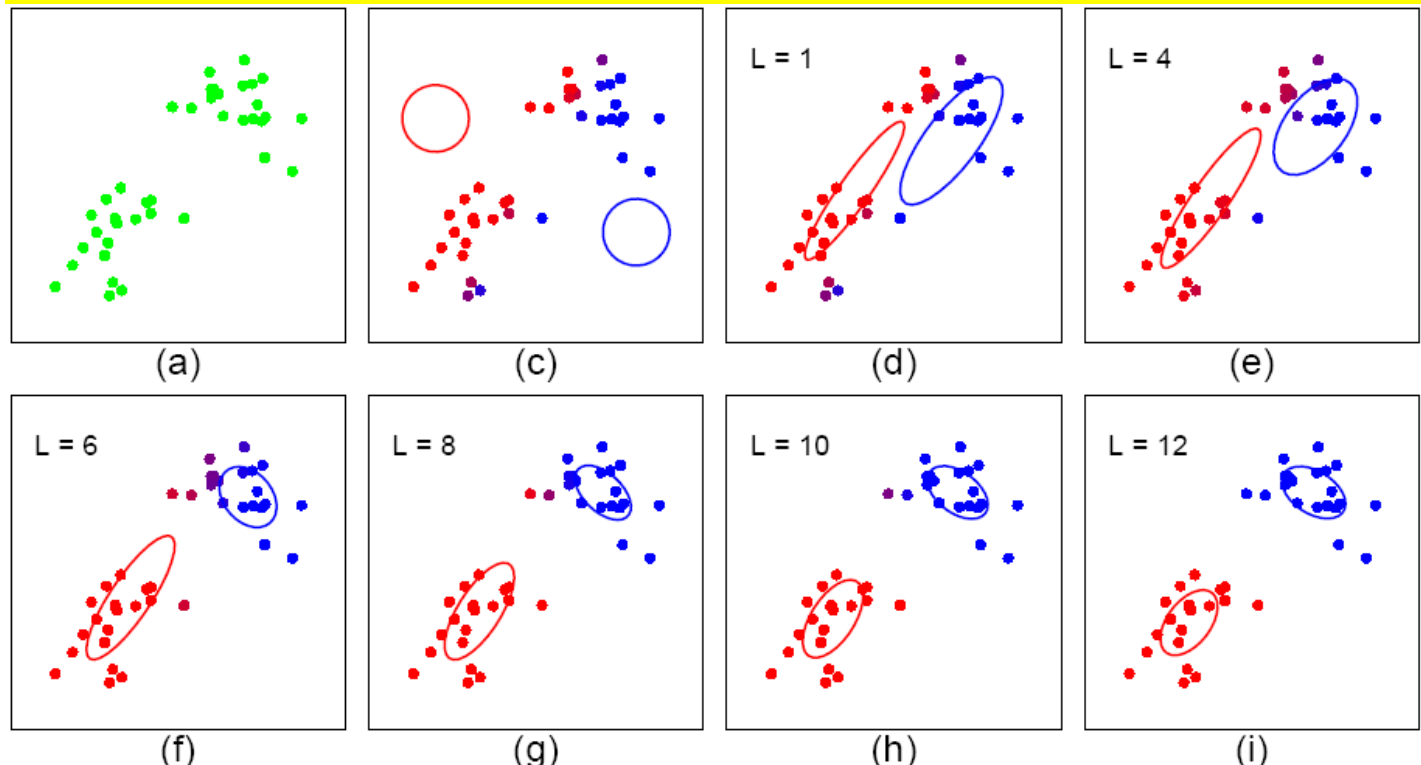
$$\sum_i \log \prod_{i=1}^n p(x = x_i) = \sum_i \log \left[\sum_{\mu_j} p(\mu = \mu_j) \frac{1}{(2\pi)^{p/2} |\Sigma_j|^{1/2}} e^{-\frac{1}{2}(\vec{x} - \vec{\mu}_j)^T \Sigma_j^{-1} (\vec{x} - \vec{\mu}_j)} \right]$$

Expectation-Maximization

for training GMM

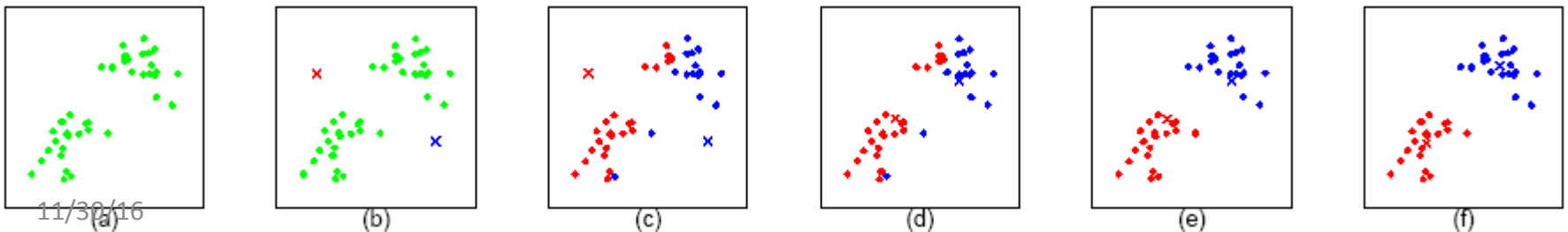
- Start:
 - "Guess" the centroid m_k and covariance S_k of each of the K clusters

- 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:



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 ?

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

What we have covered (IV)

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

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):

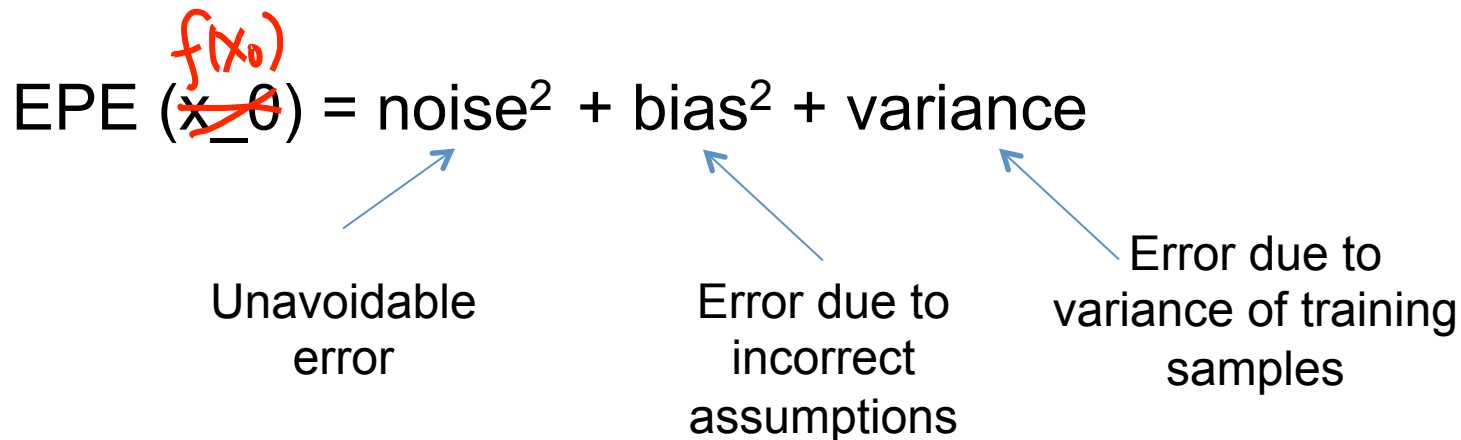
- $$\text{EPE}(f) = \mathbb{E}(L(Y, f(X))) = \int L(y, f(x)) \Pr(dx, dy)$$

$$\text{e.g.} = \int (y - f(x))^2 \Pr(dx, dy)$$

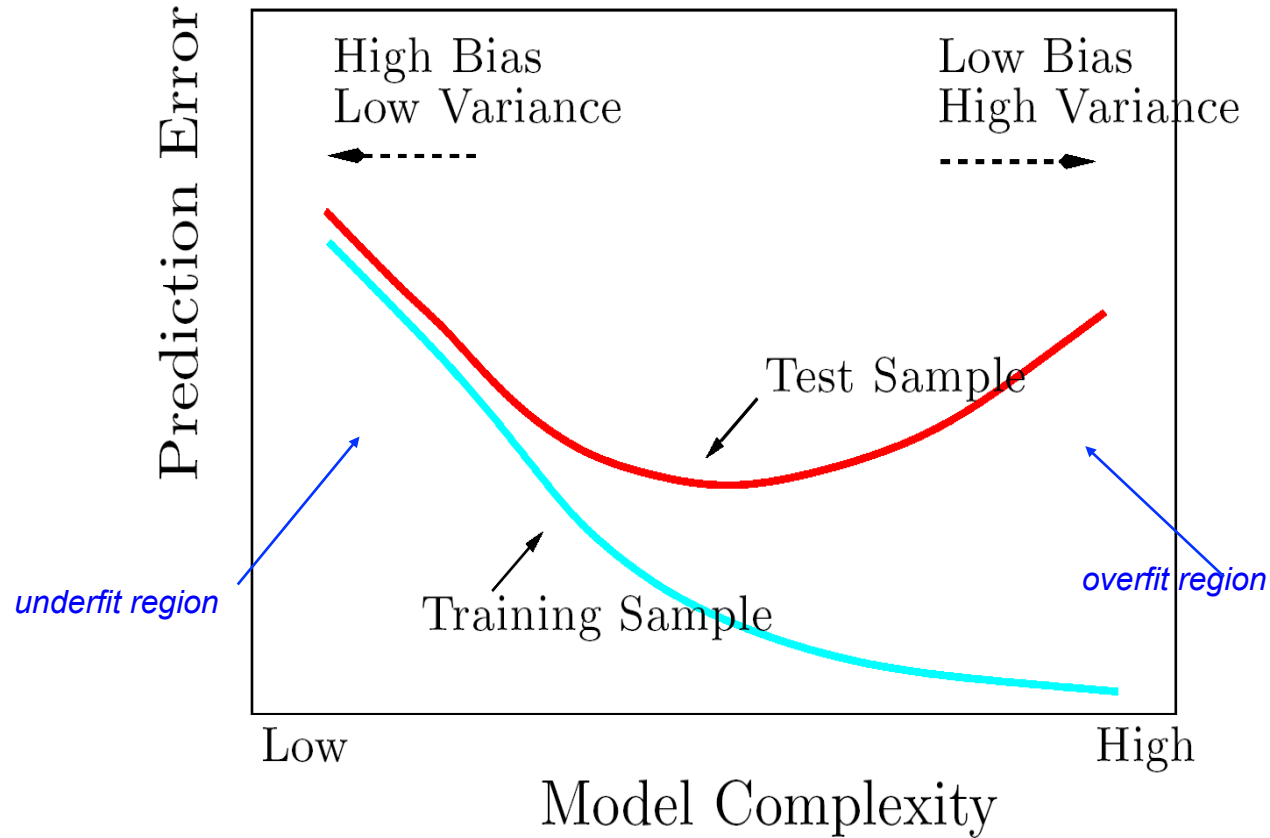
e.g. Squared error loss (also called L2 loss)

Consider
population
distribution

Bias-Variance Trade-off for EPE:



Bias-Variance Tradeoff / Model Selection



Model “bias” & Model “variance”

- Middle RED:
 - TRUE function θ [middle red]
- Error due to bias:
 - How far off in general from the middle red

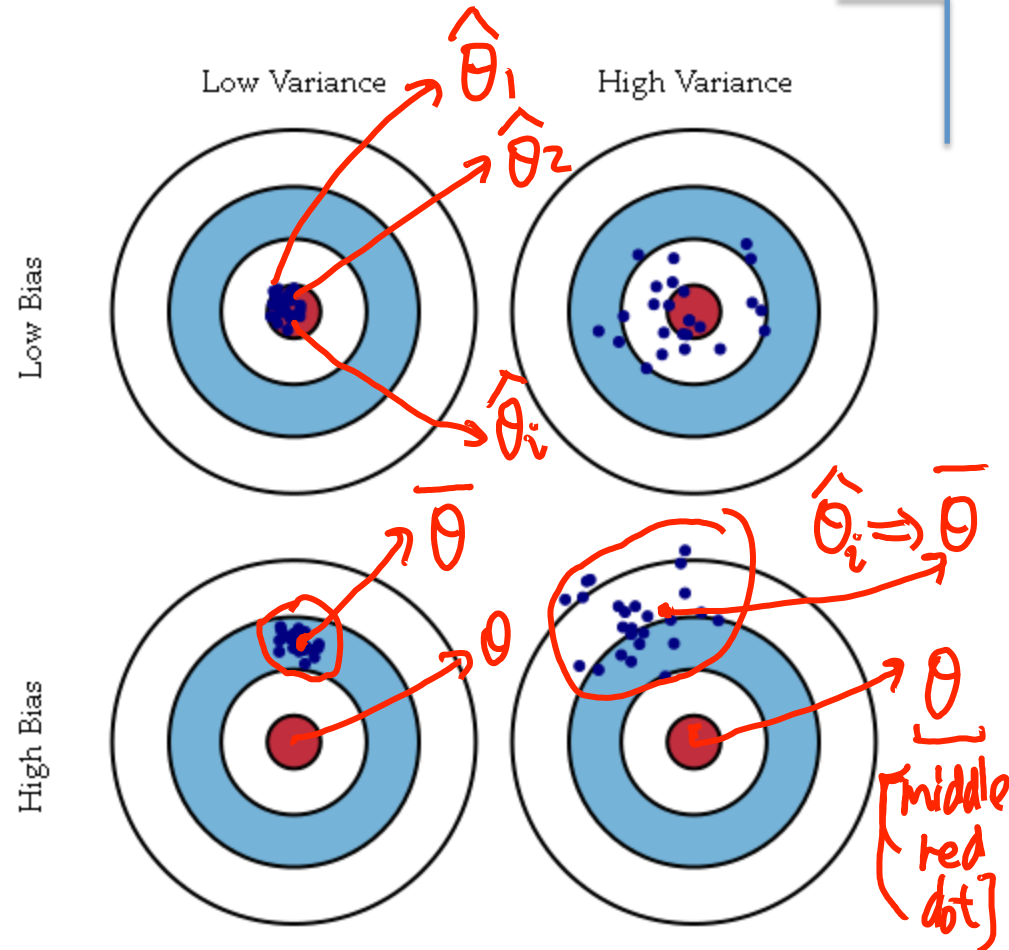
$$E(\theta - \bar{\theta})$$

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

Today



- Review of ML methods covered so far

- Regression (supervised)

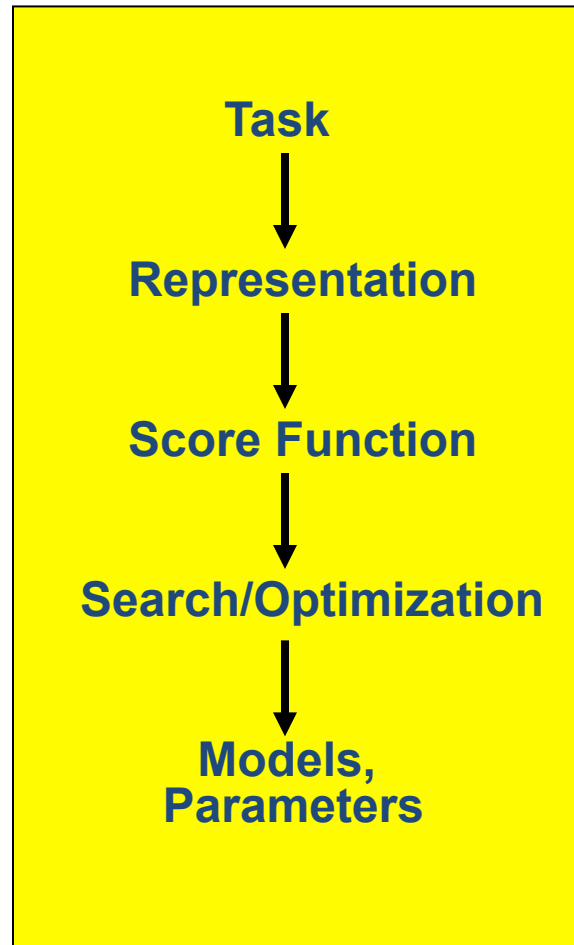
- Classification (supervised)

- Unsupervised models

- Learning theory

- Review of Assignments covered so far

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

| | |
|---------------------------------|--|
| Task | Regression, classification, clustering, dimen-reduction |
| Representation | 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, |
| Score Function | 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) , |
| Search/ Optimization | Normal equation, gradient descent, stochastic GD, Newton, Linear programming, Quadratic programming (quadratic objective with linear constraints), greedy, EM, asyn-SGD, eigenDecomp, backprop |
| Models, Parameters | 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

- ❑ Regression (supervised)

- ❑ Classification (supervised)

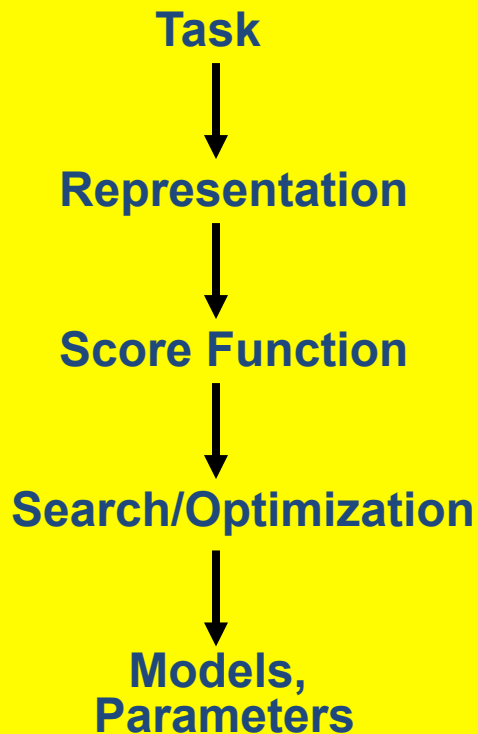
- ❑ Unsupervised models

- ❑ Learning theory



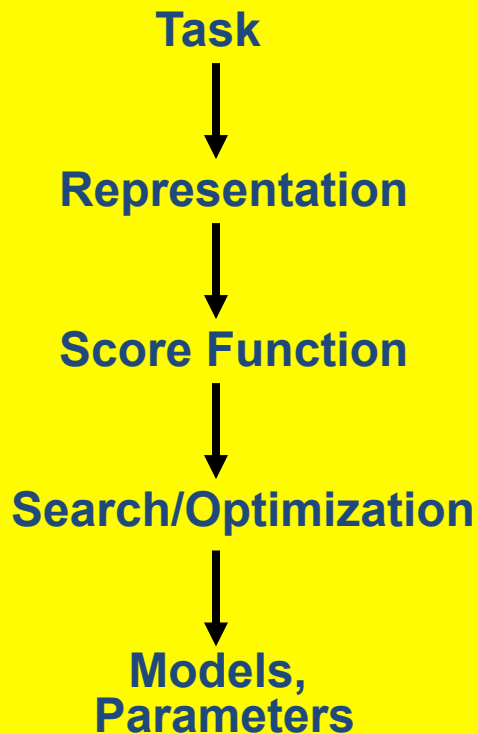
- ❑ Review of Assignments covered so far

HW1



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

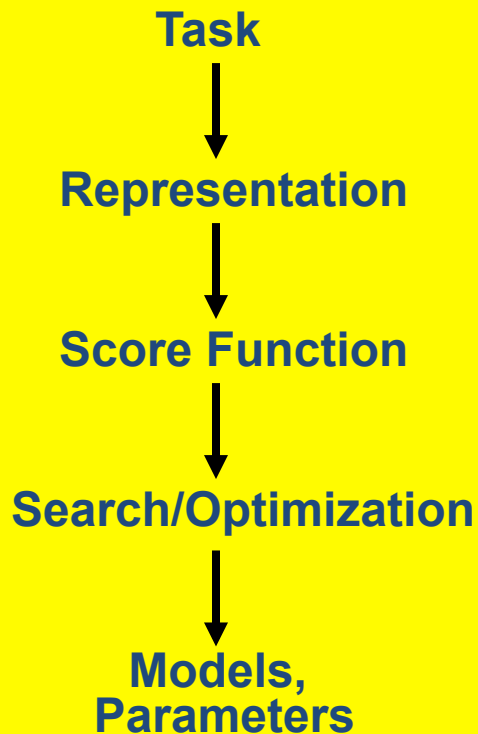
HW2



- 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

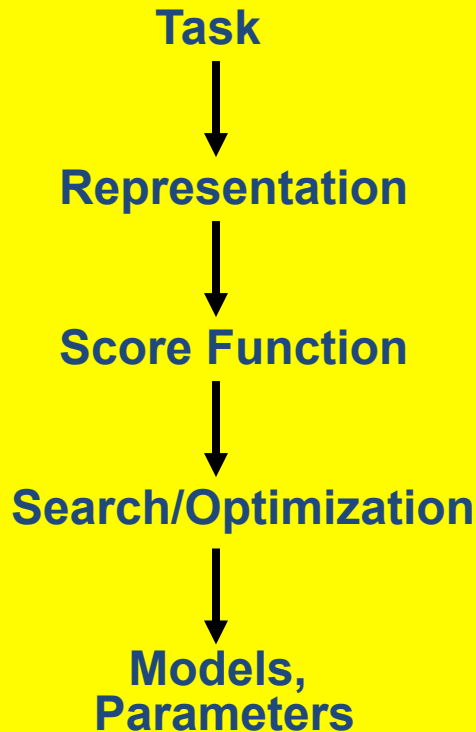
HW3

- 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

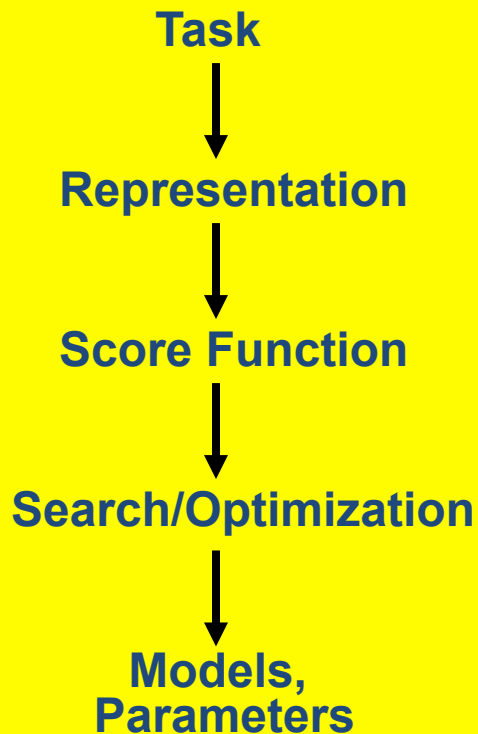


HW5

- 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



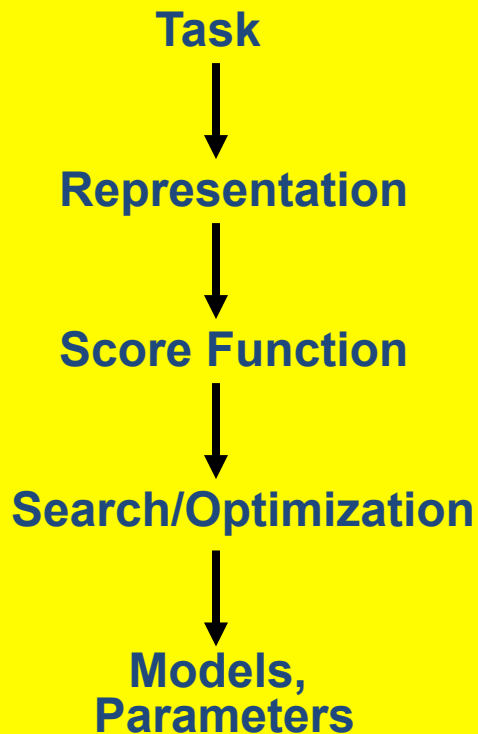
HW6



- 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