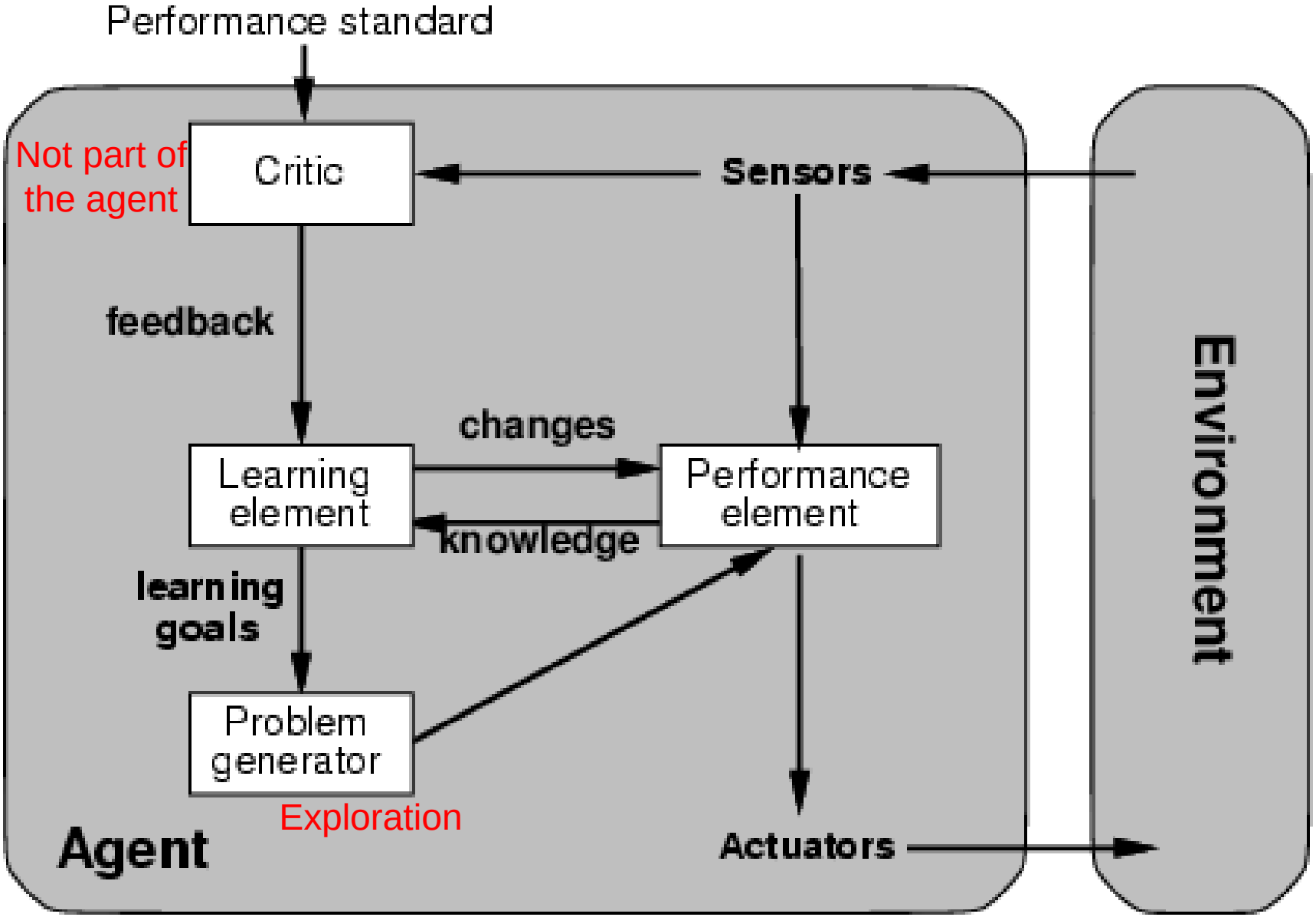
Learning

Purpose of Learning

- The agent can improve itself.
- The agent can adapt itself to different problems / scenarios.
- Why can't these improvements/abilities to handle different problems/scenarios be programmed in?
  - The designer can not program the agent for every possible problem/scenario that it may encounter.
  - The environment is stochastic or not fully observable.
  - The designer does not know how to program the agent for a task, except for letting the agent learn to solve it.

Learning Agent



Designing a Learning Agent

- Which components are to be affected by learning?
- What is already known (prior knowledge)?
- How are the components and the data represented:
  - Factored representation: A vector of attributes (numerical or categorical, continuous or discrete)
- What kind of feedback is available, if any?

Types of Learning

- **Unsupervised learning**: The agent needs to organize the object or data with no outside help and no feedback.
  - Clustering: To group objects into meaningful or useful "clusters".
- **Reinforcement leaning**: The available feedback is the outcome (reward or penalty). This can happen long after the decisions or actions that lead to the outcome.
  - Goal of learning: To minimize penalty and maximize reward.
- **Supervised learning**: The correct answers or actions are given by a "teacher" during the learning process.
  - Goal of learning: To generate "correct" answers given the inputs.

Learning from Examples

- A form of supervised learning
- A set of example cases (training samples) and their corresponding correct/desired outputs are given.
- The goal is to form a mechanism that, when given an example case, will produce the correct output.

Example of Learning from Examples

Example problem: Learning to decide whether to wait for a table when arriving at a restaurant:

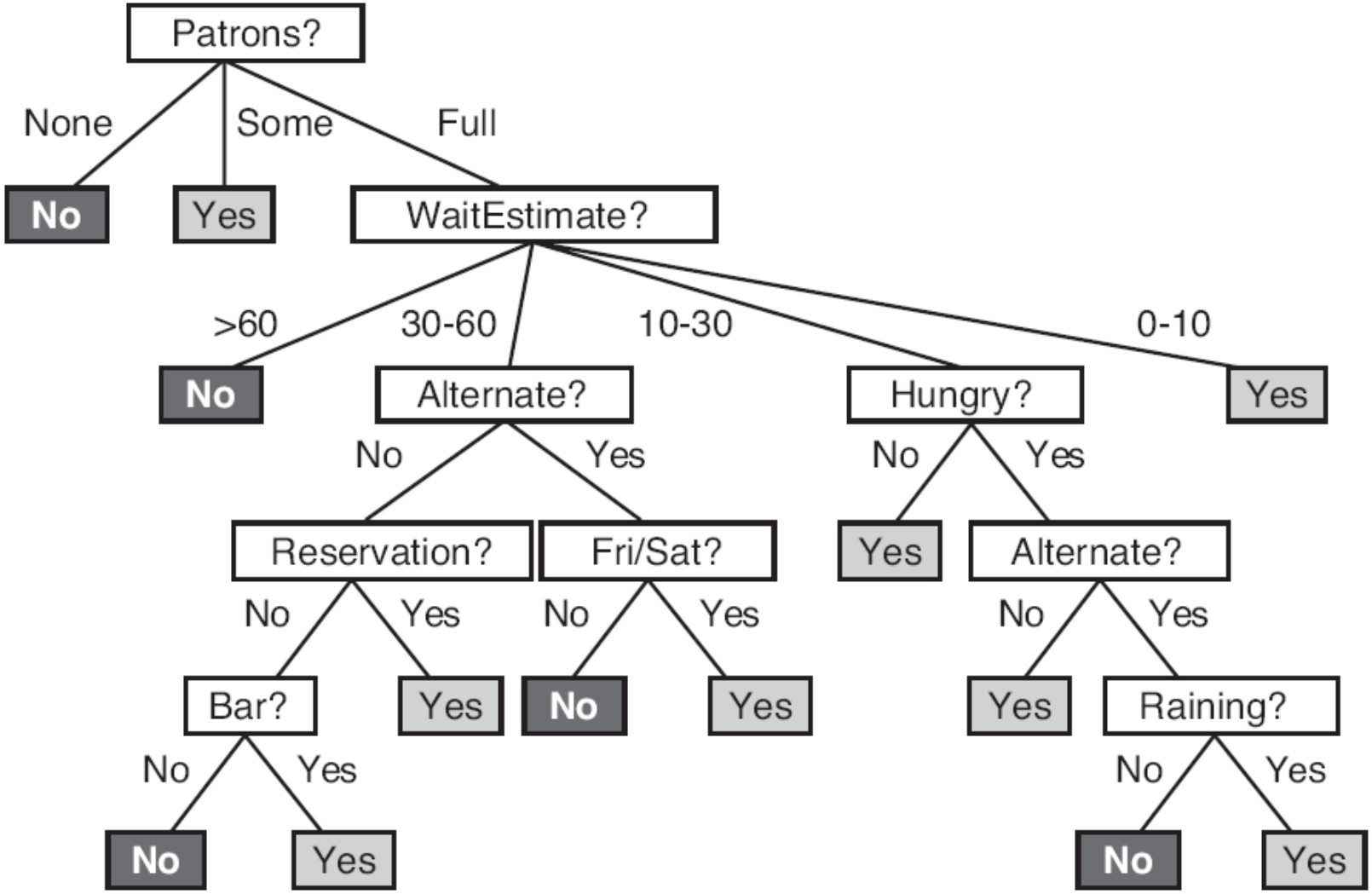
Example of Learning from Examples

The example cases:

Examples	Input Attributes										Output
	Alt.	Bar	Fri/Sat	Hun	Pat.	Price	Rain	Res.	Type	Time	Wait?
x_1	*Y*	*N*	*N*	*Y*	*Some*	*$$$*	*N*	*Y*	*French*	*0-10*	*Y*
x_2	*Y*	*N*	*N*	*Y*	*Full*	*$*	*N*	*N*	*Thai*	*30-60*	*N*
x_3	*N*	*Y*	*N*	*N*	*Some*	*$*	*N*	*N*	*Burger*	*0-10*	*Y*
x_4	*Y*	*N*	*Y*	*Y*	*Full*	*$*	*Y*	*N*	*Thai*	*10-30*	*Y*
x_5	*Y*	*N*	*Y*	*N*	*Full*	*$$$*	*N*	*Y*	*French*	*>60*	*N*
x_6	*N*	*Y*	*N*	*Y*	*Some*	*$$*	*Y*	*Y*	*Italian*	*0-10*	*Y*
x_7	*N*	*Y*	*N*	*N*	*None*	*$*	*Y*	*N*	*Burger*	*0-10*	*N*
x_8	*N*	*N*	*N*	*Y*	*Some*	*$$*	*Y*	*Y*	*Thai*	*0-10*	*Y*
x_9	*N*	*Y*	*Y*	*N*	*Full*	*$*	*Y*	*N*	*Burger*	*>60*	*N*
x_{10}	*Y*	*Y*	*Y*	*Y*	*Full*	*$$$*	*N*	*Y*	*Italian*	*10-30*	*N*
x_{11}	*N*	*N*	*N*	*N*	*None*	*$*	*N*	*N*	*Thai*	*0-10*	*N*
x_{12}	*Y*	*Y*	*Y*	*Y*	*Full*	*$*	*N*	*N*	*Burger*	*30-60*	*Y*

Decision Tree

The input-output relations are organized into a tree. Each node divides its set of samples into subsets according to a particular input attribute.



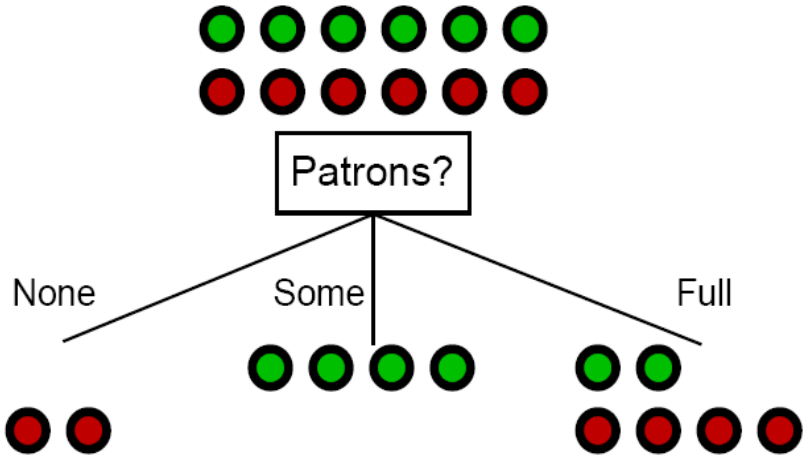
Decision Tree Learning

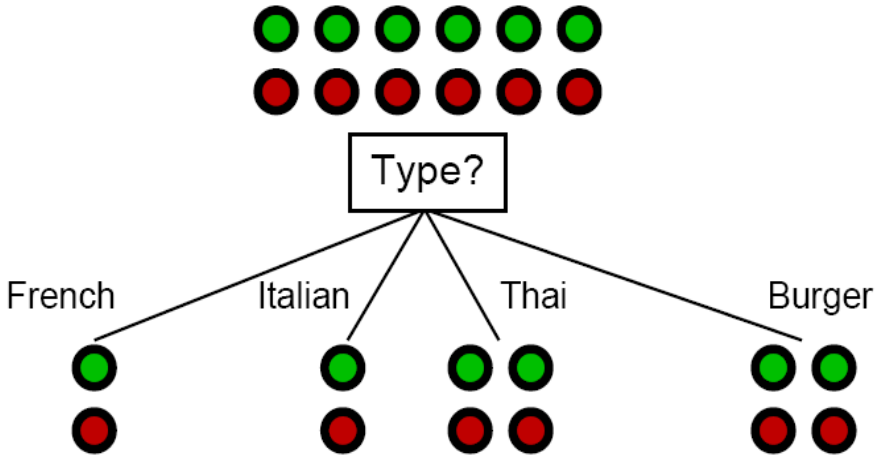
- Each tree node is associated with a set of labeled samples.
- In the beginning, we generate only the root node, which is associated with all the samples.
- The following steps are applied to each new node:
  - Select an attribute as the basis for splitting the samples of the current node.
  - Divide the values of the selected attribute in the set of samples into several groups. A new tree node is generated for each of these groups.
- The key is how to split the samples. (How to select an attribute, and how to partition the values of the selected attribute.)

Choosing Attribute Tests: The Idea

Idea: a good attribute splits the samples into subsets that (ideally) contains samples of the same labels.

Q: Which of the following two attributes are better?





Choosing Attribute Tests

- The goal of splitting is so that the sample labels (desired outputs) of the child nodes are more "pure" (or are "less uncertain") than those in the parent node.
- How to measure the "impurity" or "uncertainty" of the label distribution of a node? Some typical ones:
  - Shannon's Entropy: $H(V) = -\sum_k P(v_k) \log_2 P(v_k)$
  - Gini Index: $G(V) = 1 - \sum_k P(v_k)^2$

Choosing Attribute Tests

- The goal of splitting is so that the sample labels (desired outputs) of the child nodes are more "pure" (or are "less uncertain") than those in the parent node.
- Some representative metrics of "impurity" or "uncertainty":
  - Shannon's Entropy: $$H = -\sum_k p_k \log_2 p_k$$
  - Gini Index: $$G = 1 - \sum_k p_k^2$$

Here p_k is the ratio of items with label k.

Choosing Attribute Tests

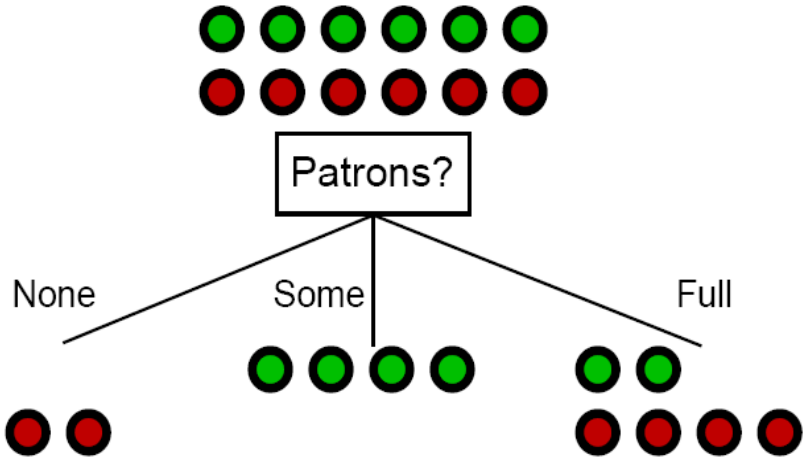
Now, consider an attribute with m possible values. Splitting a node (A) with N items on this attribute will result in m child nodes (C_1, C_2, … C_m) with N_1, N_2, … N_m items, respectively. The idea is to select the attribute that gives the most reduction in uncertainty/impurity (entropy used here):

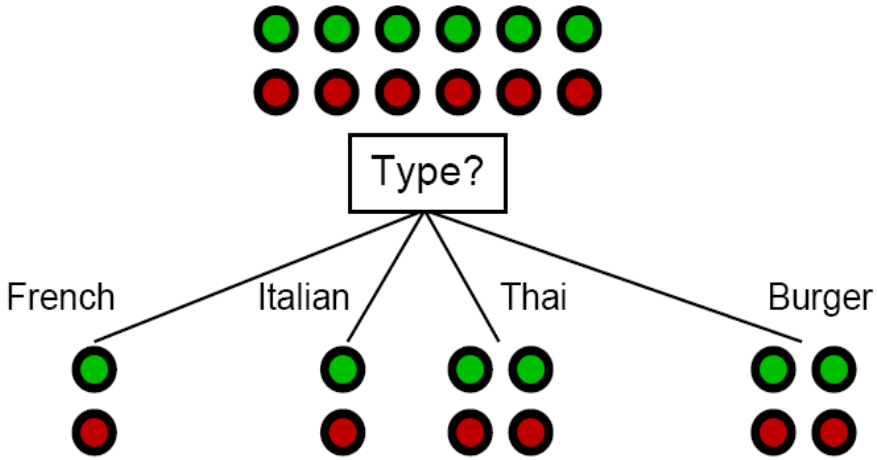
$$\Delta H = H(A) - \sum_{i=1}^{m} \frac{N_i}{N} H(C_i)$$

For entropy, this is also called the *information gain*.

Choosing Attribute Tests

Now we can try to choose an attribute again:





$$H(A) = 2\left(-\frac{1}{2}\log_2\frac{1}{2}\right) = 1$$

$$H(C_1) = H(C_2) = 0$$

$$H(C_3) = -\frac{1}{3}\log_2\frac{1}{3} - \frac{2}{3}\log_2\frac{2}{3} = 0.80$$

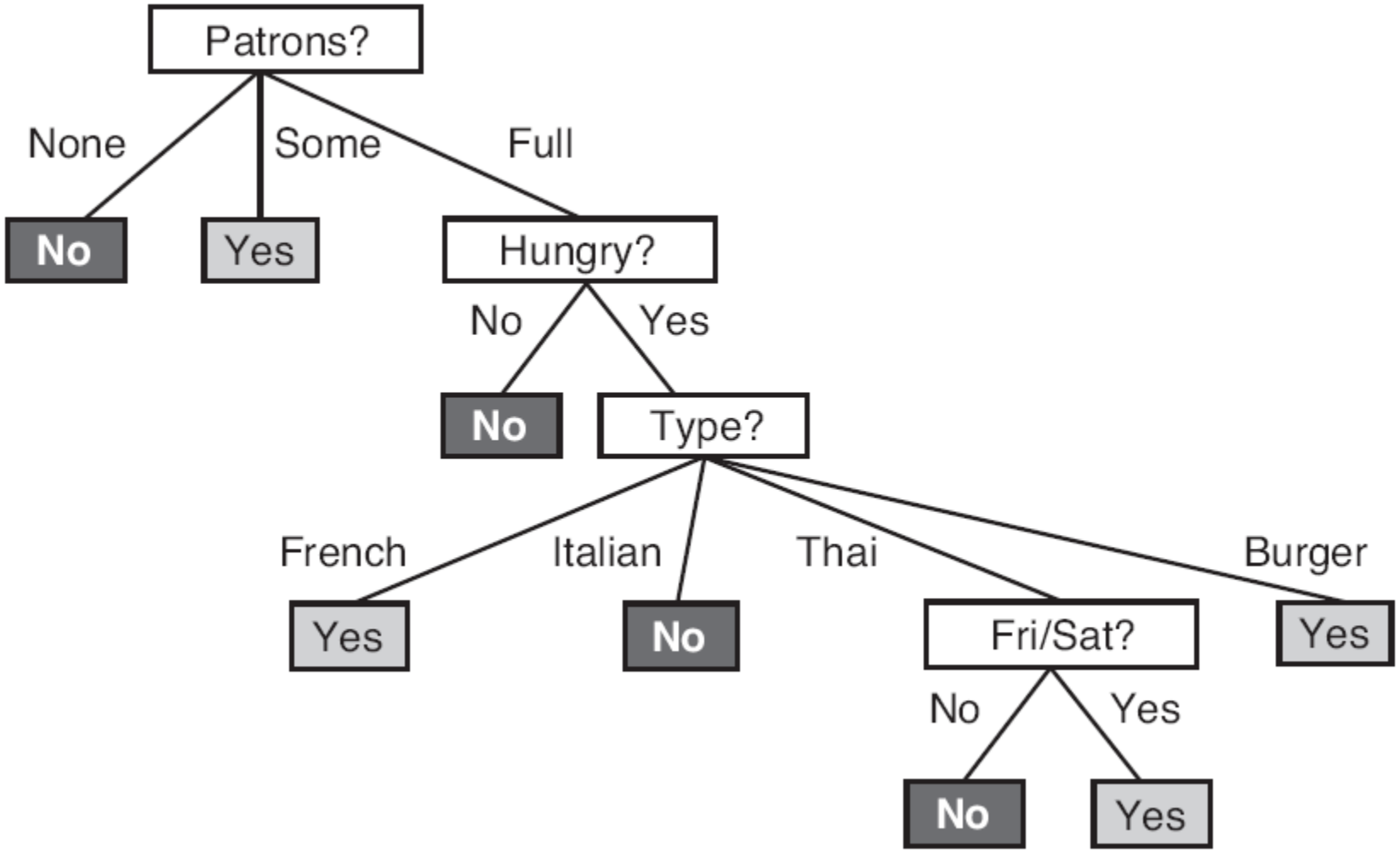
$$\Delta H = 1 - (2/12)*0 - (4/12)*0 - (6/12)*0.80$$
$$= 0.60$$

$$H(C_1) = H(C_2) = H(C_3) = H(C_4) = 1$$

$$\Delta H = 0$$

Choosing Attribute Tests

This tree is substantially smaller than the first one, but it gives the same outputs for all the training samples.



Supervised Learning Overview

- Main usages of supervised learning:
  - **Classification**: The expected output is one of several categories. Such an agent / program is called a **classifier**.
  - **Regression**: The expected output is a numerical value. Example: temperature in weather forecast.
- Both involve some input/output mapping: $f : x \rightarrow y$

Supervised Learning Overview

Training and testing:

- Training data: Collect samples in the form of $(x \rightarrow y)$.
  - For such a pair of $(x \rightarrow y)$, y is often called the ground-truth or target output of x.
  - If y represents a category (class), then it is also called the class label (or simply the label) of x.
- Training: Derive an estimated model of the mapping f using the training data.
- Testing: Using the derive model, determine y for some given x (normally not in the training data).

Supervised Learning Overview

- There are numerous possible forms (model types) to represent the mapping. Examples:
  - Rule Sets
  - Polynomials
  - Gaussian Mixtures
  - k Nearest Neighbors
  - Decision Trees
  - Neural Networks
  - …
- There are many possible forms for representing the mapping of a given set of training data. This means that the actual form used is a design choice.
- For each given form of representation, there are parameters to be determined according to the training data.

Supervised Learning Overview

- Stages of learning a model for $f : x \rightarrow y$:

Model Type

Polynomial?
Mixture of Gaussians?
Neural networks?
...

Model Design Hyperparameters

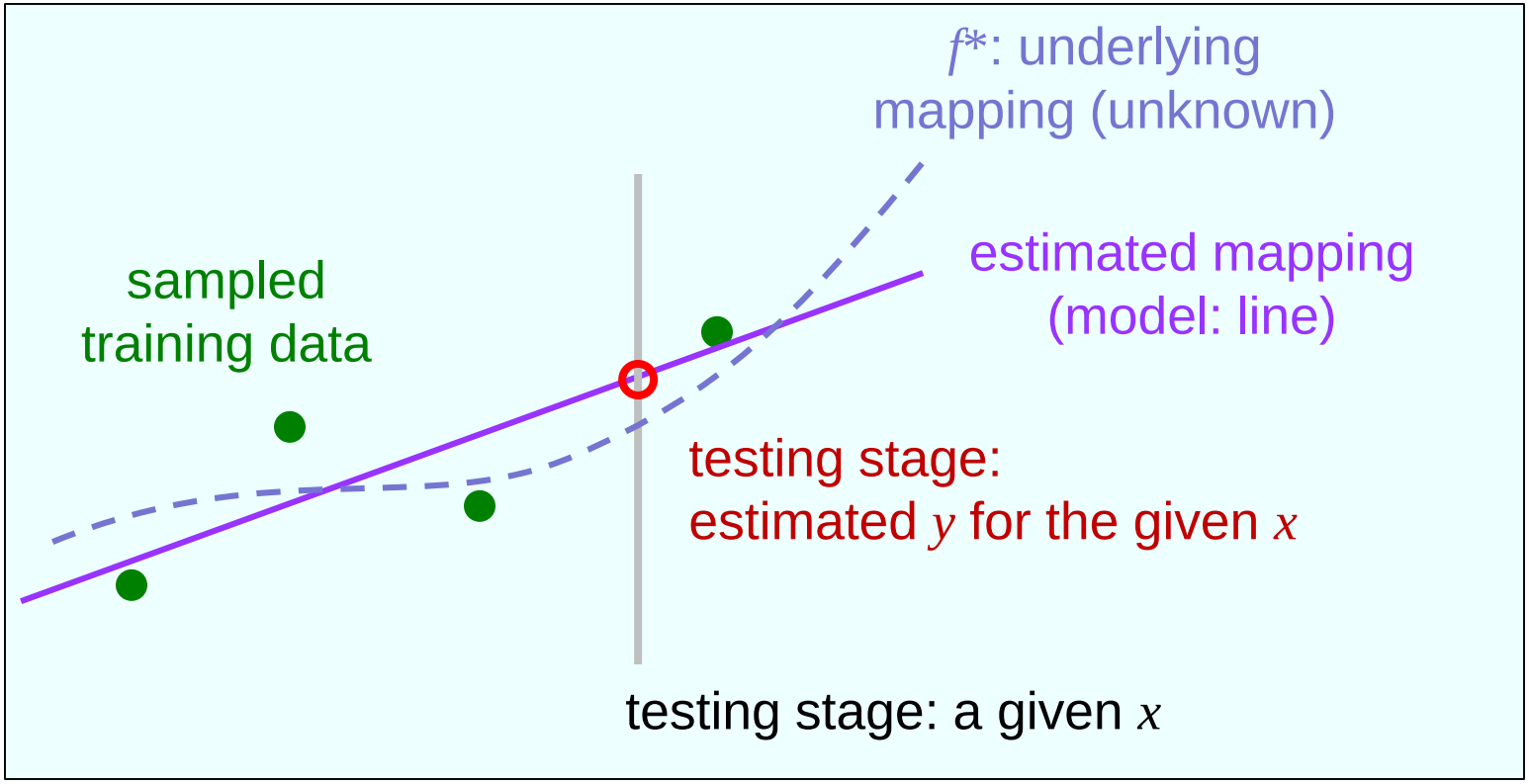
Polynomial: degree?
Mixture of Gaussians: #Gaussians?
Neural networks: #neurons?
...

Parameter Estimation

Polynomial: coefficients
Mixture of Gaussians: means/covars
Neural networks: network weights
...

Training and Testing

Here we will use regression as an example.



Bias-Variance Dilemma

Desired properties of the estimated mapping:

- Low **Bias** (goodness of fitting):
  - The estimated mapping should fit to the training data as well as possible.
  - Goal: To capture the behaviors of the underlying mapping as well as possible.
- Low **Variance** (high confidence):
  - Assume that we have several estimated mappings, each derived from a different set of training samples.
  - For a given x, each mapping gives an estimations for y.
  - The estimations for y should by as similar to each other as possible.
  - Goal: To be confident of the estimation of y.

Bias-Variance Dilemma

For supervised learning, we always need to consider the trade-off between bias and variance.

- Reason 1:

  Sampled Value (used for training) =
  Signal (from underlying mapping)
  + Noise

  Noise is a reality of life that you have to deal with.

- Reason 2: We can only have a finite number of training samples. (If we have infinite number of training samples, the noise can be averaged out.)

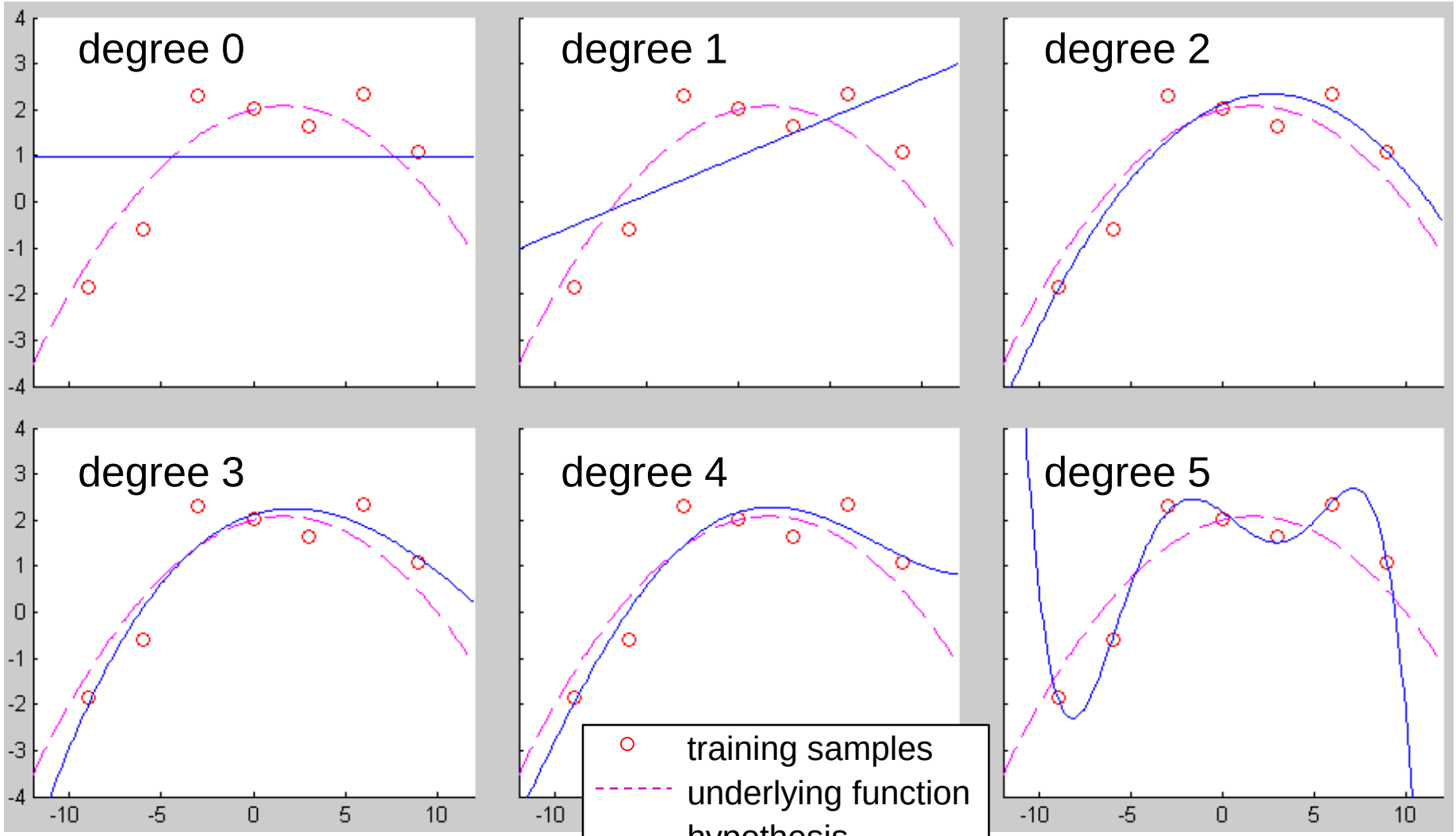
Bias-Variance Dilemma

Now, difficulties for supervised learning:

- To reduce **Bias**
  - ➔ Use more complex models
  - ➔ BOTH signal and noise are learned
  - ➔ Overfitting
- To reduce **Variance**
  - ➔ Try to avoid learning noise (variance is caused by noise)
  - ➔ Use less complex models
  - ➔ Signal is not sufficiently learned
  - ➔ Underfitting

Fitting and Model Complexity

Using polynomial regression as an example:



What to Do Now?

Several representative approaches:

- Increase the number of training samples.
- Try to determine the suitable level of model complexity.
- Regularization (the "suppression" of complexity during training)
- Consensus-based methods (ensembles)

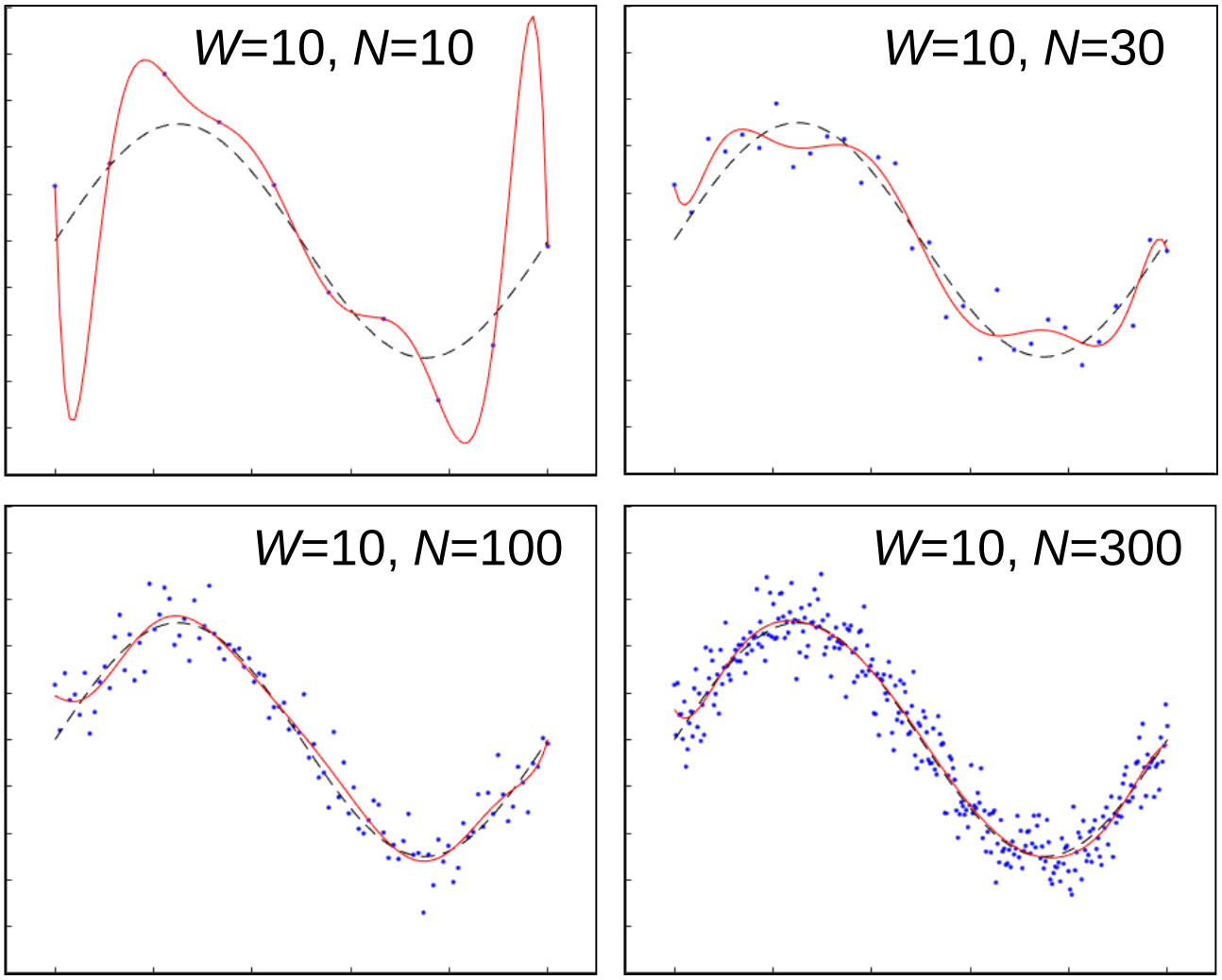
Amount of Training Data

- The usual case: The more training data, the better.
- Rule of thumb (not always suitable):

  (# training samples) $\geq$ 10 x (# free parameters in model)
- Possible difficulties:
  - Data availability
  - Increased computational cost
- When there are few training samples, some classifier types (e.g., support vector machines) generally work better than others.

Amount of Training Data

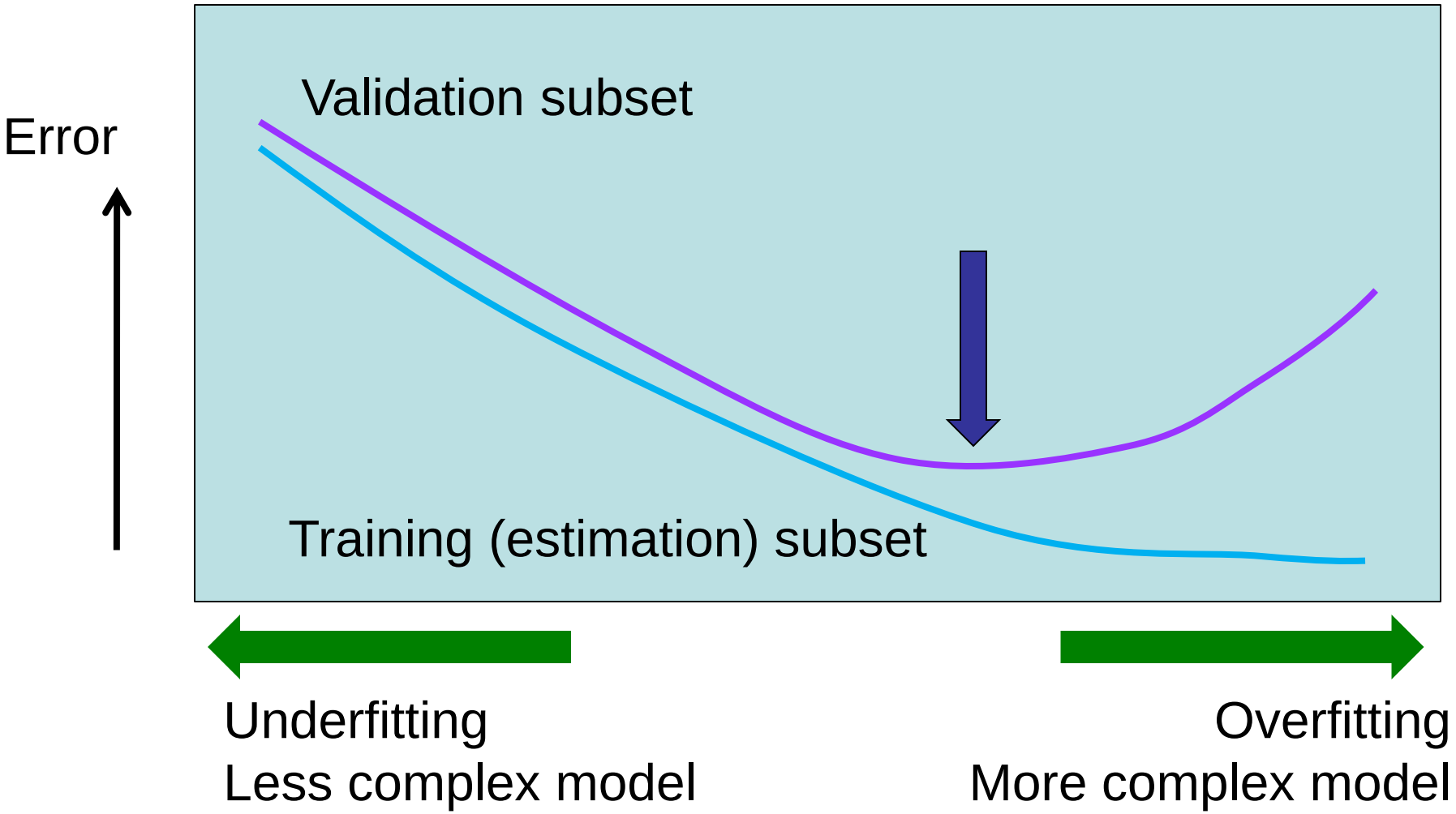
- Example (polynomial regression):



How Much Model Complexity?

- **Ockham's Razor**: Among different ways to explain the data, choose the simplest one.
- Model complexity is usually controlled / adjusted using some **hyper-parameters**.
- Example methods: **cross-validation**, post-processing model pruning.
- Many of these methods utilize **validation data** (training samples not used for model parameter estimation) to check the **generalization** ability of the built model.

Validation


Error
Validation subset
Training (estimation) subset
Underfitting
Less complex model
Overfitting
More complex model

Cross-Validation

- The N labeled samples are divided into K subsets of approximately equal sizes ($K>1$). They should have similar distributions.
- The training process (model parameter estimation) is run K times (K trials).
- In the Kth trial, the Kth subset is used for validation, and the other subsets are used for training.
- The overall performance is the combination of the performance on all the validation subsets.

Cross-Validation

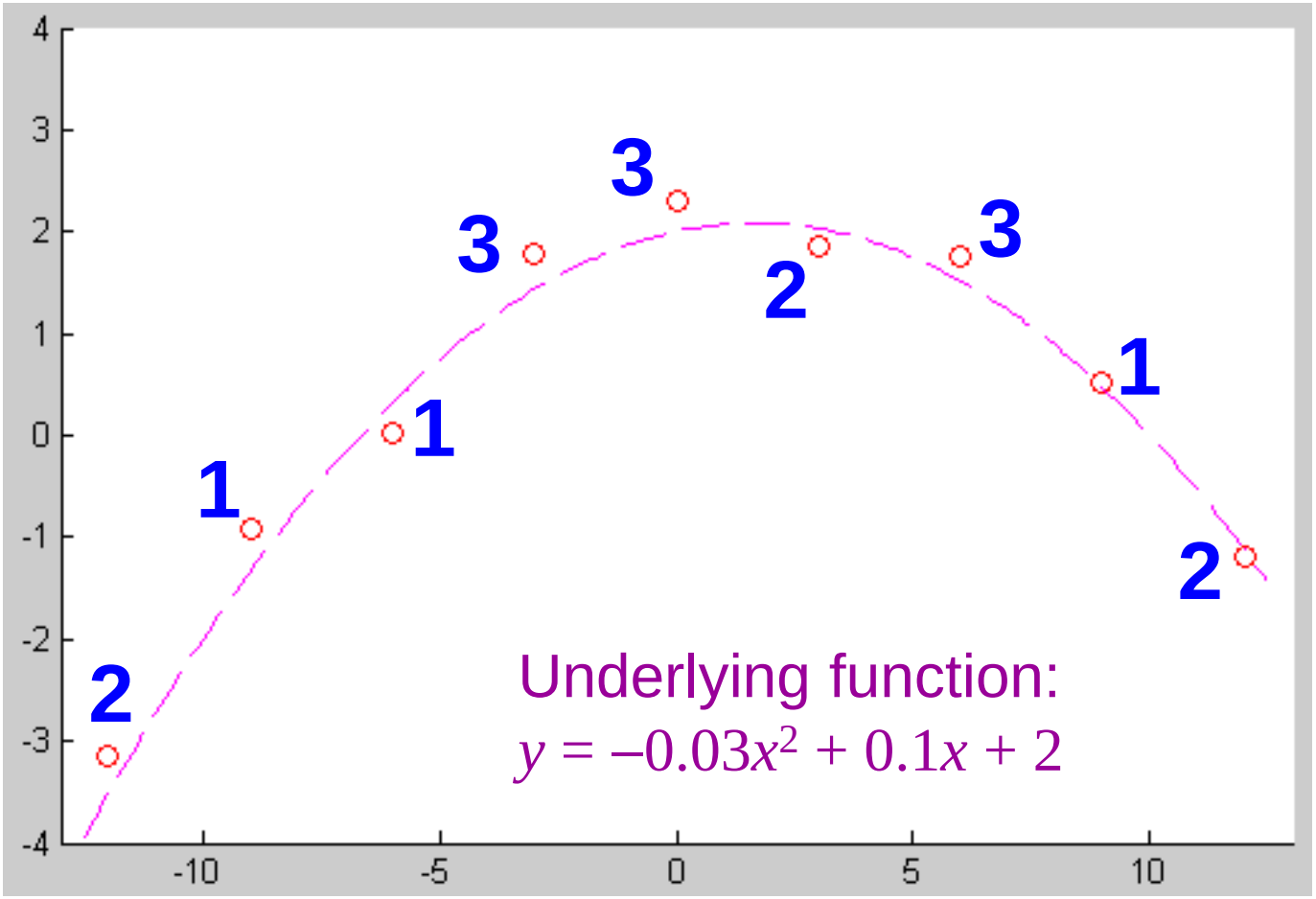
4-fold cross-validation: parameter estimation validation

Extreme case: The leave-one-out method ($K=N$).

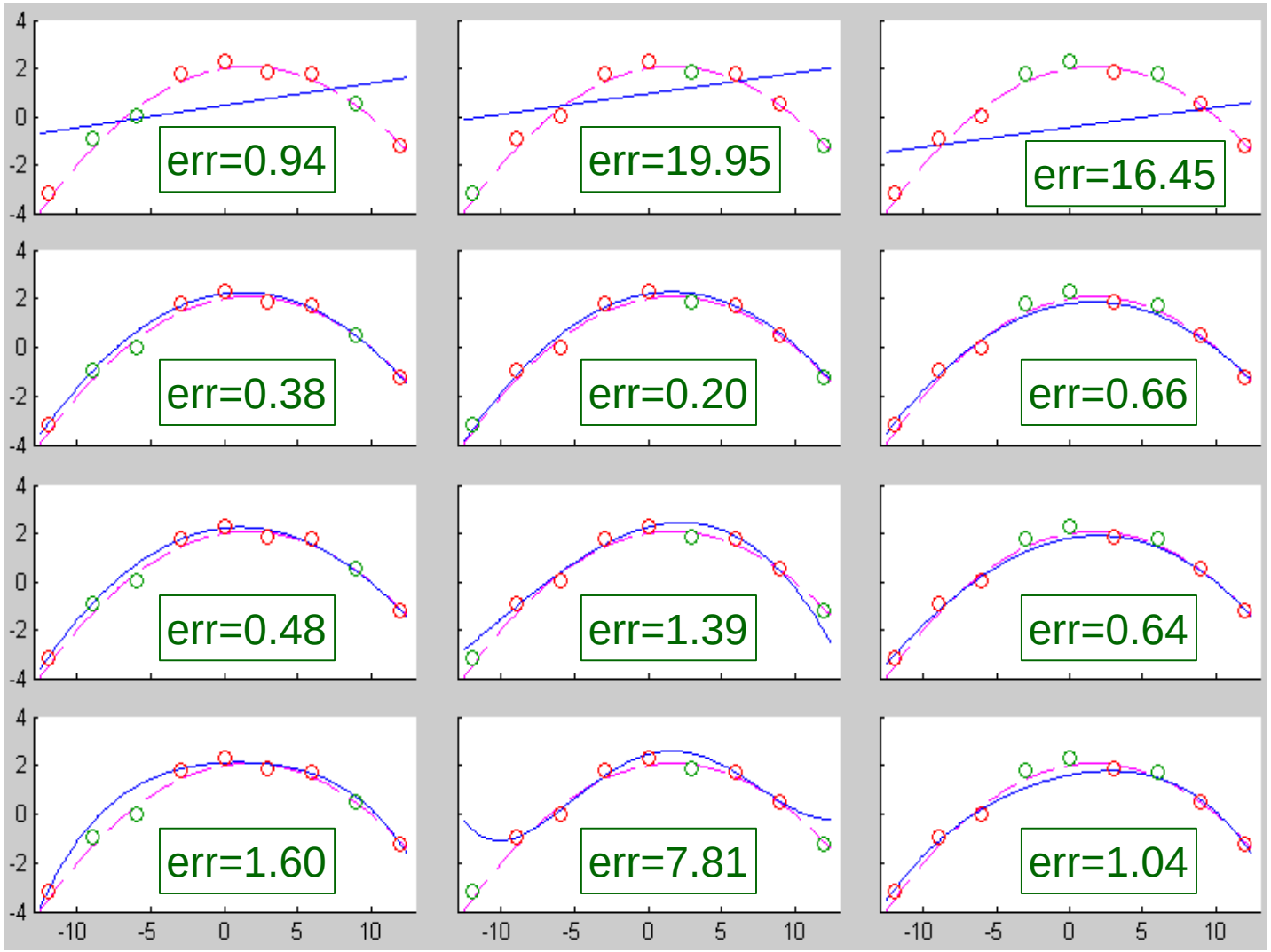
Model Selection by Cross-Validation

Example: polynomial regression:

9 training samples → 3 subsets

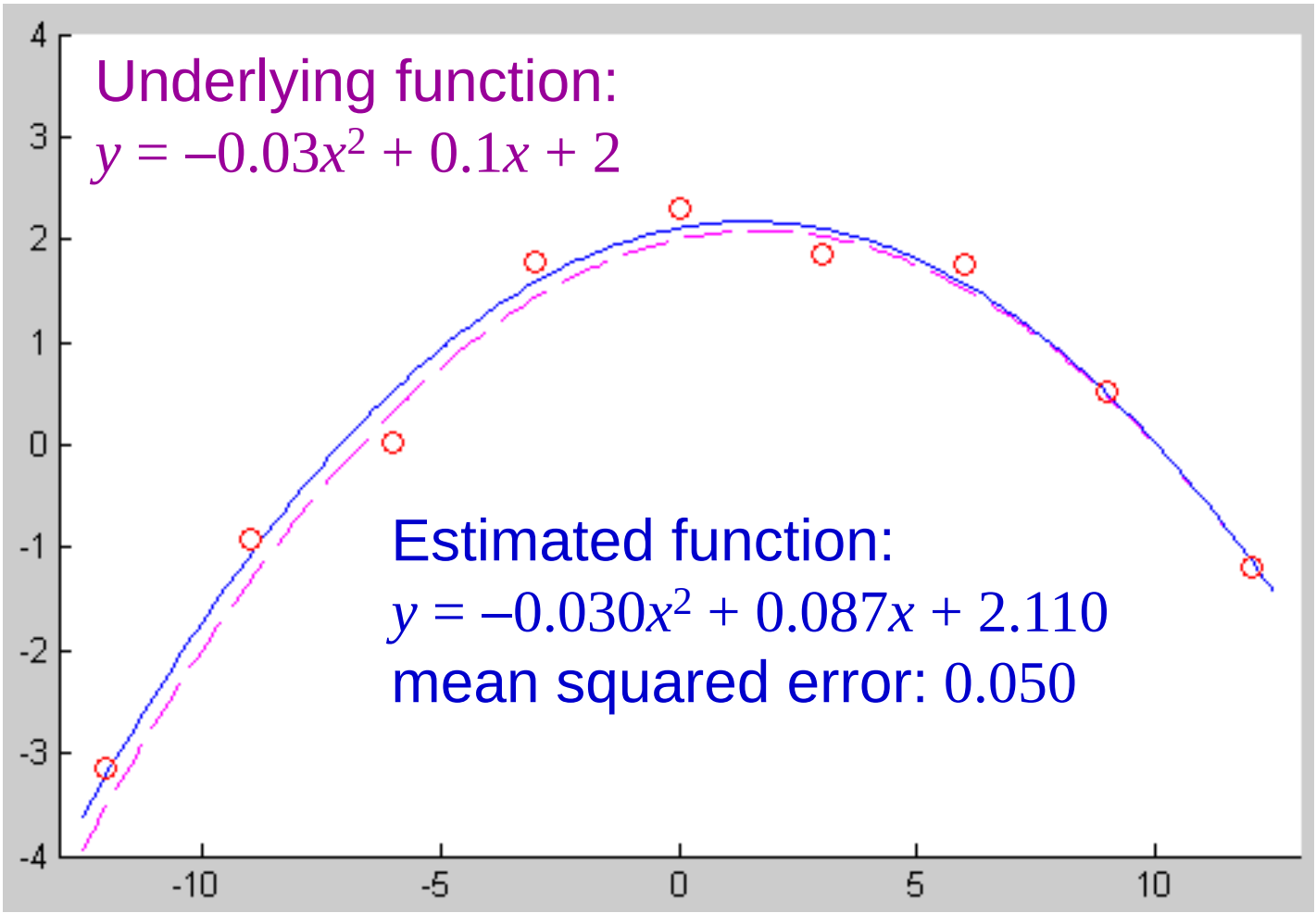


Model Selection by Cross-Validation



Model Selection by Cross-Validation

Finally, use the selected model and ALL the training samples for parameter optimization:



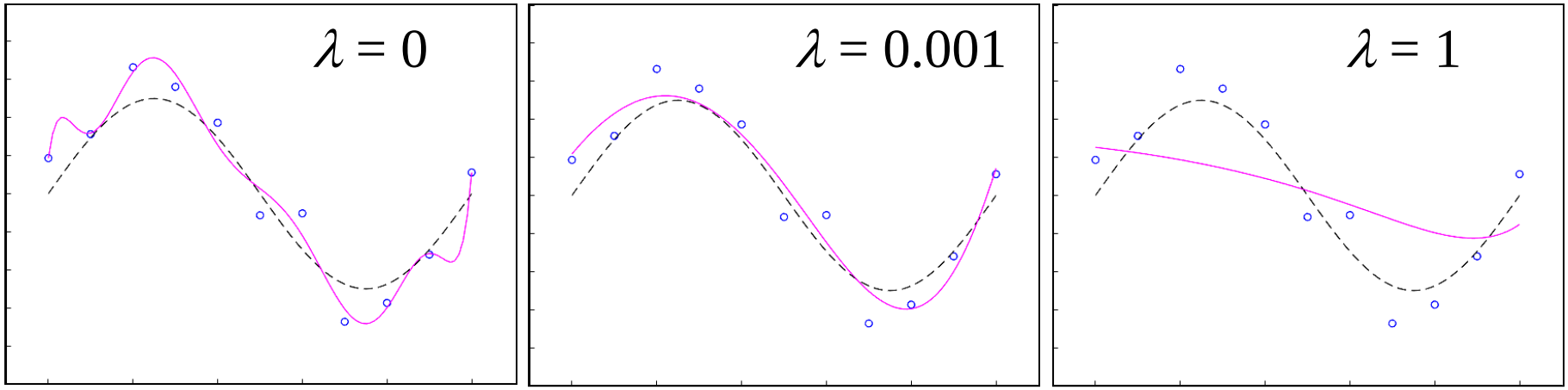
Regularization

- Include the trade-off during the learning process:
  - **Regularization**: Modify the learning objective to minimize BOTH the bias and the model complexity. (Normally, the learning process only attempts to minimize bias.)
  - Example **cost function** (to be minimized) for polynomial regression:

To minimize: $$E = \underbrace{\sum_i \left| y_i - \sum_{k=0}^{d} a_k x_i^k \right|^2}_{\text{Fitting Error}} + \underbrace{\lambda \sum_{k=0}^{d} a_k^2}_{\text{Regularization}}$$

Regularization

- Example (polynomial regression):



N=11, degree=9

Consensus Based Methods

- Build many somewhat different models (an **Ensemble**) for the same underlying mapping.
- The consensus should better represent the "signal" part, and the "noise" part is more likely to be averaged out.
- Result: Reduction of variance with minimal effect on bias.
- Common ways to create the ensemble of different models:
  - Random subset of attributes
  - Random subset of training samples

Back to Decision Trees

- Representative decision tree algorithms include:
- **ID3** (most similar to the method in the textbook)
  - Designed for categorical attributes
  - Post-processing pruning with validation data
- **C4.5** (a successor of ID3)
  - Categorical and numerical attributes
  - Use normalized information gain
- **CART** (**C**lassification **A**nd **R**egression **T**rees)
  - Categorical and numerical attributes
  - Branching factor is always two (binary tree)

Classification and Regression Trees

Node splitting criterion:

- Numerical attributes:
  - Select a threshold
  - Minimize total within-node variance
- Categorical attributes:
  - Need to find a way to partition the categories into two groups.
  - Multiple possible partitions if the items in a node are of more than two categories.
  - Minimize total Gini's impurity

Classification and Regression Trees

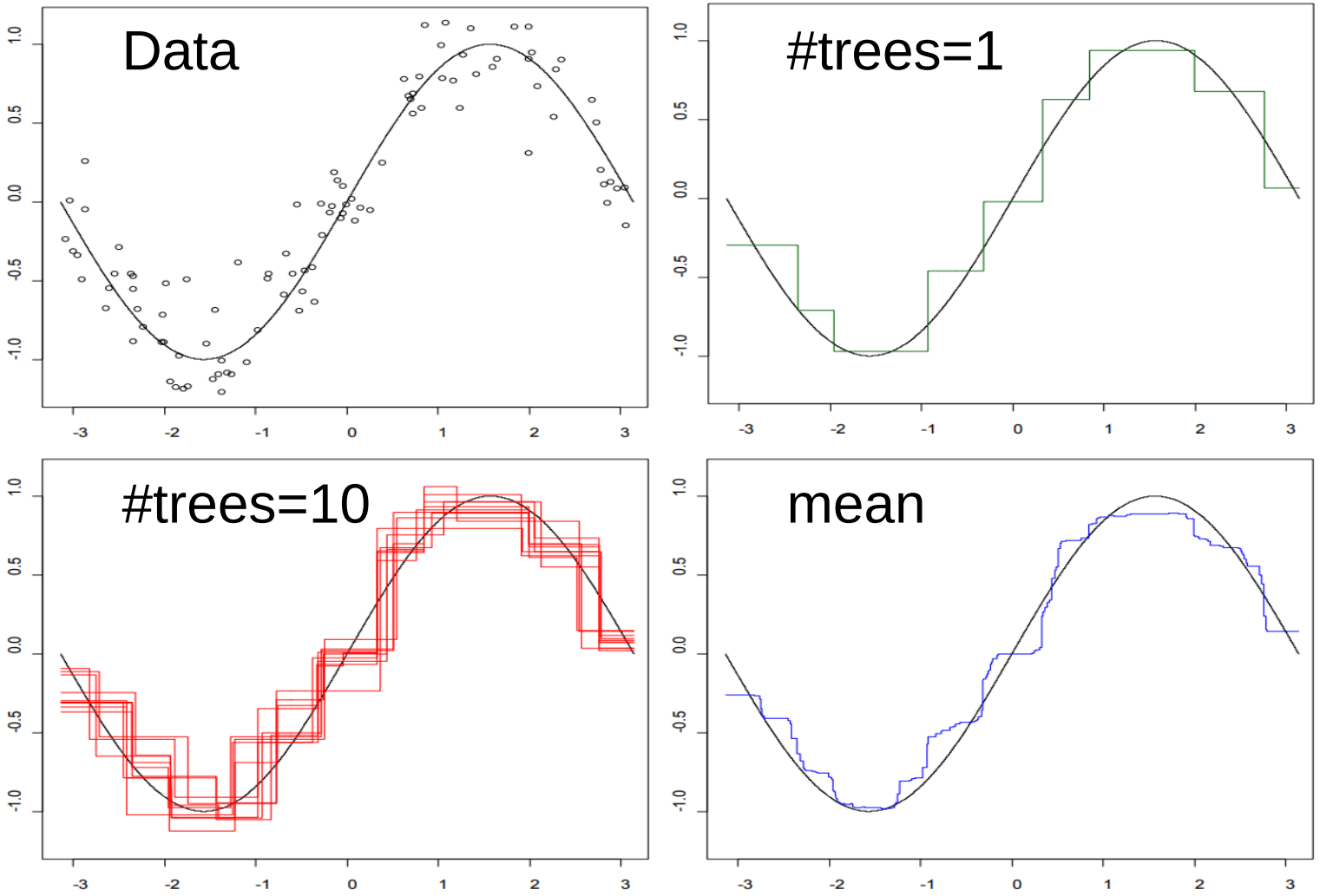
Output:

- To avoid overfitting, the growth of the tree is usually limited.
  ➔ A leaf node is often "impure" in terms of the expected outputs of its items.
- To generate an estimated output:
  - For regression: Use the mean output of the items in the node.
  - For classification: Use the majority vote of the items in the node.

Random Forests

- A representative example of ensemble learning.
- The final output is the average output of many randomized trees.
- **Bagging** = **b**ootstrap **agg**regat**ing** (*random sampling with replacement*)
- **Tree Bagging**:
  - Each tree is trained with a somewhat different set of training data (selected from a common pool of training data with bootstrap aggregation).
- **Feature/Attribute Bagging**:
  - Consider only a (small) subset of features/attributes at each node splitting.
  - Typically only $p^{1/2}$ of p features used (for classification).

Random Forests: An Example



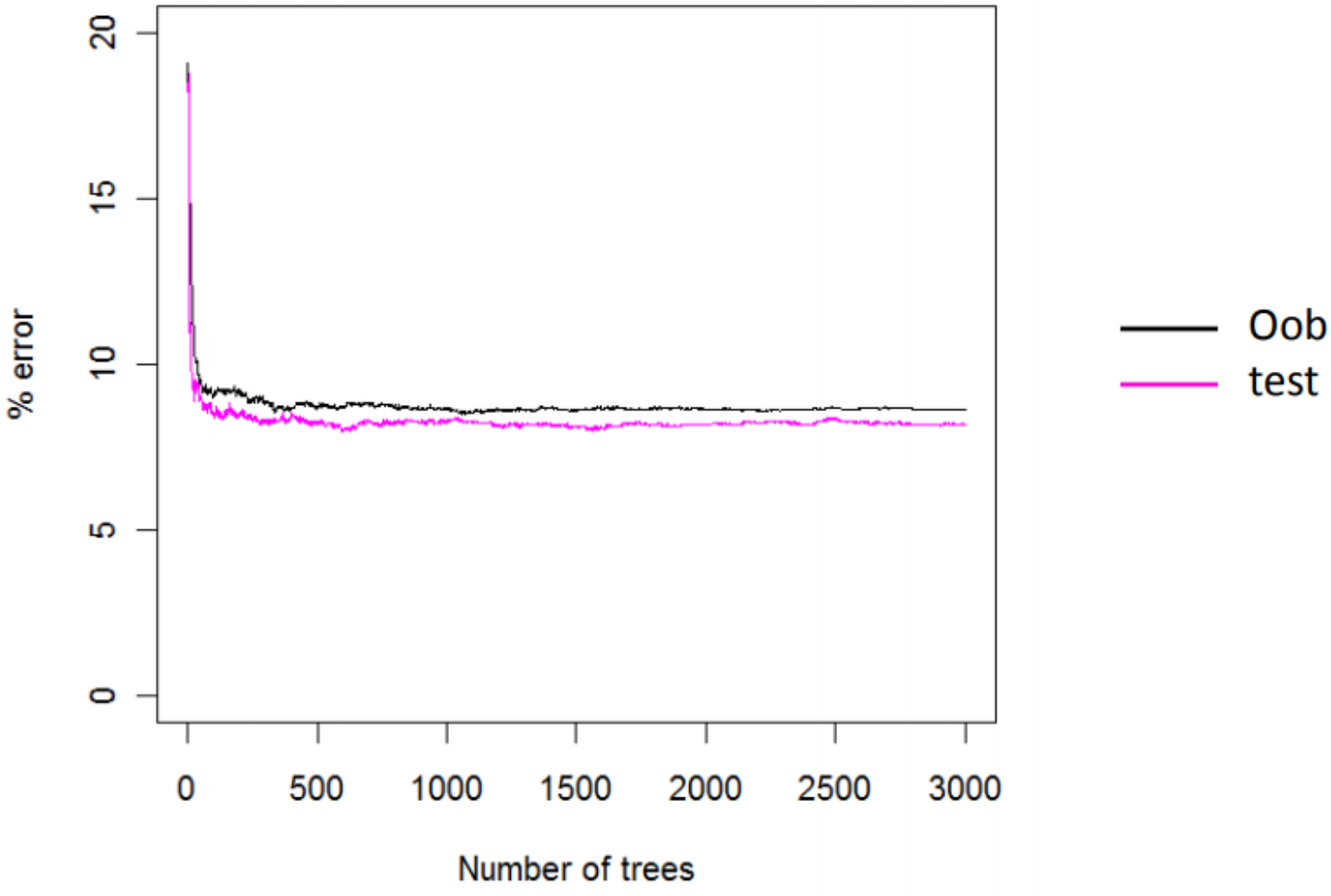
www.math.usu.edu/adele/RandomForests/Ovronnaz.pdf

Random Forests: Generalization

- For each training sample $\boldsymbol{x}$, there are some trees that do NOT consider it during tree building. It is called an out-of-bag sample for those trees.
- Use the trees for which $\boldsymbol{x}$ is out-of-bag to predict the output for $\boldsymbol{x}$. (Use averaging for regression, and use majority vote for classification.)
- Repeat the above step for all training samples. Now we have the overall out-of-bag error (mean squared error for regression, classification error rate for classification) as a measure of generalization ability.

Random Forests: Generalization

Random forests do not overfit with increased number of trees.



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