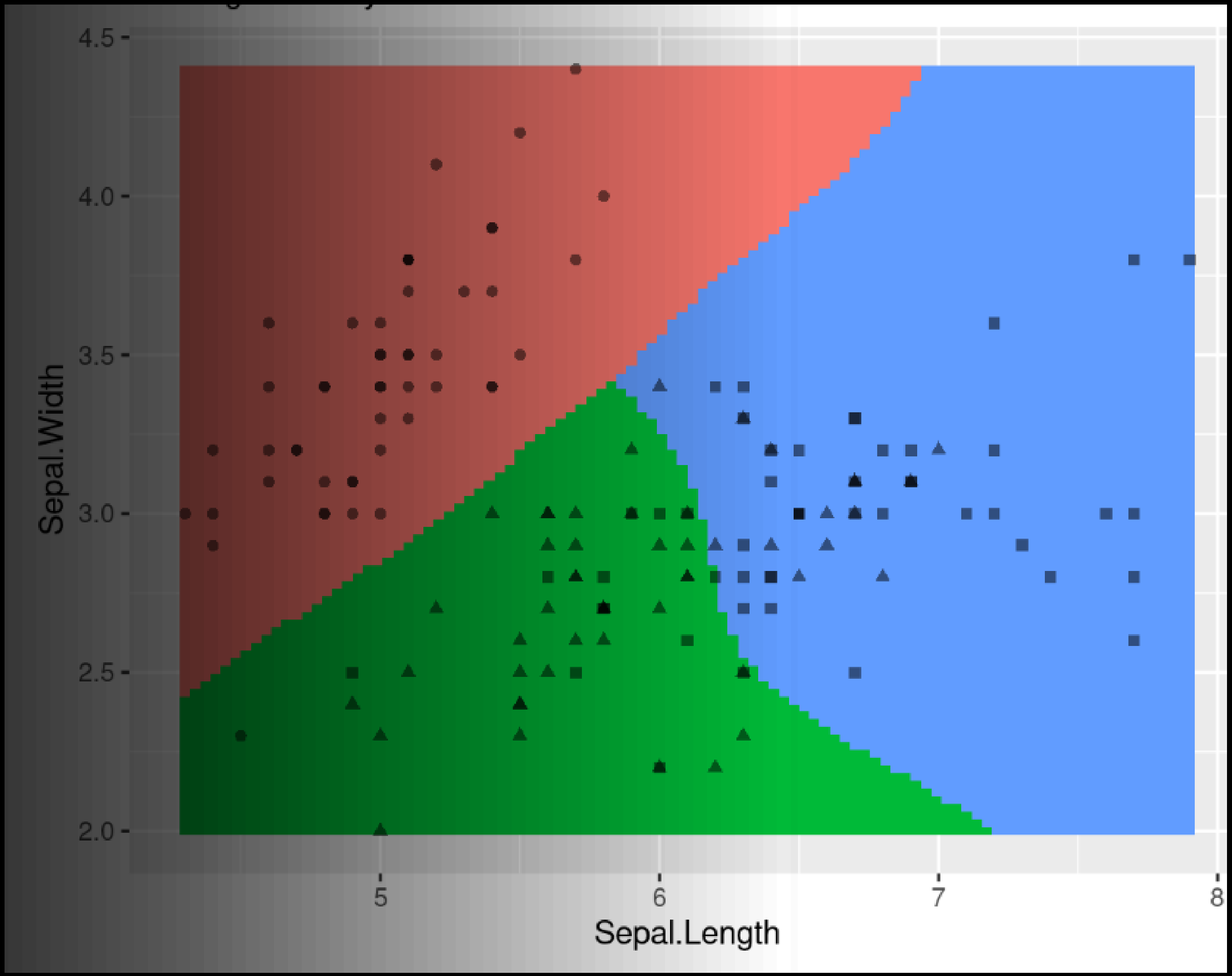
CS 5/7320
Artificial Intelligence

Learning
from Examples

AIMA Chapter 19



Slides by Michael Hahsler
Based on slides by Dan Klein, Pieter Abbeel, Sergey Levine and A. Farhadi. All CS188 materials are at http://ai.berkeley.edu with figures from the AIMA textbook.

Learning from Examples: Machine Learning

Up until now in this course:

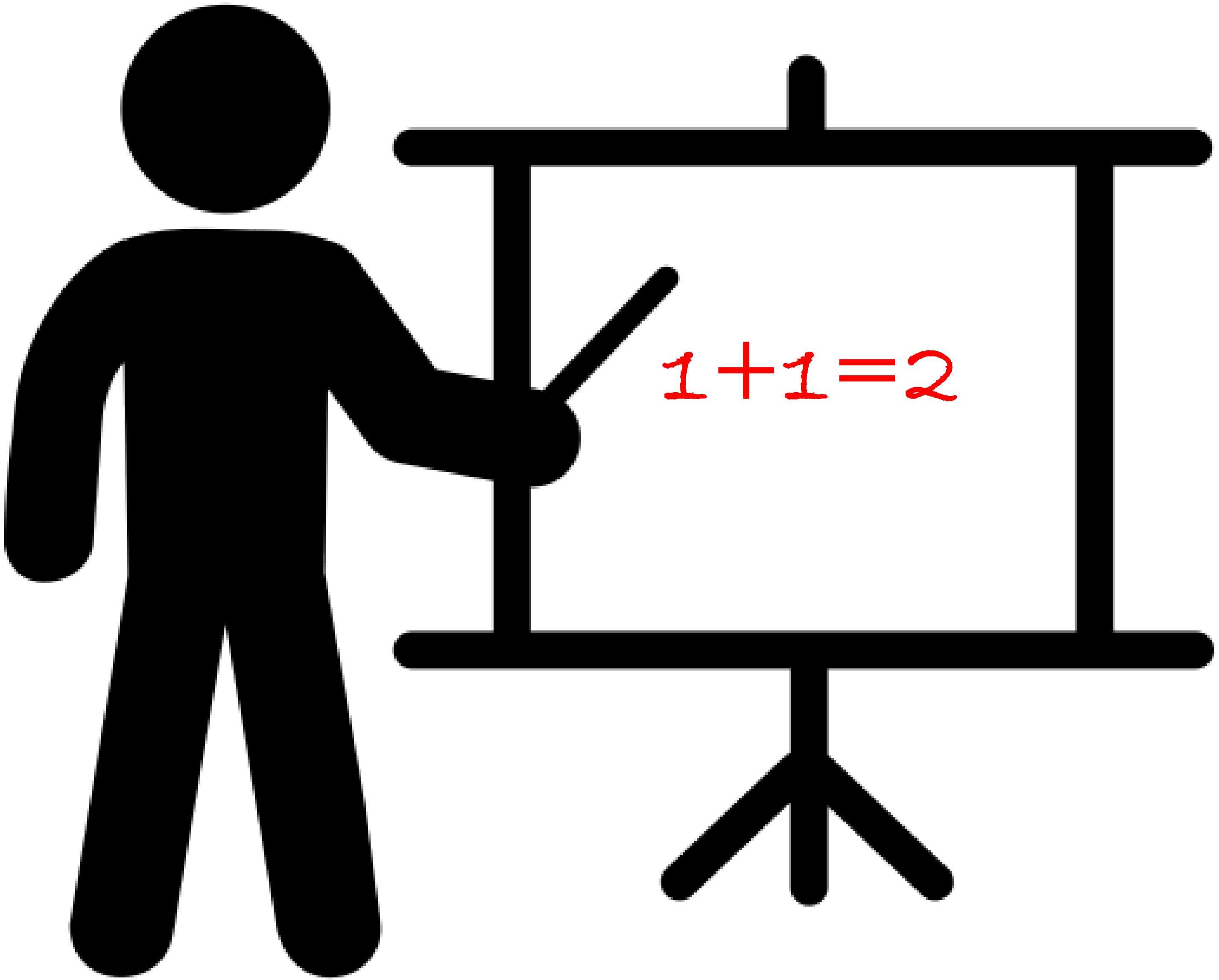
- **Hand-craft algorithms** to make rational/optimal or at least good decisions.
  Examples: Search strategies, heuristics.

Machine Learning

- **Learning**: Improve performance after making observations about the world. That is, learn what works and what doesn't.
- **How to build a model from data/experience?**
  - **Supervised Learning**: Learn a function (model) to map input to output from a training set. Examples:
    - Use a naïve Bayesian classifier to distinguish between spam/no spam
    - Learn a playout policy to simulate games (current board -> good move)
  - **Unsupervised Learning**: Organize data (e.g., clustering, embedding)
  - **Reinforcement Learning**: Learn from rewards/punishment (e.g., winning a game) obtained via interaction with the environment over time.

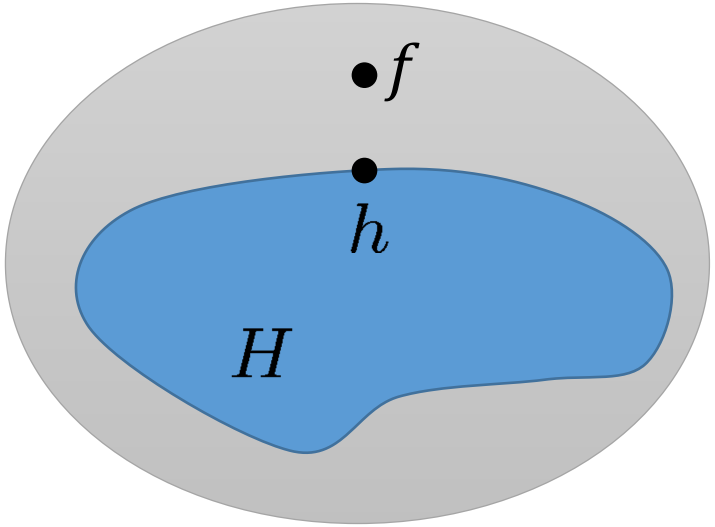
- **Learning vs. hard coding the agent function**
  - Designer cannot anticipate all possible future situations.
  - Designer may have examples but does not know how to program a solution.

Supervised Learning



Supervised Learning

- Examples
  - Input-output pairs: $\mathrm{E} = (x_1, y_1), \dots, (x_i, y_i), \dots, (x_N, y_N)$, where x is a vectors called the feature vector.
  - We assume that the examples are produced iid (with noise and errors) from a target function $y = f(x)$.

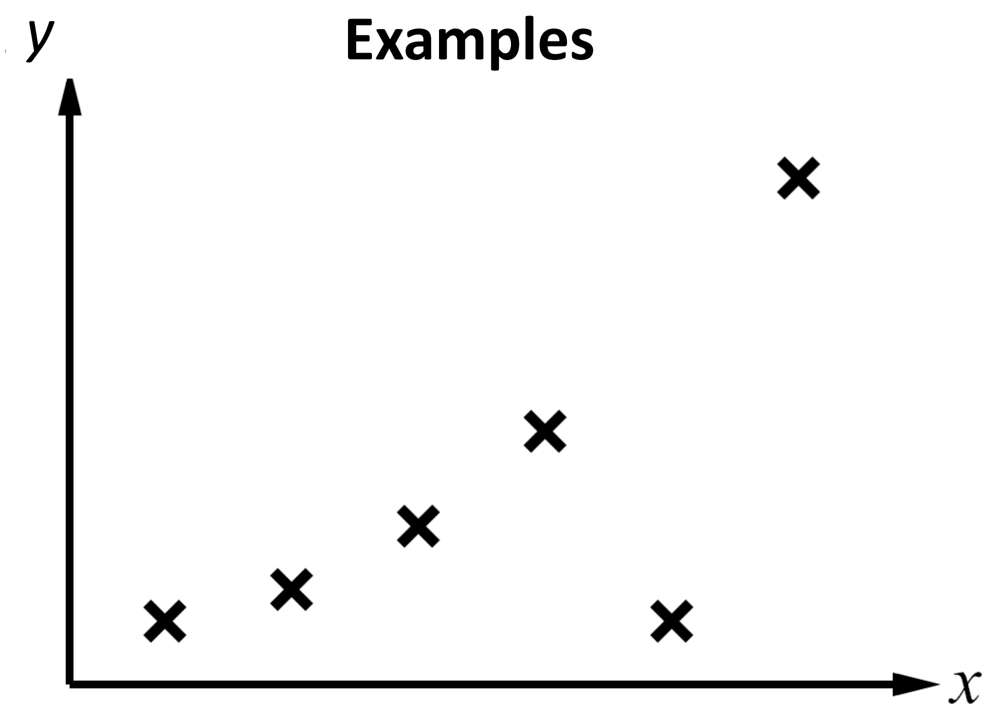


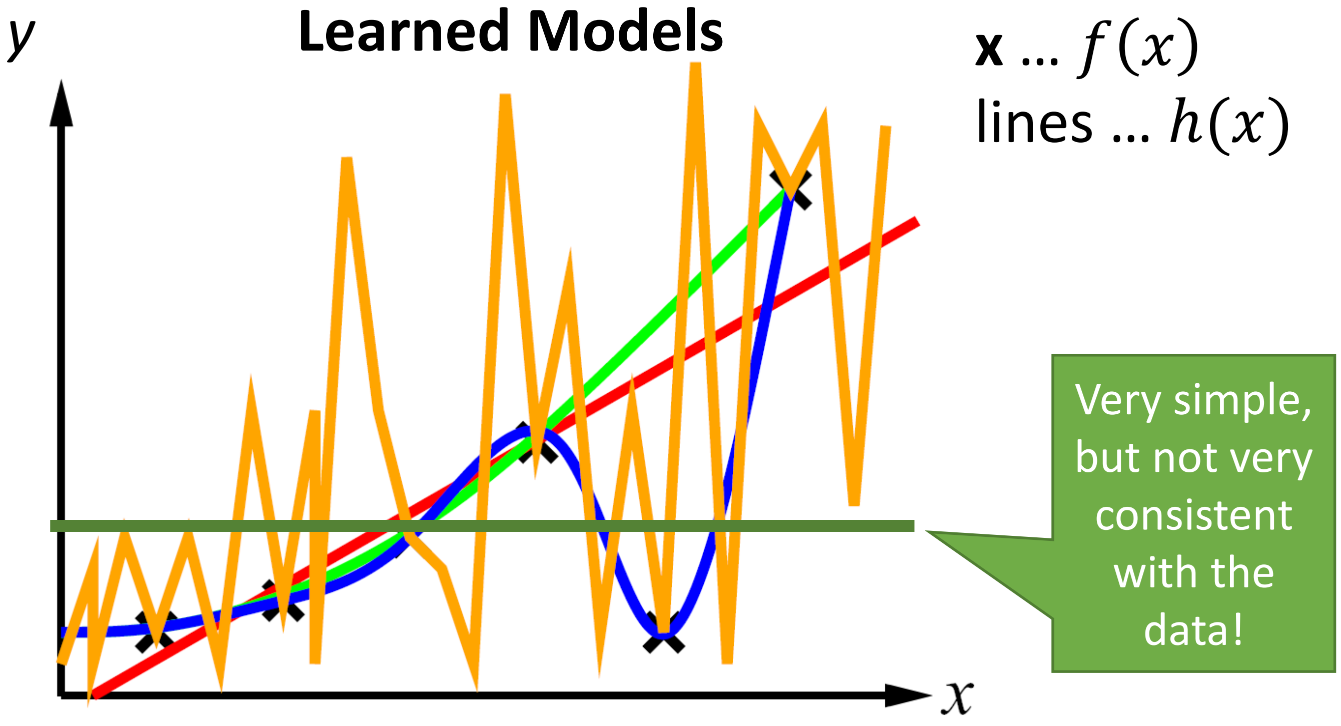
- Learning problem
  - Given a hypothesis space H of possible models.
  - Find a hypothesis $h \in H$ such that $\hat{y}_i = h(x_i) \approx y_i \; \forall i$
  - That is, we want to approximate f by h using E.

- Includes
  - Classification (outputs = class labels). E.g. x is an email and $f(x)$ is spam / ham.
  - Regression (outputs = real numbers). E.g. x is a house and $f(x)$ is its selling price.

Consistency vs. Simplicity

Example: Univariate curve fitting (regression, function approximation)





x … $f(x)$
lines … $h(x)$

Very simple, but not very consistent with the data!

- **Consistency:** $h(x_i) \approx \ y_i$
- **Simplicity:** small number of parameters often specified as the model parameter vector $\boldsymbol{\theta}$

Measuring Consistency using Loss

Goal of learning: Find a hypothesis that makes good predictions that are consistent with the examples $\mathrm{E} = (x_1, y_1), \ldots, (x_i, y_i), \ldots, (x_N, y_N)$.

That is, $\hat{y} = h(x) \approx y.$

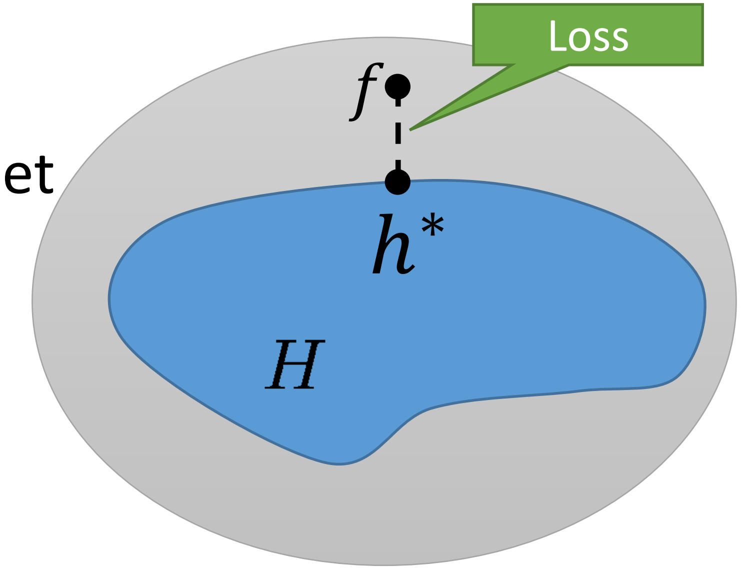
- **Measure mistakes:** Loss function $L(y, \hat{y})$
  - Absolute-value loss $L_1(y, \hat{y}) = |y - \hat{y}|$
  - Squared-error loss $L_2(y, \hat{y}) = (y - \hat{y})^2$
  - 0/1 loss $L_{0/1}(y, \hat{y}) = 0 \text{ if } y = \hat{y}, \text{else } 1$
  - Log loss, cross-entropy loss and many others…

For Regression

For Classification

- **Empirical loss:** average loss over the N examples in the dataset

$$EmpLoss_{L,E}(h) = \frac{1}{|E|} \sum_{(x,y) \in E} L(y, h(x))$$



Learning Consistent h by Minimizing the Loss

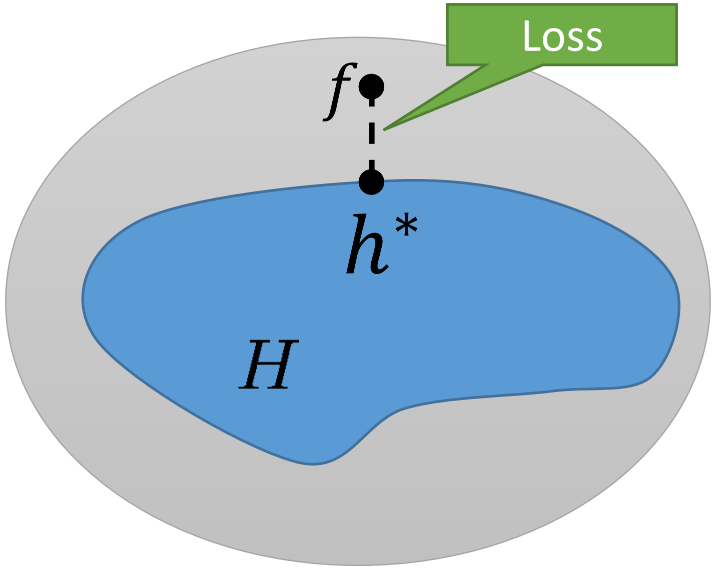
- Empirical loss

$$EmpLoss_{L,E}(h) = \frac{1}{|E|} \sum_{(x,y)\in E} L(y, h(x))$$

- Learning the best hypothesis (approximation)

$$h^* = \operatorname*{argmin}_{h\in H} EmpLoss_{L,E}(h)$$

- Reasons for $h^* \neq f$
  - a) Realizability: $f \notin H$
  - b) f is nondeterministic or examples are noisy.
  - c) Computationally intractable to search all H.



The Bayes Classifier

For 0/1 loss, the empirical loss is minimized by the model that predicts for each x the most likely class y using MAP (Maximum a posteriori) estimates. This is called the Bayes classifier.

$$\mathrm{h}^*(\mathrm{x}) = \underset{y}{\operatorname{argmax}} P(Y = y \mid X = x) = \underset{y}{\operatorname{argmax}} \frac{P(x \mid y)\, P(y)}{P(x)} = \underset{y}{\operatorname{argmax}} P(x \mid y)\, P(y)$$

Optimality: The **Bayes classifier is optimal for 0/1 loss.** It is the most consistent classifier possible with the lowest possible error called the **Bayes error rate**. No better classifier is possible!

Issue: The classifier requires to learn $P(x \mid y)\, P(y) = P(x, y)$ from the examples.

- It **needs the complete joint probability** which requires in the general case a probability table with one entry for each possible value for the feature vector x.
- This is impractical (unless a simple Bayes network exists) and most classifiers try to approximate the Bayes classifier using a simple model with fewer parameters.

Simplicity

Ease of use

- Simpler hypotheses have fewer parameters to store.
- Simpler hypotheses are easier to estimate.

Generalization: How well does the hypothesis perform on new data?

- We do not want the model to be too specific to the training examples (an issue called **overfitting**).
- Simpler models typically generalize better to new examples.

How to achieve simplicity?

a) Restrict H to simpler models (e.g., assumptions like independence, linear models). This is called **model bias.**

b) Feature selection: use fewer variables from the feature vector x

c) Regularization: penalize model for its complexity (e.g., number of parameters)

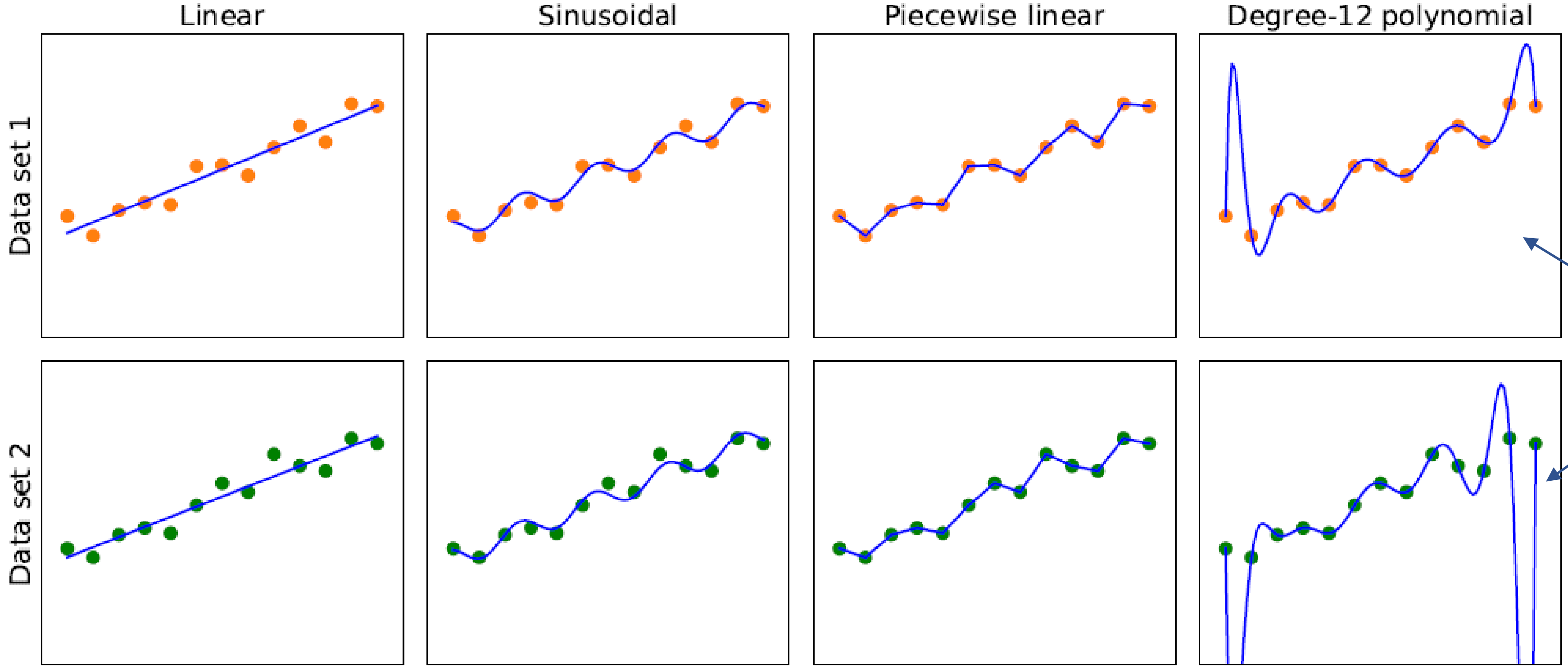
$$h^* = \underset{h \in H}{\operatorname{argmin}} \left[EmpLoss_{L,E}(h) + \underbrace{\lambda \, Complexity(h)}_{\text{Penalty term}} \right]$$

Model Selection: Bias vs. Variance

Overfitting

Simpler

More consistent



Points: Two samples from the same function f to show variance.

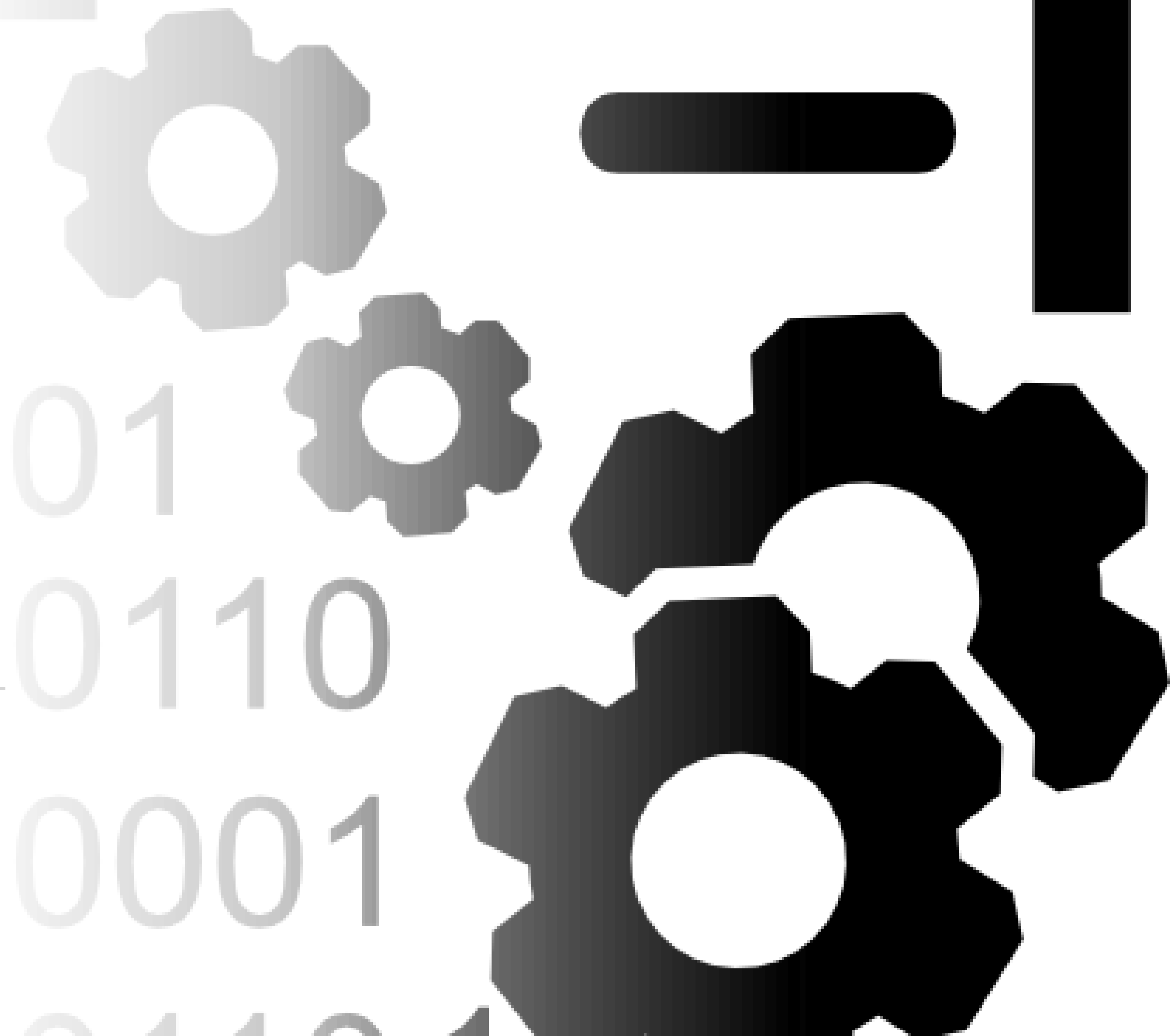
Lines: the learned function h.

High **Bias**: restrictions by the model class Low

Low **Variance**: difference in the model due to slightly different data. high

This is a tradeoff

Data

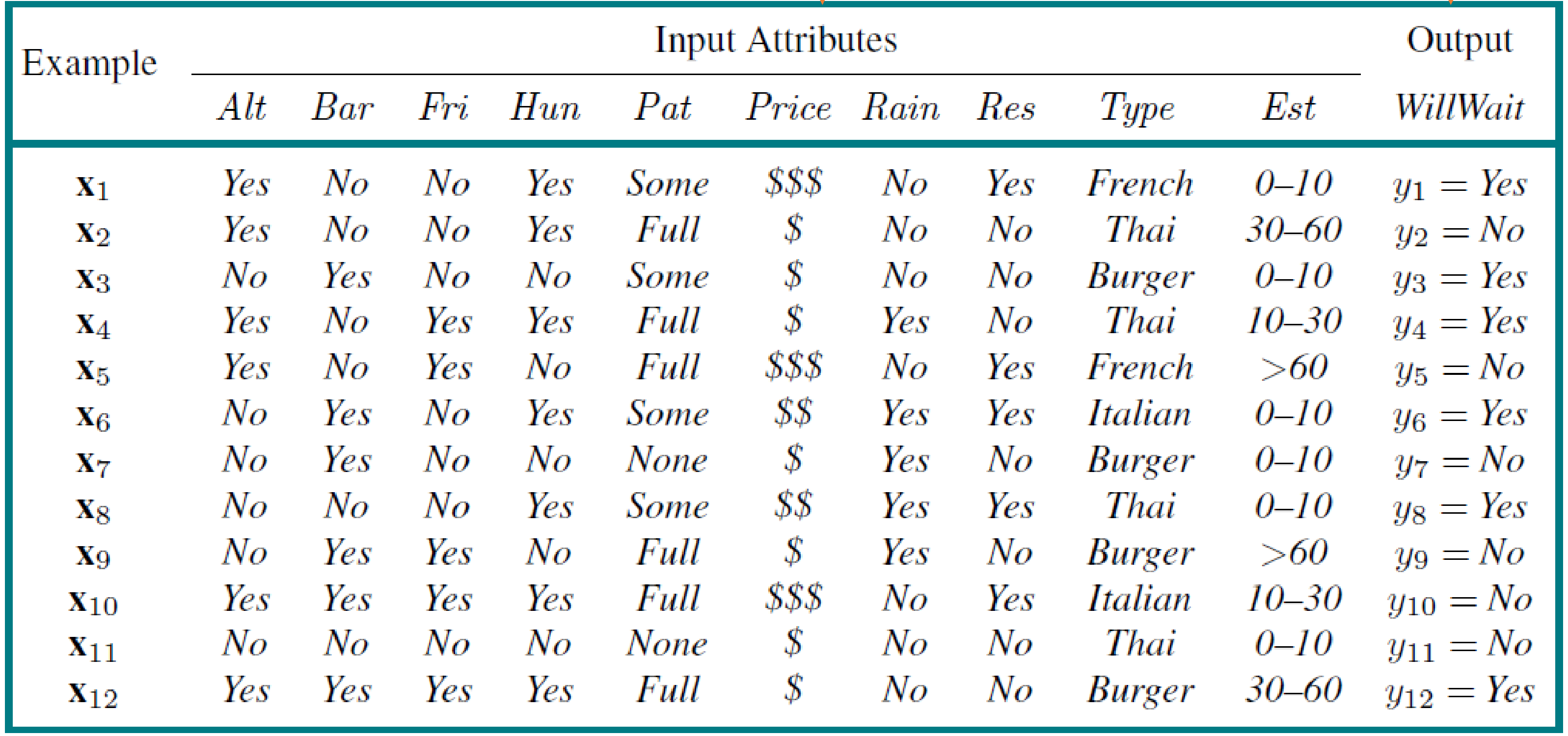


The Dataset

Features
Variables
Attributes x

Class
Label y

Examples
Instances
Observations



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Alternative

Hungry

Patrons

Reservation

Wait time

Find a hypothesis (called “model”) to predict the class given the features.

Feature Engineering

- Add information sources as new variables to the model.
- Add derived features that help the classifier (e.g., x^2).
- Embedding: E.g., convert words to vectors where vector similarity between vectors reflects semantic similarity.

- Example for Spam detection: In addition to words
  - Have you emailed the sender before?
  - Have 1000+ other people just gotten the same email?
  - Is the header information consistent?
  - Is the email in ALL CAPS?
  - Do inline URLs point where they say they point?
  - Does the email address you by (your) name?

- **Feature Selection**: Which features should be used in the model is a model selection problem (choose between models with different features).

Training and Testing

Model Evaluation (Testing)

The model was trained on the training examples E. We want to test how well the model will perform on new examples T (i.e., how well it **generalizes to new data**).

- **Testing loss**: Calculate the empirical loss for predictions on a testing data set T that is different from the data used for training.

$$EmpLoss_{L,T}(h) = \frac{1}{|T|} \sum_{(x,y) \in T} L(y, h(x))$$

- For classification we often use the **accuracy** measure, the proportion of correctly classified test examples.

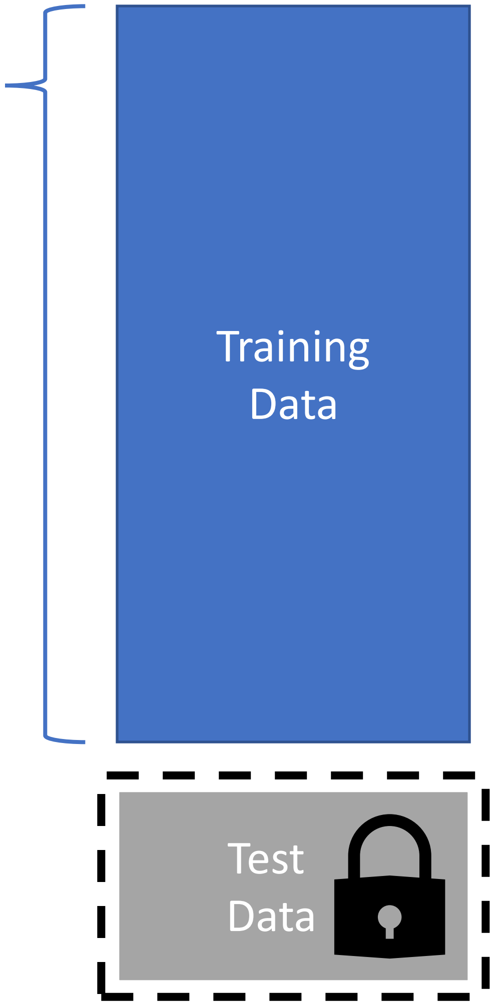
$$accuracy(h, T) = \frac{1}{|T|} \sum_{(x,y) \in T} [h(x) = y] = 1 - \ EmpLoss_{L_{0/1},T}(h)$$

$[c]$ is an indicator function returning 1 if $c \ = \ True$ and otherwise 0

Training a Model

- Models are “trained” (learned) on **the training data.** This involved estimating the model parameters (the model): E.g., probabilities, weights, factors.
- **Hyperparameters**: Many learning algorithms have choices for learning rate, regularization λ, maximal decision tree depth, selected features,... The algorithm tries to optimizes the model parameters given user-specified hyperparameters.

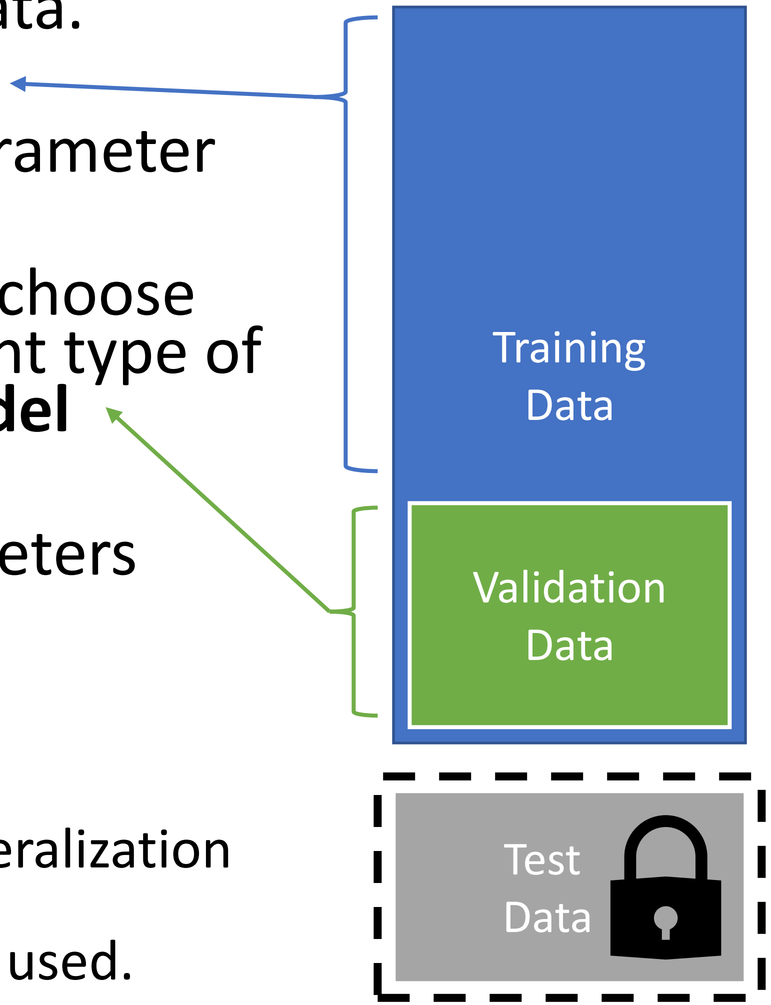
- We need to tune the hyperparameters!


Training Data

Test Data

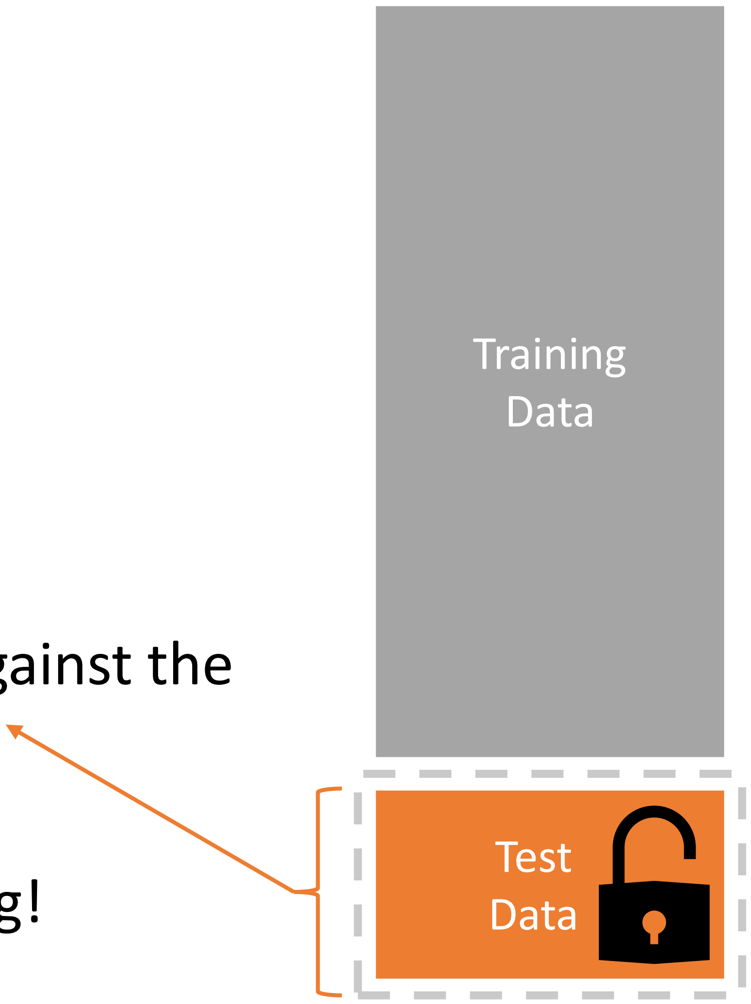
Hyperparameter Tuning/Model Selection

1. Hold a validation data set back from the training data.
2. **Learn models** using the training set with different hyperparameters. Often a grid of possible hyperparameter combinations or some greedy search is used.
3. **Evaluate the models** using the validation data and choose the model with the best accuracy. Selecting the right type of model, hyperparameters and features is called **model selection**.
4. Learn the final model with the chosen hyperparameters using all training (including validation data).



- Notes:
  - The validation set was not used for training, so we get generalization accuracy for the different hyperparameter settings.
  - If no model selection is necessary, then no validation set is used.

Testing a Model



- After the model is selected, the final model is evaluated against the test set to **estimate the final model accuracy**.
- Very important: never “peek” at the test set during training!

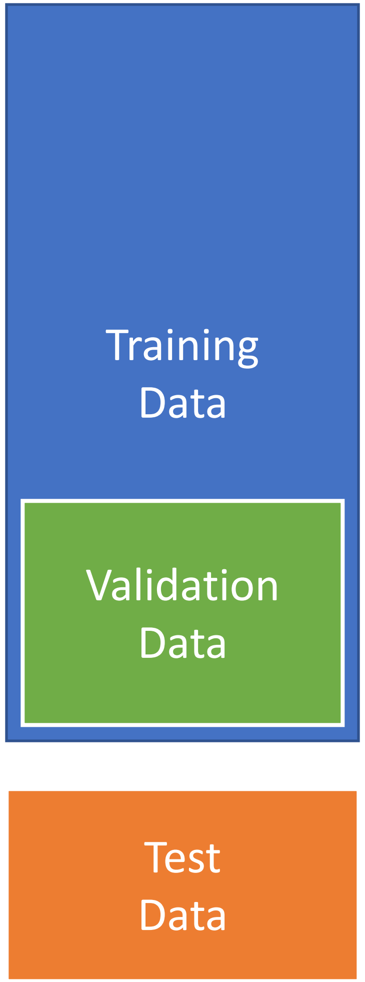
How to Split the Dataset

- **Random splits:** Split the data randomly in, e.g., 60% training, 20% validation, and 20% testing.

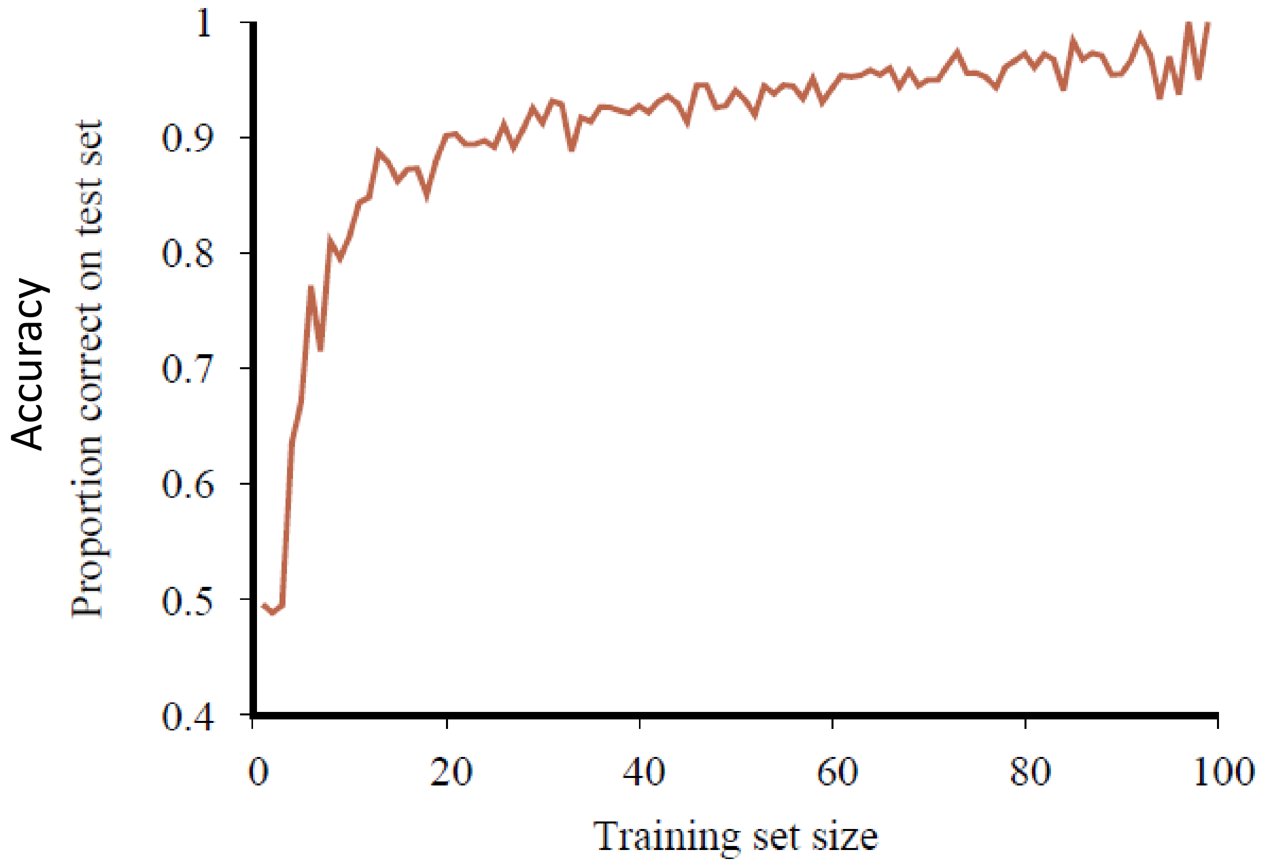
- **Stratified splits:** Like random splits, but balance classes and other properties of the examples.

- **k-fold cross validation:** Use training & validation data better
  - Split the training & validation data randomly into k folds.
  - For k rounds hold 1 fold back for testing and use the remaining $k - 1$ folds for training.
  - Use the average error/accuracy as a better estimate.
  - Some algorithms/tools do this internally.

- **LOOCV** (leave-one-out cross validation): $k = n$ used if very little data is available.



Learning Curve:
The Effect the Training Data Size



Accuracy of a classifier when the amount of available training data increases.

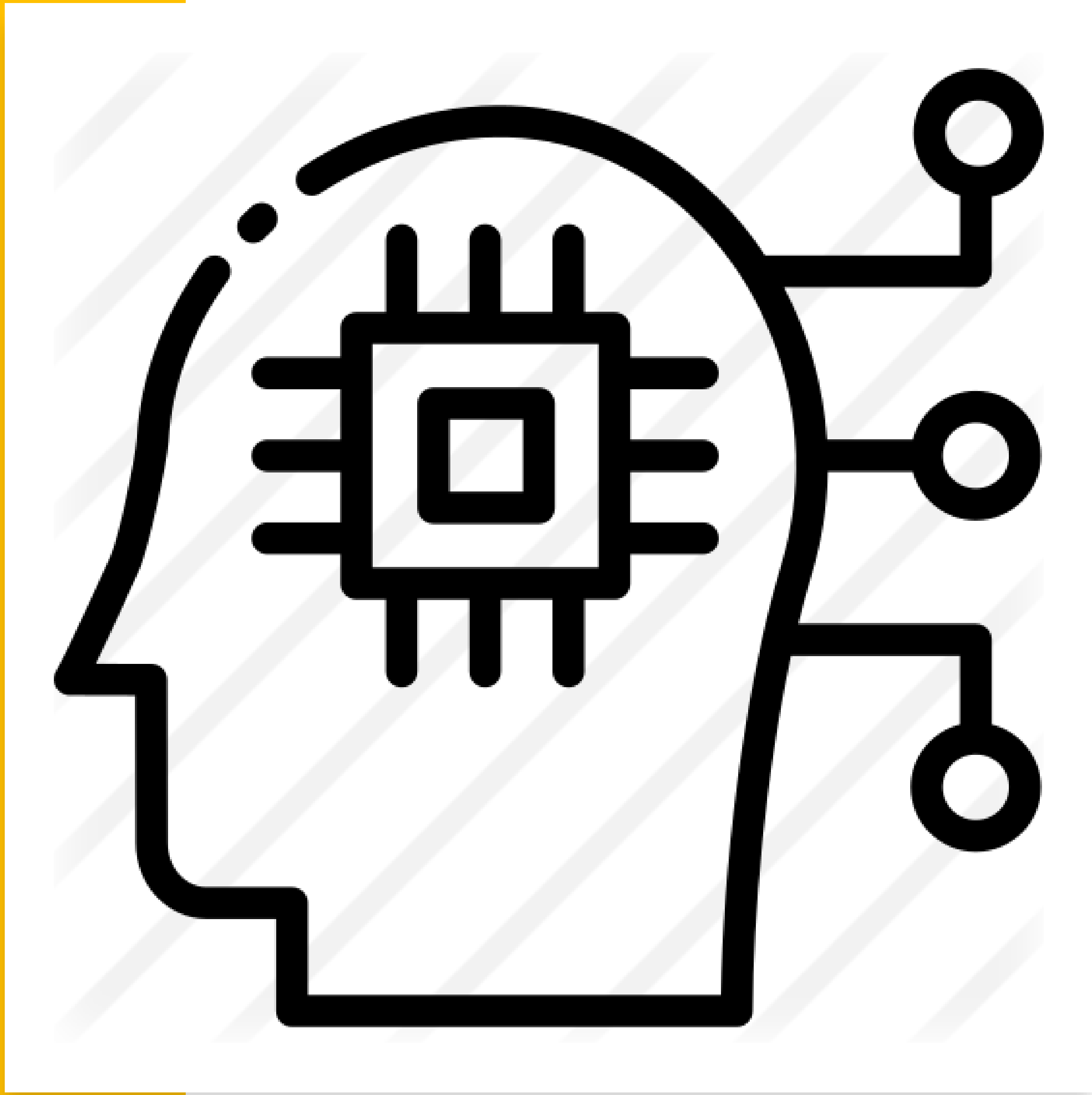
More data is better!

Comparing to a Baselines

- First step: get a **baseline**
  - Baselines are very simple straw man model.
  - Helps to determine how hard the task is.
  - Helps to find out what a good accuracy is.

- **Weak baseline**: The most frequent label classifier
  - Gives all test instances whatever label was most common in the training set.
    - Example: For spam filtering, give every message the label “ham.”
  - Accuracy might be very high if the problem is skewed (called class imbalance).
    - Example: If calling everything “ham” gets already 66% right, so a classifier that gets 70% isn’t very good…

- **Strong baseline**: For research, we typically compare to previous published state-of-the-art as a baseline.



Types of Models

Regression: Predict a number

Classification: Predict a label

Regression: Linear Regression

Model: $h_{\boldsymbol{w}}(\boldsymbol{x}_j) = w_o + w_1 x_{j,1} + \cdots + w_n x_{j,n} = \sum_i w_i x_{j,i} = \boldsymbol{w}^T \boldsymbol{x}_j$

Empirical Loss: $L(\boldsymbol{w}) = \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2$

Squared error loss over the whole data matrix $\boldsymbol{X}$

Gradient: $\nabla L(\boldsymbol{w}) = 2X^T(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$

The gradient is a vector of partial derivatives

$$\nabla L(\boldsymbol{w}) = \left[\frac{\partial L}{\partial w_1}(\boldsymbol{w}), \frac{\partial L}{\partial w_2}(\boldsymbol{w}), \dots, \frac{\partial L}{\partial w_n}(\boldsymbol{w})\right]^T$$

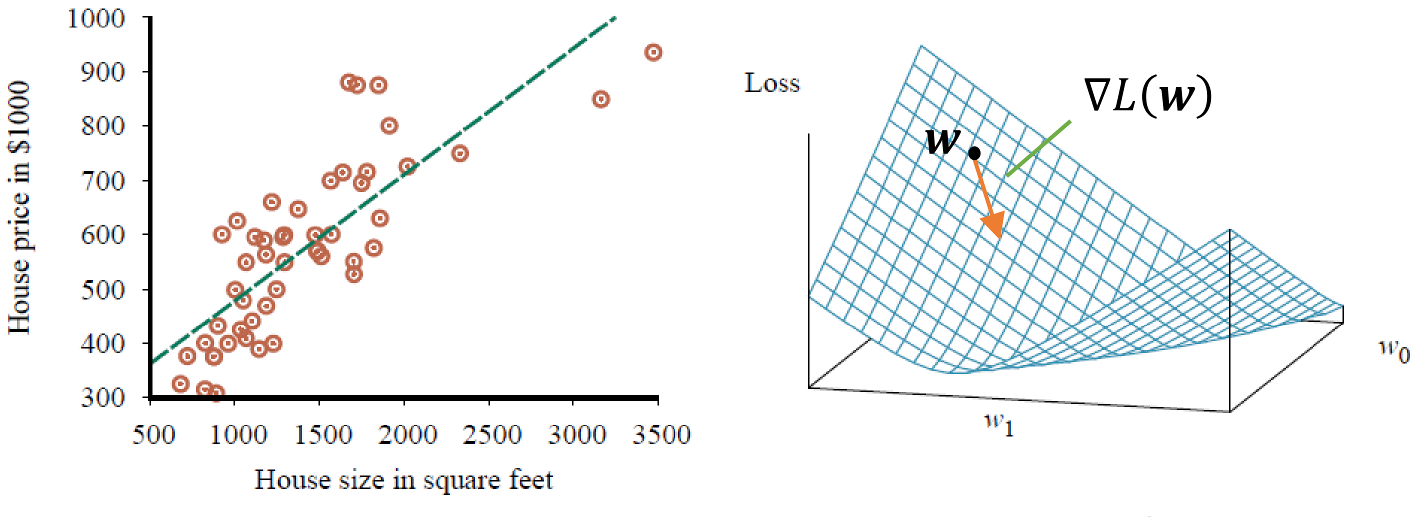
Find: $\nabla L(\boldsymbol{w}) = 0$

Gradient descend:

$$\boldsymbol{w} = \boldsymbol{w} - \alpha \nabla L(\boldsymbol{w})$$

Analytical solution:

$$\boldsymbol{w}^* = \underbrace{(\boldsymbol{X}^T\boldsymbol{X})^{-1}}_{\text{Pseudo inverse}}\boldsymbol{X}^T\boldsymbol{y}$$



(a)

(b)

Naïve Bayes Classifier

- Approximates a Bayes classifier with the **naïve independence assumption** that all n features are conditional independent given the class.

$$h(x) = \operatorname*{argmax}_{y} \; P(y) \prod_{i=1}^{n} P(x_i \mid y)$$

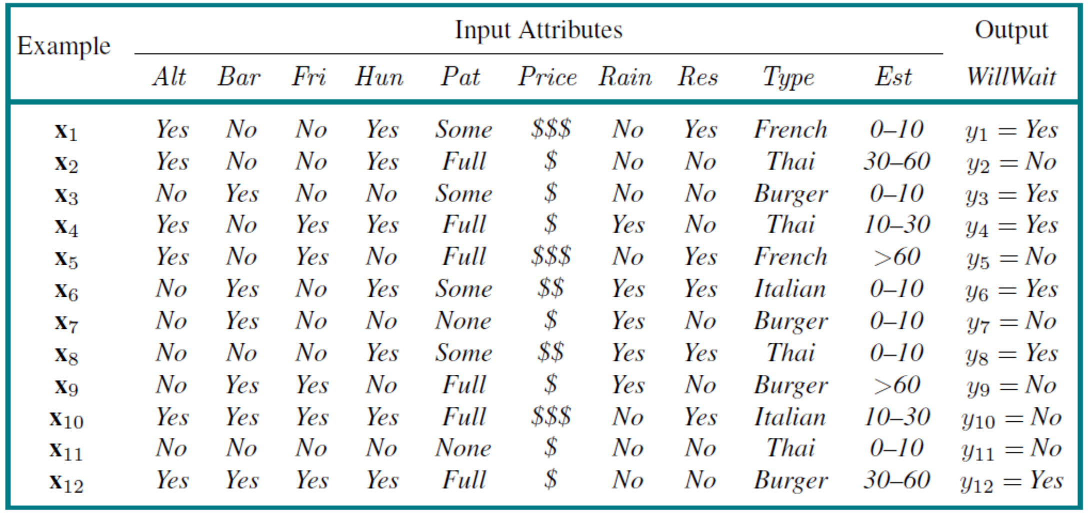
The $P(y)$s and the $P(x_i \mid y)$s are estimated from the data by counting.

- Gaussian Naïve Bayes Classifiers extend the approach to continuous features by assuming:

$$P(x_i \mid y) \sim N(\mu_y, \sigma_y)$$

The parameters for the normal distribution $N(\mu_y, \sigma_y)$ are estimated from data.

Decision Trees



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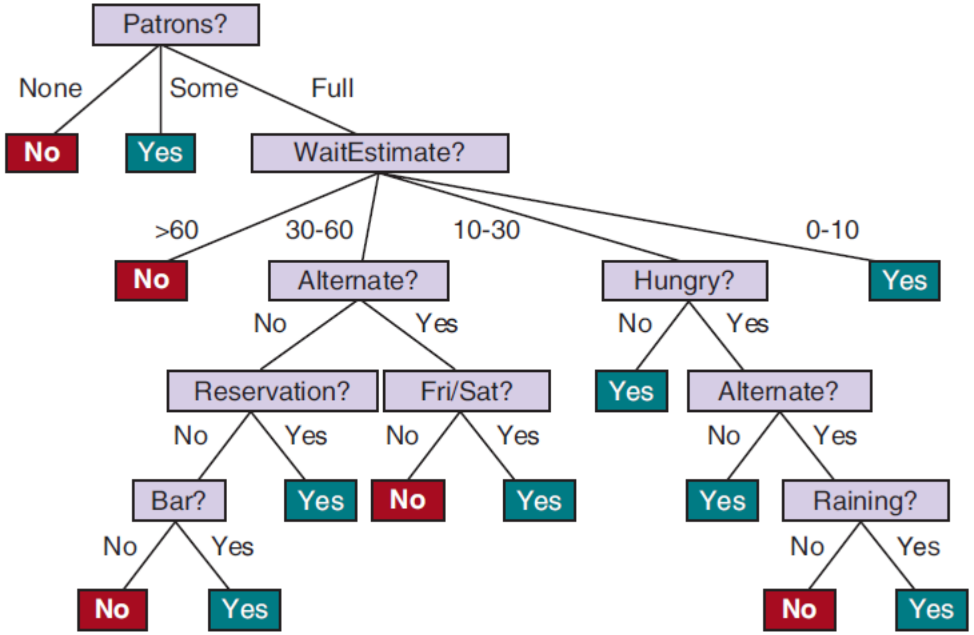
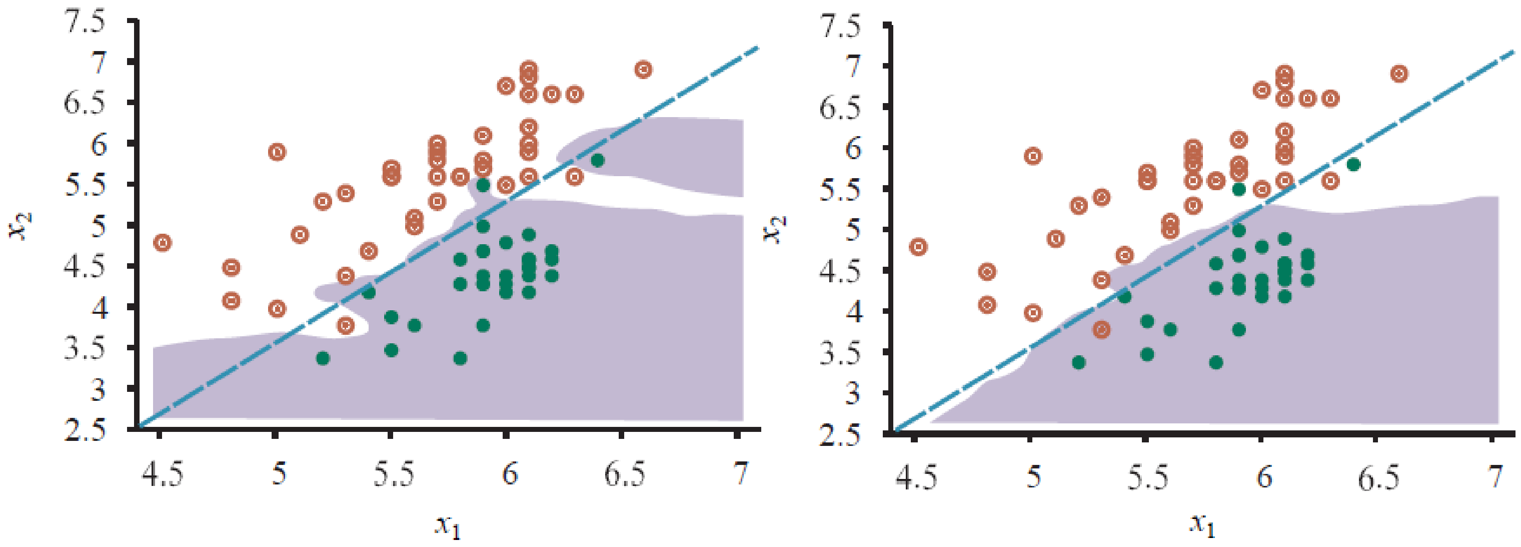


- A **sequence of decisions** represented as a tree.
- Many implementations that differ by
  - How to select features to split?
  - When to stop splitting?
  - Is the tree pruned?
- Approximates a Bayesian classifier by

$$h(x) = \underset{y}{\operatorname{argmax}}\; P(Y = y \mid \text{leafNodeMatching}(x))$$

K-Nearest Neighbors Classifier

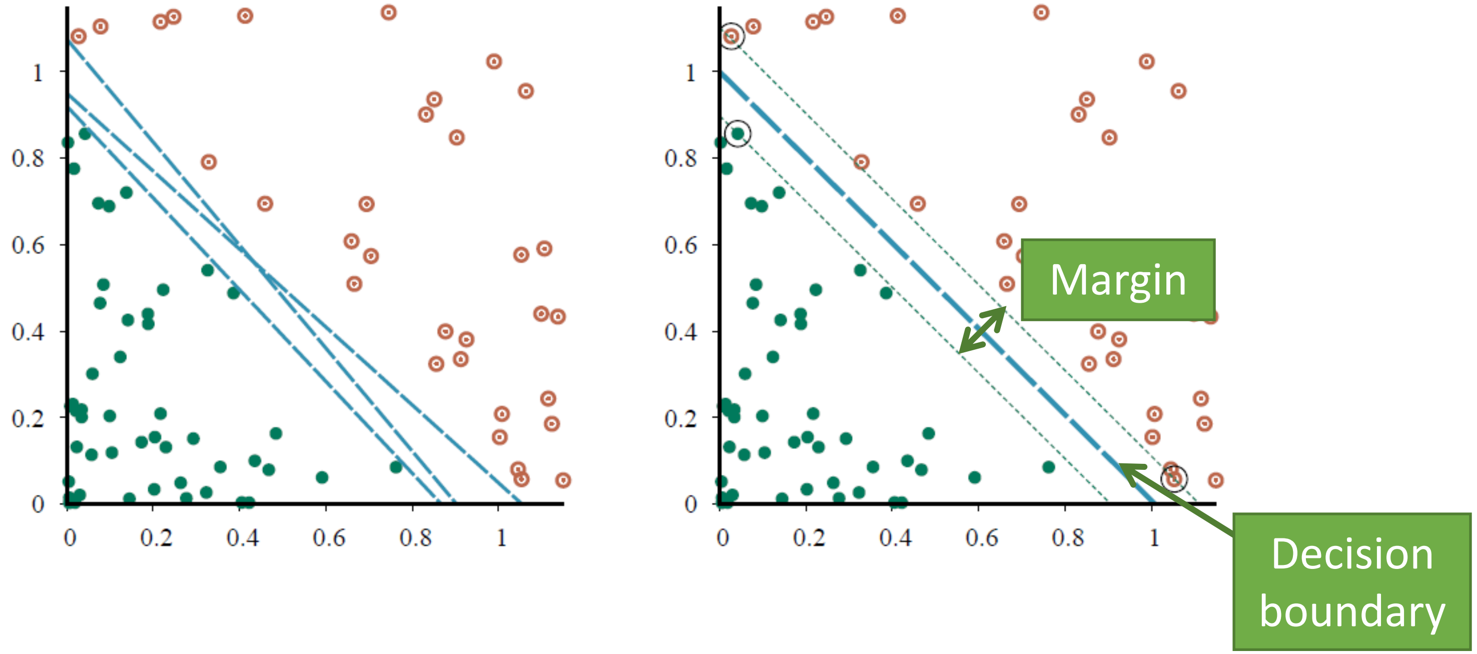


$(k = 1)$ $(k = 5)$

- Class is predicted by looking at the majority in the set of the k nearest **neighbors**. k is a hyperparameter. Larger k smooth the decision boundary.
- Neighbors are found using a distance measure (e.g., Euclidean distance between points).
- Approximates a Bayesian classifier by

$$h(x) = \underset{y}{\operatorname{argmax}}\, P(Y = y \mid \text{neighborhood}(x))$$

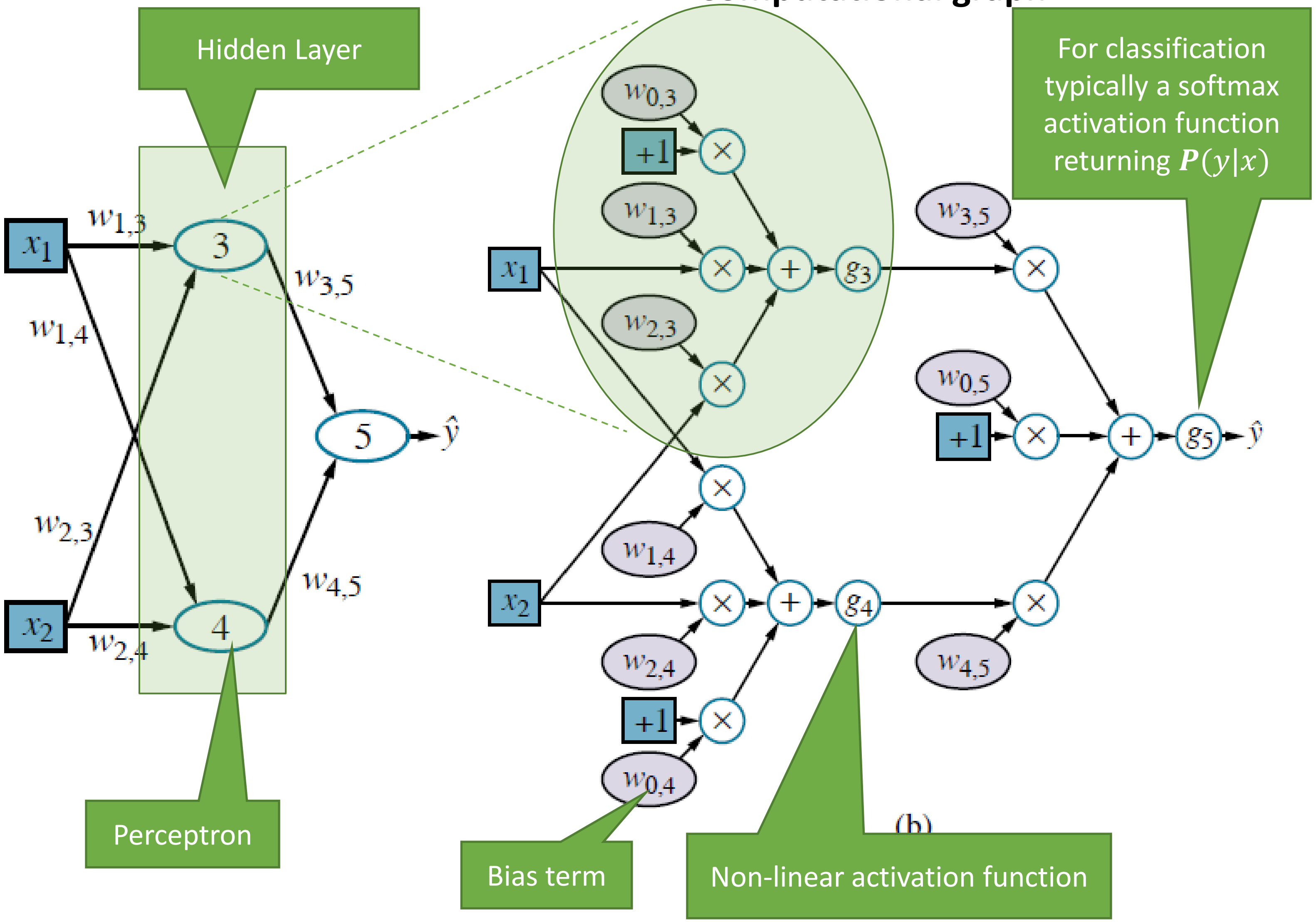
Support Vector Machine (SVM)



- Linear classifier that finds **the maximum margin separator** using only the points that are "support vectors" and quadratic optimization.
- The kernel trick can be used to learn non-linear decision boundaries.

Artificial Neural Networks/Deep Learning

Computational graph



Hidden Layer

Perceptron

Bias term

Non-linear activation function

For classification typically a softmax activation function returning $\boldsymbol{P}(y|x)$

- Represent $\hat{y} = h(x)$ as a network of weighted sums with non-linear **activation functions** g (e.g., logistic, ReLU).
- Learn weights **w** from examples using **backpropagation** of prediction errors $\mathrm{L}(\hat{y}, y)$ (gradient descend).
- ANNs are **universal approximators**. Large networks can approximate any function (no bias). **Regularization** is typically used to avoid overfitting.
- **Deep learning** adds more hidden layers and layer types (e.g., convolution layers) for better learning.

Other Popular Models and Methods

Many other models exist

- **Generalized linear model (GLM):** This important model family includes **linear regression** and the classification method **logistic regression.**

Often used methods

- **Regularization:** enforce simplicity by using a penalty for complexity.
- **Kernel trick:** Let a linear classifier learn non-linear decision boundaries (= a linear boundary in a high dimensional space).
- **Ensemble Learning:** Use many models and combine the results (e.g., random forest, boosting).
- **Embedding and Dimensionality Reduction:** Learn how to represent data in a simpler way.

Example Use of ML for Intelligent Agents

Learn Actions

- Directly learn the best action from examples.

$action$Example Use of ML for Intelligent Agents$= h(state)$

- This model can also be used as a **playout policy** for Monte Carlo tree search with data from self-play.

Learn Heuristics

- Learn evaluation functions for states.

$$eval = h(state)$$

- Can learn a **heuristic** for minimax search from examples.

Perception

- **Natural language processing:** Use deep learning / word embeddings / language models to understand concepts, translate between languages, or generate text.
- Speech recognition: Identify the most likely sequence of words.
- Vision: Object recognition in images/videos. Generate images/video.

Example Use of ML for Intelligent Agents

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$$action = h(state)$$

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Perception

- **Natural language processing:** Use deep learning / word embeddings / language models to understand concepts, translate between languages, or generate text.
- Speech recognition: Identify the most likely sequence of words.
- Vision: Object recognition in images/videos. Generate images/video.

Bottom line: Learning a function is often more effective than hard-coding it, but we do not always know how it performs in very rare cases!