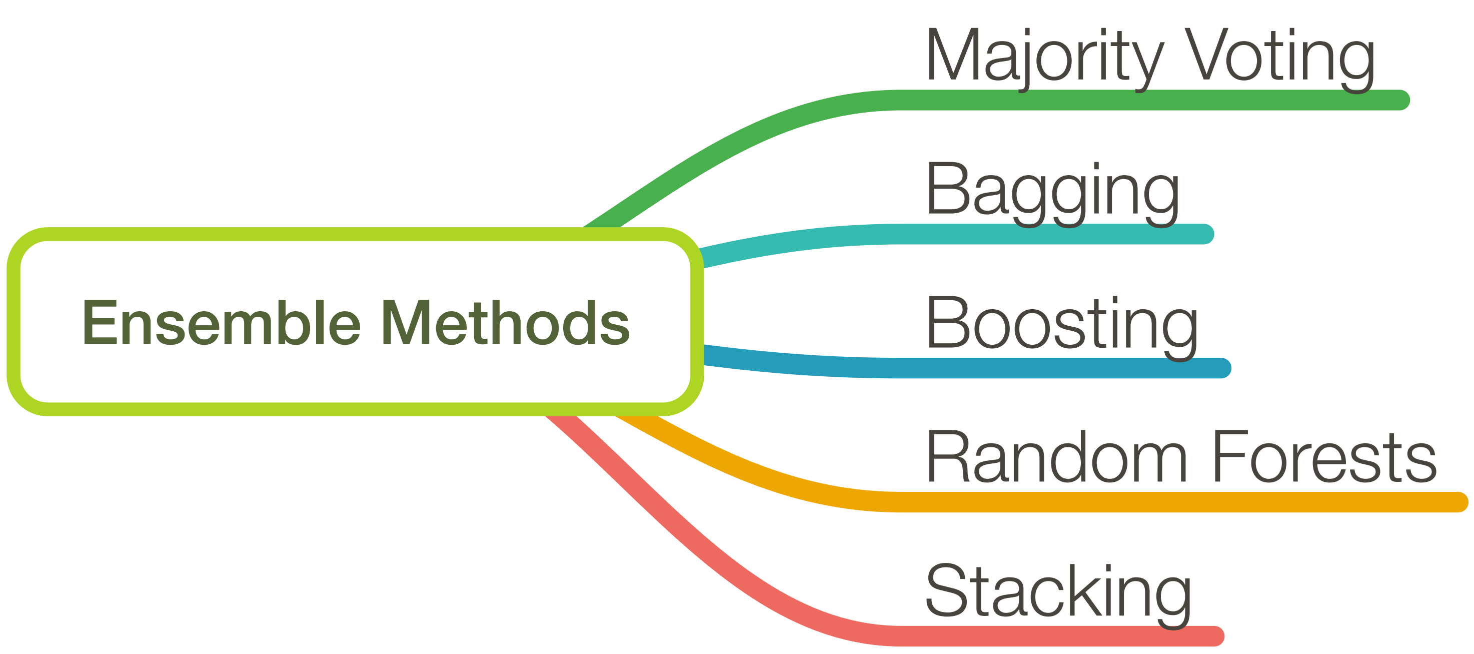
Lecture 07

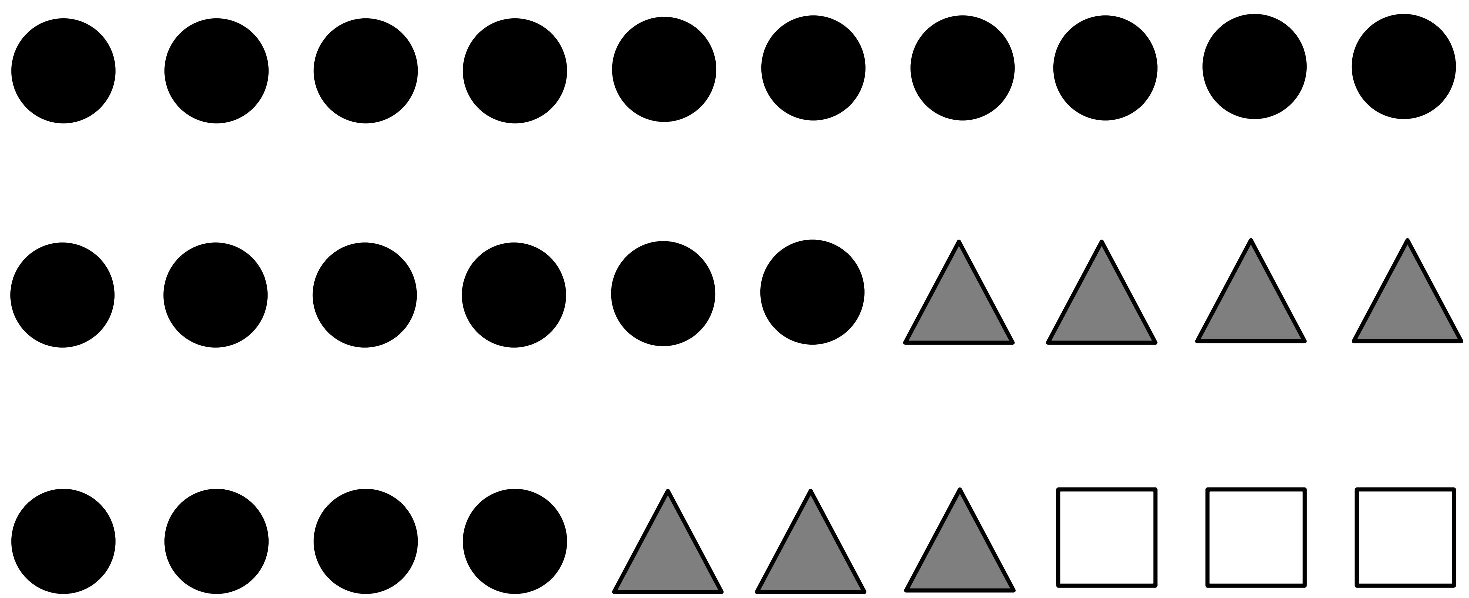
Ensemble Methods

STAT 479: Machine Learning, Fall 2018
Sebastian Raschka
http://stat.wisc.edu/~sraschka/teaching/stat479-fs2018/

Overview


Ensemble Methods
Majority Voting
Bagging
Boosting
Random Forests
Stacking

Majority Voting

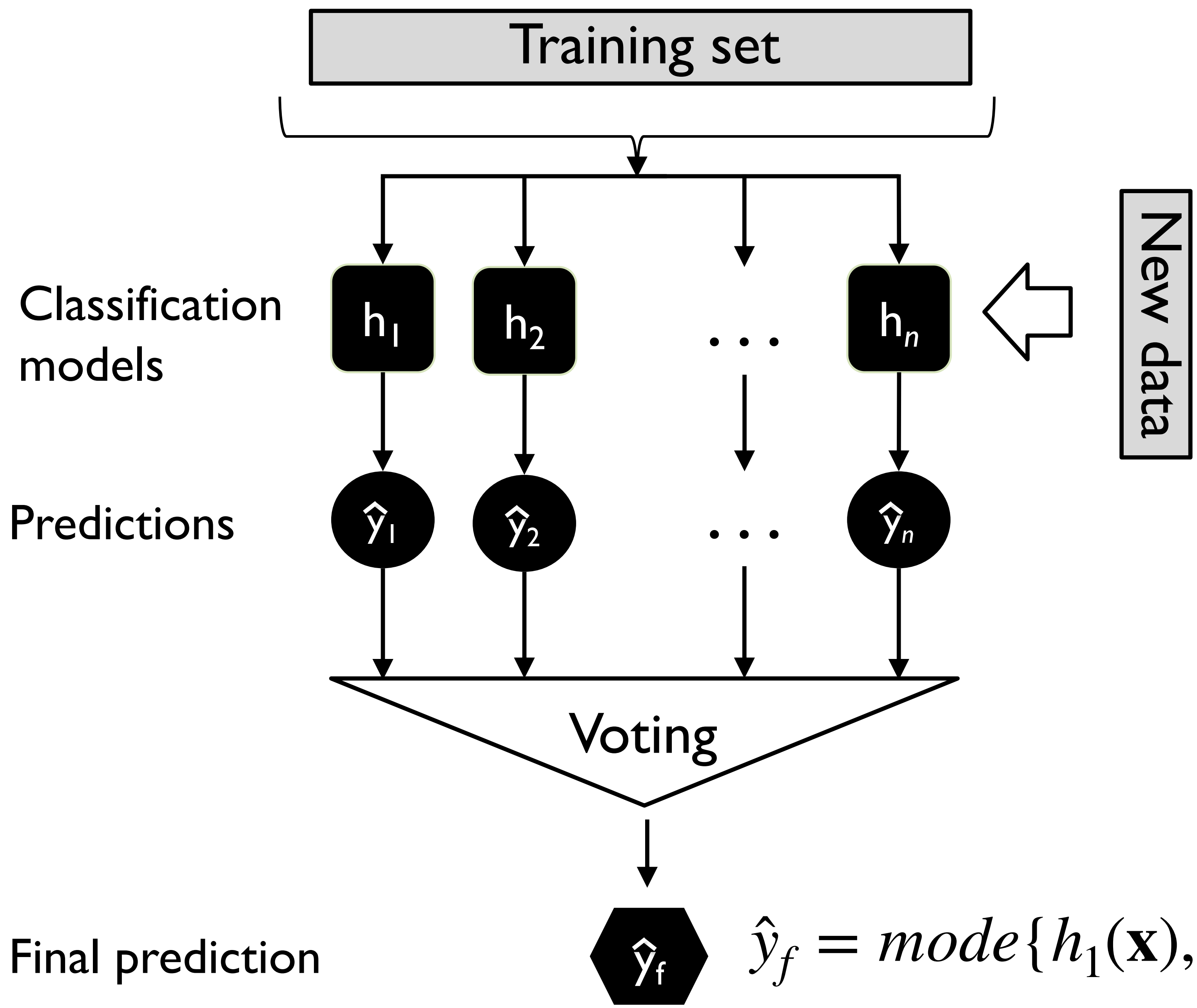


Unanimity

Majority

Plurality

Majority Vote Classifier



$$\hat{y}_f = mode\{h_1(\mathbf{x}), h_2(\mathbf{x}), \dots h_n(\mathbf{x})\}$$

where $h_i(\mathbf{x}) = \hat{y}_i$

Why Majority Vote?

- assume *n* independent classifiers with a base error rate ϵ
- here, independent means that the errors are uncorrelated
- assume a binary classification task
- assume the error rate is better than random guessing (i.e., lower than 0.5 for binary classification)

$$\forall \epsilon_i \in \{\epsilon_1, \epsilon_2, \ldots, \epsilon_n\}, \epsilon_i < 0.5$$

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The probability that we make a wrong prediction via the ensemble if *k* classifiers predict the same class label

$$P(k) = \binom{n}{k} \epsilon^k (1-\epsilon)^{n-k} \qquad\qquad k > \lceil n/2 \rceil$$

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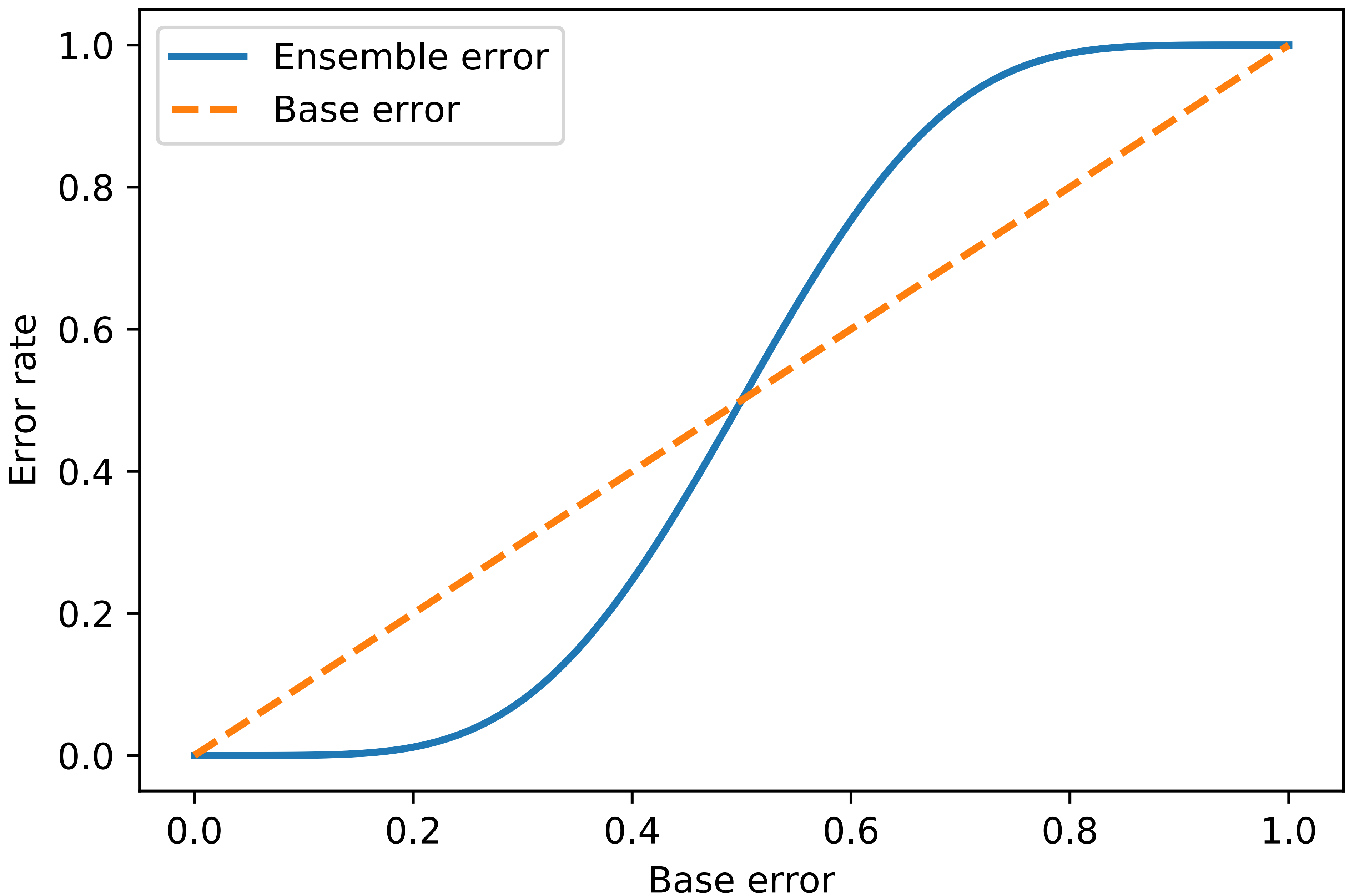
Ensemble error:

$$\epsilon_{ens} = \sum_{k}^{n} \binom{n}{k} \epsilon^k (1 - \epsilon)^{n-k}$$

$$\epsilon_{ens} = \sum_{k=6}^{11} \binom{11}{k} 0.25^k (1 - 0.25)^{11-k} = 0.034$$

$$\epsilon_{ens} = \sum_{k}^{n} \binom{n}{k} \epsilon^k (1-\epsilon)^{n-k}$$



"Soft" Voting

$$\hat{y} = \arg\max_{j} \sum_{i=1}^{n} w_i p_{i,j}$$

$p_{i,j}$: predicted class membership probability of the *i*th classifier for class label *j*

w_j: optional weighting parameter, default $w_i = 1/n, \forall w_i \in \{w_1, \ldots, w_n\}$

"Soft" Voting

Use only for well-calibrated classifiers!

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"Soft" Voting

$$\hat{y} = \arg\max_j \sum_{i=1}^{n} w_i p_{i,j}$$

Binary classification example

$j \in \{0,1\}$ $\quad h_i(i \in \{1,2,3\})$

$$h_1(\mathbf{x}) \rightarrow [0.9, 0.1]$$
$$h_2(\mathbf{x}) \rightarrow [0.8, 0.2]$$
$$h_3(\mathbf{x}) \rightarrow [0.4, 0.6]$$

"Soft" Voting $\hat{y} = \arg\max_j \sum_{i=1}^{n} w_i p_{i,j}$

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$$h_2(\mathbf{x}) \rightarrow [0.8, 0.2]$$

$$h_3(\mathbf{x}) \rightarrow [0.4, 0.6]$$

$$p(j = 0 \,|\, \mathbf{x}) = 0.2 \cdot 0.9 + 0.2 \cdot 0.8 + 0.6 \cdot 0.4 = 0.58$$

$$p(j = 1 \,|\, \mathbf{x}) = 0.2 \cdot 0.1 + 0.2 \cdot 0.2 + 0.6 \cdot 0.6 = 0.42$$

$$\hat{y} = \arg\max_j \left\{ p(j = 0 \,|\, \mathbf{x}), p(j = 1 \,|\, \mathbf{x}) \right\}$$

Bagging

(Bootstrap Aggregating)

Breiman, L. (1996). Bagging predictors. *Machine learning*, *24*(2), 123-140.

Algorithm 1 Bagging

```
Let $n$ be the number of bootstrap samples

for i=1 to $n$ do
    Draw bootstrap sample of size $m$, $\mathcal{D}_i$
    Train base classifier $h_i$ on $\mathcal{D}_i$
$\hat{y} = mode\{h_1(\mathbf{x}), ..., h_n(\mathbf{x})\}$
```

Bootstrap Sampling

Bootstrap Sampling

$$P(\textbf{not chosen}) = \left(1 - \frac{1}{n}\right)^n,$$

$$\frac{1}{e} \approx 0.368, \quad n \to \infty .$$

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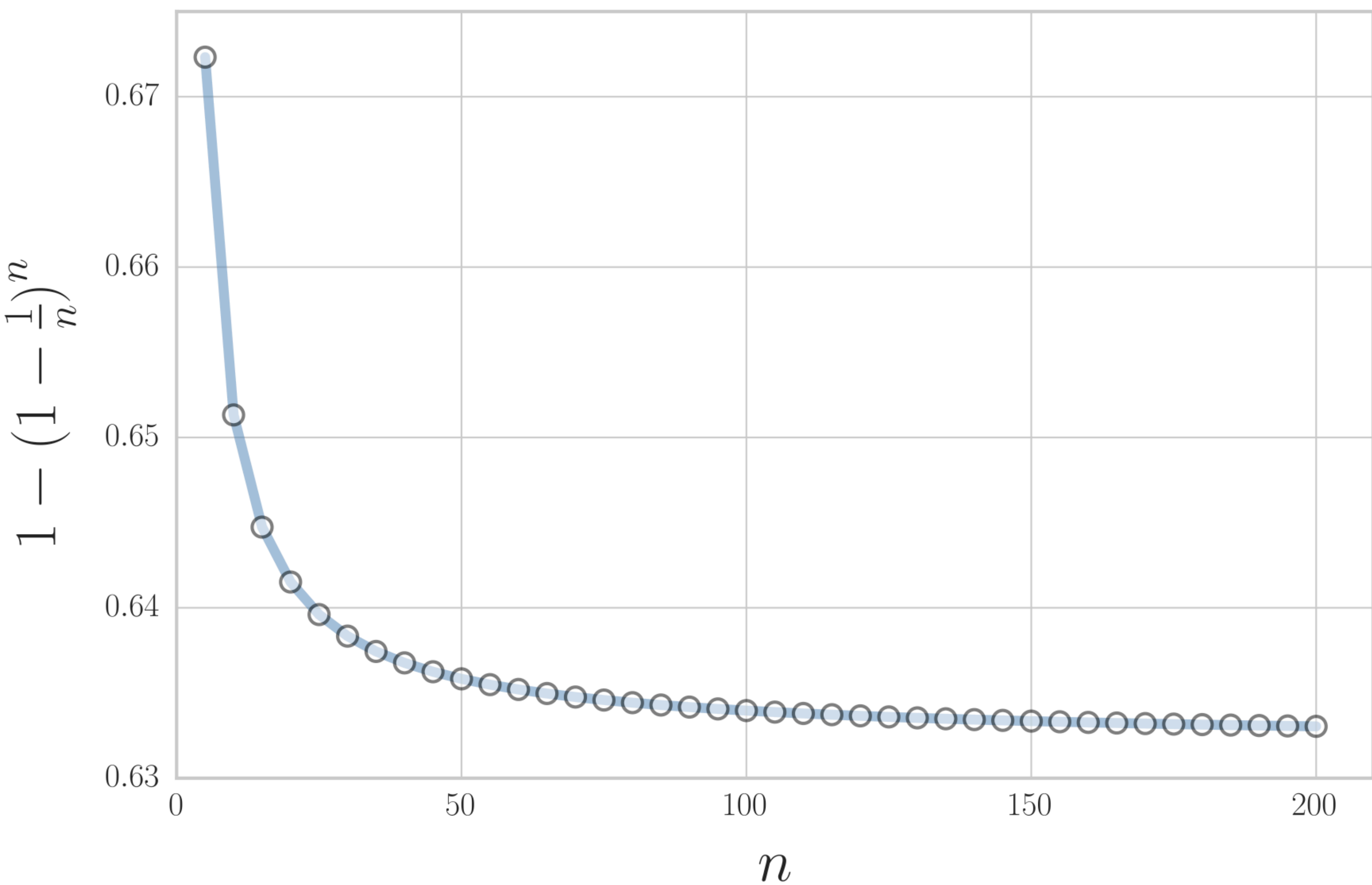
$$P(\textbf{chosen}) = 1 - \left(1 - \frac{1}{n}\right)^n \approx 0.632$$

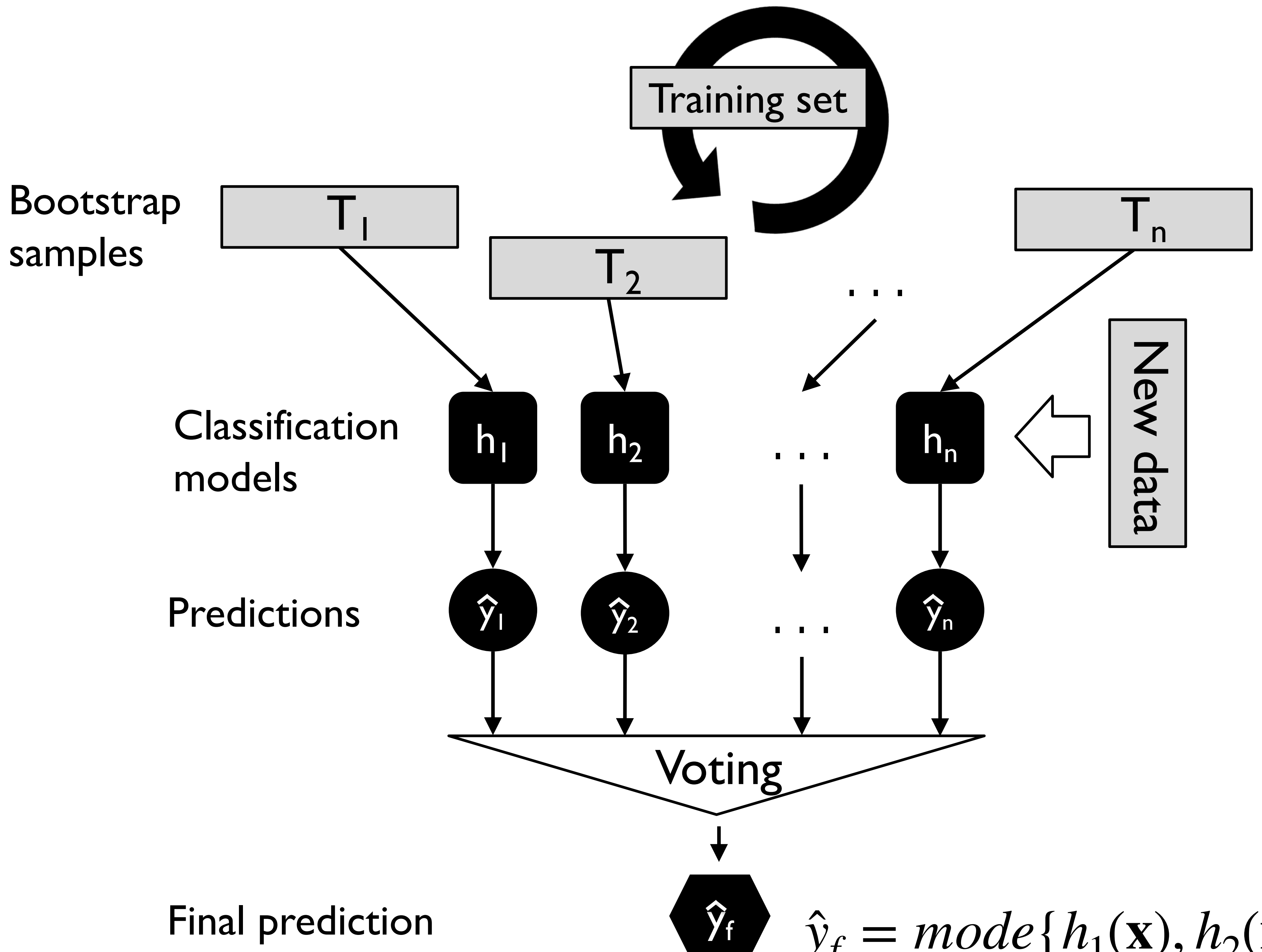


Bootstrap Sampling

Training example indices	Bagging round 1	Bagging round 2	…
1	2	7	…
2	2	3	…
3	1	2	…
4	3	1	…
5	7	1	…
6	2	7	…
7	4	7	…

h_1 h_2 h_n

Bagging Classifier



$$\hat{y}_f = mode\{h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots h_n(\mathbf{x})\}$$

where $h_i(\mathbf{x}) = \hat{y}_i$

Bias-Variance Decomposition

Loss = Bias + Variance + Noise

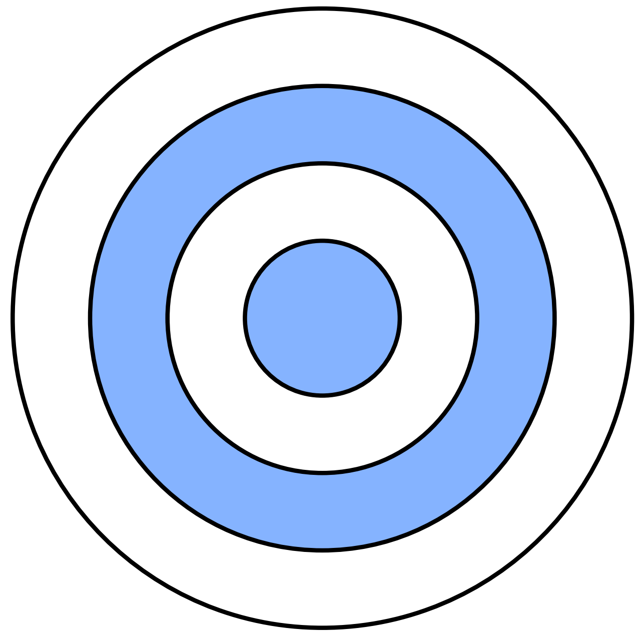
(more technical details in next lecture on model evaluation)

Bias-Variance Intuition

Low Variance
(Precise)

High Variance
(Not Precise)

Low Bias
(Accurate)



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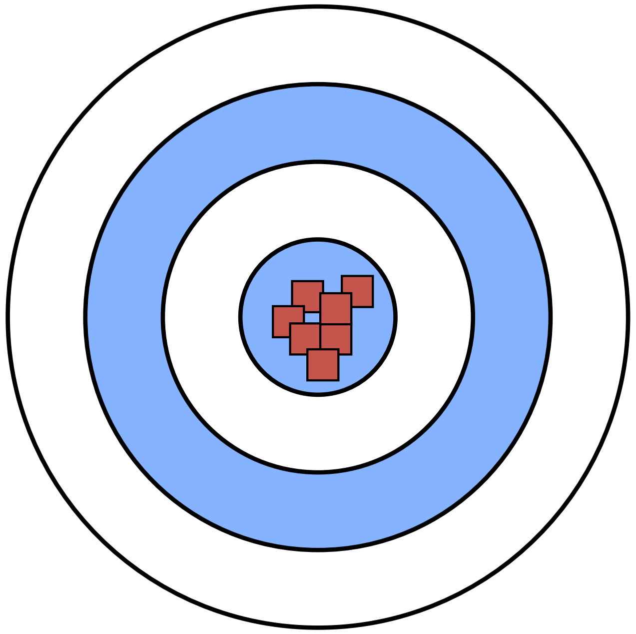

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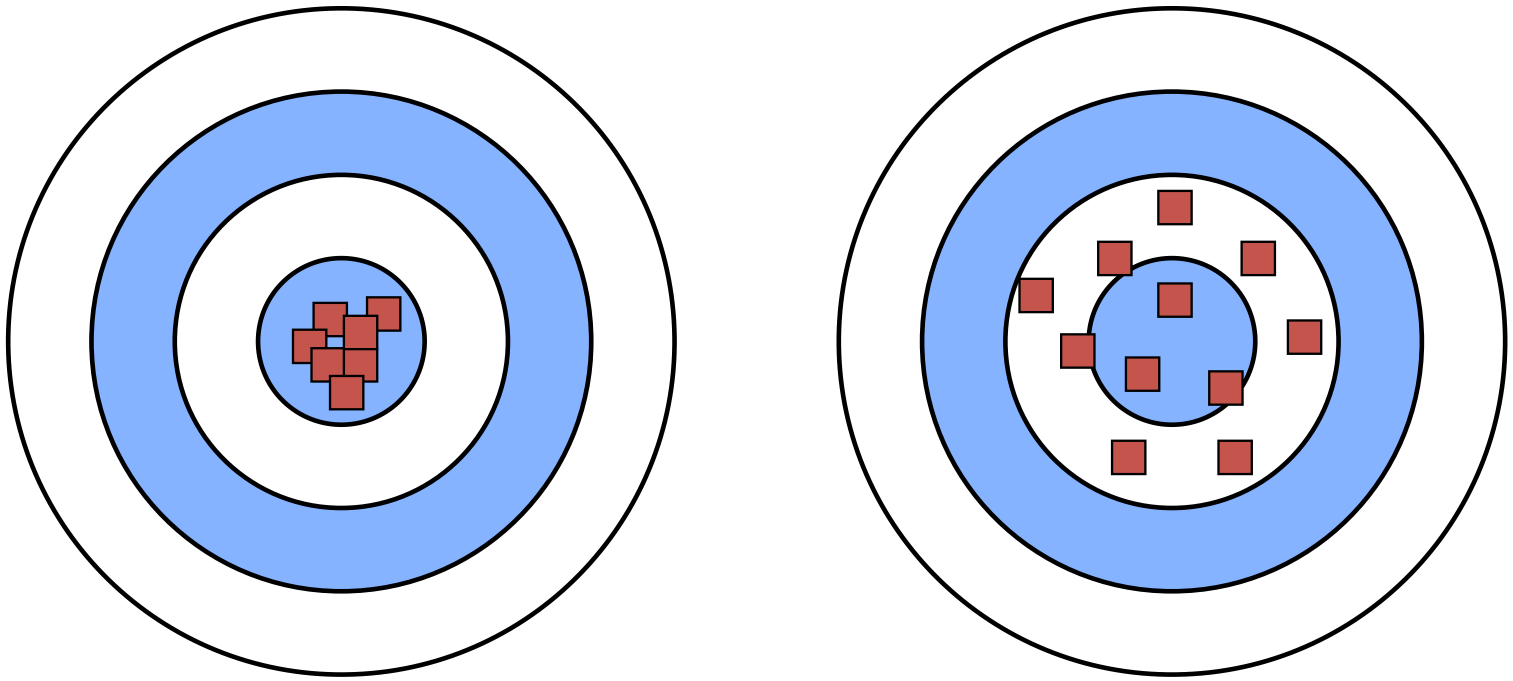

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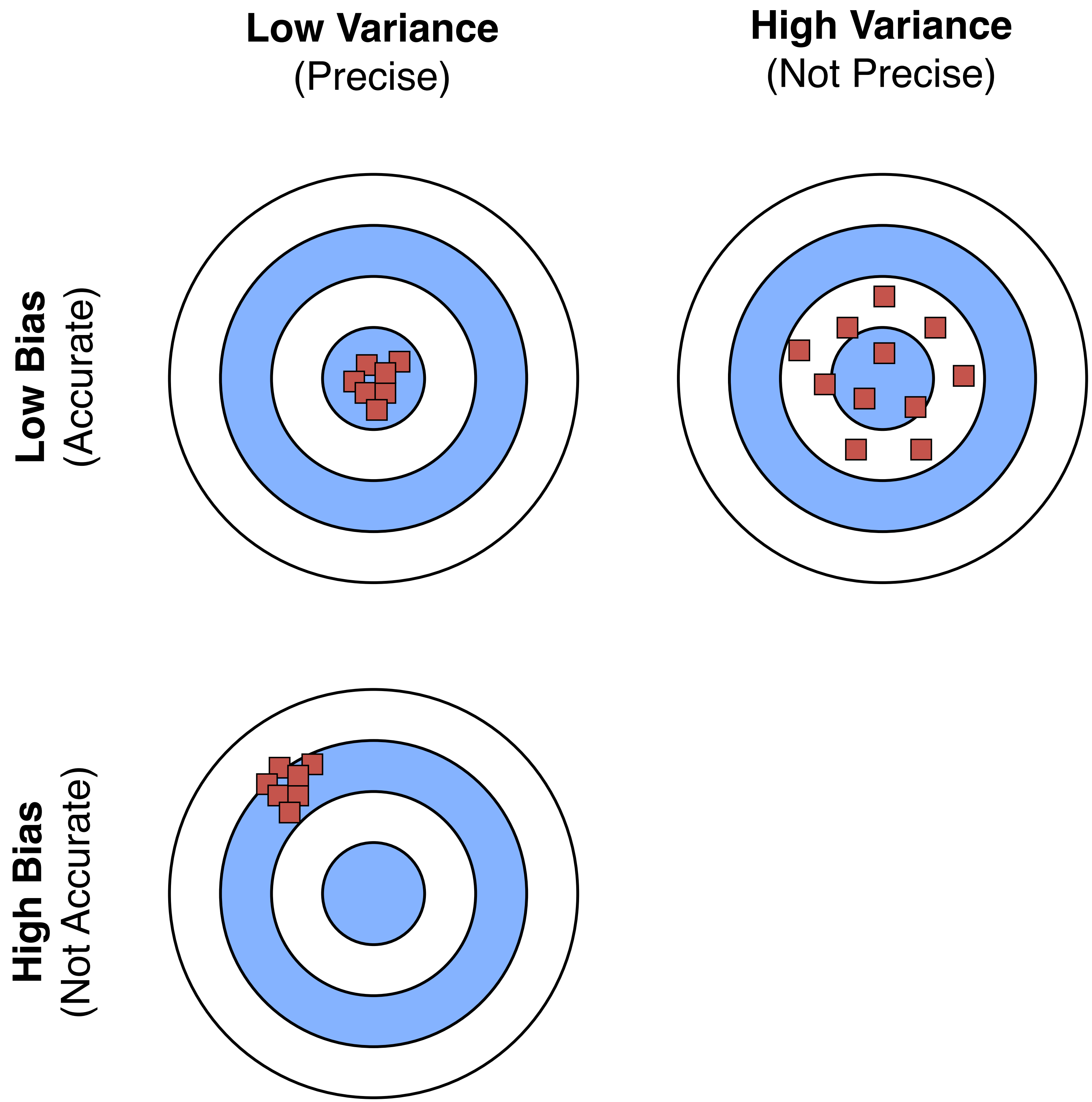
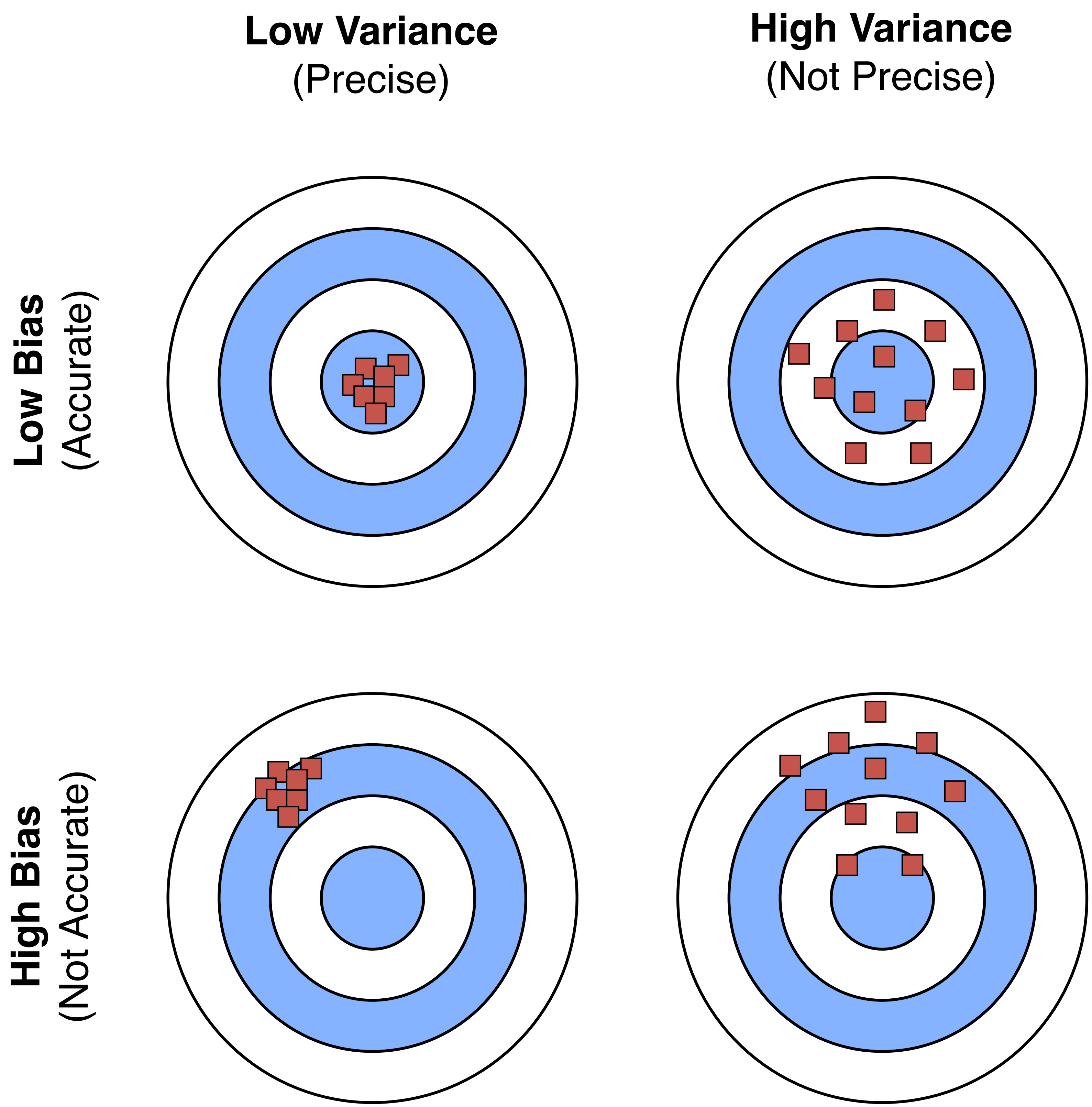
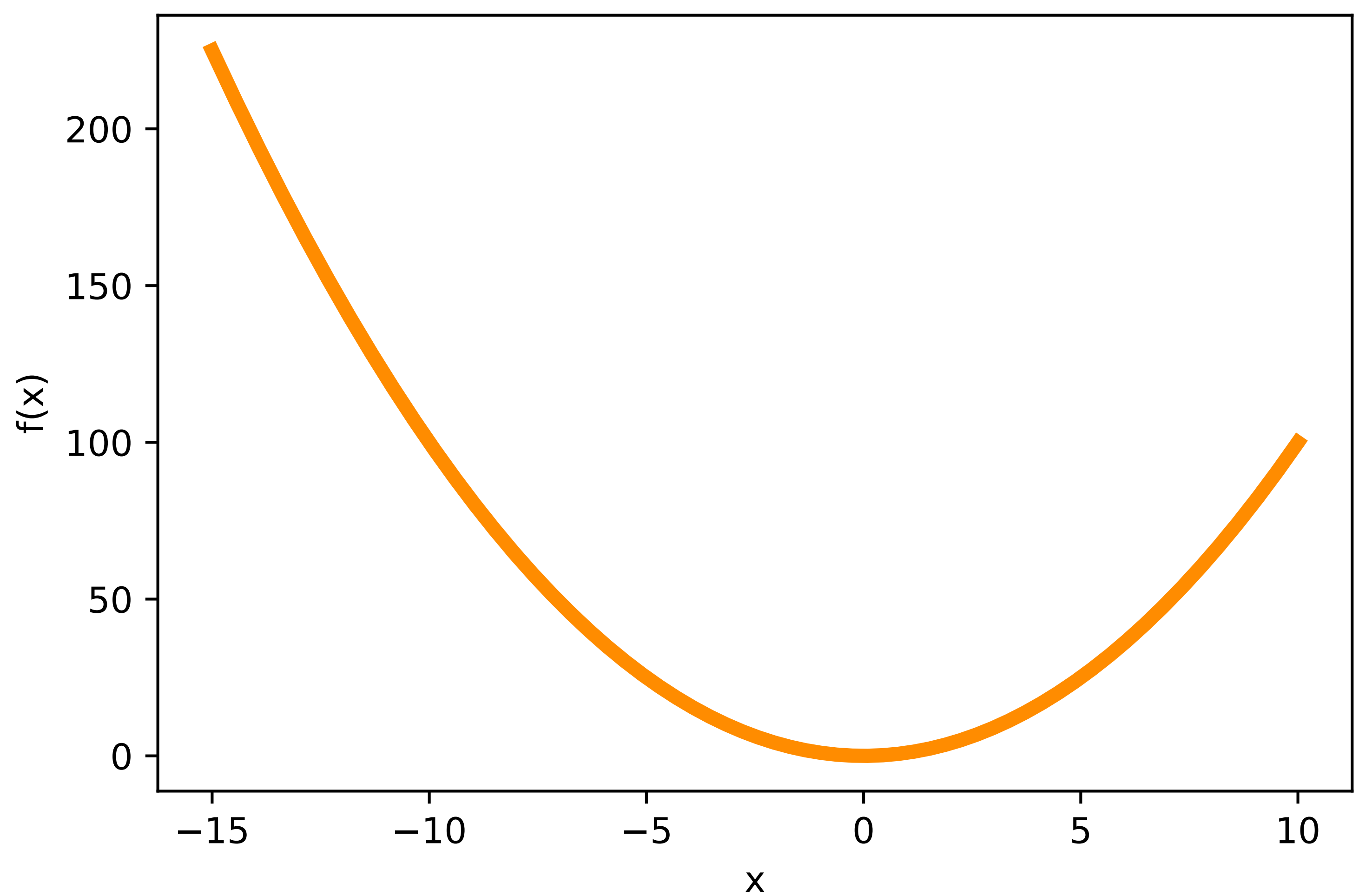


Bias-Variance Intuition

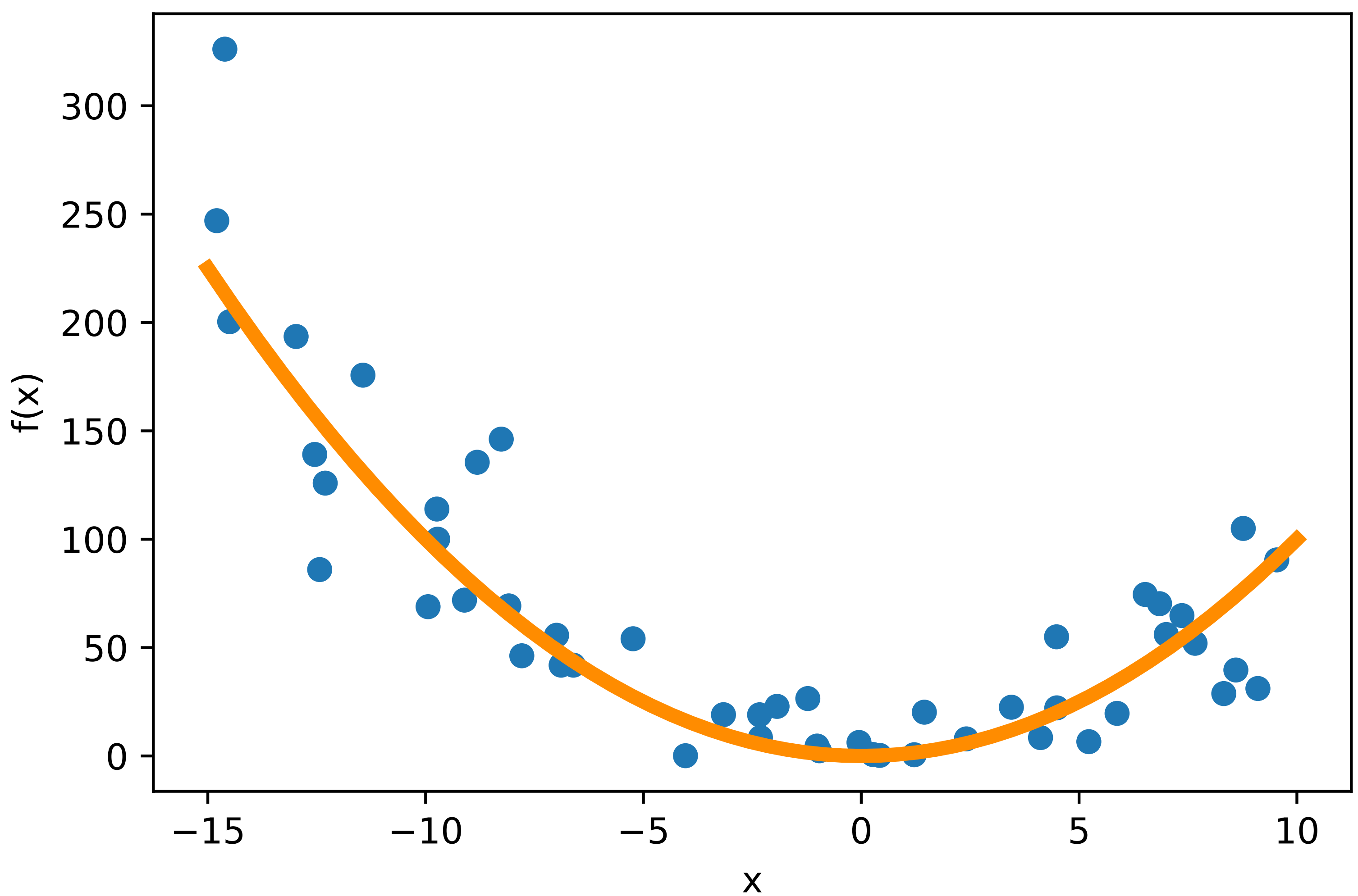


Bias and Variance Example



where f(x) is some true (target) function

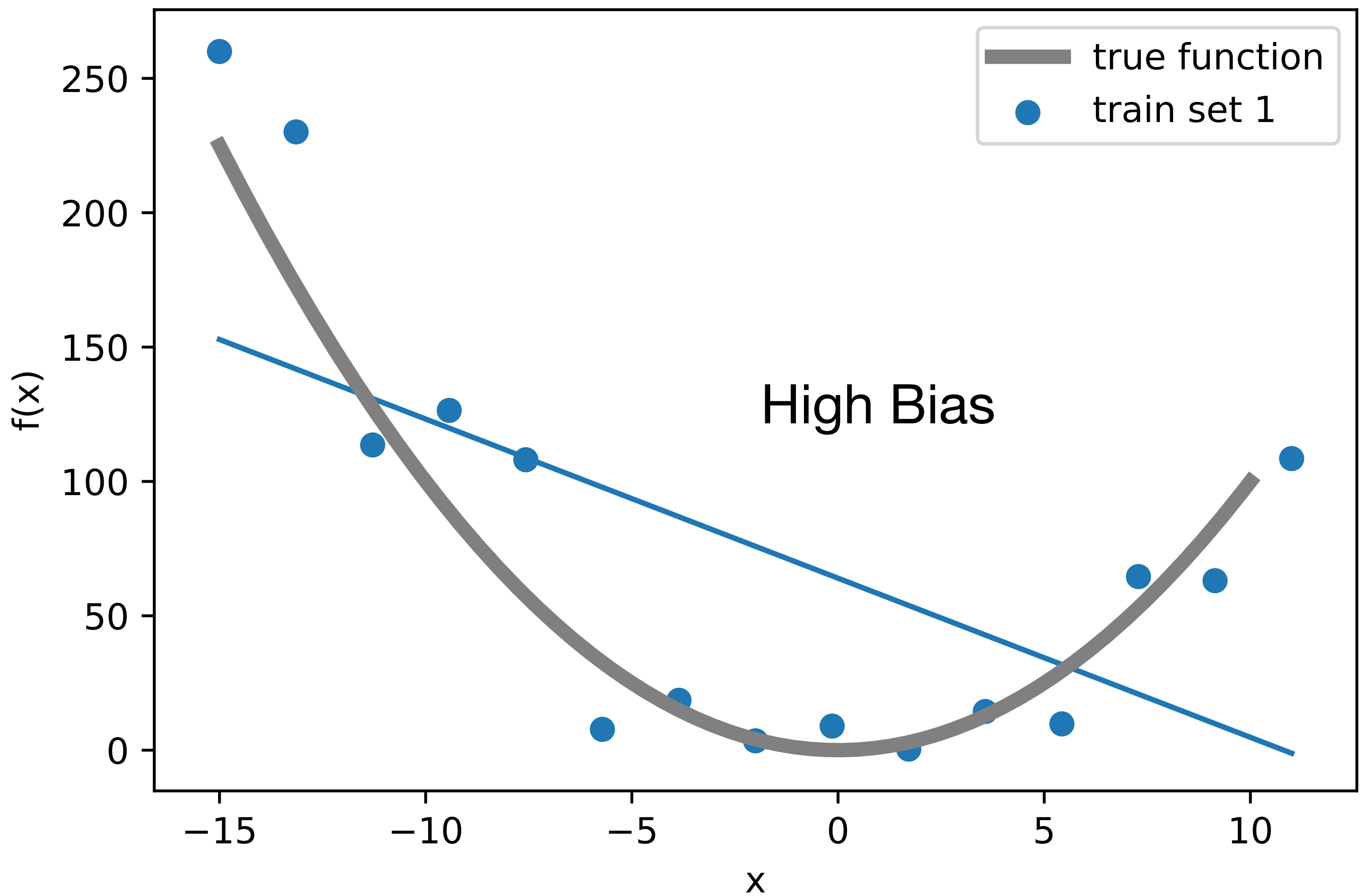
Bias and Variance Example



where f(x) is some true (target) function

the blue dots are a training dataset;
here, I added some random Gaussian noise

Bias and Variance Example

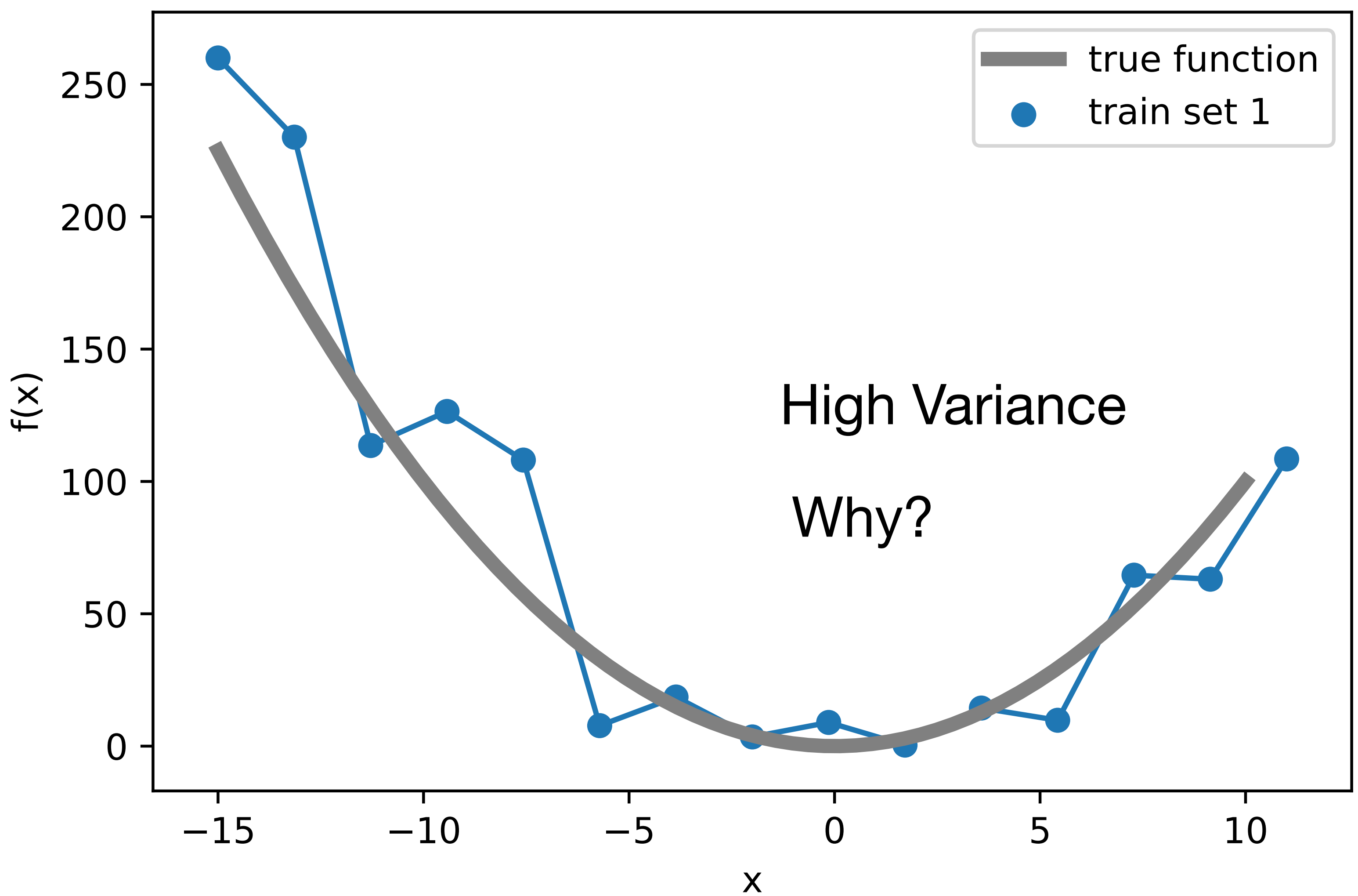


where f(x) is some true (target) function

the blue dots are a training dataset;
here, I added some random Gaussian noise

here, suppose I fit a simple linear model (linear regression)
or a decision tree stump

Bias and Variance Example

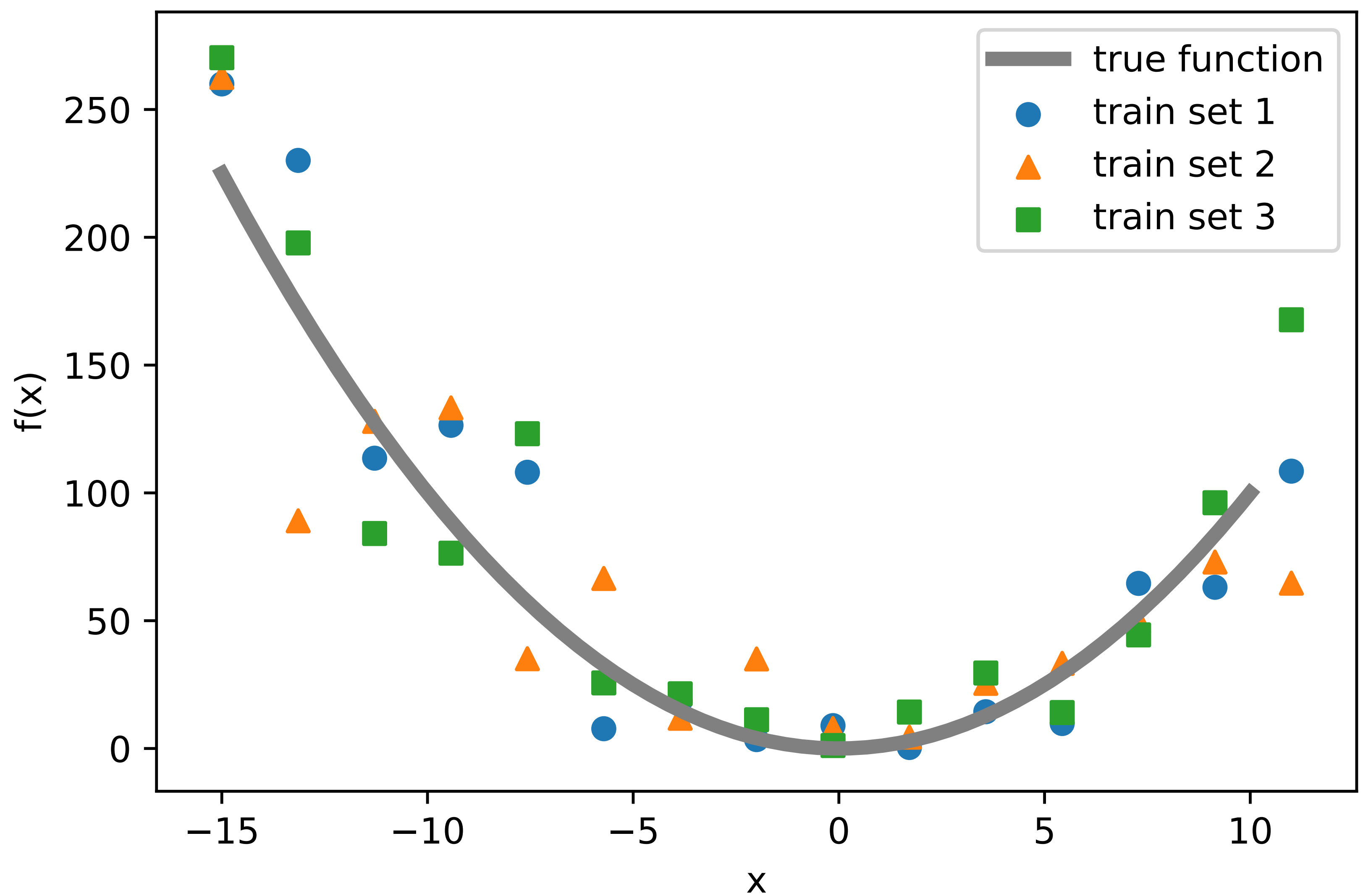


where f(x) is some true (target) function

the blue dots are a training dataset;
here, I added some random Gaussian noise

here, suppose I fit an unpruned decision tree

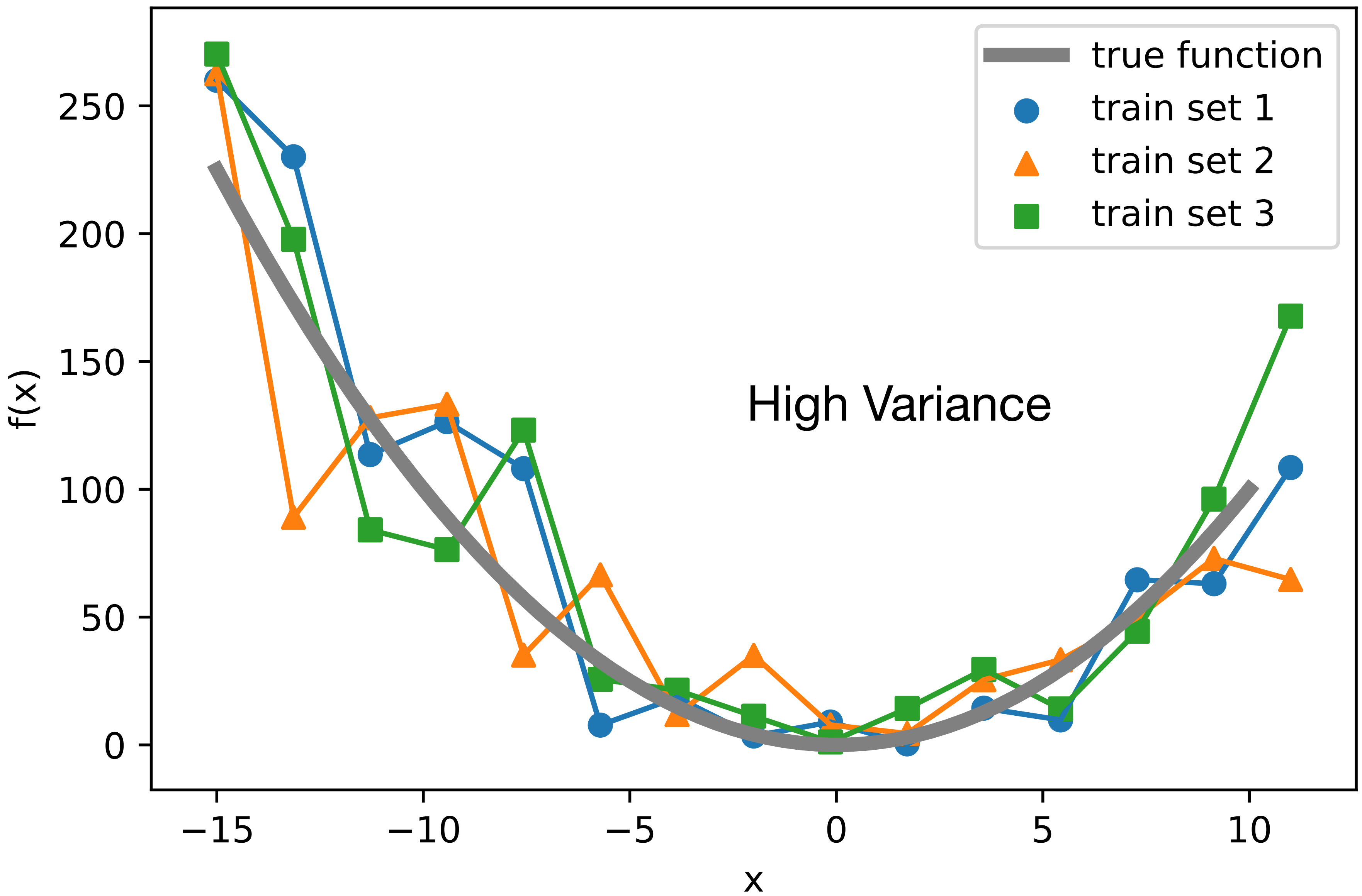
Bias and Variance Example



where f(x) is some true (target) function

suppose we have multiple training sets

Bias and Variance Example



So, why does bagging work/what does it do?

Boosting

Adaptive Boosting

e.g., AdaBoost (here!)

Freund, Y., & Schapire, R. E. (1997). A decision-theoretic generalization of on-line learning and an application to boosting. *Journal of computer and system sciences*, *55*(1), 119-139.

Gradient Boosting

e.g., XGBoost

Friedman, J. H. (2001). Greedy function approximation: a gradient boosting machine. *Annals of statistics*, 1189-1232.

Chen, T., & Guestrin, C. (2016). Xgboost: A scalable tree boosting system. In *Proceedings of the 22nd ACM SIGKDD International conference on knowledge discovery and data mining* (pp. 785-794). ACM.

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Differ mainly in terms of how
- weights are updated
- classifiers are combined

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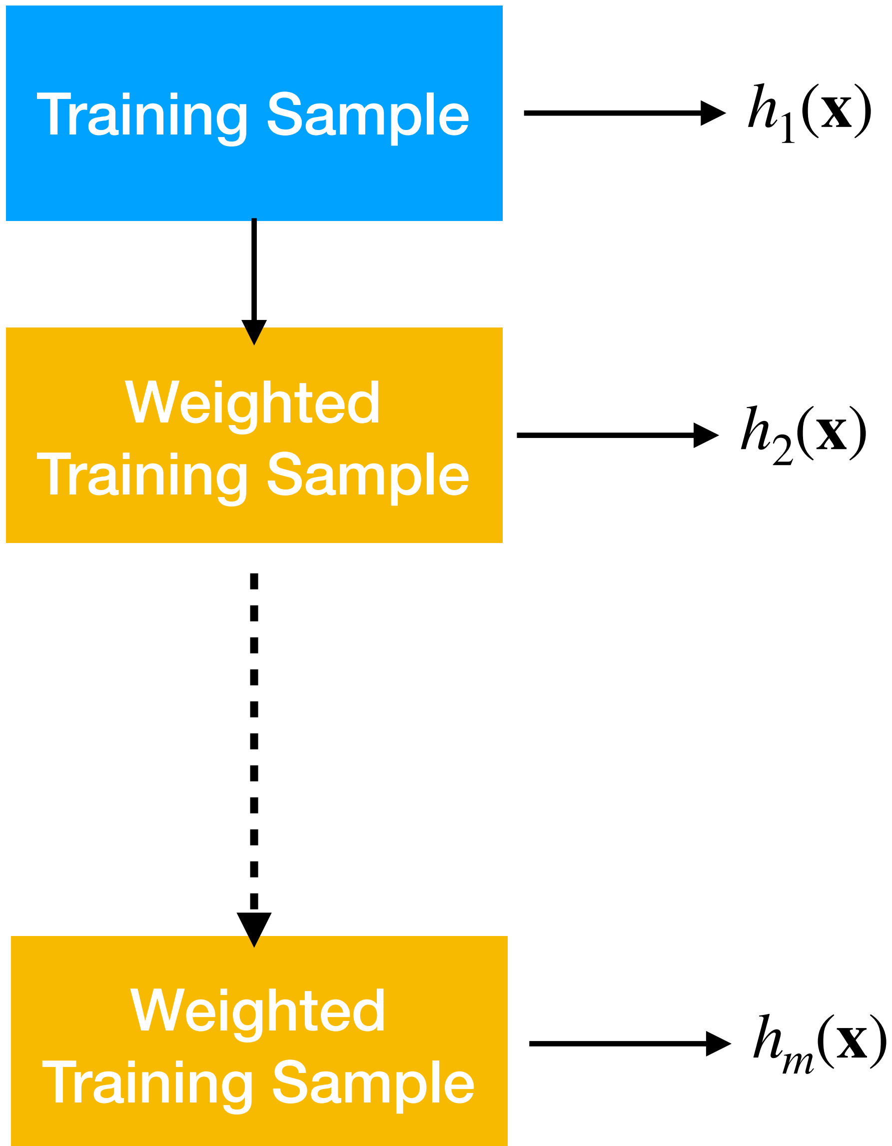
General Boosting



$$h_m(\mathbf{x}) = sign\left(\sum_{j=1}^{m} w_j \, h_j(\mathbf{x})\right) \quad \text{for} \quad h(\mathbf{x}) \in \{-1, 1\}$$

or $$h_m(\mathbf{x}) = \arg\max_i \left(\sum_{j=1}^{m} w_j \, \mathbf{1}[h_j(\mathbf{x}) = i]\right) \quad \text{for} \quad h(\mathbf{x}) = i, \qquad i \in \{1, \ldots, n\}$$

General Boosting

- Initialize a weight vector with uniform weights

- Loop:
    - Apply weak learner* to weighted training examples (instead of orig. training set, may draw bootstrap samples with weighted probability)
    - Increase weight for misclassified examples

- (Weighted) majority voting on trained classifiers

* a learner slightly better than random guessing

AdaBoost

Algorithm 1 AdaBoost

Initialize k: the number of AdaBoost rounds
Initialize $\mathcal{D}$: the training dataset, $\mathcal{D} = \{\langle \mathbf{x}^{[1]}, y^{[1]} \rangle, ..., \mathbf{x}^{[n]}, y^{[n]} \rangle\}$
Initialize $w_1(i) = 1/n, \quad i = 1, ..., n, \ \mathbf{w}_1 \in \mathbb{R}^n$

for r=1 to k **do**
    For all $i : \mathbf{w}_r(i) := w_r(i) / \sum_i w_r(i)$ [normalize weights]
    $h_r := FitWeakLearner(\mathcal{D}, \mathbf{w}_r)$
    $\epsilon_r := \sum_i w_r(i) \, \mathbf{1}(h_r(i) \neq y_i)$ [compute error]
    if $\epsilon_r > 1/2$ then stop
    $\alpha_r := \frac{1}{2} \log[(1 - \epsilon_r)/\epsilon_r]$ [small if error is large and vice versa]
    $w_{r+1}(i) := w_r(i)/z_r \times \begin{cases} \mathrm{e}^{-\alpha_r} & \text{if } h_r(\mathbf{x}^{[i]}) = y^{[i]} \\ \mathrm{e}^{\alpha_r} & \text{if } h_r(\mathbf{x}^{[i]}) \neq y^{[i]} \end{cases}$
Predict: $h_k(\mathbf{x}) = \arg\max_j \sum_r \alpha_r \mathbf{1}[h_r(\mathbf{x}) = j]$

Modify AdaBoost w. Bootstrap

Algorithm 1 AdaBoost

Initialize k: the number of AdaBoost rounds
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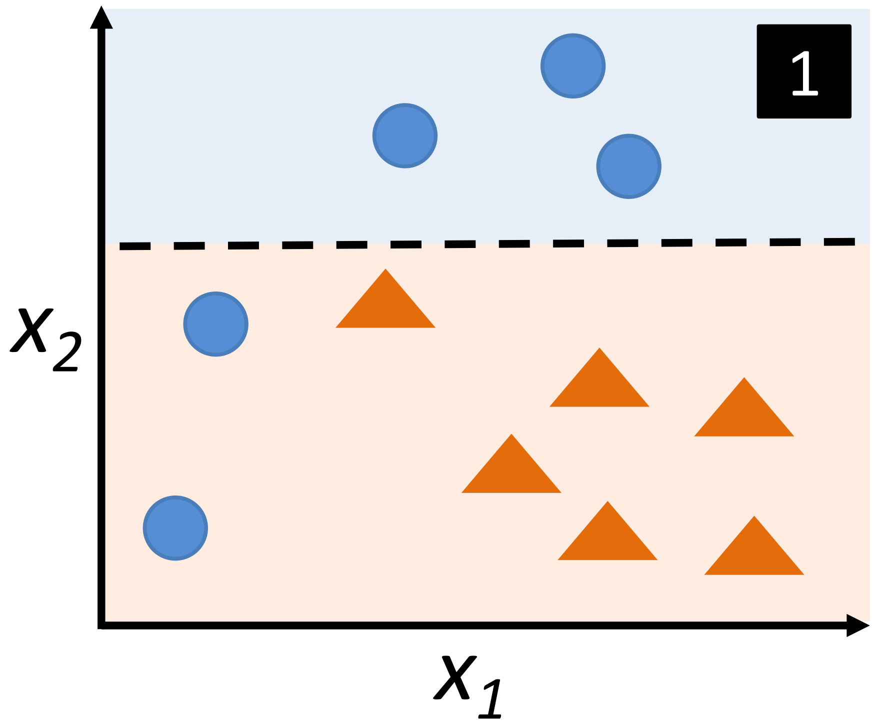
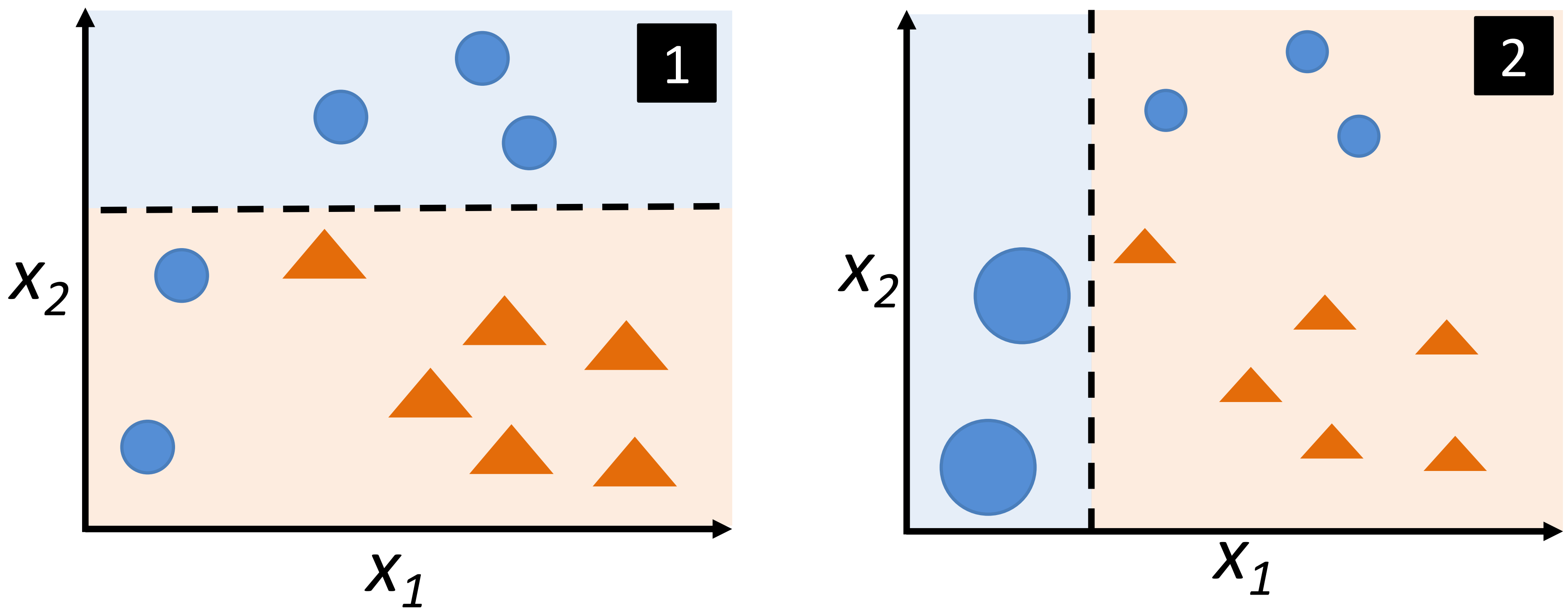
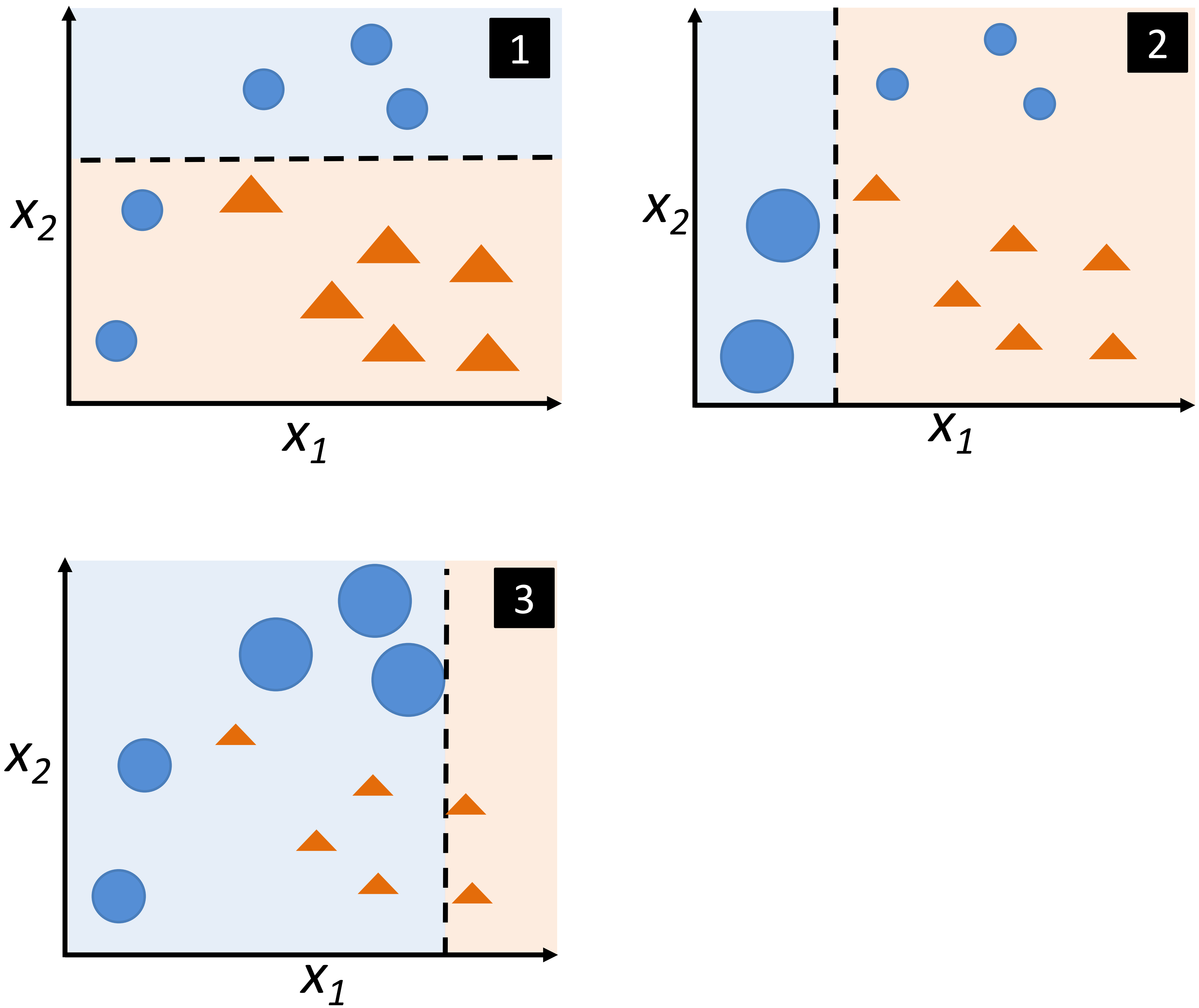
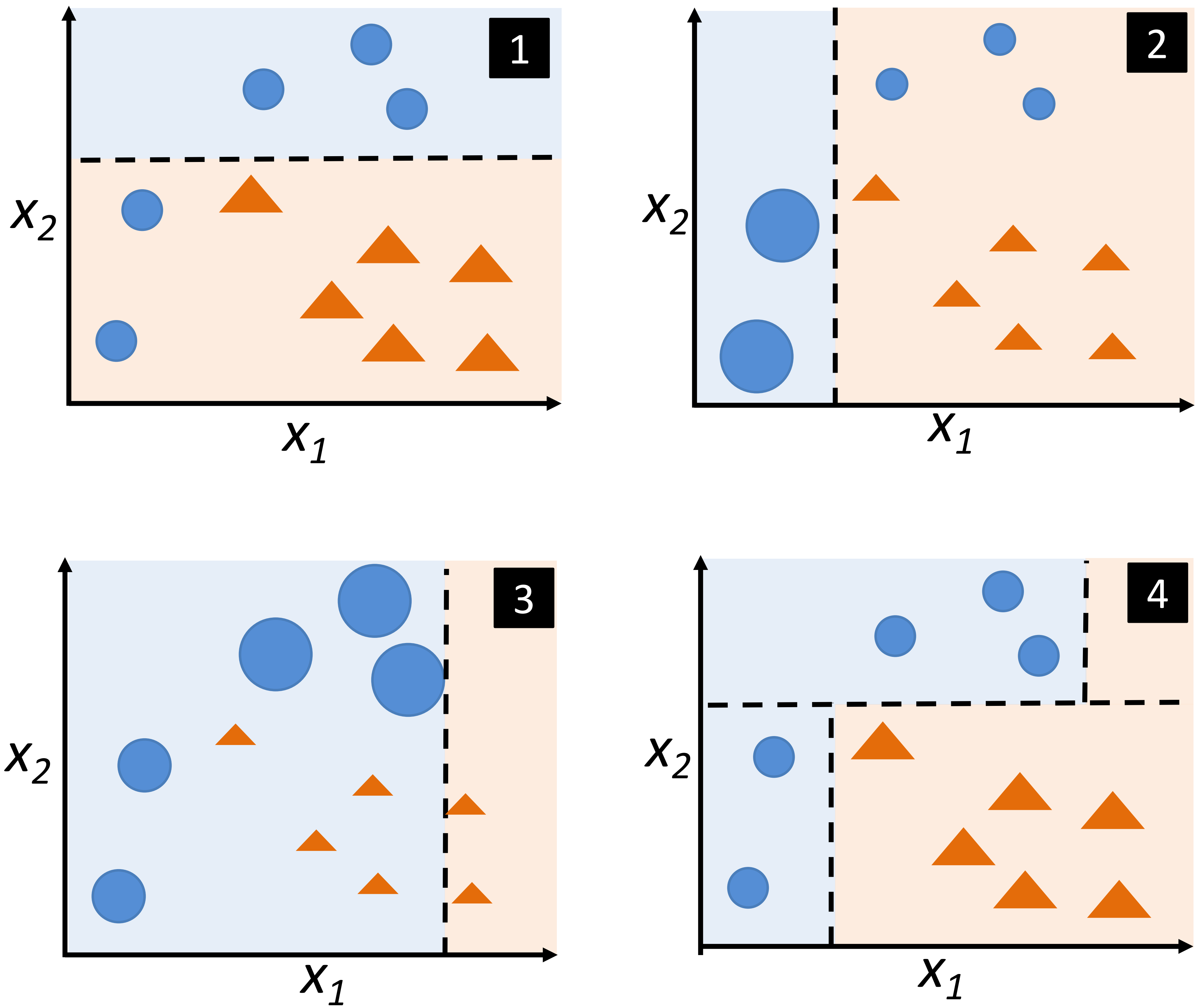
Decision Tree Stumps


1
x_2
x_1


1
2
x_1
x_2
x_1
x_2


1
2
3
x_1
x_2


1
2
3
4
x_2
x_1
x_2
x_1
x_2
x_1
x_2
x_1

Random Forests

Random Forests

= Bagging w. trees + random feature subsets

Random Feature Subset for each Tree or Node?

Tin Kam Ho used the "**random subspace method,**" where each tree got a random subset of features.

"Our method relies on an autonomous, pseudo-random procedure to select a small number of dimensions from a given feature space …"

- Ho, Tin Kam. "The random subspace method for constructing decision forests." IEEE transactions on pattern analysis and machine intelligence 20.8 (1998): 832-844.

"Trademark" random forest:

"… random forest with random features is formed by selecting at random, at each node, a small group of input variables to split on."

- **Breiman**, Leo. "Random Forests" Machine learning 45.1 (2001): 5-32.

Random Feature Subset for each Tree or Node?

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“Our method relies on an autonomous, pseudo-random procedure to select a small number of dimensions from a given feature space …”

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“Trademark” random forest:

“… random forest with random feature … *andom, at each node, a small group of input variab* …

- Breiman, Leo. “Random Forests” Ma … 2.

num features $= \log_2 m + 1$

where m is the number of input features

In contrast to the original publication
[Breiman, “Random Forests”, Machine Learning, 45(1), 5-32, 2001]
the scikit-learn implementation combines classifiers by averaging their probabilistic prediction, instead of letting each classifier vote for a single class.

"Soft Voting"

Will discuss Random Forests and feature importance in *Feature Selection* lecture

(Loose) Upper Bound for the Generalization Error

Breiman, “Random Forests”, Machine Learning, 45(1), 5-32, 2001

$$\textbf{PE} \leq \frac{\bar{\rho} \cdot (1 - s^2)}{s^2}$$

$\bar{\rho}$: Average correlation among trees

s : "Strength" of the ensemble

Extremely Randomized Trees (ExtraTrees)

Geurts, P., Ernst, D., & Wehenkel, L. (2006). Extremely randomized trees. *Machine learning*, *63*(1), 3-42.

Random Forest random components:

1) ______________

2) ______________

ExtraTrees algorithm adds one more random component

3) ______________

Stacking

Stacking Algorithm

Wolpert, David H. "Stacked generalization." Neural networks 5.2 (1992): 241-259.

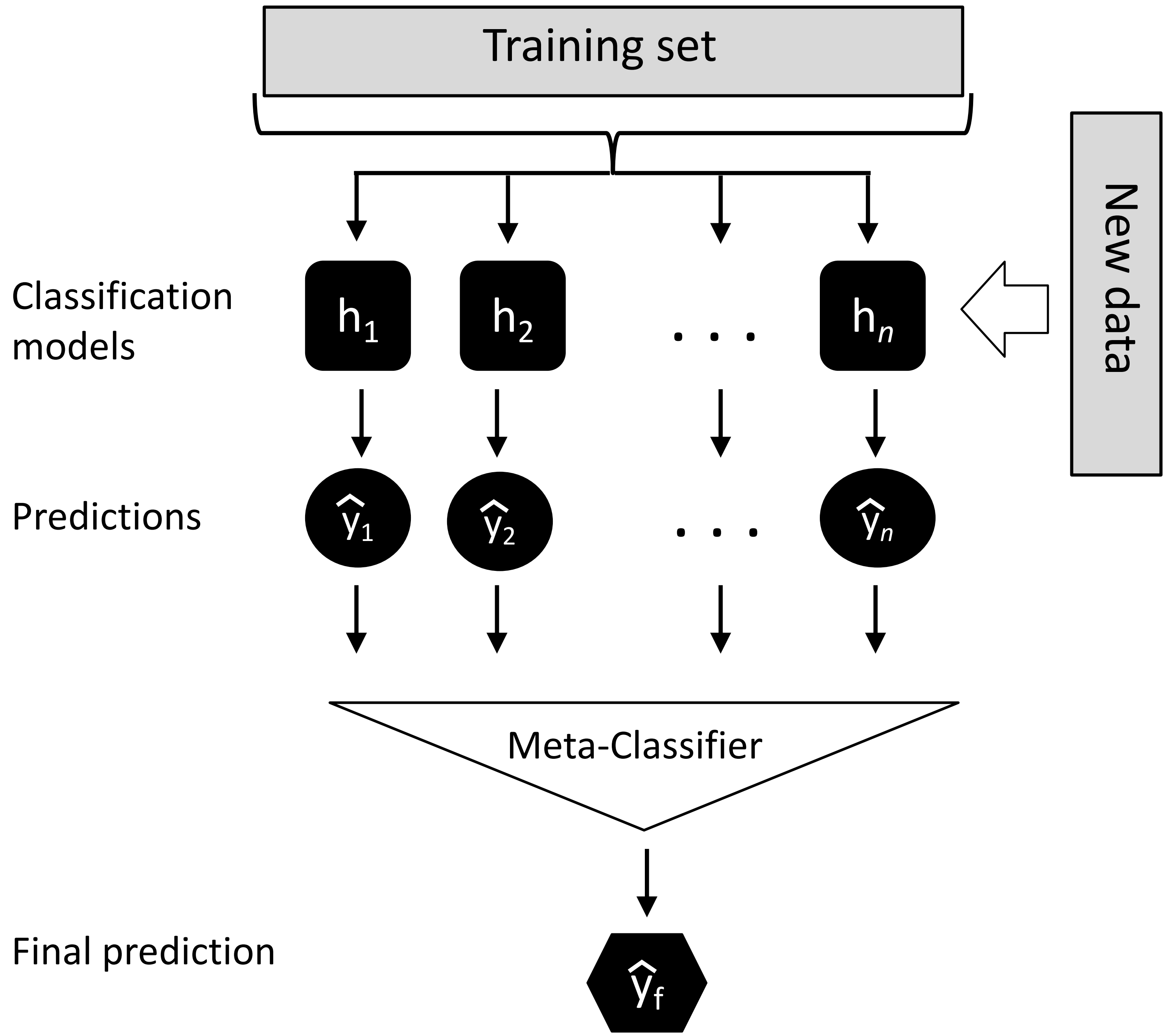
Algorithm 19.7 Stacking

Input: Training data $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^{m}$ ($\mathbf{x}_i \in \mathbb{R}^n$, $y_i \in \mathcal{Y}$)
Output: An ensemble classifier H

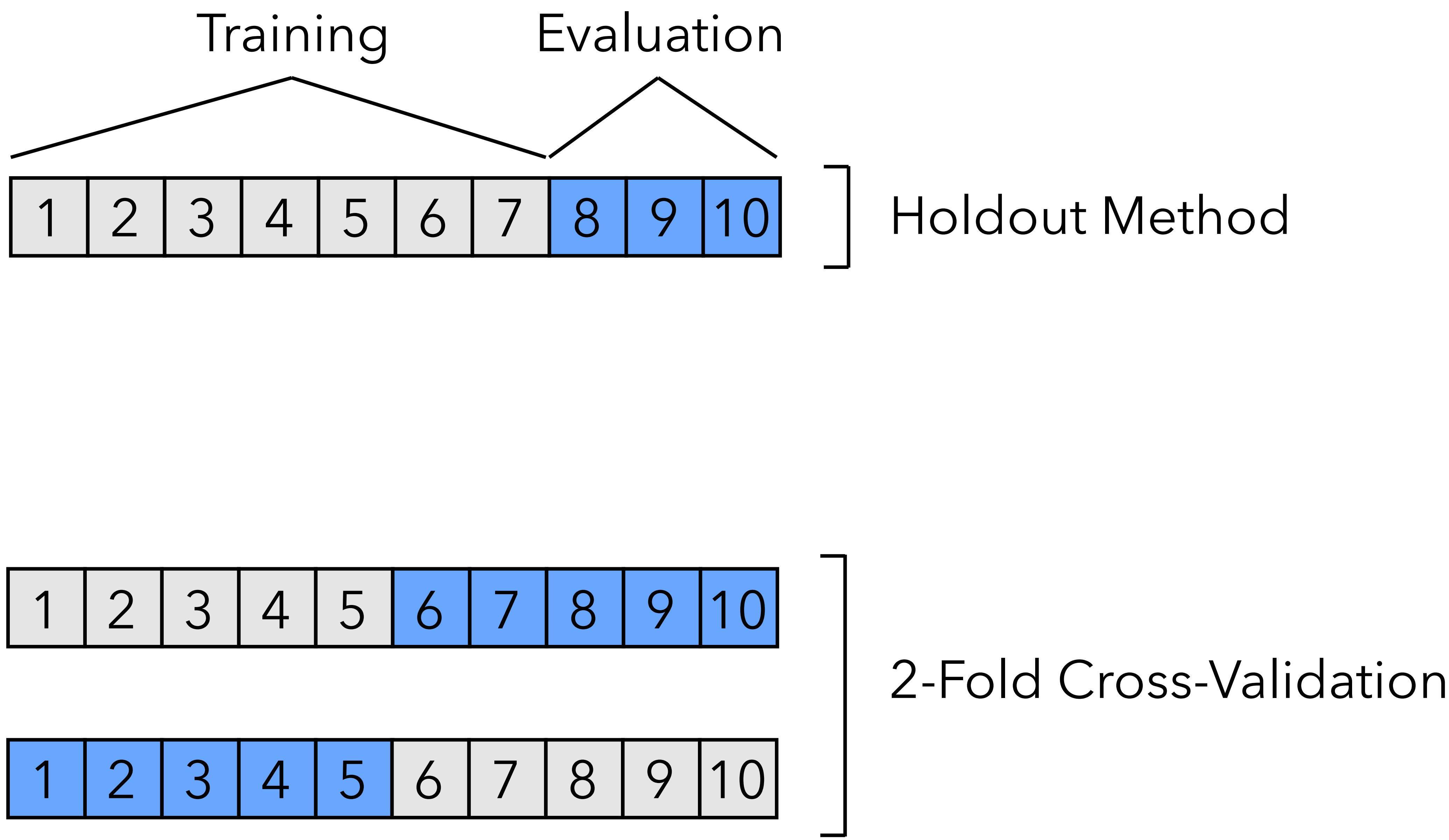
Step 1: Learn first-level classifiers
for $t \leftarrow 1$ to T **do**
    Learn a base classifier h_t based on $\mathcal{D}$
end for
Step 2: Construct new data sets from $\mathcal{D}$
for $i \leftarrow 1$ to m **do**
    Construct a new data set that contains $\{\mathbf{x}'_i, y_i\}$, where $\mathbf{x}'_i = \{h_1(\mathbf{x}_i), h_2(\mathbf{x}_i), \ldots, h_T(\mathbf{x}_i)\}$
end for
Step 3: Learn a second-level classifier
Learn a new classifier h' based on the newly constructed data set
return $H(\mathbf{x}) = h'(h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots, h_T(\mathbf{x}))$

Tang, J., S. Alelyani, and H. Liu. "Data Classification: Algorithms and Applications." Data Mining and Knowledge Discovery Series, CRC Press (2015): pp. 498-500.

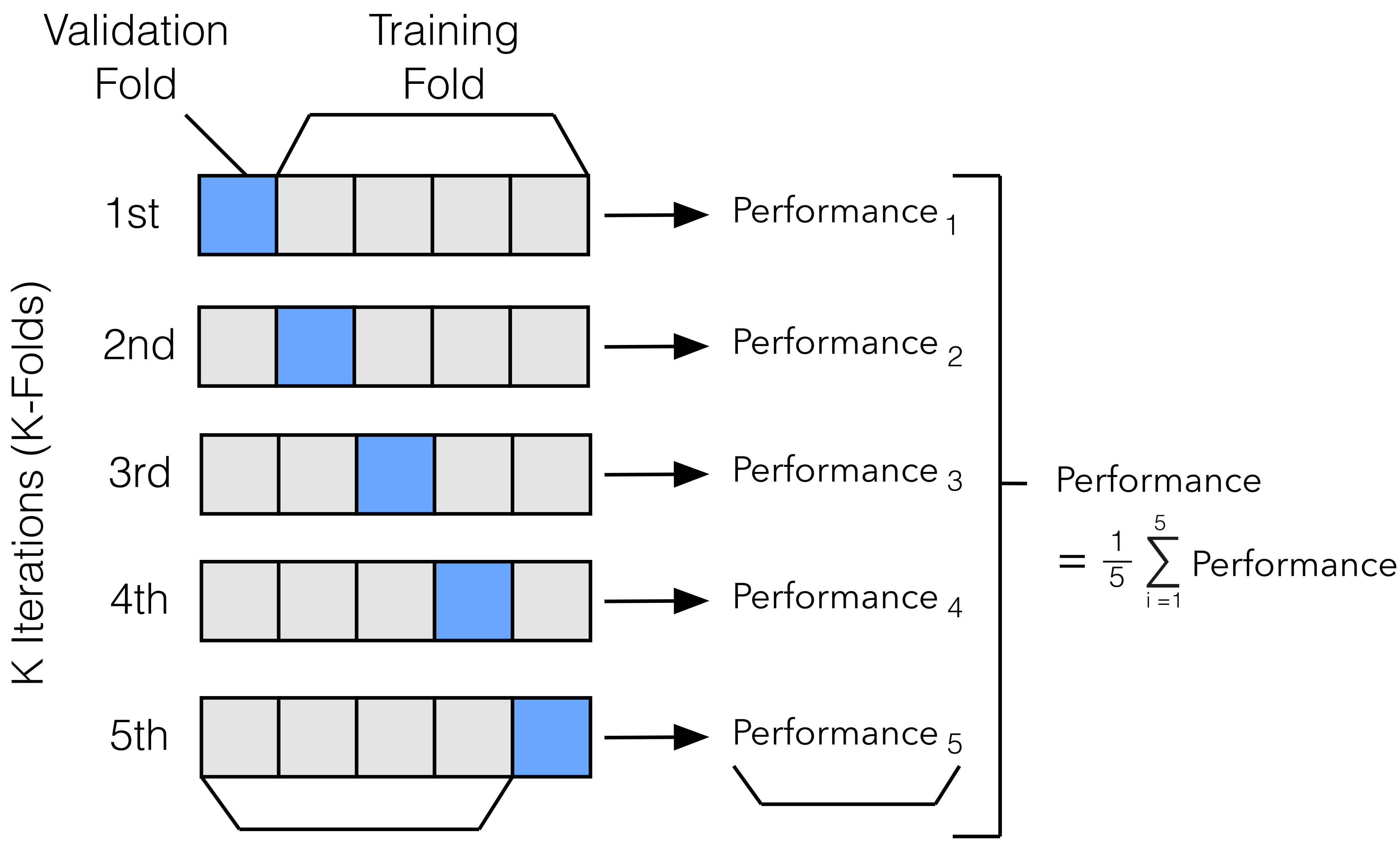
Stacking Algorithm

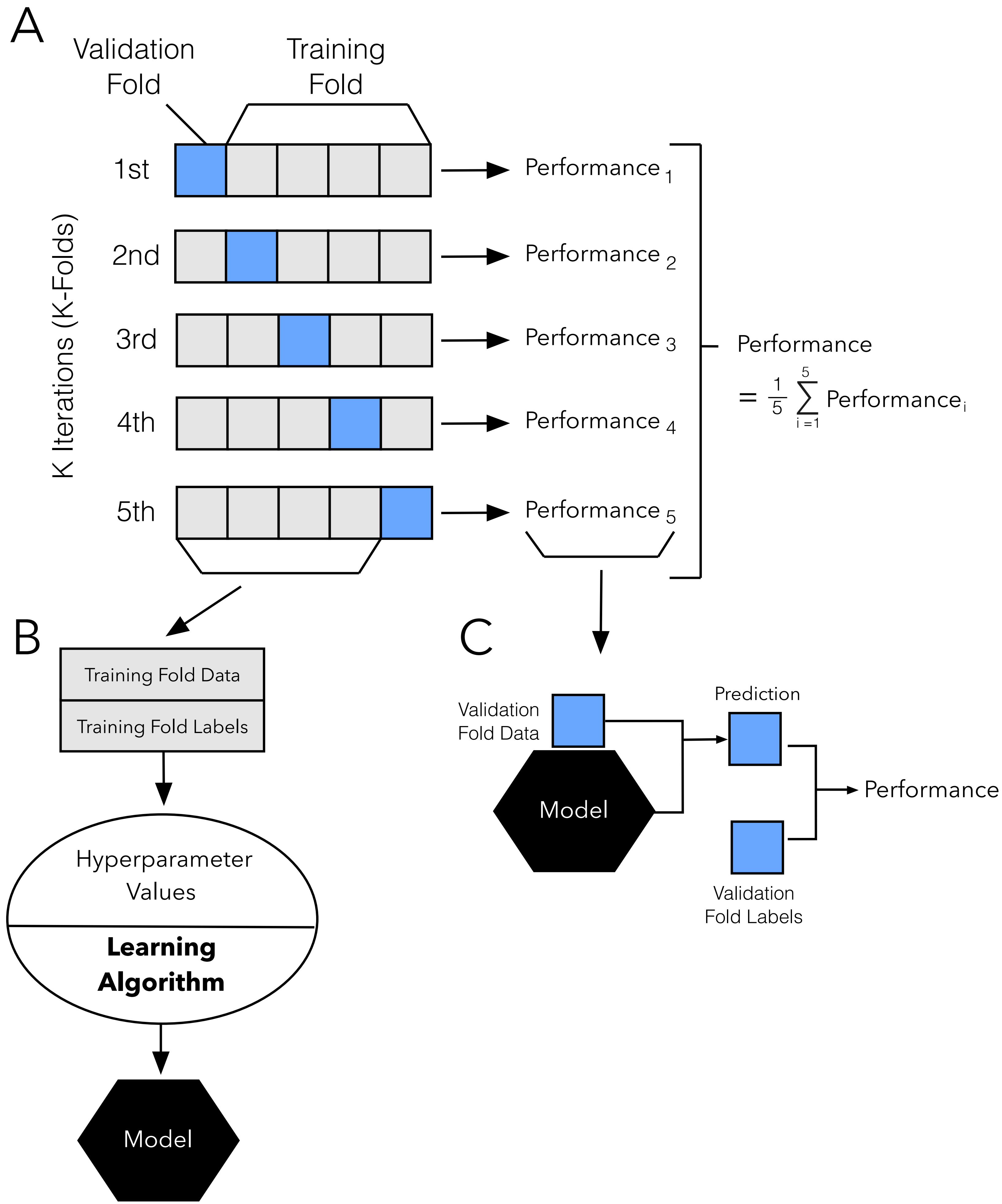


Cross-Validation



k-fold Cross-Validation




A
Validation Fold
Training Fold
K Iterations (K-Folds)
1st
2nd
3rd
4th
5th
Performance 1
Performance 2
Performance 3
Performance 4
Performance 5
Performance
$= \frac{1}{5} \sum_{i=1}^{5} \text{Performance}_i$
B
Training Fold Data
Training Fold Labels
Hyperparameter Values
Learning Algorithm
Model
C
Validation Fold Data
Model
Prediction
Performance
Validation Fold Labels

Stacking Algorithm with Cross-Validation

Wolpert, David H. "Stacked generalization." Neural networks 5.2 (1992): 241-259.

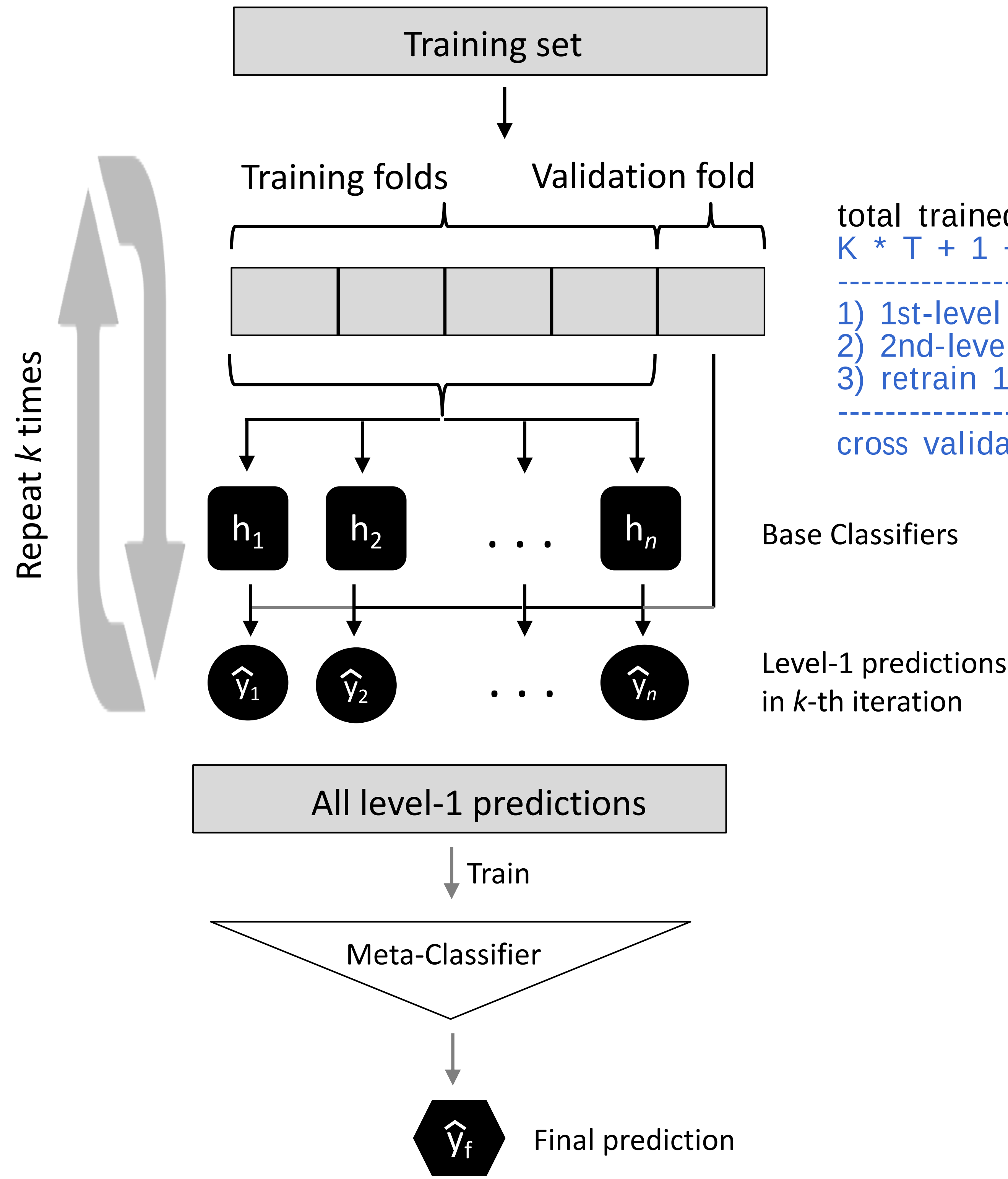
Algorithm 19.8 Stacking with K-fold Cross Validation

Input: Training data $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^{m}$ ($\mathbf{x}_i \in \mathbb{R}^n$, $y_i \in \mathcal{Y}$)
Output: An ensemble classifier H

Step 1: Adopt cross validation approach in preparing a training set for second-level classifier
Randomly split $\mathcal{D}$ into K equal-size subsets: $\mathcal{D} = \{\mathcal{D}_1, \mathcal{D}_2, \ldots, \mathcal{D}_K\}$
for $k \leftarrow 1$ to K **do**
  Step 1.1: Learn first-level classifiers
  for $t \leftarrow 1$ to T **do**
    Learn a classifier h_{kt} from $\mathcal{D} \setminus \mathcal{D}_k$
  end for
  Step 1.2: Construct a training set for second-level classifier
  for $\mathbf{x}_i \in \mathcal{D}_k$ **do**
    Get a record $\{\mathbf{x}'_i, y_i\}$, where $\mathbf{x}'_i = \{h_{k1}(\mathbf{x}_i), h_{k2}(\mathbf{x}_i), \ldots, h_{kT}(\mathbf{x}_i)\}$
  end for
end for
Step 2: Learn a second-level classifier
Learn a new classifier h' from the collection of $\{\mathbf{x}'_i, y_i\}$
Step 3: Re-learn first-level classifiers
for $t \leftarrow 1$ to T **do**
  Learn a classifier h_t based on $\mathcal{D}$
end for
return $H(\mathbf{x}) = h'(h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots, h_T(\mathbf{x}))$

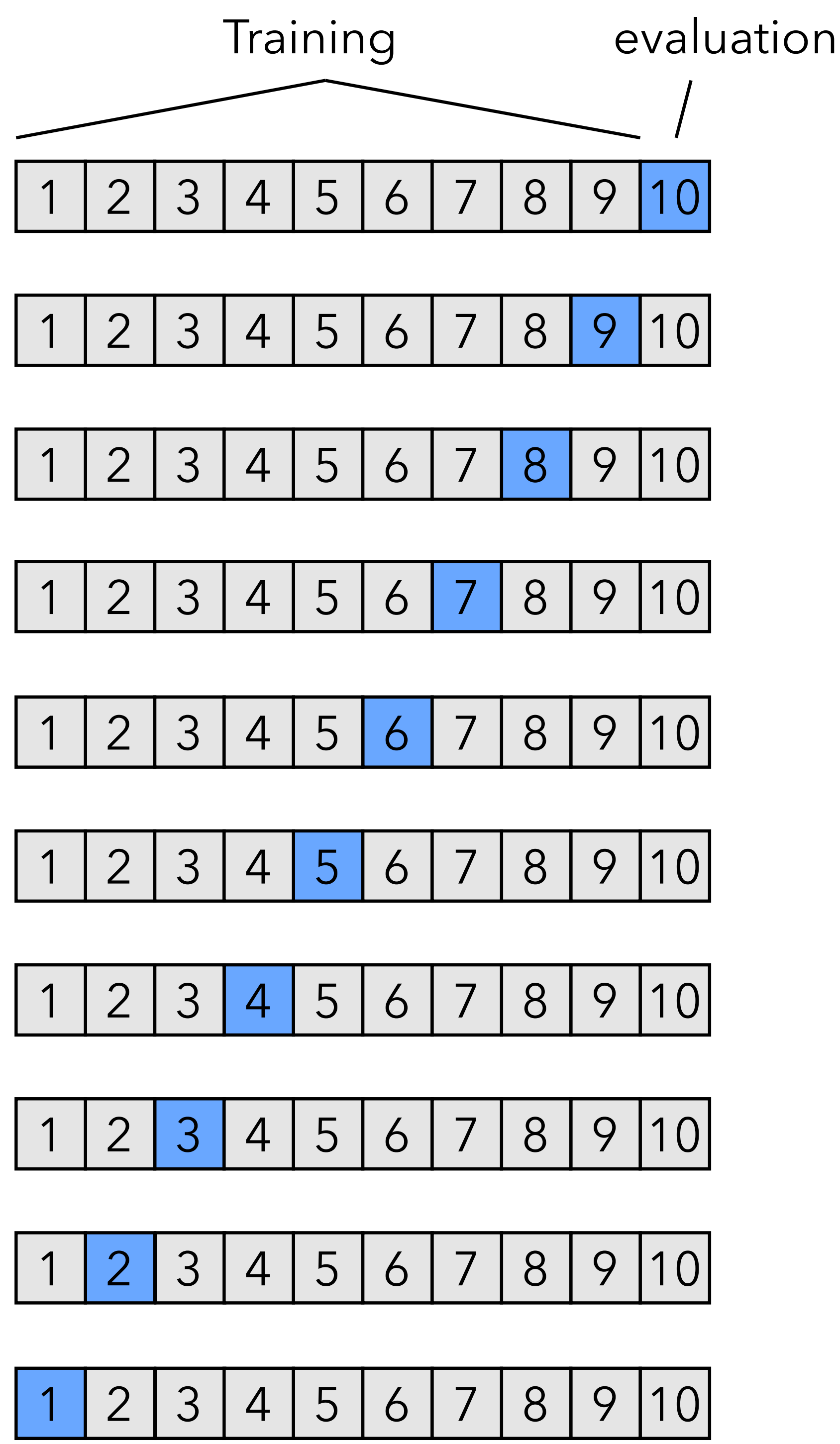
Tang, J., S. Alelyani, and H. Liu. "Data Classification: Algorithms and Applications." Data Mining and Knowledge Discovery Series, CRC Press (2015): pp. 498-500.

Stacking Algorithm with Cross-Validation



total trained models:
K * T + 1 + T
----
1) 1st-level K-fold cross validation
2) 2nd-level classifier
3) retrain 1st-level model
----
cross validation is adopt to avoid overfitting

Leave-One-Out CV



Demo

07_ensembles_demo.ipynb

Reading Assignments

Python Machine Learning, 2nd Ed., Ch07