Bias/Variance Tradeoff and Ensemble Methods

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Acknowledgement: Nick Rouzzi, Vibhav Gogate, David Sontag, Killian Weinberger, Aarti Singh

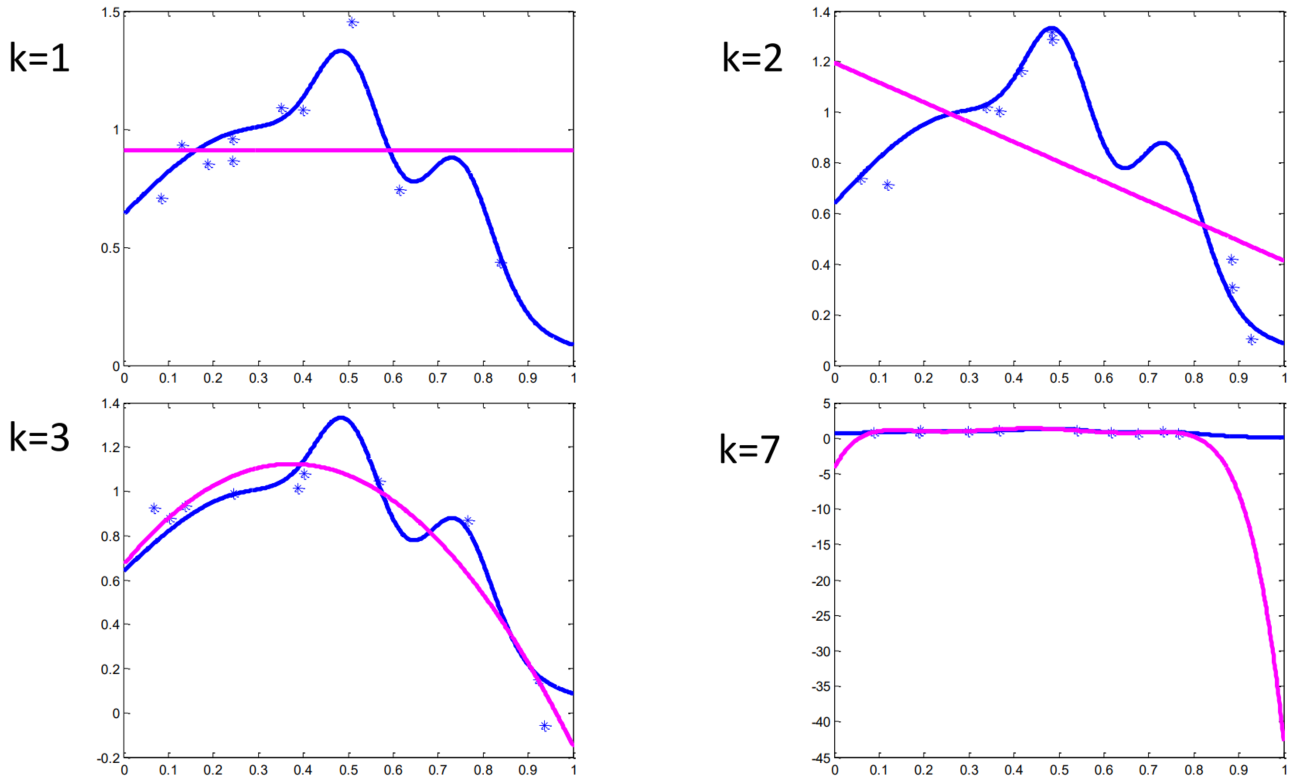
Last Time

- PAC learning
- Bias/variance tradeoff
  - small hypothesis spaces (not enough flexibility) can have high bias
  - rich hypothesis spaces (too much flexibility) can have high variance
- Today: more on this phenomenon and how to get around it

High Variance or Overfitting

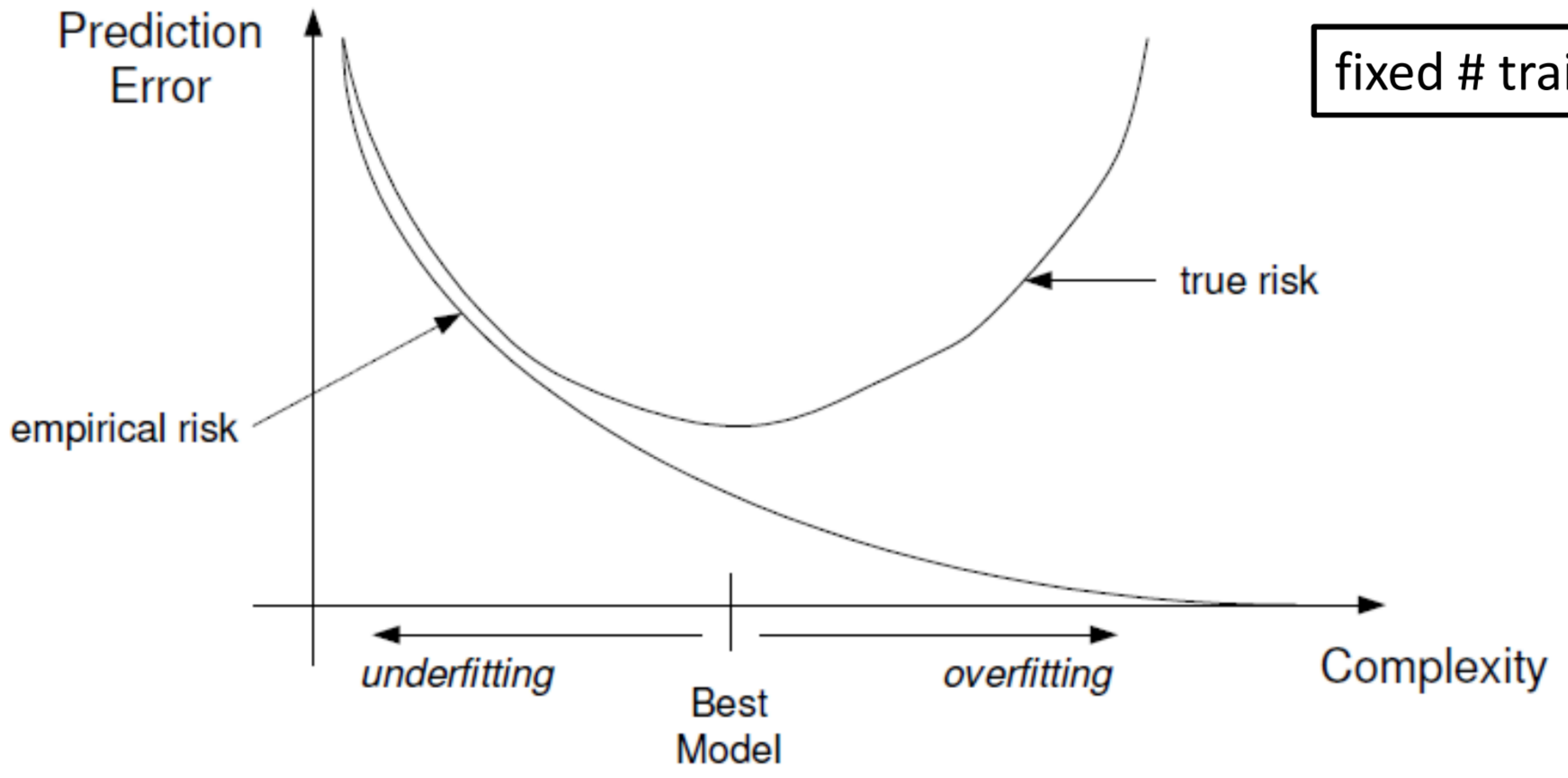
If we allow very complicated predictors, we could overfit the training data.

Examples: Regression (Polynomial of order k – degree up to k-1)



Effect of Model Complexity

If we allow very complicated predictors, we could overfit the training data.



fixed # training data

Intuition

- Bias
  - Measures the accuracy or quality of the algorithm
  - High bias means a poor match
- Variance
  - Measures the precision or specificity of the match
  - High variance means a weak match
- We would like to minimize each of these
- Unfortunately, we can’t do this independently, there is a trade-off

Bias-Variance Analysis in Regression

- Dataset: $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$

- True function is $y = f(x) + \epsilon$
  - Where noise, ϵ, is normally distributed with zero mean and standard deviation σ

- Given a set of training examples, $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})$, we fit a hypothesis $g(x) = w^T x + b$ to the data to minimize the squared error

$$\sum_i \left[y^{(i)} - g\left(x^{(i)}\right)\right]^2$$

Some Terminology

Expected Label (given $\mathbf{x} \in \mathbb{R}^d$):

$$\bar{y}(\mathbf{x}) = E_{y|\mathbf{x}}[Y] = \int\limits_y y \Pr(y|\mathbf{x}) \partial y.$$

Expected Test Error (given h_D):

$$E_{(\mathbf{x},y)\sim P}\left[(h_D(\mathbf{x}) - y)^2\right] = \int\limits_x \int\limits_y (h_D(\mathbf{x}) - y)^2 \Pr(\mathbf{x}, y) \partial y \partial \mathbf{x}.$$

Expected Classifier (given $\mathcal{A}$):

$$\bar{h} = E_{D\sim P^n}[h_D] = \int h_D \Pr(D) \partial D$$

Expected Test Error (given $\mathcal{A}$):

$$E_{\substack{(\mathbf{x},y)\sim P \\ D\sim P^n}}\left[(h_D(\mathbf{x}) - y)^2\right] = \int_D \int_{\mathbf{x}} \int_y (h_D(\mathbf{x}) - y)^2 \mathrm{P}(\mathbf{x}, y) \mathrm{P}(D) \partial \mathbf{x} \partial y \partial D$$

Probability Reminder

- Variance of a random variable, Z

$$\begin{aligned} Var(Z) &= E[(Z - E[Z])^2] \\ &= E[Z^2 - 2ZE[Z] + E[Z]^2\ ] \\ &= E[Z^2] - E[Z]^2 \end{aligned}$$

- Properties of $Var(Z)$

$$Var(aZ) = E[a^2Z^2] - E[aZ]^2 = a^2Var(Z)$$

Bias-Variance-Noise Decomposition

$$E_{\mathbf{x},y,D}\left[[h_D(\mathbf{x}) - y]^2\right] = E_{\mathbf{x},y,D}\left[\left[\left(h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right) + \left(\bar{h}(\mathbf{x}) - y\right)\right]^2\right]$$

$$= E_{\mathbf{x},D}\left[(\bar{h}_D(\mathbf{x}) - \bar{h}(\mathbf{x}))^2\right] + 2\ E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x}) - y\right)\right]$$

$$+ E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x}) - y\right)^2\right]$$

Bias-Variance-Noise Decomposition

$$
\begin{aligned}
E_{\mathbf{x},y,D}\left[[h_D(\mathbf{x}) - y]^2\right] &= E_{\mathbf{x},y,D}\left[\left[(h_D(\mathbf{x}) - \bar{h}(\mathbf{x})) + (\bar{h}(\mathbf{x}) - y)\right]^2\right] \\
&= E_{\mathbf{x},D}\left[(\bar{h}_D(\mathbf{x}) - \bar{h}(\mathbf{x}))^2\right] + 2\ E_{\mathbf{x},y,D}\left[(h_D(\mathbf{x}) - \bar{h}(\mathbf{x}))\,(\bar{h}(\mathbf{x}) - y)\right] \\
&\quad + E_{\mathbf{x},y}\left[(\bar{h}(\mathbf{x}) - y)^2\right]
\end{aligned}
$$

The middle term of the above equation is 0 as we show below

$$
\begin{aligned}
E_{\mathbf{x},y,D}\left[(h_D(\mathbf{x}) - \bar{h}(\mathbf{x}))\,(\bar{h}(\mathbf{x}) - y)\right] &= E_{\mathbf{x},y}\left[E_D\left[h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right]\,(\bar{h}(\mathbf{x}) - y)\right] \\
&= E_{\mathbf{x},y}\left[(E_D\left[h_D(\mathbf{x})\right] - \bar{h}(\mathbf{x}))\,(\bar{h}(\mathbf{x}) - y)\right] \\
&= E_{\mathbf{x},y}\left[(\bar{h}(\mathbf{x}) - \bar{h}(\mathbf{x}))\,(\bar{h}(\mathbf{x}) - y)\right] \\
&= E_{\mathbf{x},y}\left[0\right] \\
&= 0
\end{aligned}
$$

Adapted from Killian Weinberger (Cornell)

Bias-Variance-Noise Decomposition

Returning to the earlier expression, we're left with the variance and another term

$$E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x}) - y\right)^2\right] = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}} + E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x}) - y\right)^2\right]$$

Adapted from Killian Weinberger (Cornell)

Bias-Variance-Noise Decomposition

Returning to the earlier expression, we're left with the variance and another term

$$E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x})-y\right)^2\right] = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}} + E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-y\right)^2\right]$$

We can break down the second term in the above equation as follows:

$$\begin{aligned} E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-y\right)^2\right] &= E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)+\left(\bar{y}(\mathbf{x})-y\right)^2\right] \\ &= \underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x})-y\right)^2\right]}_{\text{Noise}} + \underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2} + 2\ E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\left(\bar{y}(\mathbf{x})-y\right)\right] \end{aligned}$$

Adapted from Killian Weinberger (Cornell)

Bias-Variance-Noise Decomposition

Returning to the earlier expression, we're left with the variance and another term

$$E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x})-y\right)^2\right] = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}} + E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-y\right)^2\right]$$

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The third term in the equation above is 0

Adapted from Killian Weinberger (Cornell)

Bias-Variance-Noise Decomposition

The third term in the equation above is 0, as we show below

$$\begin{aligned}
E_{\mathbf{x},y}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\left(\bar{y}(\mathbf{x})-y\right)\right] &= E_{\mathbf{x}}\left[E_{y|\mathbf{x}}\left[\bar{y}(\mathbf{x})-y\right]\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[E_{y|\mathbf{x}}\left[\bar{y}(\mathbf{x})-y\right]\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[\left(\bar{y}(\mathbf{x})-E_{y|\mathbf{x}}\left[y\right]\right)\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[\left(\bar{y}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)\right] \\
&= E_{\mathbf{x}}\left[0\right] \\
&= 0
\end{aligned}$$

This gives us the decomposition of expected test error as follows

$$\underbrace{E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x})-y\right)^2\right]}_{\text{Expected Test Error}} = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}} + \underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x})-y\right)^2\right]}_{\text{Noise}} + \underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2}$$

Adapted from Killian Weinberger (Cornell)

Bias, Variance, and Noise

This gives us the decomposition of expected test error as follows

$$\underbrace{E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x})-y\right)^2\right]}_{\text{Expected Test Error}} = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x})-\bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}} + \underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x})-y\right)^2\right]}_{\text{Noise}}$$

$$+ \underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2}$$

Variance: Captures how much your classifier changes if you train on a different training set. How "over-specialized" is your classifier to a particular training set (overfitting)? If we have the best possible model for our training data, how far off are we from the average classifier?

Bias: What is the inherent error that you obtain from your classifier even with infinite training data? This is due to your classifier being "biased" to a particular kind of solution (e.g. linear classifier). In other words, bias is inherent to your model.

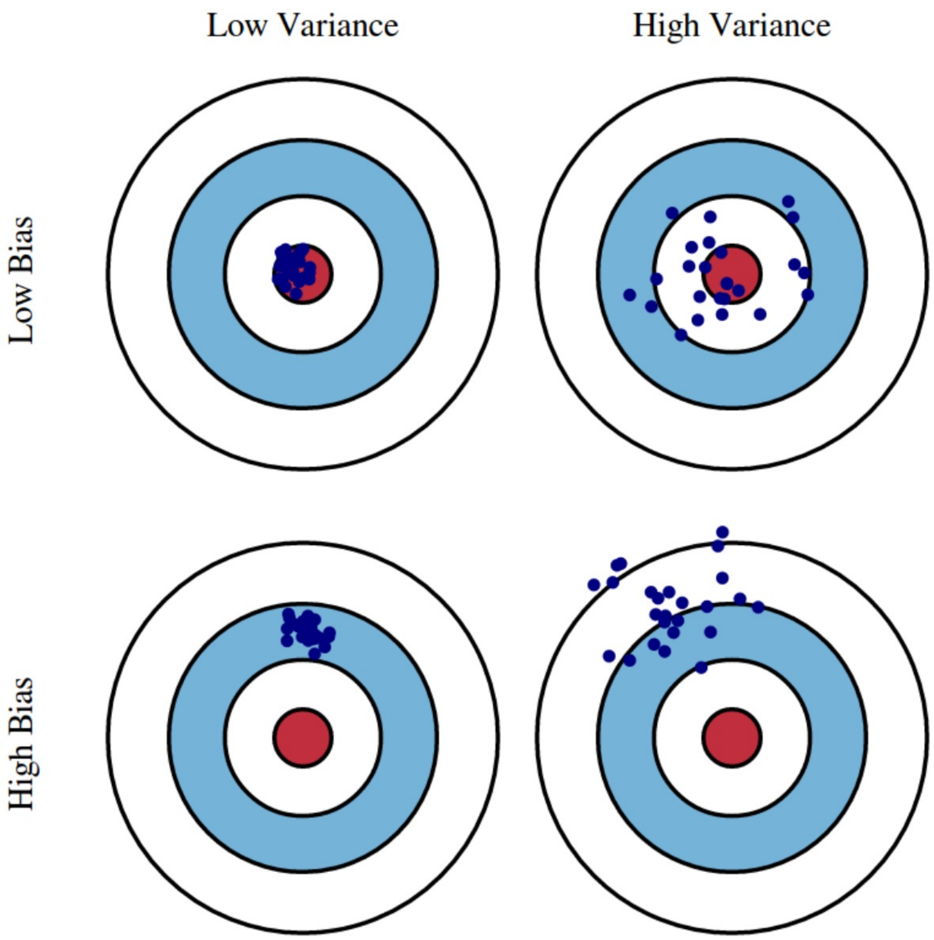
Noise: How big is the data-intrinsic noise? This error measures ambiguity due to your data distribution and feature representation. You can never beat this, it is an aspect of the data.

Bias, Variance, and Noise

$$\underbrace{E_{\mathbf{x},y,D}\left[\left(h_D(\mathbf{x}) - y\right)^2\right]}_{\text{Expected Test Error}} = \underbrace{E_{\mathbf{x},D}\left[\left(h_D(\mathbf{x}) - \bar{h}(\mathbf{x})\right)^2\right]}_{\text{Variance}}$$

$$+ \underbrace{E_{\mathbf{x},y}\left[\left(\bar{y}(\mathbf{x}) - y\right)^2\right]}_{\text{Noise}}$$

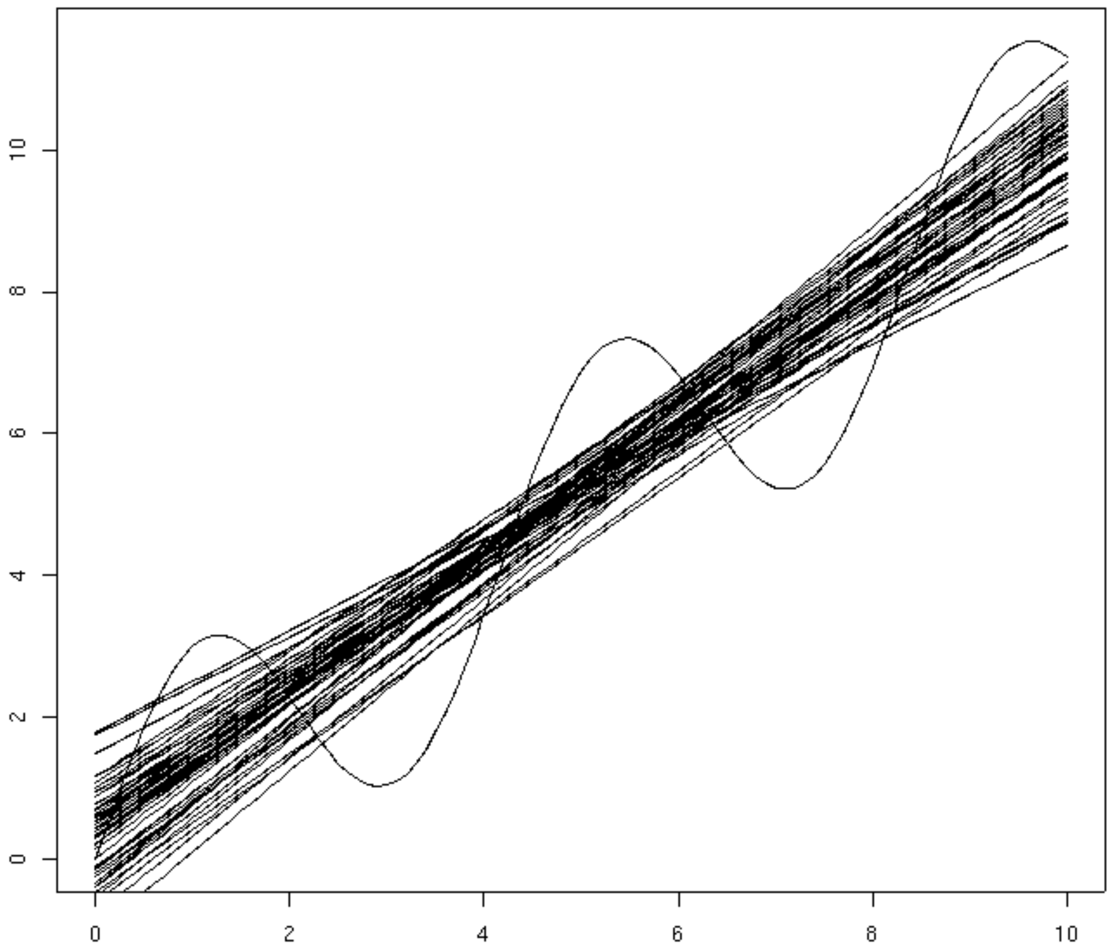
$$+ \underbrace{E_{\mathbf{x}}\left[\left(\bar{h}(\mathbf{x}) - \bar{y}(\mathbf{x})\right)^2\right]}_{\text{Bias}^2}$$



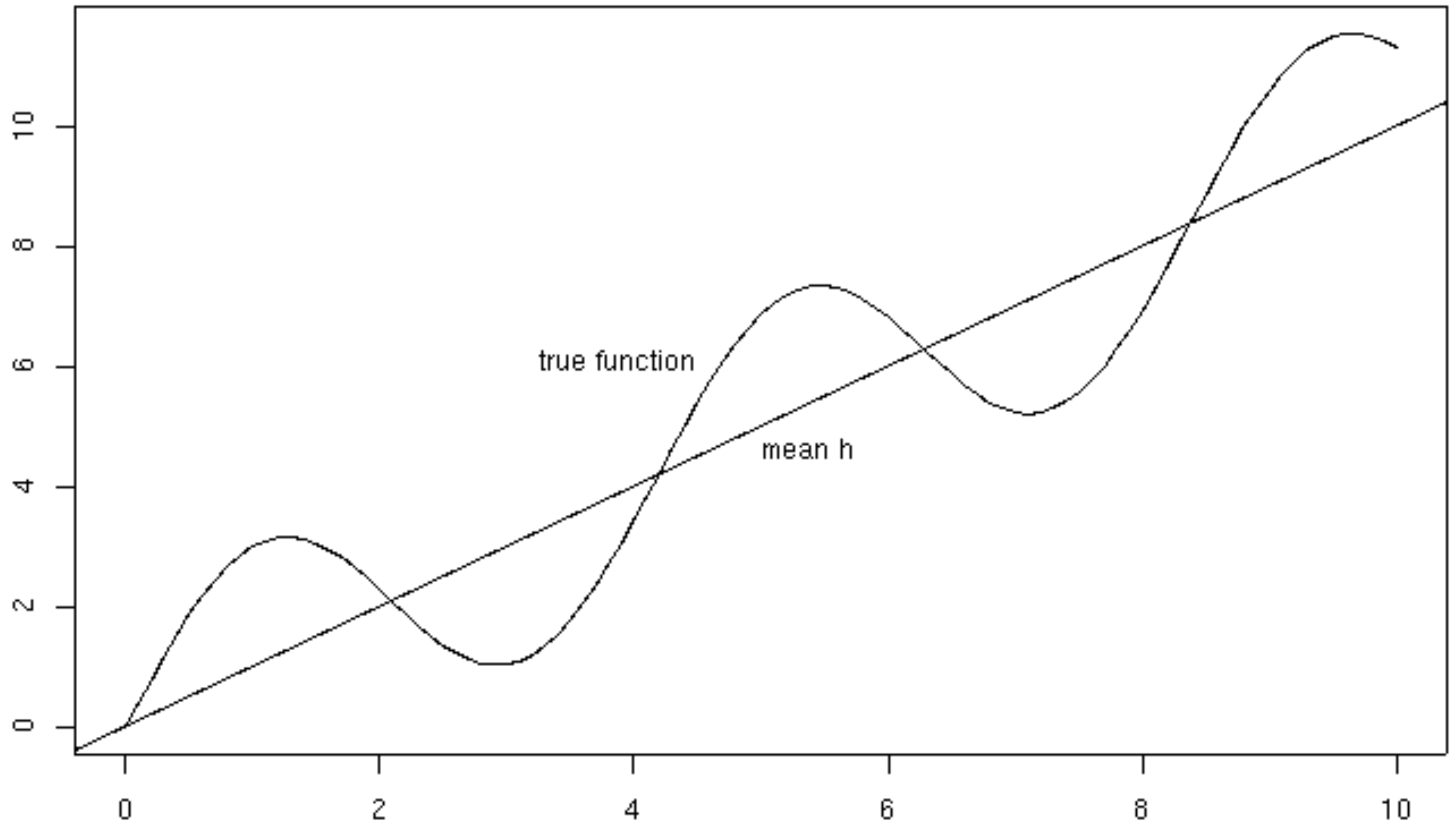
Adapted from Killian Weinberger (Cornell)

2-D Example

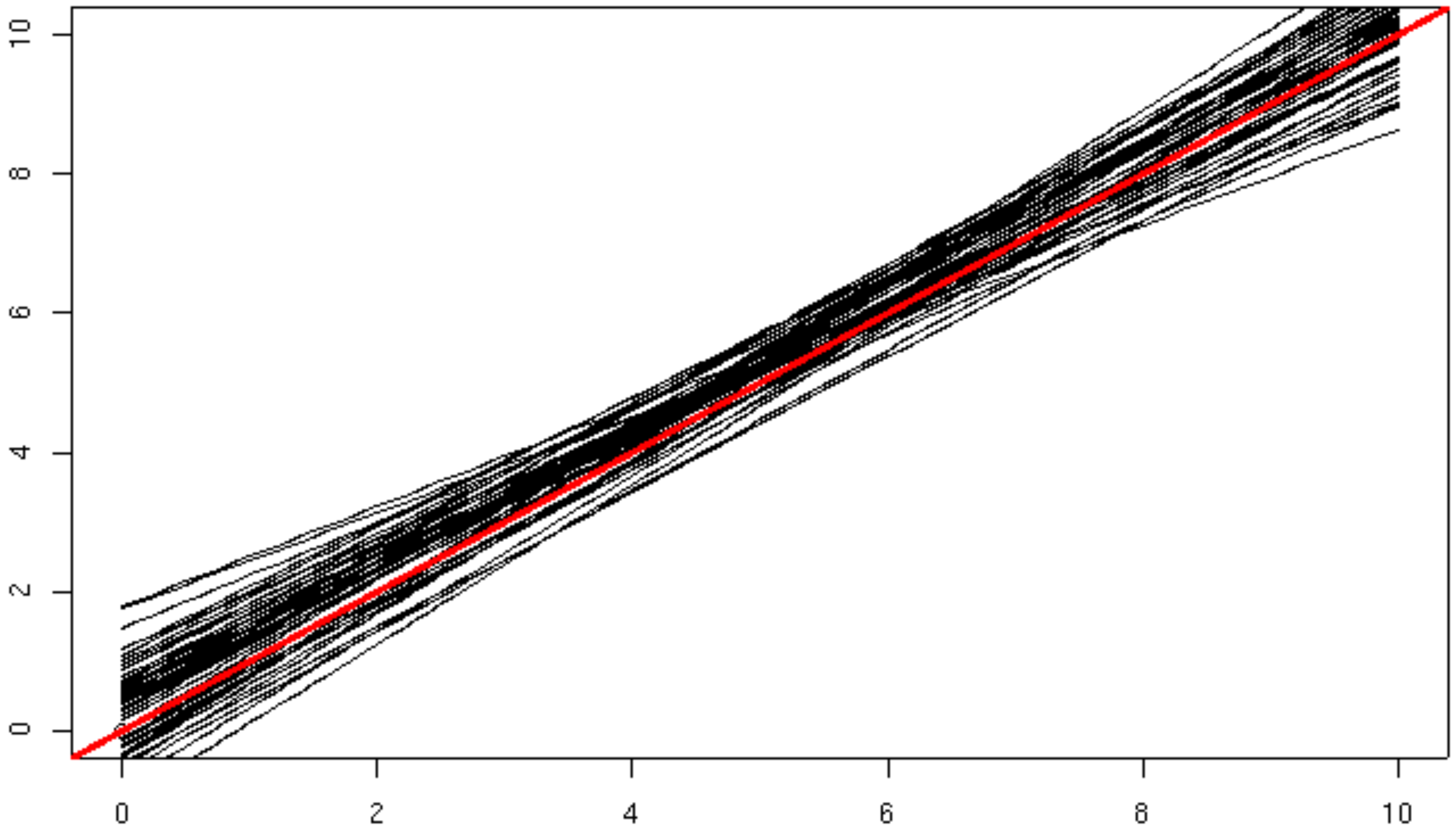
50 fits (20 examples each)



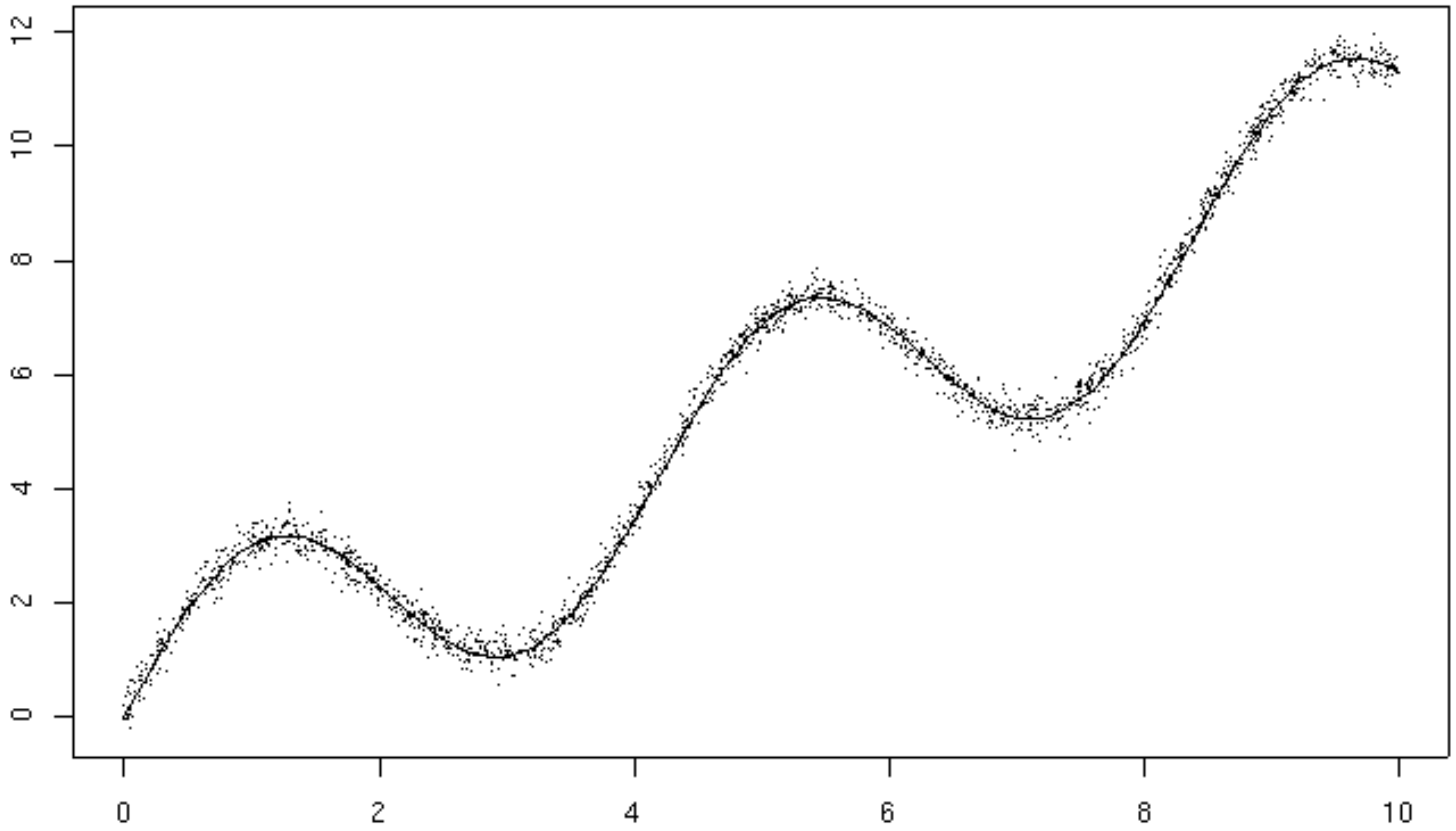
Bias



Variance

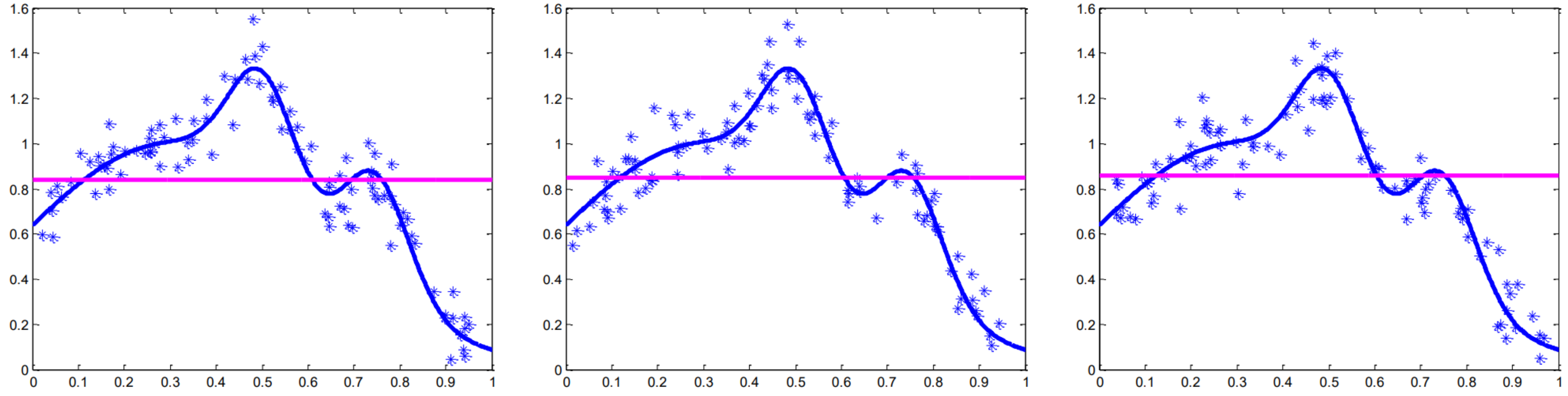


Noise

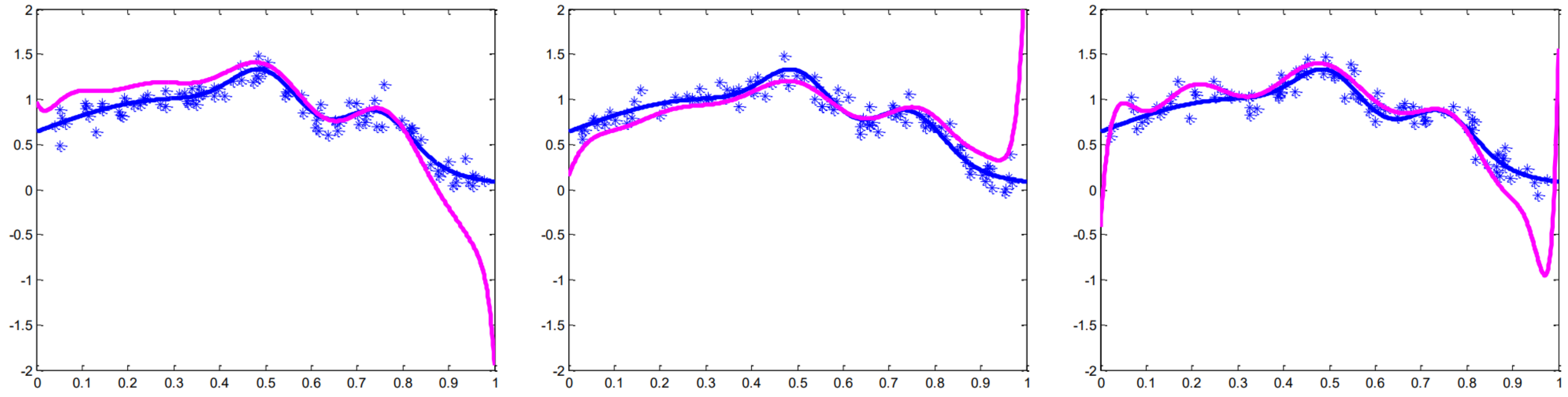


Bias-Variance Tradeoff

Large bias, Small variance – poor approximation but robust/stable



Small bias, Large variance – good approximation but instable



Bias

- Low bias
  - ?
- High bias
  - ?

Bias

- Low bias
  - Linear regression applied to linear data
  - 2nd degree polynomial applied to quadratic data
- High bias
  - Constant function applied to non-constant data
  - Linear regression applied to highly non-linear data

Variance

- Low variance
  - ?
- High variance
  - ?

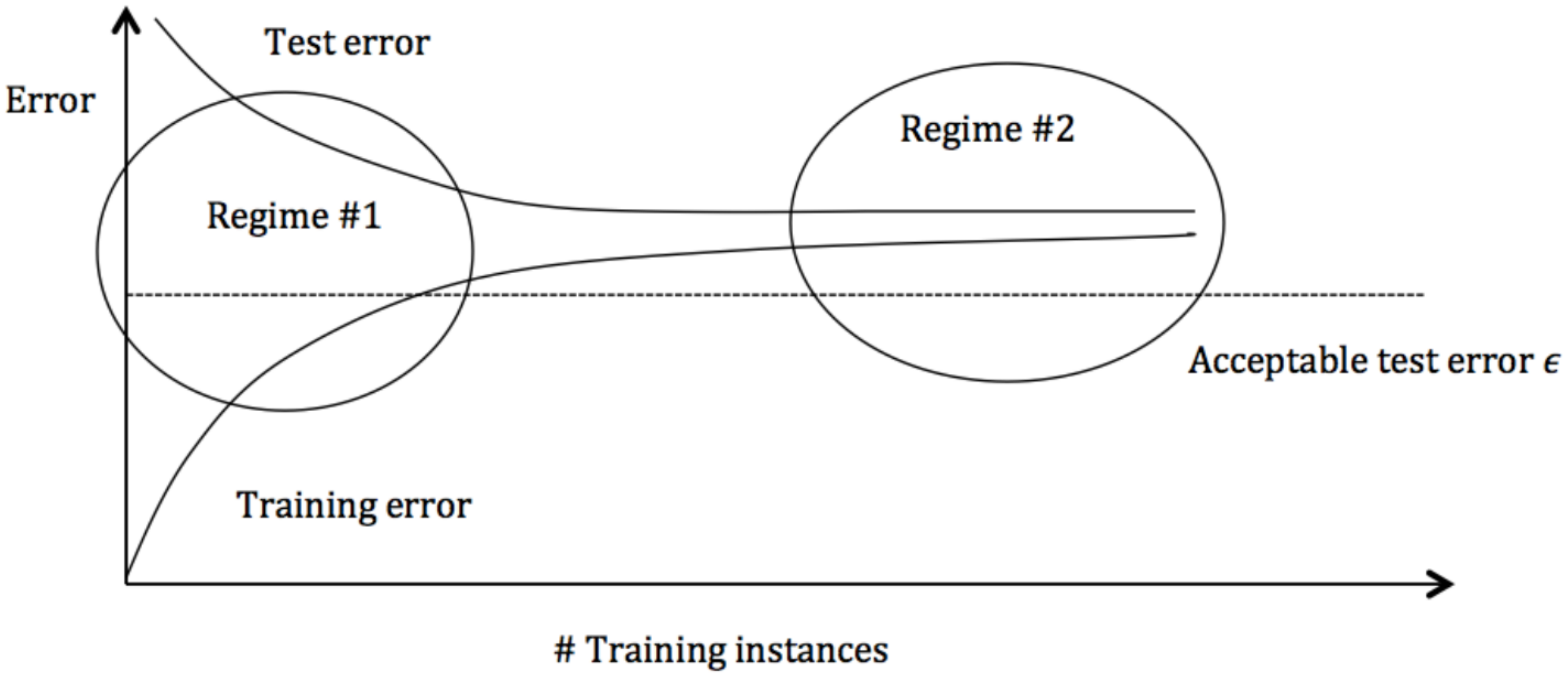
Variance

- Low variance
  - Constant function
  - Model independent of training data
- High variance
  - High degree polynomial

Bias/Variance Tradeoff

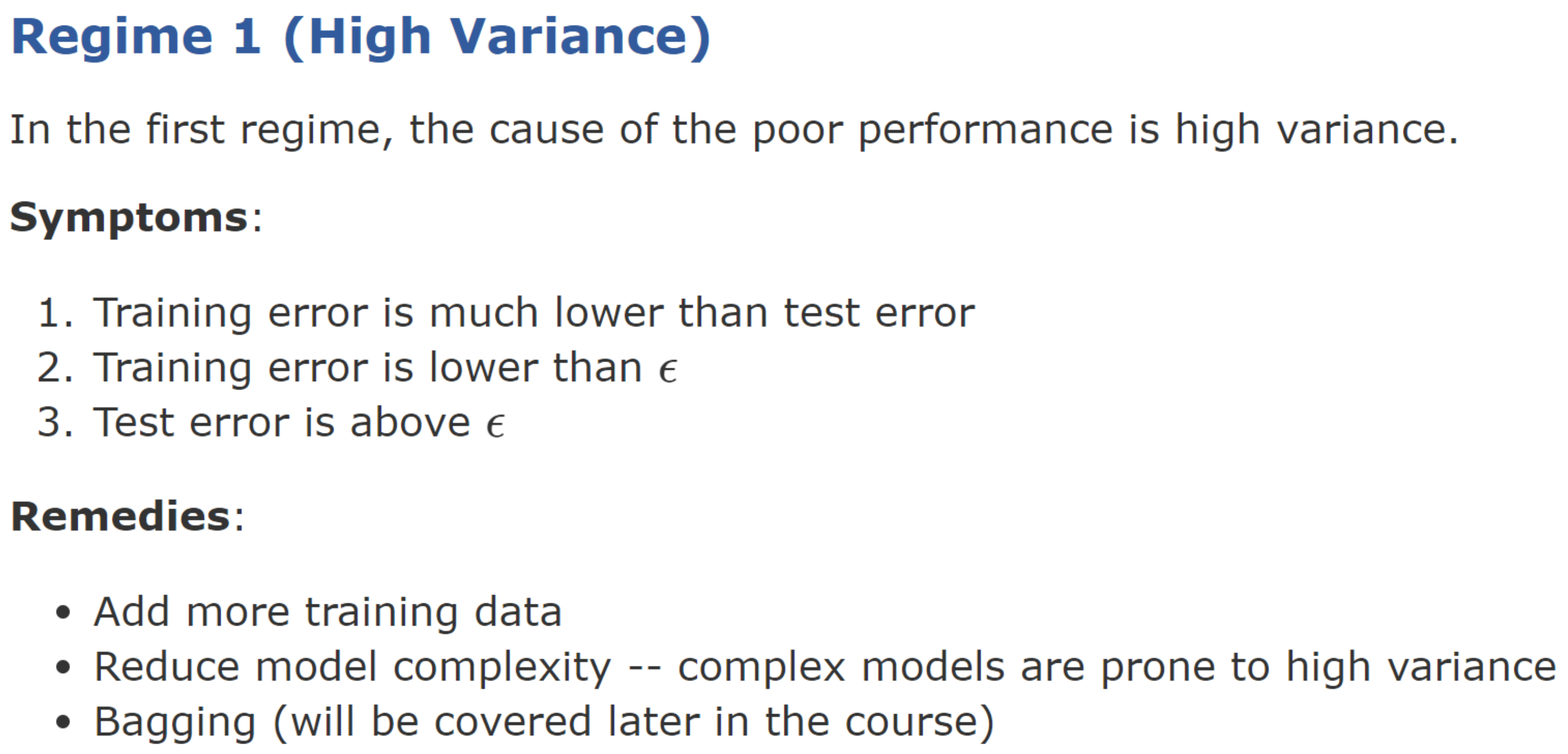
- (bias^2+variance) is what counts for prediction
- As we saw in PAC learning, we often have
  - Low bias $\Rightarrow$ high variance
  - Low variance $\Rightarrow$ high bias
  - How can we deal with this in practice?

Detecting High Variance/Bias



Adapted from Killian Weinberger (Cornell)

Detecting High Variance



Regime 1 (High Variance)

In the first regime, the cause of the poor performance is high variance.

Symptoms:

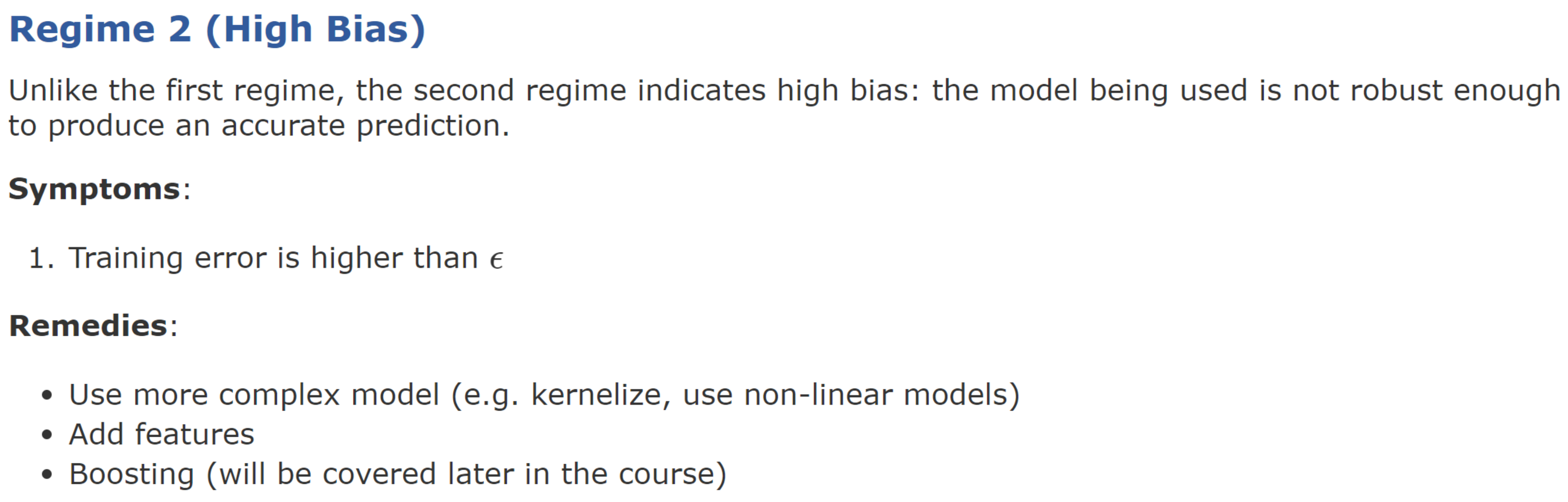
1. Training error is much lower than test error
2. Training error is lower than ϵ
3. Test error is above ϵ

Remedies:

- Add more training data
- Reduce model complexity -- complex models are prone to high variance
- Bagging (will be covered later in the course)

Adapted from Killian Weinberger (Cornell)

Detecting High Bias



Regime 2 (High Bias)

Unlike the first regime, the second regime indicates high bias: the model being used is not robust enough to produce an accurate prediction.

Symptoms:

1. Training error is higher than ϵ

Remedies:

- Use more complex model (e.g. kernelize, use non-linear models)
- Add features
- Boosting (will be covered later in the course)

Adapted from Killian Weinberger (Cornell)

How to select the right model?

Model Spaces with increasing complexity:

- Nearest-Neighbor classifiers with varying neighborhood sizes k = 1,2,3,…
  Small neighborhood => Higher complexity

- Decision Trees with depth k or with k leaves
  Higher depth/ More # leaves => Higher complexity

- Regression with polynomials of order k = 0, 1, 2, …
  Higher degree => Higher complexity

- Kernel Regression with bandwidth h
  Small bandwidth => Higher complexity

How can we select the right complexity model ?

Held out Validation Set

We would like to pick the model that has smallest generalization error.

Can judge generalization error by using an independent sample of data.

Hold – out procedure:

n data points available $D \equiv \{X_i, Y_i\}_{i=1}^{n}$

1) Split into two sets: Training dataset $D_T = \{X_i, Y_i\}_{i=1}^{m}$ Validation dataset $D_V = \{X_i, Y_i\}_{i=m+1}^{n}$ NOT test Data !!

2) Use D_T for training a predictor from each model class:

$$\widehat{f}_\lambda = \arg\min_{f \in \mathcal{F}_\lambda} \underbrace{\widehat{R}_T(f)}$$

→ Evaluated on training dataset D_T

Held out Validation Set

3) Use *Dv* to select the model class which has smallest empirical error on D_V

$$\widehat{\lambda} = \arg\min_{\lambda \in \Lambda} \widehat{R}_V(\widehat{f}_\lambda) \xrightarrow{} \text{Evaluated on validation dataset } D_V$$

4) Hold-out predictor

$$\widehat{f} = \widehat{f}_{\widehat{\lambda}}$$

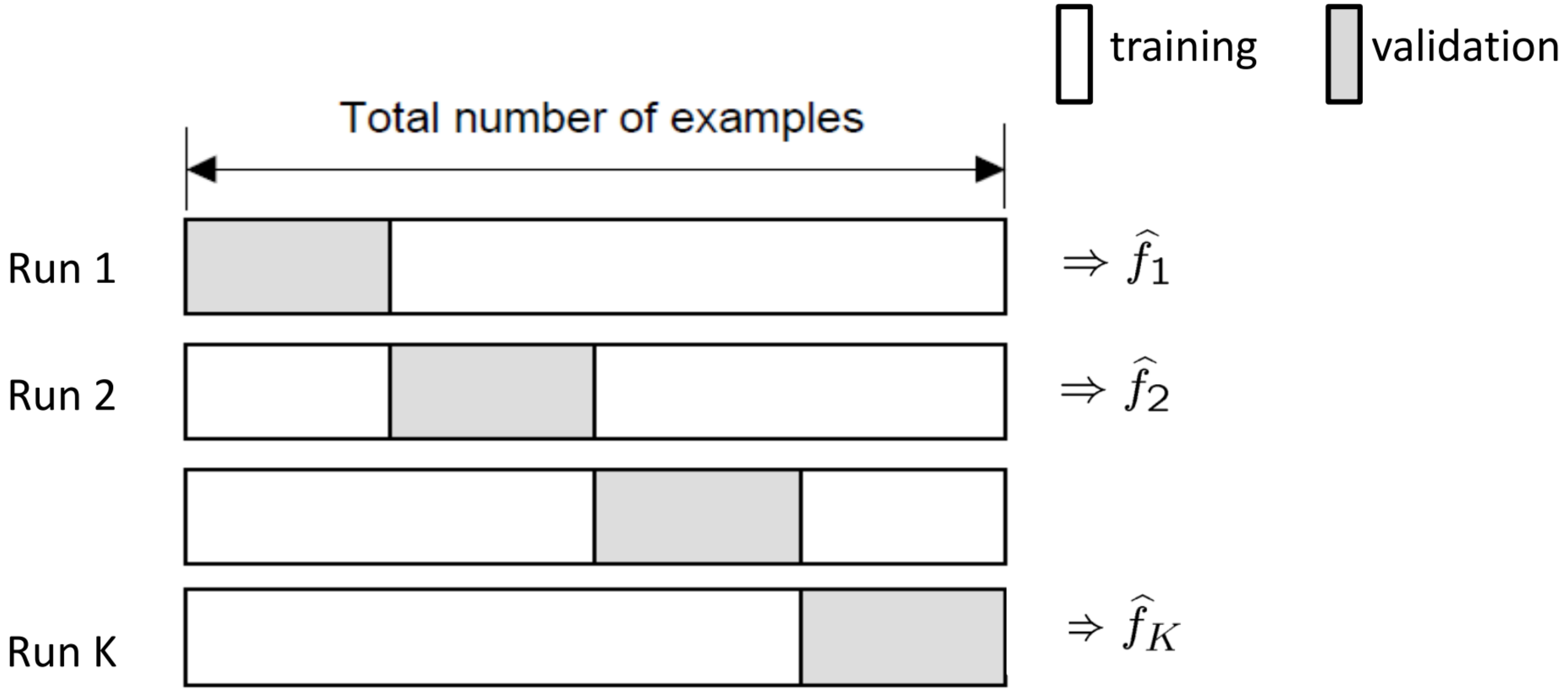
Intuition: Small error on one set of data will not imply small error on a randomly sub-sampled second set of data

Ensures method is "stable"

Cross Validation

K-fold cross-validation

Create K-fold partition of the dataset.
Form K hold-out predictors, each time using one partition as validation and rest K-1 as training datasets.
Final predictor is average/majority vote over the K hold-out estimates.



Ensemble Methods

Reduce Variance Without Increasing Bias

- Averaging reduces variance: let $Z_1, \dots, Z_N$ be i.i.d random variables

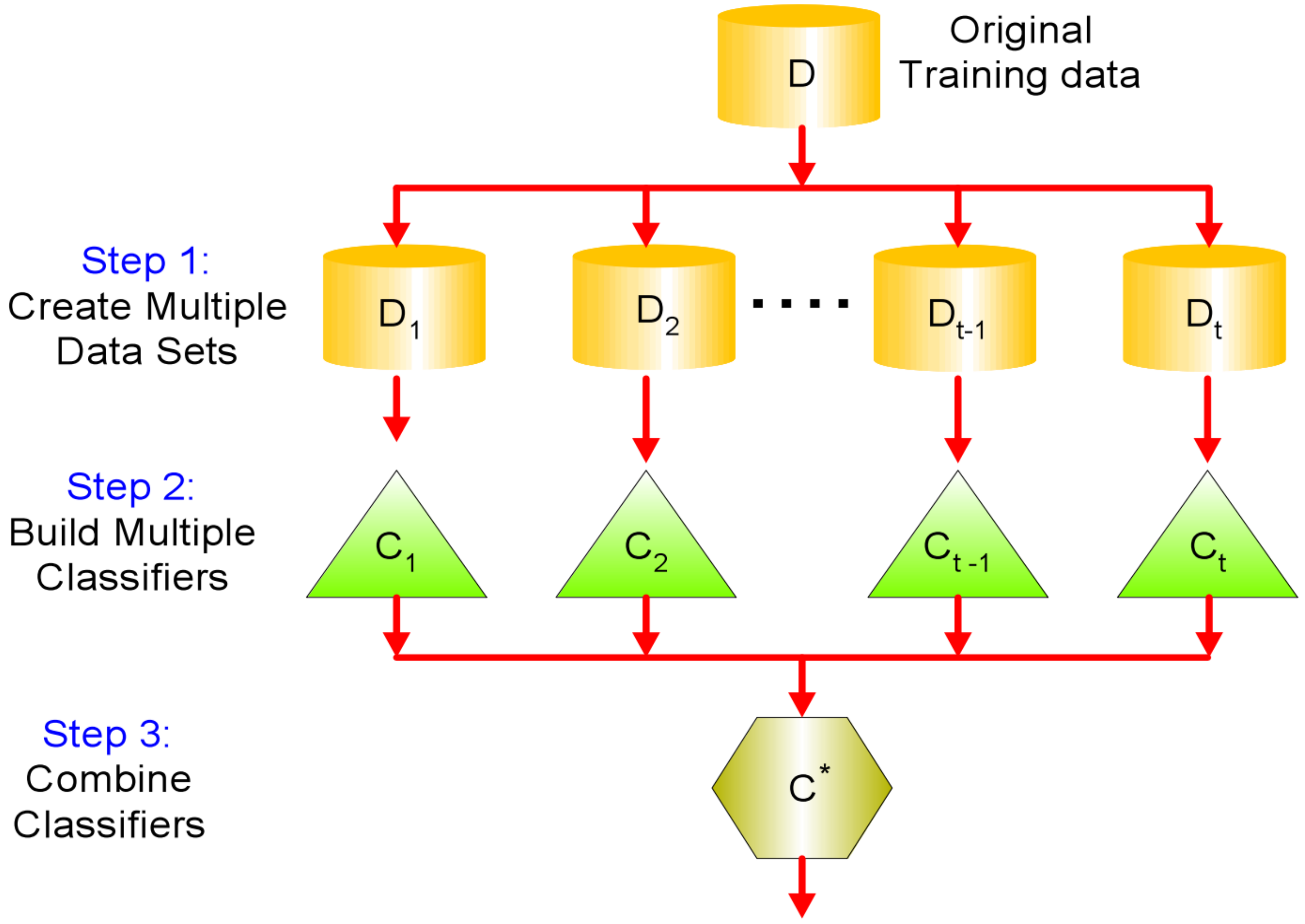
$$Var\left(\frac{1}{N}\sum_i Z_i\right) = \frac{1}{N} Var(Z_i)$$

- Idea: average models to reduce model variance
- How to apply it to our setting?
  - Only one training set
  - Where do multiple models come from?

Bagging: Bootstrap Aggregation

- Take repeated bootstrap samples from training set D (Breiman, 1994)
- Bootstrap sampling: Given set D containing N training examples, create D' by drawing N examples at random **with replacement** from D
- Bagging:
  - Create k bootstrap samples $D_1, \ldots, D_k$
  - Train distinct classifier on each D_i
  - Classify new instance by majority vote / average

Bagging: Bootstrap Aggregation



D
Original Training data
Step 1: Create Multiple Data Sets
D_1
D_2
D_{t-1}
D_t
Step 2: Build Multiple Classifiers
C_1
C_2
C_{t-1}
C_t
Step 3: Combine Classifiers
C^*

[image from the slides of David Sontag]

Bagging

Data	1	2	3	4	5	6	7	8	9	10
BS 1	7	1	9	10	7	8	8	4	7	2
BS 2	8	1	3	1	1	9	7	4	10	1
BS 3	5	4	8	8	2	5	5	7	8	8

- Build a classifier from each bootstrap sample
- In each bootstrap sample, each data point has probability $\left(1-\frac{1}{N}\right)^N$ of not being selected
    - Expected number of distinct data points in each sample is then

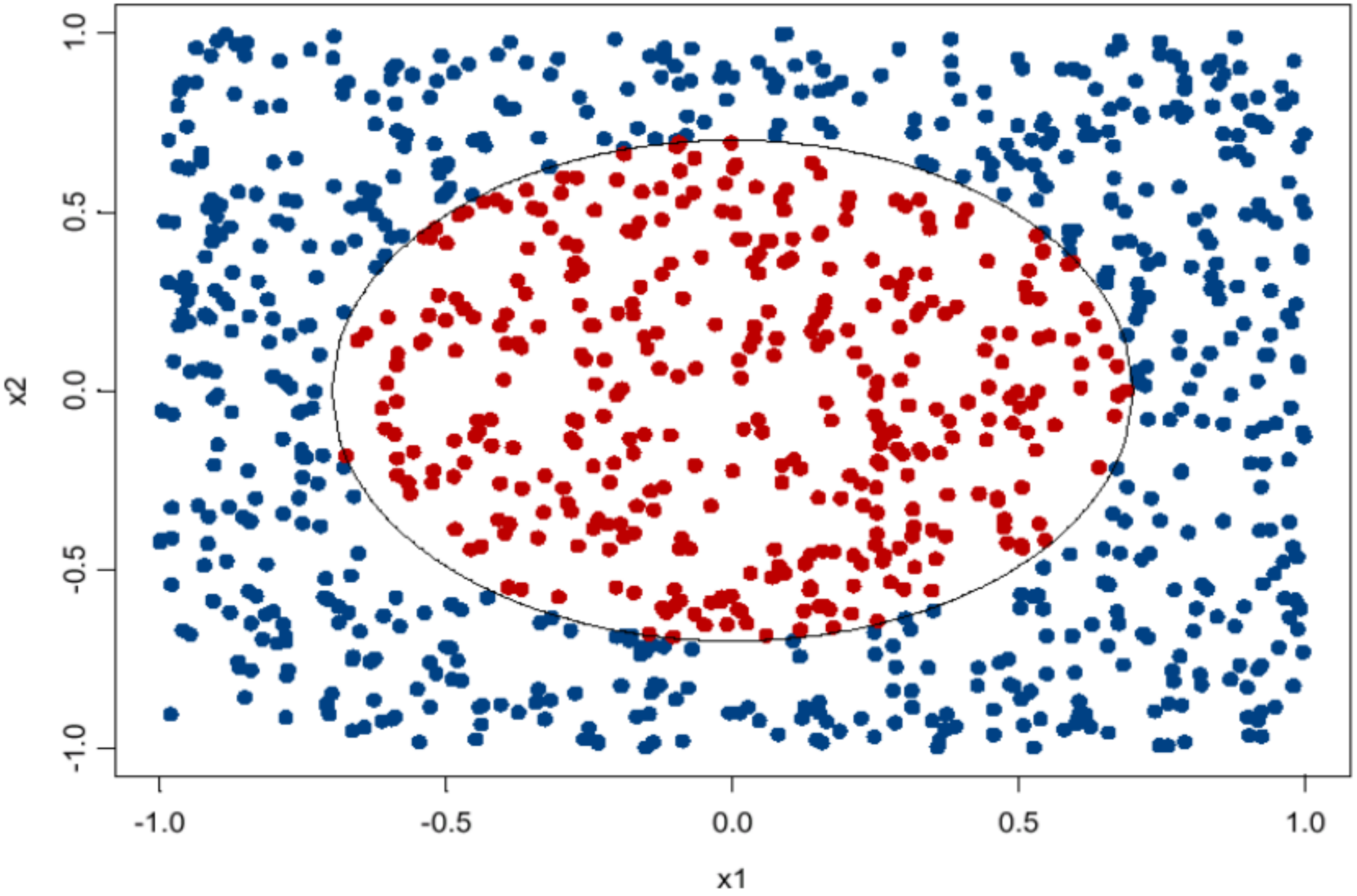
$$N \cdot \left(1 - \left(1 - \frac{1}{N}\right)^N\right) \approx N \cdot (1 - \exp(-1)) = .632 \cdot N$$

Bagging

Data	1	2	3	4	5	6	7	8	9	10
BS 1	7	1	9	10	7	8	8	4	7	2
BS 2	8	1	3	1	1	9	7	4	10	1
BS 3	5	4	8	8	2	5	5	7	8	8

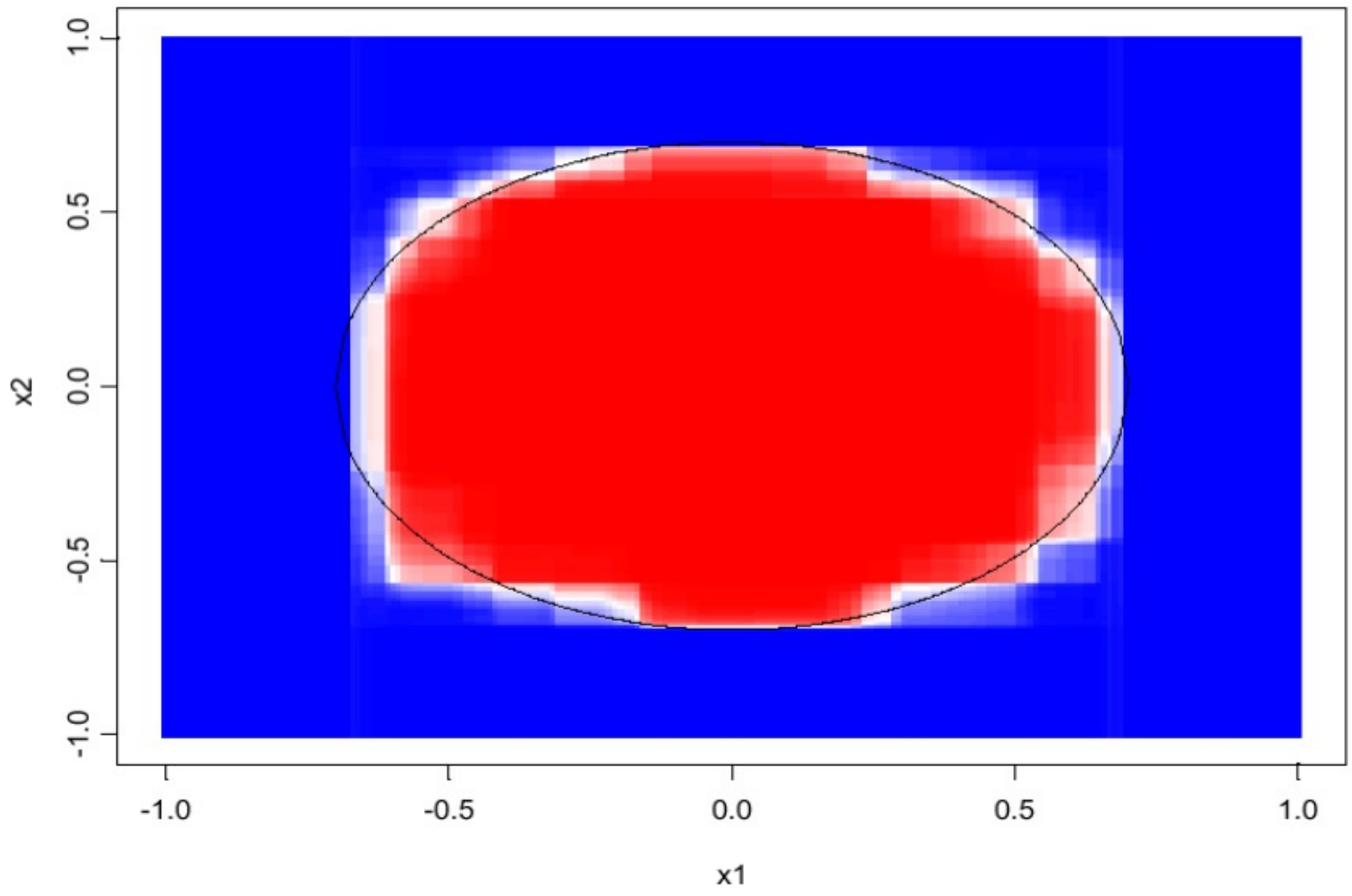
- Build a classifier from each bootstrap sample
- In each bootstrap sample, each data point has probability $\left(1 - \frac{1}{N}\right)^N$ of not being selected
  - If we have 1 TB of data, each bootstrap sample will be ~ 632GB (this can present computational challenges, e.g., you shouldn't replicate the data)

Decision Tree Bagging



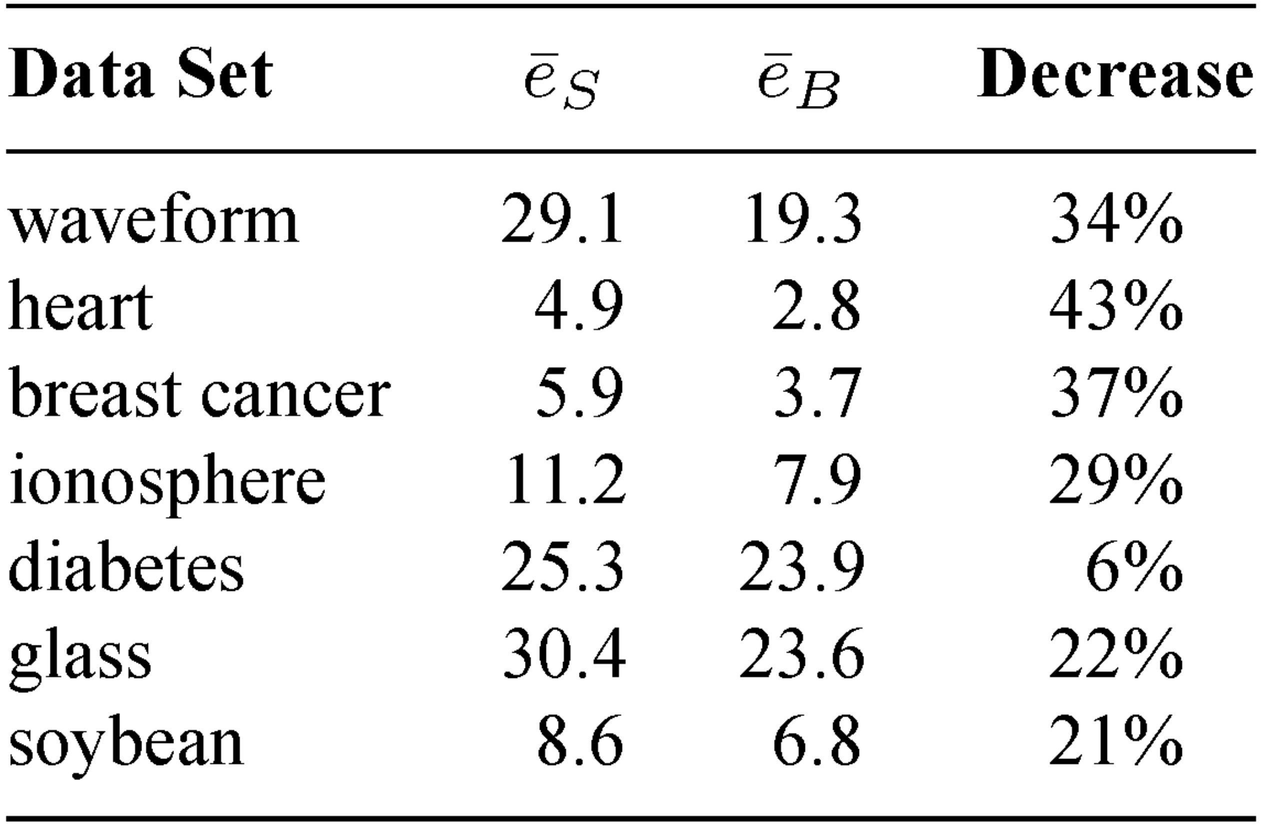
[image from the slides of David Sontag]

Decision Tree Bagging (100 Bagged Trees)



[image from the slides of David Sontag]

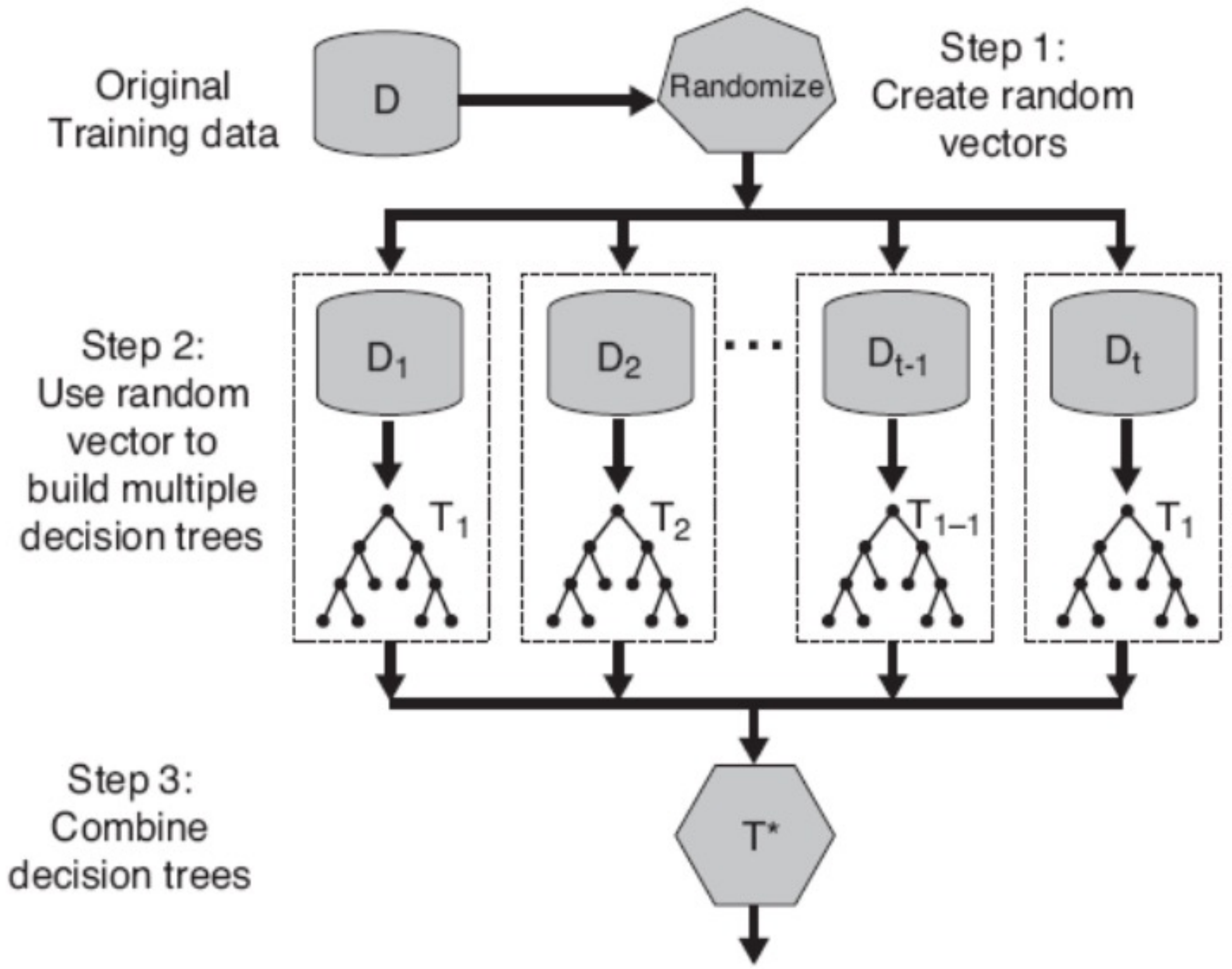
Bagging Results



	Without Bagging	With Bagging	
Data Set	$\bar{e}_S$	$\bar{e}_B$	**Decrease**
waveform	29.1	19.3	34%
heart	4.9	2.8	43%
breast cancer	5.9	3.7	37%
ionosphere	11.2	7.9	29%
diabetes	25.3	23.9	6%
glass	30.4	23.6	22%
soybean	8.6	6.8	21%

Breiman “Bagging Predictors” Berkeley Statistics Department TR#421, 1994

Random Forests



Original Training data
D
Randomize
Step 1: Create random vectors
Step 2: Use random vector to build multiple decision trees
D_1
D_2
D_{t-1}
D_t
T_1
T_2
T_{1-1}
T_1
Step 3: Combine decision trees
T*

Random Forests

- Ensemble method specifically designed for decision tree classifiers
- Introduce two sources of randomness: “bagging” and “random input vectors”
  - Bagging method: each tree is grown using a bootstrap sample of training data
  - Random vector method: best split at each node is chosen from a random sample of m attributes instead of all attributes

Random Forest Algorithm

- For $b = 1$ to B
  - Draw a bootstrap sample of size N from the data
  - Grow a tree T_b using the bootstrap sample as follows
    - Choose m attributes uniformly at random from the data
    - Choose the best attribute among the m to split on
    - Split on the best attribute and recurse (until partitions have fewer than s_{min} number of nodes)

- Prediction for a new data point x
  - Regression: $\frac{1}{B}\sum_b T_b(x)$
  - Classification: choose the majority class label among $T_1(x), \dots, T_B(x)$

Random Forest Demo

A demo of random forests implemented in JavaScript

When Will Bagging Improve Accuracy?

- Depends on the stability of the base-level classifiers
- A learner is unstable if a small change to the training set causes a large change in the output hypothesis
  - If small changes in D cause large changes in the output, then there will likely be an improvement in performance with bagging
- Bagging can help unstable procedures, but could hurt the performance of stable procedures
  - Decision trees are unstable
  - k-nearest neighbor is stable