Variance Reduction and Ensemble Methods

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Based on the slides of Vibhav Gogate and David Sontag

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

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

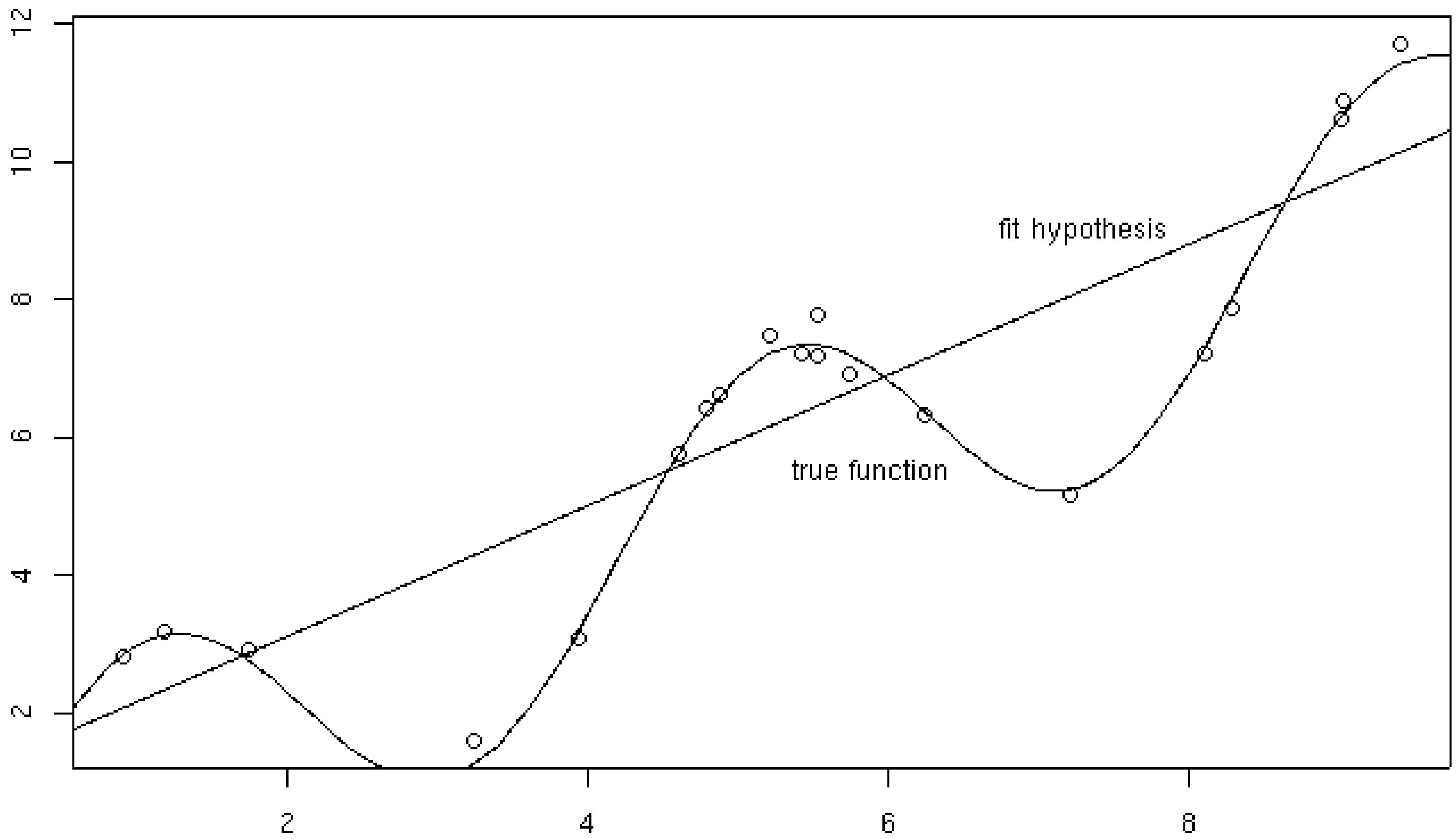
- True function is $y = f(x) + \epsilon$
  - where ϵ is normally distributed with zero mean and standard deviation σ
- Given a set of training examples, $\left(x^{(1)}, y^{(1)}\right), \dots, \left(x^{(n)}, y^{(n)}\right)$, we fit a hypothesis $g(x) = w^T x + b$ to the data to minimize the squared error

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

2-D Example

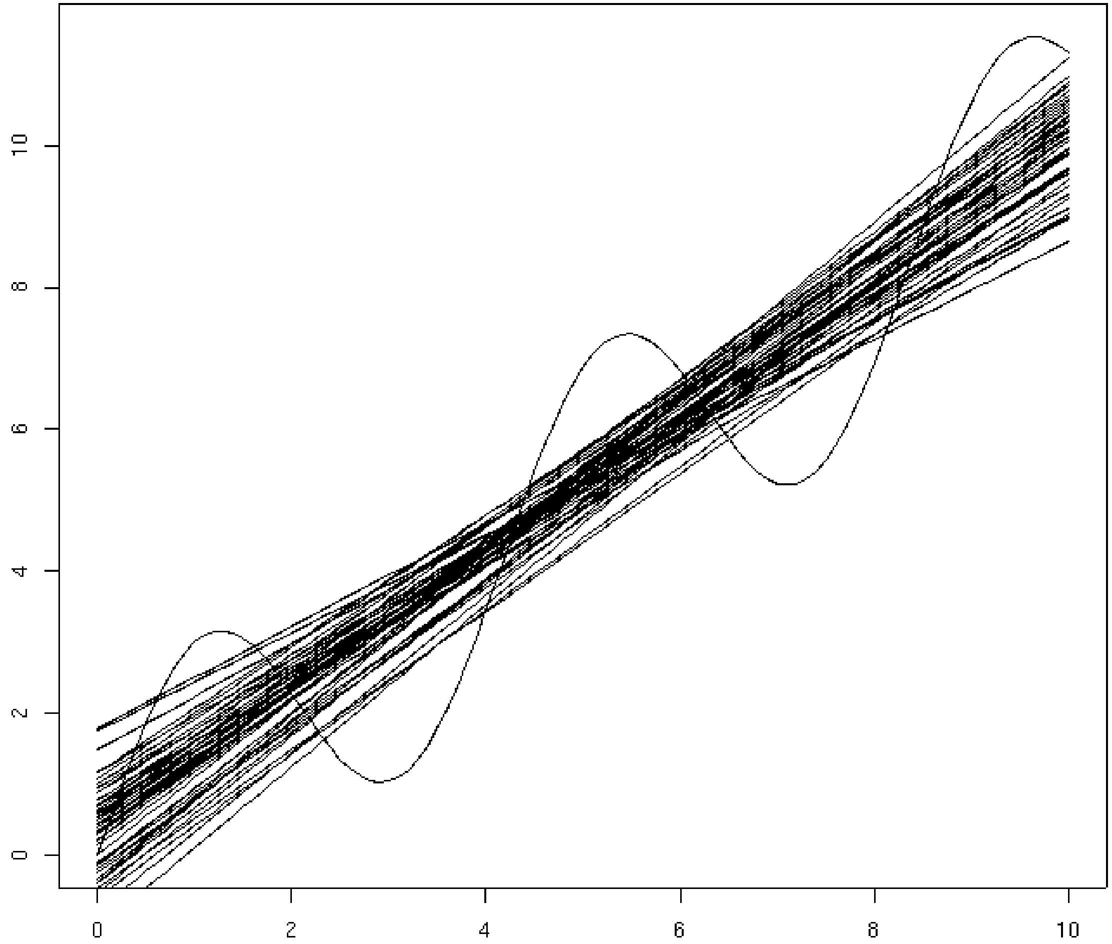
Sample 20 points from

$$f(x) = x + 2\sin(1.5x) + N(0,0.2)$$



2-D Example

50 fits (20 examples each)



Bias-Variance Analysis

- Given a new data point x' with observed value $y' = f(x') + \epsilon$, want to understand the expected prediction error

- Suppose that training samples are drawn independently from a distribution $p(S)$, want to compute

$$E\left[\left(y' - g_S(x')\right)^2\right]$$

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

$$
\begin{aligned}
E\left[\left(y' - g_S(x')\right)^2\right] &= E[g_S(x')^2 - 2g_S(x')y' + y'^2] \\
&= E[g_S(x')^2] - 2E[g_S(x')]E[y'] + E\left[y'^2\right] \\
&= Var\left(g_S(x')\right) + E[g_S(x')]^2 - 2E[g_S(x')]f(x') \\
&\qquad + Var(y') + f(x')^2 \\
&= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + Var(\epsilon) \\
&= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + \sigma^2
\end{aligned}
$$

Bias-Variance-Noise Decomposition

$$E\left[\left(y' - g_S(x')\right)^2\right] = E[g_S(x')^2 - 2g_S(x')y' + y'^2]$$

$$= E[g_S(x')^2] - 2E[g_S(x')]E[y'] + E\left[y'^2\right]$$

The samples S and the noise ϵ are independent

$$= Var\left(g_S(x')\right) + E[g_S(x')]^2 - 2E[g_S(x')]f(x') + Var(y') + f(x')^2$$

$$= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + Var(\epsilon)$$

$$= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + \sigma^2$$

Bias-Variance-Noise Decomposition

$$E\left[\left(y' - g_S(x')\right)^2\right] = E[g_S(x')^2 - 2g_S(x')y' + y'^2]$$

$$= E[g_S(x')^2] - 2E[g_S(x')]E[y'] + E\left[y'^2\right]$$

Follows from definition of variance

$$= Var\left(g_S(x')\right) + E[g_S(x')]^2 - 2E[g_S(x')]f(x')$$

$$+ Var(y') + f(x')^2$$

$$= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + Var(\epsilon)$$

$$= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + \sigma^2$$

Bias-Variance-Noise Decomposition

$$E\left[\left(y' - g_S(x')\right)^2\right] = E[g_S(x')^2 - 2g_S(x')y' + y'^2]$$

$$= E[g_S(x')^2] - 2E[g_S(x')]E[y'] + E\left[y'^2\right]$$

$E[y'] = f(x')$

$$= Var\left(g_S(x')\right) + E[g_S(x')]^2 - 2E[g_S(x')]f(x')$$
$$+ Var(y') + f(x')^2$$

$$= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + Var(\epsilon)$$

$$= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + \sigma^2$$

Bias-Variance-Noise Decomposition

$$E\left[\left(y' - g_S(x')\right)^2\right] = E[g_S(x')^2 - 2g_S(x')y' + y'^2]$$

$$= E[g_S(x')^2] - 2E[g_S(x')]E[y'] + E\left[y'^2\right]$$

$$= Var\left(g_S(x')\right) + E[g_S(x')]^2 - 2E[g_S(x')]f(x')$$

$$+ Var(y') + f(x')^2$$

$$= Var\left(g_S(x')\right) + \left(E[g_S(x')] - f(x')\right)^2 + Var(\epsilon)$$

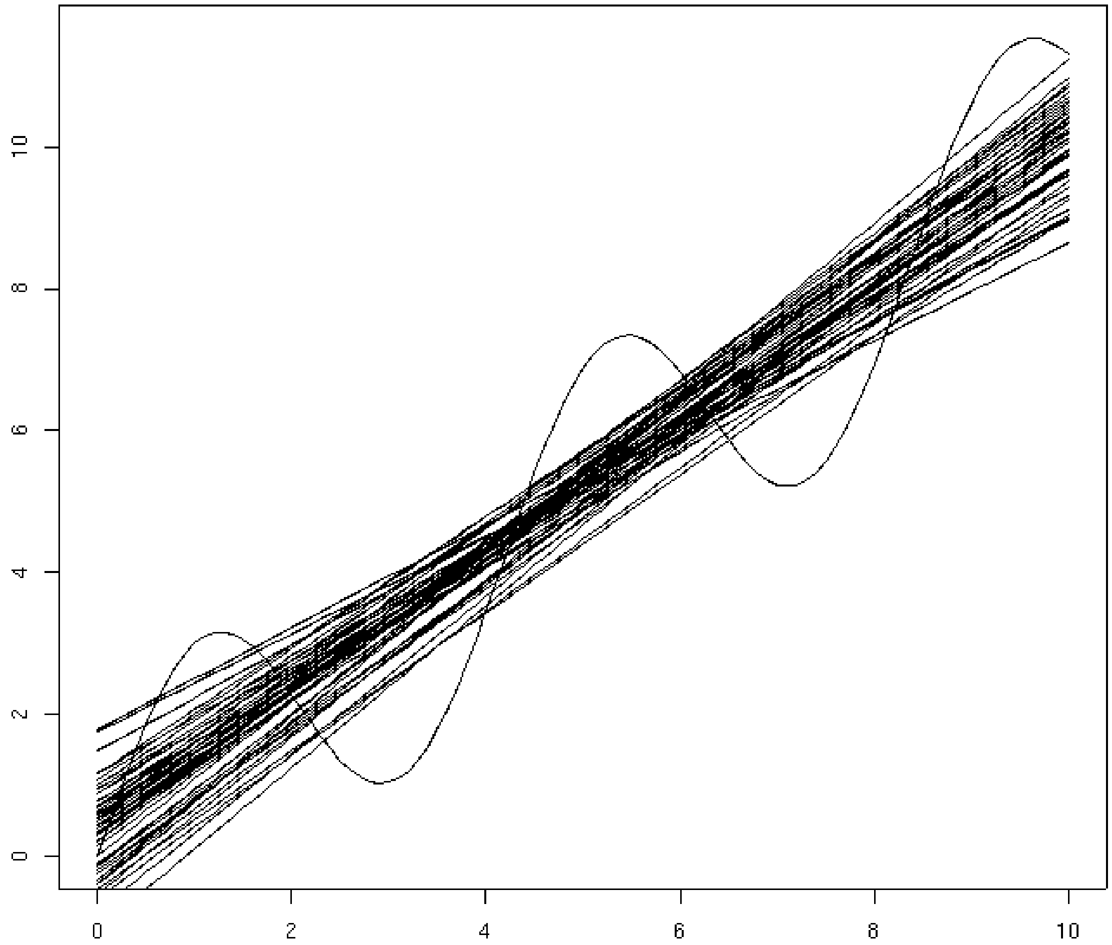
$$= \underbrace{Var\left(g_S(x')\right)}_{\text{Variance}} + \underbrace{\left(E[g_S(x')] - f(x')\right)^2}_{\text{Bias}} + \underbrace{\sigma^2}_{\text{Noise}}$$

Bias, Variance, and Noise

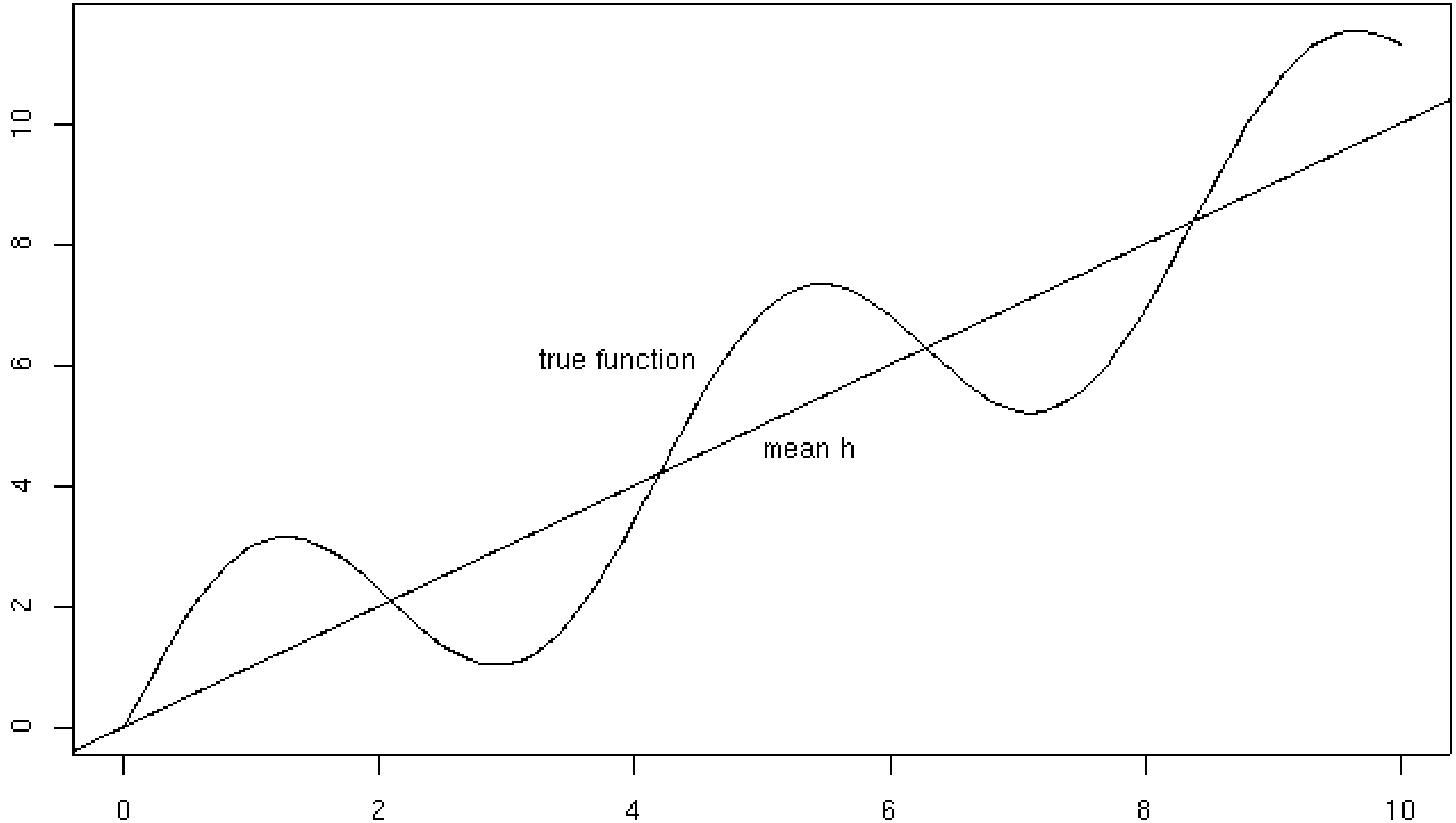
- Variance: $E[\,(g_S(x') - E[g_S(x')])^2\,]$
  – Describes how much $g_S(x')$ varies from one training set S to another
- Bias: $E[g_S(x')] - f(x')$
  – Describes the average error of $g_S(x')$
- Noise: $E\left[\left(y' - f(x')\right)^2\right] = E[\epsilon^2] = \sigma^2$
  – Describes how much y' varies from $f(x')$

2-D Example

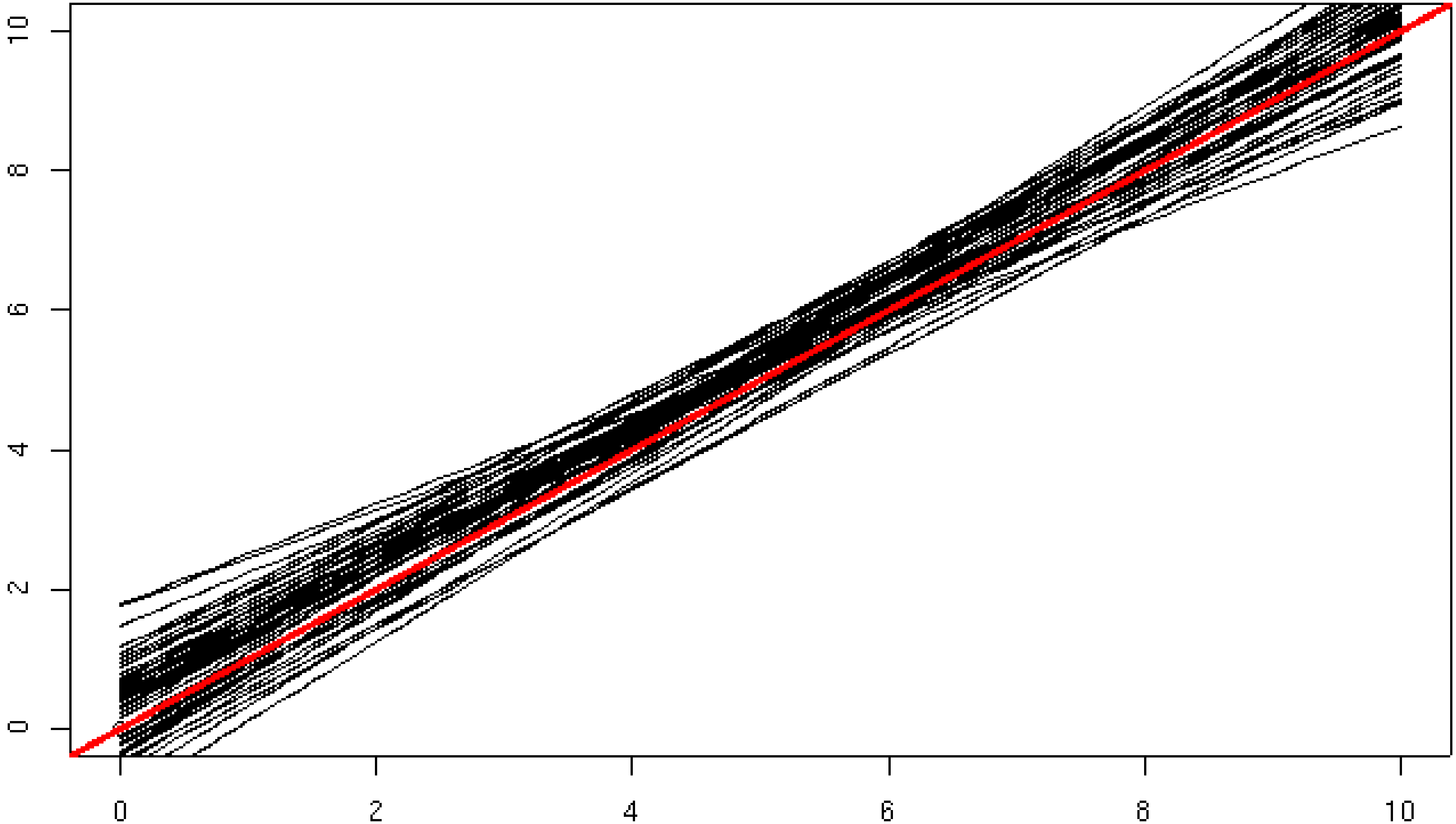
50 fits (20 examples each)



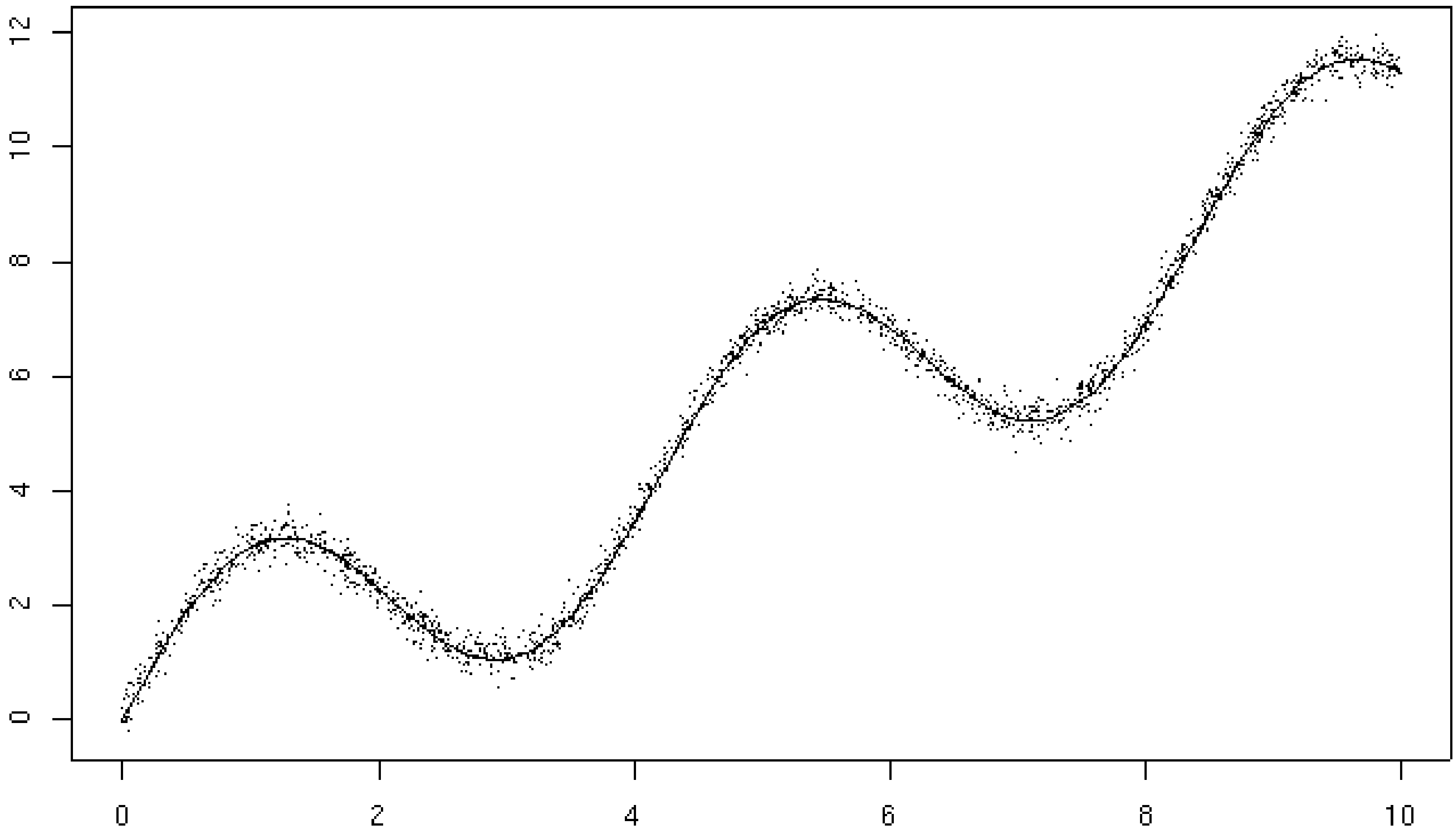
Bias



Variance



Noise



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
  - Linear regression applied to 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
  - Is this a firm rule?

Reduce Variance Without Increasing Bias

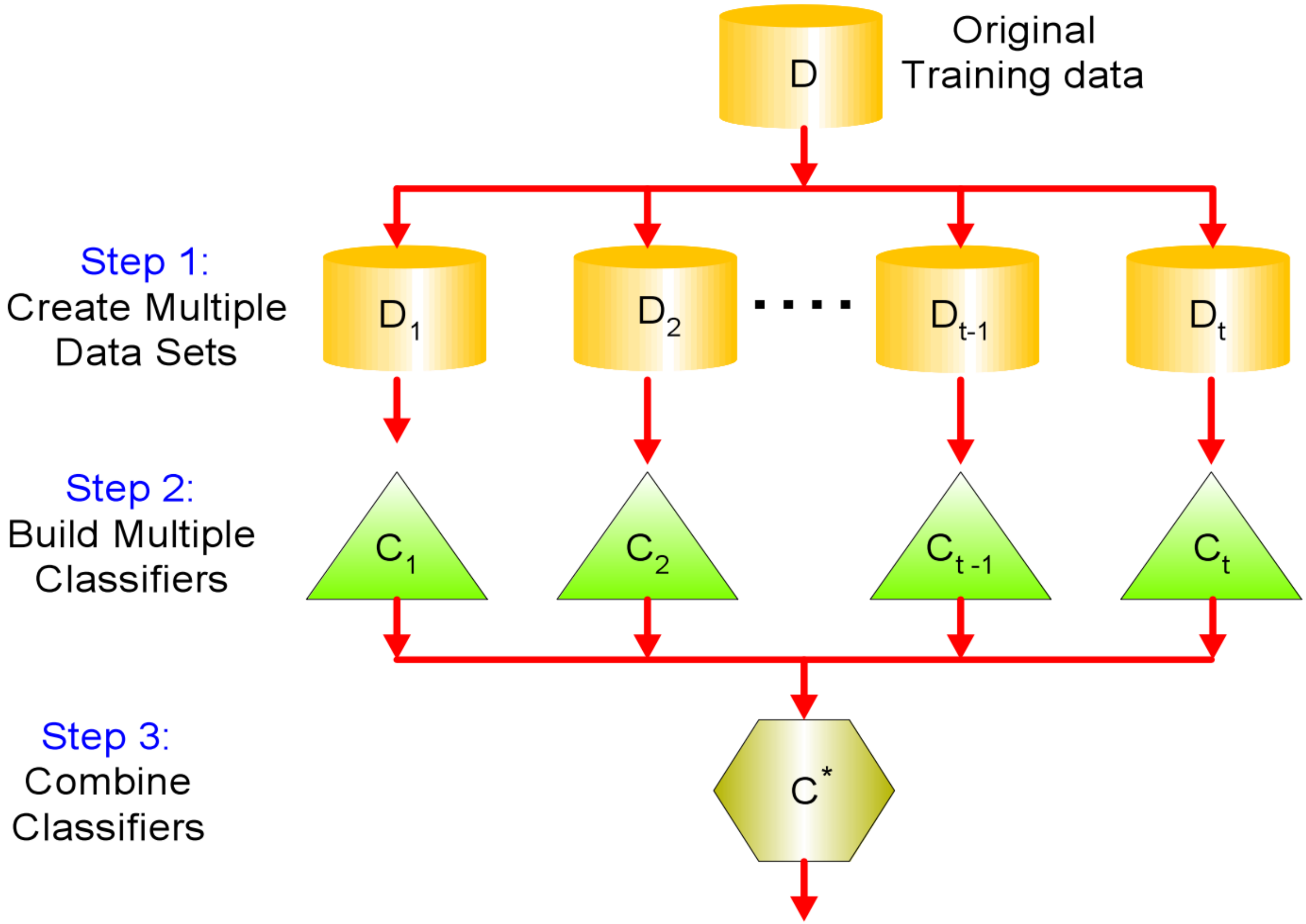
- Averaging reduces variance: let $Z_1, \ldots, Z_N$ be i.i.d random variables

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

- Idea: average models to reduce model variance
- The problem
  - 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



[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 data points in each sample is then

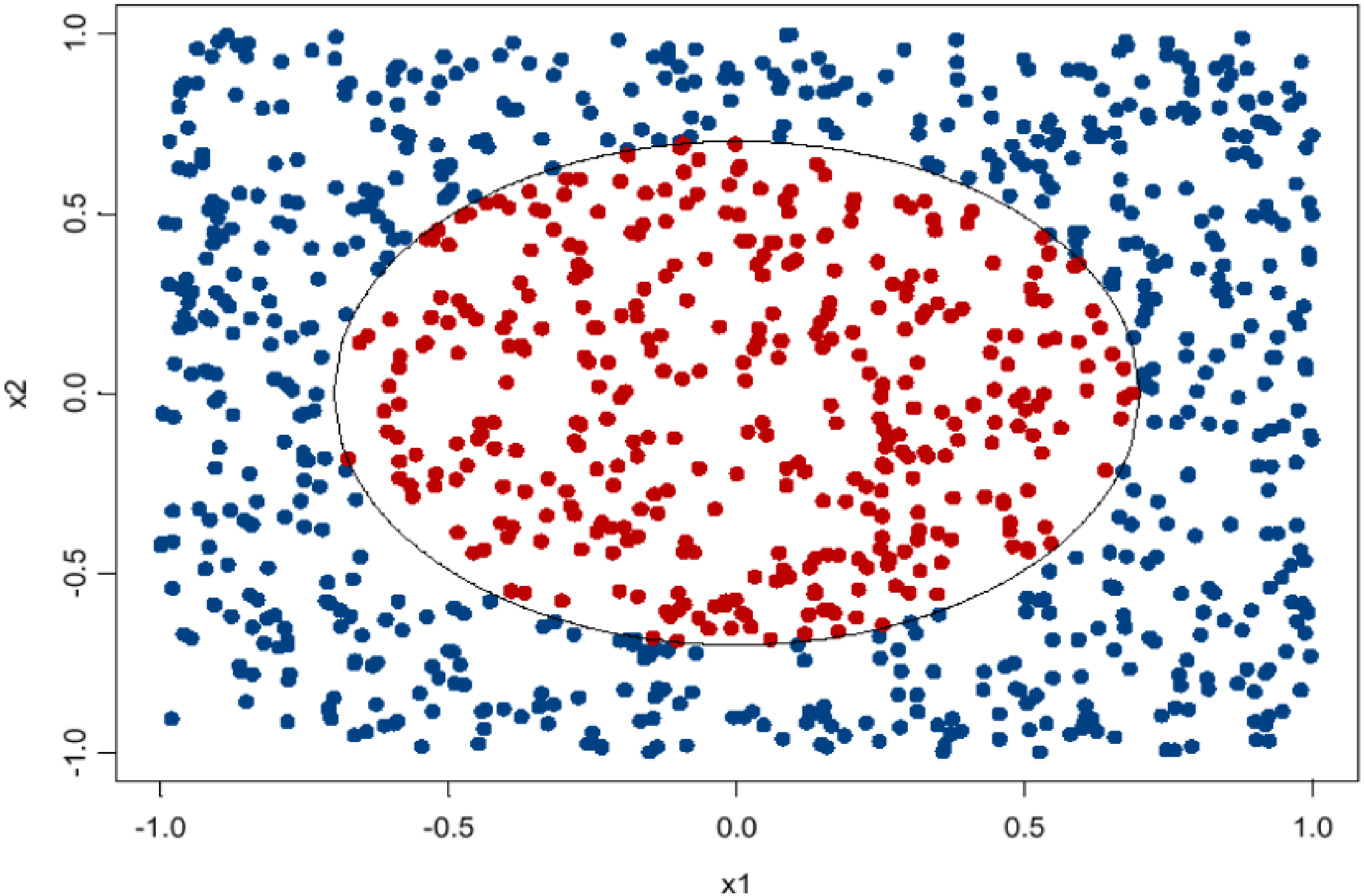
$$N \cdot \left(1-\left(1-\frac{1}{N}\right)^N\right) \approx N \cdot (1-\exp(-1)) = .632 \cdot N$$

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

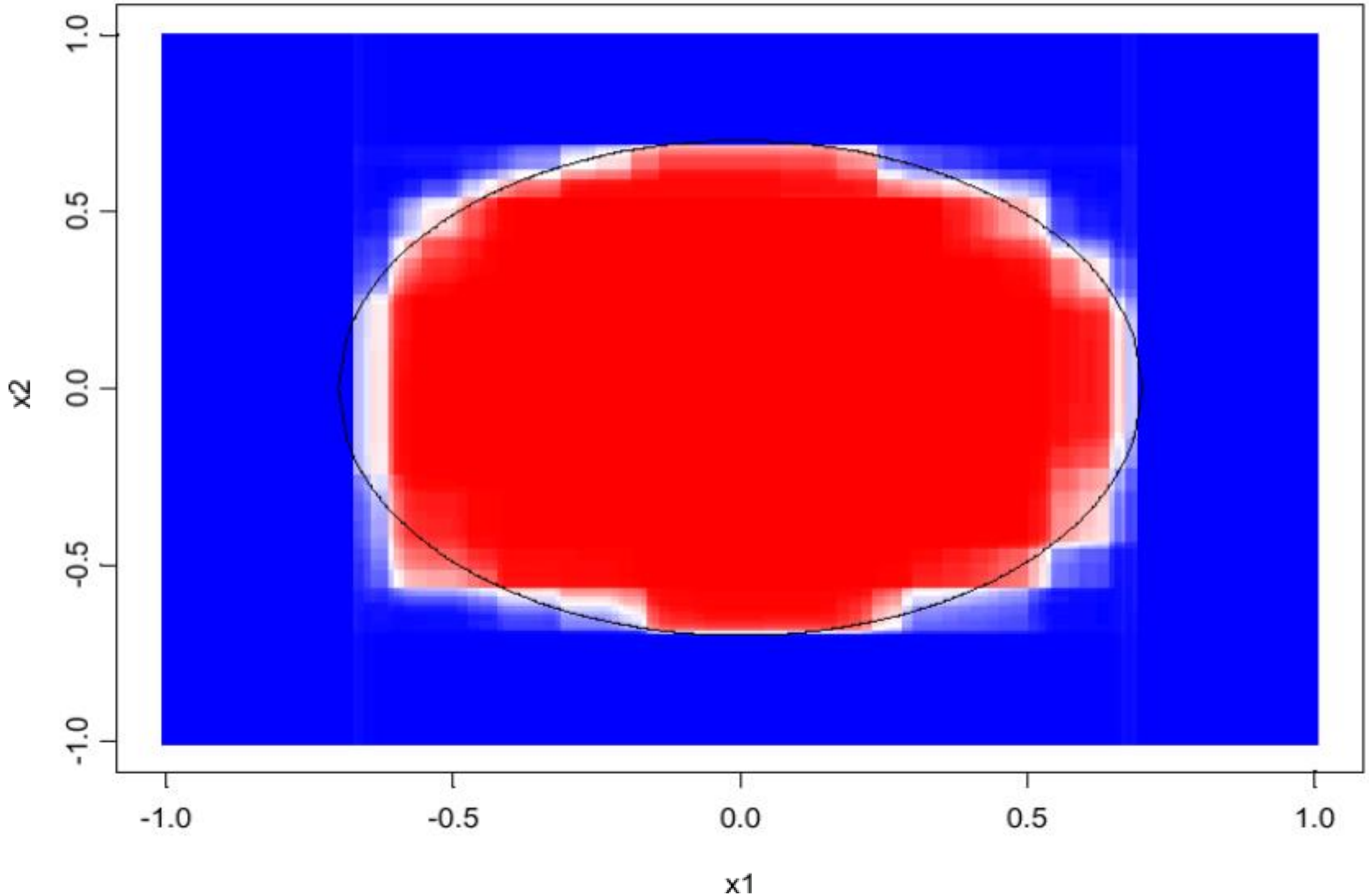
- Build a classifier from each bootstrap sample
- In each bootstrap sample, each data point has probability $\left(1 - \frac{1}{N}\right)^N$ of not being selected
  - If we have 1 TB of data, each bootstrap sample will be ~ 632GB (this can present computational challenges)

Decision Tree Bagging



[image from the slides of David Sontag]

Decision Tree Bagging (100 Bagged Trees)



[image from the slides of David Sontag]

Bagging Experiments

i) The data set is randomly divided into a test set $\mathcal{T}$ and a learning set $\mathcal{L}$. In the real data sets $\mathcal{T}$ is 10% of the data. In the simulated waveform data, 1800 samples are generated. $\mathcal{L}$ consists of 300 of these, and $\mathcal{T}$ the remainder.

ii) A classification tree is constructed from $\mathcal{L}$ using 10-fold cross-validation. Running the test set $\mathcal{T}$ down this tree gives the misclassification rate $e_S(\mathcal{L}, \mathcal{T})$.

iii) A bootstrap sample $\mathcal{L}_B$ is selected from $\mathcal{L}$, and a tree grown using $\mathcal{L}_B$. The original learning set $\mathcal{L}$ is used as test set to select the best pruned subtree (see Section 4.3). This is repeated 50 times giving tree classifiers $\phi_1(\boldsymbol{x}), \ldots, \phi_{50}(\boldsymbol{x})$.

iv) If $(j_n, \boldsymbol{x}_n) \in \mathcal{T}$, then the estimated class of $\boldsymbol{x}_n$ is that class having the plurality in $\phi_1(\boldsymbol{x}_n), \ldots, \phi_{50}(\boldsymbol{x}_n)$. If there is a tie, the estimated class is the one with the lowest class label. The proportion of times the estimated class differs from the true class is the bagging misclassification rate $e_B(\mathcal{L}, \mathcal{T})$.

v) The random division of the data into $\mathcal{L}$ and $\mathcal{T}$ is repeated 100 times and the reported $\bar{e}_S, \bar{e}_B$ are the averages over the 100 iterations. For the waveform data, 1800 new cases are generated at each iteration. Standard errors of $\bar{e}_S$ and $\bar{e}_B$ over the 100 iterations are also computed.

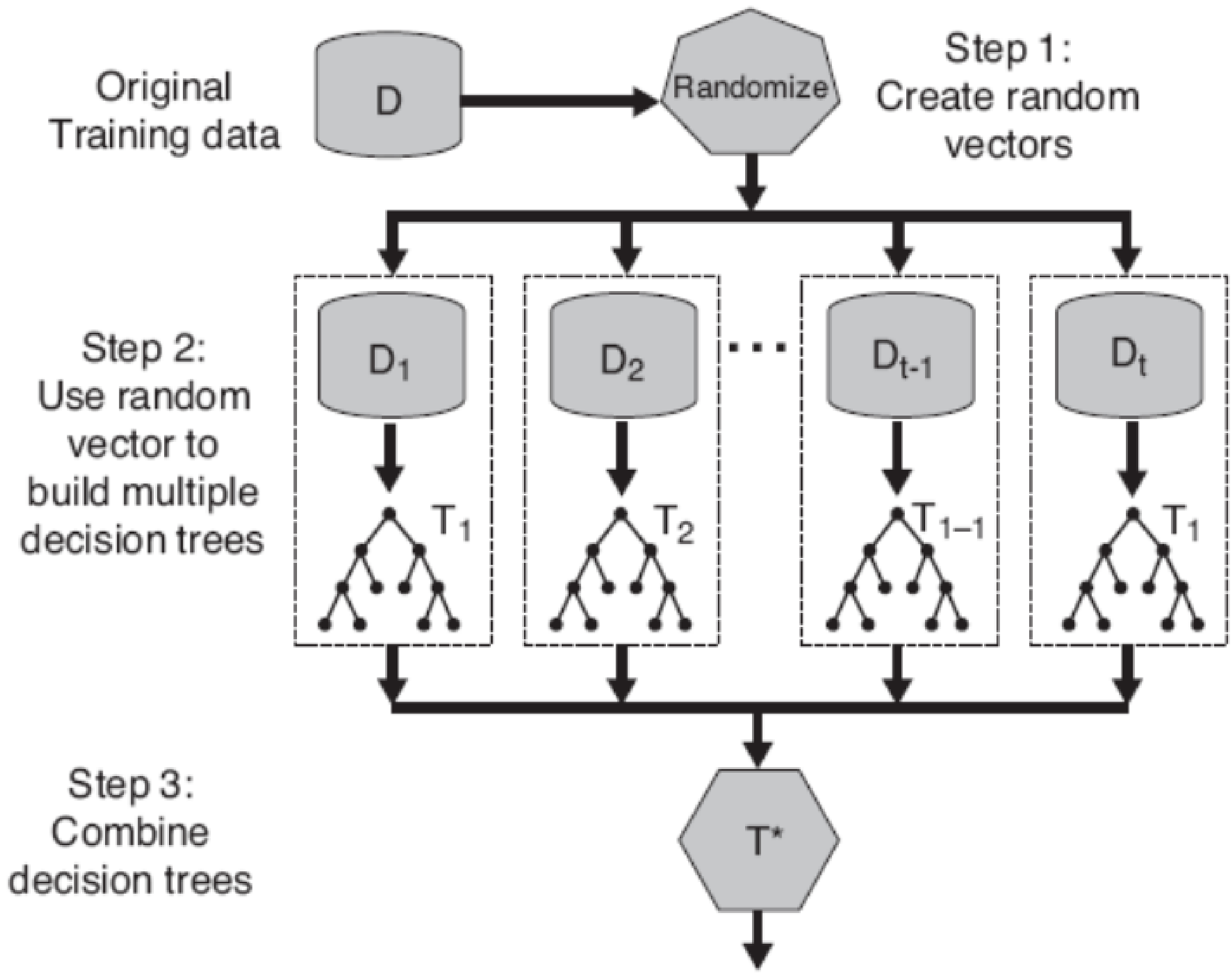
Bagging Results

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

UTD

Random Forests



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 $T_1(x), \ldots, T_B(x)$

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 be an improvement in performance with bagging
- Bagging helps unstable procedures, but could hurt the performance of stable procedures
  - Decision trees are unstable
  - k-nearest neighbor is stable