# Machine Learning

## Ensemble Methods

# Bias, Variance, Noise

- Classification errors have different sources
  - Choice of hypothesis space and algorithm
  - Training set
  - Noise in the data
- The expected error sources are often characterized using
  - Bias – Error due to the algorithm and hypothesis
  - Variance – Error due to training data
  - Noise – Noise in the data

# Bias, Variance, Noise

- In regression we can show the decomposition of the error into these components
  - Assume that a data point *(x,y)* and training sets *D* are drawn randomly from a data distribution
  - The squared regression error for a data point *x* is

$$
\begin{aligned}
E_{D,y}\left[\left(y-h(x)\right)^2\right] &= E_{D,y}\left[y^2-2yh(x)+h(x)^2\right] \\
&= E_{D,y}\left[y^2\right]-2E_{D,y}[y]E_{D,y}\left[h(x)\right]+E_{D,y}\left[h(x)^2\right] \\
&= E_{D,y}\left[y^2\right]-E_y\left[y\right]^2 \\
&\quad +E_y\left[y\right]^2-2E_y[y]E_D\left[h(x)\right]+E_D\left[h(x)\right]^2 \\
&\quad +E_D\left[h(x)^2\right]-E_D\left[h(x)\right]^2
\end{aligned}
$$

# Bias, Variance, Noise

- Using the relation $E[(x-E[x])^2]=E[x^2]-E[x]^2$ we can transform this:

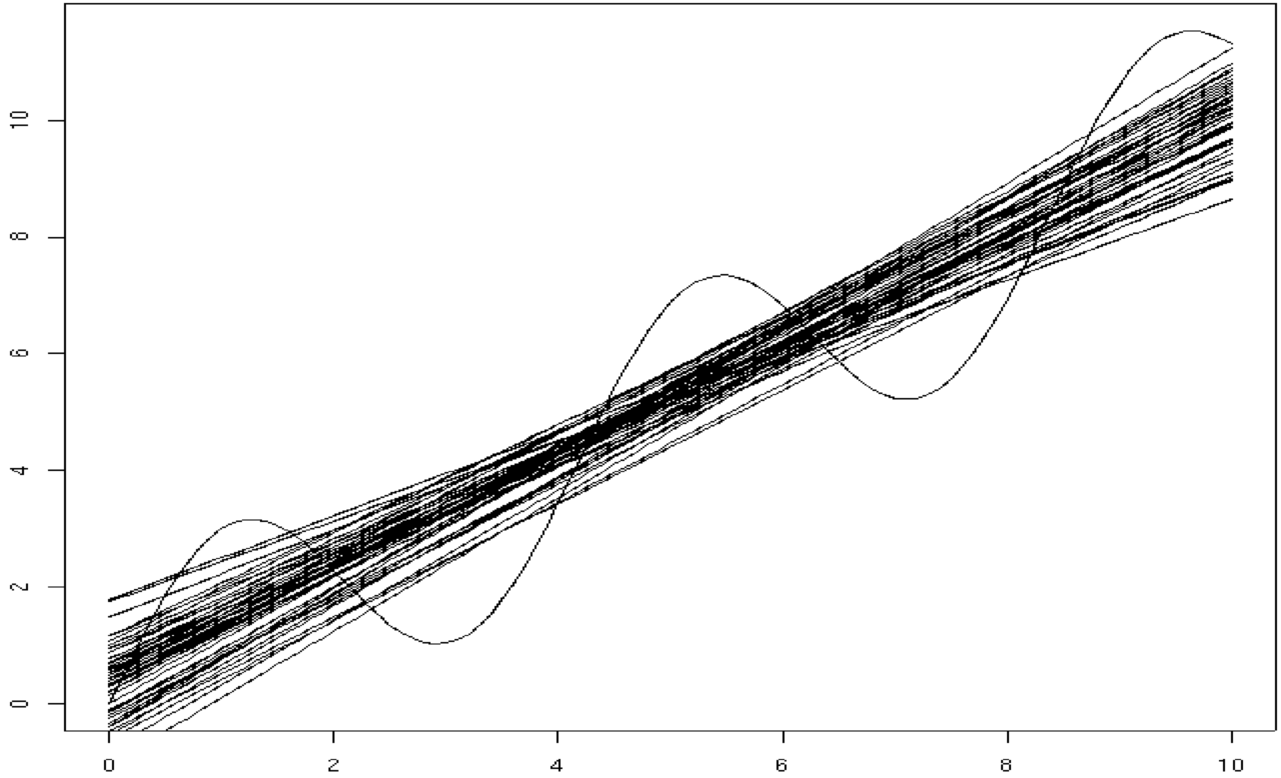
$$
\begin{aligned}
E_{D,y}\left[\left(y-h(x)\right)^2\right] &= E_y\left[y^2\right]-E_y\left[y\right]^2 \\
&\quad +E_y\left[y\right]^2-2E_y[y]E_D\left[h(x)\right]+E_D\left[h(x)\right]^2 \\
&\quad +E_D\left[h(x)^2\right]-E_D\left[h(x)\right]^2 \\
&= E_y\left[\left(y-f(x)\right)^2\right] && \leftarrow \text{Noise} \\
&\quad +\left(f(x)-E_D\left[h(x)\right]\right)^2 && \leftarrow \text{Bias}^2 \\
&\quad +E_D\left[\left(h(x)-E_D\left[h(x)\right]\right)^2\right] && \leftarrow \text{Variance}
\end{aligned}
$$

# Bias, Variance, Noise

- Each of the terms explains a different part of the expected error
  - Noise describes how much the target value varies form the true function value
  - Bias describes how much different the average (best) learned hypothesis is from the true function
  - Variance describes how much the learned hypotheses vary with changes in the training data

# Linear Regression Example

- 50 datasets with 20 data points each

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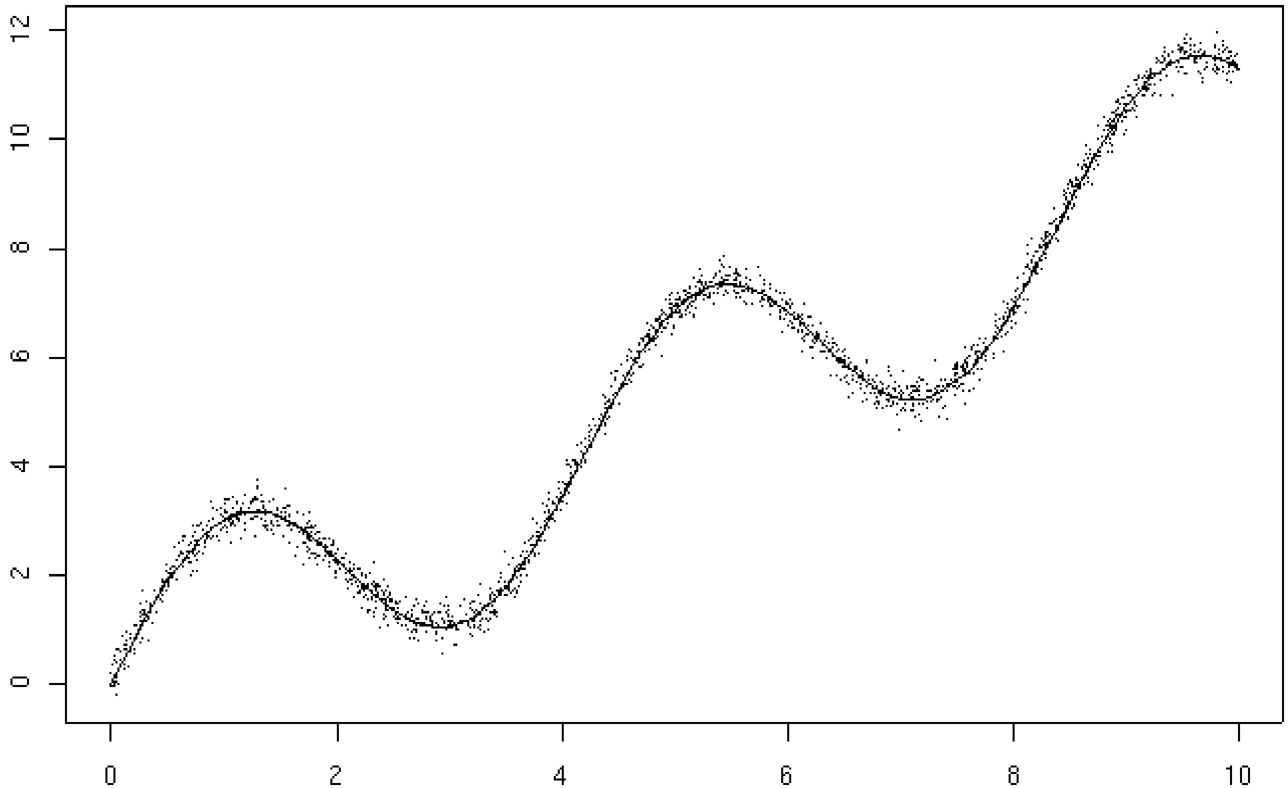
# Linear Regression Example

- Noise

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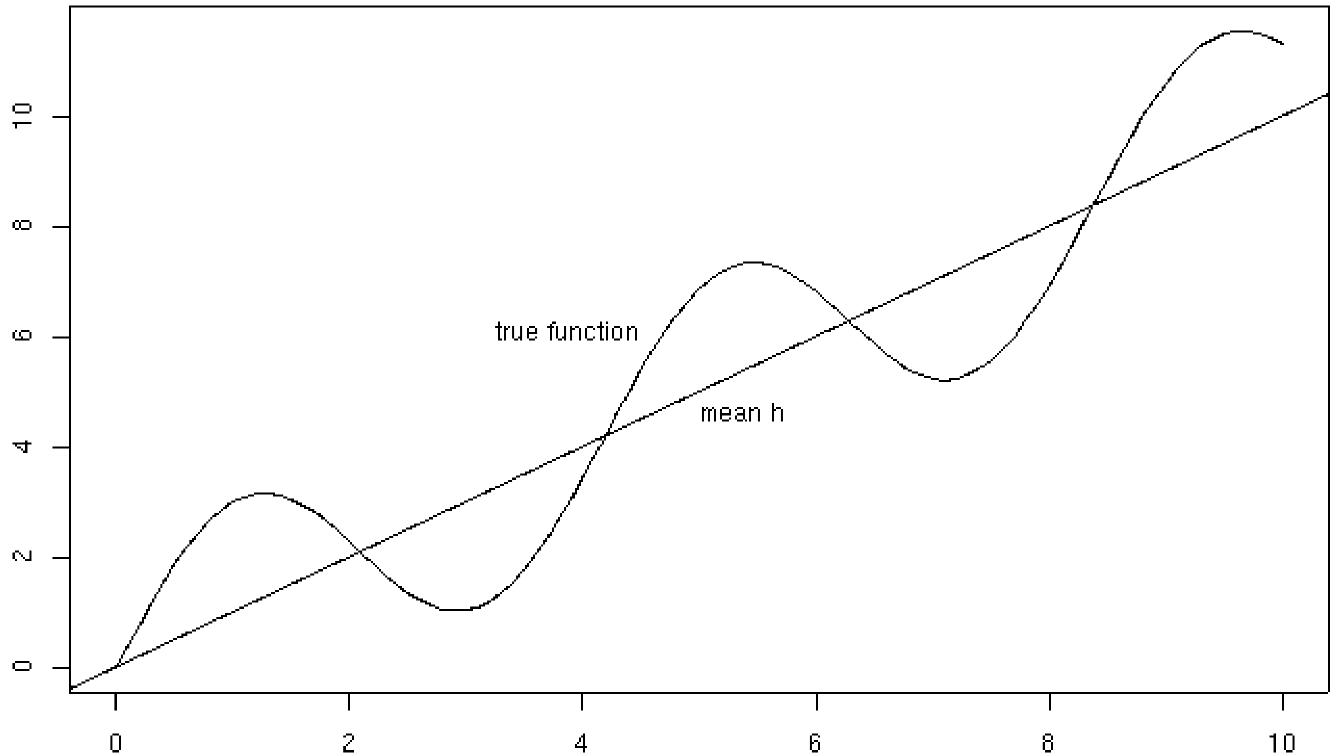
# Linear Regression Example

- Bias

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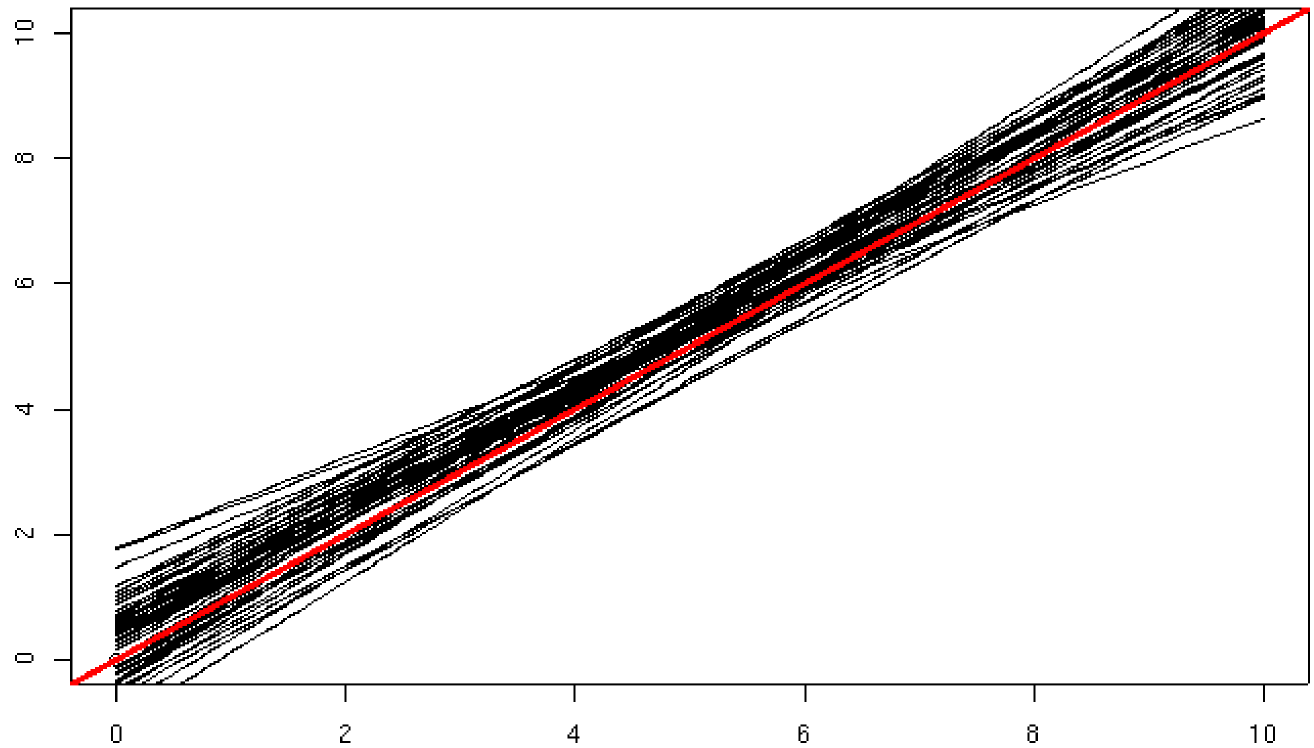
# Linear Regression Example

- Variance

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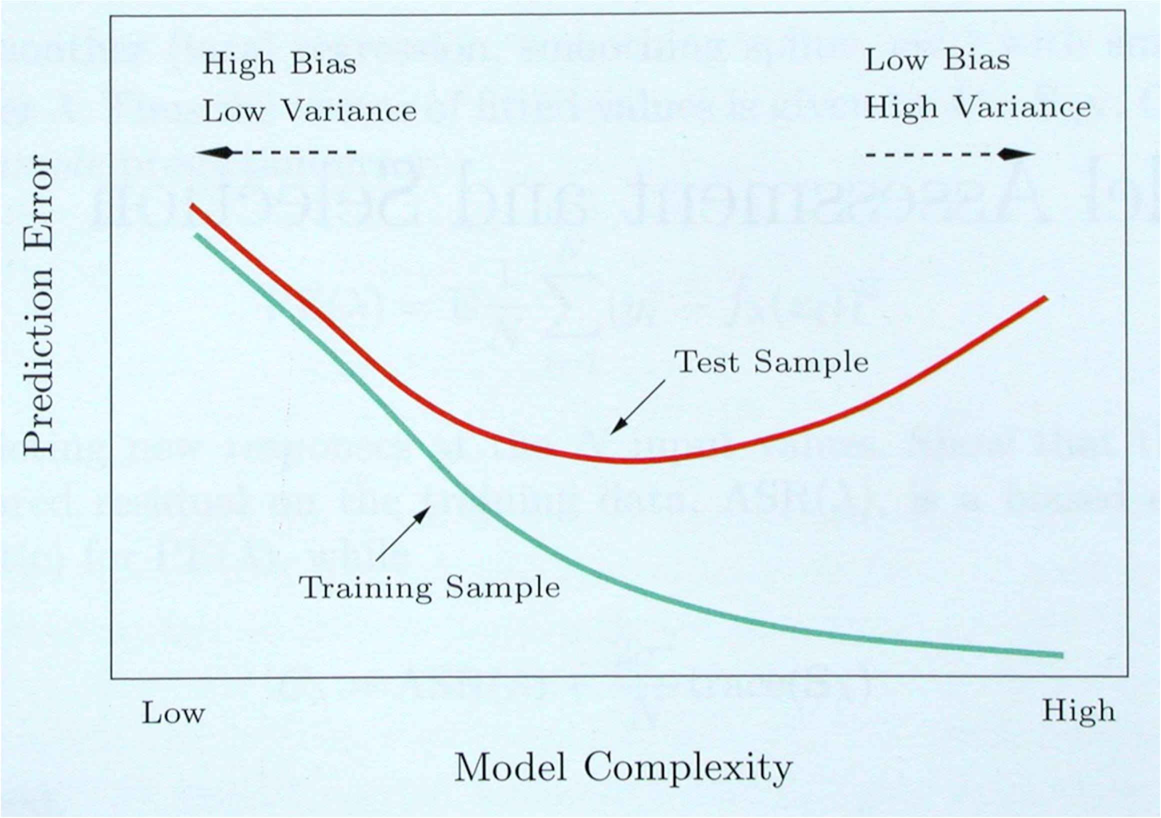
# Bias Variance Tradeoff

- Bias can be minimized by appropriate hypothesis spaces (containing the function) and algorithm
  - Requires knowledge of the function or a more complex hypothesis space
- Variance can be minimized by a hypothesis space that requires little data and does not overfit
  - Requires knowledge of function or use of a simpler hypothesis space
- Bias and variance often trade off against each other and are hard to optimize at the same time

# Bias Variance Tradeoff

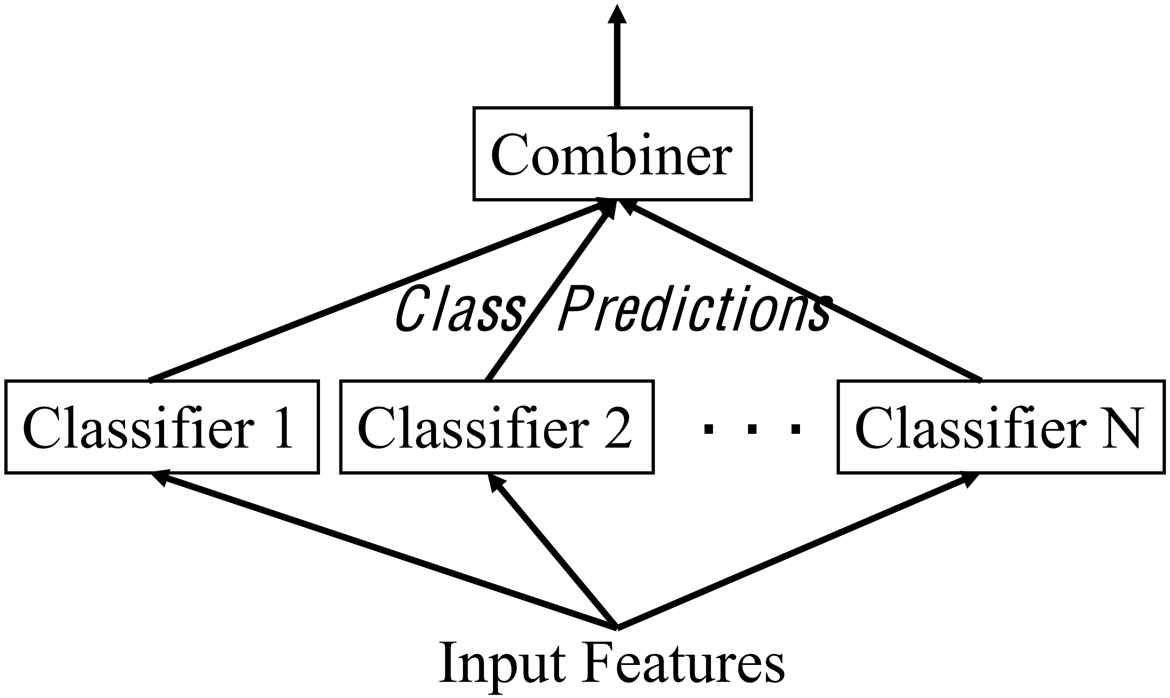
- Typical bias/variance tradeoff:




Hastie, Tibshirani, Friedman

# Influencing Bias and/or Variance: Ensemble Methods

- Ensemble methods can change bias and/or variance of an existing classifiers



# Bagging

- One way to address variance is by averaging over multiple learned hypotheses
  - Bagging samples the initial n training examples with replacement to generate k bootstrap sample sets (usually of the same set size, n)
  - A classifier/regression function is learned on each of the k training sets
  - The final classification/regression function is determined through majority vote or averaging

# Bagging

- The variance of the ensemble classifier/regression function can have lower variance
  - Resulting variance depends on correlation between the hypotheses
    - If all classifiers are the same there is no gain
    - If the classifiers change strongly there will be gain of up to a factor of 1/k
  - Bootstrap sampling could lead to a small degradation in the learned classifiers/functions
- Bagging mainly helps with methods that are very sensitive to changes in the data set

# Bagging

- Bagging generally has no influence on bias
  - Does only average the hypotheses
- Reduces bias for classifiers/regression approaches that are sensitive to training data
  - Averaging the hypotheses can reduce the variance of the final classifier/regression function
- Can we also influence bias using ensemble classification ?

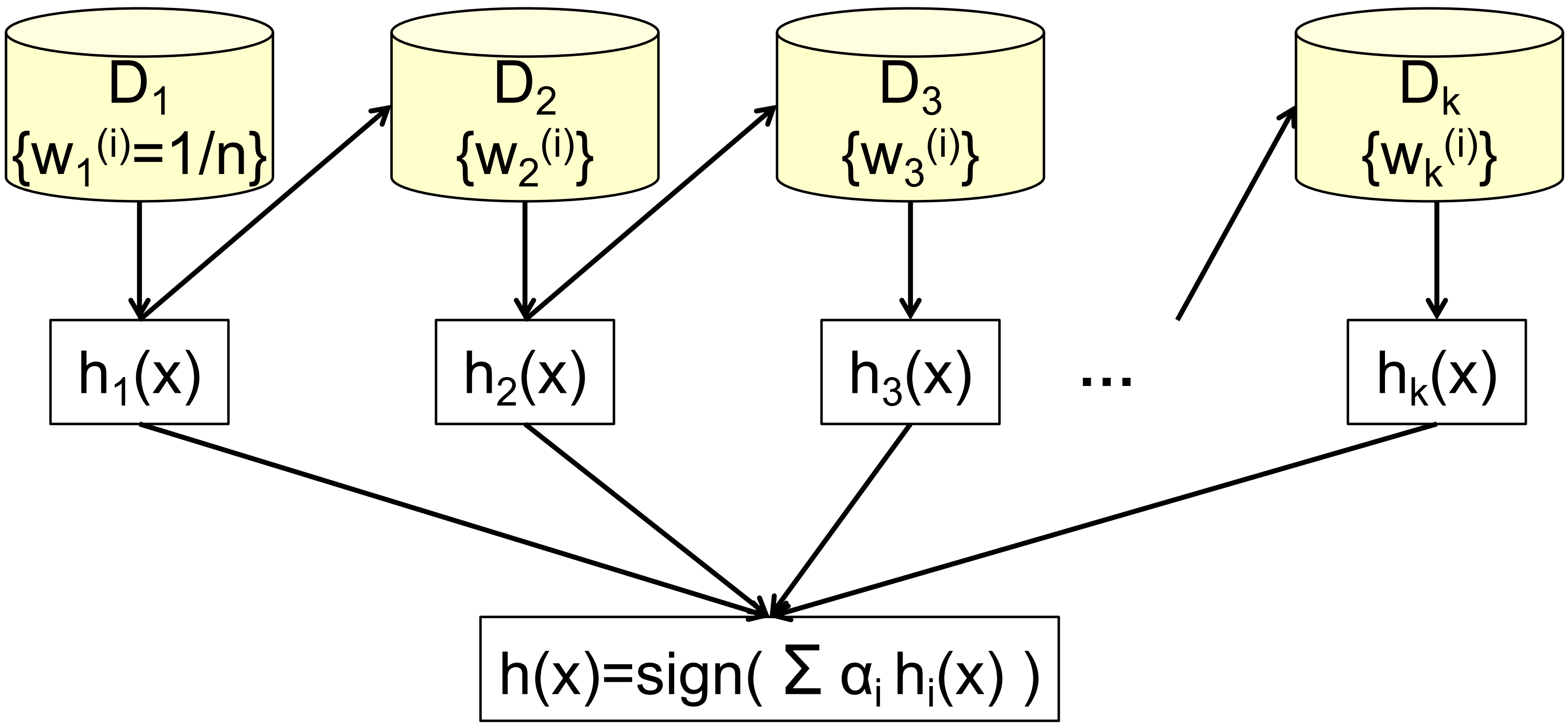
# Boosting

- Boosting takes a different approach by modifying the training set systematically to allow subsequent classifiers to focus on misclassified examples
  - Originally proposed in the theory of weak learners
    - Even minimally better than random performance can be used to build better learners as an ensemble
  - Only used for classification
  - Whole ensemble formed by weighted voting

# Boosting

- Start with equally weighted samples
- Learn a classifier on the weighted data
    - Weight indicates contribution to the error function
  - Compute the error on the training set
  - Increase weight of samples that were misclassified
  - Go back to learning a new classifier until sufficient are learned (often more than 100)
- Perform classification as the weighted sum or predictions of all the models

# Boosting



$D_1$
$\{w_1^{(i)}=1/n\}$
$D_2$
$\{w_2^{(i)}\}$
$D_3$
$\{w_3^{(i)}\}$
$D_k$
$\{w_k^{(i)}\}$
$h_1(x)$
$h_2(x)$
$h_3(x)$
...
$h_k(x)$
$h(x)=\text{sign}(\ \Sigma\ \alpha_i\, h_i(x)\ )$

# Boosting Example: AdaBoost

- Assuming classes as *1* and *-1*, the normalized error of the *m*^th^ classifier is

$$\varepsilon_m = \sum_{i=1}^{n} \omega_m^{(i)} (1 - \delta_{h(x^{(i)}),y^{(i)}}) \Big/ \sum_{i=1}^{n} \omega_m^{(i)}$$

  - Learn the $m^{th}$ classifier and continue if $\varepsilon_m < ½$

$$h_m = \operatorname{argmin}_h E_m$$

  - From this we can compute the classifier weight

$$\alpha_m = \frac{1}{2} \ln\left(1 - \varepsilon_m / \varepsilon_m\right)$$

  - And adjust the weights for the data items

$$\omega_{m+1} = \omega_m e^{-\alpha_m y^{(i)} h_m(x^{(i)})}$$

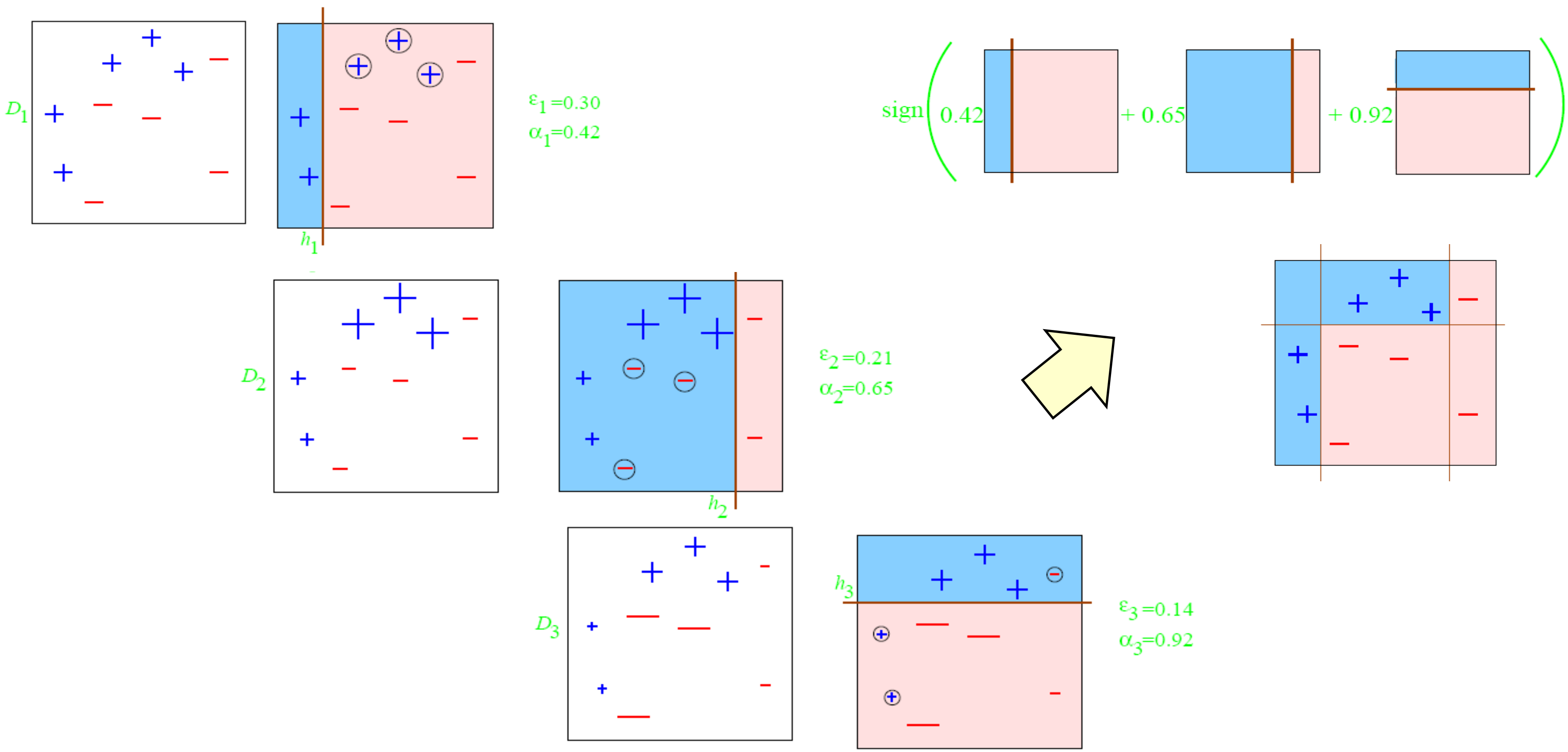
# Boosting Example: AdaBoost

- The final classifier produces

$$h(x) = sign\left(\sum_{j=1}^{k} \alpha_j h_j(x)\right)$$

  - Construction iteratively minimizes an exponential energy function over the misclassifications and with it the misclassification rate

# Boosting Example



# Boosting

- Boosting can improve bias and variance
  - Usually leads to larger improvements than bagging
  - Boosting can lead to improvements even with stable classifiers (as opposed to bagging)
  - But:
    - Boosting can hurt performance on very noisy data
    - Boosting is also more common to lead to degraded performance than bagging
- Instead of weights on data samples, boosting can also use resampling

# Ensemble Methods

- Ensemble methods can be used to improve the performance of existing classifiers
  - Bagging improves variance by averaging solutions
  - Boosting can improve bias and variance through weighing of data samples for each classifier to focus on misclassified items
- A range of other ensemble methods have been proposed and built to achieve better performance than a single classifier
  - E.g Mixture of Experts