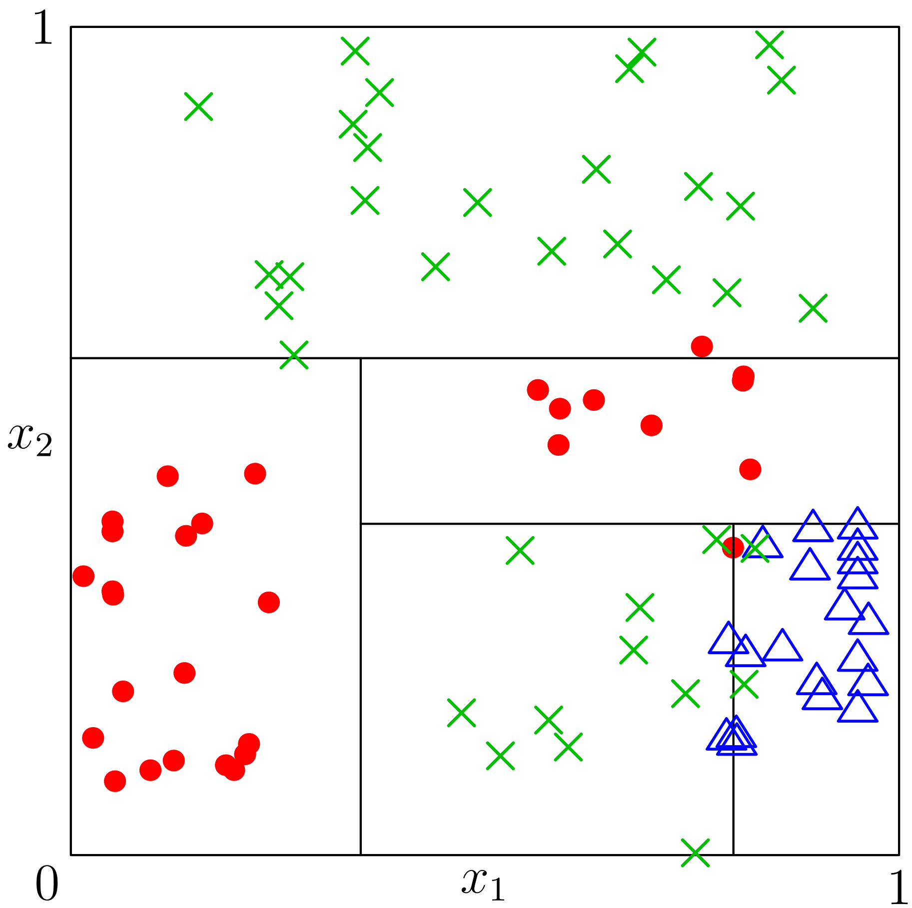
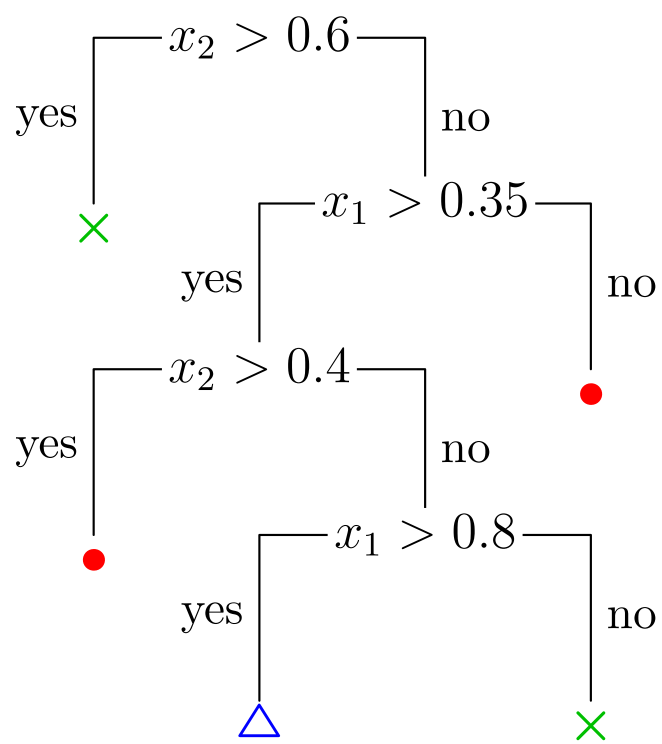
Advanced Machine Learning

Ensemble Methods

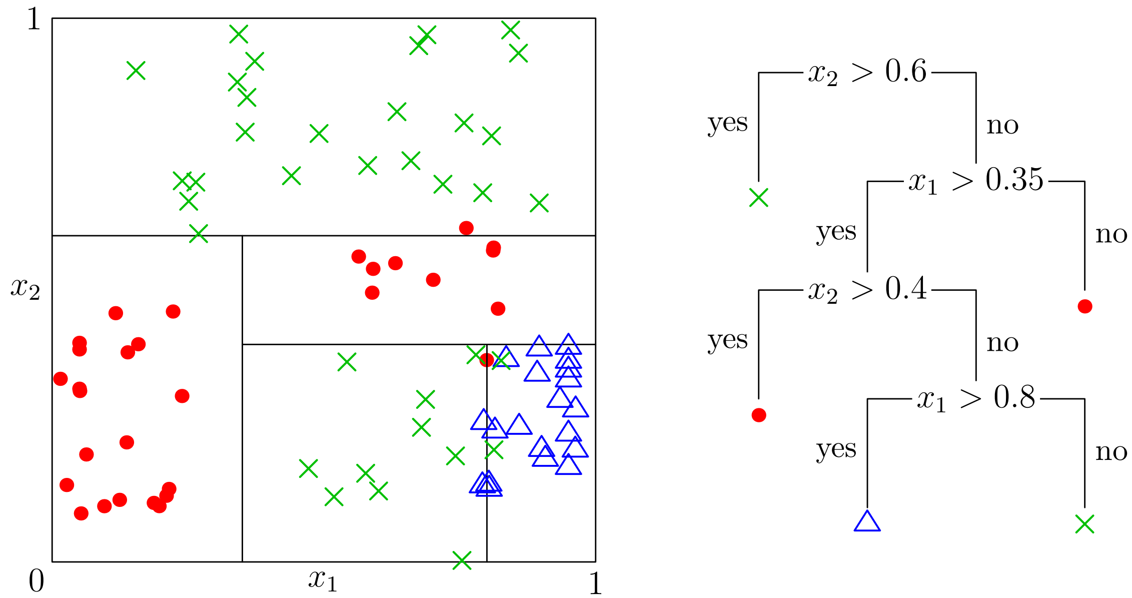




Decision Trees, Bagging, Boosting

Outline

1. **Decision Trees**
2. Bagging
3. Boosting



Removing Variance By Averaging

- We can reduce the variance and hence improve our generalisation error by averaging over different learning machines
- There are a number of different techniques for doing this that go by the name of **ensemble methods** or **ensemble learning**
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- (nevertheless, even for deep learning taking the average response of many machines is usually done to win competitions)

Ensembling of Decision Trees

- One set of algorithms where ensembling are common place are decision trees

- These are particularly good for handling messy data
  - ⋆ categorical data
  - ⋆ mixture of data types
  - ⋆ missing data
  - ⋆ large data sets
  - ⋆ multiclass

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Decision Trees

- Decision trees builds a binary tree to partition the data, $\mathcal{D} = \{(\boldsymbol{x}_i, y_i) | i = 1, \ldots, m\}$, into the leaves of the tree

- Each decision rule depends on a single feature

- At each step the rule is chosen that maximise the "$purity$" of the leaf nodes

- Decisions can be made on numerical values or categories

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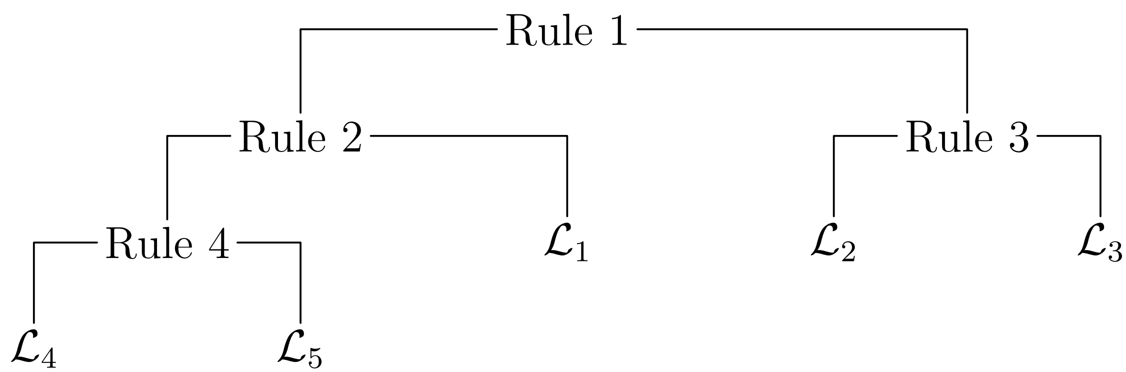
Partitioning

- Consider a classification problems with examples $(\boldsymbol{x}, y)$ belonging to some classes $y \in \mathcal{C}$

- The data is partitioned by the tree into leaves



- The proportion of data points in leaf $\mathcal{L}$ belonging to class c is

$$p_c(\mathcal{L}) = \frac{1}{|\mathcal{L}|} \sum_{(\boldsymbol{x},y)\in\mathcal{L}} [\![y = c]\!]$$

where $[\![y = c]\!] = 1$ if $y = c$ and 0 otherwise

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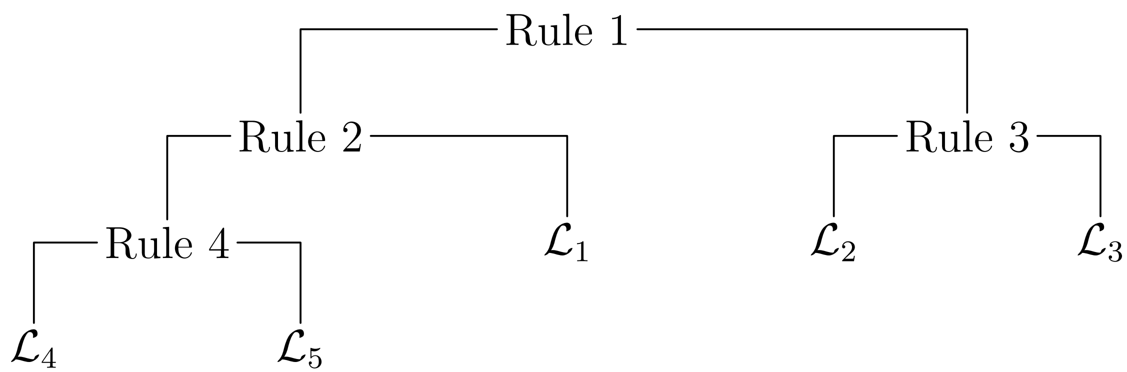

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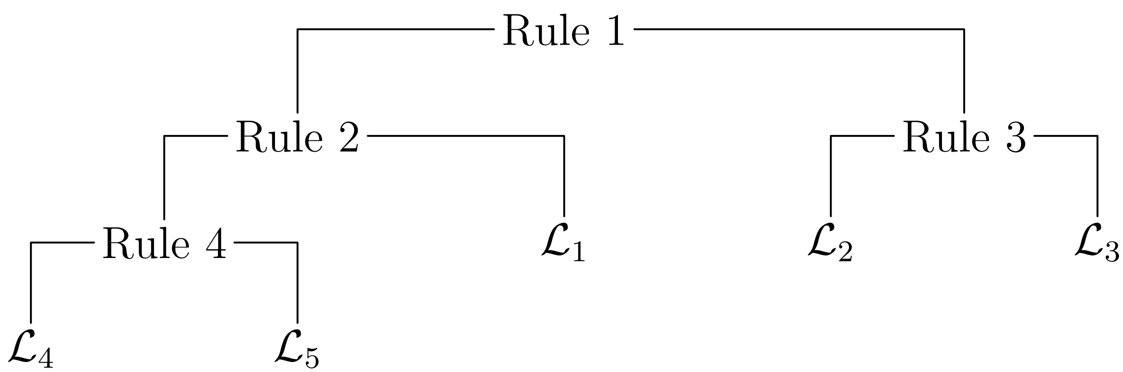

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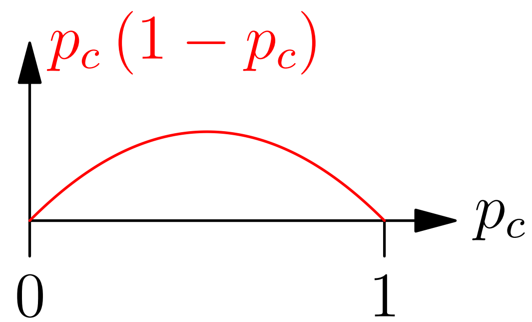
Leaf Purity

- Two different purity measures, $Q_m(\mathcal{L})$, for a leaf node $\mathcal{L}$ are commonly used
  - **Gini index**

$$Q_m^g(\mathcal{L}) = \sum_{c \in \mathcal{C}} p_c(\mathcal{L})\ (1 - p_c(\mathcal{L}))$$



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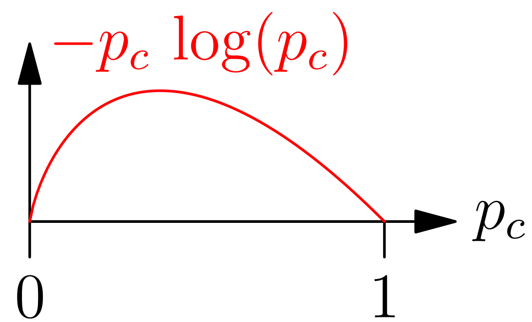

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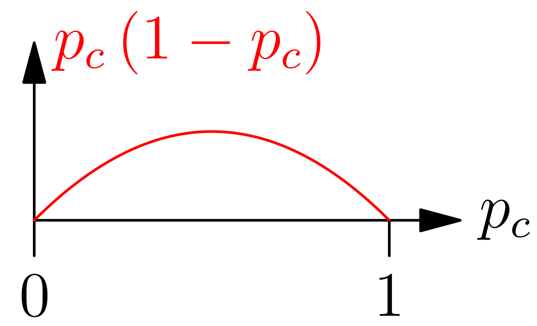

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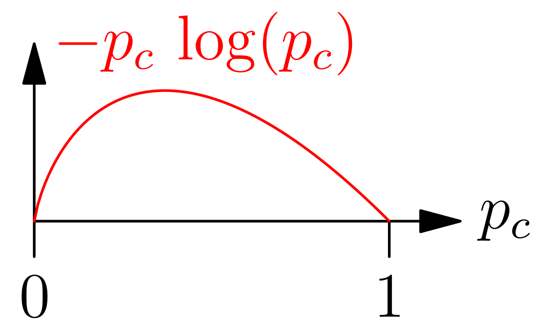

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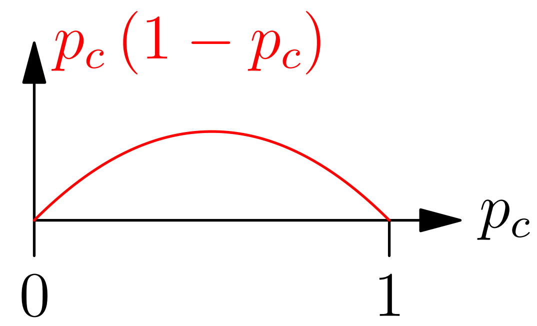

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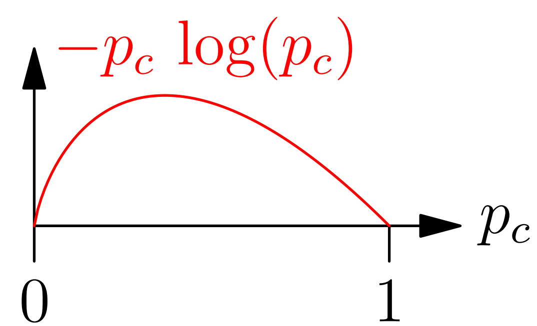
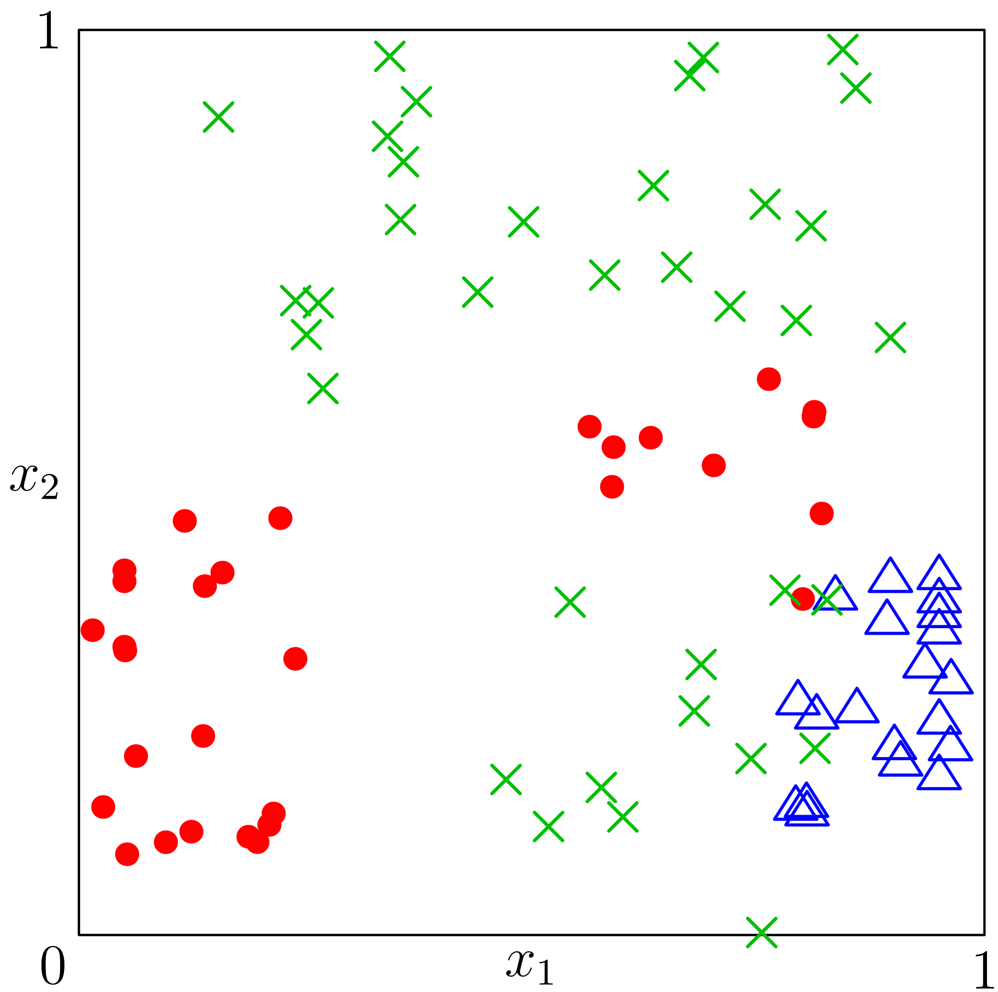


Building Decision Trees



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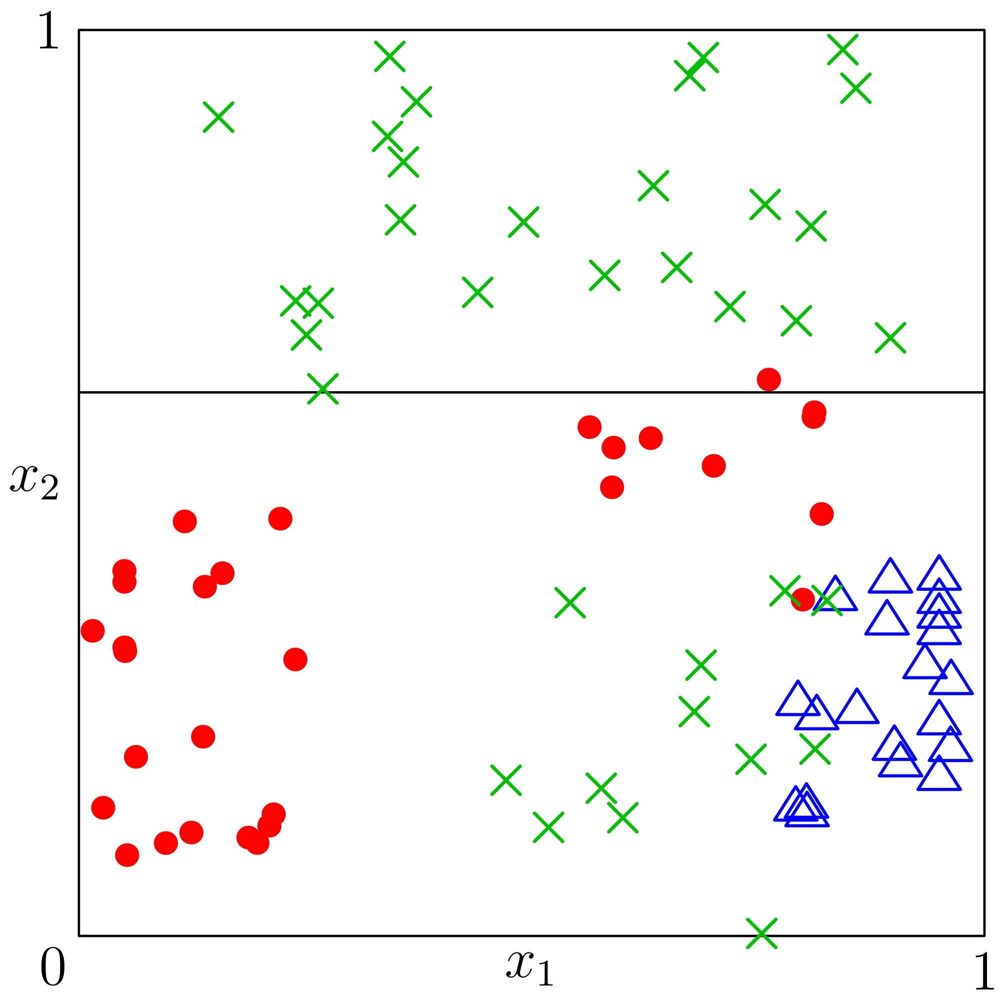

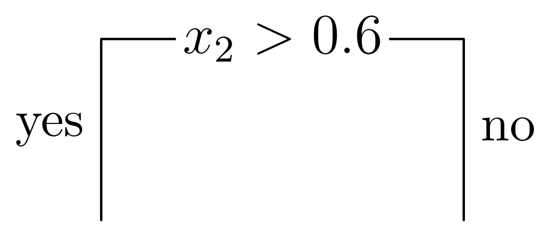

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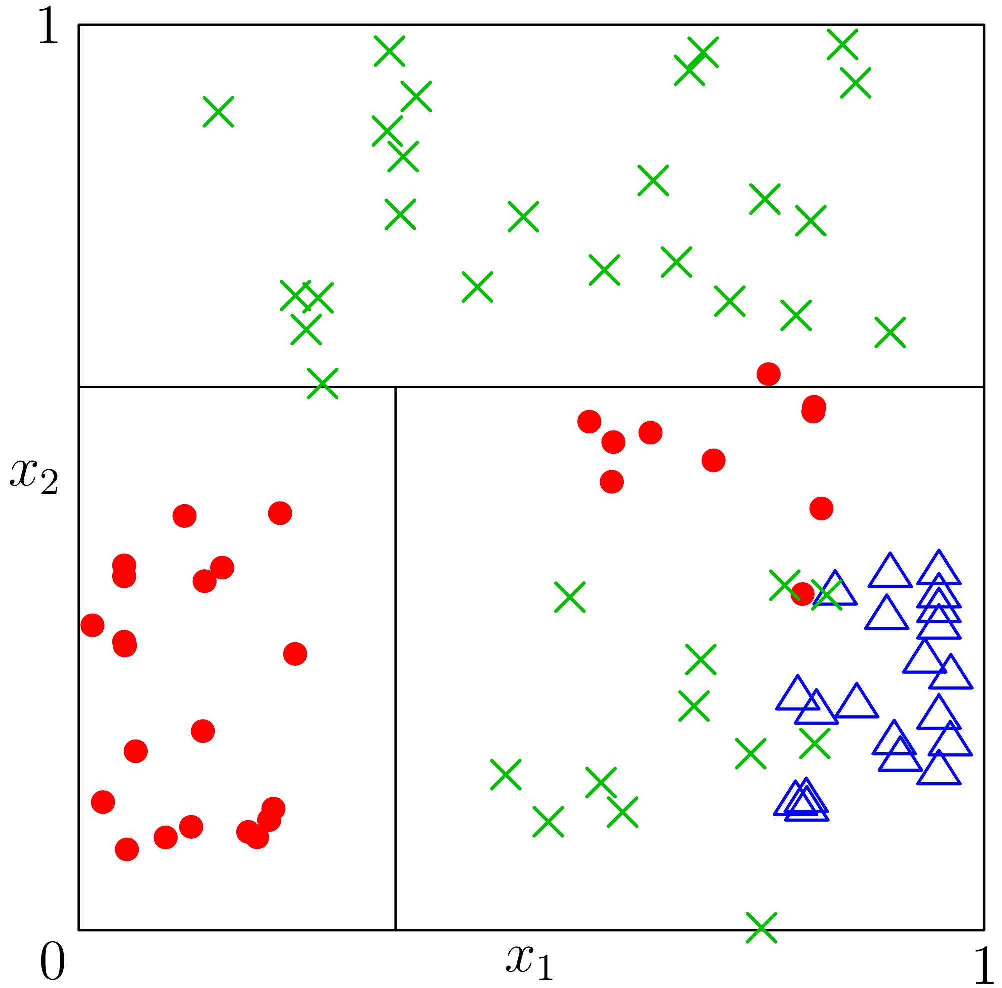

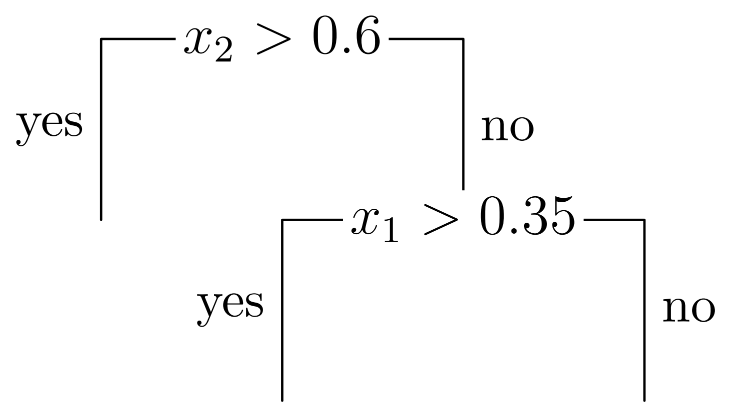

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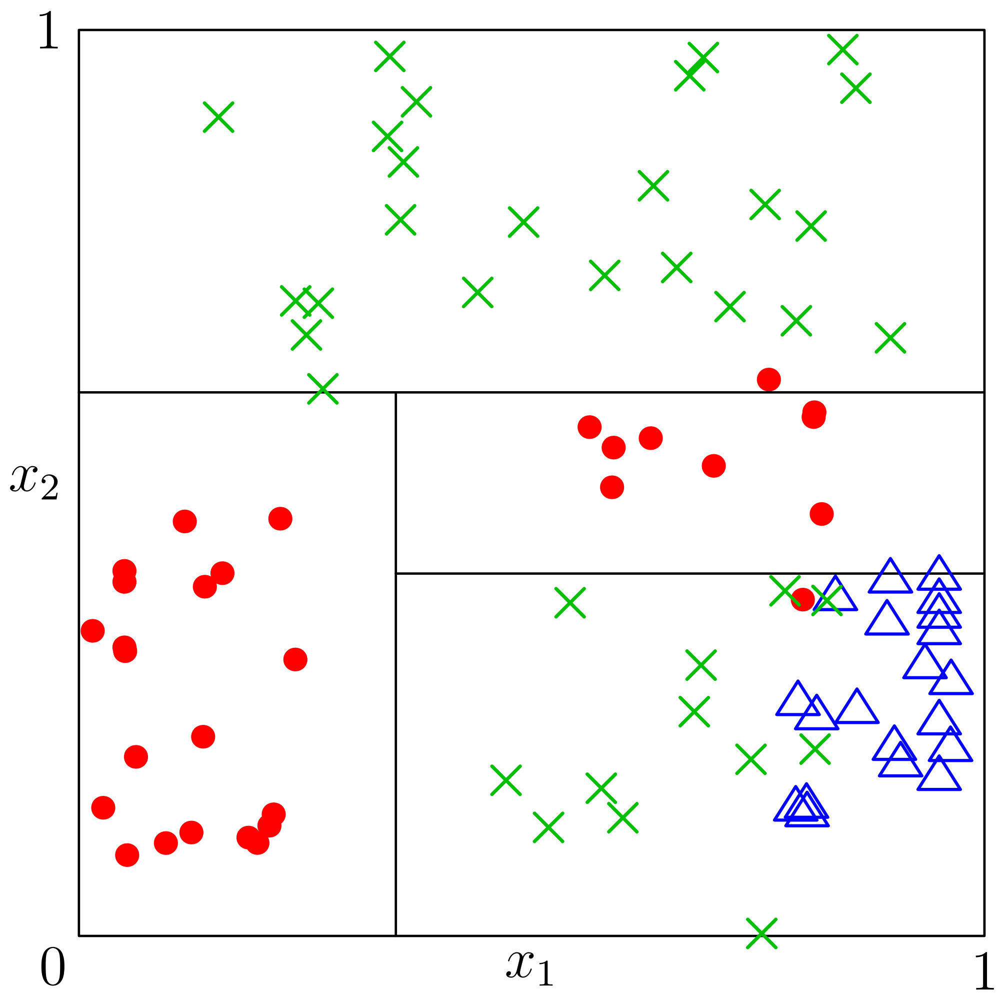

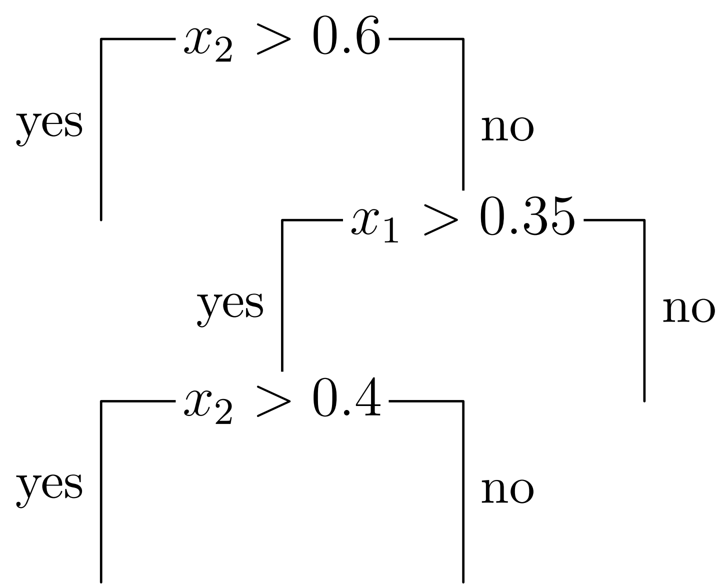

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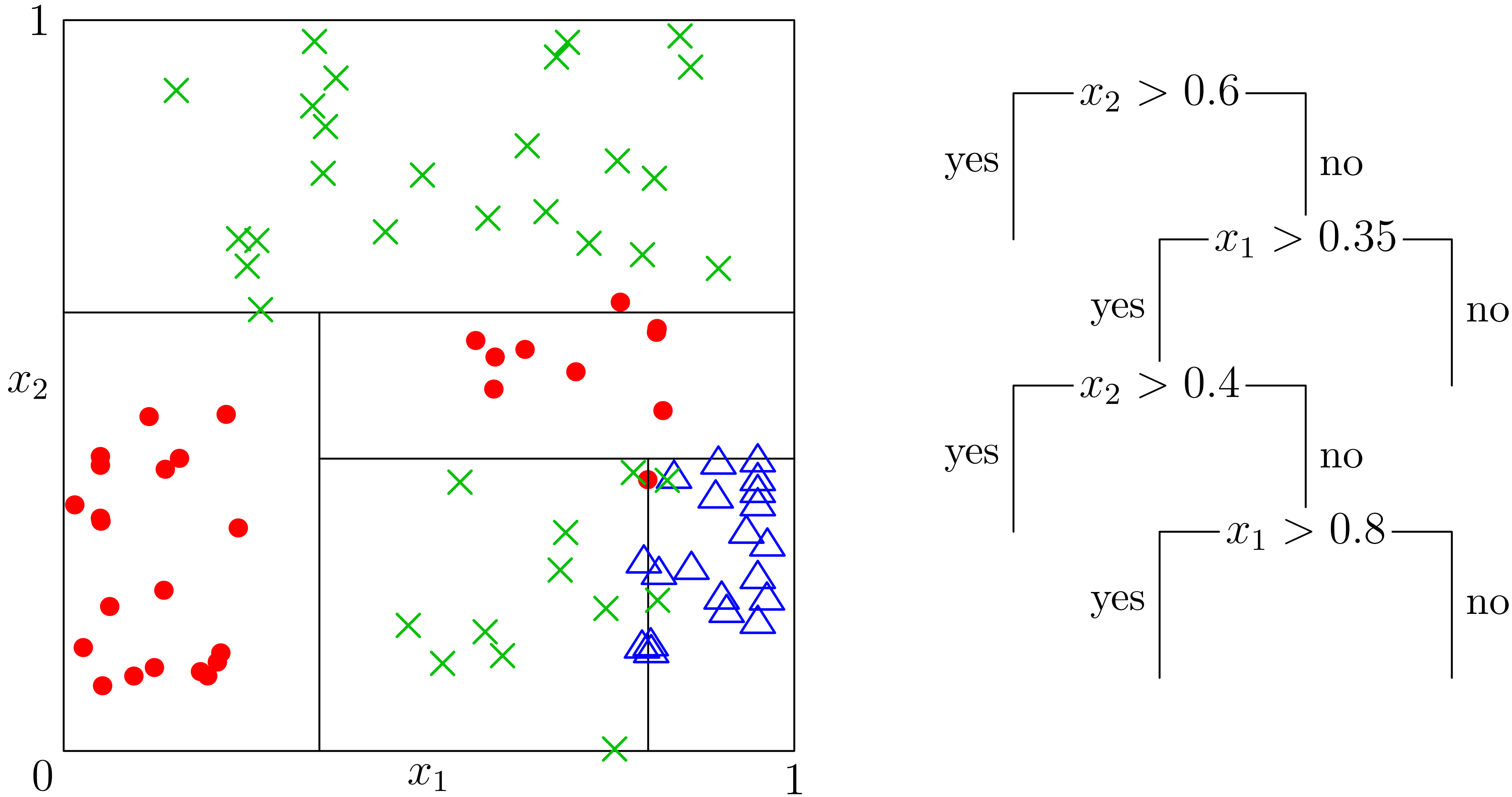

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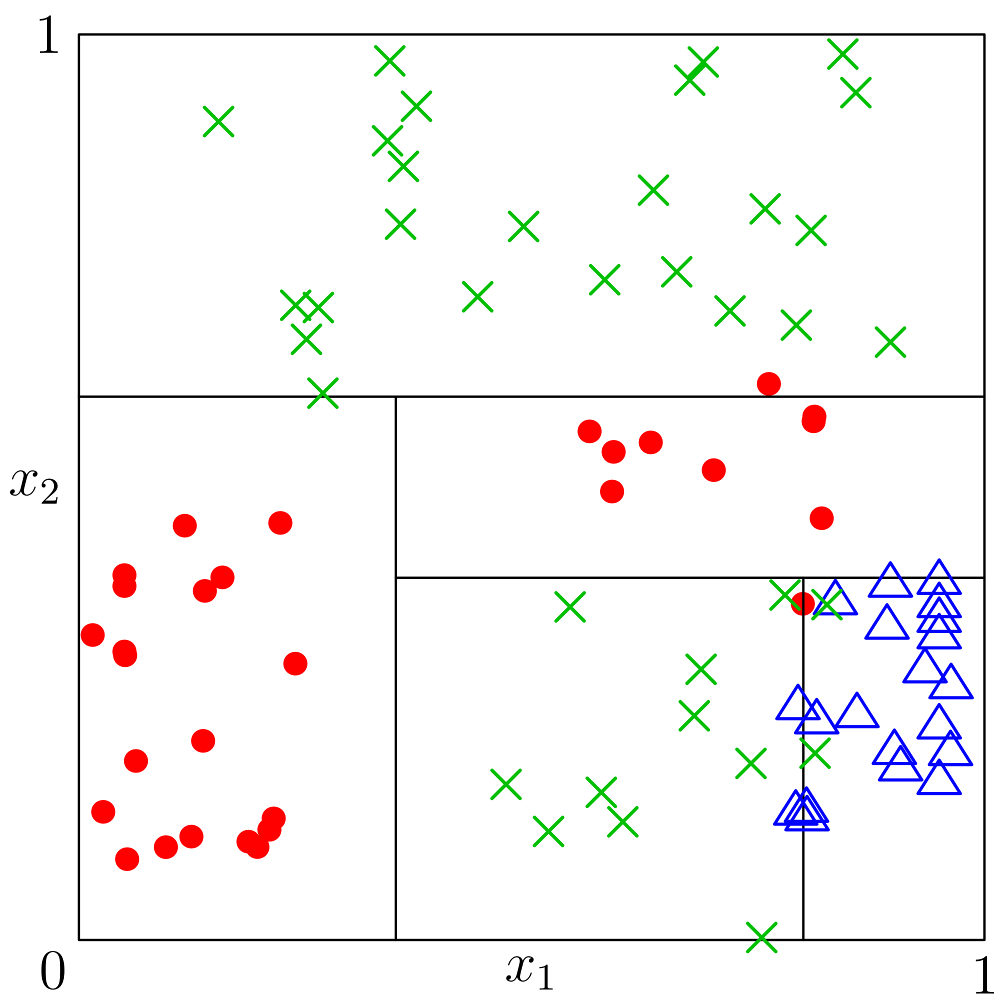

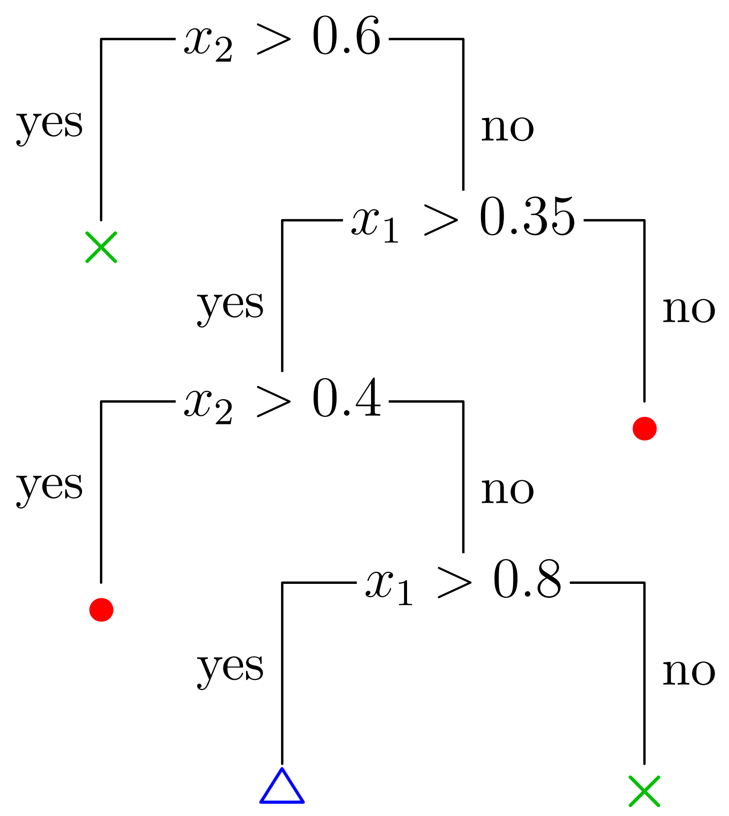

Observations

- Decision trees are very useful for exploring new data sets—the tree shows what features are most important

- Decision trees can also be used for regression problems
  - ⋆ Approximate function by a series of steps
  - ⋆ Reduce variance between data points assigned to leaf nodes

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- Decision trees depend strongly on the early decisions and so vary a lot for slightly different data sets—high variance

Outline

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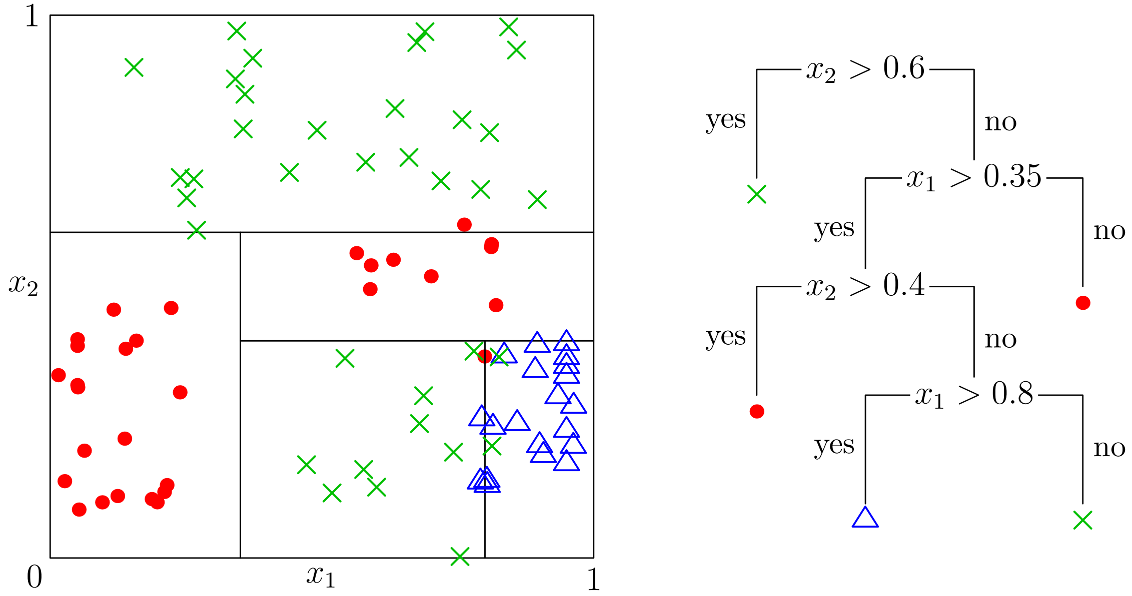
2. **Bagging**

3. Boosting



Error In The Means

- By taking the mean over many samples we can reduce out variance and thus improve our generalisation performance

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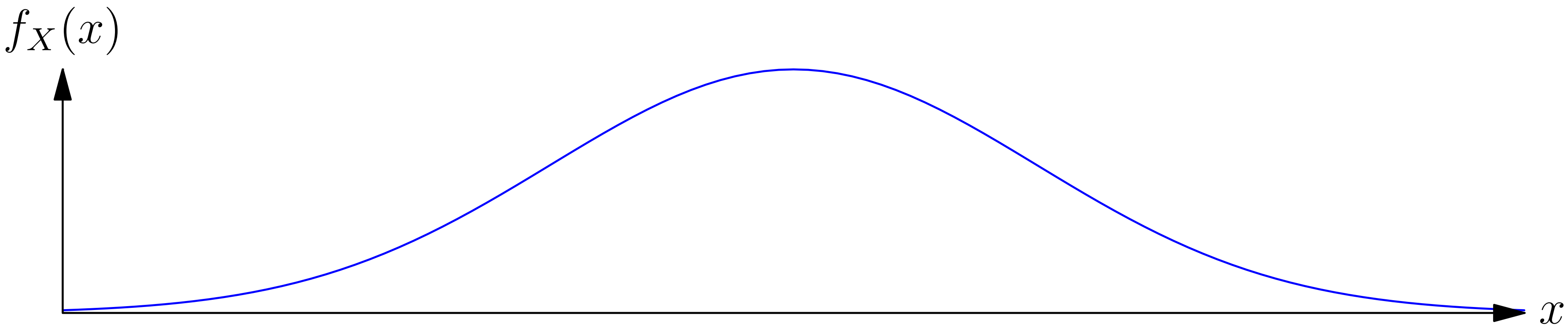

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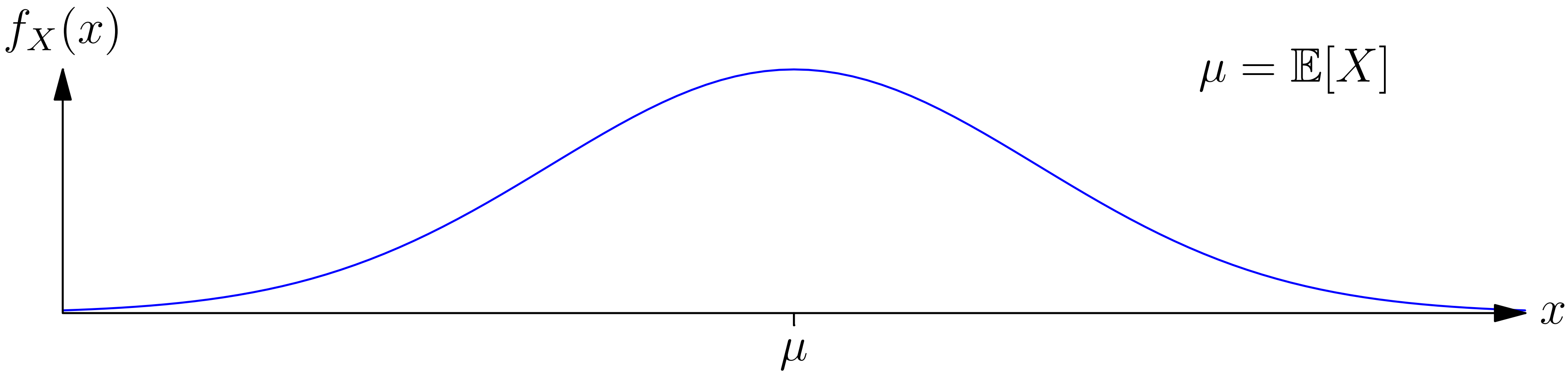

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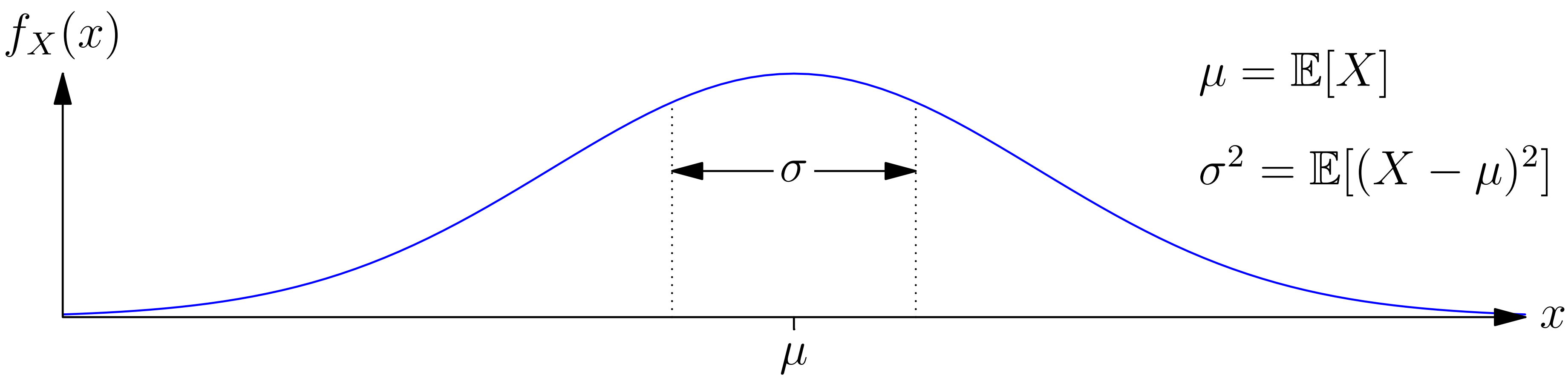

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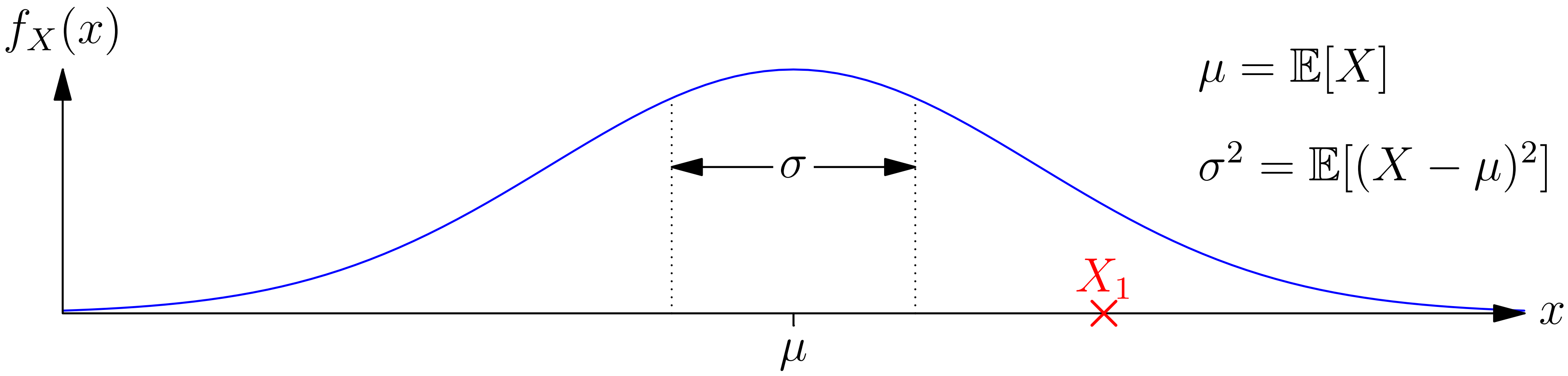

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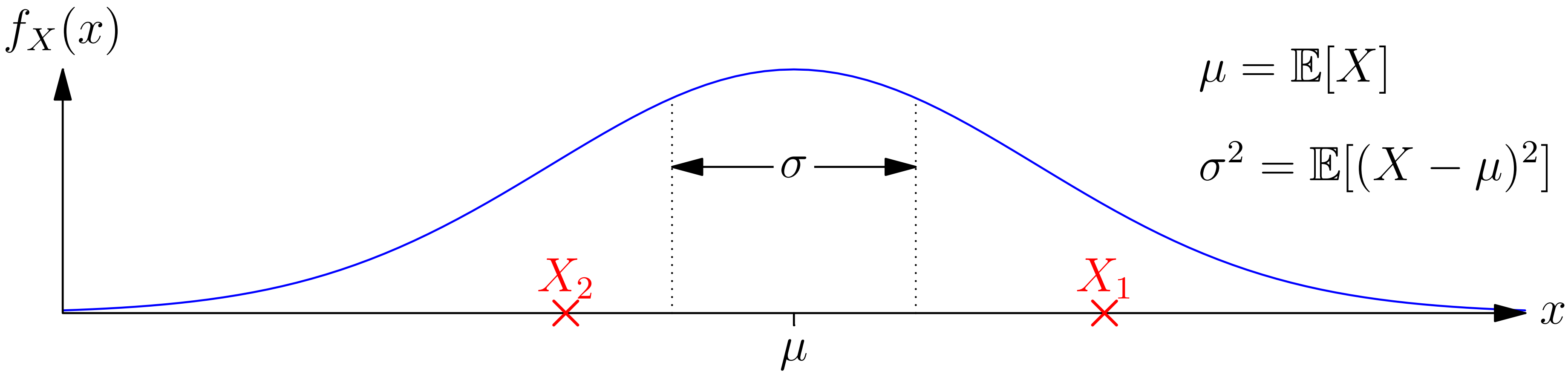

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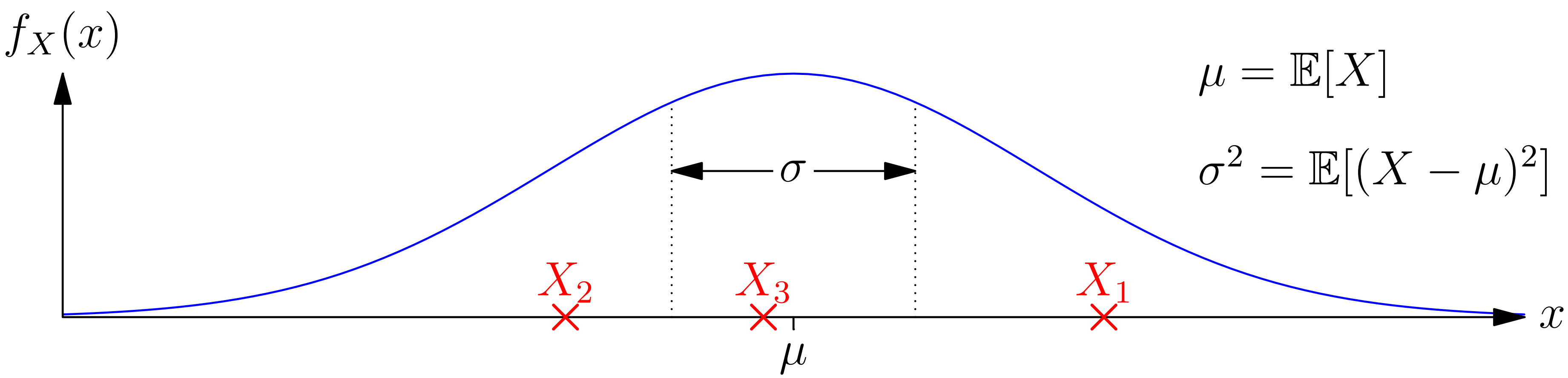

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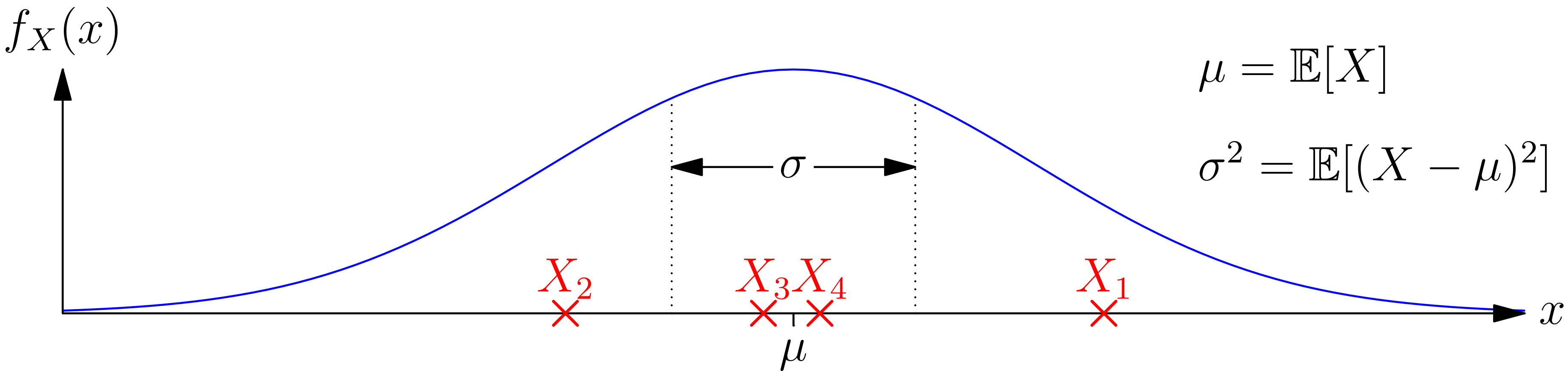

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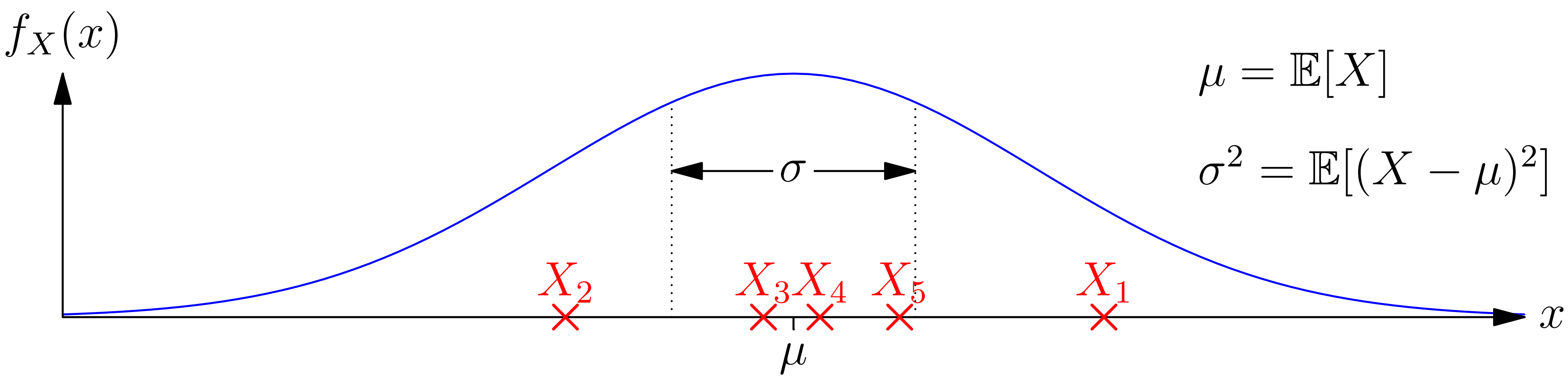

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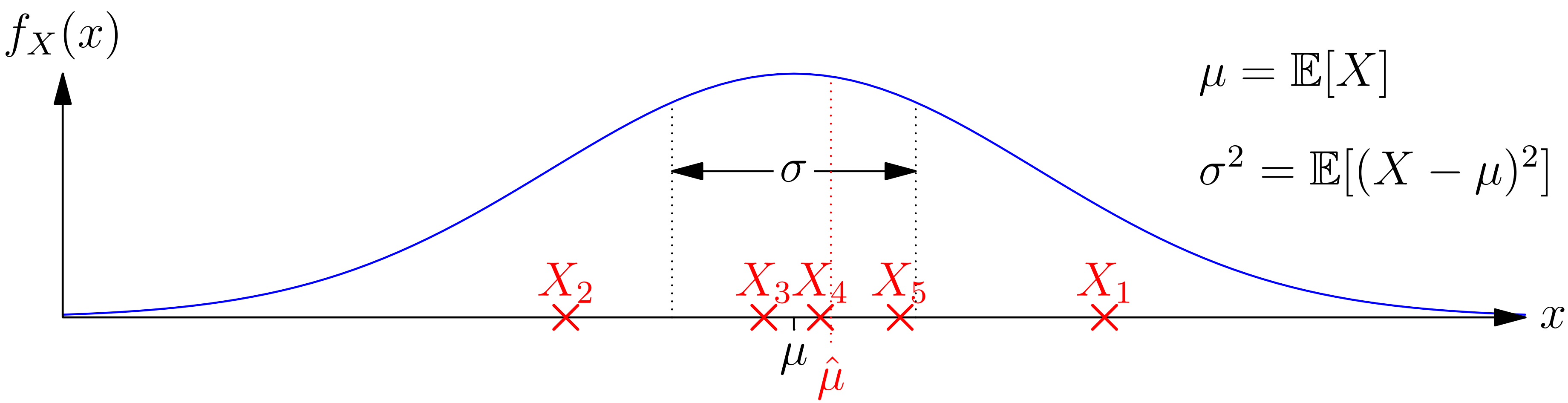

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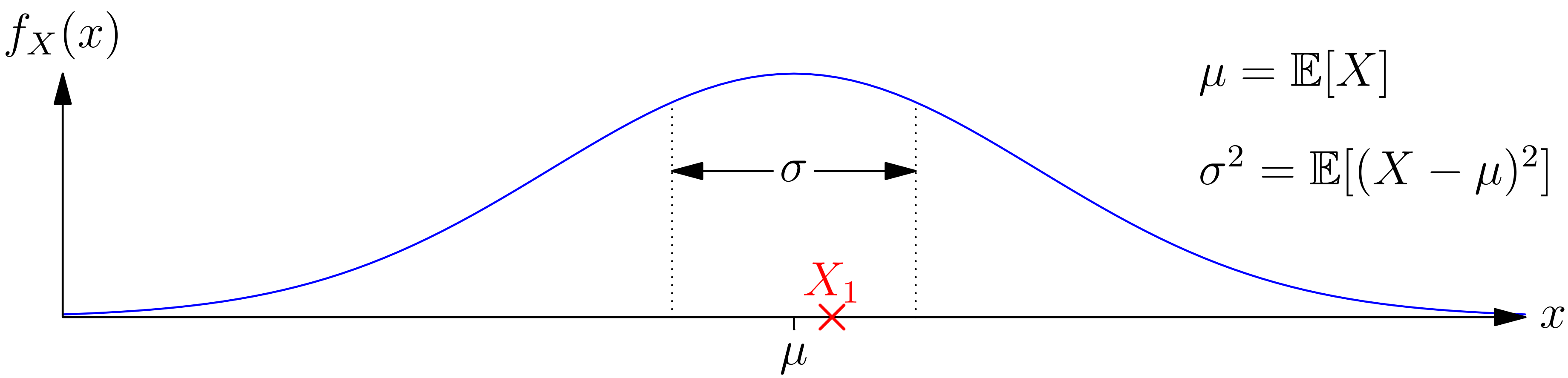

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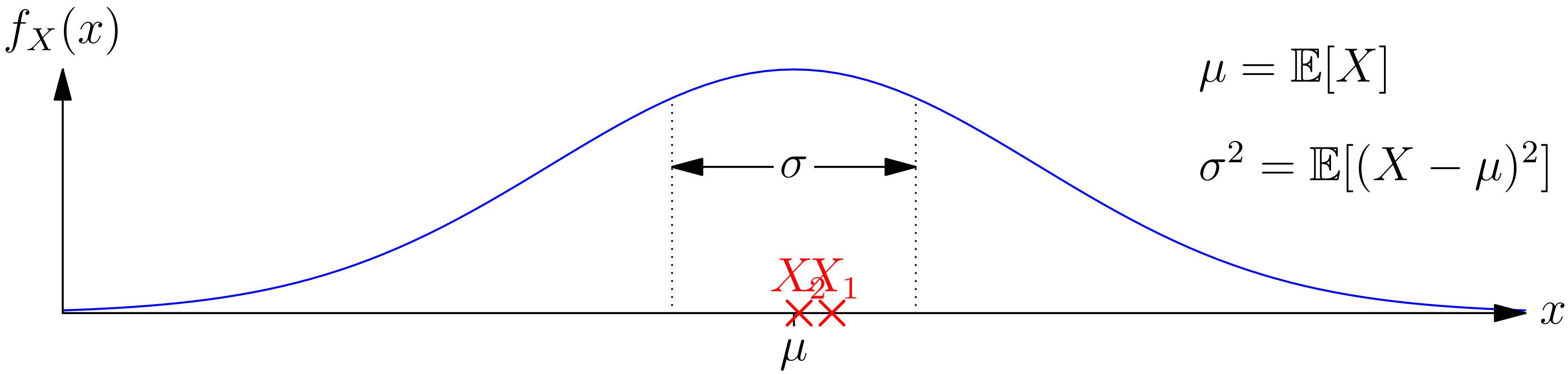

$\mu = \mathbb{E}[X]$

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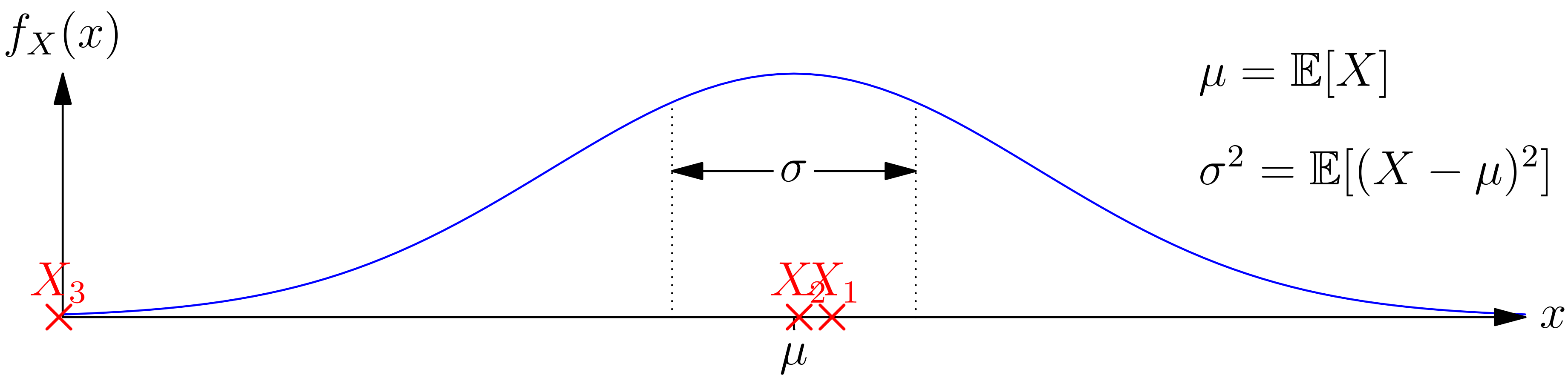

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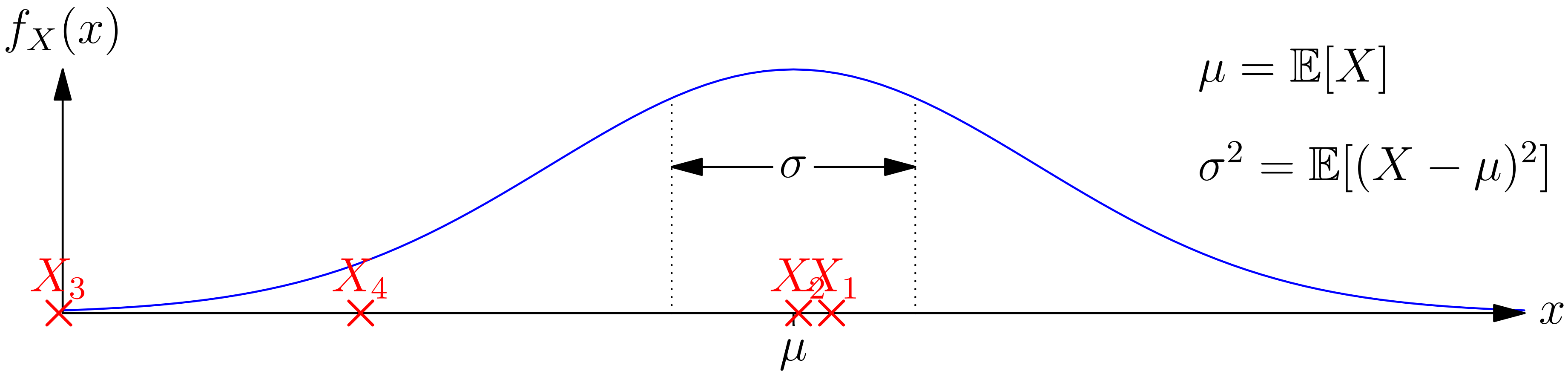

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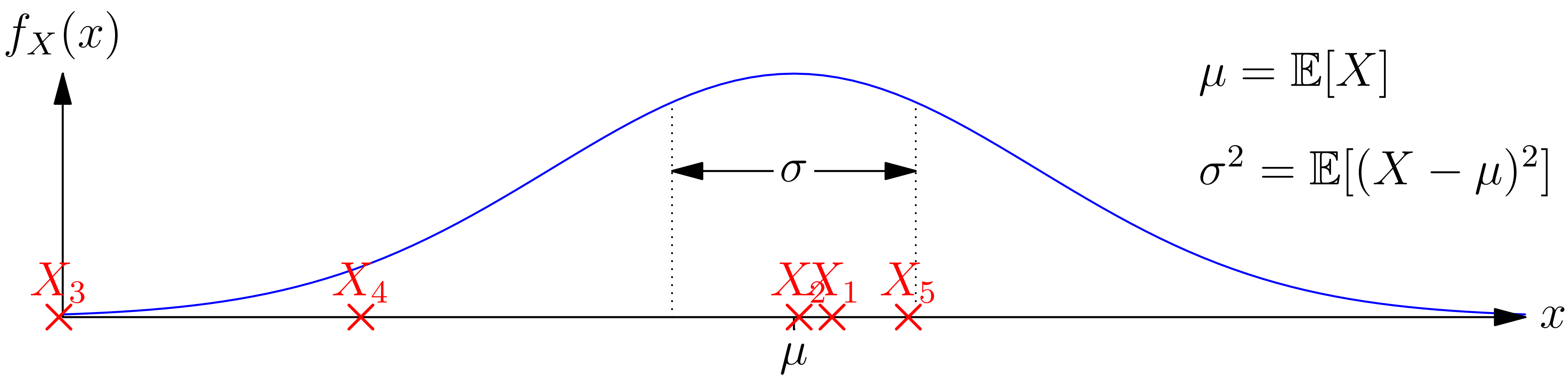

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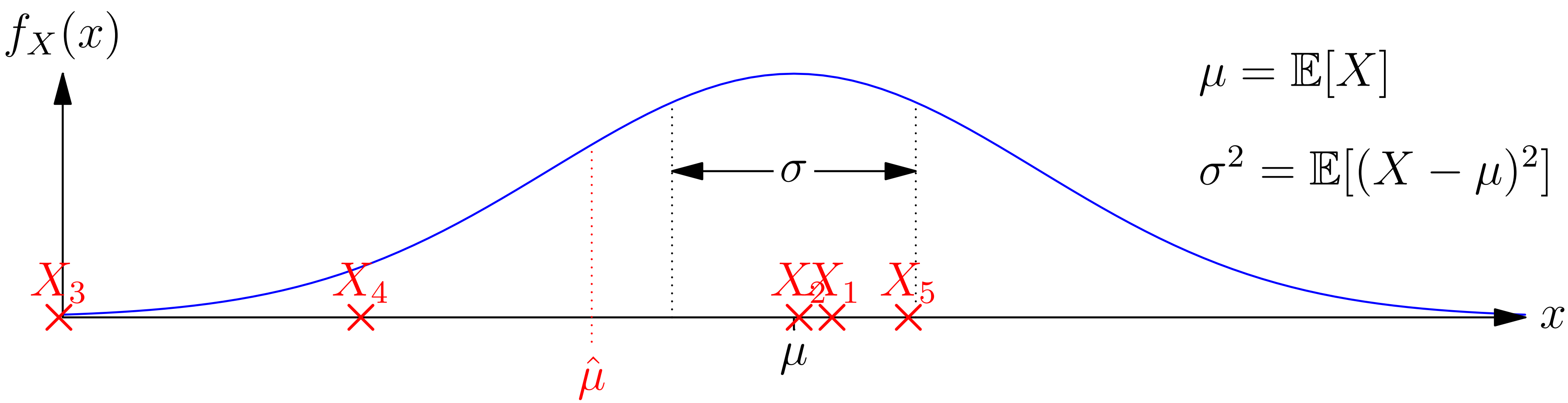

Mean and Variance

- The expected value of the mean, $\hat{\mu}_n$ of n random **independent** variables, X_i, is the expected value $\mu = \mathbb{E}[X_i]$

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$$\frac{1}{n^2}\mathbb{E}\left[\left(\sum_{i=1}^{n}(X_i - \mu)\right)^2\right] = \frac{1}{n^2}\mathbb{E}\left[\sum_{i=1}^{n}(X_i - \mu)^2 + \sum_{i=1}^{n}\sum_{\substack{j=1\\ j\neq i}}^{n}(X_i - \mu)\,(X_j - \mu)\right]$$

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- To reduce the variance in a learning machine (such as a decision tree) we can average over many machines
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Performance of Bagging

- For classification we get our different machines to vote
- For regression we can average the prediction of different machines
- Bagging improves the performance of decision trees
- However, we can usually do better using Boosting
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- If we calculate the variance of the mean of positively correlated variables with correlation ρ we find

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$(\rho = \mathbb{E}[(X_i - \mu)\,(X_j - \mu)]\,/\sigma^2)$

- As $n \to \infty$ the second term vanishes, but we are left with the first term

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Random Forest

- In random forests we average much less correlated trees
- We do this for each tree we choose a subset of $p' \ll p$ of the features on which to split the tree
- Typically p' can range from 1 to $\sqrt{p}$
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- By averaging over a huge number of trees (order of 1000) we typically get good results
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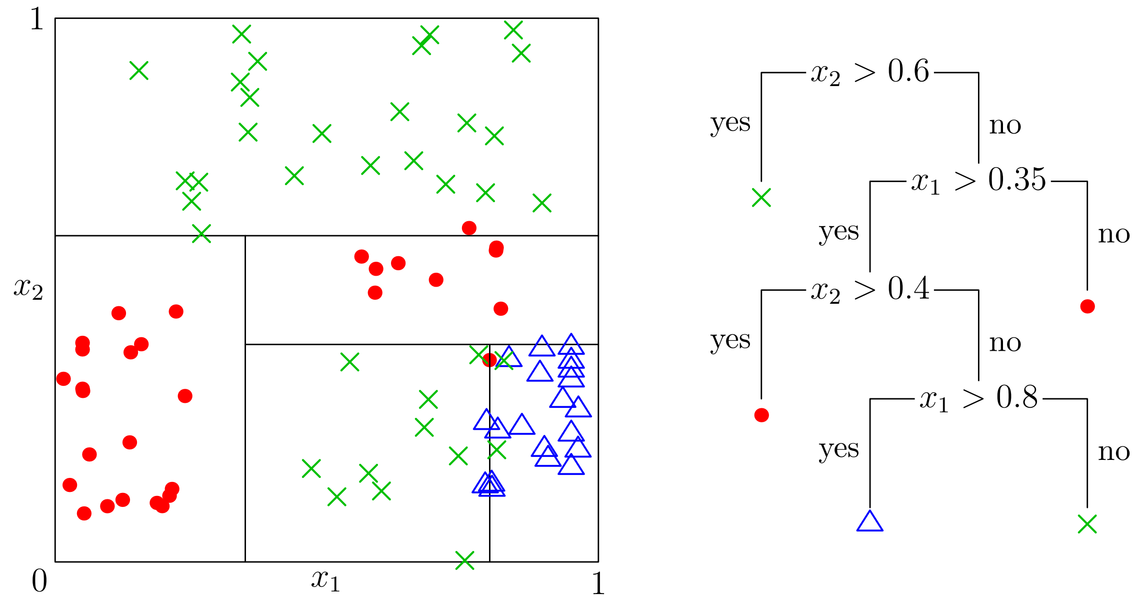
Outline

1. Decision Trees
2. Bagging
3. **Boosting**



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- In boosting we make a **strong learner** by using a weighted sum of **weak learners**

$$C_n(\boldsymbol{x}) = \sum_{i=1}^{n} \alpha_i \, \hat{h}_i(\boldsymbol{x})$$

- Weak learners, $\hat{h}_i(\boldsymbol{x})$, are learning machine that do a little better than chance

- The trick is to choose the weights, α_i

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Shallow Trees

- One of the most effective type of weak learner are very shallow trees
- Sometimes we just use one variable (the stump)
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  - ⋆ adaboost
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Boosting a Binary Classifier

- Suppose we have a binary classification task with data $\mathcal{D} = \{(\boldsymbol{x}^\mu, y^\mu) | \mu = 1, 2, \ldots, m\}$ with $y^\mu \in \{-1, 1\}$
- Our i^{th} weak learner provides a prediction $\hat{h}_i(\boldsymbol{x}^\mu) \in \{-1, 1\}$
- We ask, can we find a linear combination

$$C_n(\boldsymbol{x}) = \alpha_1 \hat{h}_1(\boldsymbol{x}) + \alpha_2 \hat{h}_2(\boldsymbol{x}) + \cdots + \alpha_n \hat{h}_n(\boldsymbol{x})$$

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- AdaBoost is a classic solution to this problem

- It assigns an "loss function"

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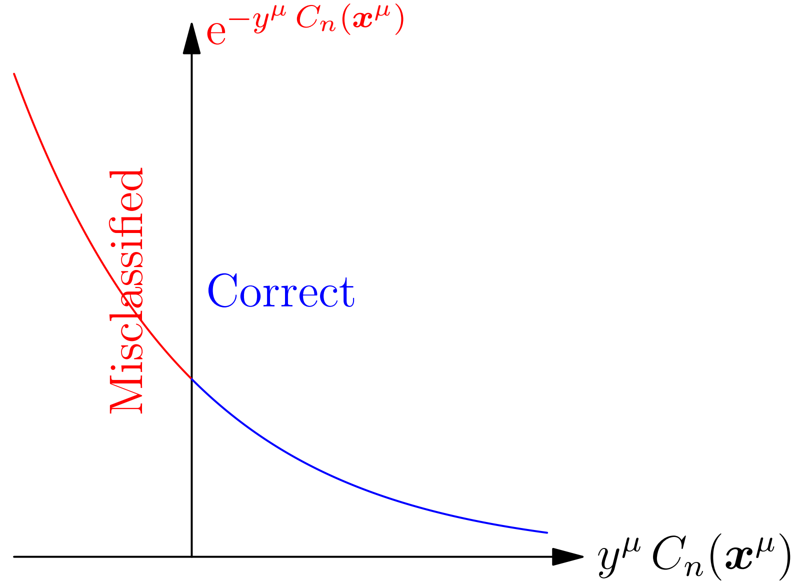

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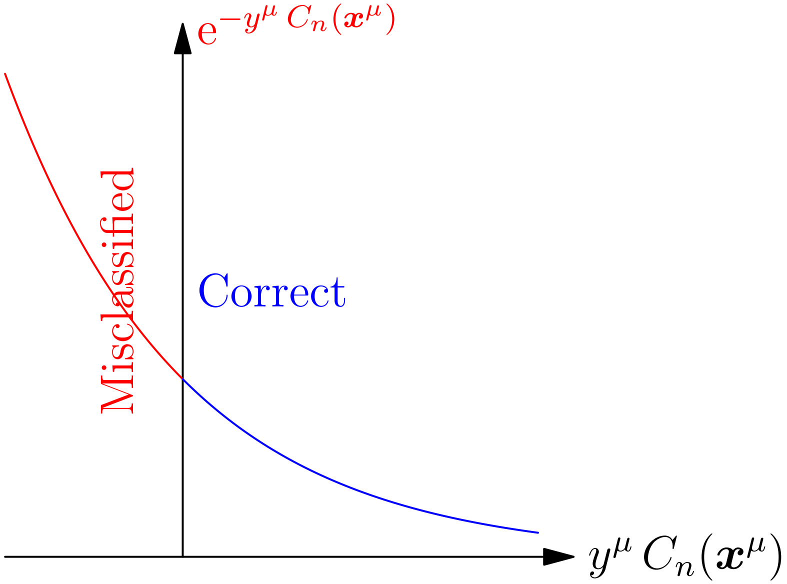

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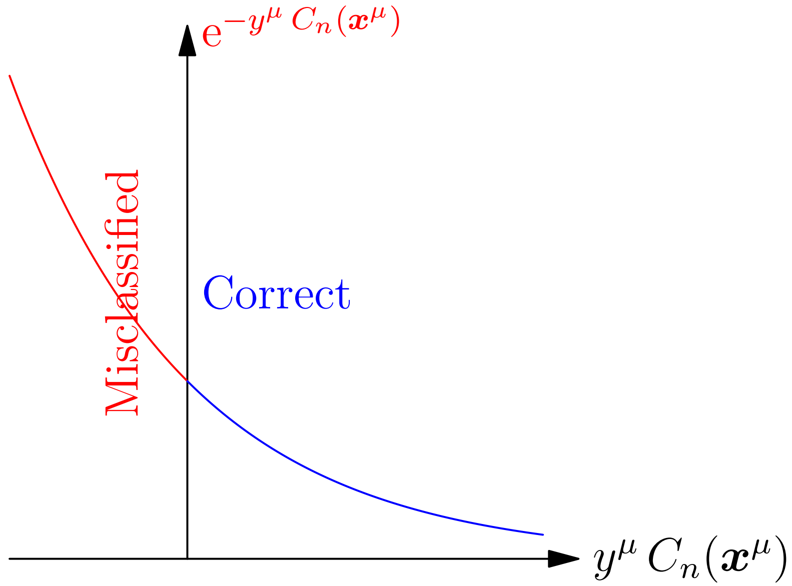

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Iterative Learning

- We build up a strong learner iteratively (greedily)

$$C_n(\boldsymbol{x}) = C_{n-1}(\boldsymbol{x}) + \alpha_n \, \hat{h}_n(\boldsymbol{x})$$

- Defining $w_1^\mu = 1$ and $w_n^\mu = \mathrm{e}^{-y^\mu C_{n-1}(\boldsymbol{x}^\mu)}$ then

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- To minimise the error

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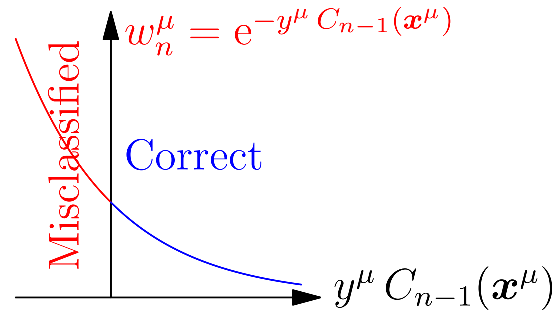

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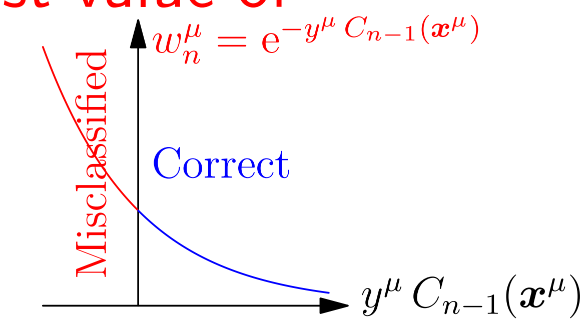

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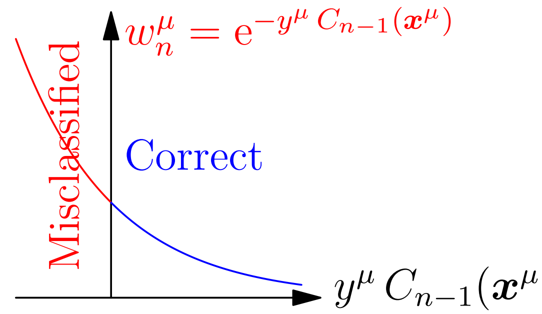

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Algorithm

1. Start with a set of weak learners $\mathcal{W}$
2. Associate a weight, w_n^μ, with every data point $(\boldsymbol{x}^\mu, y^\mu)$, $\mu = 1, 2, \ldots, m$
3. Initially $w_0^\mu = 1$
4. Choose the weak learning, $\hat{h}_n(\boldsymbol{x}) \in \mathcal{W}$, that minimises $\displaystyle\sum_{\mu: y^\mu \neq \hat{h}_n(\boldsymbol{x}^\mu)} w_n^\mu$
5. Update predictor $C_n(\boldsymbol{x}) = C_{n-1}(\boldsymbol{x}) + \alpha_n\, \hat{h}_n(\boldsymbol{x})$ where
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4. Choose the weak learning, $\hat{h}_n(\boldsymbol{x}) \in \mathcal{W}$, that minimises $\displaystyle\sum_{\mu : y^\mu \neq \hat{h}_n(\boldsymbol{x}^\mu)} w_n^\mu$
5. Update predictor $C_n(\boldsymbol{x}) = C_{n-1}(\boldsymbol{x}) + \alpha_n \, \hat{h}_n(\boldsymbol{x})$ where
$$\alpha_n = \frac{1}{2} \log \left(\frac{\sum_{\mu : y^\mu = \hat{h}_n(\boldsymbol{x}^\mu)} w_n^\mu}{\sum_{\mu : y^\mu \neq \hat{h}_n(\boldsymbol{x}^\mu)} w_n^\mu} \right)$$
6. Update $w_{n+1}^\mu = w_n^\mu \, \mathrm{e}^{-y^\mu \, \alpha_n \, \hat{h}_n(\boldsymbol{x}^\mu)}$
7. Go to 4

Algorithm

1. Start with a set of weak learners $\mathcal{W}$
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Performance

- Adaboost works well with weak learners, usually out-performing bagging
- It doesn't work well with strong learners (tends to over-fit)
- It is limited to binary classification (there are generalisation, but they are difficult to get to work)
- It has fallen from fashion
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Gradient Boosting

- In gradient boosting we again build a strong learner as a linear combination of weak learners

$$C_n(\boldsymbol{x}) = C_{n-1}(\boldsymbol{x}) + \hat{h}_n(\boldsymbol{x})$$

- At each step $\hat{h}_n(\boldsymbol{x})$ is trained to predict the residual error, $\Delta_{n-1} = y - C_{n-1}(\boldsymbol{x})$, (i.e. the target minus the current prediction)

- (This difference looks a bit like a gradient hence the rather confusing name)

- Gradient boosting also mainly used with regression decision trees

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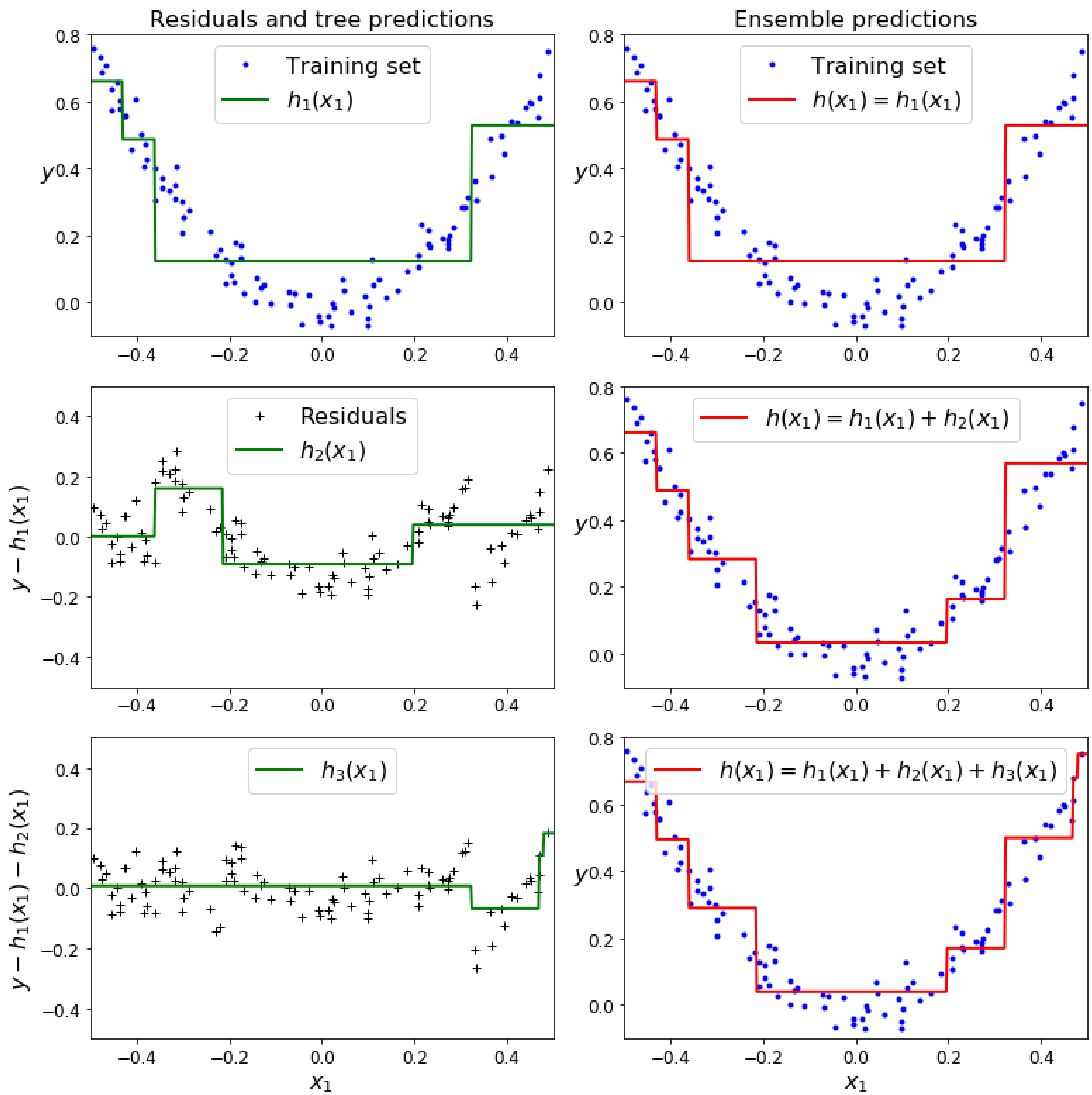
Residuals and tree predictions
Training set
$h_1(x_1)$
Ensemble predictions
Training set
$h(x_1) = h_1(x_1)$
Residuals
$h_2(x_1)$
$h(x_1) = h_1(x_1) + h_2(x_1)$
$h_3(x_1)$
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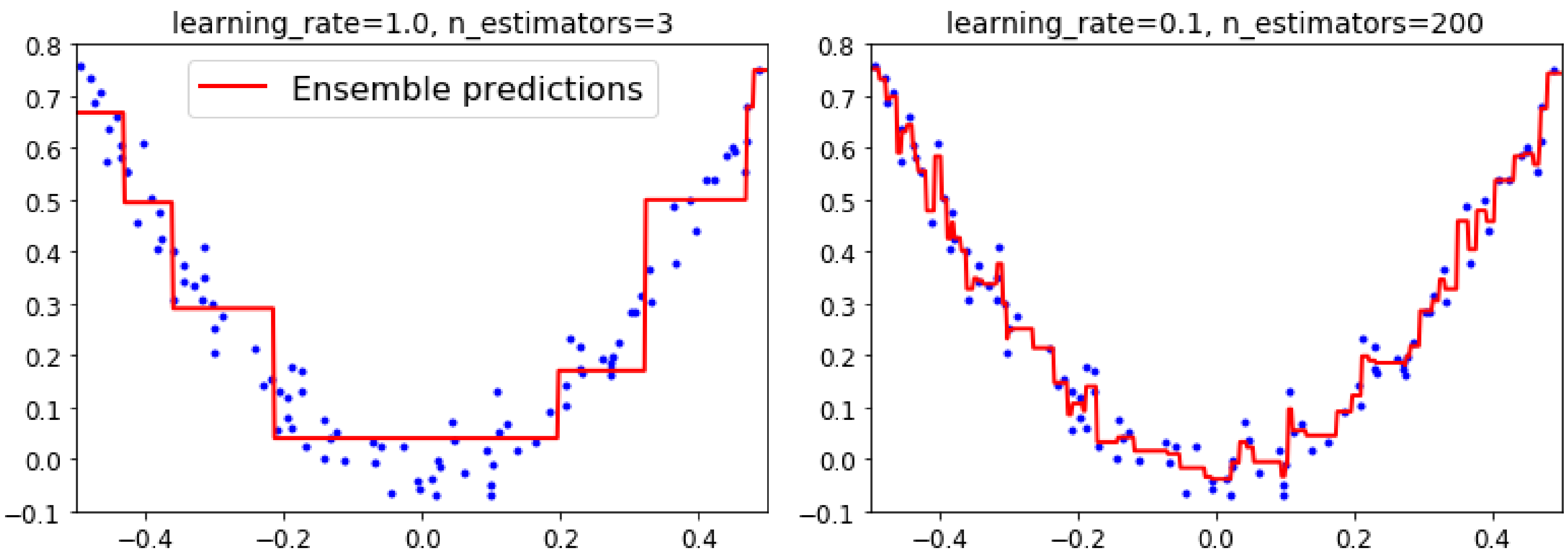
y
$y - h_1(x_1)$
$y - h_1(x_1) - h_2(x_1)$
x_1

Keep On Going

- We can keep on going



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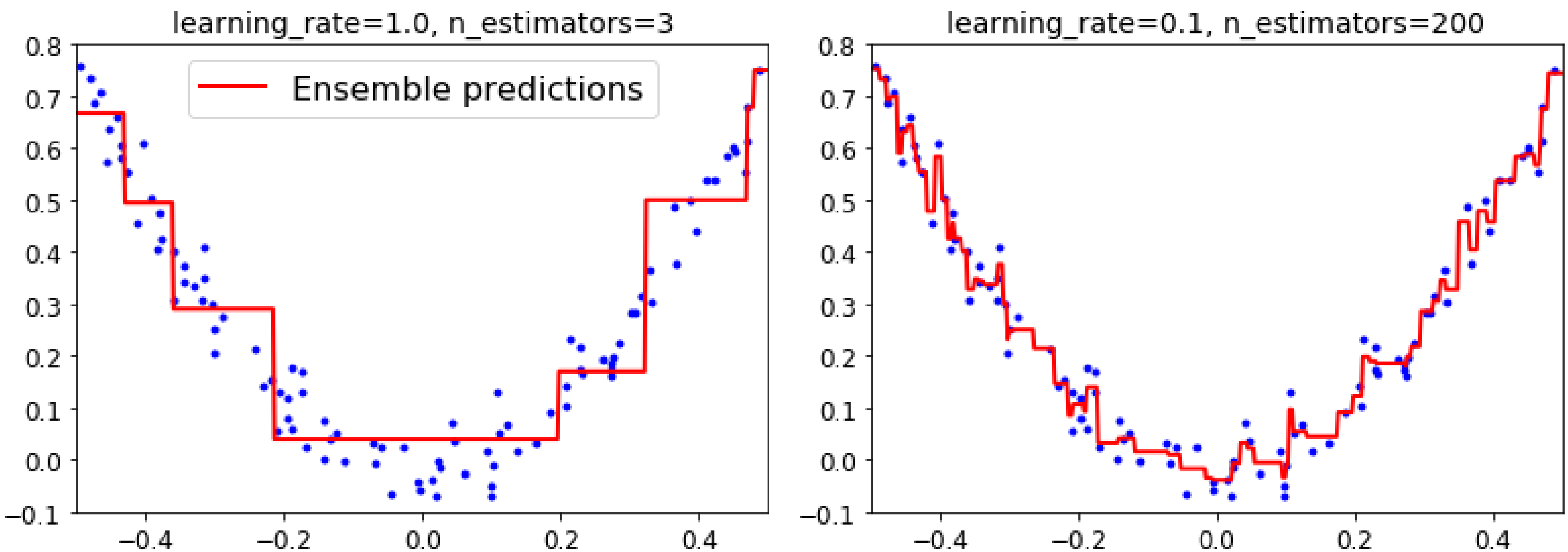
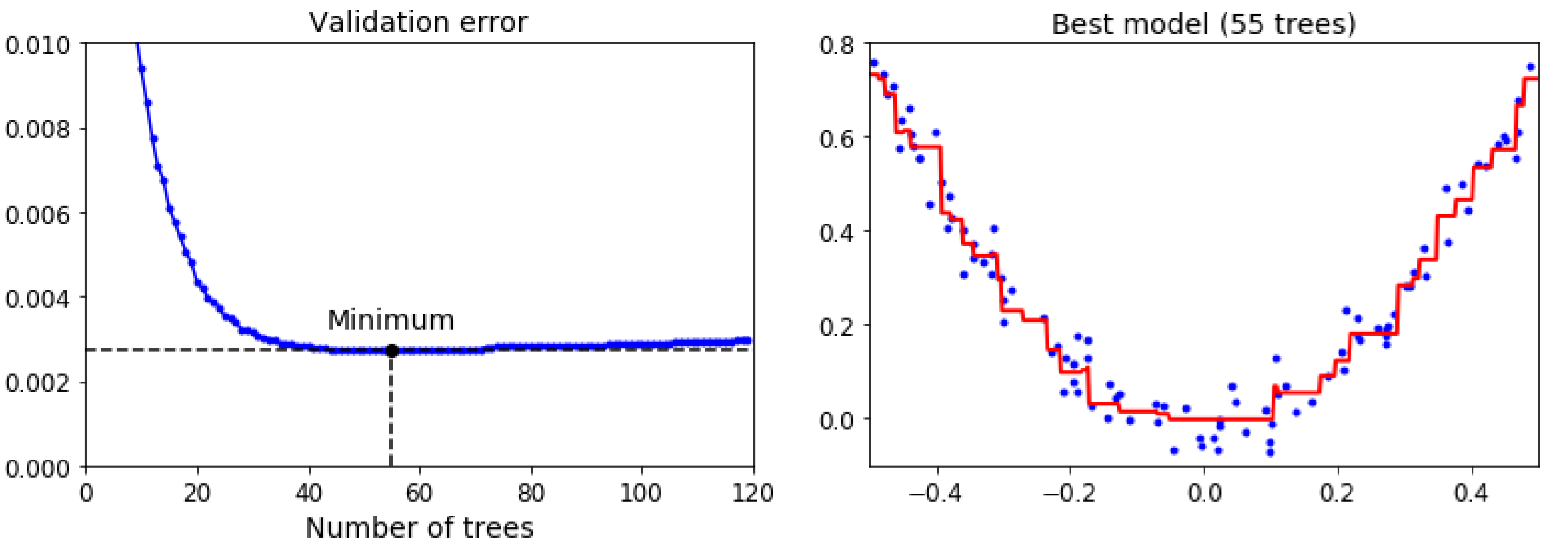


- But we will over-fit eventually

Early Stopping

- Like many algorithms we often get better results by early stopping



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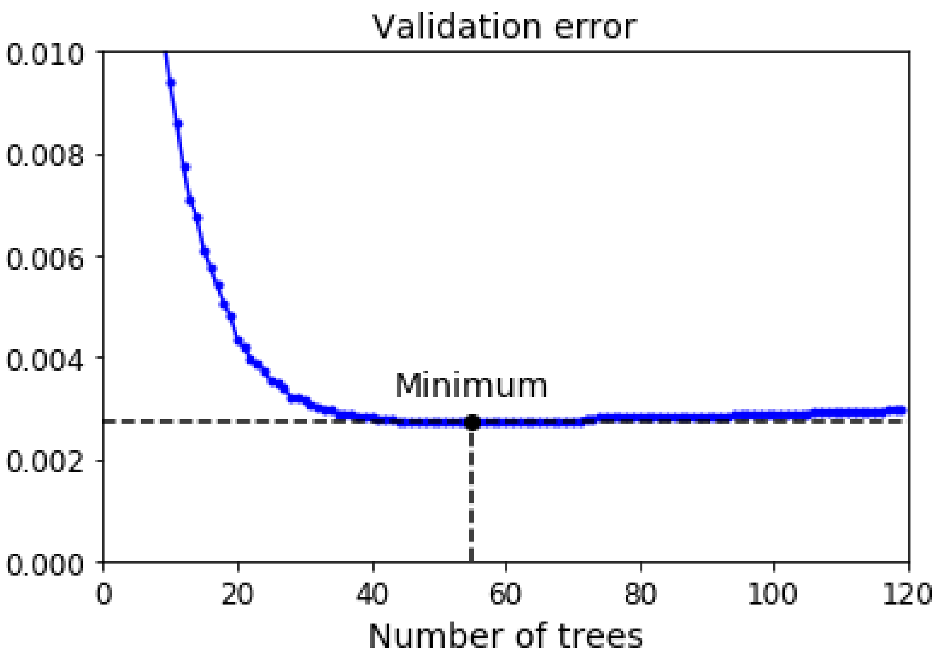

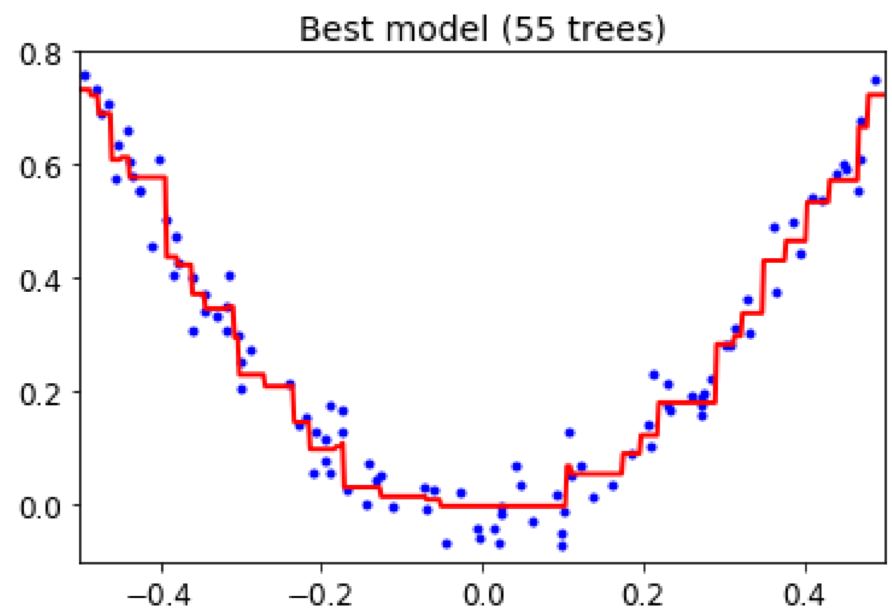

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XGBoost

- XGBoost is an implementation of gradient boosting that won the Higg's Boson challenge and regularly wins Kaggle competitions
- XGBoost stands for eXtreme Gradient Boosting
- It was much faster than most gradient boosting algorithms and scales to billions of training data points—although GBM is often better
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- Rather a bodge of optimisation hacks

Conclusion

- Ensemble methods have proved themselves to be very powerful
- Tend to work best with very simple models (true of random forest and boosting)
- XGBoost or GBM are currently the best methods for tabular data (particular for large training sets)
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