Lecture 0: Intro;
Optional: Trees, ensembles.

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Outline

1. Linear models and metrics recap
2. Decision trees in classification and regression.
3. Information criterions.
4. Pruning.
5. Ensembling methods
6. Optional: advanced ensembling methods

Linear models recap

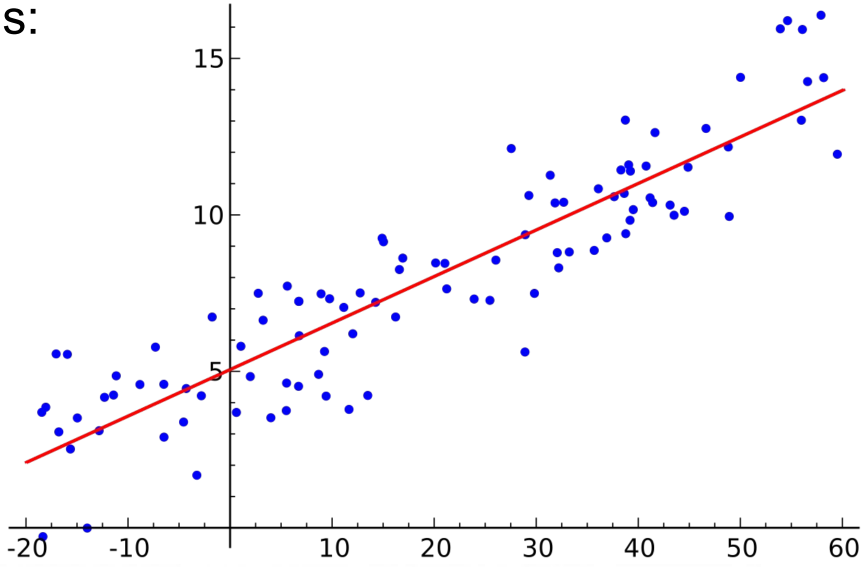
Linear models

$$Y = \underbrace{X_1 + X_2 + X_3}$$

Dependent Variable	Independent Variable
Outcome Variable	Predictor Variable
Response Variable	Explanatory Variable

Linear models

- Predictive models:



Estimated (or predicted) Y value for observation i

Estimate of the regression intercept

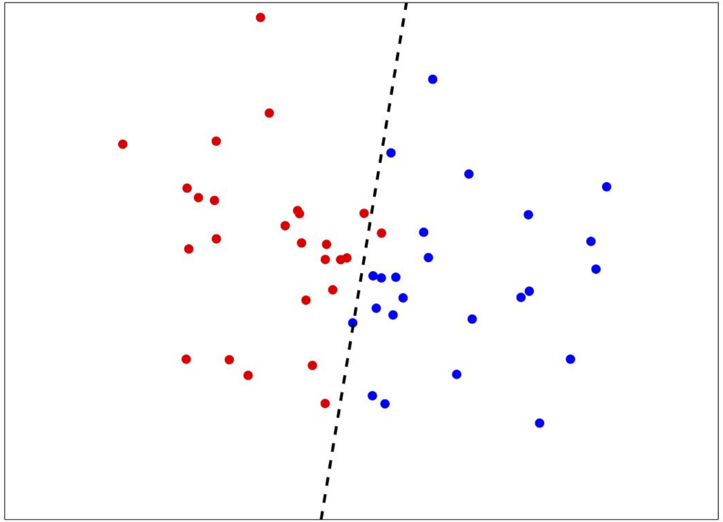
Estimate of the regression slope

Value of X for observation i

$$\hat{Y}_i = b_0 + b_1 X_i$$

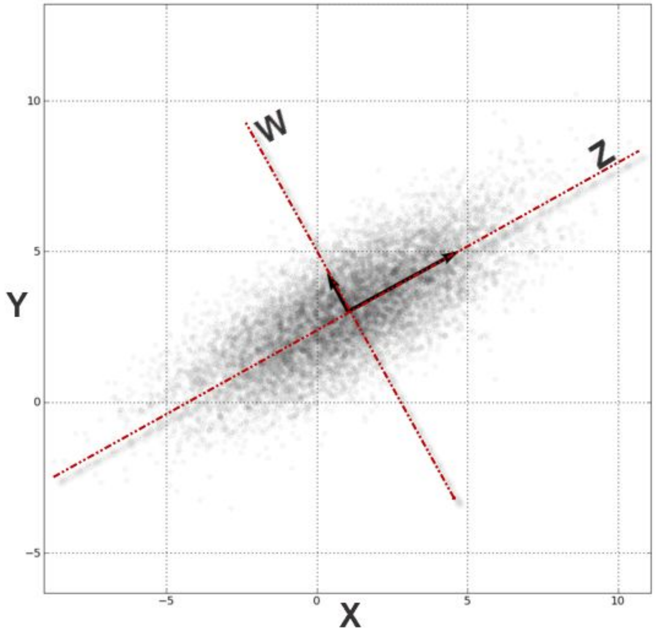
Linear models

- Predictive models:
- Classification models:



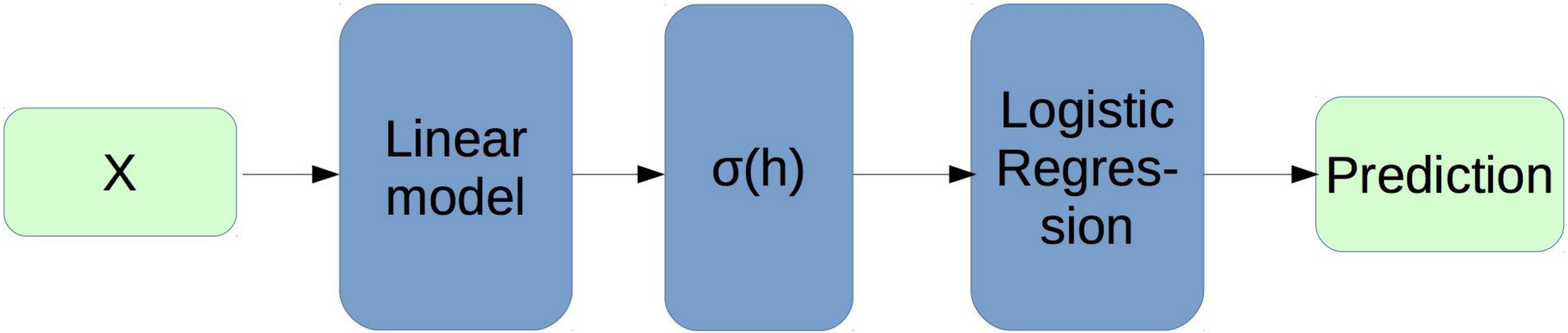
Linear models

- Predictive models:
- Classification models:
- Unsupervised models (e.g. PCA analysis)



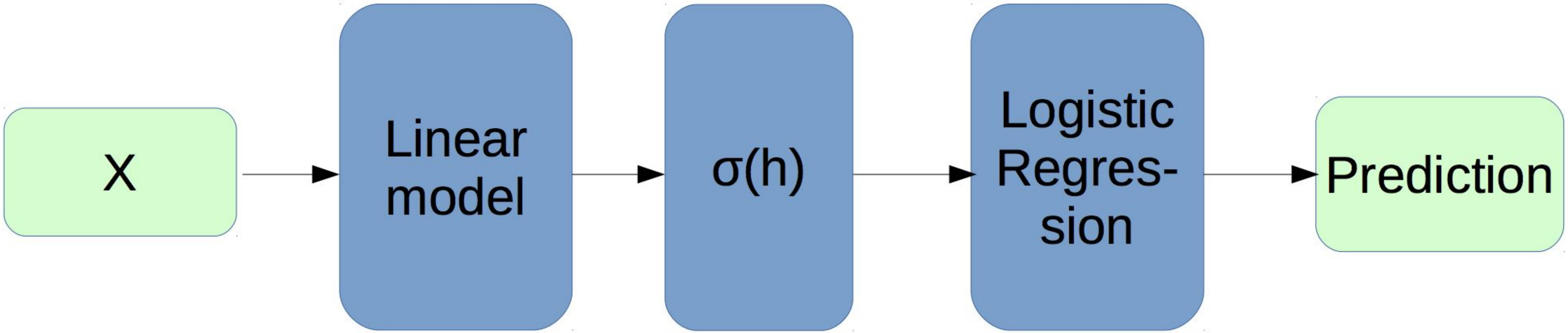
Linear models

- Predictive models:
- Classification models:
- Unsupervised models (e.g. PCA analysis)
- Building block of other models (ensembles, NNs, etc.)



Linear models

- Predictive models:
- Classification models:
- Unsupervised models (e.g. PCA analysis)
- Building block of other models (ensembles, NNs, etc.)



Actually, it's a neural network. We will meet it later.

Quality functions in classification

Quality functions in classification

- Accuracy
- Precision
- Recall
- F-score
- ROC-curve, ROC-AUC
- PR-curve

Accuracy

Number of right classifications

target: 1 0 1 0 0 0 0 1 0 0

Accuracy

Number of right classifications

target: 1 0 1 0 0 0 0 1 0 0

predicted: 0 0 1 0 0 0 0 1 1 0

Accuracy

Number of right classifications

target: 1 0 1 0 0 0 0 1 0 0

predicted: 0 0 1 0 0 0 0 1 1 0

Accuracy

Number of right classifications

target: 1 0 1 0 0 0 0 1 0 0

predicted: 0 0 1 0 0 0 0 1 1 0

accuracy = 8/10 = 0.8

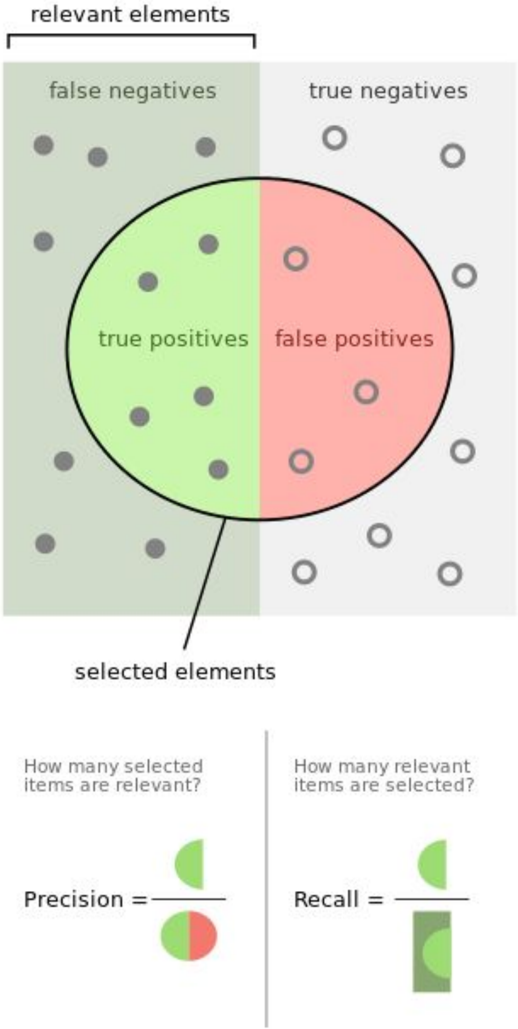
Precision and recall

		Actual Class	
		Yes	No
Predicted Class	Yes	**T**rue **P**ositive	**F**alse **P**ositive
	No	**F**alse **N**egative	**T**rue **N**egative

$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

Precision and recall



		Actual Class	
		Yes	No
Predicted Class	Yes	**T**rue **P**ositive	**F**alse **P**ositive
	No	**F**alse **N**egative	**T**rue **N**egative

$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

F-score

Harmonic mean of precision and recall.
Closer to the smallest one.

$$F_1 = \left(\frac{\mathrm{recall}^{-1} + \mathrm{precision}^{-1}}{2} \right)^{-1} = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}$$

F-score

Harmonic mean of precision and recall.
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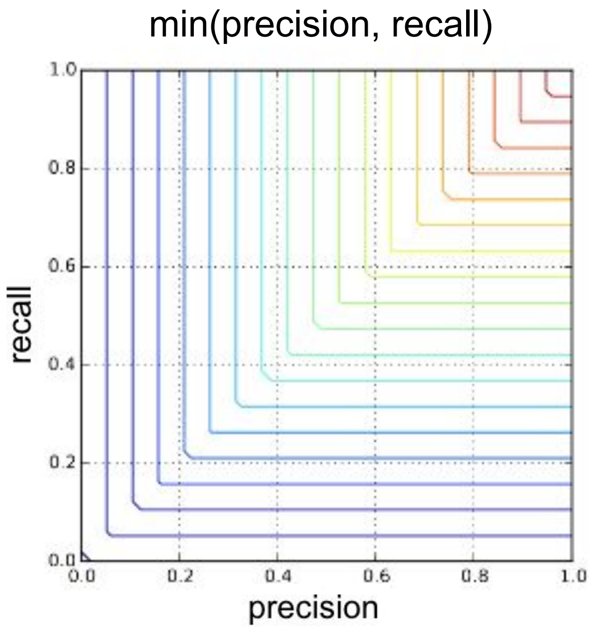
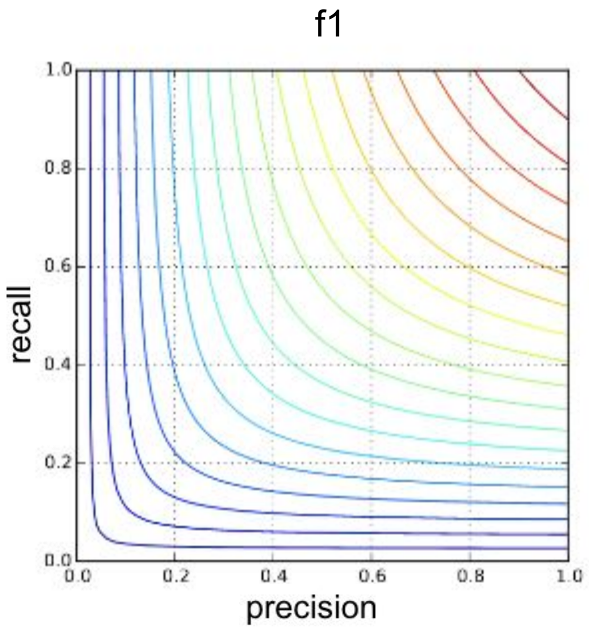
$$F_\beta = (1 + \beta^2) \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{(\beta^2 \cdot \mathrm{precision}) + \mathrm{recall}}$$

F-score



min(precision, recall)
recall
precision
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0



f1
recall
precision
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0

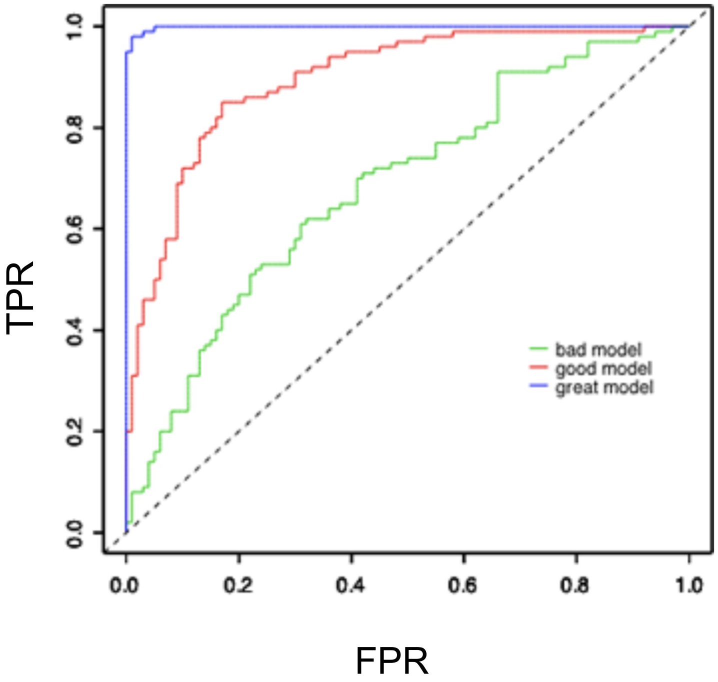
ROC - receiver operating characteristic

		Actual Class	
		Yes	No
Predicted Class	Yes	**T**rue **P**ositive	**F**alse **P**ositive
	No	**F**alse **N**egative	**T**rue **N**egative

$$TPR = \frac{True\ positives}{True\ positives + False\ negatives}$$

$$FPR = \frac{False\ positives}{False\ positives + True\ negatives}.$$

ROC - receiver operating characteristic



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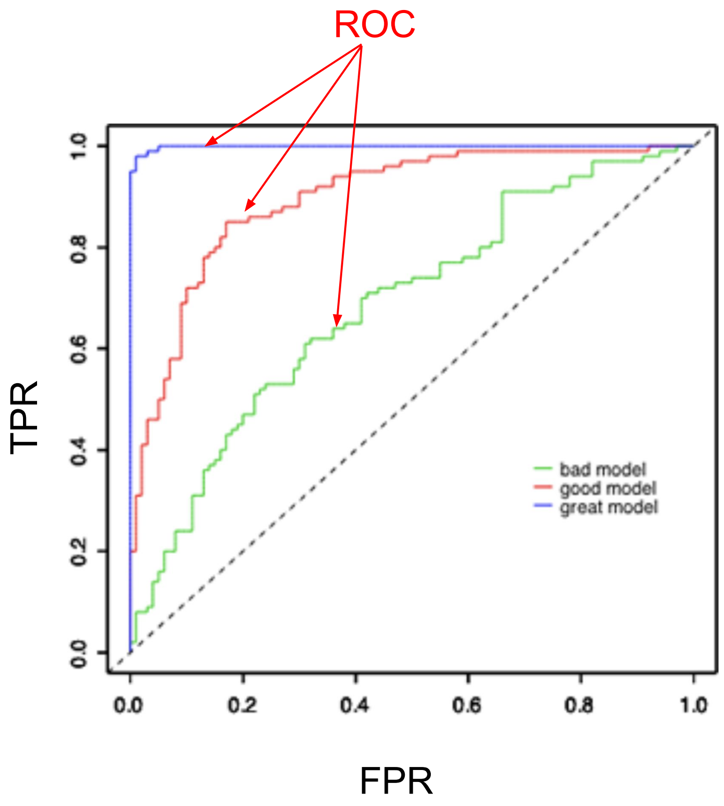
ROC



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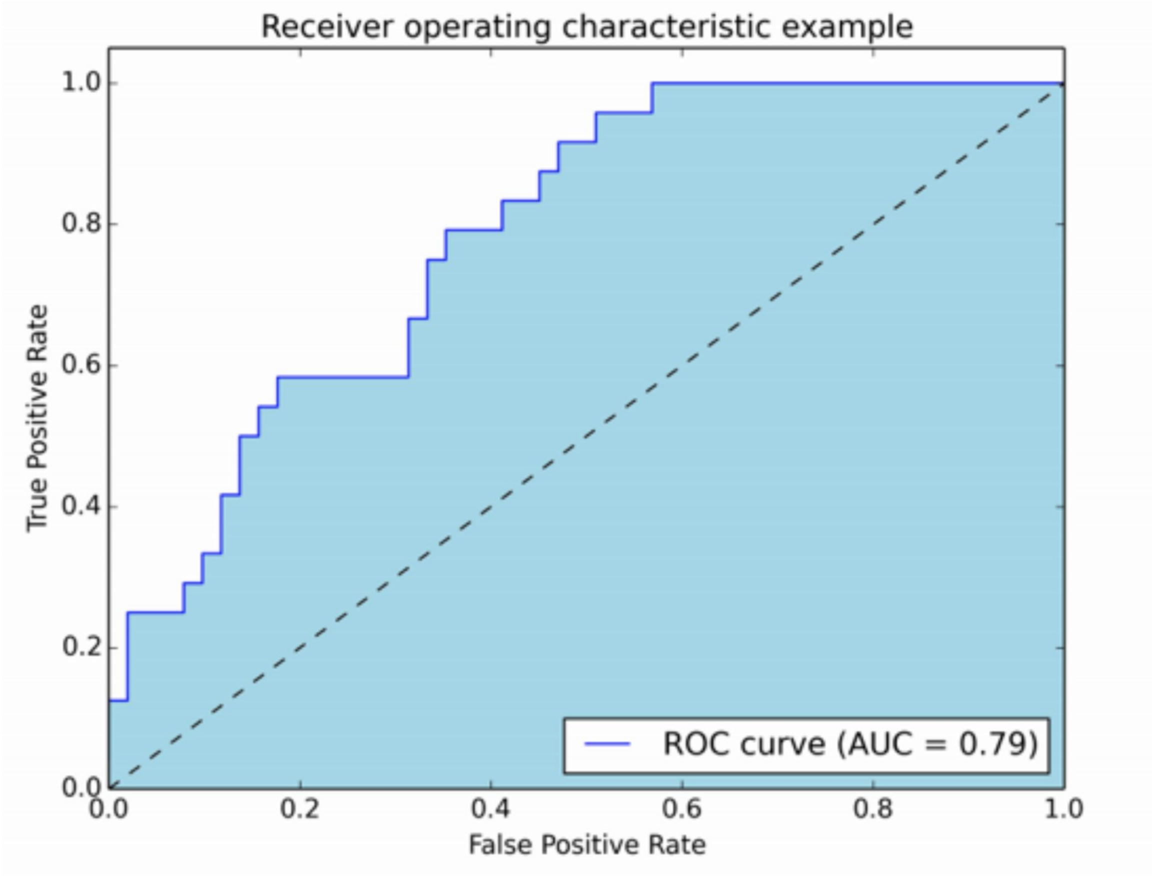
$$TPR = \frac{True\ positives}{True\ positives + False\ negatives}$$

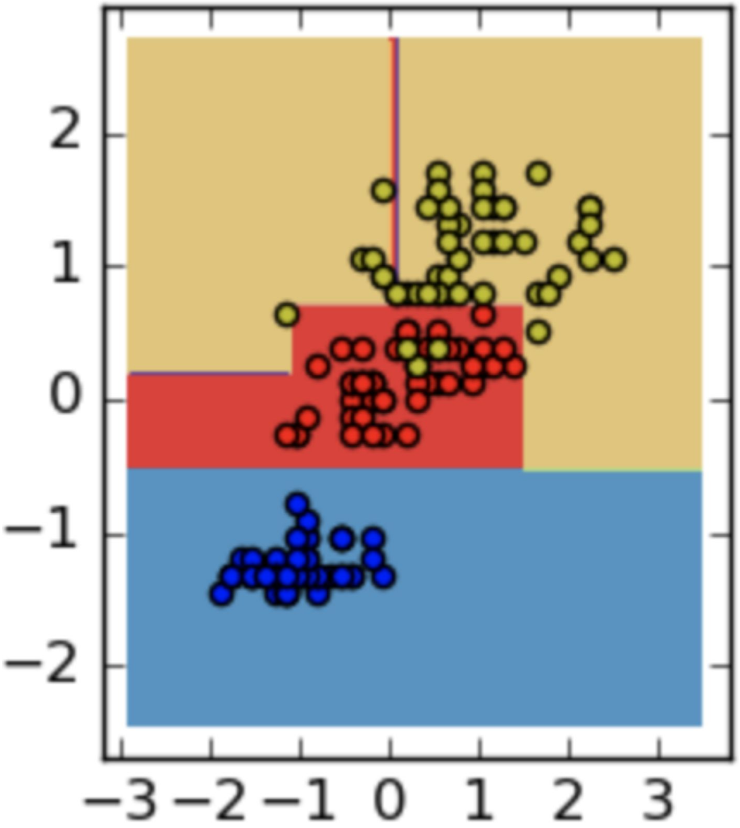
$$FPR = \frac{False\ positives}{False\ positives + True\ negatives}.$$

ROC-AUC - area under curve



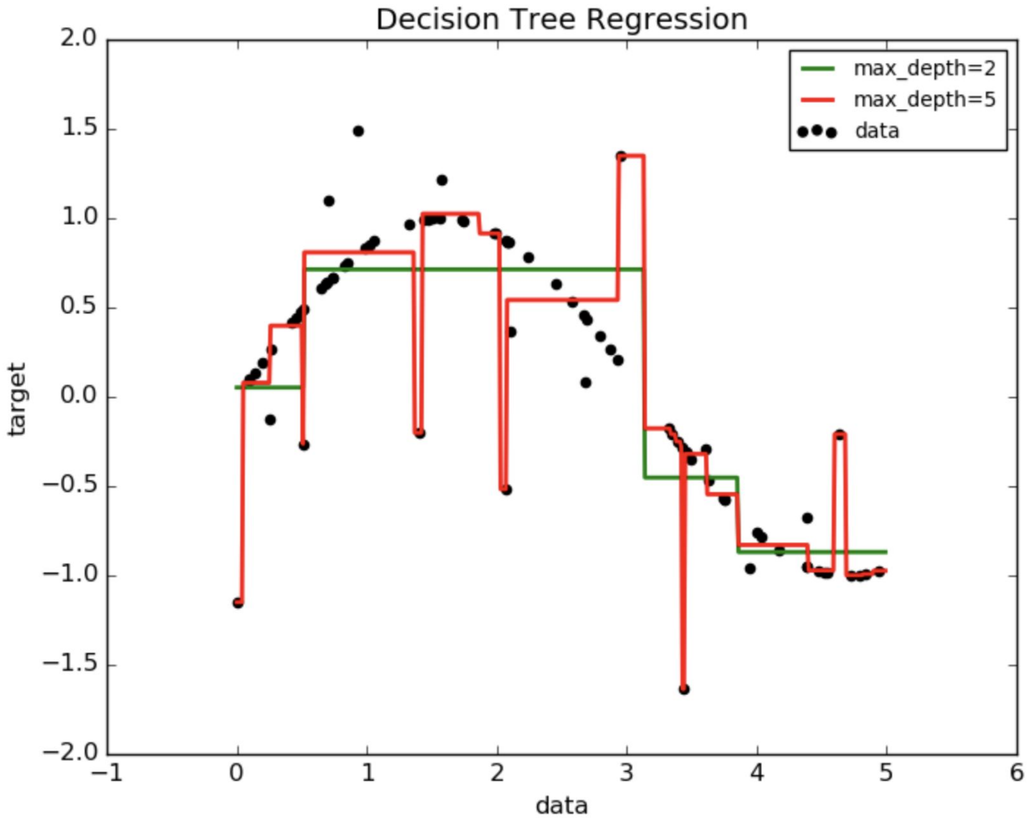
Decision trees

Decision tree in classification



Classification problem with 3 classes and 2 features.

Decision tree in regression



Green - decision tree of depth 2
Red - decision tree of depth 5

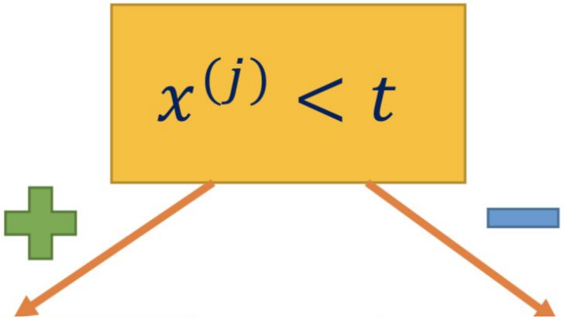
Every leaf corresponds to some constant.

Constructing decision trees

$$\boxed{x^{(j)} < t}$$

1. Make a split

Constructing decision trees



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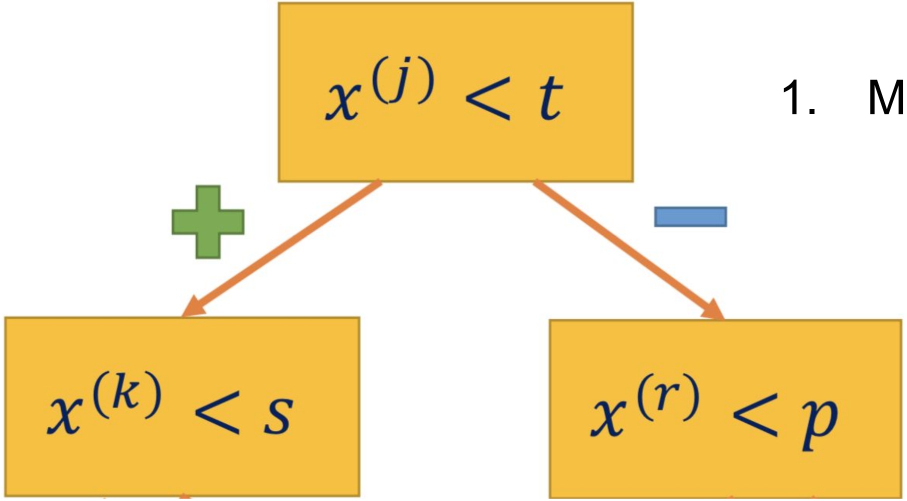
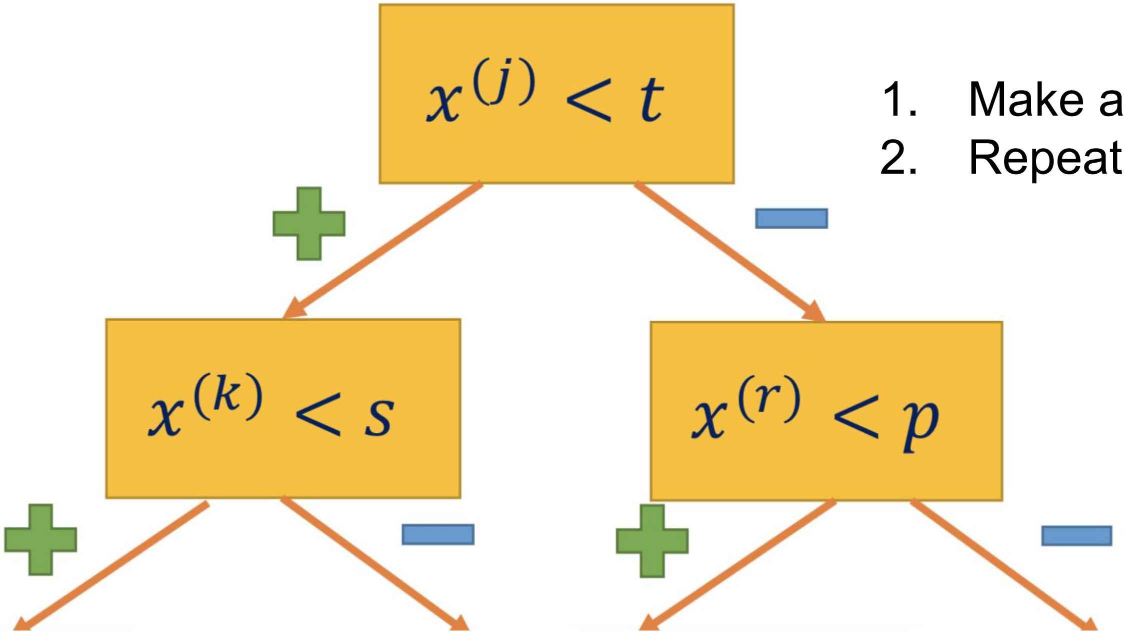
Constructing decision trees



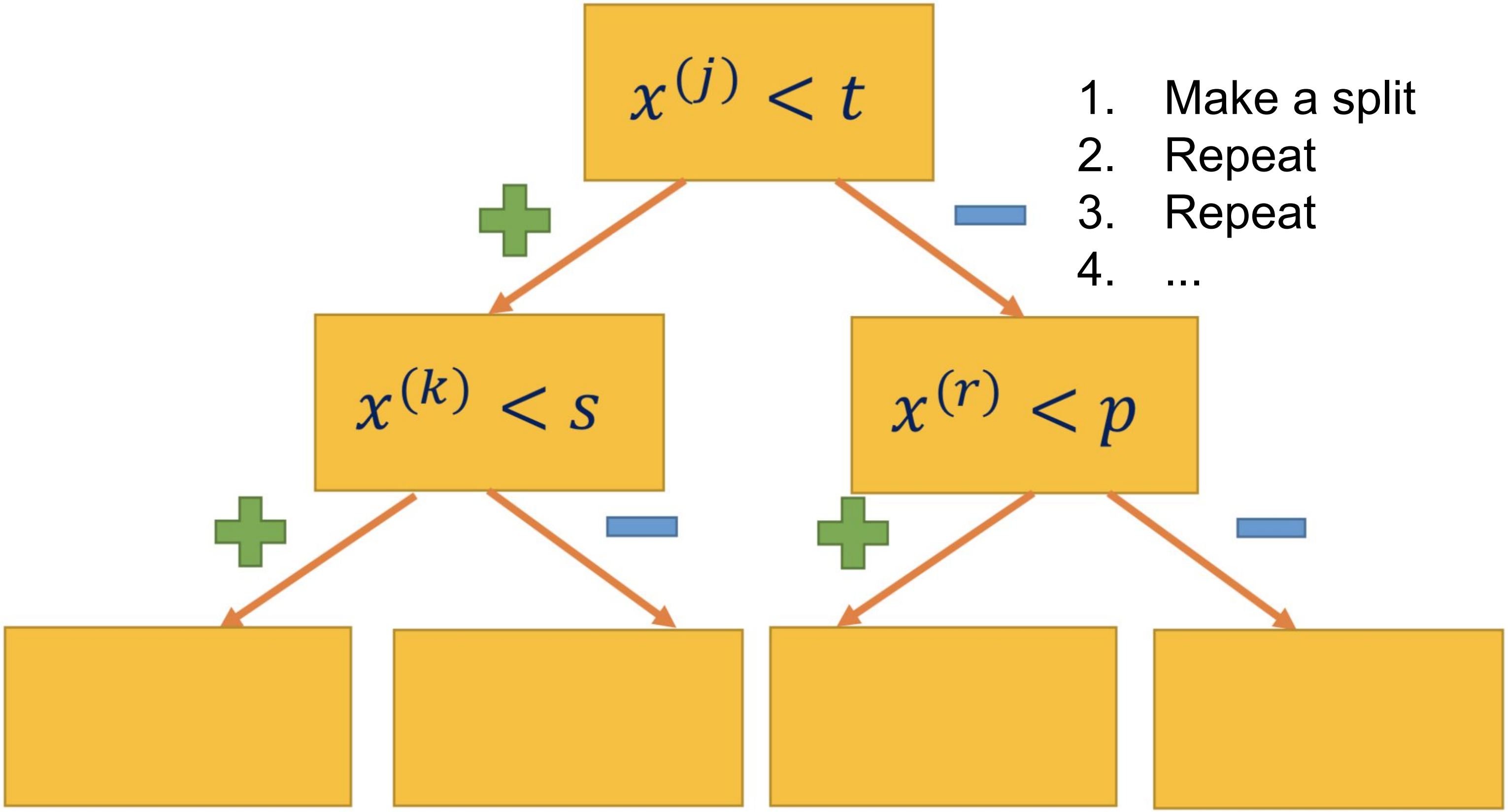
1. Make a split

Constructing decision trees



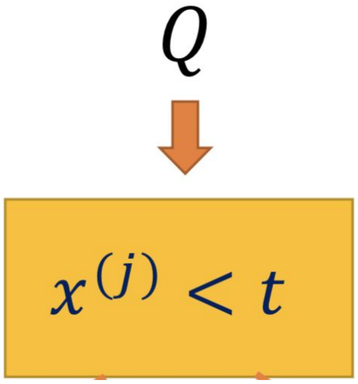
1. Make a split
2. Repeat

Constructing decision trees



1. Make a split
2. Repeat
3. Repeat
4. ...

How to split data properly?



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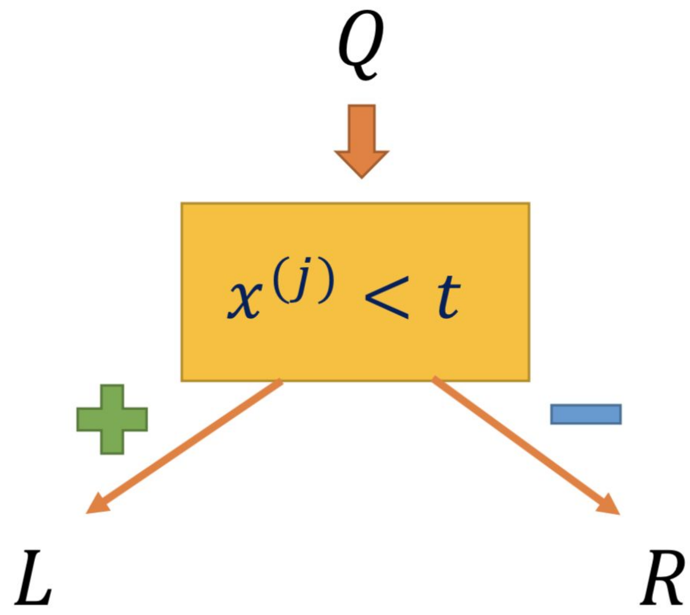

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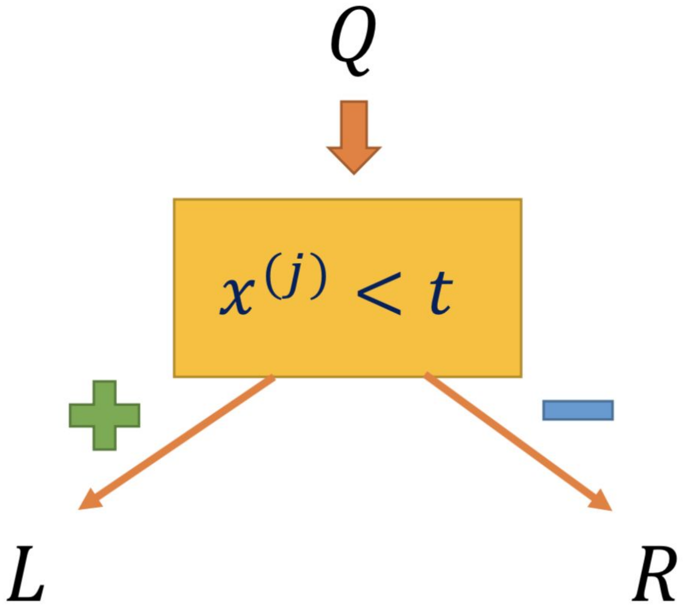
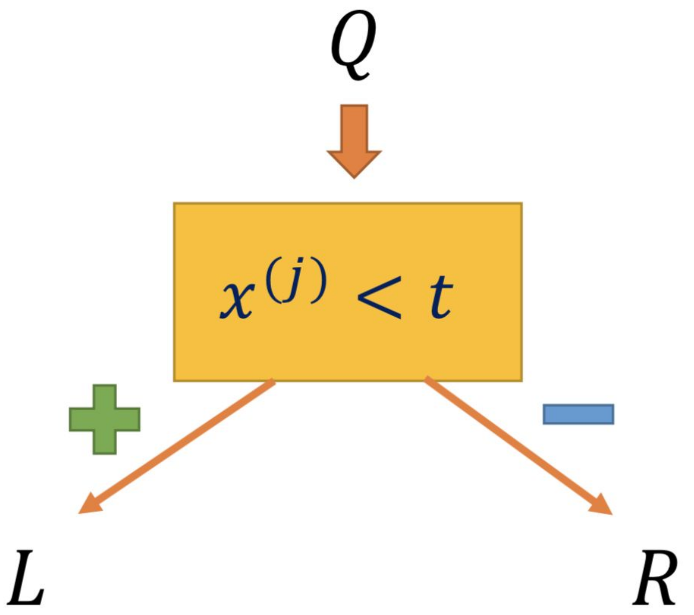


$$G(j,t) = \frac{|L|}{|Q|} H(L) + \frac{|R|}{|Q|} H(R)$$

How to split data properly?



What is H()?

$$G(j,t) = \frac{|L|}{|Q|}H(L) + \frac{|R|}{|Q|}H(R) \rightarrow \min_{j,t}$$

Information criteria

H(R) is measure of “heterogeneity” of our data.
Consider binary classification problem:

1. Misclassification criteria: $$H(R) = 1 - \max\{p_0, p_1\}$$

2. Entropy criteria: $$H(R) = -p_0 \log_2 p_0 - p_1 \log_2 p_1$$

3. Gini impurity: $$H(R) = 1 - p_0^2 - p_1^2 = 1 - 2p_0p_1$$

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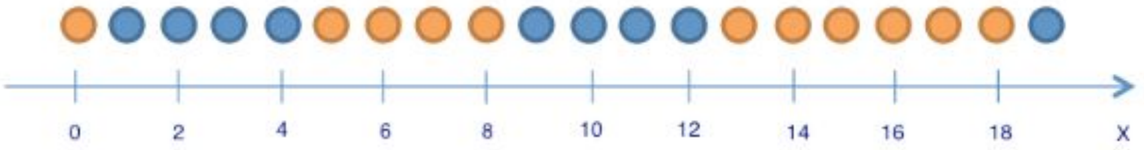
Consider binary classification problem:



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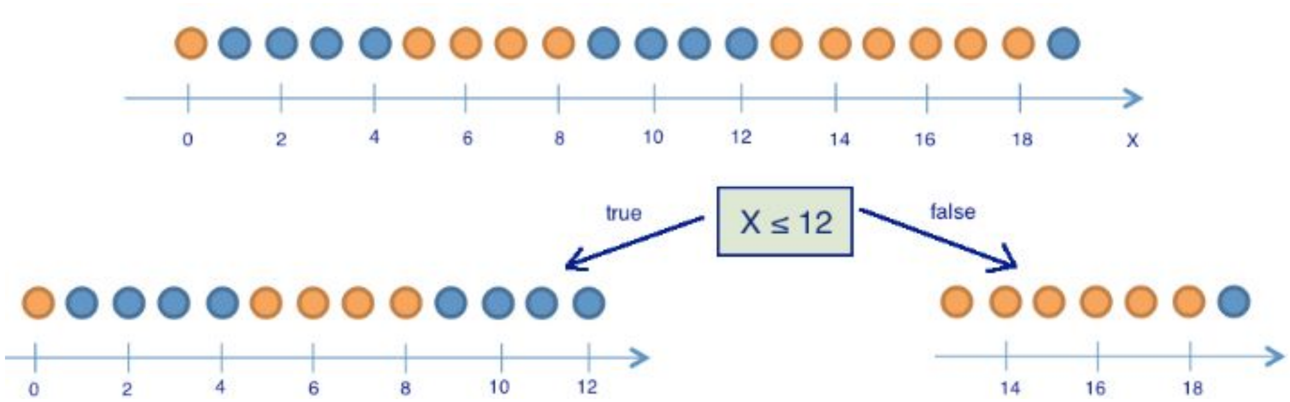
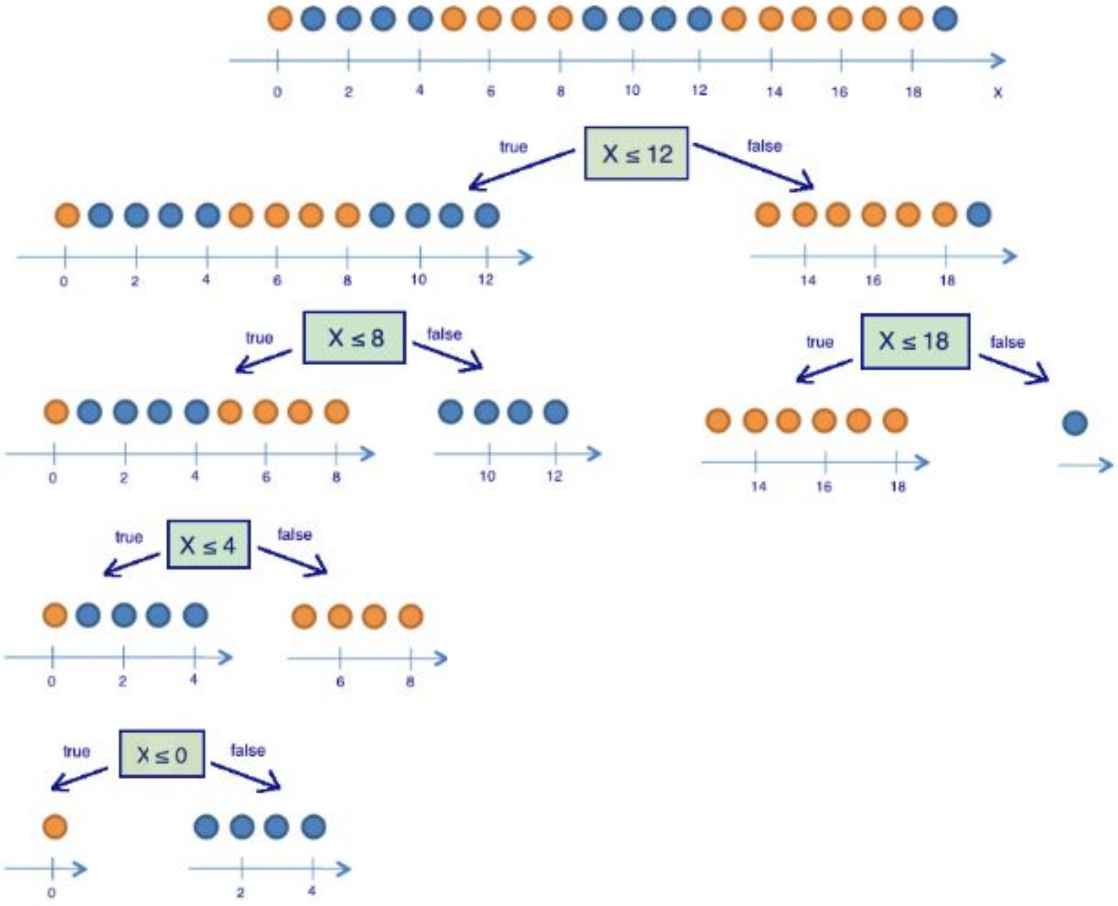
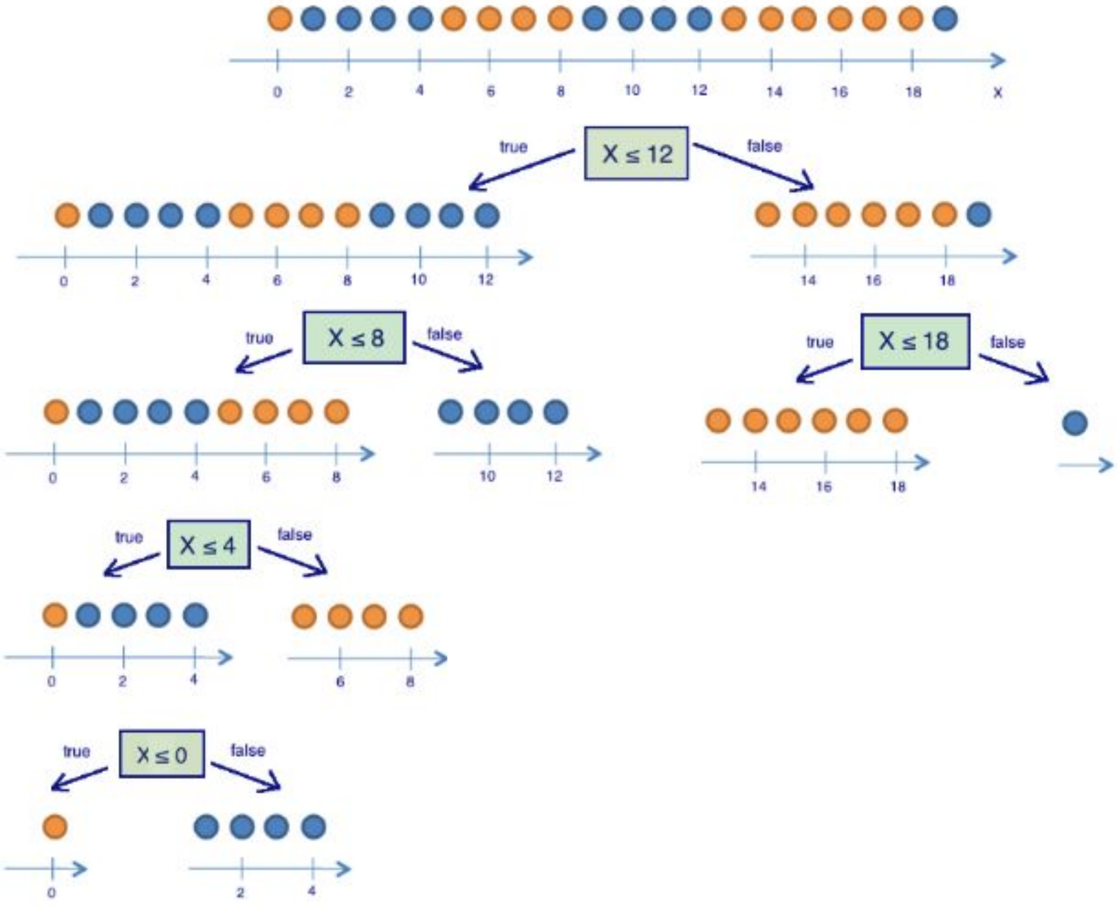


Information criteria: Entropy



source: https://habr.com/ru/company/ods/blog/322534/



Information criteria: Entropy

$$S = -\sum_k p_k \log_2 p_k$$

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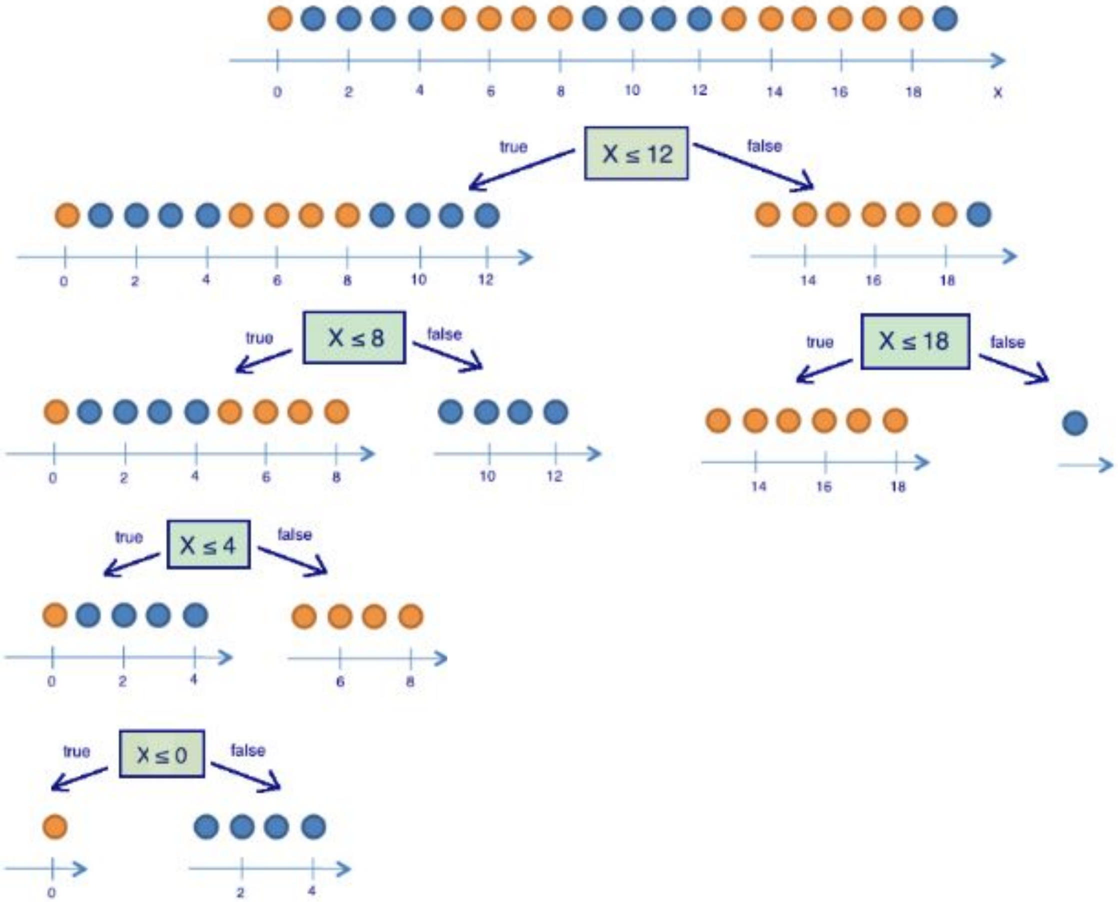
Information criteria: Entropy



$$S = -\sum_k p_k \log_2 p_k$$

In binary case N = 2

$$S = -p_+ \log_2 p_+ - p_- \log_2 p_- = -p_+ \log_2 p_+ - (1 - p_+) \log_2 (1 - p_+)$$

source: https://habr.com/ru/company/ods/blog/322534/

Information criteria

H(R) is measure of “heterogeneity” of our data.
Consider multiclass classification problem:

1. Misclassification criteria: $$H(R) = 1 - \max_k \{p_k\}$$

2. Entropy criteria: $$H(R) = -\sum_k p_k \log_2 p_k$$

3. Gini impurity: $$H(R) = 1 - \sum_k (p_k)^2$$

Information criteria

H(R) is measure of “heterogeneity” of our data.
Consider regression problem:

1. Mean squared error $$H(R) = \min_c \frac{1}{|R|} \sum_{(x_i, y_i) \in R} (y_i - c)^2$$

Information criteria

H(R) is measure of “heterogeneity” of our data.
Consider regression problem:

1. Mean squared error $$H(R) = \min_{c} \frac{1}{|R|} \sum_{(x_i, y_i) \in R} (y_i - c)^2$$

What is the constant?

Information criteria

H(R) is measure of “heterogeneity” of our data.
Consider regression problem:

1. Mean squared error

$$H(R) = \min_c \frac{1}{|R|} \sum_{(x_i, y_i) \in R} (y_i - c)^2$$

$$c^* = \frac{1}{|R|} \sum_{y_i \in R} y_i$$

Bootstrap

Bootstrap

Consider dataset X containing N objects.

Pick l objects with return from X and repeat in N times to get N datasets.

Error of model trained on Xj: $$\varepsilon_j(x) = b_j(x) - y(x), \qquad j = 1, \dots, N,$$

Then $$\mathbb{E}_x(b_j(x) - y(x))^2 = \mathbb{E}_x \varepsilon_j^2(x).$$

The mean error of N models: $$E_1 = \frac{1}{N}\sum_{j=1}^{N} \mathbb{E}_x \varepsilon_j^2(x).$$

Bootstrap

Consider the errors unbiased and uncorrelated:

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$
$$\mathbb{E}_x \varepsilon_i(x) \varepsilon_j(x) = 0, \quad i \neq j.$$

The final model averages all predictions:

$$a(x) = \frac{1}{N} \sum_{j=1}^{N} b_j(x).$$

Bootstrap

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$$a(x) = \frac{1}{N} \sum_{j=1}^{N} b_j(x).$$

$$E_N = \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^{n} b_j(x) - y(x) \right)^2 =$$
$$= \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^{N} \varepsilon_j(x) \right)^2 =$$
$$= \frac{1}{N^2} \mathbb{E}_x \left(\sum_{j=1}^{N} \varepsilon_j^2(x) + \underbrace{\sum_{i \neq j} \varepsilon_i(x) \varepsilon_j(x)}_{=0} \right) =$$
$$= \frac{1}{N} E_1.$$

Bootstrap

Consider the errors unbiased and uncorrelated:

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$
$$\mathbb{E}_x \varepsilon_i(x)\varepsilon_j(x) = 0, \quad i \neq j.$$

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$$E_N = \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{n} b_j(x) - y(x)\right)^2 =$$
$$= \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{N} \varepsilon_j(x)\right)^2 =$$
$$= \frac{1}{N^2}\mathbb{E}_x\left(\sum_{j=1}^{N} \varepsilon_j^2(x) + \underbrace{\sum_{i\neq j} \varepsilon_i(x)\varepsilon_j(x)}_{=0}\right) =$$
$$\boxed{= \frac{1}{N}E_1.}$$

Error decreased by N times!

Bootstrap

Consider the errors ~~unbiased and uncorrelated~~:

Because this is a lie

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$
$$\mathbb{E}_x \varepsilon_i(x)\varepsilon_j(x) = 0, \quad i \neq j.$$

The final model averages all predictions:

$$a(x) = \frac{1}{N}\sum_{j=1}^{N} b_j(x).$$

$$E_N = \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{n} b_j(x) - y(x)\right)^2 =$$
$$= \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{N} \varepsilon_j(x)\right)^2 =$$
$$= \frac{1}{N^2}\mathbb{E}_x\left(\sum_{j=1}^{N} \varepsilon_j^2(x) + \underbrace{\sum_{i\neq j} \varepsilon_i(x)\varepsilon_j(x)}_{=0}\right) =$$

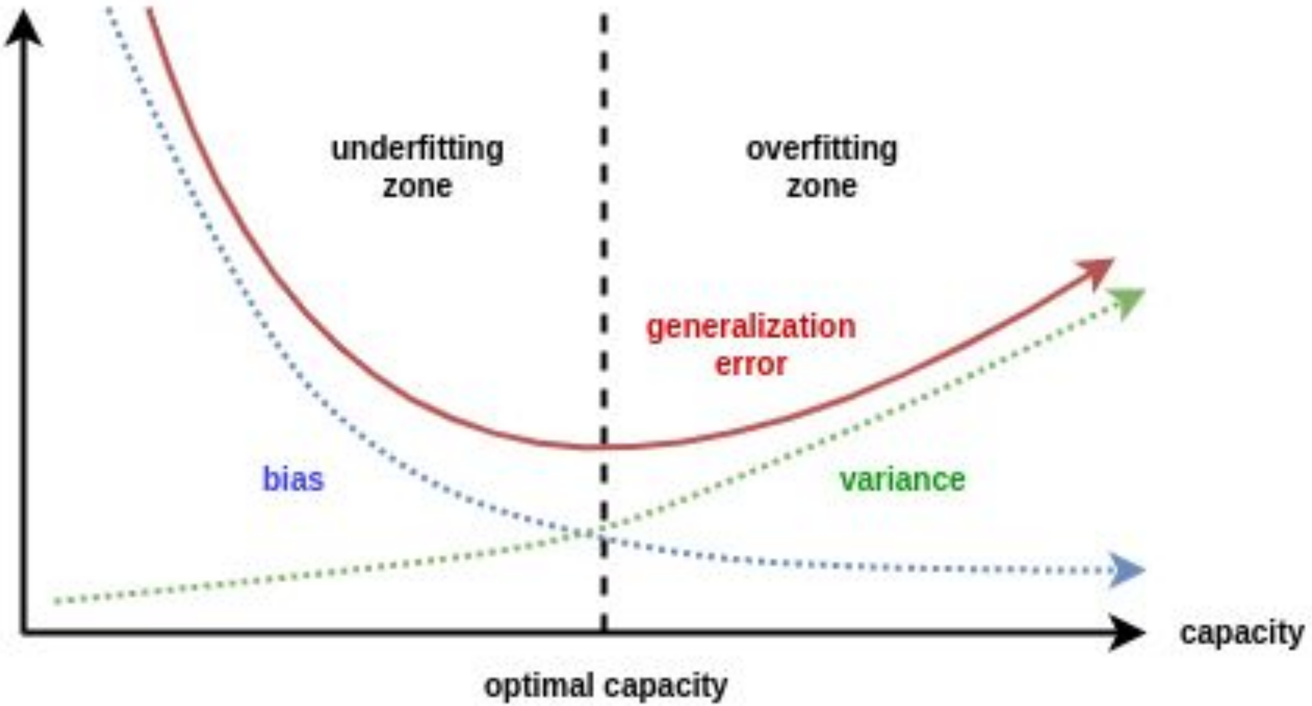
Error decreased by N times!

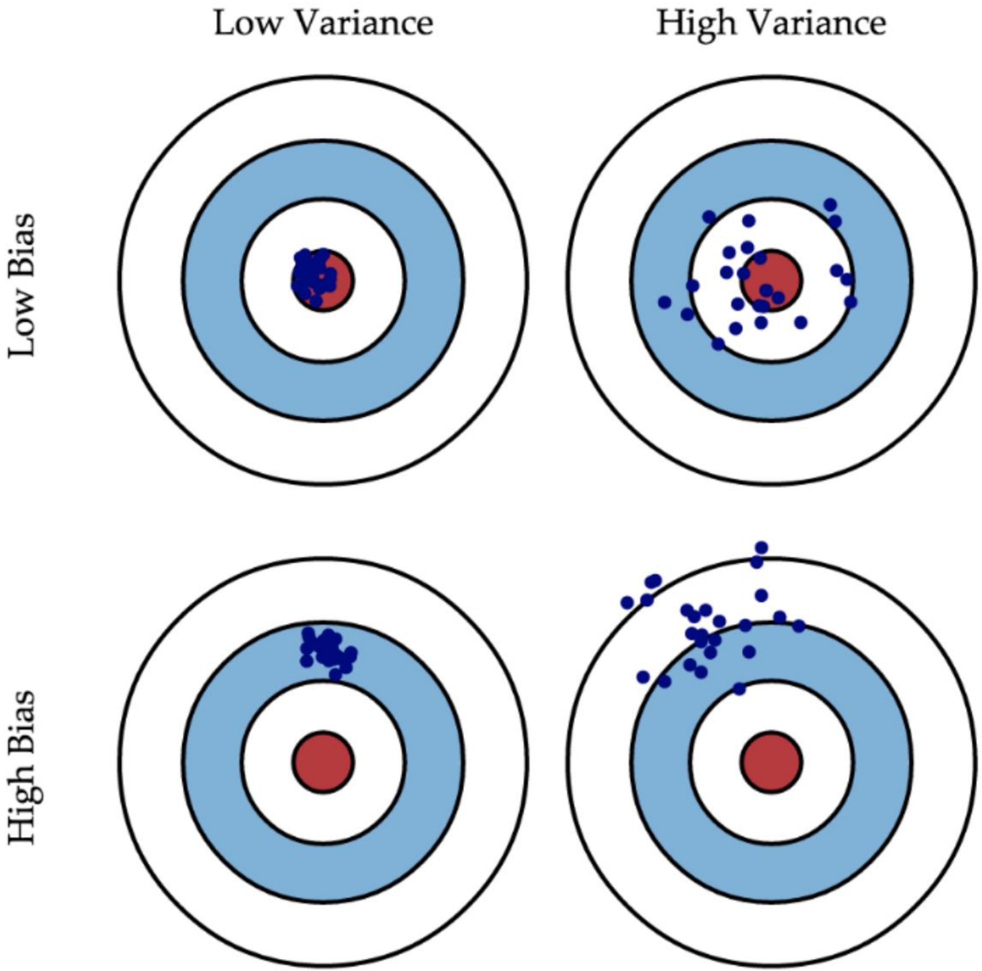
$$\boxed{= \frac{1}{N}E_1.}$$


Original Dataset
x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10}
Bootstrap 1
x_8 x_6 x_2 x_9 x_5 x_8 x_1 x_4 x_8 x_2
x_3 x_7 x_{10}
Bootstrap 2
x_{10} x_1 x_3 x_5 x_1 x_7 x_4 x_2 x_1 x_8
x_6 x_9
Bootstrap 3
x_6 x_5 x_4 x_1 x_2 x_4 x_2 x_6 x_9 x_2
x_3 x_7 x_8 x_{10}
Training Sets
Test Sets

Bias-variance decomposition

Bias-variance tradeoff




Low Variance
High Variance
Low Bias
High Bias

Bias-variance decomposition

The dataset $X = (x_i, y_i)_{i=1}^{\ell}$ with $y_i \in \mathbb{R}$ for regression problem.

Denote loss function $L(y, a) = \big(y - a(x)\big)^2$

The corresponding risk estimation is

$$R(a) = \mathbb{E}_{x,y}\Big[\big(y - a(x)\big)^2\Big] = \int_{\mathbb{X}} \int_{\mathbb{Y}} p(x, y)\big(y - a(x)\big)^2 dx dy.$$

Denote $\mu : (\mathbb{X} \times \mathbb{Y})^\ell \to \mathcal{A}$, where $\mathcal{A}$ is some family of algorithms.

So $L(\mu) = \mathbb{E}_X\left[\mathbb{E}_{x,y}\left[\left(y - \mu(X)(x)\right)^2\right]\right]$, where X dataset.

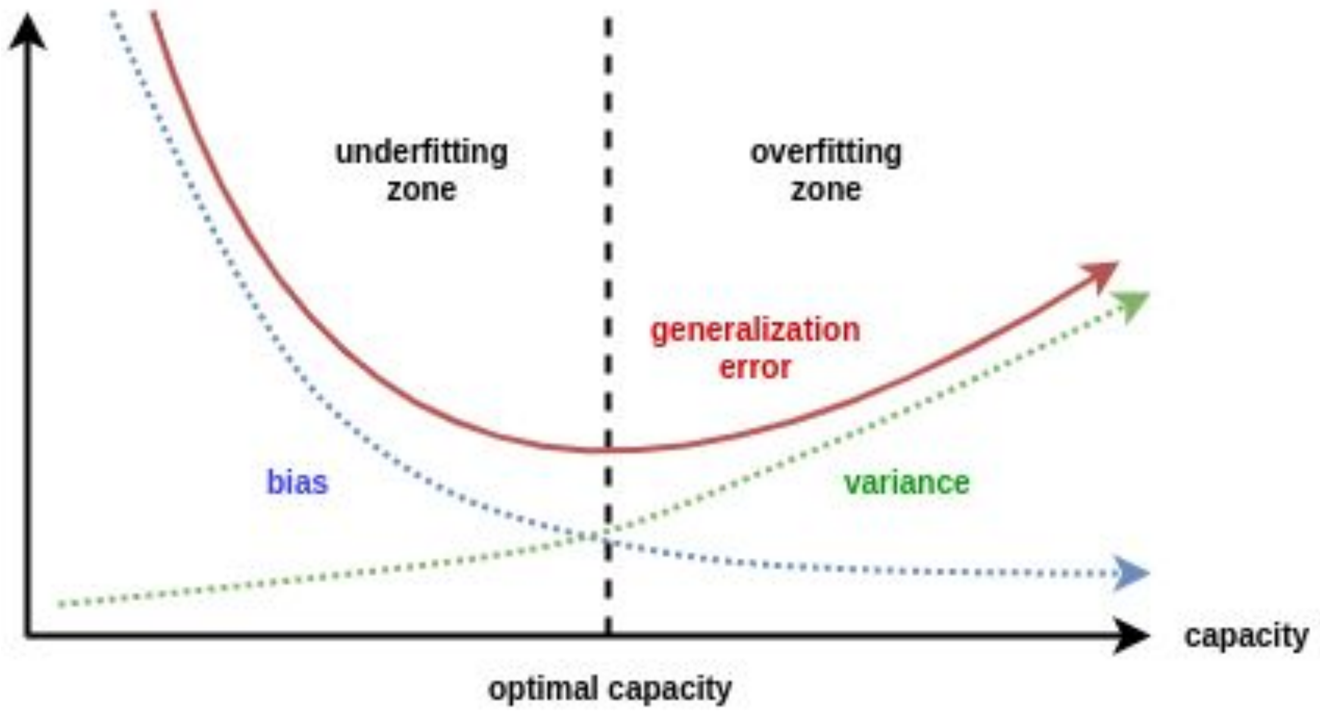
$$L(\mu) = \underbrace{\mathbb{E}_{x,y}\left[\left(y - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{noise}} +$$

$$+ \underbrace{\mathbb{E}_x\left[\left(\mathbb{E}_X\left[\mu(X)\right] - \mathbb{E}[y \mid x]\right)^2\right]}_{\text{bias}} + \underbrace{\mathbb{E}_x\left[\mathbb{E}_X\left[\left(\mu(X) - \mathbb{E}_X\left[\mu(X)\right]\right)^2\right]\right]}_{\text{variance}}.$$

This exact form of bias-variance decomposition is correct for square loss in regression.

However, it is much more general. See extra materials for more exotic cases.

Bias-variance tradeoff



Bagging = Bootstrap aggregating

Denote dataset $\tilde{X}$ bootstrapped from X.

Denote μ: $\tilde{\mu}(X) = \mu(\tilde{X})$. Let $b_n(x)$ be basic algorithm.

Denote the ensemble:

$$a_N(x) = \frac{1}{N}\sum_{n=1}^{N} b_n(x) = \frac{1}{N}\sum_{n=1}^{N} \tilde{\mu}(X)(x).$$

The bias term takes the following form:

$$\mathbb{E}_{x,y}\left[\left(\mathbb{E}_X\left[\frac{1}{N}\sum_{n=1}^{N}\tilde{\mu}(X)(x)\right] - \mathbb{E}[y \mid x]\right)^2\right] =$$

$$= \mathbb{E}_{x,y}\left[\left(\frac{1}{N}\sum_{n=1}^{N}\mathbb{E}_X[\tilde{\mu}(X)(x)] - \mathbb{E}[y \mid x]\right)^2\right] =$$

$$= \boxed{\mathbb{E}_{x,y}\left[\left(\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right] - \mathbb{E}[y \mid x]\right)^2\right]}.$$

One algorithm bias

The variance:

$$\mathbb{E}_{x,y}\Big[\mathbb{E}_X\Big[\frac{1}{N^2}\sum_{n=1}^{N}\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)^2+$$

$$+\frac{1}{N^2}\sum_{n_1\neq n_2}\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)\Big]\Big]=$$

$$=\frac{1}{N^2}\mathbb{E}_{x,y}\Big[\mathbb{E}_X\Big[\sum_{n=1}^{N}\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)^2\Big]\Big]+$$

$$+\frac{1}{N^2}\mathbb{E}_{x,y}\Big[\mathbb{E}_X\Big[\sum_{n_1\neq n_2}\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)\times$$

$$\times\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)\Big]\Big]=$$

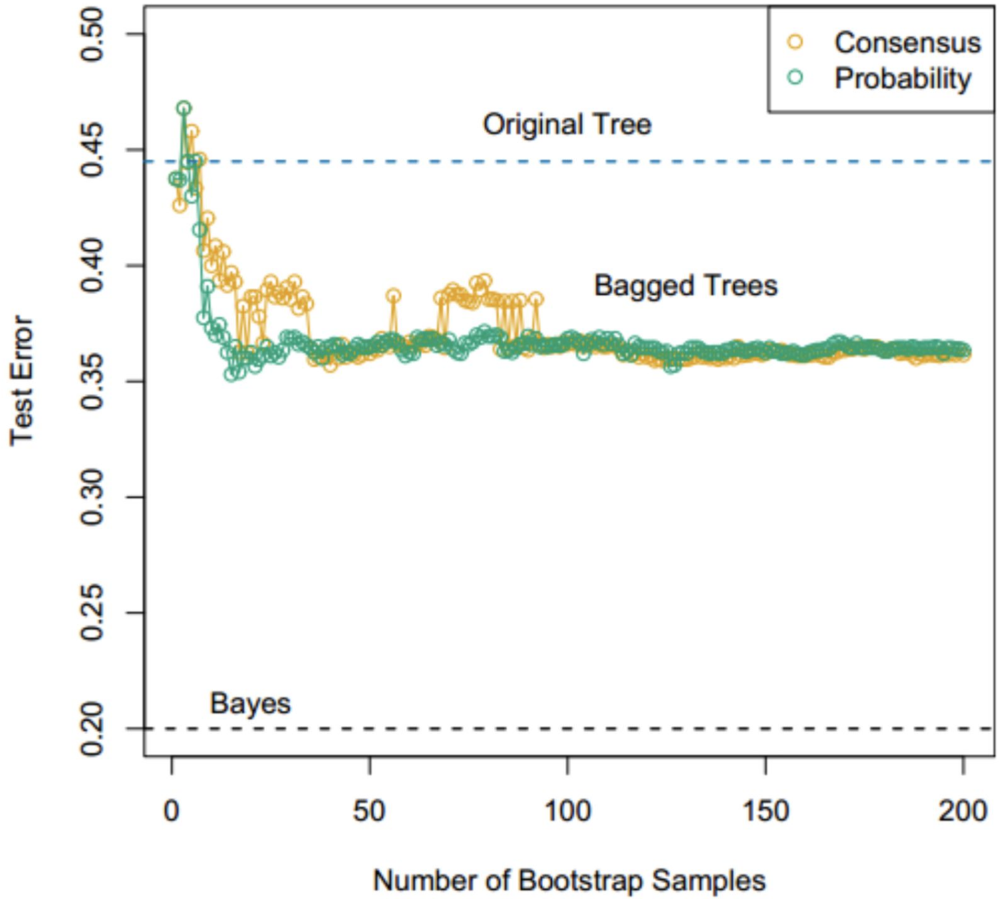
One algorithm variance * 1/N

$$=\boxed{\frac{1}{N}\mathbb{E}_{x,y}\Big[\mathbb{E}_X\Big[\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)^2\Big]\Big]}+$$

$$\boxed{+\frac{N(N-1)}{N^2}\mathbb{E}_{x,y}\Big[\mathbb{E}_X\Big[\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)\times\Big(\tilde{\mu}(X)(x)-\mathbb{E}_X\left[\tilde{\mu}(X)(x)\right]\Big)\Big]\Big]}$$

Basic algorithms covariance

Bagging = Bootstrap aggregating



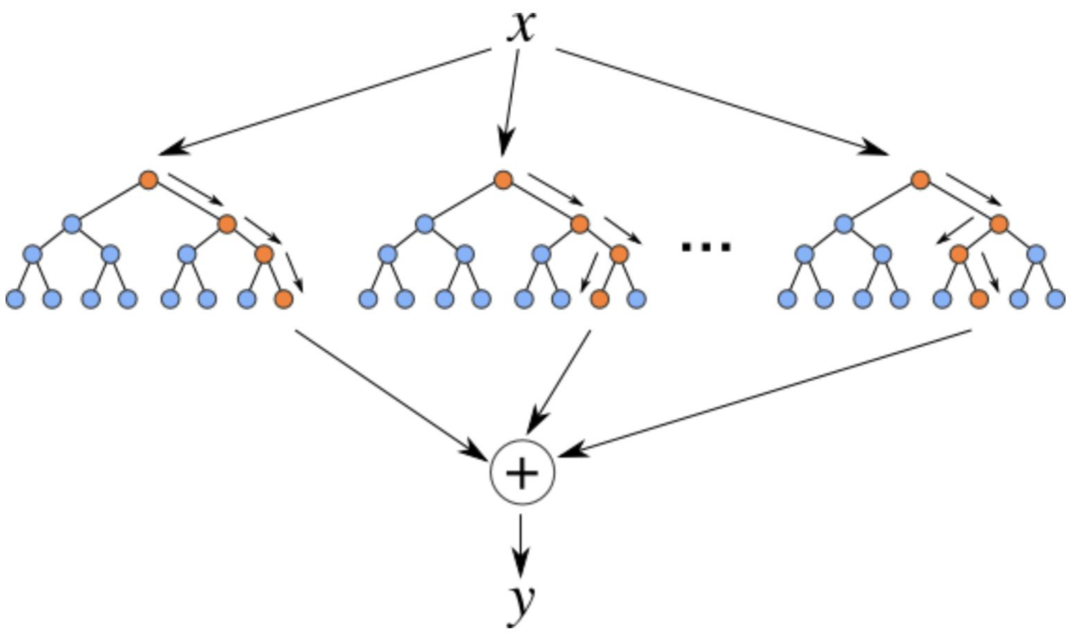
Bagging = Bootstrap aggregating

Decreases the variance if the basic algorithms are not correlated.

RSM - Random Subspace Method

Same approach, but with features.

Bagging + RSM = Random Forest



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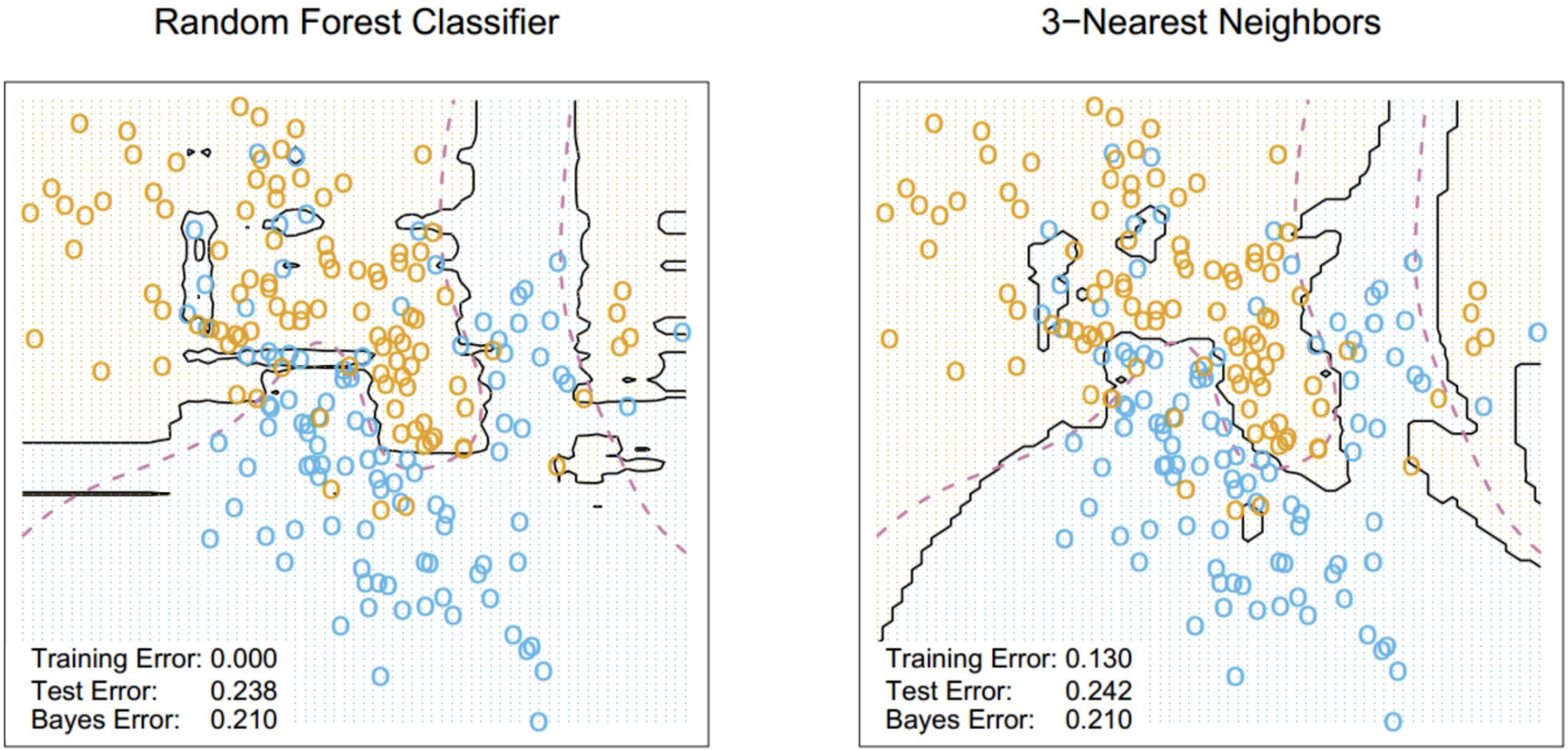
$$\mathrm{OOB} = \sum_{i=1}^{\ell} L\left(y_i, \frac{1}{\sum_{n=1}^{N}[x_i \notin X_n]} \sum_{n=1}^{N}[x_i \notin X_n] b_n(x_i)\right)$$


Random Forest Classifier
Training Error: 0.000
Test Error: 0.238
Bayes Error: 0.210
3−Nearest Neighbors
Training Error: 0.130
Test Error: 0.242
Bayes Error: 0.210