Machine Learning
Lecture 3: Linear Classification

Harbour.Space University
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Outline

1. Linear regression recap
2. Linear classification
    - Margin in linear classification
    - Loss functions
3. Gradient descent recap
4. Logistic regression
5. Measuring the quality in classification
6. Model validation and evaluation.

Linear regression problem statement:

- Dataset $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{N}$, where $\mathbf{x}_i \in \mathbb{R}^n, \quad y_i \in \mathbb{R}$.
- The model is linear:

$$\hat{y} = w_0 + \sum_{k=1}^{p} x_k \cdot w_k = //\mathbf{x} = [1, x_1, x_2, \ldots, x_p]// = \mathbf{x}^T \mathbf{w}$$

where $\mathbf{w} = (w_0, w_1, \ldots, w_n)$, w_0 is bias term.

- Least squares method (MSE minimization) provides a solution:

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|Y - \hat{Y}\|_2^2 = \arg\min_{\mathbf{w}} \|Y - X\mathbf{w}\|_2^2$$

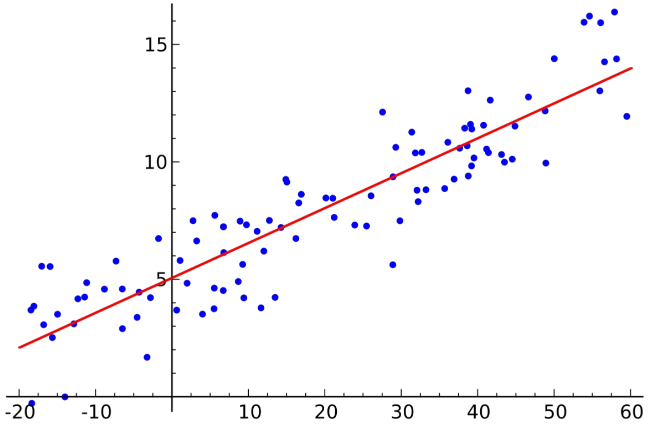
From regression to classification

From regression to classification

Regression:

$$\hat{y} = f(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$$

$$Q = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$



How can we use the same technique to solve the *classification* problem?

From regression to classification

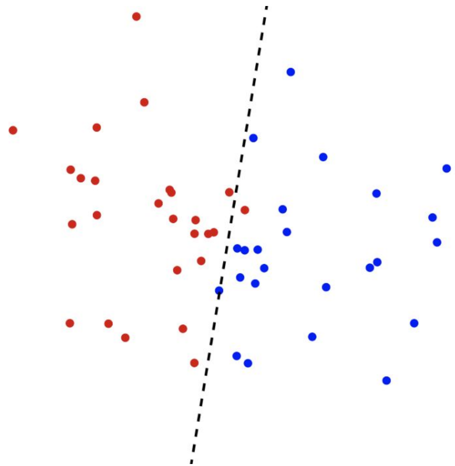
Classification:

$$\hat{y} = f(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$$

$$a(\mathbf{x}) = +1 \ \text{ if } f(\mathbf{x}) > 0$$
$$a(\mathbf{x}) = -1 \ \text{ if } f(\mathbf{x}) < 0$$

$$Q = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{y}_i)$$

Let's say we predict the class label now



What about loss function?

From regression to classification

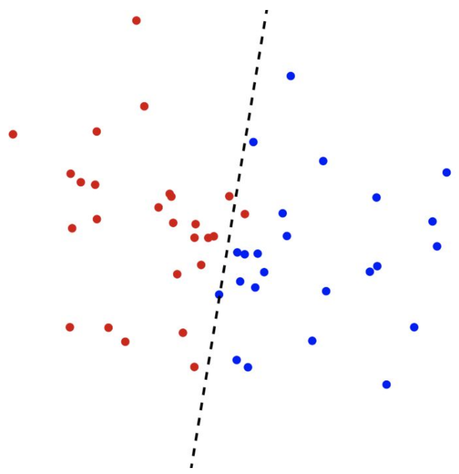
Classification:

$$\hat{y} = f(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$$

$$a(\mathbf{x}) = +1 \ \text{ if } f(\mathbf{x}) > 0$$
$$a(\mathbf{x}) = -1 \ \text{ if } f(\mathbf{x}) < 0$$

$$Q = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{y}_i)$$

Let's say we predict the class label now



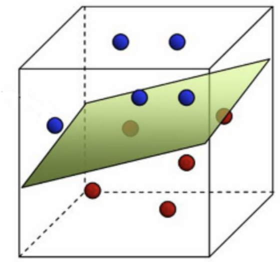
Loss function could be just number of misclassifications

Linear classification

$$a(\mathbf{x}) = +1 \ \text{ if } f(\mathbf{x}) > 0$$
$$a(\mathbf{x}) = -1 \ \text{ if } f(\mathbf{x}) < 0$$

$$f(\mathbf{x}) = \mathbf{x}^T \mathbf{w}$$

Geometrical interpretation:
Linearly separable case



Margin

Denote algorithm $a(\mathbf{x}) = \operatorname{sign}(f(\mathbf{x}))$

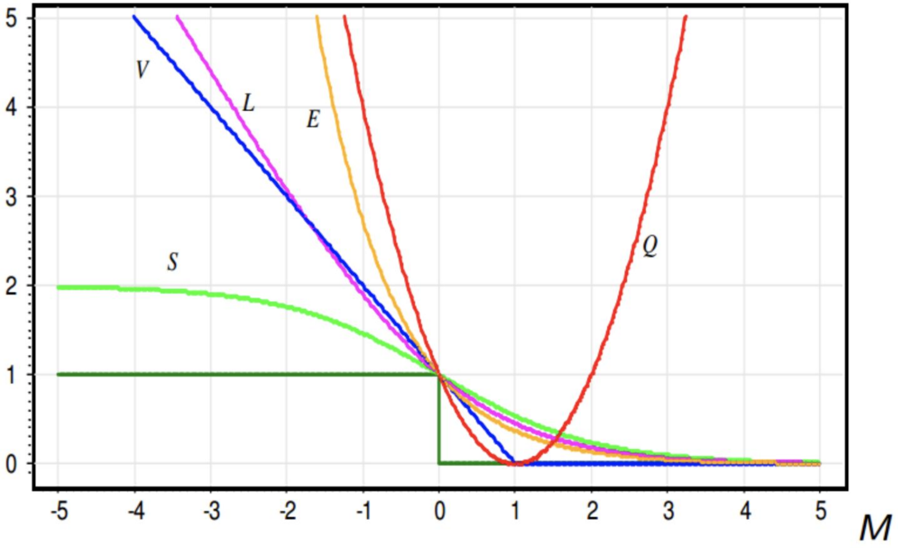
Let's call $M_i = y_i a(\mathbf{x}_i)$ algorithm ***margin*** on object $\mathbf{x}_i$.

$$M_i \le 0 \iff y_i \ne a(\mathbf{x}_i)$$
$$M_i > 0 \iff y_i = a(\mathbf{x}_i)$$

Loss functions in classification

$$Q = \frac{1}{N}\sum_{i=1}^{N}[M_i \leq 0] \leq \widetilde{Q} = \frac{1}{N}\sum_{i=1}^{N} L(M_i)$$

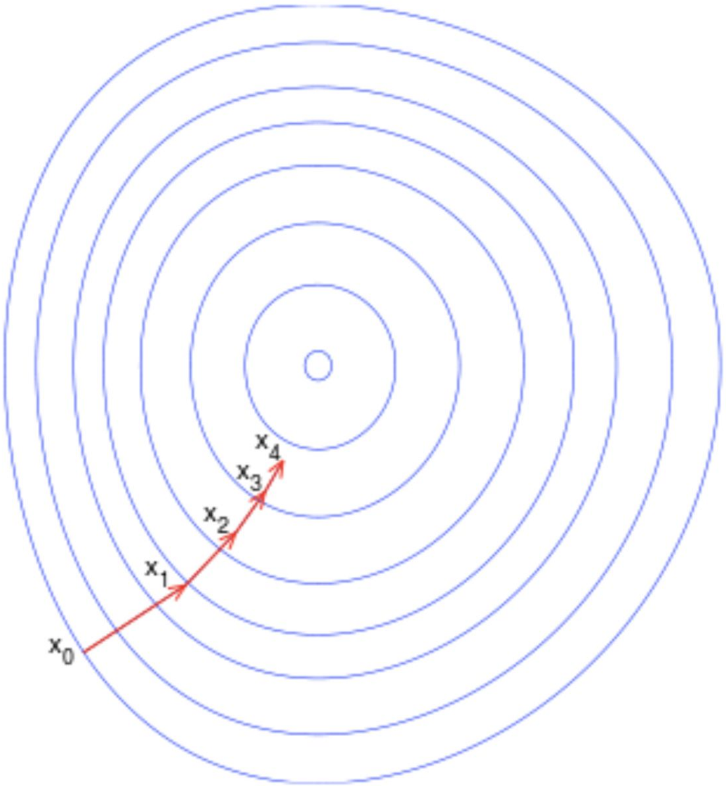
$$\widetilde{Q} \longrightarrow \min \implies Q \longrightarrow \min$$



$$Q(M) = (1-M)^2$$
$$V(M) = (1-M)_+$$
$$S(M) = 2(1+e^M)^{-1}$$
$$L(M) = \log_2(1+e^{-M})$$
$$E(M) = e^{-M}$$

Loss functions

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \gamma_n \nabla F(\mathbf{x}_n),\ n \geq 0.$$



$$\nabla_w \tilde{Q} = \sum_{i=1}^{l} \nabla L(M_i)$$

$$\nabla \tilde{Q} = \sum_{i=1}^{l} L'(M_i) \frac{\partial M_i}{\partial w}$$

$$\frac{\partial M_i}{\partial w} = y_i x_i$$

$$\nabla \tilde{Q} = \sum_{i=1}^{l} y_i x_i L'(M_i)$$

$$\boxed{w_{n+1} = w_n - \gamma_n \sum_{i=1}^{l} y_i x_i L'(M_i)}$$

Logistic regression

$y_i \in \{0, 1\}$

$$Q = -\sum_{i=1}^{\ell} y_i \ln p_i + (1 - y_i) \ln(1 - p_i) \to \min_w$$

$$p_i = \sigma(\langle w, x_i \rangle) = \frac{1}{1 + e^{-\langle w, x_i \rangle}} = P(y = 1|x)$$

logistic loss

L1 or L2 regularization terms are usually used along the *logistic loss* function.
The optimization problem is solved by SGD or Newton-Raphson's method.

Logistic regression optimization problem

$$Q = -\sum_{i=1}^{\ell} y_i \ln \frac{1}{1+e^{-\langle w, x_i \rangle}} + (1-y_i) \ln \frac{1}{1+e^{\langle w, x_i \rangle}} \to \min_w$$

$$-y_i \ln \frac{1}{1+e^{-\langle w, x_i \rangle}} - (1-y_i) \ln \frac{1}{1+e^{\langle w, x_i \rangle}} = \begin{cases} \ln\left(1+e^{-\langle w, x_i \rangle}\right), y_i = 1 \\ \ln\left(1+e^{\langle w, x_i \rangle}\right), y_i = 0 \end{cases}$$

$$Q = \sum_{i=1}^{\ell} \underbrace{\ln\left(1+e^{-y_i \langle w, x_i \rangle}\right)}_{L(M) = \ln(1+e^{-M_i})} \to \min_w \qquad y_i \in \{-1, 1\}$$

Measuring the quality in classification

Quality functions in classification

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

Accuracy

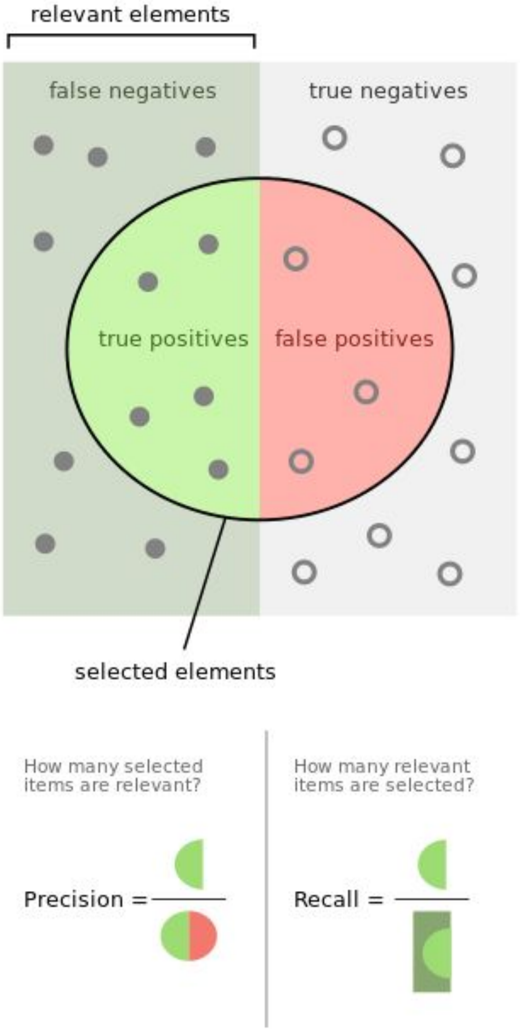
Number of right classifications

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

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

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

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

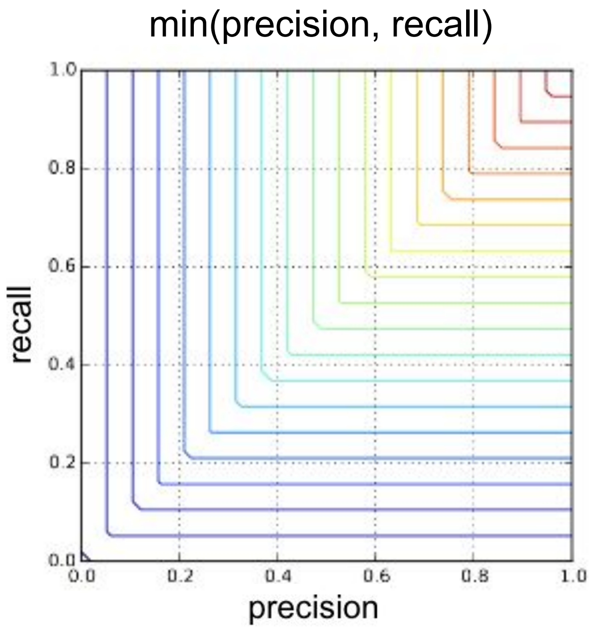
F-score

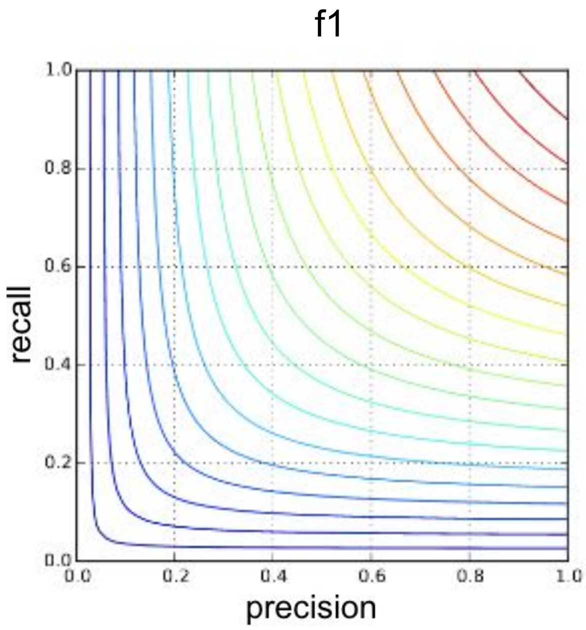
Harmonic mean of precision and recall.
Closer to the smallest one.

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

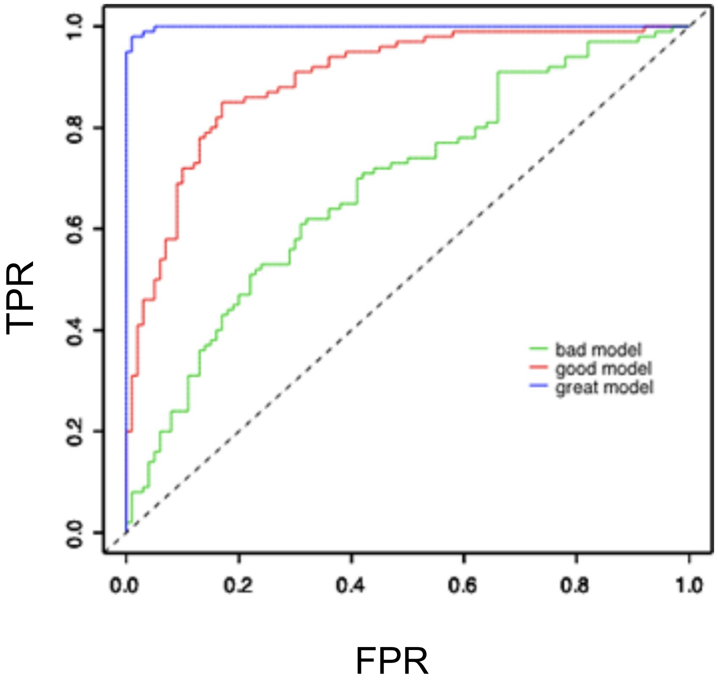
$$F_\beta = (1 + \beta^2) \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{(\beta^2 \cdot \mathrm{precision}) + \mathrm{recall}}$$

F-score


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


f1
recall
precision
0.0
0.2
0.4
0.6
0.8
1.0

ROC - receiver operating characteristic

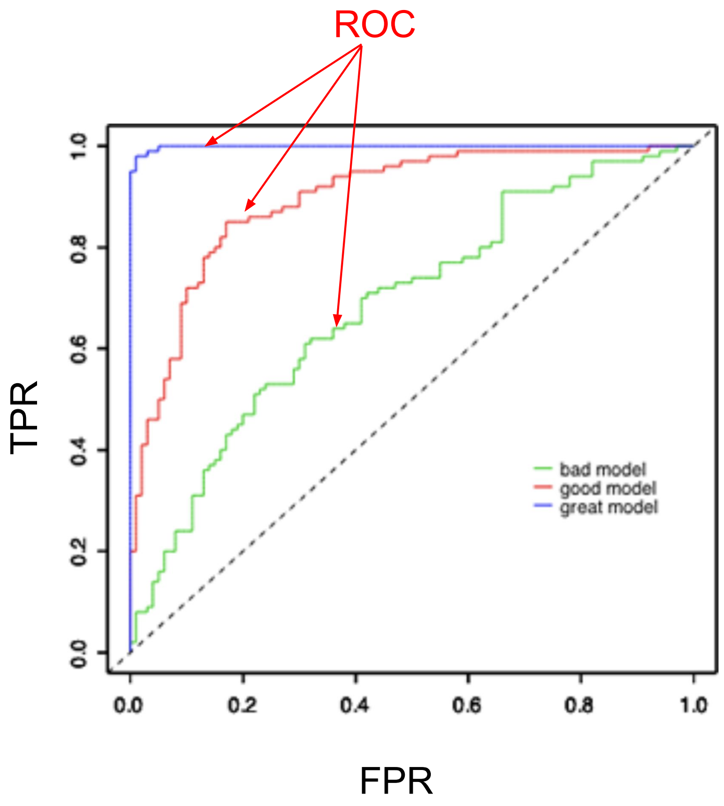


		Actual Class	
		Yes	No
Predicted Class	Yes	**T**rue **P**ositive	**F**alse **P**ositive
	No	**F**alse **N**egative	**T**rue **N**egative

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

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

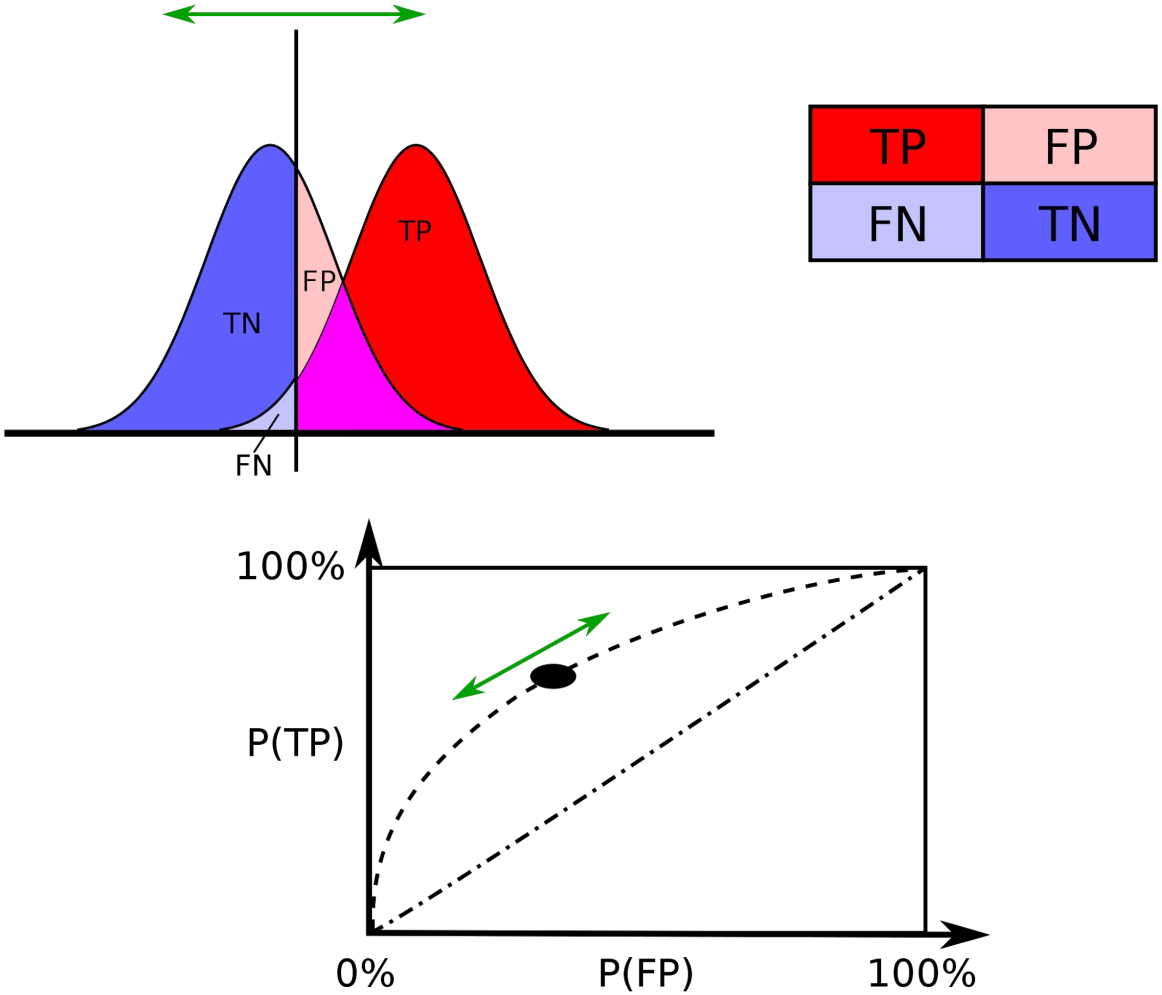
ROC



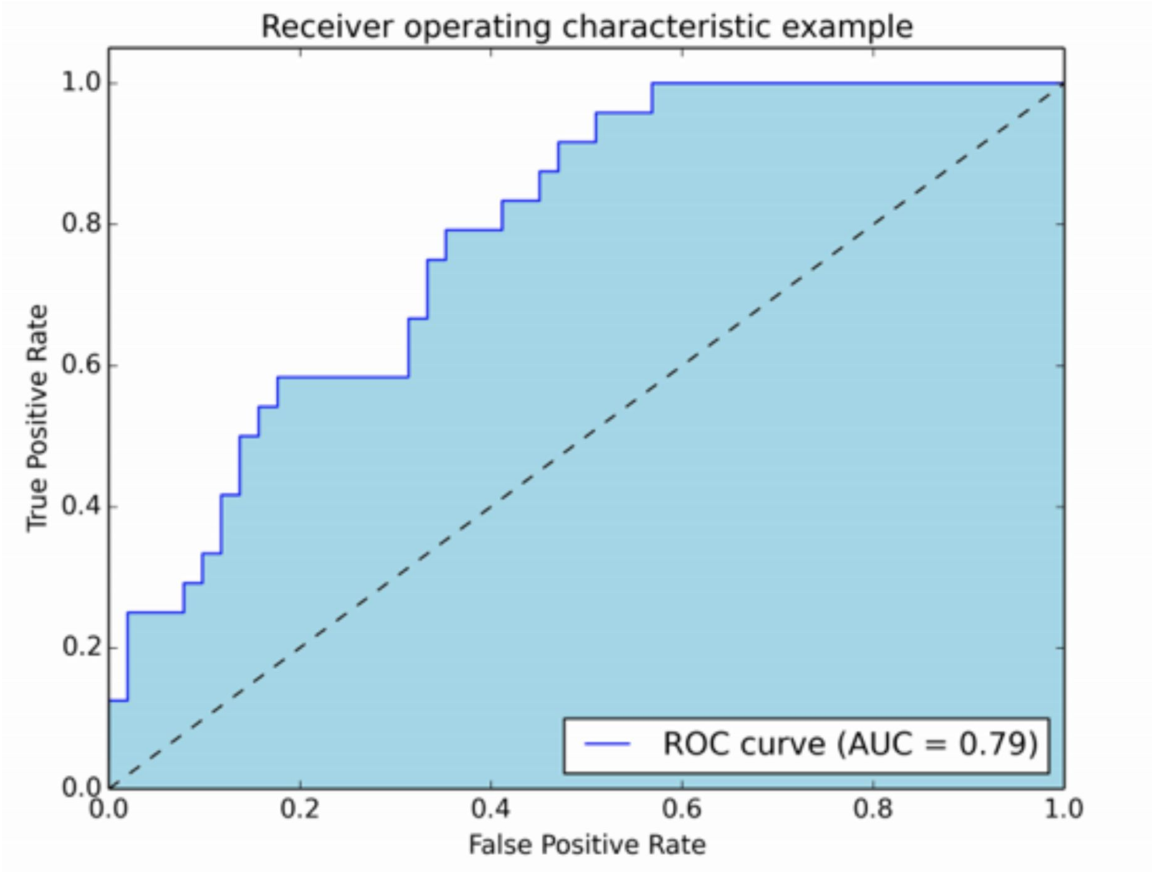
		Actual Class	
		Yes	No
Predicted Class	Yes	**T**rue **P**ositive	**F**alse **P**ositive
	No	**F**alse **N**egative	**T**rue **N**egative

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

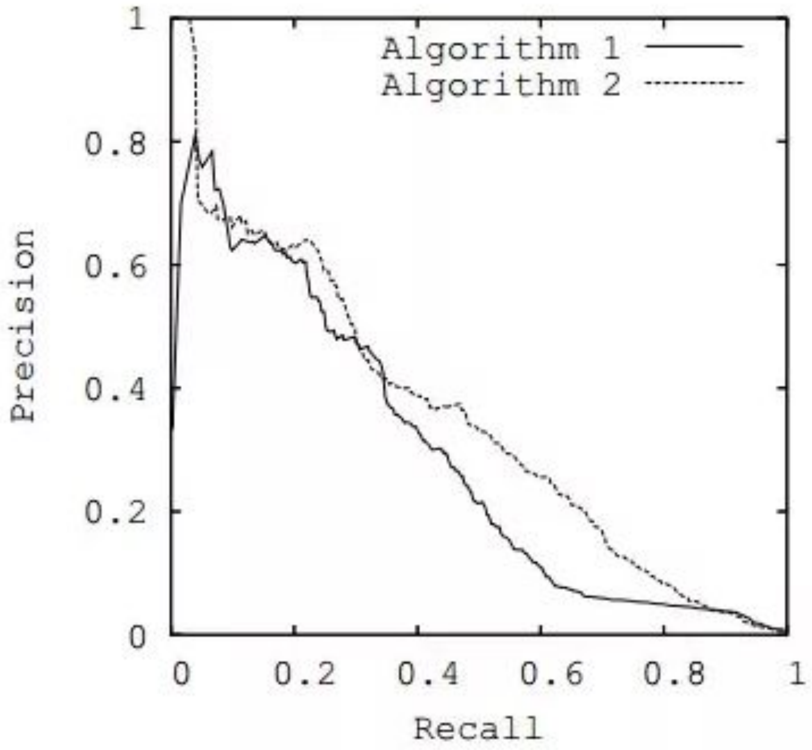
$$FPR = \frac{False\ positives}{False\ positives + True\ negatives}.$$


TP
FP
TN
FN
TP
FP
FN
TN
100%
P(TP)
0%
P(FP)
100%

ROC-AUC - area under curve



PR-curve



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

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

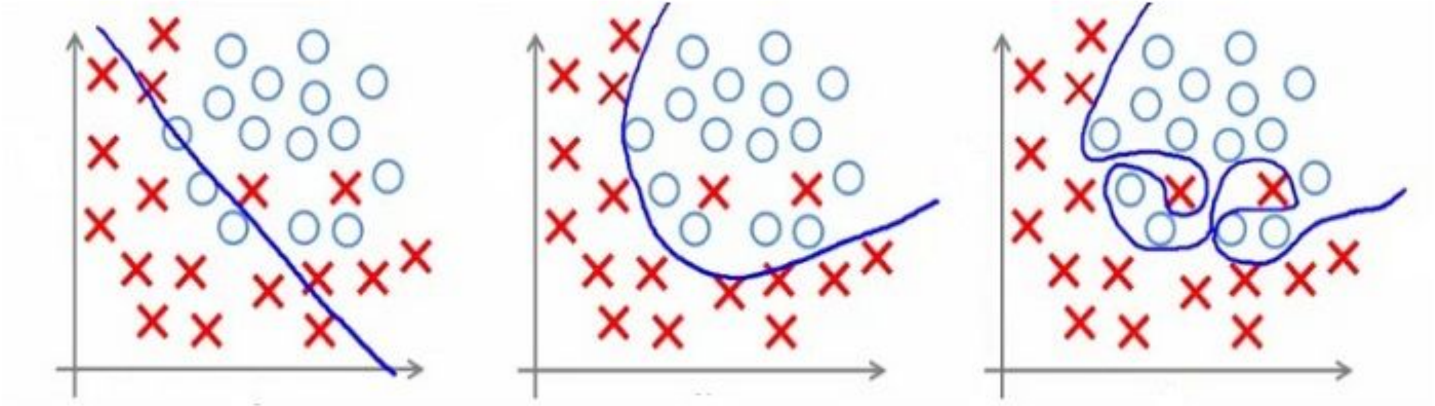
Model validation and evaluation

Supervised learning problem statement

Let's denote:

- Training set $\mathcal{L} = \{\mathbf{x}_i, y_i\}_{i=1}^{n}$, where
  - $(\mathbf{x} \in \mathbb{R}^p,\ y \in \mathbb{R}\ )$ for regression
  - $\mathbf{x}_i \in \mathbb{R}^p$, $y_i \in \{+1, -1\}$ for binary classification
- Model $f(\mathbf{x})$ predicts some value for every object
- Loss function $Q(\mathbf{x}, y, f)$ that should be minimized

Overfitting vs. underfitting



Under-fitting

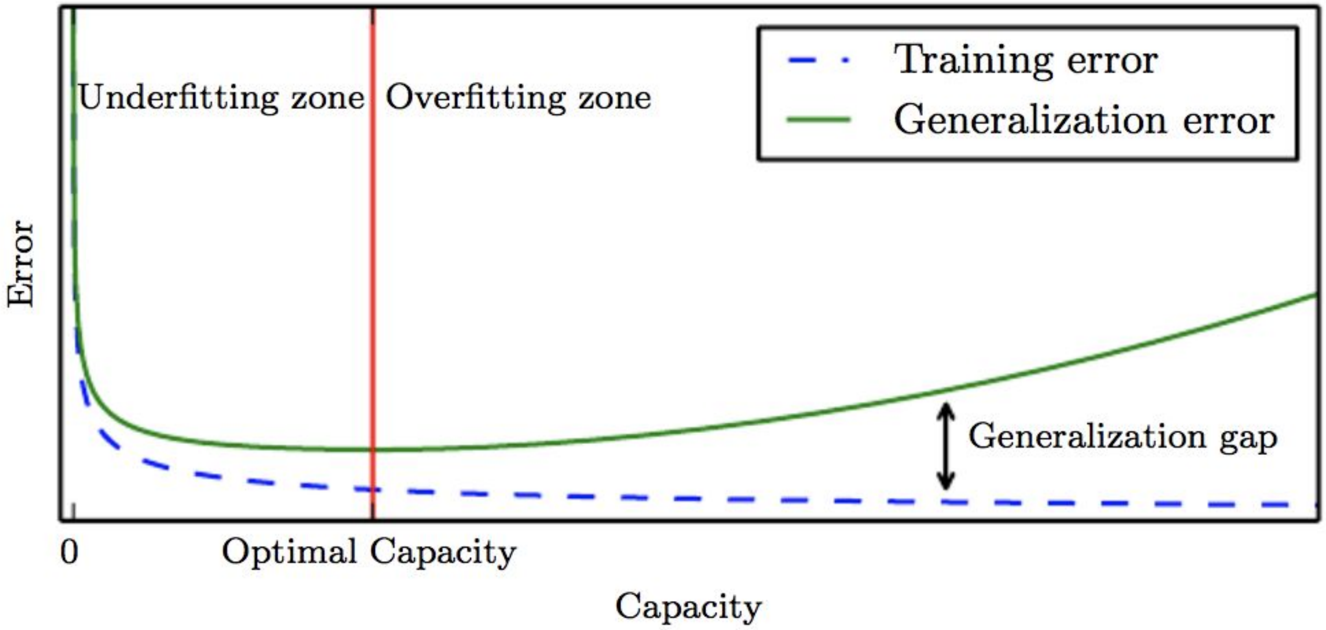
(too simple to explain the variance)

Appropriate-fitting

Over-fitting

(forcefitting -- too good to be true)

Overfitting vs. underfitting



Overfitting vs. underfitting

- We can control overfitting / underfitting by altering model's capacity (ability to fit a wide variety of functions):
- select appropriate hypothesis space
- learning algorithm's effective capacity may be less than the representational capacity of the model family

Evaluating the quality

Image credit: Joseph Nelson [@josephofiowa]

Evaluating the quality

Is it good enough?

Image credit: Joseph Nelson @josephofiowa

Evaluating the quality

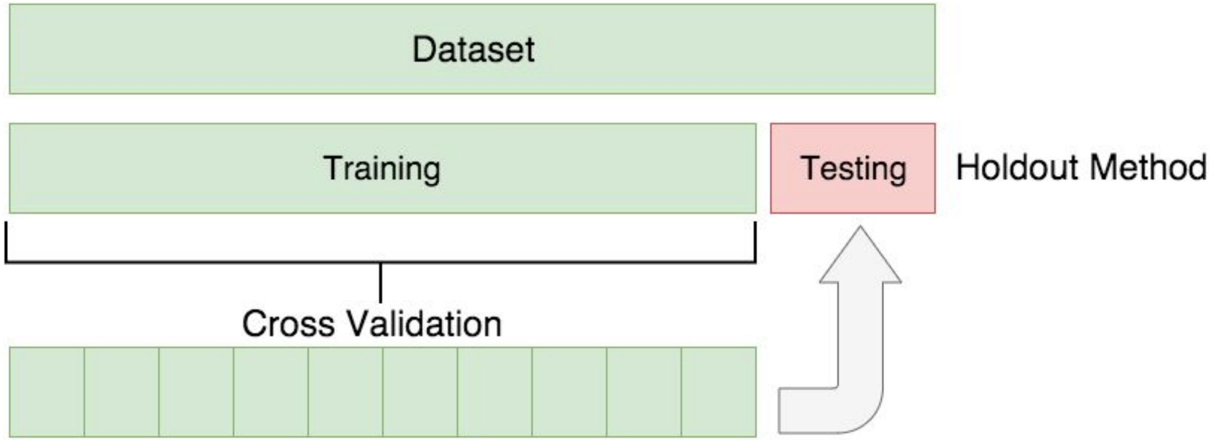
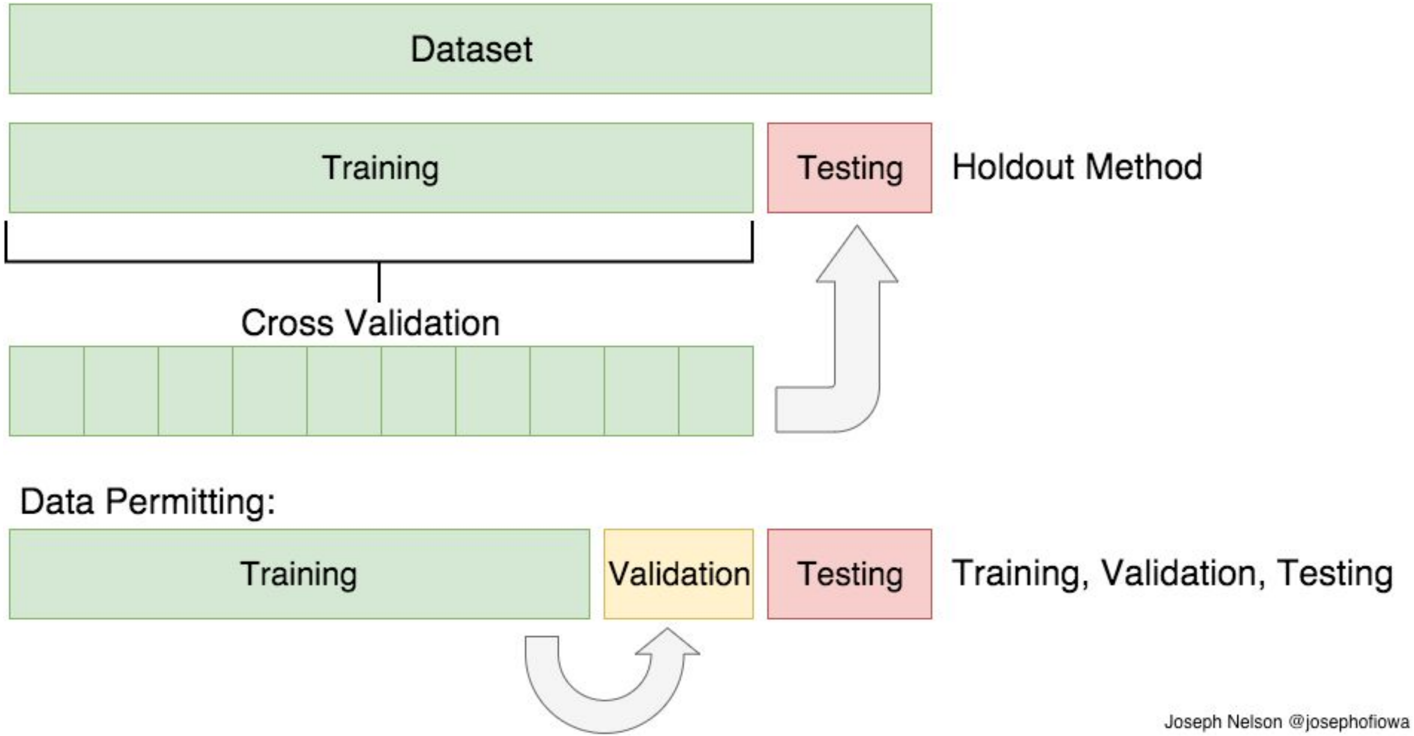


Image credit: Joseph Nelson @josephofiowa

Evaluating the quality



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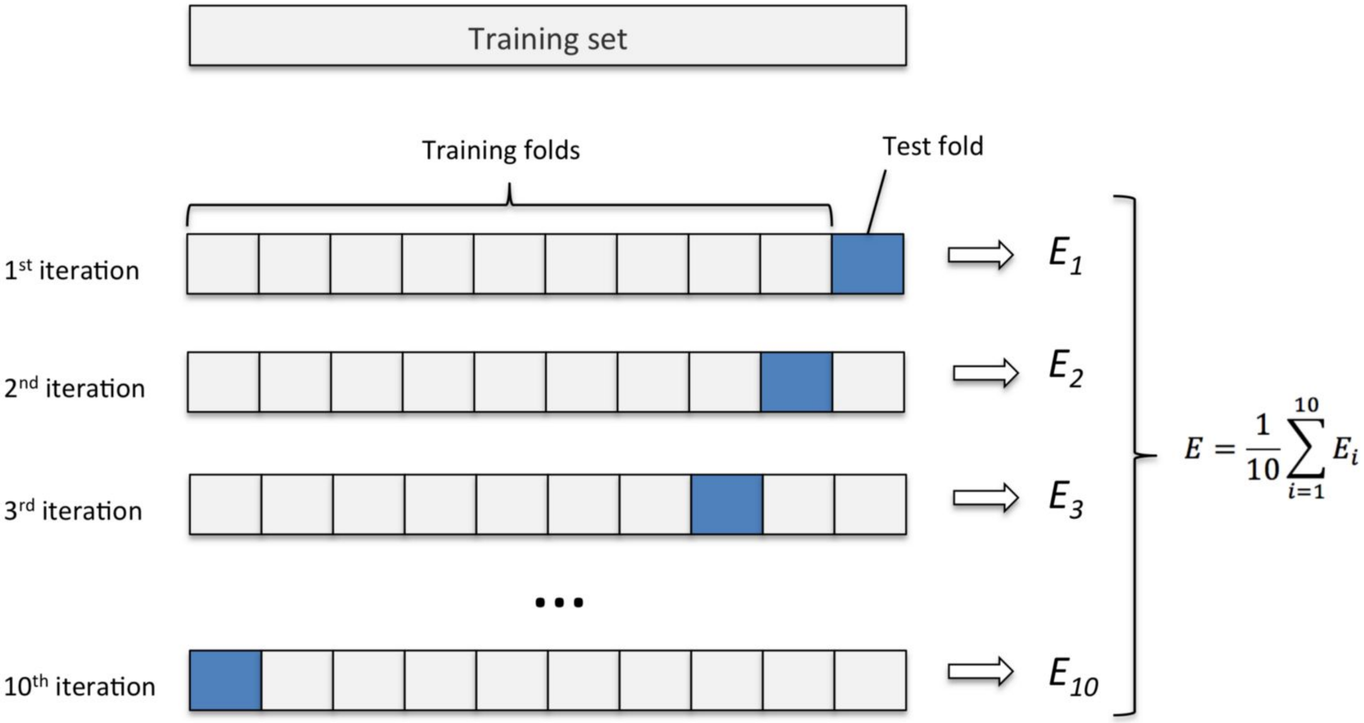
Cross-validation



$$E = \frac{1}{10}\sum_{i=1}^{10} E_i$$