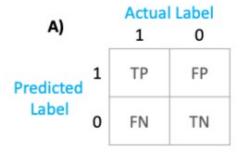
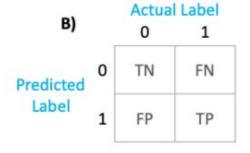
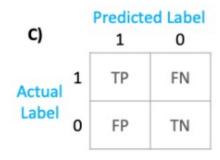
Confusion Matrix

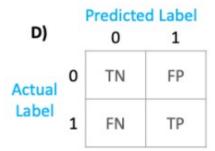
Sklearn Representation

<u>Scikit learn documentation says</u> — Wikipedia and other references may use a different convention for axes.









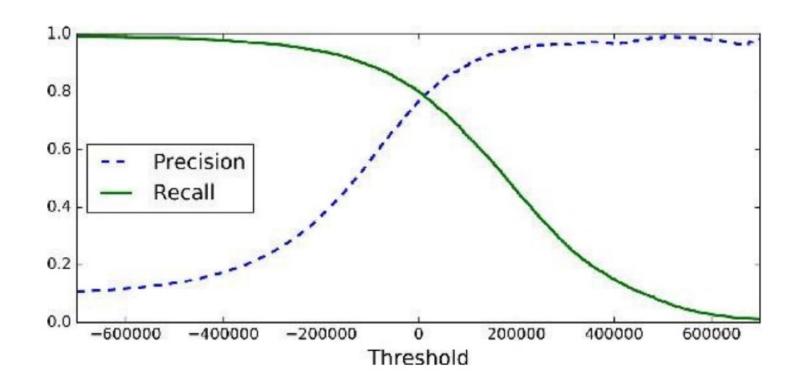
F_{β} -Score

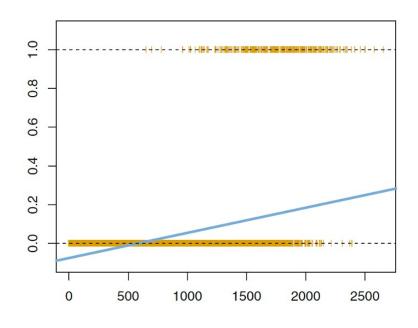
$$F_eta = (1 + eta^2) \cdot rac{ ext{precision} \cdot ext{recall}}{(eta^2 \cdot ext{precision}) + ext{recall}}$$

$$eta = 1$$
 $F_1 = rac{2}{ ext{recall}^{-1} + ext{precision}^{-1}} = 2rac{ ext{precision} \cdot ext{recall}}{ ext{precision} + ext{recall}} = rac{ ext{tp}}{ ext{tp} + rac{1}{2}(ext{fp} + ext{fn})}$

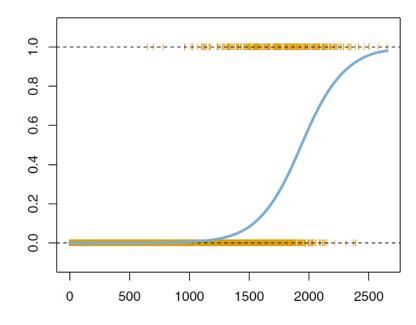
harmonic mean

Precission – Racall Trade off





$$p(X) = \beta_0 + \beta_1 X$$



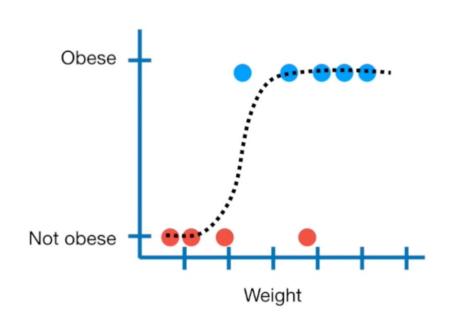
$$p(X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

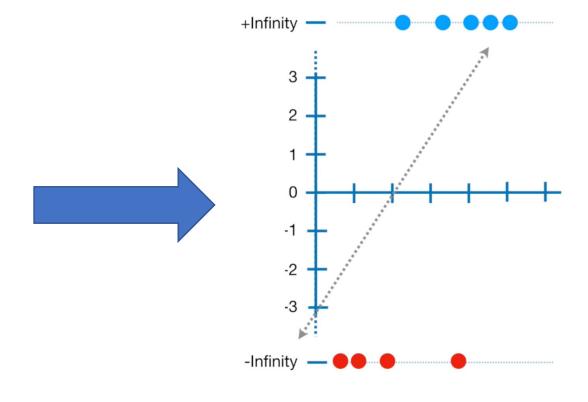
$$h_{\theta}(x) = \frac{1}{1 + e^{-(\theta^T x)}} = \frac{1}{1 + e^{-(\theta_0 + \theta_1 x)}}$$

$$\frac{h_{\theta}(x)}{1 - h_{\theta}(x)} = e^{(\theta_0 + \theta_1 x)}$$

$$\log\left(\frac{h_{\theta}(x)}{1 - h_{\theta}(x)}\right) = \theta_0 + \theta_1 x$$

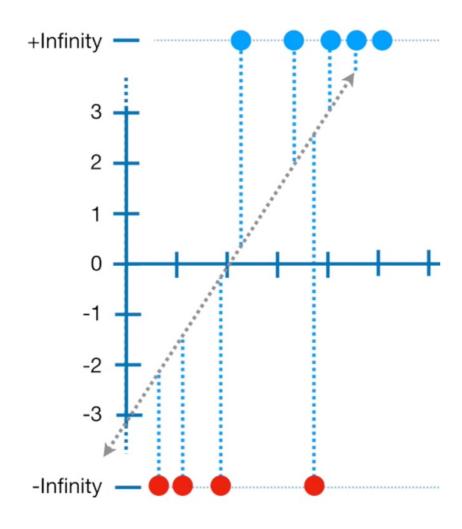
(log odds)

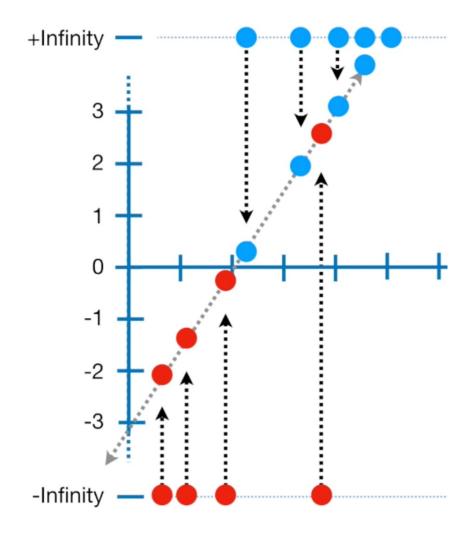


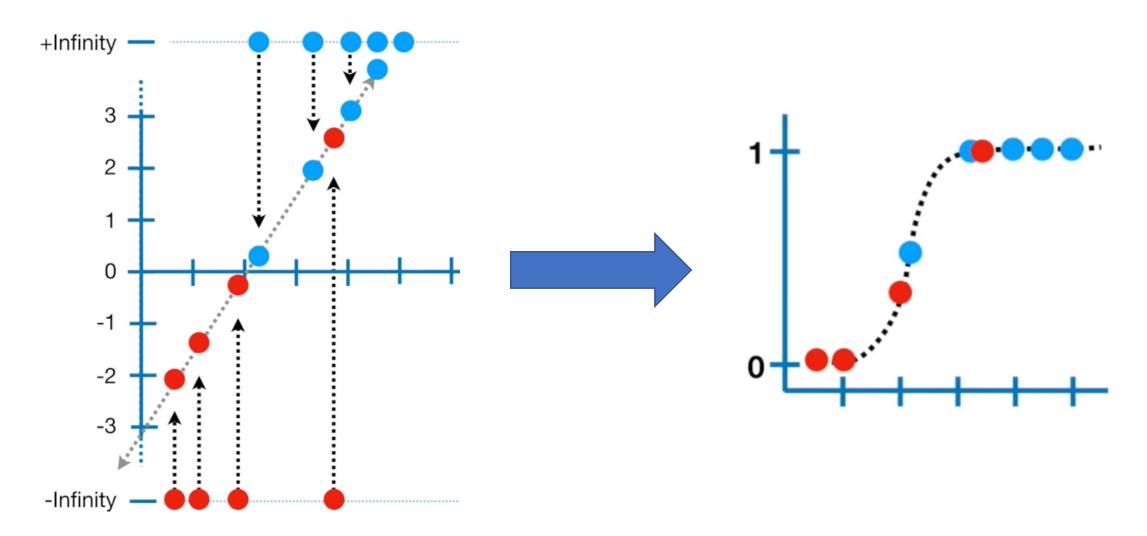


$$h_{\theta}(x) = \frac{1}{1 + e^{-(\theta_0 + \theta_1 x)}}$$

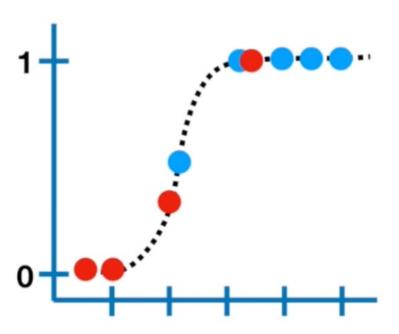
$$\log\left(\frac{h_{\theta}(x)}{1 - h_{\theta}(x)}\right) = \theta_0 + \theta_1 x$$







MLE – maximum likelihood estimation:



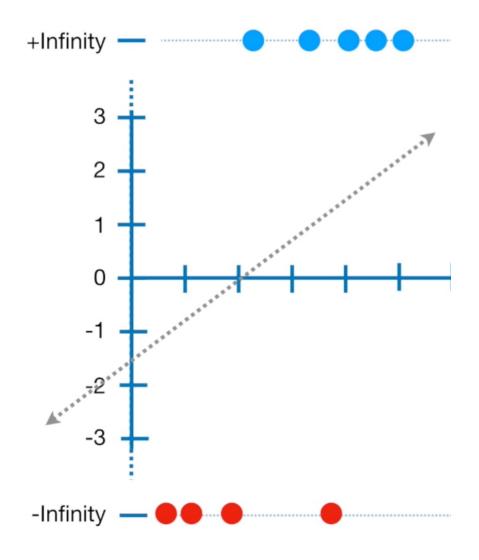
Likelihood:

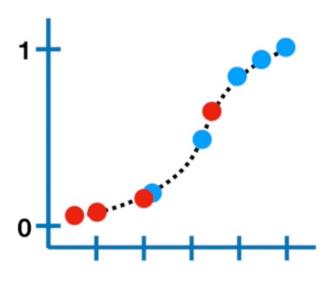
$$\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_{i'}=0} (1 - p(x_{i'}))$$

Log-likelihood:

$$\log \ell(\beta_0, \beta_1) = \sum_{i: y_i = 1} \log p(x_i) + \sum_{i: y_{i'} = 0} \log(1 - p(x_{i'}))$$

$$= \log(0.49) + \log(0.9) + \log(0.91) + \log(0.91) + \log(0.92) + \log(1 - 0.9) + \log(1 - 0.3) + \log(1 - 0.01) + \log(1 - 0.01)$$





$$= \log(0.22) + \log(0.4) + \log(0.8) + \log(0.89) + \log(0.92) + \log(1 - 0.6) + \log(1 - 0.2) + \log(1 - 0.1) + \log(1 - 0.05)$$

Logistic Regression – Loss function

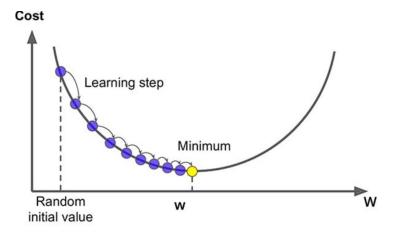
Linear Regression:

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \frac{1}{2} \left(h_{\theta}(x^{(i)}) - y^{(i)} \right)^{2}$$

$$\operatorname{Cost}(h_{\theta}(x^{(i)}), y^{(i)}) = \frac{1}{2} \left(h_{\theta}(x^{(i)}) - y^{(i)} \right)^{2} \quad \text{non-convex}$$

$$\begin{aligned} & \operatorname{Cost}(h_{\theta}(x), y) = \begin{cases} & -\log(h_{\theta}(x)) & \text{if } y = 1 \\ & -\log(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases} \\ & J(\theta) = \frac{1}{m} \sum_{i=1}^{m} \operatorname{Cost}(h_{\theta}(x^{(i)}), y^{(i)}) \\ & = -\frac{1}{m} [\sum_{i=1}^{m} y^{(i)} \log h_{\theta}(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_{\theta}(x^{(i)}))] \end{aligned}$$

Gradient prosty Gradient descent



$$\theta_j \coloneqq \theta_j - \eta \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$$

 η – learning rate (0.01)

$$X = \begin{bmatrix} x_{1,1} & \dots & x_{1,n} \\ x_{2,1} & \dots & x_{2,n} \\ \vdots & \ddots & \vdots \\ x_{m,1} & \dots & x_{m,n} \end{bmatrix}$$

$$\boldsymbol{x_i} = \begin{bmatrix} x_{i,1} & x_{i,2} & \dots & x_{i,n} \end{bmatrix}$$

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} (y_i \log(h_{\theta}(x_i)) - (1 - y_i) \log(1 - h_{\theta}(x_i)))$$

$$h_{\theta}(x_i) = g(\theta^T x_i)$$

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^{m} (h_{\theta}(x_i) - y_i) x_{i,j}$$

$$\text{eta = 0.1 } \# \text{ learning rate }$$

$$\text{n_iterations = 1000}$$

$$\text{m = 100}$$

$$\text{theta = np.random.randn(2,1)} \# \text{ random initialization}$$

$$\text{for iteration in range(n_iterations):}$$

$$\text{gradients = 2/m * X_b.T.dot(X_b.dot(theta) - y)}$$

$$\text{theta = theta - eta * gradients}$$

Stochastyczny Gradient Stochastic Gradient Descent



$$\theta_j \coloneqq \theta_j - \eta \frac{\partial}{\partial \theta_i} J_i(\theta_0, \theta_1)$$

 η – learning rate (0.01)

$$X = \begin{bmatrix} x_{1,1} & \dots & x_{1,n} \\ x_{2,1} & \dots & x_{2,n} \\ \vdots & \ddots & \vdots \\ x_{m,1} & \dots & x_{m,n} \end{bmatrix}$$

$$\boldsymbol{x_i} = \begin{bmatrix} x_{i,1} & x_{i,2} & \dots & x_{i,n} \end{bmatrix}$$

i-ustalone, losowe

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} (y_i \log(h_{\theta}(x_i)) - (1 - y_i) \log(1 - h_{\theta}(x_i)))$$

$$h_{\theta}(x_i) = g(\theta^T x_i)$$

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x_i) - y_i) x_{i,j}$$

for epoch in range(n_epochs):
 for i in range(m):
 random_index = np.random.randint(m)
 xi = X_b[random_index:random_index+1]
 yi = y[random_index:random_index+1]
 gradients = 2 * xi.T.dot(xi.dot(theta) - yi)
 eta = learning_schedule(epoch * m + i)
 theta = theta - eta * gradients

Gradient z minigrupami Mini-batch Gradient Descent



$$\theta_j \coloneqq \theta_j - \eta \frac{\partial}{\partial \theta_j} J_I(\theta_0, \theta_1)$$

 η – learning rate (0.01)

$$X = \begin{bmatrix} x_{1,1} & \dots & x_{1,n} \\ x_{2,1} & \dots & x_{2,n} \\ \vdots & \ddots & \vdots \\ x_{m,1} & \dots & x_{m,n} \end{bmatrix}$$

$$\boldsymbol{x_i} = \begin{bmatrix} x_{i,1} & x_{i,2} & \dots & x_{i,n} \end{bmatrix}$$

I-ustalone, losowy podzbiór X

$$J(\theta) = -\frac{1}{m} \sum_{i=1}^{m} (y_i \log(h_{\theta}(x_i)) - (1 - y_i) \log(1 - h_{\theta}(x_i)))$$

$$h_{\theta}(x_i) = \boldsymbol{g}(\boldsymbol{\theta}^T \boldsymbol{x}_i)$$

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{1}{m} \sum_{i=1}^m (h_{\theta}(x_i) - y_i) x_{i,j}$$

Workflow

DATA

TRAIN DATASET



CLEANSING



(...)



TRANSFORMATION

SCALING

NORMALISATION

ENCODING

DIM. REDUCTION

DISCRETISATION



REGRESSION

SUPPORT VECTOR

TREES



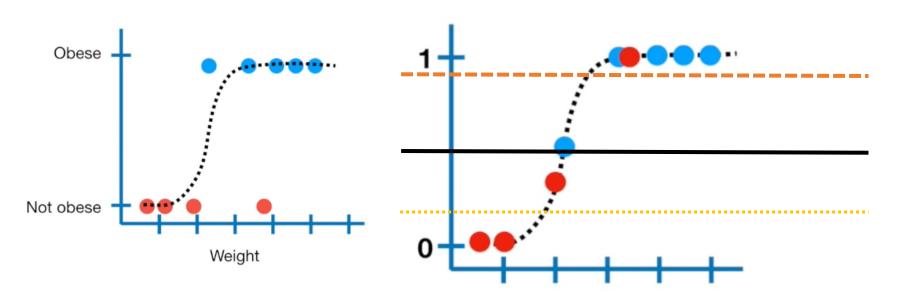
TRAIN DATASET

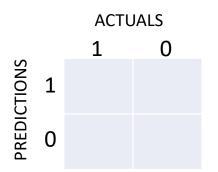


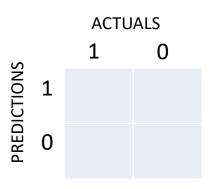
PIPELINE

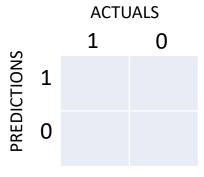


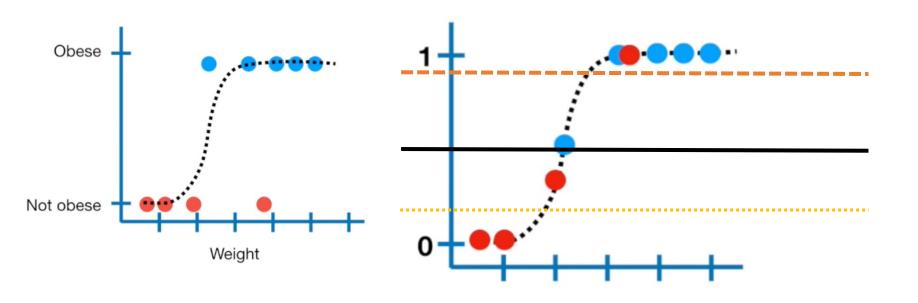
MODEL PERFORMANCE







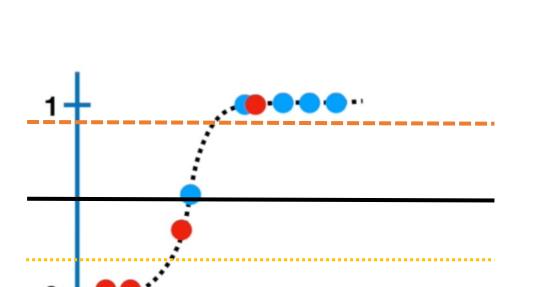


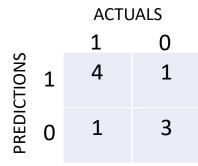


		ACTUALS			
		1	0		
PREDICTIONS	1	4	1		
PREDI	0	1	3		

		ACTUALS			
S		1	0		
PREDICTIONS	1	5	0		
PRED	0	1	3		

		ACTUALS			
S		1	0		
PREDICTIONS	1	5	0		
PRED	0	2	2		



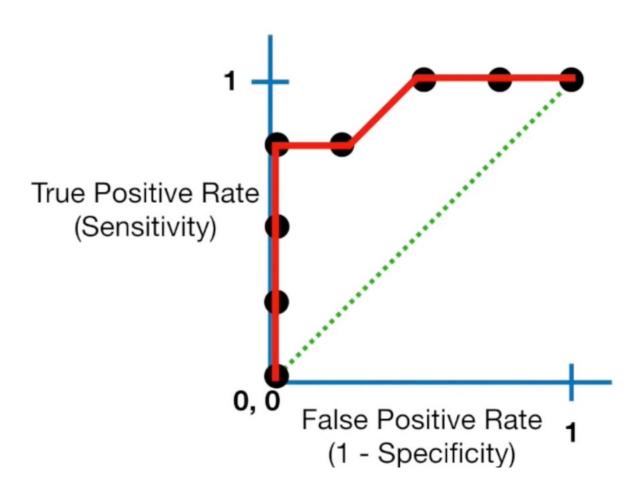


$$TPR = \frac{TP}{TP + FN} = \frac{4}{4+1}$$

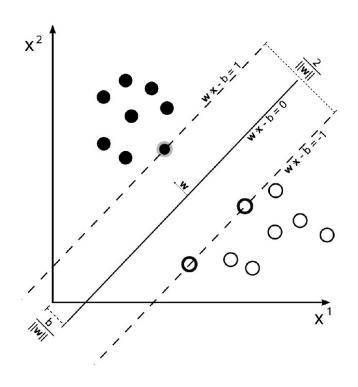
$$FPR = 1 - TPR = \frac{FP}{FP + TN} = \frac{1}{1+3}$$

$$TPR = \frac{5}{5+1}$$
$$FPR = \frac{0}{0+3}$$

$$TPR = \frac{5}{5+2}$$
$$FPR = \frac{0}{3+2}$$



SVM – Hard Margin



$$f(x)=w^Tx-b$$

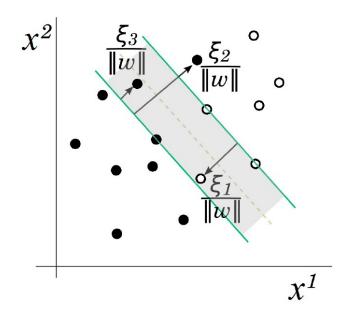
$$(w,b) = \underset{w,b}{\arg\min} ||w||^2$$

Constraints:

$$w^T x_i - b \ge 1$$
, $x_i \in Class$
 $w^T x_i - b \le -1$, $x_i \notin Class$

$$(w^T x_i - b) y_i \ge 1$$

SVM – Soft Margin



Constraints, for each *i*:

$$\xi_i \ge 0$$

$$(w^T x_i - b) y_i \ge 1 - \xi_i$$

$$\xi_{i} = \max \{1 - f(x_{i})y_{i}, 0\}$$
 Hinge loss
$$f(x) = w^{T}x - b$$

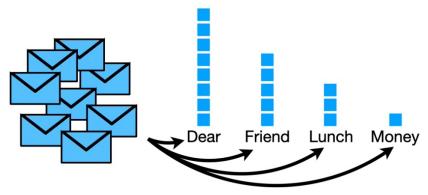
$$(w, b) = \arg \min_{w, b} \sum_{i} \xi_{i} + \lambda ||w||^{2}$$

$$\lambda > 0$$

Likelihoods

Naïve Bayes

$$p(word|N) = \frac{\#word}{\#total\ words\ in\ N}$$



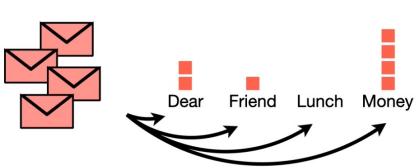
$$p(Dear | N) = 0.47$$

p(**Friend**
$$|$$
 N $) = 0.29$

$$p(Lunch | N) = 0.18$$

$$p(Money | N) = 0.06$$

Prior probability
$$p(N) = \frac{\#N}{\#total\ emails}$$



$$p(word|S) = \frac{\#word}{\#total\ words\ in\ S}$$

$$p(| Dear | S) = 0.29$$

p(**Friend**
$$|$$
 S) = 0.14

$$p(Lunch | S) = 0.00$$

$$p(Money | S) = 0.57$$

Prior probability
$$p(S) = \frac{\#S}{\#total\ emails}$$



$$p(N) \times p(Dear \mid N) \times p(Friend \mid N)$$

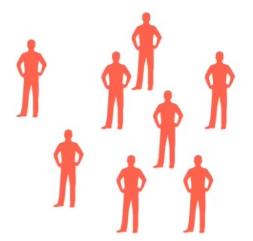
$$p(S) \times p(Dear | S) \times p(Friend | S)$$

Naïve Bayes - Gaussian



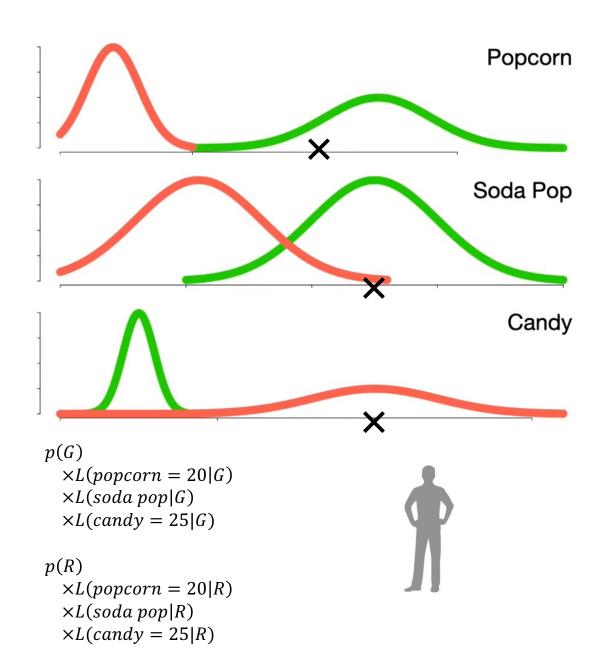
p(G)	_	# <i>G</i>
p(a)	_	#total

Popcorn (grams)	Soda Pop (ml)	Candy (grams)
24.3	750.7	0.2
28.2	533.2	50.5
etc.	etc.	etc.



$$p(R) = \frac{\#R}{\#total}$$

Popcorn (grams)	Soda Pop (ml)	Candy (grams)
2.1	120.5	90.7
4.8	110.9	102.3
etc.	etc.	etc.



Decission Tree - CART

Gini:

$$H(Q_m) = \sum_k p_{mk} (1-p_{mk})$$

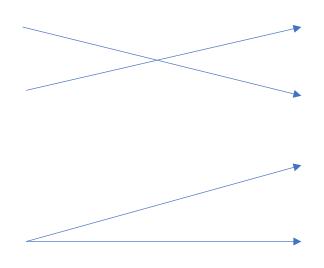
Log Loss or Entropy:

$$H(Q_m) = -\sum_k p_{mk} \log(p_{mk})$$

Step 1: Bootstraping

Original Dataset

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	No	Yes	167	Yes



Bootstrapped Dataset

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	Yes	Yes	180	Yes
No	No	No	125	No
Yes	No	Yes	167	Yes
Yes	No	Yes	167	Yes

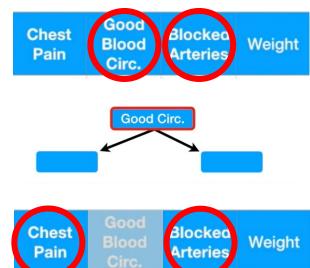
Step 2: Create Decision Tree.

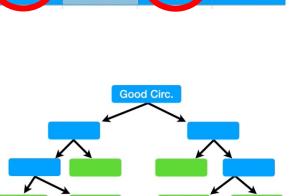
Randomly select subset of features.

Find best split.

Randomly select subset of features to node split.

Create Tree considering subset of features.

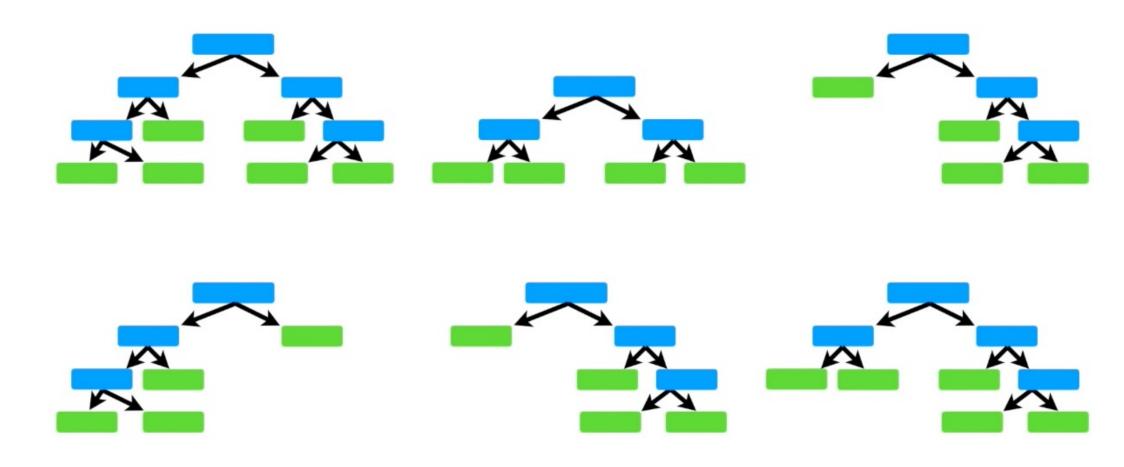




Bootstrapped Dataset

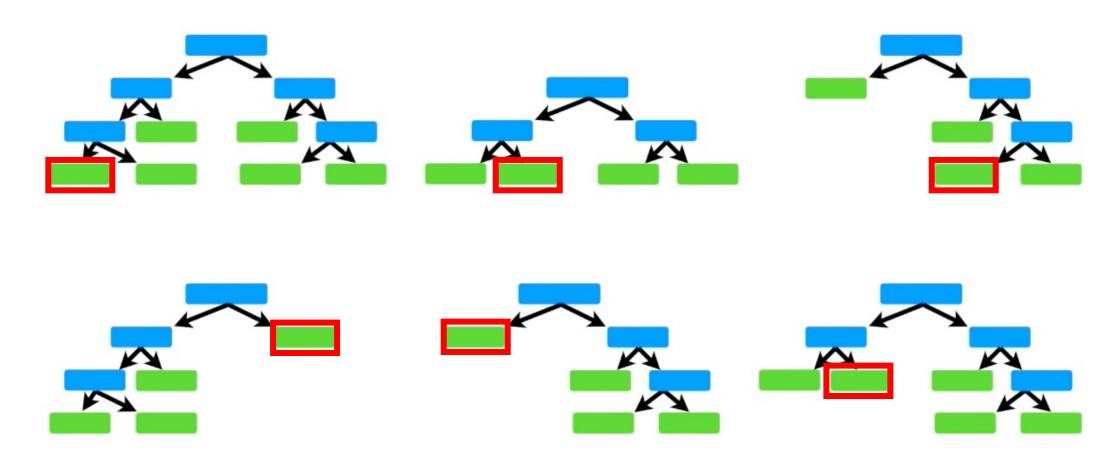
Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	Yes	Yes	180	Yes
No	No	No	125	No
Yes	No	Yes	167	Yes
Yes	No	Yes	167	Yes

Repeat Step 1 & Step 2 creating next trees.



Predictions.

Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	No	No	168	



Out-Of-Bag Dataset

Original Dataset



Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Sugar
Yes	Yes	No	210	No

We can make predictions for *oob* subset and calculate metrics.

In sklearn module sklearn.ensemble. RandomForestClassifier has **oob_score_** attrbiiute returning accuracy.

oob_score_ : float

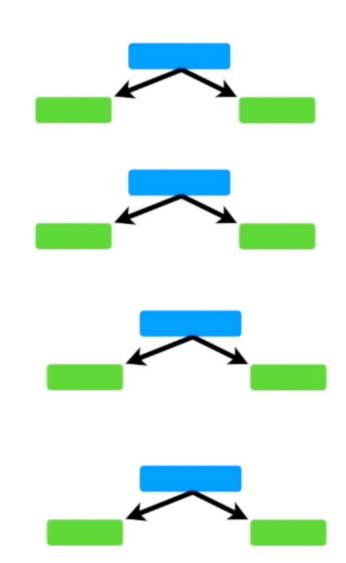
Score of the training dataset obtained using an out-of-bag estimate. This attribute exists only when oob_score is True.

Bootstrapped Dataset

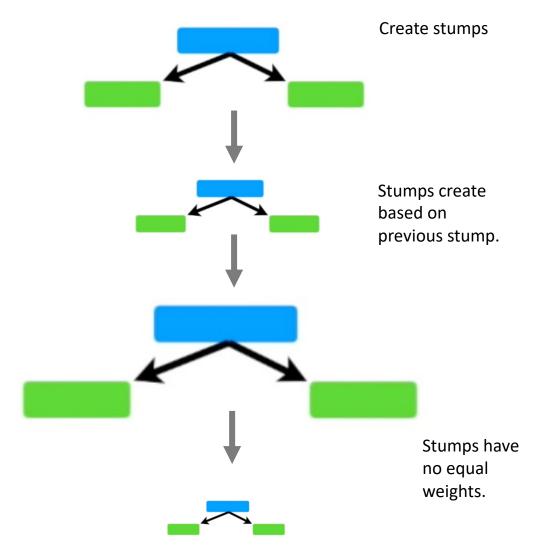
Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
Yes	Yes	Yes	180	Yes
No	No	No	125	No
Yes	No	Yes	167	Yes
Yes	No	Yes	167	Yes

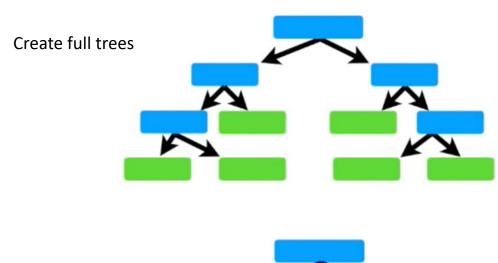
Original Dataset

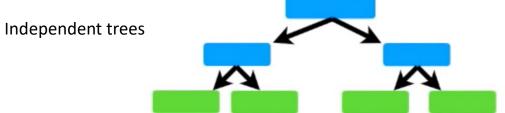
Chest Pain	Good Blood Circ.	Blocked Arteries	Weight	Heart Disease
No	No	No	125	No
Yes	Yes	Yes	180	Yes
Yes	Yes	No	210	No
Yes	No	Yes	167	Yes

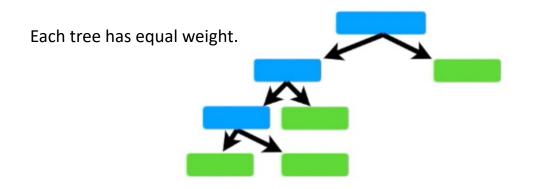


stump









Chest Pain	Blocked Arteries	Patient Weight	Heart Disease
Yes	Yes	205	Yes
No	Yes	180	Yes
Yes	No	210	Yes
Yes	Yes	167	Yes
No	Yes	156	No
No	Yes	125	No
Yes	No	168	No
Yes	Yes	172	No

Sample Weight

1/8

1/8

1/8

1/8

1/8

1/8

1/8

1/8

Step 1. Find best split minimizing Gini



Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	New Weight
Yes	Yes	205	Yes	0.05
No	Yes	180	Yes	0.05
Yes	No	210	Yes	0.05
Yes	Yes	167	Yes	0.33
No	Yes	156	No	0.05
No	Yes	125	No	0.05
Yes	No	168	No	0.05
Yes	Yes	172	No	0.05

Step 1. Find best split minimizing Gini

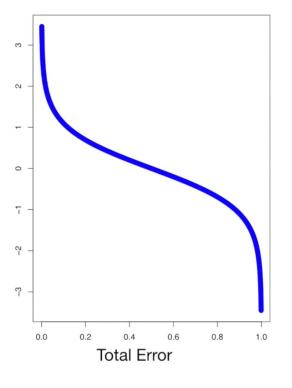
Step 2. Update sample weights.

$$I = \frac{1}{2}\log(\frac{1 - total_error}{total_error})$$

total_error - sum of incorrect
classified samples weights

New weigth = $weight \times e^{I}$ - True

New weigth = weight $\times e^{-I}$ - False



Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	0.07
No	Yes	180	Yes	0.07
Yes	No	210	Yes	0.07
Yes	Yes	167	Yes	0.49
No	Yes	156	No	0.07
No	Yes	125	No	0.07
Yes	No	168	No	0.07
Yes	Yes	172	No	0.07

Step 1. Find best split minimizing Gini

Step 2. Update sample weights.

Step 3. Normalize sample weights.

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease
Yes	Yes	205	Yes
No	Yes	180	Yes
Yes	No	210	Yes
Yes	Yes	167	Yes
No	Yes	156	No
No	Yes	125	No
Yes	No	168	No
Yes	Yes	172	No

Sample Weight
0.07
0.07
0.07
0.49
0.07
0.07
0.07
0.07

Step 1. Find best split minimizing Gini

Step 2. Update sample weights.

Step 3. Normalize sample weights.

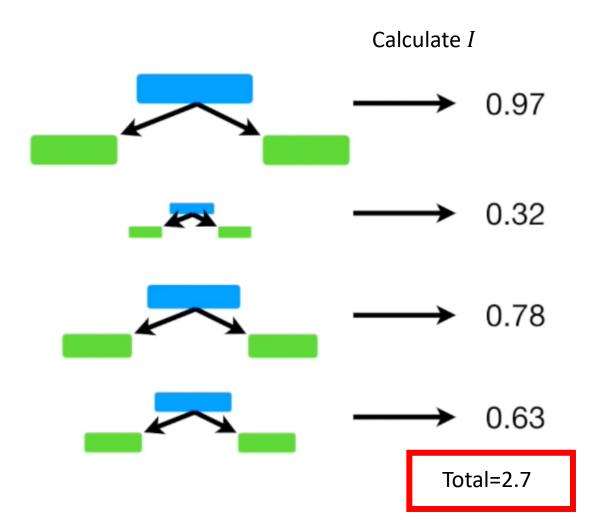
Step 3. Bootstrap dataset using new sample weights.

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
No	Yes	156	No	1/8
Yes	Yes	167	Yes	1/8
No	Yes	125	No	1/8
Yes	Yes	167	Yes	1/8
Yes	Yes	167	Yes	1/8
Yes	Yes	172	No	1/8
Yes	Yes	205	Yes	1/8
Yes	Yes	167	Yes	1/8

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
No	Yes	156	No	1/8
Yes	Yes	167	Yes	1/8
No	Yes	125	No	1/8
Yes	Yes	167	Yes	1/8
Yes	Yes	167	Yes	1/8
Yes	Yes	172	No	1/8
Yes	Yes	205	Yes	1/8
Yes	Yes	167	Yes	1/8

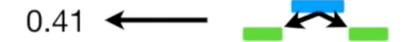
- Step 1. Find best split minimizing Gini
- Step 2. Update sample weights.
- Step 3. Normalize sample weights.
- Step 4. Bootstrap dataset using new sample weights.
- Step 5. Repeat using bootstrap dataset.

$$I = \frac{1}{2}\log(\frac{1-total_error}{total_error})$$



Chest	Blocked	Patient	Heart
Pain	Arteries	Weight	Disease
No	Yes	156	No

Calculate *I*





Input: Data $\{(x_i, y_i)\}_{i=1}^n$, and a differentiable **Loss Function** $L(y_i, F(x))$

Step 1: Initialize model with a constant value: $F_0(x) = \operatorname{argmin} \sum_{i=1}^{n} L(y_i, \gamma)$

Step 2: for m = 1 to M:

(A) Compute
$$r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x) = F_{m-1}(x)}$$
 for $i = 1,...,n$

- **(B)** Fit a regression tree to the r_{im} values and create terminal regions R_{im} , for $j = 1...J_m$
- (C) For $j = 1...J_m$ compute $\gamma_{jm} = \underset{\gamma}{\operatorname{argmin}} \sum_{x_i \in R_{ij}} L(y_i, F_{m-1}(x_i) + \gamma)$ (D) Update $F_m(x) = F_{m-1}(x) + \nu \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$

Step 3: Output $F_M(x)$

$$\sum_{i=1}^{N} \mathbf{y}_{i} \times \log(\mathbf{p}) + (1 - \mathbf{y}_{i}) \times \log(1 - \mathbf{p})$$

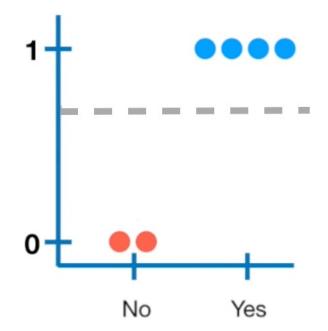
Chest Pain	Age	Color	Heart Disease	Residual
Yes	12	Blue	Yes	0.3
Yes	87	Green	Yes	0.3
No	44	Blue	No	-0.7
Yes	19	Red	No	-0.7
No	32	Green	Yes	0.3
No	14	Blue	Yes	0.3

1. Initialise predication value

$$\log(\text{odds}) = \log \frac{\#p}{\#n} = 0.69314 \approx 0.7$$

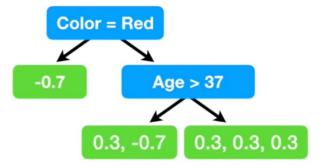
$$p(X) = \frac{e^{\log\frac{\#p}{\#n}}}{1 + e^{\log\frac{\#p}{\#n}}} = 0.667 \approx 0.7$$

2. Calculate (pseudo) residuals

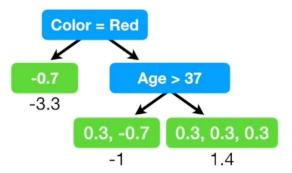


Chest Pain	Age	Color	Heart Disease	Residual
Yes	12	Blue	Yes	0.3
Yes	87	Green	Yes	0.3
No	44	Blue	No	-0.7
Yes	19	Red	No	-0.7
No	32	Green	Yes	0.3
No	14	Blue	Yes	0.3

3. Build tree to predict residuals



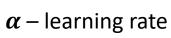
4. Calculate output value

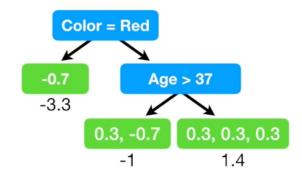


Chest Pain	Age	Color	Heart Disease	Predicted Prob.
Yes	12	Blue	Yes	0.9
Yes	87	Green	Yes	0.5
No	44	Blue	No	0.5
Yes	19	Red	No	0.1
No	32	Green	Yes	0.9
No	14	Blue	Yes	0.9

5. Update log-odds.

$$new \log(odds) = \\ \log(odds) + \alpha \times$$





6. Calculate probabilities.

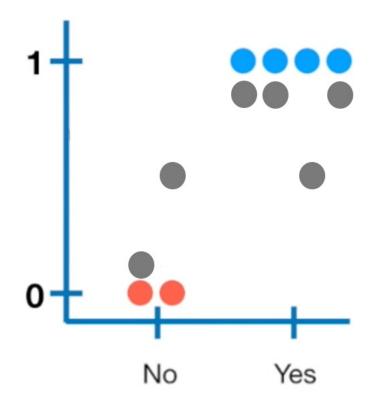
$$p_{new}(X) = \frac{e^{\log(odds)}}{1 + e^{\log(odds)}}$$

7. Calculate residuals.

Grsdient Boost

Chest Pain	Age	Color	Heart Disease	Predicted Prob.	Resid
Yes	12	Blue	Yes	0.9	0.1
Yes	87	Green	Yes	0.5	0.5
No	44	Blue	No	0.5	-0.
Yes	19	Red	No	0.1	-0.
No	32	Green	Yes	0.9	0.1
No	14	Blue	Yes	0.9	0.1

R	Residual		
	0.1		
	0.5		
	-0.5		
	-0.1		
	0.1		
	0.1		



No

14

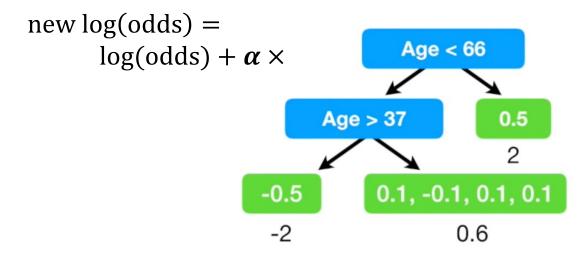
Chest Pain	Age	Color	Heart Disease	Residual
Yes	12	Blue	Yes	0.1
Yes	87	Green	Yes	0.5
No	44	Blue	No	-0.5
Yes	19	Red	No	-0.1
No	32	Green	Yes	0.1

Blue

Yes

8. Repeat.

0.1

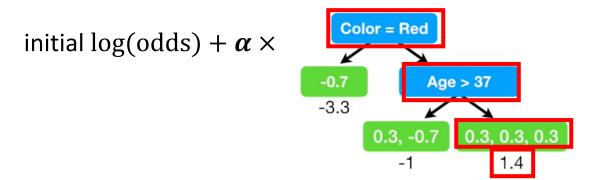


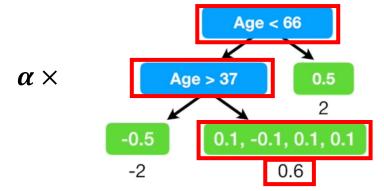
$$p_{new}(X) = \frac{e^{\log(odds)}}{1 + e^{\log(odds)}}$$

residuals

Chest Pain	Age	Color	
Yes	25	Green	

Predictions





pred log(odds)

$$p_{pred}(X) = \frac{e^{\text{pred log(odds)}}}{1 + e^{\text{pred log(odds)}}}$$

Summary

Metrics:

- Confusion Matrix (TP/FP/TN/FN)
- Accuracy
- Precision/Recall/F-score
- ROC-AUC

Machine Learning:

- Logistic Regression
- Support Vector Machine (+kernel trick)
- K Nearest Neighbours
- Naïve Bayes (Gaussian/Multinomial)
- Decision Tree
- Random Forrest
- Boosting (AdaBoost/Gradient Boost)

SVM vs. Logistic Regression Random Forrest vs. Decision Trees Random Forrest vs. Gradient Boost Boosting vs. Bagging

Random in Random Forrest

Imbalanced Dataset

Regularisation:

- Lasso (L1)
- Ridge (L2)
- ElasticNet

Sklearn

- Pipelines
- Grid Search
- Custom Estimator

TODO:

XGBoost

(Stochastic) Gradient Descent



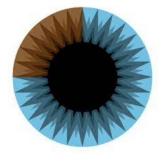
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Machine Learning Study Groups

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