Linear Classification & Logistic Regression

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Questions

1. перечислите 3-5 известных вам задач машинного обучения
2. Метод максимального правдоподобия: формулировка, использование свойства iid и переход к логарифму
3. Постановка задачи регрессии. Что добавляется в случае линейной регрессии?
4. В чём состоит наивность наивного байесовского классификатора?
5. Выписать аналитическое решение задачи линейной регрессии. Какие могут быть проблемы при его использовании?
6. Теорема Гаусса-Маркова: формулировка
7. Регуляризация: перечислить известные типы, для чего нужна и как изменится аналитическое решение в этом случае?
8. Запишите функции потерь в задаче регрессии. (3-5 шт)
9. Что такое переобучение и как его можно обнаружить?
10. Параметры и гиперпараметры: их свойства и отличия (кратко)
11. Техники валидации модели: перечислить 3-5 известных способа
12. * kNN - алгоритм: к чему может привести разный масштаб признаков, что делать в таком случае?

Recap

Lecture 2:
Linear Regression

- Linear Models overview
- Regression problem statement
- Linear Regression analytical solution
  - Gauss-Markov theorem (BLUE)
  - Instability
- Regularization
  - L2 aka Ridge
    - Analytical solution
  - L1 aka LASSO
    - Weights decay rule
  - Elastic Net
- Metrics in regression
- Model building cycle
  - Train
  - Validation
  - Test

Outline

- Linear classification
  - margin
  - loss functions
- Logistic regression
  - sigmoid derivation
  - Maximum Likelihood Estimation (MLE)
  - logistic loss
  - probability calibration
- Multiclass aggregation strategies
  - One vs Rest
  - One vs One
- Metrics in classification
  - Accuracy, Balanced accuracy
  - Precision, Recall, F-score
  - ROC curve, PR curve, AUC
  - Confusion matrix

Linear Classification

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01

Classification problem

$$X \in R^{n \times p}$$

$$Y \in C^n \qquad \text{e.g. } C = \{-1, 1\}$$

$$|C| < +\infty$$

$$c(X) = \hat{Y} \approx Y$$

Linear classifier

The most simple linear classifier

$$c(x) = \begin{cases} 1, & \text{if } f(x) \geq 0 \\ -1, & \text{if } f(x) < 0 \end{cases}$$

or equivalently

$$c(x) = \operatorname{sign}(f(x)) = \operatorname{sign}(x^T w)$$

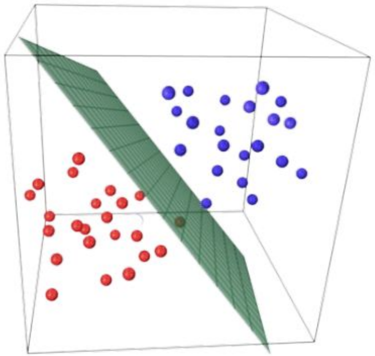
Geometrical interpretation:

hyperplane dividing space into two

subspaces

Why cutoff value is fixed?

(bias term is implied)



Margin

Let's define linear model's Margin as

$$M_i = y_i \cdot f(x_i) = y_i \cdot x_i^T w$$

main property:

negative margin reveals misclassification

$$M_i > 0 \Leftrightarrow y_i = c(x_i)$$

$$M_i \leq 0 \Leftrightarrow y_i \neq c(x_i)$$

Weights choice

Remembering old paradigm

$$\text{Empirical risk} = \sum_{\text{by object}} \text{Loss on object} \longrightarrow \min_{\text{model params}}$$

Essential loss is misclassification

$$L_{\text{mis}}(y_i^t, y_i^p) = [y_i^t \neq y_i^p] = \\ = [M_i \leq 0]$$

Disadvantages

- Not differentiable
- Overlooks confidence

Solution:

estimate it with a smooth function

Iverson bracket $[P] = \begin{cases} 1, & \text{if } P \text{ is true} \\ 0, & \text{otherwise} \end{cases}$

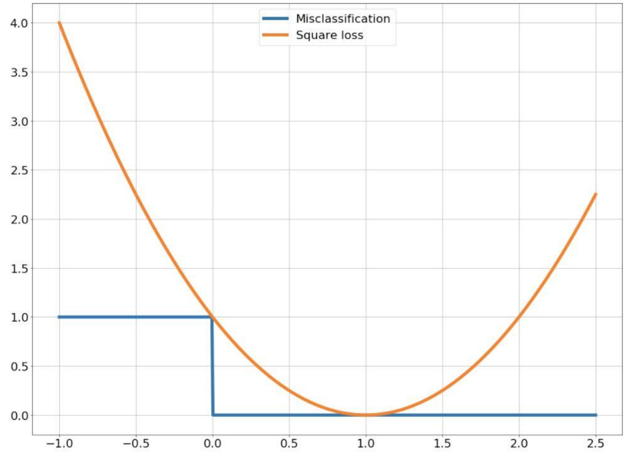
Square loss

Let's treat classification problem as regression problem:

$$Y \in \{-1, 1\} \mapsto Y \in R$$

thus we optimize MSE

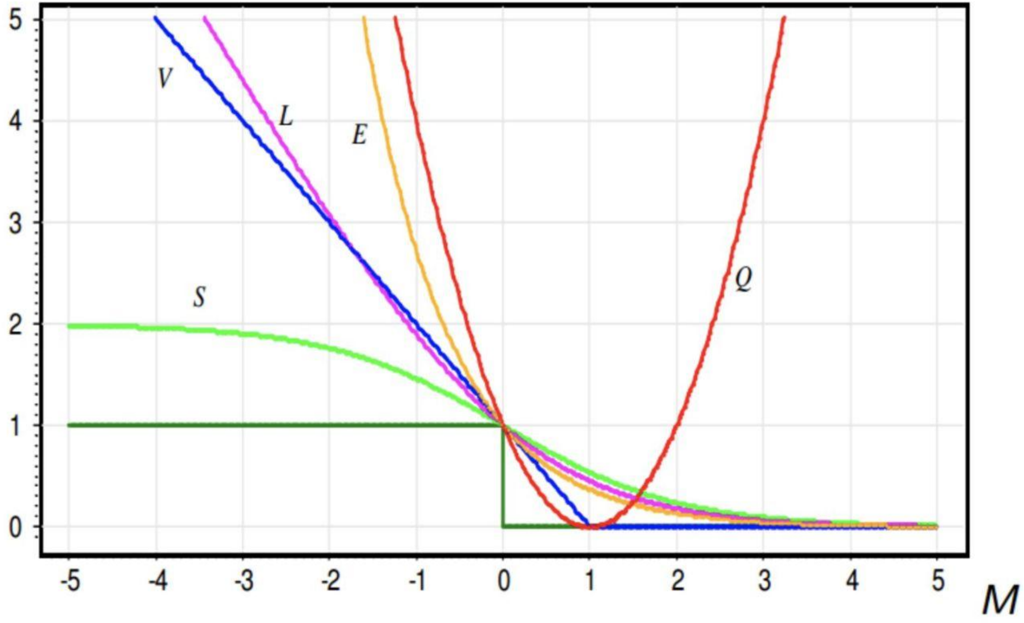
$$L_{\text{MSE}} = (y_i - x_i^T w)^2 = \frac{(y_i^2 - y_i \cdot x_i^T w)^2}{y_i^2} = $$
$$= (1 - y_i \cdot x_i^T w)^2 = (1 - M_i)^2$$



Advantage: already solved

Disadvantage: penalizes for high confidence

Other losses



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

Loss functions for classification

Logistic Regression

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Intuition

I. Let's try to predict probability of an object to have positive class

$$p_+ = P(y = 1|x) \in [0, 1]$$

II. But all we can predict is a real number!

$$y = x^T w \in R$$

III. Time for some tricks

$$\frac{p_+}{1 - p_+} \in [0, +\infty)$$

$$\log \frac{p_+}{1 - p_+} \in R$$

Here is the match

This is called **logit** or **log-odds**

IV. Reverse to closed form

$$\frac{p_+}{1 - p_+} = \exp(x^T w)$$

$$p_+ = \frac{1}{1 + exp(-x^T w)} = \sigma(x^T w)$$

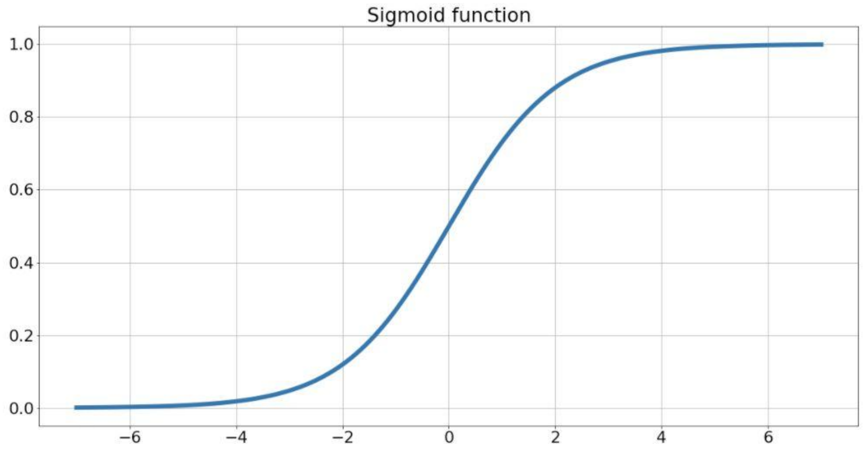
Sigmoid (aka logistic) function

$$\sigma(x) = \frac{1}{1 + exp(-x)}$$

Sigmoid is odd relative to (0, 0.5) point

Symmetric property:

$$1 - \sigma(x) = \sigma(-x)$$



Derivative: $\sigma'(x) = \sigma(x) \cdot (1 - \sigma(x))$

MLE for Logistic Regression

Just to remind

$$\log L(w|X,Y) = \log P(X,Y|w) = \log \prod_{i=1}^{n} P(x_i, y_i|w)$$

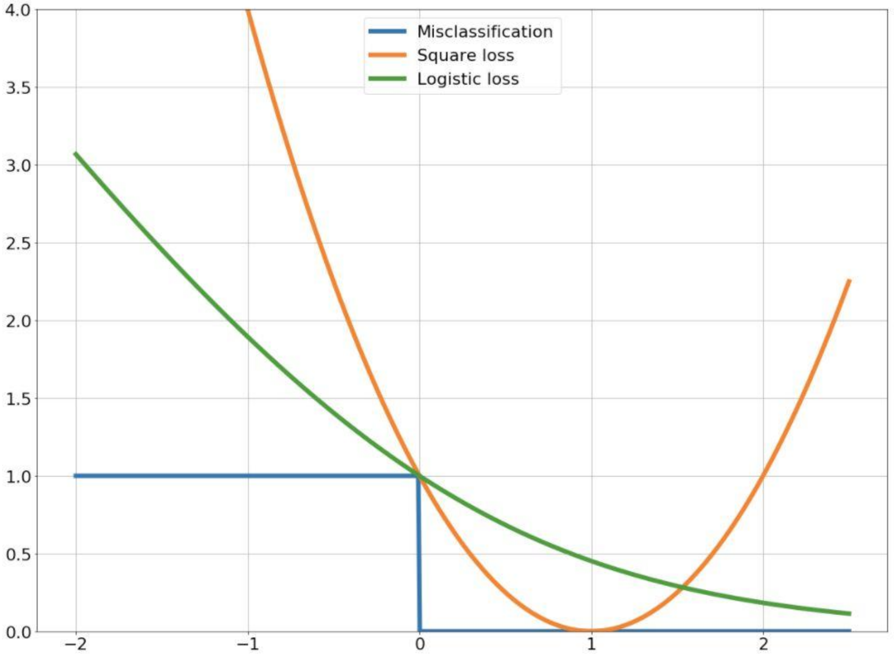
Calculating probabilities for objects (which are modelled as Bernoulli variables)

$$\begin{aligned} \text{if } y_i = 1: &\quad P(x_i, 1|w) = \sigma_w(x_i) = \sigma_w(M_i) \\ \text{if } y_i = -1: &\quad P(x_i, -1|w) = 1 - \sigma_w(x_i) = \sigma_w(-x_i) = \sigma_w(M_i) \end{aligned}$$

$$\log L(w|X,Y) = \sum_{i=1}^{n} \log \sigma_w(M_i) = \boxed{-\sum_{i=1}^{n} \log(1 + \exp(-M_i)) \to \min_w}$$

Logistic loss

$$L_{Logistic} = \log(1 + \exp(-M_i))$$



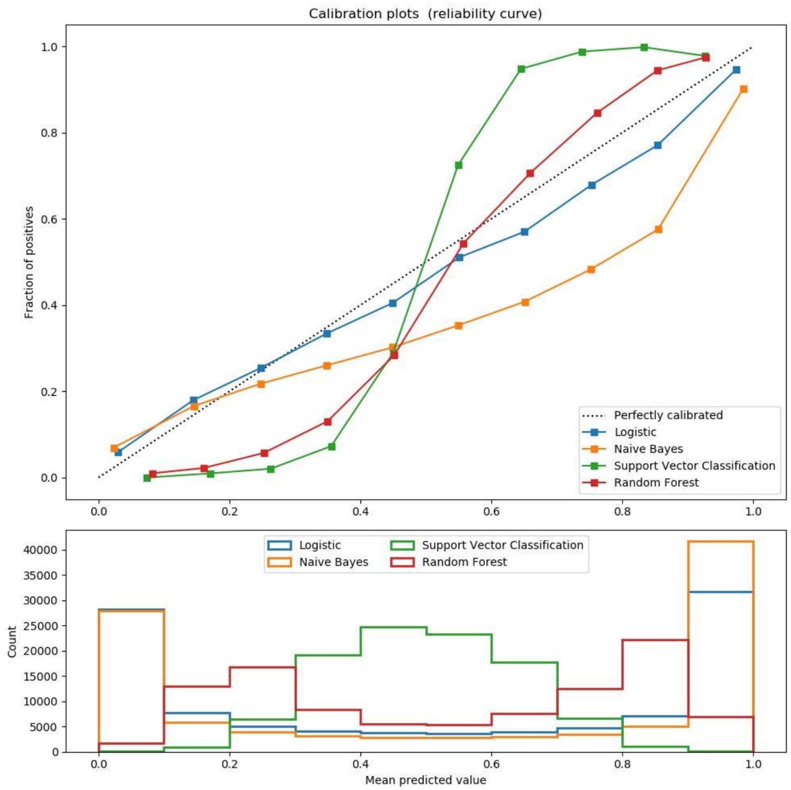
Probability calibration

By using Logistic Regression

we generate a Bernoulli distribution

in each point of space

[Calibration discussion]



Multiclass aggregation strategies

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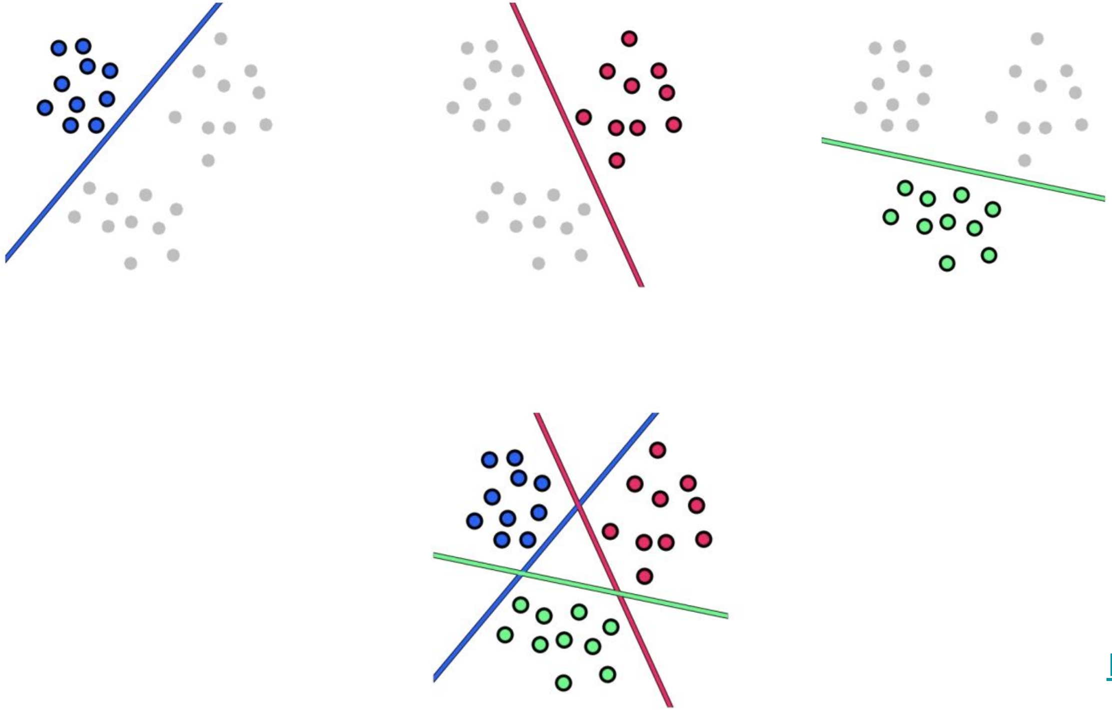
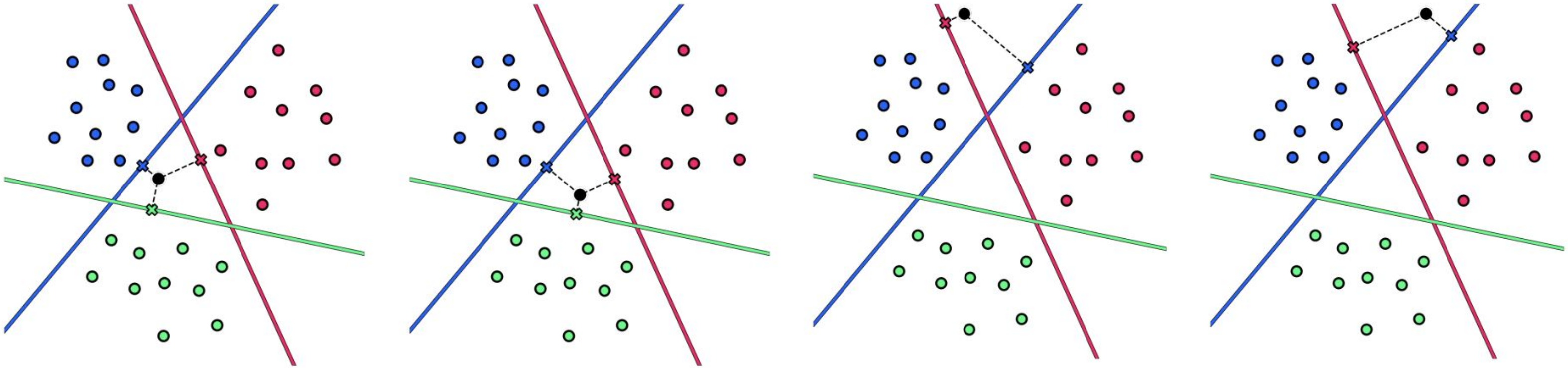
One vs Rest

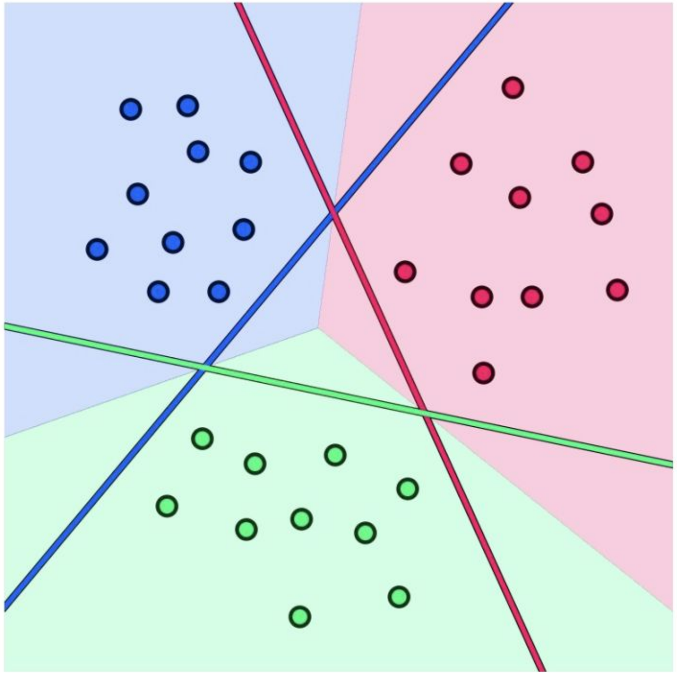


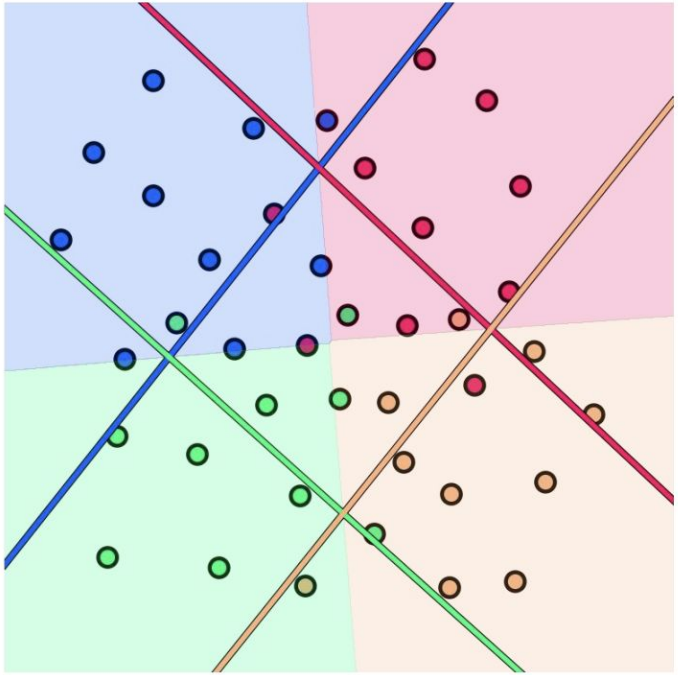
[Images source](#)

One vs Rest: unclassified regions

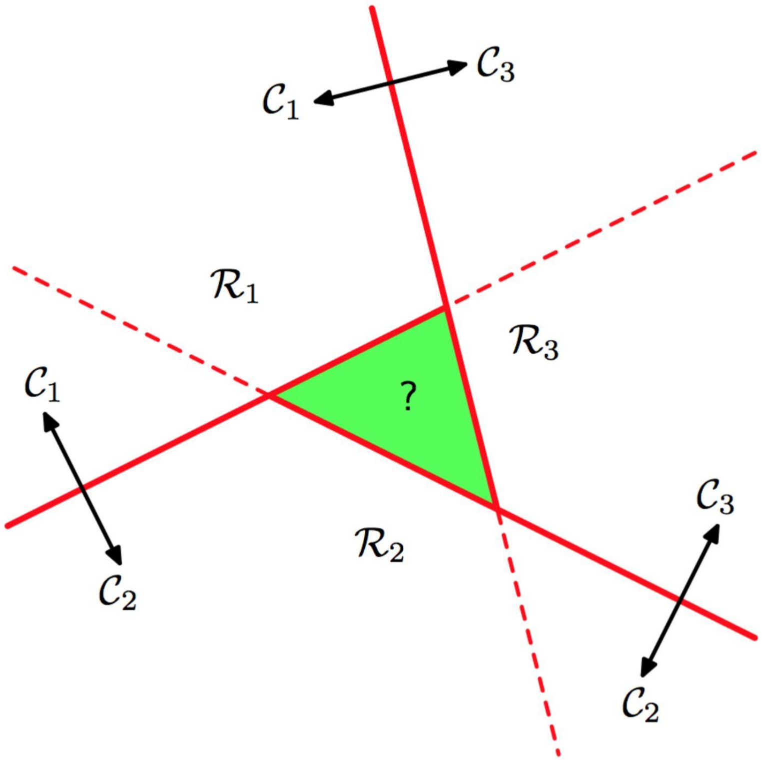


One vs Rest: final result



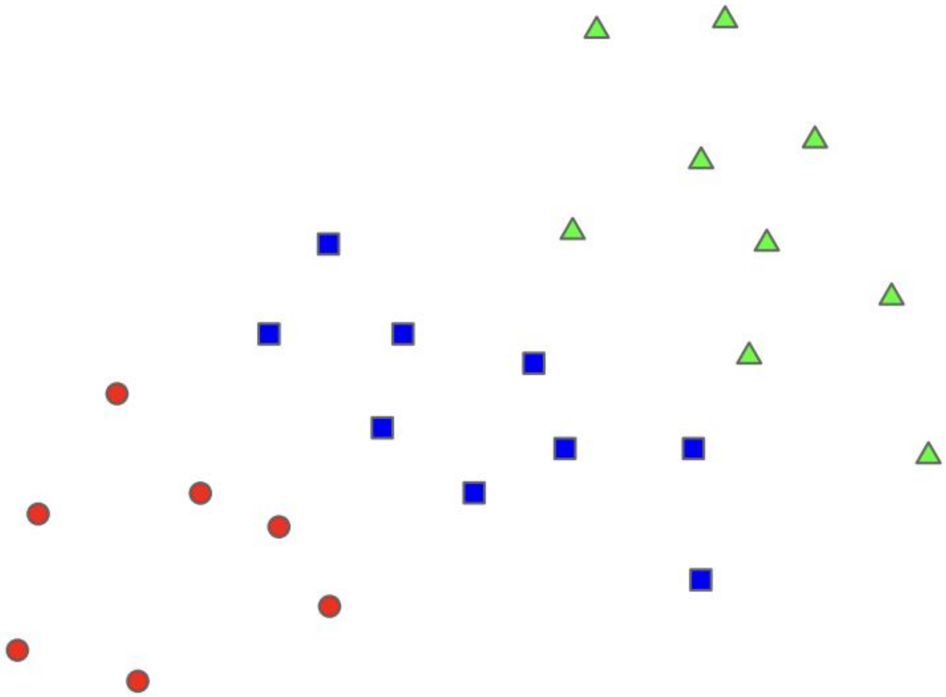


One vs One



$\mathcal{C}_1$
$\mathcal{C}_3$
$\mathcal{R}_1$
$\mathcal{R}_3$
$\mathcal{C}_1$
?
$\mathcal{C}_3$
$\mathcal{C}_2$
$\mathcal{R}_2$
$\mathcal{C}_2$

Failure case?



Summary

	One vs Rest	One vs One
#classifiers	k	k(k-1)/2
dataset for each	full	subsampled

Metrics in classification

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Metrics

- Accuracy
  - Balanced accuracy
- Precision
- Recall
- F-score
- ROC curve
  - ROC-AUC
- PR curve
  - PR-AUC
- Multiclass generalizations
- Confusion matrix

Accuracy

Number of right classifications

$$\text{Accuracy} = \frac{1}{n}\sum_{i=1}^{n}[y_i^t = y_i^p]$$

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

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

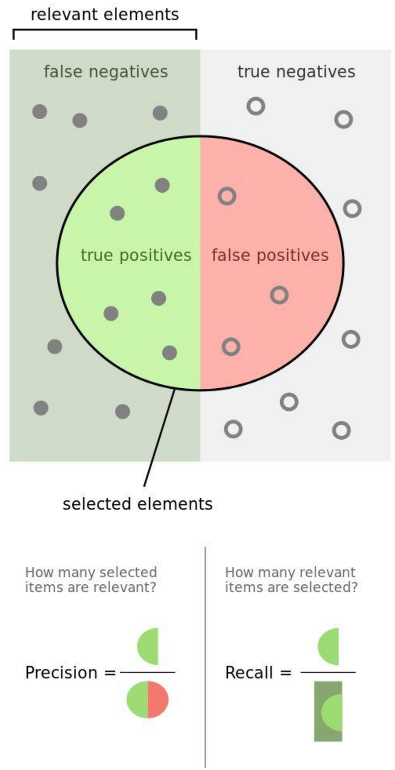
accuracy = 8/10 = 0.8

$$\text{Balanced accuracy} = \frac{1}{C}\sum_{k=1}^{C}\frac{\sum_i [y_i^t = k \text{ and } y_i^t = y_i^p]}{\sum_i [y_i^t = k]}$$

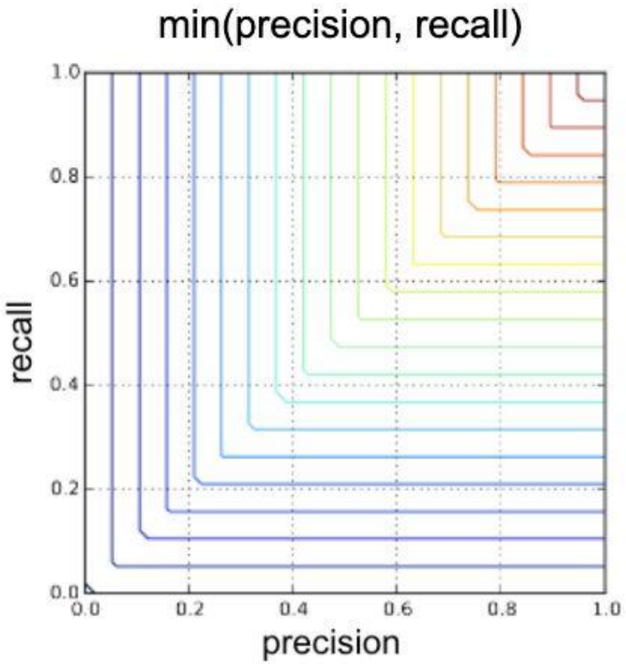
Precision and Recall

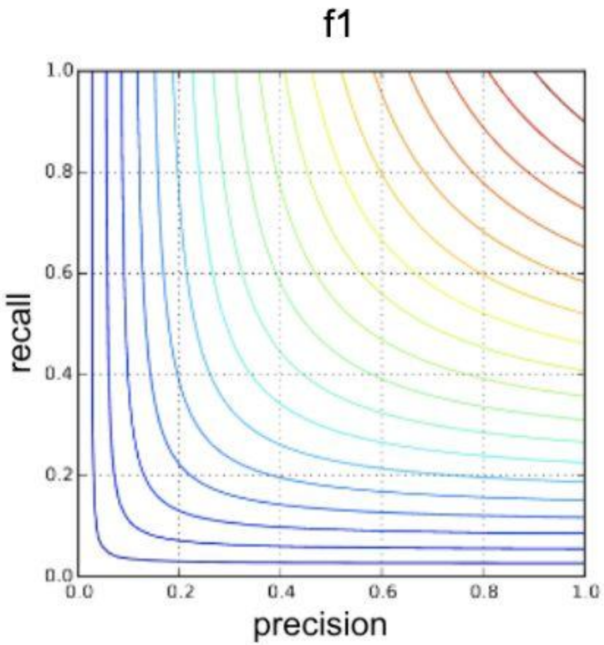
		True condition	
	Total population	Condition positive	Condition negative
Predicted condition	Predicted condition positive	**True positive**	**False positive**, Type I error
	Predicted condition negative	**False negative**, Type II error	**True negative**

$$\text{Precision} = \frac{TP}{TP + FP} \quad \text{Recall} = \frac{TP}{TP + FN}$$



F-score motivation





F-score

Harmonic mean of precision and recall

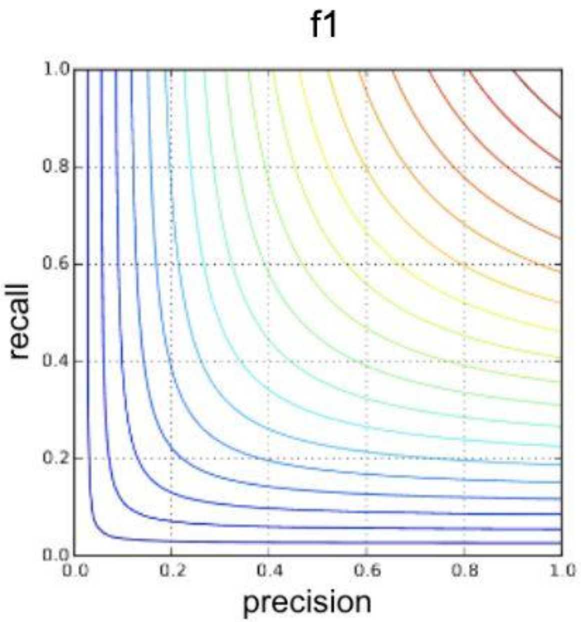
Closer to smaller one

$$F_1 = \frac{2}{\mathrm{precision}^{-1} + \mathrm{recall}^{-1}} = 2\,\frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}$$

Generalization to different ratio between

Precision and Recall

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

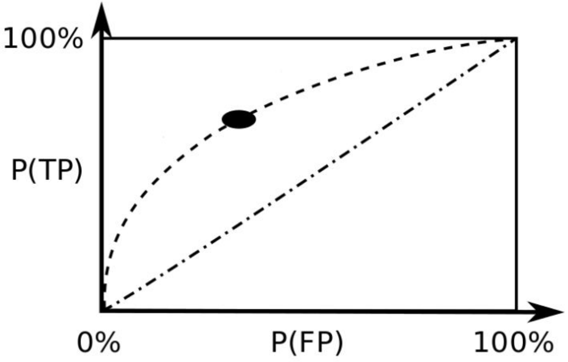


Receiver Operating Characteristic (ROC)

		True condition	
	Total population	Condition positive	Condition negative
Predicted condition	Predicted condition positive	**True positive**	**False positive**, Type I error
	Predicted condition negative	**False negative**, Type II error	**True negative**

$$\mathrm{FPR} = \frac{FP}{FP + TN}$$

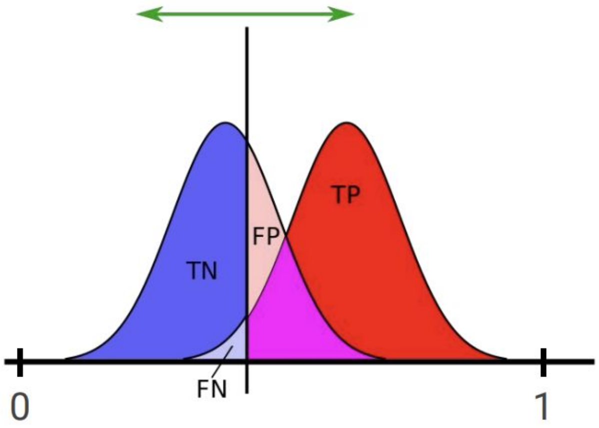
$$\mathrm{TPR} = \frac{TP}{TP + FN} (= \mathrm{Recall})$$

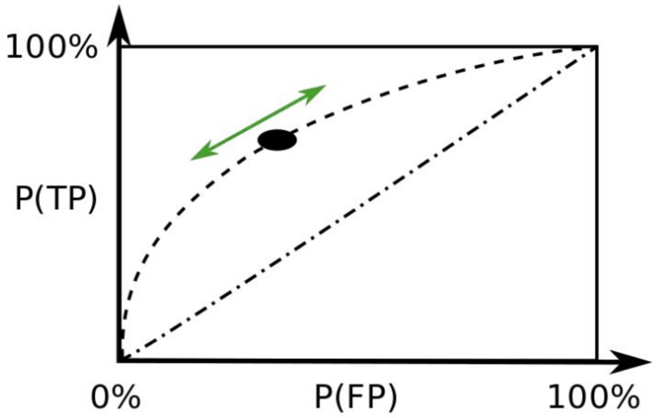


Receiver Operating Characteristic (ROC)

Classifier needs to predict probabilities

Objects get sorted by positive probability





Line is plotted as threshold moves

Receiver Operating Characteristic (ROC)

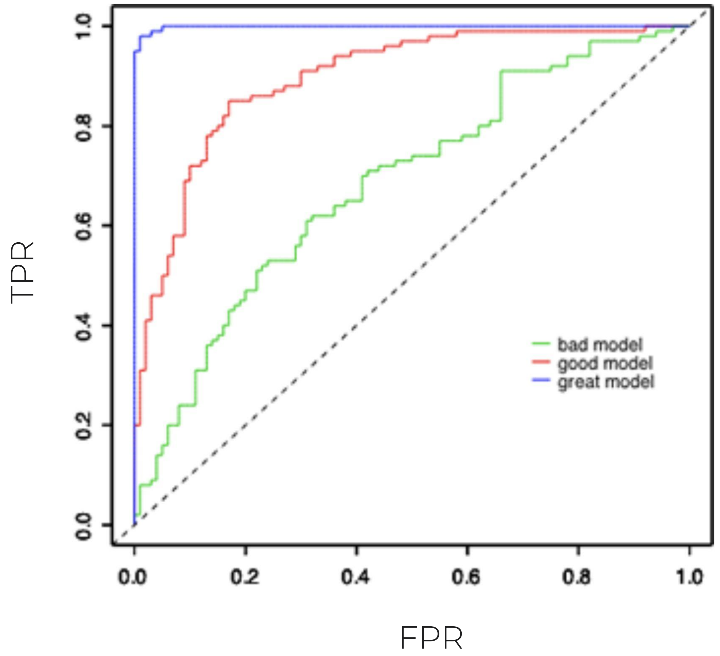
Baseline is random predictions

Always above diagonal (for reasonable classifier)

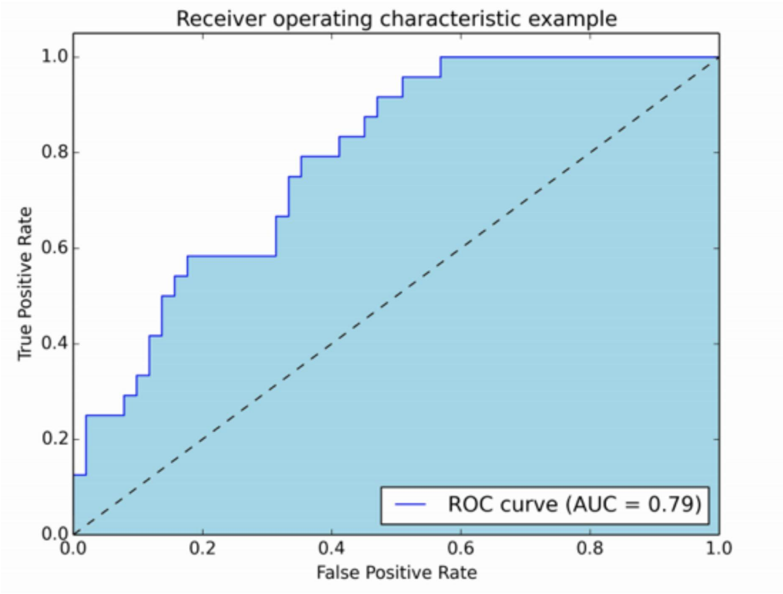
If below - change sign of predictions

Strictly higher curve means better classifier

Number of steps (thresholds) not bigger than dataset



ROC Area Under Curve (ROC-AUC)

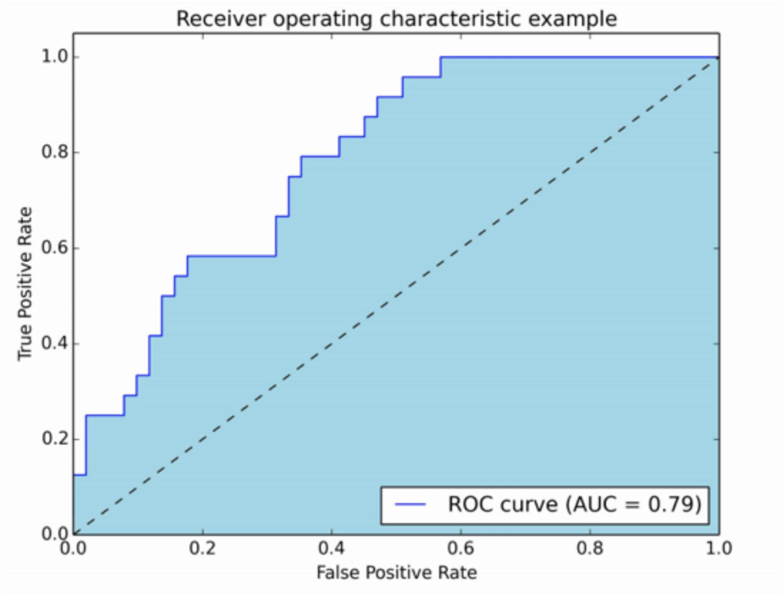


Effectively lays in (0.5, 1)

Bigger ROC-AUC doesn't imply higher curve everywhere

More explanations with pictures

ROC-AUC properties



Equal to fraction of correctly sorted paris
Because we compute it over predictions sorted by score.

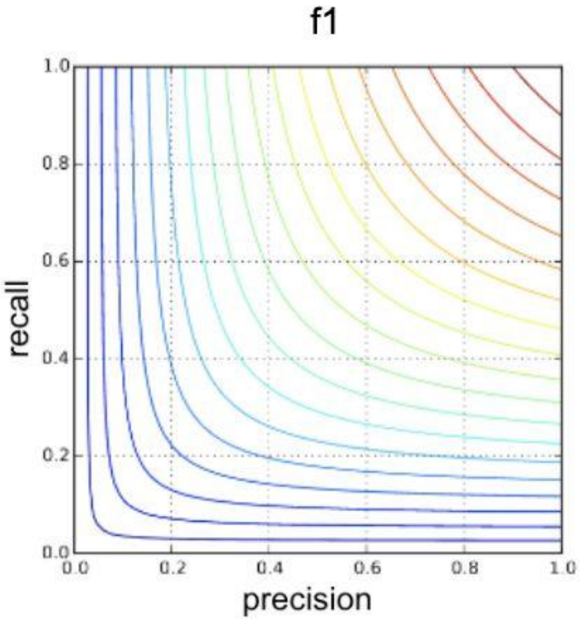
Scale-invariant
It measures how well predictions are ranked, rather than their absolute values.
If we multiply all predictions by constant metric will not change.

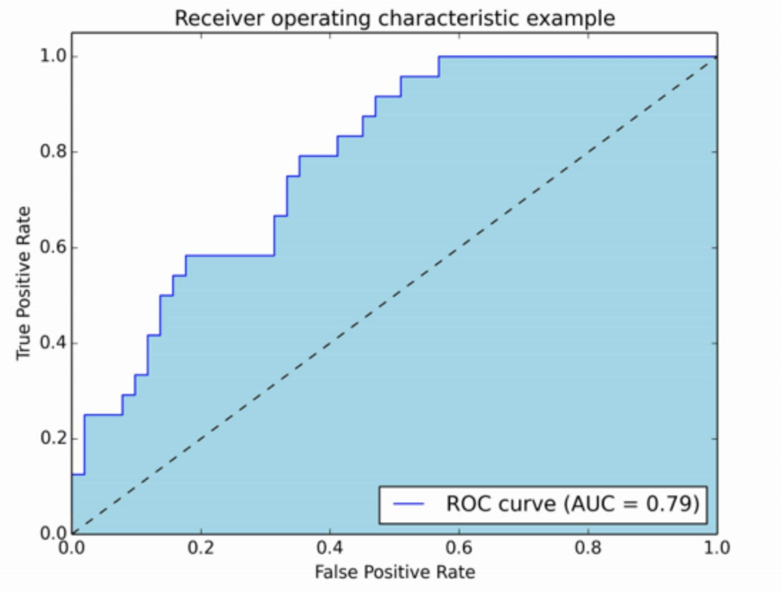
Classification-threshold-invariant
It measures the quality of the model's predictions irrespective of what classification threshold is chosen.

[Source]

F-score vs ROC-AUC

Which one to tune?





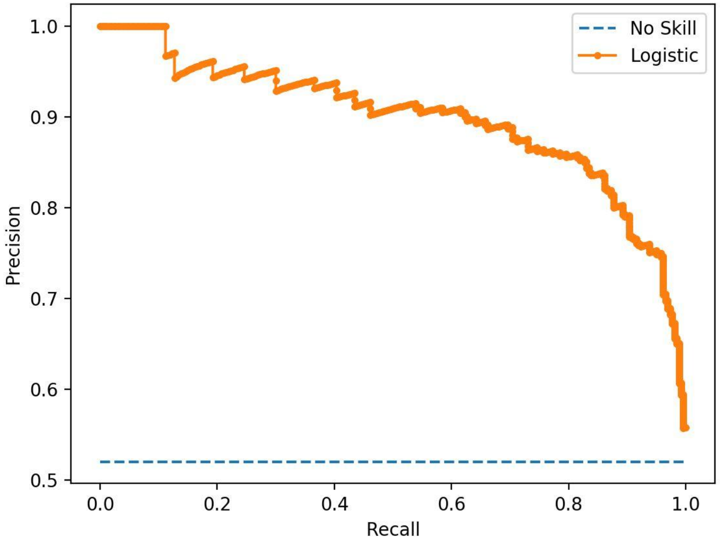
Precision-Recall Curve

AUC is in (0, 1)

Source of AP metric

(important for next semester)

[Nice article]



Multiclass metrics

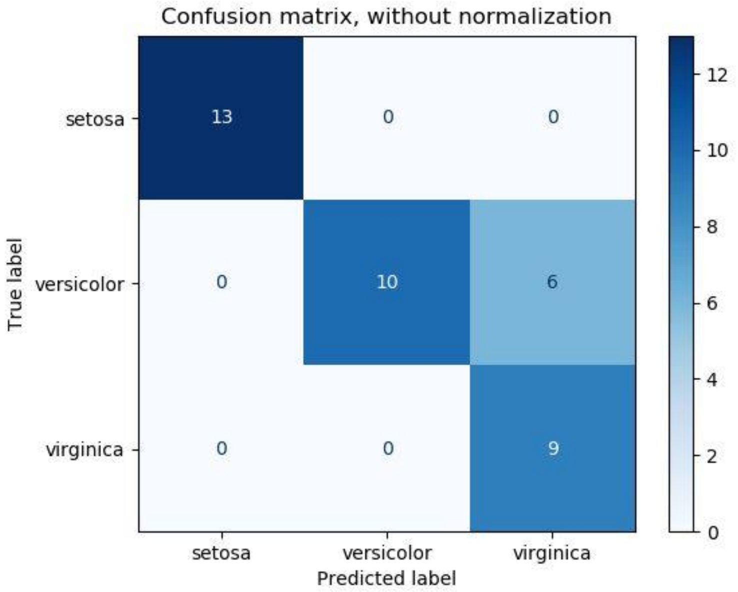
As with linear models we need some magic to measure multiclass problems

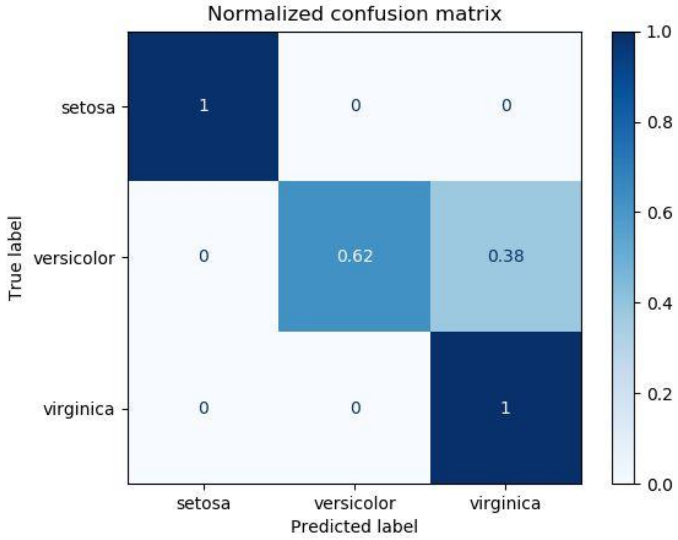
Basically it's mean of one or another kind

Detailed info here and here

average	Precision	Recall	F_beta
"micro"	$P(y, \hat{y})$	$R(y, \hat{y})$	$F_\beta(y, \hat{y})$
"samples"	$\frac{1}{\|S\|} \sum_{s \in S} P(y_s, \hat{y}_s)$	$\frac{1}{\|S\|} \sum_{s \in S} R(y_s, \hat{y}_s)$	$\frac{1}{\|S\|} \sum_{s \in S} F_\beta(y_s, \hat{y}_s)$
"macro"	$\frac{1}{\|L\|} \sum_{l \in L} P(y_l, \hat{y}_l)$	$\frac{1}{\|L\|} \sum_{l \in L} R(y_l, \hat{y}_l)$	$\frac{1}{\|L\|} \sum_{l \in L} F_\beta(y_l, \hat{y}_l)$
"weighted"	$\frac{1}{\sum_{l \in L} \|\hat{y}_l\|} \sum_{l \in L} \|\hat{y}_l\| P(y_l, \hat{y}_l)$	$\frac{1}{\sum_{l \in L} \|\hat{y}_l\|} \sum_{l \in L} \|\hat{y}_l\| R(y_l, \hat{y}_l)$	$\frac{1}{\sum_{l \in L} \|\hat{y}_l\|} \sum_{l \in L} \|\hat{y}_l\| F_\beta(y_l, \hat{y}_l)$

Confusion matrix





Revise

- Linear classification
  - margin
  - loss functions
- Logistic regression
  - sigmoid derivation
  - Maximum Likelihood Estimation
  - Logistic loss
  - probability calibration
- Multiclass aggregation strategies
  - One vs Rest
  - One vs One
- Metrics in classification
  - Accuracy, Balanced accuracy
  - Precision, Recall, F-score
  - ROC curve, PR curve, AUC
  - Confusion matrix

Next time

- Support Vector Machines
- Principal Component Analysis
- Linear Discriminant Analysis

Thanks for attention!

Questions?

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