

Machine Learning – winter term 2016/17 –

Chapter 01: Introduction

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Outline



1. Motivation

- 2. Machine Learning Basics
- 3. Machine Learning vs X
- 4. Benchmarking ML Systems

Machine Learning ("ML") and Big Data $_{\scriptscriptstyle images\,from\,[16]}$



(June 2016)

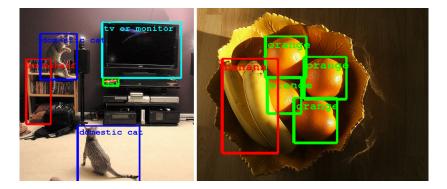


There is more and more unstructured data around (web 2.0, mobile devices, IoT, self-driving cars, ...)

Machine Learning: Some recent Achievements image from [17]

"Imagine a historian of science writing about computer vision in the year 2100. They will identify the years 2011 to 2015 (and probably a few years beyond) as a time of **huge breakthroughs**, driven by deep convolutional nets."

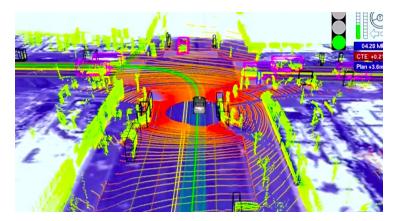
(M. Nielsen, "Neural Networks and Deep Learning")



Machine Learning: Some recent Achievements image from [12]

"In the past decade, machine learning has given us self-driving cars, practical speech recognition, effective web search, and a vastly improved understanding of the human genome."

(Andrew Ng, Stanford University)



Machine Learning: Some recent Achievements image from [3]

"A survey carried out among AI experts recently shows they think machines will be as intelligent as humans by the year 2040."

(Nick Bostrom)



Atlas, The Next Generation

Machine Learning: Motivation

"If data had mass, the earth would be a black hole."

(Steven Marsland)

"As more data becomes available, more ambitious problems can be tackled. As a result, machine learning is **widely used in computer science** and other fields. However, developing successful machine learning applications requires a substantial amount of 'black art' that is hard to find in textbooks."

(P. Domingos, A few Useful Things to Know about Machine Learning)

Example Applications

kaggle

Have a look on kaggle.com

Flight Quest

optimize flight routes based on wheather and traffic

- TFI Restaurant Revenue Prediction predict annual sales of restaurants to open
- Job Recommendation Challenge predict which jobs users will apply to
- Whale Detection Challenge detect whale calls from audio, prevent collision with ship traffic
- Discovering trolling in user comments
- ► ...

There's also the 'classics'

- OCR, handwriting recognition, object recognition
- search engines, recommender systems, targeted advertising
- natural language processing, spam filtering

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An ML Sample Application images from [4] [13]

- A computer system is to make a non-trivial decision
- Example: spam filtering
- Why not hard-code the decision logic?

Problems

- high effort to grasp problem's complexity
- easy to code *something*, difficult to reach the **optimal** program
- feasibility checking: What accuracy can be reached by a decision?
- code is extremely difficult to maintain
- keeping track of data changes (e.g., when spammers change strategies) is almost impossible
- there is no way to take user feedback into account



Machine Learning: Definition

"Machine learning is a scientific discipline that explores the construction and study of **algorithms that can learn from data**. Such algorithms operate by building a **model** from **example inputs** and using that to make **predictions or decisions**, rather than following strictly static program instructions."

(en.wikipedia.org)

"The field of study that gives computers the ability to learn without being explicitly programmed."

(Arthur Samuel (1959))

"A computer program is said to **learn** from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with Experience E."

(Tom Mitchell (1998))

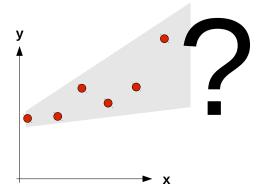
Remark

These definitions are entirely non-operational!



Machine Learning's Hello World





- Goal: predict a person's weight in the future
- ► Given: a set of 2D samples (x₁, y₁), ..., (x_n, y_n) (x is time, y is person's weight)
- Approach (linear regression): fit a line to the points and use this line for prediction
- Does this qualify as machine learning?

Machine Learning's Hello World

Linear Regression

We define a line as a function

$$\mathcal{M}_{\theta}(x) = a \cdot x + b$$

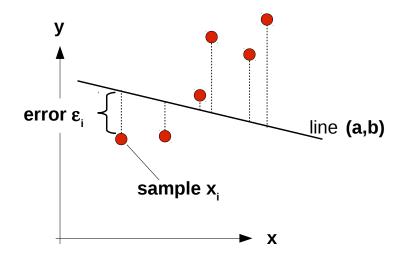
We measure the quality of a particular line θ = (a, b) using an error function E:

$$E(\theta) = \sum_{i=1}^{n} \underbrace{\left(\underbrace{a \cdot x_i + b}_{\mathcal{M}(x_i)} - y_i\right)^2}_{exp}$$

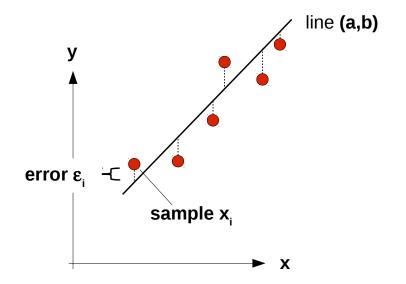
• The **best line** is the one that **minimizes** *E*:

$$(a^*,b^*) = rg\min_{ heta \in \mathbb{R}^2} E(heta)$$

Machine Learning's Hello World a bad line: The errors $\epsilon_1^2, ..., \epsilon_n^2$ are high $\rightarrow E$ is high



Machine Learning's Hello World a good line: The errors $\epsilon_1^2, ..., \epsilon_n^2$ are low $\rightarrow E$ is low





Machine Learning's Hello World

We minimize E by settings its gradient to zero, followed by a bit of algebra:

$$\frac{\partial E}{\partial b} = \partial \left(\sum_{i} (a \cdot x_{i} + b - y_{i})^{2} \right) / \partial b = 0$$

$$2 \cdot \sum_{i} (a \cdot x_{i} + b - y_{i}) = 0$$

$$n \cdot b = \sum_{i} y_{i} - a \cdot \sum_{i} x_{i}$$

$$b = \overline{y} - a\overline{x}$$

$$\frac{\partial E}{\partial a} = \partial \left(\sum_{i} (a \cdot x_{i} + b - y_{i})^{2} \right) / \partial a = 0$$

$$2 \cdot \sum_{i} (a \cdot x_{i} + b - y_{i}) \cdot x_{i} = 0$$

$$\sum_{i} (a \cdot x_{i} + (\bar{y} - a\bar{x}) - y_{i}) \cdot x_{i} = 0$$

$$a \left(\sum_{i} x_{i}^{2} - \bar{x} \sum_{i} x_{i} \right) = \sum_{i} y_{i} x_{i} - \bar{y} \sum_{i} x_{i} \quad //:n$$

$$a = s_{xy} / s_{x}^{2}$$

- The problem above is a regression problem: It is about predicting a real-valued variable y.
- We call the points $(x_1, y_1), ..., (x_n, y_n)$ the training samples.
- We call our line function $\mathcal{M}(x) = a \cdot x + b$ the **model**.
- ► We call the process of estimating the model parameters (here, *a* and *b*) training.
- ► A typical training strategy is to formulate an error criterion (here, E) and **optimize** this criterion.
- In our example, we were able to pin down the solution by hand (we say: there is an *analytical* solution). In practice, optimization can be much trickier. Not all functions are easy to optimize.
- Therefore, learning is often done by **local search**.

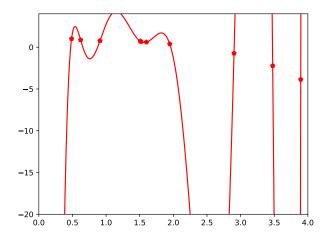
- Obviously, picking the right model for the right data is tricky. It is the core problem in machine learning, actually.
- Example: Would those be better models?

$$\mathcal{M}_{a,b,c,d}(x) = a + b \cdot sin(c \cdot x + d)$$

 $\mathcal{M}_{a,b,c,d,e}(x) = a + b \cdot sin(c \cdot x + d) + e \cdot x$
 $\mathcal{M}_{a_0,a_1,\dots,a_{100}}(x) = \sum_{i=0}^{100} a_i \cdot x^i$

Example: Runge's Phenomenon

Fitting an 8-degree polynomial to 9 points



"The real value of a scientific explanation lies not in its ability to explain (what one has already seen), but in predicting events that have yet to (be seen)"

(Blumer et al. 1987)

"With four parameters I can fit an elephant and with five I can make him wiggle his trunk."

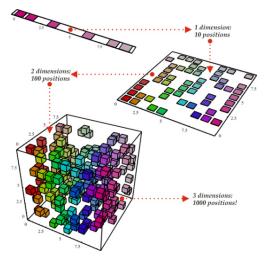
(John von Neumann)

- Our polynomial model works well on the training data but generalizes poorly to novel data. The model overfits.
- We call θ = (a, b) the model's parameters. In practical models there may be thousands of parameters.
- Overfitting is usually more severe...
 - ... the more parameters a model has.
 - ... the fewer training samples we have.



Machine Learning: The Curse of Dimensionality image from [10]

- Overfitting is also more severe the **more dimensions** we have.
- Reason: As the number of dimensions increases, we require more and more data to populate our input space!



Machine Learning: Challenges images from [14] [9] [2] [1]



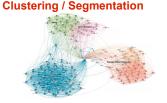
Regression



Classification



(decorption): "ABIERTOW!, "local": "es"



Data Reduction Beer Market Perceptual Mapping



Recommendation

amazon.com

Recommended for You

Amazon.com has new recommendations for you based on items you purchased or told us you own.



Anomaly Detection



Machine Learning: Small Example image from [15]

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7	

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9		0		Palsson, Master. Gosta Leonard	male	2	3			349909			S
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Some more ML Terminology

- ML's goal is to make predictions about real-world objects
 - **SPAM filtering**: objects = e-mails
 - route planning: objects = routes to drive
- Our goal is to make a prediction regarding an object.
 We call this prediction a label or target
 - ▶ SPAM filtering: label ∈ {*spam*/*ham*}
 - route planning: label $\in \mathbb{R}^+_0$ (= time to destination)
- We describe each object by a number of features
 - ▶ **Titanic**: features = gender, ticket price, passenger class, ...
- The collection of the features describing an object is called a feature vector (and usually denoted with x).
- Features can be categorial or numerical.
- In case of numerical features, the object can be interpreted as a **point** in a (high-dimensional) space!



ML: Feature Engineering / Feature Extraction

Often, we prepare the input data before applying ML

- Features may be missing, i.e. x is incomplete.
 Approach: estimate missing values (imputation)
- 2. Categorical features may have to be transformed into numerical ones, typically by introducing dummy variables (one-hot encoding)

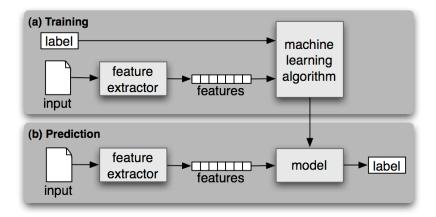
dummy variables

				uun	inty variable	:5	
	PS	color	PS	is_green	ist_silver	ist_red	
Prof. Ulges' car	70	white	73	0	0	0	
Prof. Ulges' wives' car	690	red	690	0	0	1	

- 3. Often, we discard outliers
- 4. Often, we try to pre-select 'important' features.

A Basic ML System Pipeline image from [?]

- 1. We train the system in an off-line phase, obtaining a model
- 2. We apply the system in an on-line phase



Types of Machine Learning

classification vs. regression
 in classification, the labels y₁, ..., y_n are categorical.
 In regression, they are real-valued.

supervised learning

learning from samples $\mathbf{x}_1, ..., \mathbf{x}_n$ with labels $y_1, ..., y_n$

unsupervised learning

learning only from samples $\mathbf{x}_1, ..., \mathbf{x}_n$, <u>no labels</u>

semi-supervised learning

learning from samples $\mathbf{x}_1, ..., \mathbf{x}_n$, some with labels

active learning

. . .

the system can pick which samples to label

ensemble learning

... is about combining learners for a more robust decision

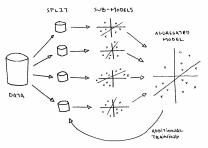
reinforcement learning

... is about learning from feedback instead of labels

Types of Machine Learning (cont'd) image from [5]

Online Learning

- Perspective so far: batch learning (train off-line, apply on-line)
- What if data is too large for memory? Does the model allow a sharding of training data? example: linear regression



What if data come in dynamic streams?
 (→ data stream mining / online learning)

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ML vs. Statistics image from [11]

⊁

"Statistics is the science of learning from data. Machine Learning is the science of learning from data. These fields are identical in intent, although they differ in their history, conventions, emphasis and culture."

("The rise of the machines" - Larry Wasserman, CMU)

ML vs. Statistics

- The term "machine learning" has a negativ overtone in statistics ("Why do Statisticians hate us?")
- Both fields address the same problems with similar methods

model parameters
parameters
fitting
test set performance
regression/classification
density estimation, clustering
large grant = \$50,000
nice place to have a meeting: Las Vegas in August

ML: Relation to other Fields (cont'd)

⊁

ML vs. Artificial Intelligence (AI)

- Machine Learning is a subfield of **subsymbolic** AI
- The other part of AI symbolic AI is about logic, discrete search and rule-based inference.

ML vs. Optimization

- Machine learning techniques usually employ optimization
- "Machine learning = optimization + generalization"

ML vs. Data Mining

- Data mining focuses on exploratory data analysis (by a human expert), machine learning on automatic inference.
- Data mining experts use machine learning, and machine learning experts use data mining.

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Why is Benchmarking so important?

- Machine Learning = iterative re-design of...
 - data
 - features
 - models
 - parameters
- ► Key Driver: Evaluation / Benchmarking



Benchmarking ML Systems: Motivation image from [7]

⊁

Example: YouTube recommender

- We add a **"user history" feature** to the recommender.
- For example, the feature could merge some videos from the user's history into the recommendations.
- ► YouTube redirects some volume of **traffic** to the new system.
- ► YouTube benchmarks the new system against the old one.



Benchmarking: Ground Rule image from [6]

"The most common mistake among machine learning beginners is to test on the training data and have the illusion of success."



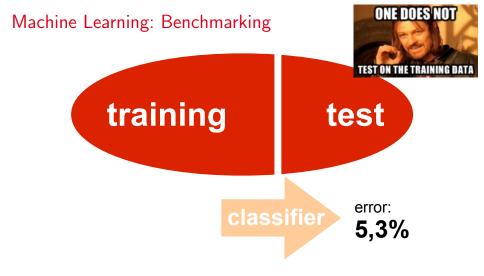
(P. Domingos, A few Useful Things to Know about Machine Learning)

Why?

- All classifiers are prone to overfitting
- Achieving perfect accuracy on the training samples is quite simple (by simply memorizing them).
- It is the generalization to new data that matters!
- When building classifiers, always set some test data aside!

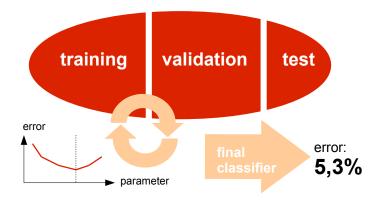
Adhering to the Ground Rule is trickier than you think!

- Example: neural network training
- Example: standard datasets in research



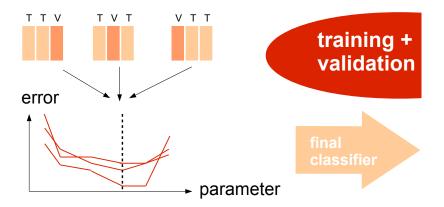
- We separate our dataset into training and testing data
- ▶ Tip 1: choose 'just enough' test data, use the rest for training
- Tip 2: use a roughly balanced class distribution

Machine Learning: Benchmarking



- Some of a classifiers' parameters are usually learned, other (free) parameters are set manually
- Typical approach: grid search
- ▶ **Example**: decision tree (later today) → *parameter* = *depth*
- Approach: train \rightarrow validate \rightarrow test

Machine Learning: Benchmarking



- If there is small training data, we apply cross-validation: Split the data into subsets ("folds"), train/validate multiple times, and average the results
- Extreme case: leave-one-out validation

Accuracy Measures: Loss



- In the following, we focus on benchmarking classification systems
- Basic idea: Count the samples for which the classification system chooses the correct/wrong class.
- But: Some misclassifications are more expensive than others!
- Example: spam filtering
 - misclassifying ham as spam: really bad
 - misclassifying spam as ham: not so bad
- We model the cost of specific misclassifications via a loss function L (assuming possible classes 1, ..., C'):

$$L:\{1,...,C'\}\times\{1,...,C'\}\rightarrow\mathbb{R}$$

• The loss function is often provided by a **business expert**.

Accuracy Measures: Loss



The loss function is usually modeled as a $C' \times C'$ matrix:

L(i,j) := cost for misclassifying a sample from class i as class j

$$\begin{array}{c} \text{picked class } j \\ \text{true} \\ \text{class} \\ i \end{array} \begin{pmatrix} L(1,1) & L(1,2) & \dots & L(1,C') \\ L(2,1) & L(2,2) & \dots & L(2,C') \\ \dots \\ L(C',1) & L(C',2) & \dots & L(C',C') \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 & \dots & 1 \\ 1 & 0 & \dots & 1 \\ \dots \\ 1 & 1 & \dots & 0 \end{pmatrix} \\ \text{zero-one-loss} \end{array}$$

Remark

One standard loss function is zero-one loss (right): any error costs 1

Average Loss, Error Rate, Accuracy

- ▶ Let $\mathbf{x}_1, ..., \mathbf{x}_n$ be a set of **test samples** with **labels** $y_1, ..., y_n \in \{1, ..., C'\}$, and $\phi(\mathbf{x}_1), ..., \phi(\mathbf{x}_n) \in \{1, ..., C'\}$ the **predictions** of our classifier.
- We measure the classifier's average loss:

$$\frac{1}{n}\sum_{i=1}^{n}L(y_i,\phi(\mathbf{x}_i))$$

In case of zero-one-loss, this is equivalent to the error rate:

$$\frac{1}{n}\sum_{i=1}^n\mathbf{1}_{\phi(\mathbf{x}_i)\neq y_i}$$

The error rate's counterpart is the (classification) accuracy:

$$\frac{1}{n}\sum_{i=1}^{n}\mathbf{1}_{\phi(\mathbf{x}_i)=y_i}$$

Obviously: accuracy = 1 – error rate

The Confusion Matrix image from [8]

- Sometimes, it is interesting to check which classes the classifier confuses most often.
- ▶ Therefore, we define the **confusion matrix** $C \in \mathbb{R}^{C' \times C'}$ with

$$C_{jk} := \#\{ i \in \{1, ..., n\} \mid y_i = j \land \phi(\mathbf{x}_i) = k \}$$

Example

		Estimated Emotion							
		Anger	Boredom	Disgust	Fear	Happiness	Sadness	Neutral	Emotion Recog. Rate
True Emotion	Anger	19	0	2	0	3	0	0	79.2%
	Boredom	1	8	1	1	0	1	7	42.1%
	Disgust	0	1	6	0	1	0	3	54.5%
	Fear	1	3	2	7	2	0	1	43.8%
	Happiness	3	0	3	2	5	0	2	33.3%
	Sadness	0	0	0	0	0	14	0	100.0%
	Neutral	0	5	1	0	0	0	13	68.4%
	HMM Recog. Rate	79.2%	47.1%	40.0%	70.0%	45.5%	93.3%	50.0%	



True/False Positives/Negatives

- Binary classifiers are frequent in practice! We can think of them as detectors (information retrieval, spam filtering, medical expert systems, face detection, fraud detection, ...)
- Often, binary classification problems are highly imbalanced, with very few positive samples vs. many negative ones.
- For binary classifiers, the terms in the confusion matrix have specific names.

$$C = \begin{pmatrix} TP & FN \\ FP & TN \end{pmatrix}$$

- TP = true positives
- TN = true negatives
- ► FP = false positives
- ► FN = false negatives

True/False Positive/Negative Rate

Common Quality Measures

- error rate := $\frac{FP+FN}{FP+FN+TP+TN}$
- false positive rate (FPR) := $\frac{FP}{FP+TN}$
- false negative rate (FNR) := $\frac{FN}{TP+FN}$
- true positive rate (TPR) := $\frac{TP}{TP+FN} \left(= 1 FNR$, aka sensitivity

▶ true neg. rate
$$(\mathsf{TNR}) := \frac{\mathsf{TN}}{\mathsf{FP}+\mathsf{TN}} \Big(= 1 - \mathsf{FPR},$$
 aka specificity $\Big)$

Quality Measures from Information Retrieval

• recall :=
$$\frac{TP}{TP+FN}$$
 (= sensitivity)

• precision := $\frac{TP}{TP+FP}$



TPs+FPs+FNs+TNs: Do-it-Yourself









- false positive rate =
- ▶ false negative rate =
- ▶ recall =
- precision =
- error rate =

The F-Measure



Which of the two classifiers is better?

- We introduce the **F-measure** as a global quality indicator.
- Given recall *r* and precision *p*, we define:

$$F(r,p) := 2 \cdot \frac{p \cdot r}{p+r}$$

► The F-measure is the harmonic mean of precision and recall.

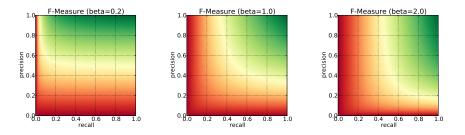
The F-Measure



We can extend the F-measure with a parameter β to emphasize precision or recall:

$$F_{\beta}(r,p) := \left(1+\beta^2\right) \cdot rac{p \cdot r}{\beta^2 \cdot p + r}$$

The higher β, the more important is recall (β = 1 → recall and precision are equally important)



Score-based Benchmarking

 Often, classifiers compute an internal score for each sample, s(x), and threshold these scores to obtain their final decision:

$$\phi({f x})=1 \quad \Leftrightarrow \quad s({f x})\geq T$$

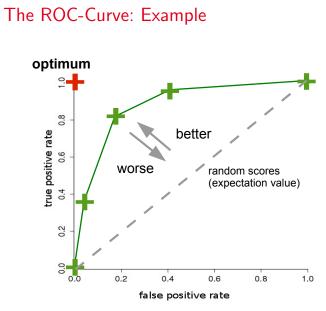
- ► The **lower** the threshold *T*, the **more positives** the classifier generates.
- ▶ How do we benchmark the classifier **independent** of *T*?
- Goal: Measure how well the scores discriminate positive samples from negative ones.

Approach

- ► We vary the threshold *T* and measure the FPR and FNR for each value of *T*.
- We obtain a curve, the Receiver-Operator-Characteristic (ROC) curve.

Т	FPR	TPR
1.0	0.00	0.00
0.9	0.05	0.38
0.1	0.41	0.96
0.0	1.00	1.00





T FPR TPR 1.0 0.00 0.00 0.9 0.05 0.38 0.1 0.41 0.96 0.0 1.00 1.00

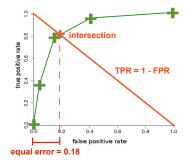
The ROC-Curve: Equal Error

We observe: When lowering the threshold T, the ...

- ▶ ... false-positive-rate (FPR) increases from 0 to 1
- ► ... false-negative-rate (FNR) decreases from 1 to 0. We derive a single quality measure from the ROC curve: The **Equal Error Rate (EER)**.
 - For some value T* holds:

 $FNR \approx FPR.$

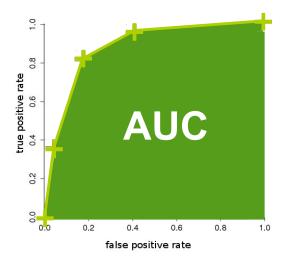
- This error rate is the EER.
- Graphically, we obtain the EER by intersecting the ROC curve with TPR = 1 - FPR.





The ROC-Curve: AUC

We derive another quality measure from the ROC curve: The **Area Under Curve (AUC)**



RPC Curves

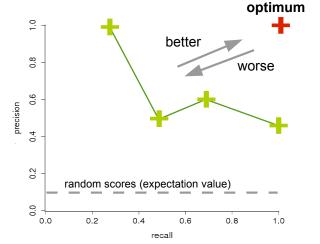
- ⊁
- For retrieval/recommender systems, we often derive a curve similar to the ROC curve, but based on precision and recall.
- Varying the threshold T corresponds to traversing the ranked result list from top to bottom.
- Whenever we encounter a **new positive**, we add a new point with coordinates (*recall*, *precision*) to the curve.

Example

recall	precision
0.25	1.00
0.50	0.50
0.75	0.60
1.00	0.44

RPC Curves

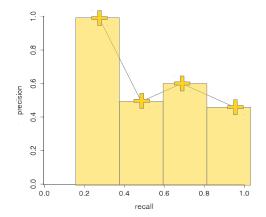
The resulting graph is called the **Recall-Precision-Curve (RPC)**.



recall	precision
0.25	1.00
0.50	0.50
0.75	0.60
1.00	0.44

RPC Curves \rightarrow Average Precision

We derive another indicator from the RPC curve: The **Average Precision**.



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