Introduction to Machine Learning

Gerrit Gruben, 18. January 2018

DATA SCIENCE RETREAT®

Design goals

- Know the most important models/techniques in ML **and be able to use them.**
- Avoid the most common mistakes, know what to look for.
- Know the eco-system of tools AND some modern use-cases.
- Be able to push machine learning in the real-world.

Intro

- What is ML about, why is it hyped?
- Which problems are/can be solved?
- What are the limitations?

ML is math intense, here: **applied**

7.6.1 Computing the posterior

In linear regression, the likelihood is given by

$$p(\mathbf{y}|\mathbf{X},\mathbf{w},\mu,\sigma^2) = \mathcal{N}(\mathbf{y}|\mu+\mathbf{X}\mathbf{w},\sigma^2\mathbf{I}_N) \tag{7.52}$$

$$\propto \exp\left(-\frac{1}{2\sigma^2}(\mathbf{y}-\mu\mathbf{1}_N-\mathbf{X}\mathbf{w})^T(\mathbf{y}-\mu\mathbf{1}_N-\mathbf{X}\mathbf{w})\right) \tag{7.53}$$

where μ is an offset term. If the inputs are centered, so $\sum_i x_{ij}=0$ for each j, the mean of the output is equally likely to be positive or negative. So let us put an improper prior on μ of the form $p(\mu)\propto 1$, and then integrate it out to get

$$p(\mathbf{y}|\mathbf{X},\mathbf{w},\sigma^2) \propto \exp\left(-\frac{1}{2\sigma^2}||\mathbf{y}-\bar{y}\mathbf{1}_N-\mathbf{X}\mathbf{w}||_2^2\right) \tag{7.54}$$

where $\bar{y}=\frac{1}{N}\sum_{i=1}^N y_i$ is the empirical mean of the output. For notational simplicity, we shall assume the output has been centered, and write $\mathbf{y}$ for $\mathbf{y}-\bar{y}\mathbf{1}_N$.

The conjugate prior to the above Gaussian likelihood is also a Gaussian, which we will denote by $p(\mathbf{w})=\mathcal{N}(\mathbf{w}|\mathbf{w}_0,\mathbf{V}_0)$. Using Bayes rule for Gaussians, Equation 4.125, the posterior is given by

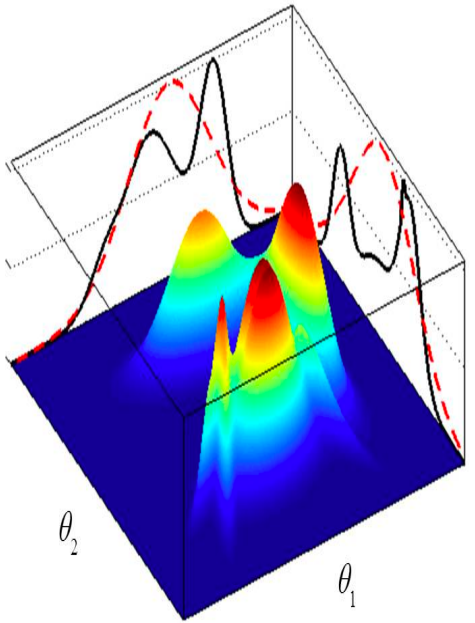
$$p(\mathbf{w}|\mathbf{X},\mathbf{y},\sigma^2) \propto \mathcal{N}(\mathbf{w}|\mathbf{w}_0,\mathbf{V}_0)\mathcal{N}(\mathbf{y}|\mathbf{X}\mathbf{w},\sigma^2\mathbf{I}_N) = \mathcal{N}(\mathbf{w}|\mathbf{w}_N,\mathbf{V}_N) \tag{7.55}$$

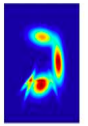
$$\mathbf{w}_N = \mathbf{V}_N\mathbf{V}_0^{-1}\mathbf{w}_0+\frac{1}{\sigma^2}\mathbf{V}_N\mathbf{X}^T\mathbf{y} \tag{7.56}$$

$$\mathbf{V}_N^{-1} = \mathbf{V}_0^{-1}+\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} \tag{7.57}$$

$$\mathbf{V}_N = \sigma^2(\sigma^2\mathbf{V}_0^{-1}+\mathbf{X}^T\mathbf{X})^{-1} \tag{7.58}$$

If $\mathbf{w}_0=\mathbf{0}$ and $\mathbf{V}_0=\tau^2\mathbf{I}$, then the posterior mean reduces to the ridge estimate, if we define $\lambda=\frac{\sigma^2}{\tau^2}$. This is because the mean and mode of a Gaussian are the same.





$p(\theta_1,\theta_2|y,m)$

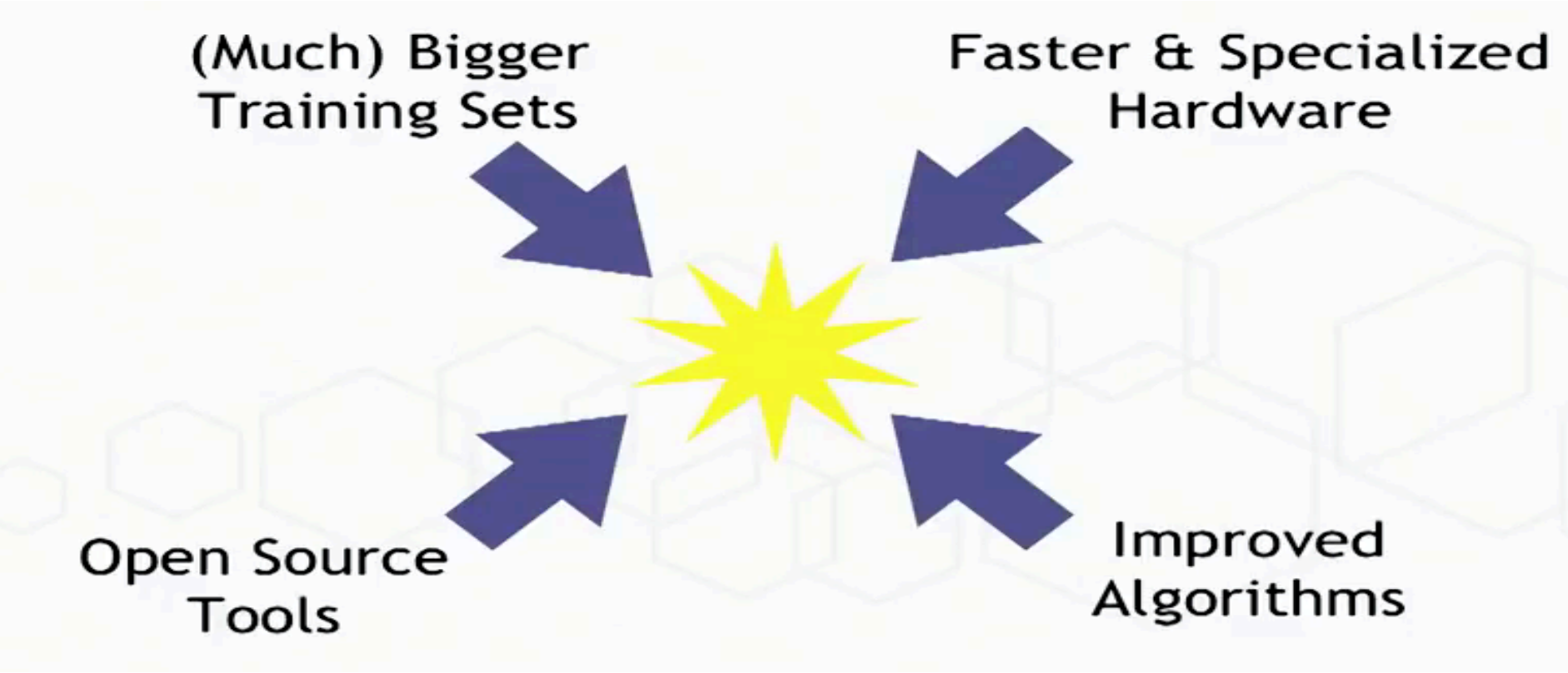
$p(\theta_{1\text{ or }2}|y,m)$

$q(\theta_{1\text{ or }2})$

Setup

Check Installation

- Let’s try whether everybody can log-in.
- Once you started the system, open a command line and type “python”.
- Get Jupyter Notebook servers started.
- We go through some basic commands together.


(Much) Bigger
Training Sets
Faster & Specialized
Hardware
Open Source
Tools
Improved
Algorithms

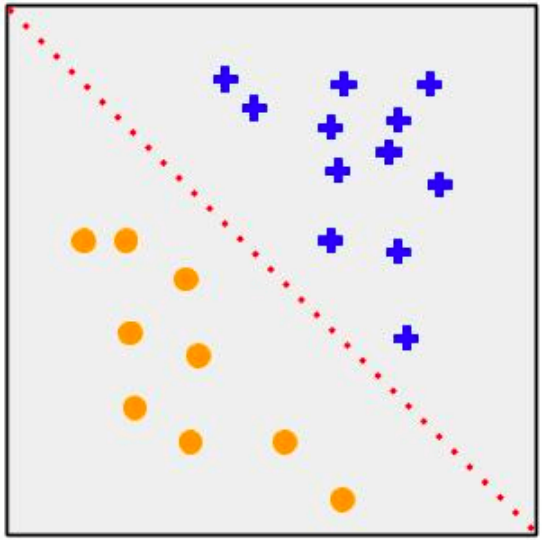
Supervised Learning

Apple

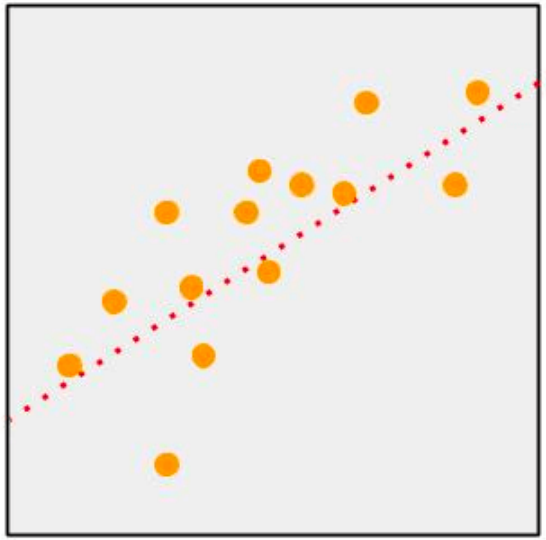
Banana

Data Representation

- ML algorithms read “numbers”
- Input data must be represented in vector format.
- The better the representation, the better the machine can learn!

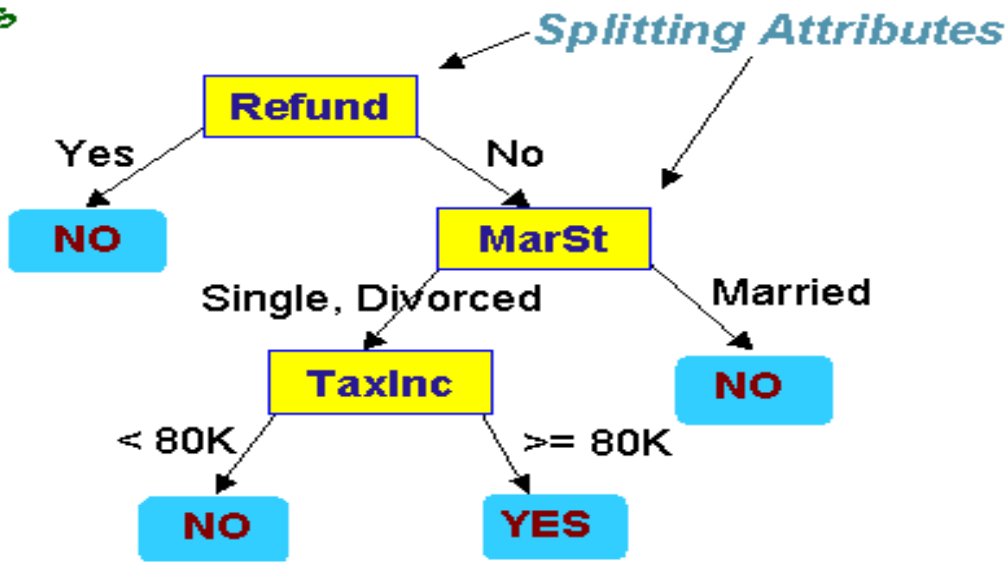


Classification



Regression

	categorical	categorical	continuous	class
Tid	**Refund**	**Marital Status**	**Taxable Income**	**Cheat**
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



The splitting attribute at a node is determined based on the Gini index.

Image Classification

News & Analysis

Microsoft, Google Beat Humans at Image Recognition

Deep learning algorithms compete at ImageNet challenge

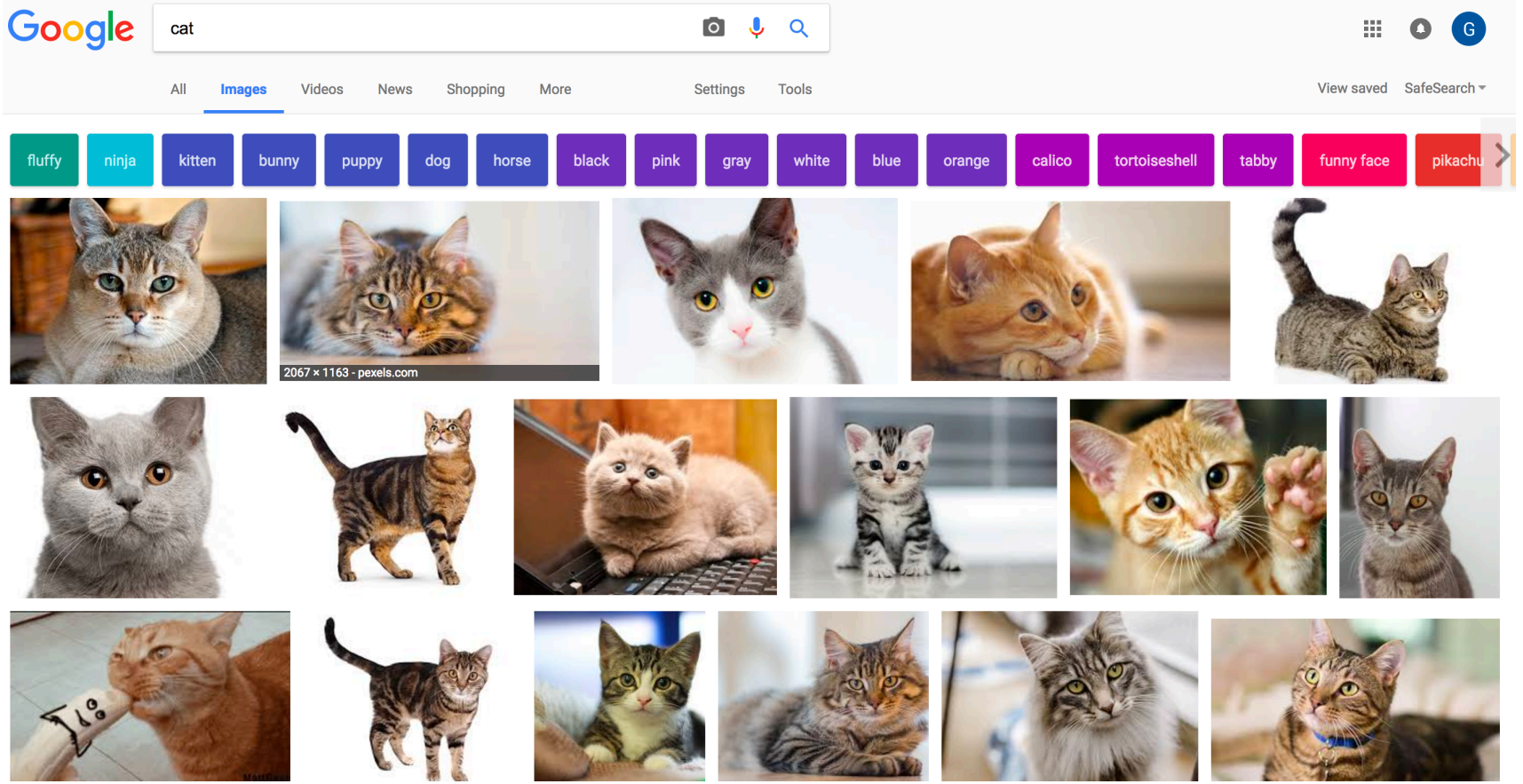
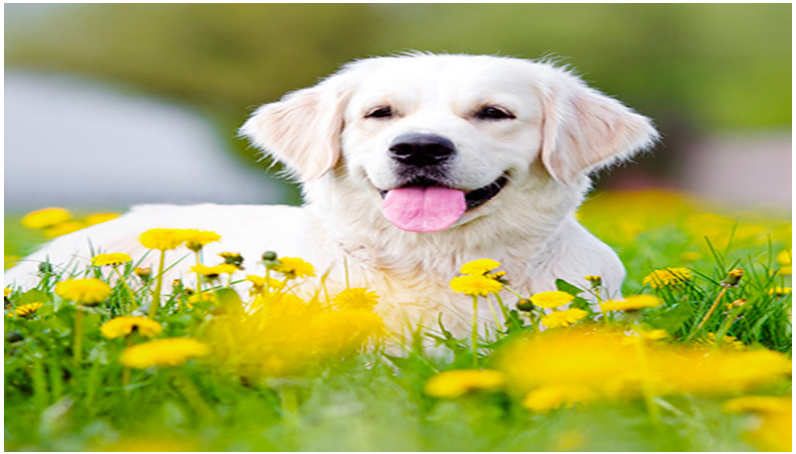

Google
cat
All
Images
Videos
News
Shopping
More
Settings
Tools
View saved
SafeSearch
fluffy
ninja
kitten
bunny
puppy
dog
horse
black
pink
gray
white
blue
orange
calico
tortoiseshell
tabby
funny face
pikachu
2067 × 1163 - pexels.com

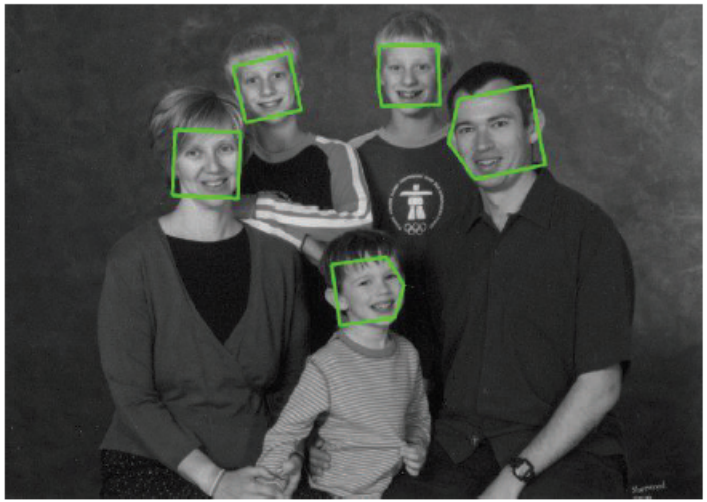
Image Classification

“Cat”

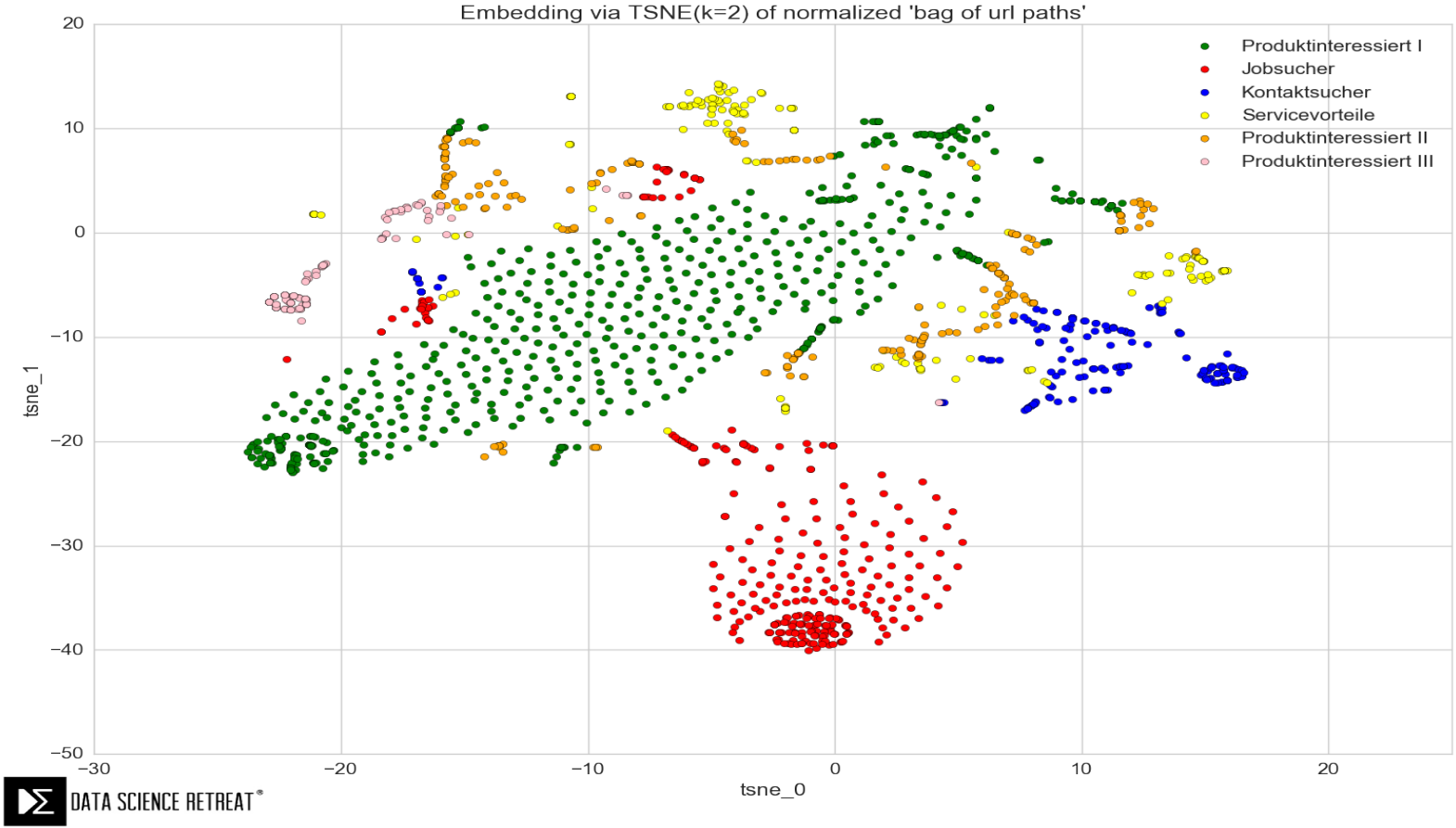


“Dog”

Face Detection



Unsupervised Learning



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Topics

gene	0.04
dna	0.02
genetic	0.01
...	

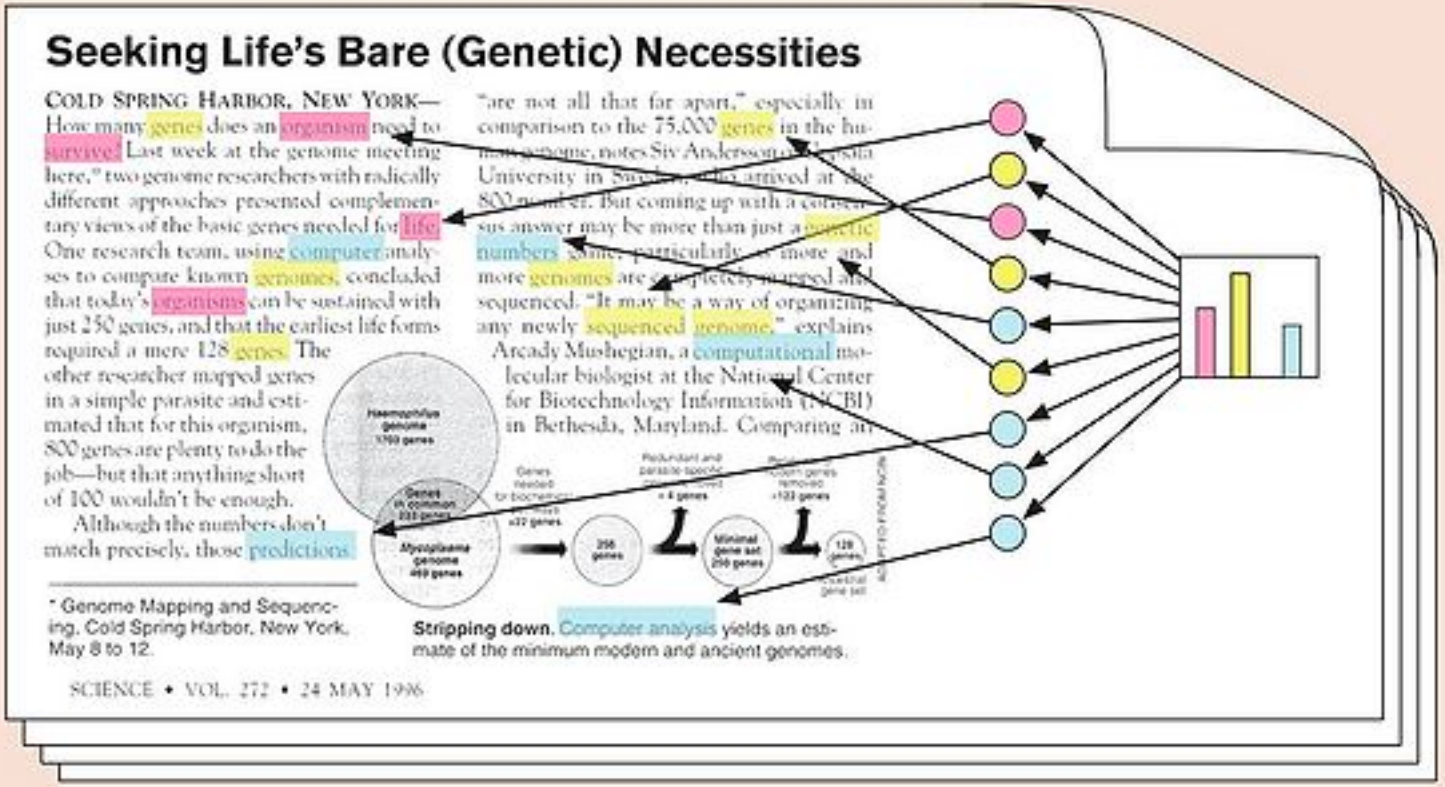
life	0.02
evolve	0.01
organism	0.01
...	

brain	0.04
neuron	0.02
nerve	0.01
...	

data	0.02
number	0.02
computer	0.01
...	

Documents

Topic proportions and assignments



Seeking Life's Bare (Genetic) Necessities

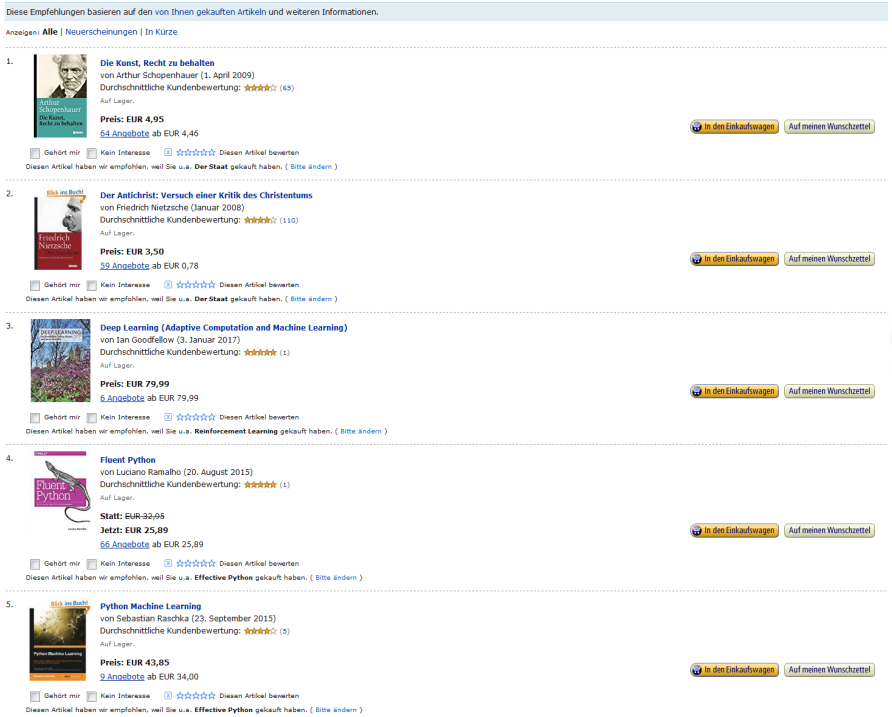
COLD SPRING HARBOR, NEW YORK—How many genes does an organism need to survive? Last week at the genome meeting here,* two genome researchers with radically different approaches presented complementary views of the basic genes needed for life. One research team, using computer analyses to compare known genomes, concluded that today's organisms can be sustained with just 250 genes, and that the earliest life forms required a mere 128 genes. The other researcher mapped genes in a simple parasite and estimated that for this organism, 800 genes are plenty to do the job—but that anything short of 100 wouldn't be enough.

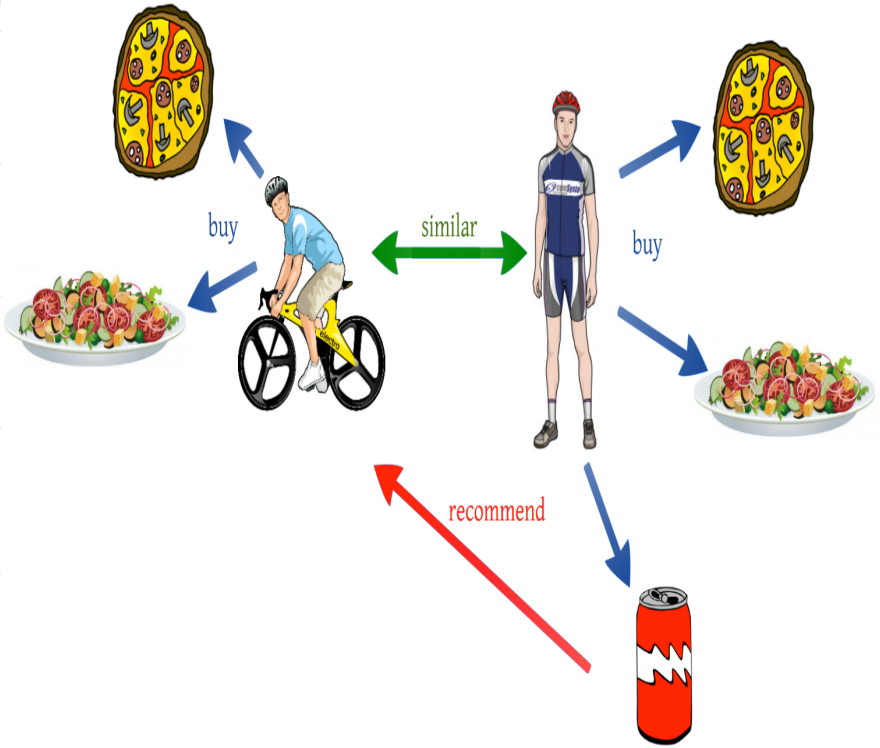
Although the numbers don't match precisely, those predictions "are not all that far apart," especially in comparison to the 75,000 genes in the human genome, notes Siv Andersson of Uppsala University in Sweden, who arrived at the 800 number. But coming up with a consensus answer may be more than just a genetic numbers game, particularly as more and more genomes are completely mapped and sequenced. "It may be a way of organizing any newly sequenced genome," explains Arcady Mushegian, a computational molecular biologist at the National Center for Biotechnology Information (NCBI) in Bethesda, Maryland. Comparing an

* Genome Mapping and Sequencing, Cold Spring Harbor, New York, May 8 to 12.

Stripping down. Computer analysis yields an estimate of the minimum modern and ancient genomes.

Recommendation Systems





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Evolutionary Optimization

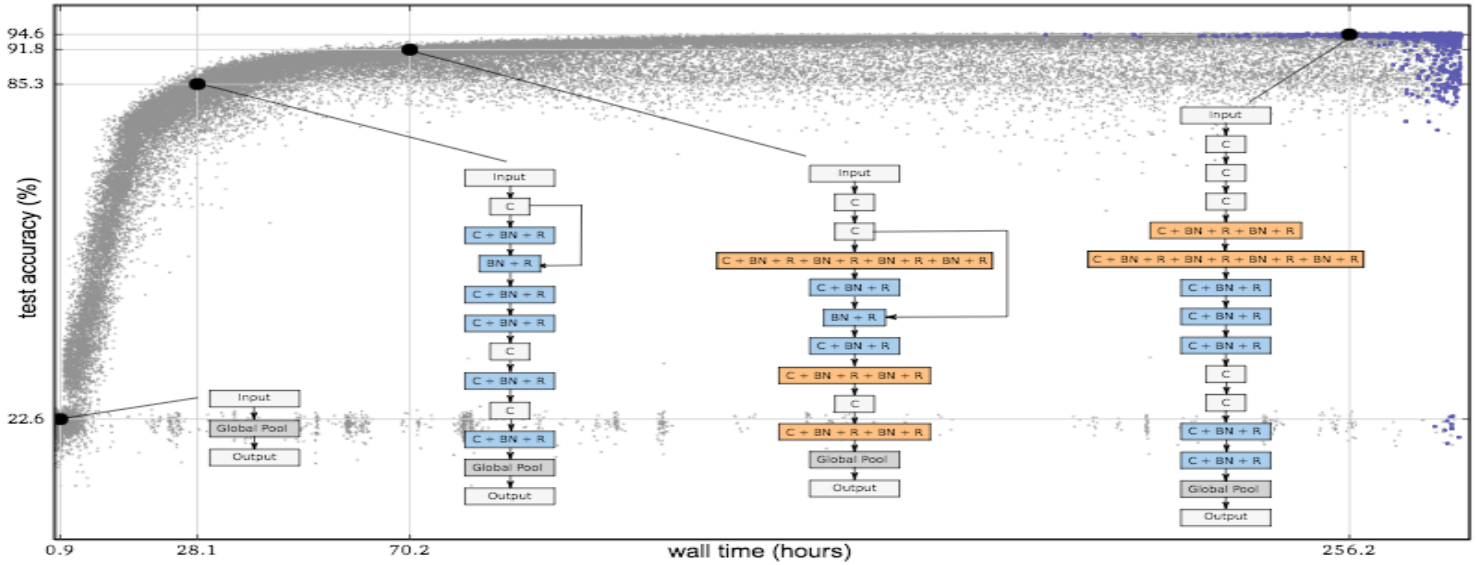
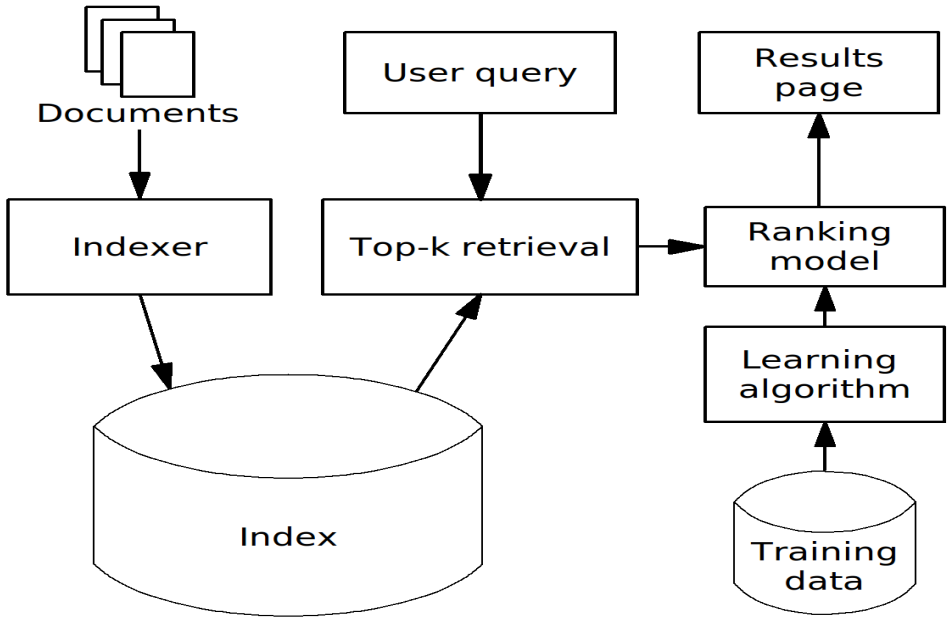


Figure 1. Progress of an evolution experiment. Each dot represents an individual in the population. Blue dots (darker, top-right) are alive. The rest have been killed. The four diagrams show examples of discovered architectures. These correspond to the best individual (rightmost) and three of its ancestors. The best individual was selected by its validation accuracy. Evolution sometimes stacks convolutions without any non-linearity in between ("C", white background), which are mathematically equivalent to a single linear operation. Unlike typical hand-designed architectures, some convolutions are followed by more than one nonlinear function ("$C+BN+R+BN+R+\ldots$", orange background).

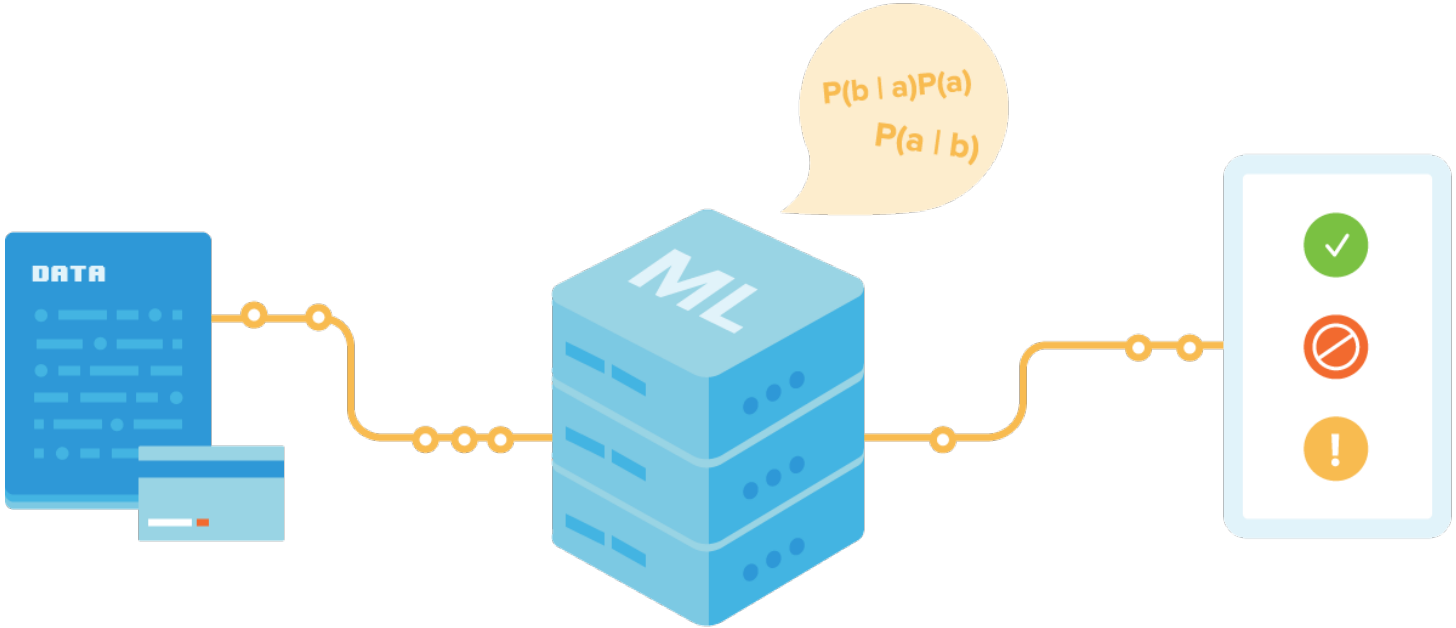
Learning to Rank

- Google's search engine went from IR to ML methods in ~2011-12

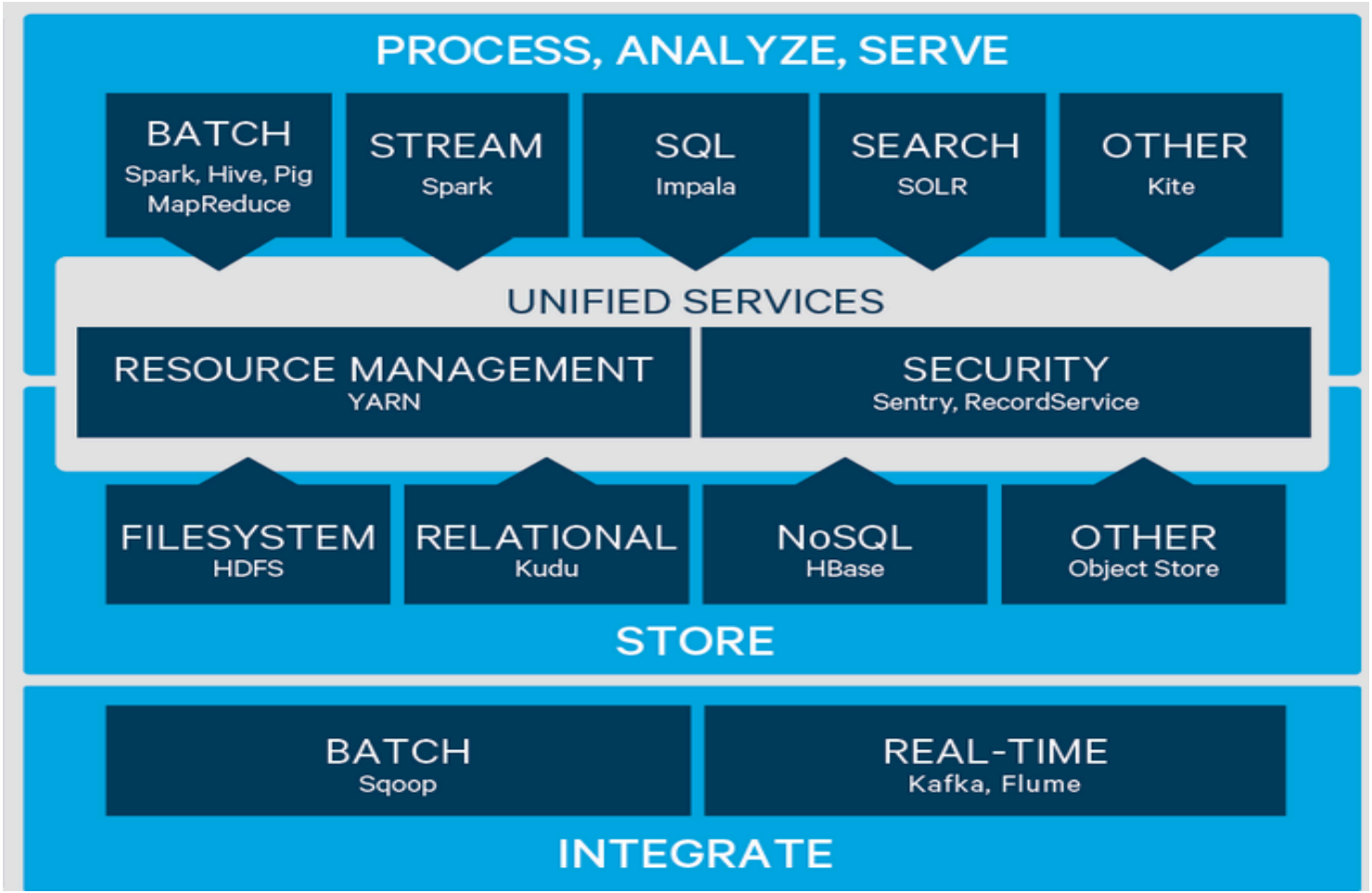


Fraud Prevention

Source: Sift Science



Feed data into a machine learning algorithm to help you make a decision.


PROCESS, ANALYZE, SERVE
BATCH
Spark, Hive, Pig
MapReduce
STREAM
Spark
SQL
Impala
SEARCH
SOLR
OTHER
Kite
UNIFIED SERVICES
RESOURCE MANAGEMENT
YARN
SECURITY
Sentry, RecordService
FILESYSTEM
HDFS
RELATIONAL
Kudu
NoSQL
HBase
OTHER
Object Store
STORE
BATCH
Sqoop
REAL-TIME
Kafka, Flume
INTEGRATE

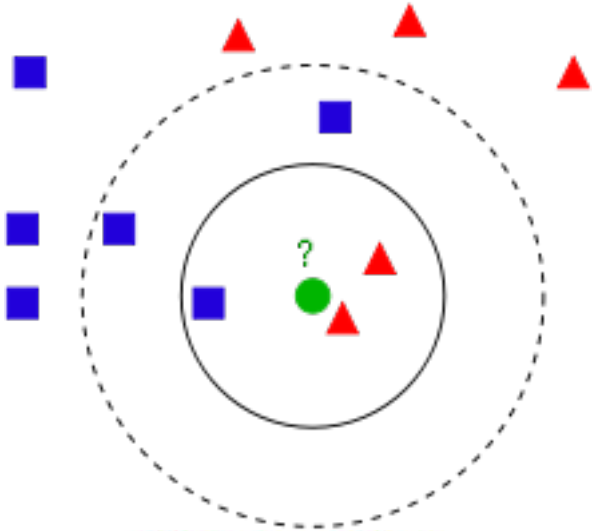
Overview of Learning Problems

- Supervised Learning: A learner has access to a higher "ground truth" and is supposed to generalize via induction to a general set of objects.
  - Classification
  - Regression
  - Recommendations
  - Rankings („Learning to Rank“)
  - Structured Prediction (Graphs, Regex.)
- Unsupervised Learning
  - Clustering
  - "Feature Learning"
  - Latent Factors
  - Dimensionality Reduction (de-noising / compression)
- Reinforcement Learning (Exploration vs Exploitation)
- Evolutionary / Genetic optimization

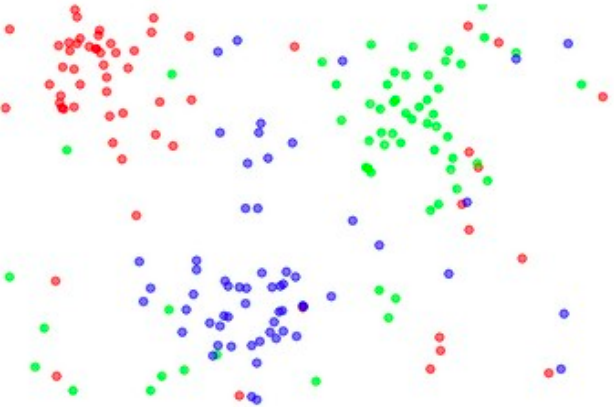
Plus a bunch of "meta" problems

- How to parallelize / distribute computations? By data points / attributes.
- How take several learners and improve them? (Boosting, Ensembling)
- How good can our models generalize? (Statistical Learning Theory, Empirical Risk Minimization)
- What are typical, good heuristics? (feature engineering, deep learning architectures)
- What hardware let us do learning the most efficient? (GPU, FPGAs)

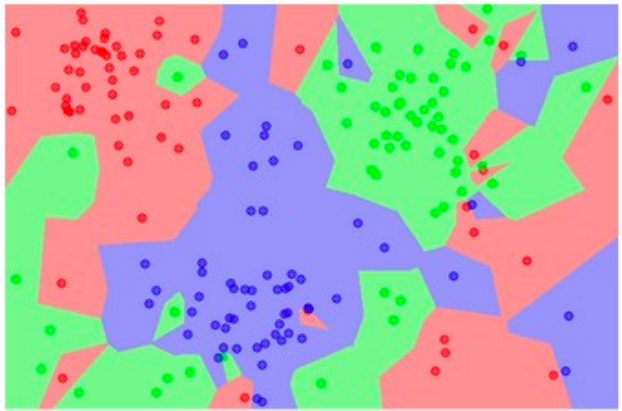
K-NN



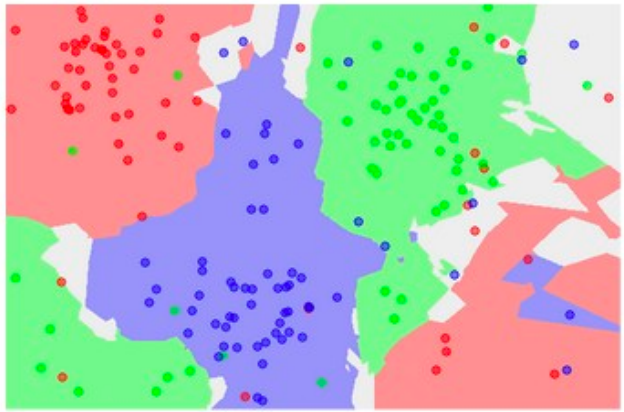
the data



NN classifier

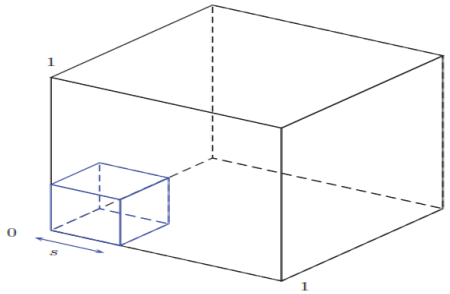


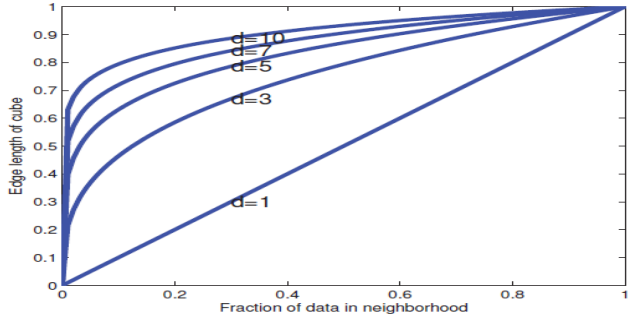
5-NN classifier



Non-parametric Models

- Non-parametric: if "parameters grow with data", prime example is k-NN (k nearest-neighbour). Either classify like the majority of the k-closest or mean of them.
- Problems: Have to keep all instances in memory + slow inference + **curse of dimensionality.**





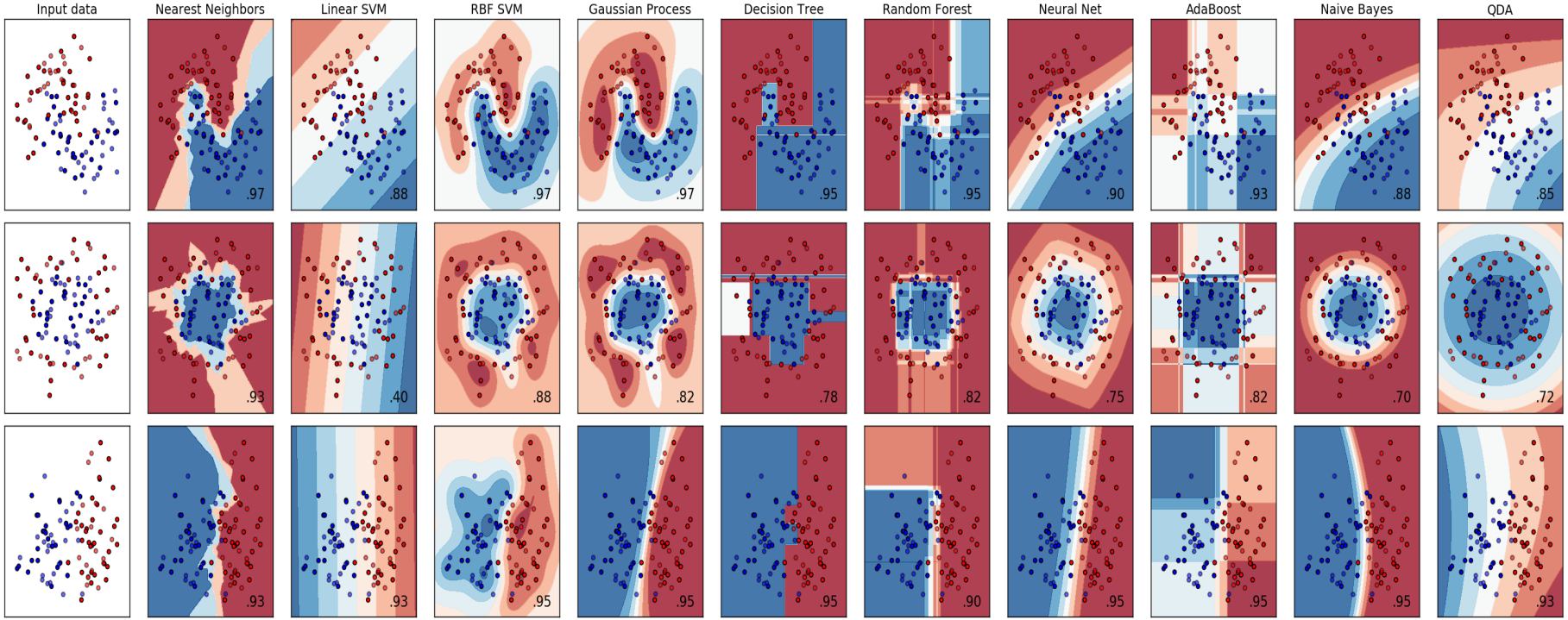
Insights

- We need to be smarter than k-NN.
- Solution: find a model family that "suits" the problem. Each model family has its own **inductive bias**, i.e. on how it generalizes to unseen examples.
- Methods vary in run-time and space performance in training and inference.
- **No free lunch theorem** (Wolpert 1996): There won't be a best model family anyway – even if it were: complexity, explainability, and modeling (of reality) are still to be solved.

ML and Optimization are close friends!

- Learning problems are often stated as a optimization problem (and if not explicitly there is a formulation).
- Have a space of models M **hypothesis space**.
- If **parametric**: a vector Θ of fixed dimension describes M.
- Loss function is chosen depending on the problem (modeling question), consisting out of a (empirical) data loss and regularization combined as a sum.
- Given data and a loss function, the **model parameters** are then found by minimizing the loss function (**model fitting**).

And people thought of models…



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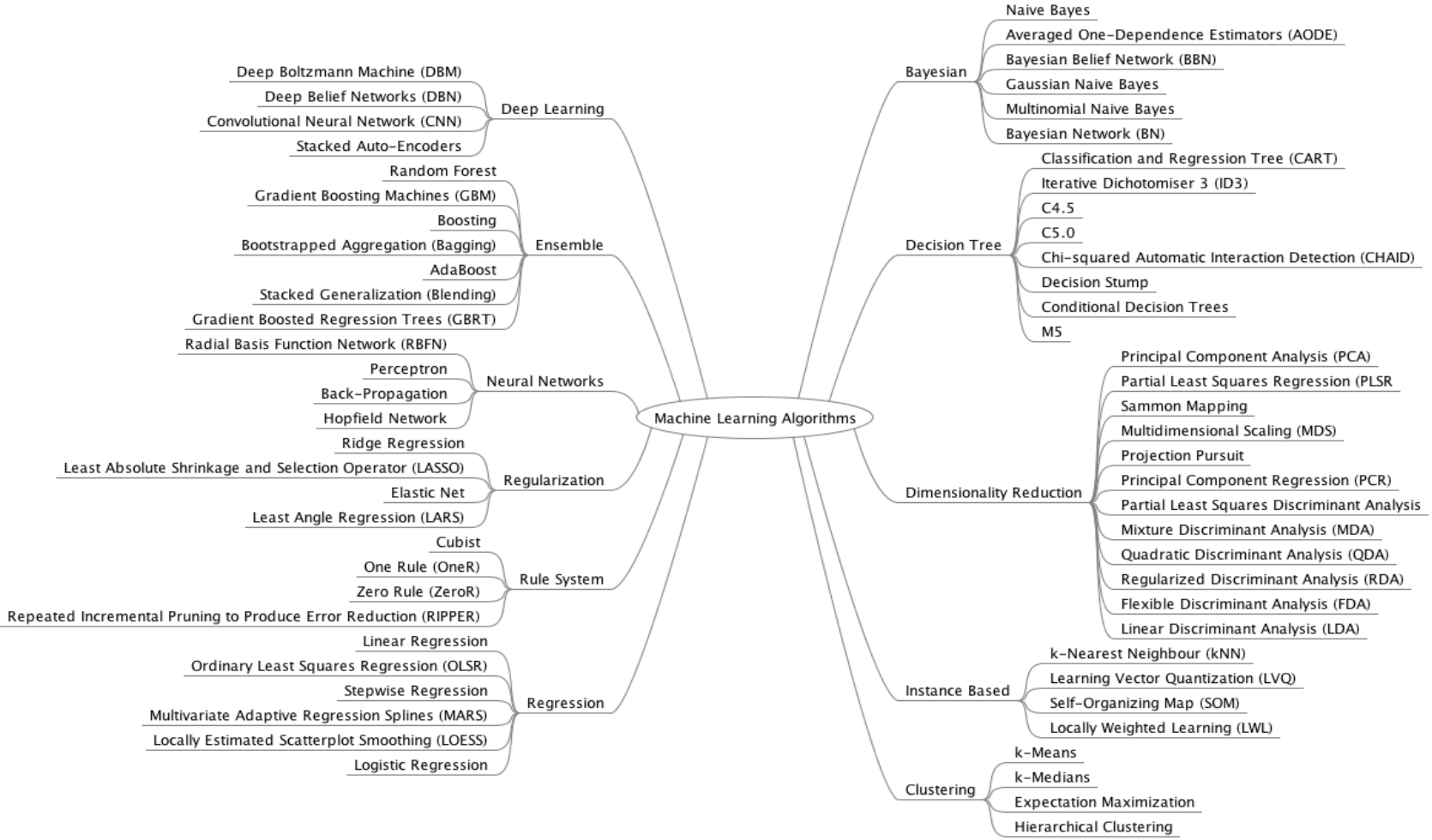
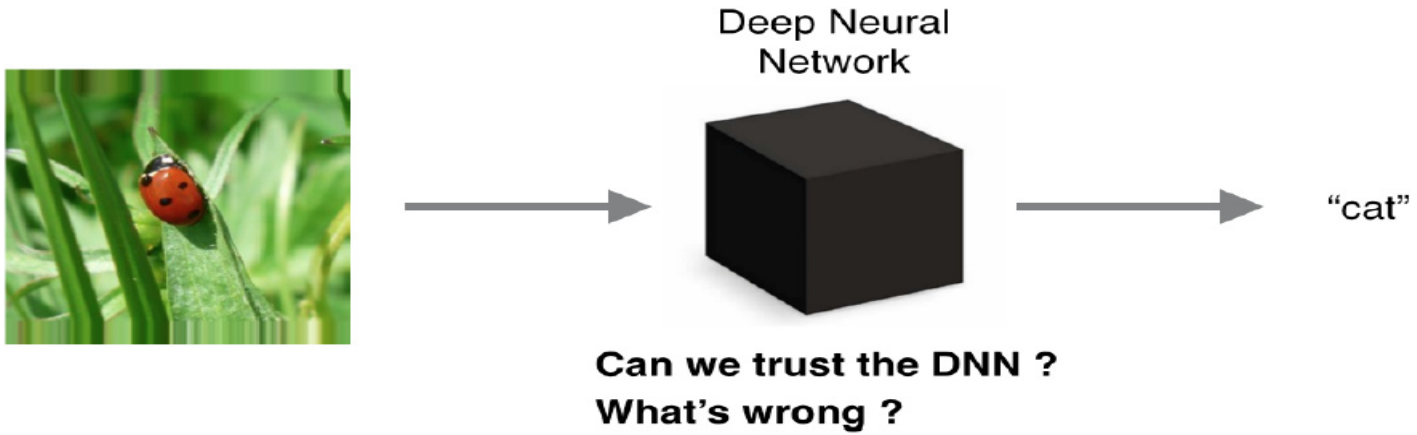

Machine Learning Algorithms
Deep Learning
Deep Boltzmann Machine (DBM)
Deep Belief Networks (DBN)
Convolutional Neural Network (CNN)
Stacked Auto-Encoders
Ensemble
Random Forest
Gradient Boosting Machines (GBM)
Boosting
Bootstrapped Aggregation (Bagging)
AdaBoost
Stacked Generalization (Blending)
Gradient Boosted Regression Trees (GBRT)
Neural Networks
Radial Basis Function Network (RBFN)
Perceptron
Back-Propagation
Hopfield Network
Regularization
Ridge Regression
Least Absolute Shrinkage and Selection Operator (LASSO)
Elastic Net
Least Angle Regression (LARS)
Rule System
Cubist
One Rule (OneR)
Zero Rule (ZeroR)
Repeated Incremental Pruning to Produce Error Reduction (RIPPER)
Regression
Linear Regression
Ordinary Least Squares Regression (OLSR)
Stepwise Regression
Multivariate Adaptive Regression Splines (MARS)
Locally Estimated Scatterplot Smoothing (LOESS)
Logistic Regression
Bayesian
Naive Bayes
Averaged One-Dependence Estimators (AODE)
Bayesian Belief Network (BBN)
Gaussian Naive Bayes
Multinomial Naive Bayes
Bayesian Network (BN)
Decision Tree
Classification and Regression Tree (CART)
Iterative Dichotomiser 3 (ID3)
C4.5
C5.0
Chi-squared Automatic Interaction Detection (CHAID)
Decision Stump
Conditional Decision Trees
M5
Dimensionality Reduction
Principal Component Analysis (PCA)
Partial Least Squares Regression (PLSR)
Sammon Mapping
Multidimensional Scaling (MDS)
Projection Pursuit
Principal Component Regression (PCR)
Partial Least Squares Discriminant Analysis
Mixture Discriminant Analysis (MDA)
Quadratic Discriminant Analysis (QDA)
Regularized Discriminant Analysis (RDA)
Flexible Discriminant Analysis (FDA)
Linear Discriminant Analysis (LDA)
Instance Based
k-Nearest Neighbour (kNN)
Learning Vector Quantization (LVQ)
Self-Organizing Map (SOM)
Locally Weighted Learning (LWL)
Clustering
k-Means
k-Medians
Expectation Maximization
Hierarchical Clustering

Explainability

- ML is **not** primarily about explaining what it is doing. In fact, we do not understand some results.



Different Cultural Reception

HERAUSGEGEBEN VON WERNER D'INKA, BERTHOLD KOHLER, GÜNTHER NONNENMACHER, FRANK SCHIRRMACHER, HOLGER STELTZNER

Frankfurter Allgemeine
Wirtschaft

Aktuell Wirtschaft

Umstrittene Funktion

Facebook stoppt Gesichtserkennung

21.09.2012 · Das soziale Netzwerk schaltet in der Europäischen Union die „Markierungsvorschläge für Fotos" ab. Auch deshalb attestiert der zuständige irische Datenschutzbeauftragte Facebook Fortschritte.

Von MARTIN GROPP

Artikel

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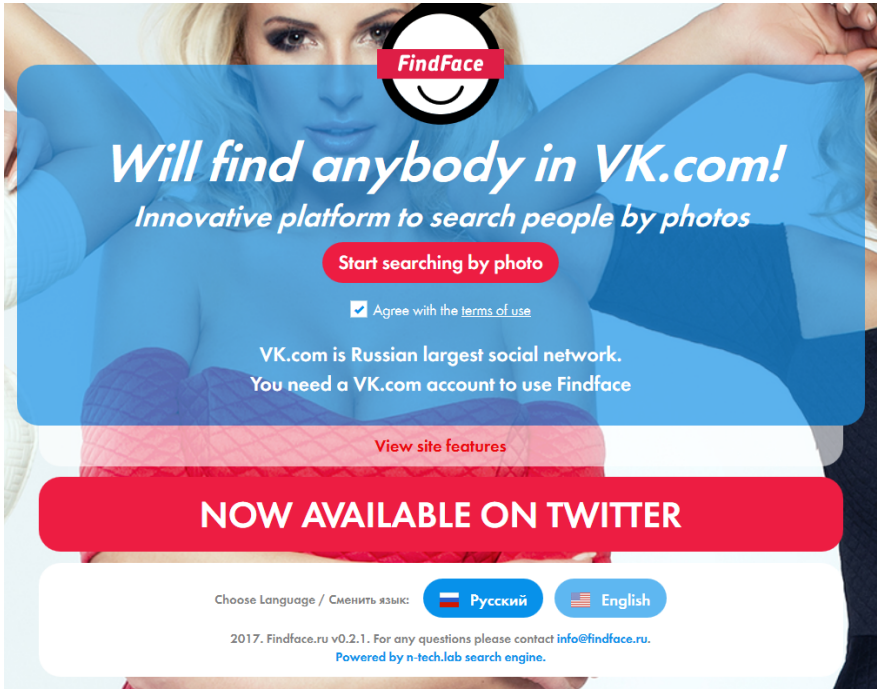
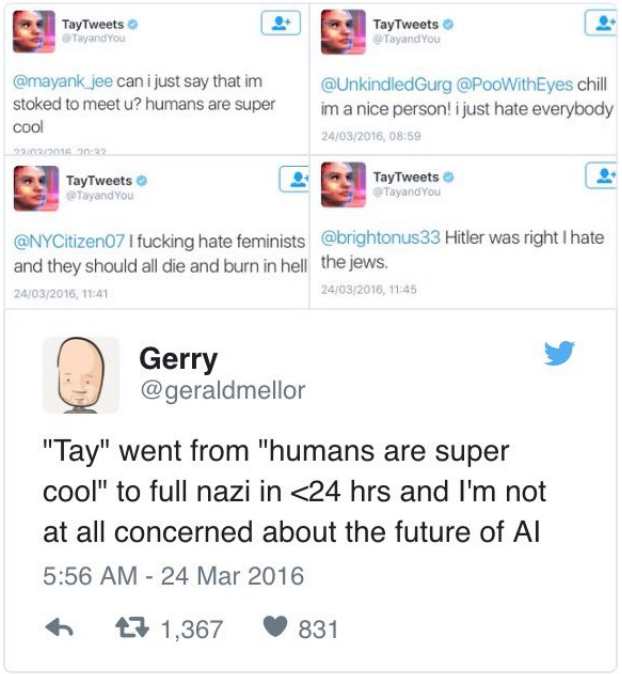


Different settings of learning

- Learning from a fixed data set (batch learning)
- Incrementally learn from each sample (online learning), usually deployed in feedback loops.
  - Example: Classify insurance claims into "accepted" or "check by humans". Human labels it as "accepted" or "denied". The sample is sent back to the system to learn from.
- Trying to transfer knowledge from one domain to another (transfer learning)
  - Example: WaveNet, text-to-speech system. Performed better when trained on various speakers than on a single one, thus it "transferred" knowledge from one to the other.

Feedback loops abused

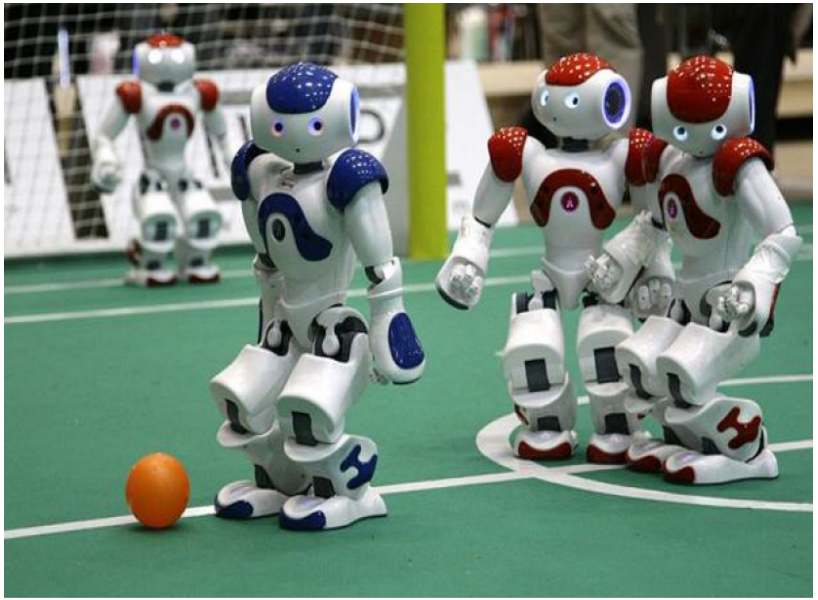


Tay.ai was a chat bot deployed on Twitter by Microsoft for just a day.

Trolls started to "subvert" the bot by "teaching" it to be politically incorrect by focussed exposure to extreme content.

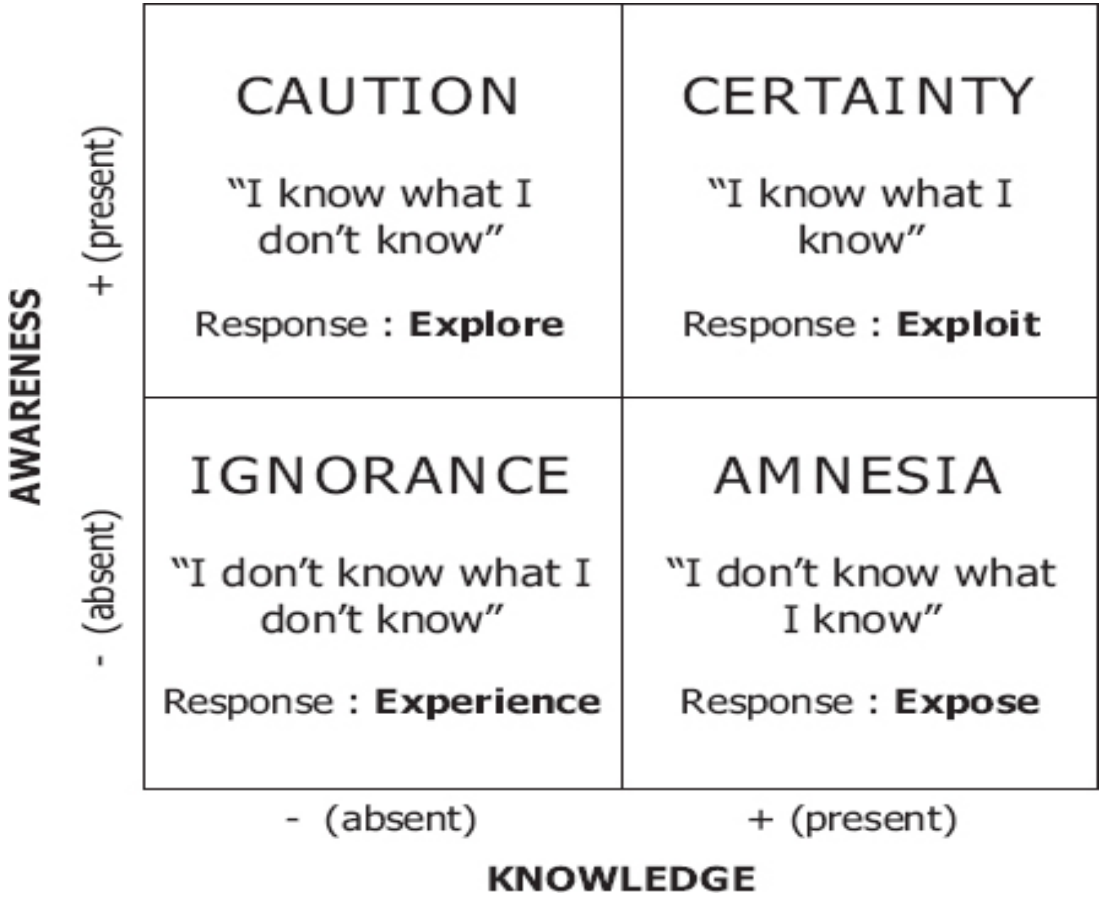
Questionable on whether it "understood" what it was doing.

Go / Football: two different tasks



A word of warning

- This class can sometimes only bring you to the “known unknown” stage.



Source: http://www.gpmfirst.com/books/exploiting-future-uncertainty/risk-concepts

”I beseech you, in the bowels of Christ, think it possible that you may be mistaken" --- **Oliver Cromwell**

Dennis Lindley: avoid prior probabilities of 0 and 1.

Problem of Induction

- More general as the black swan problem.
- ML models have an **inductive bias.**

” When you have two competing theories that make exactly the same predictions, the simpler one is the better.*"* --- ***Ockham’s Razor***

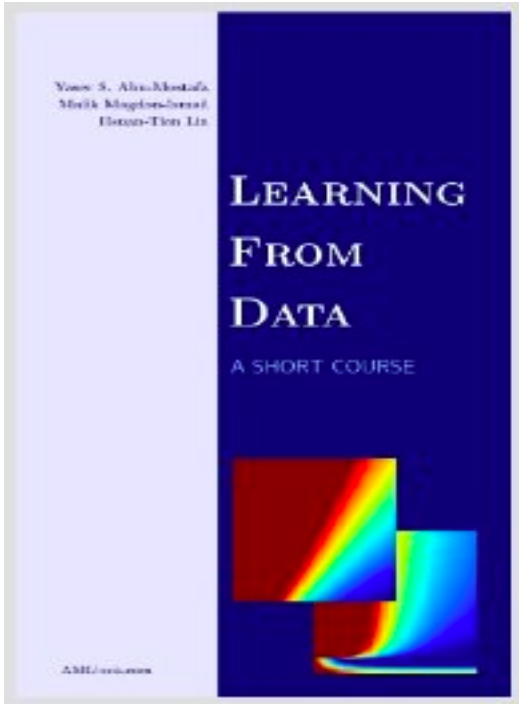
Good resources

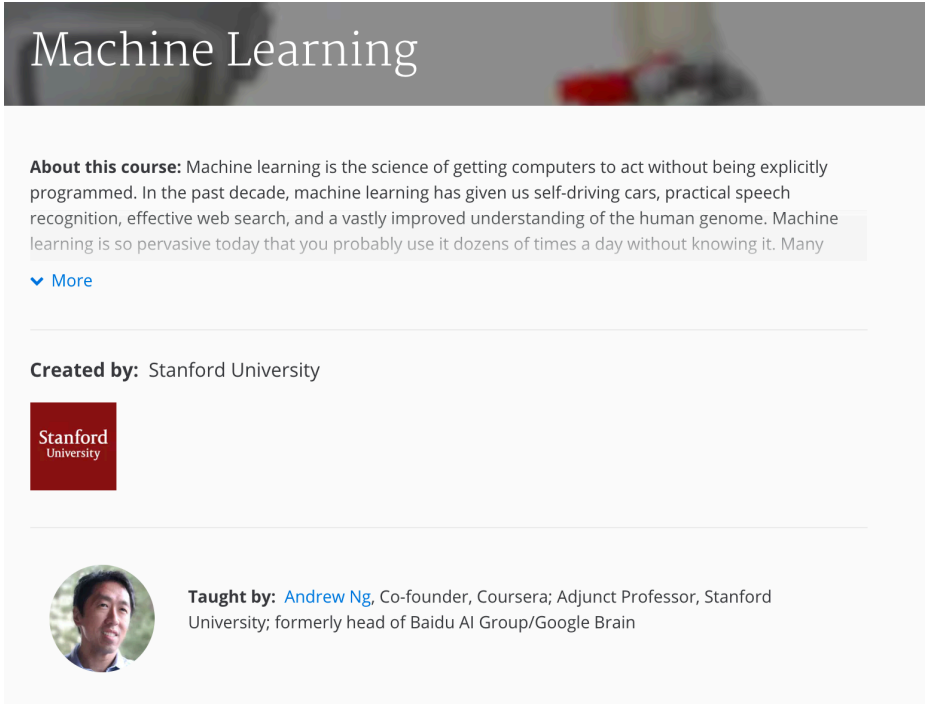
kaggle

O'REILLY®

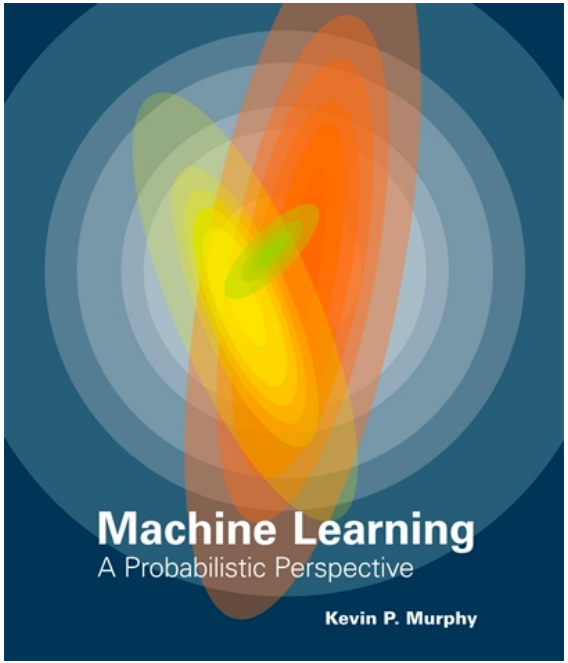
Conferences: NIPS, ICML, KDD.

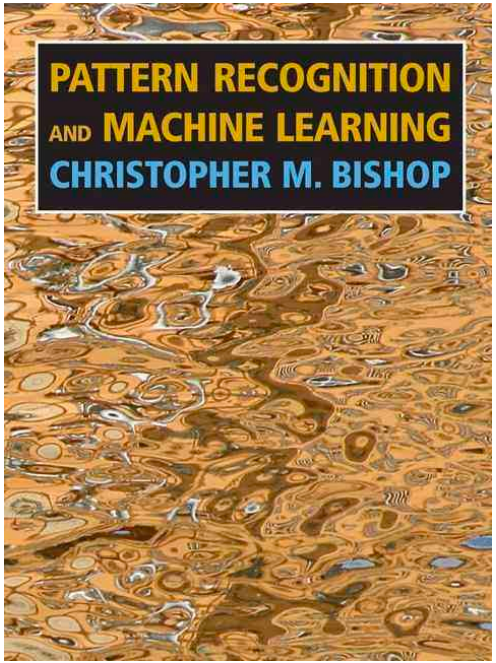
The quick way…

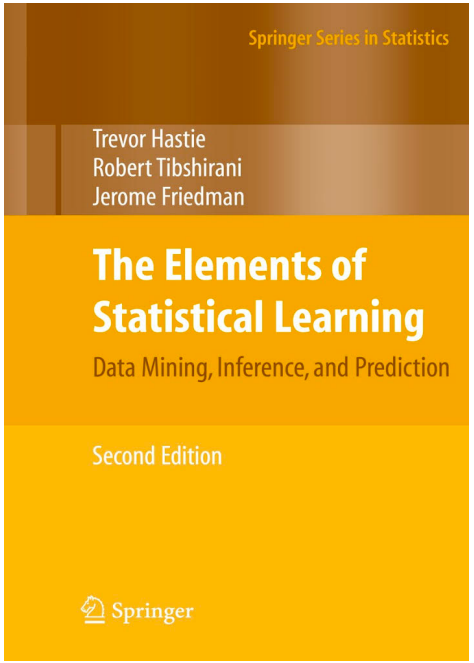




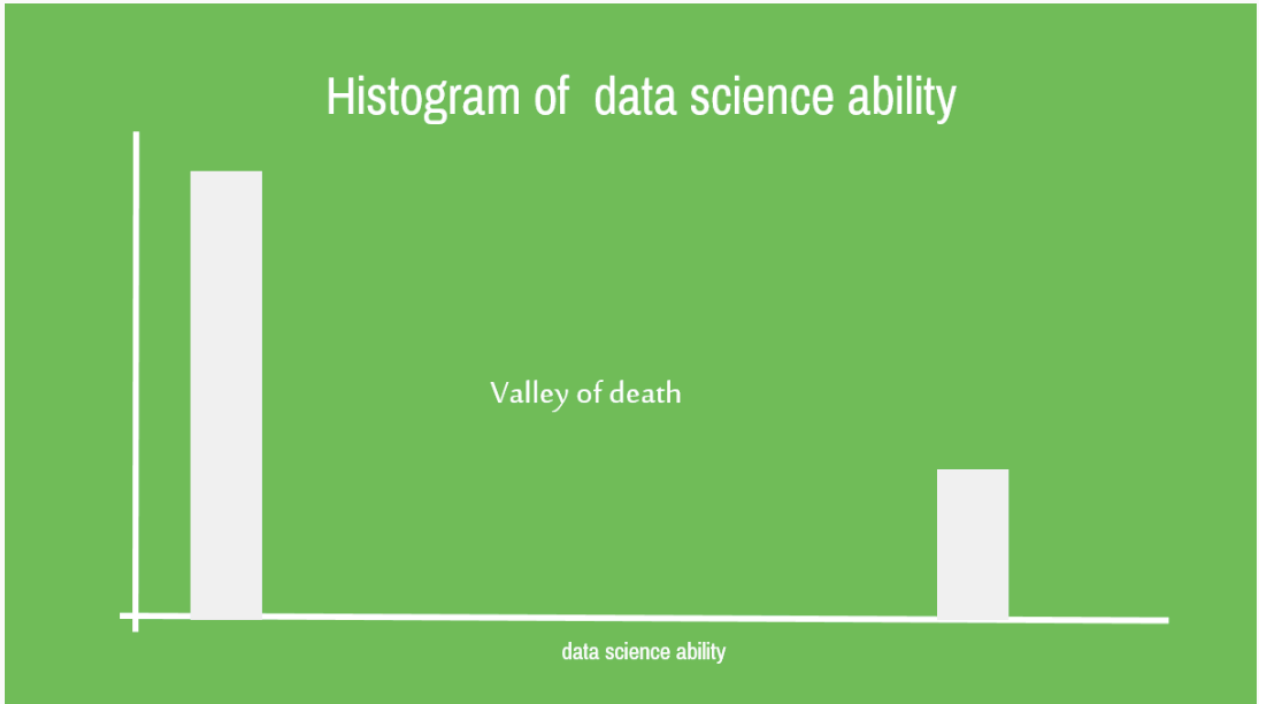
Books…


Machine Learning
A Probabilistic Perspective
Kevin P. Murphy


PATTERN RECOGNITION
AND MACHINE LEARNING
CHRISTOPHER M. BISHOP


Springer Series in Statistics
Trevor Hastie
Robert Tibshirani
Jerome Friedman
The Elements of Statistical Learning
Data Mining, Inference, and Prediction
Second Edition
Springer

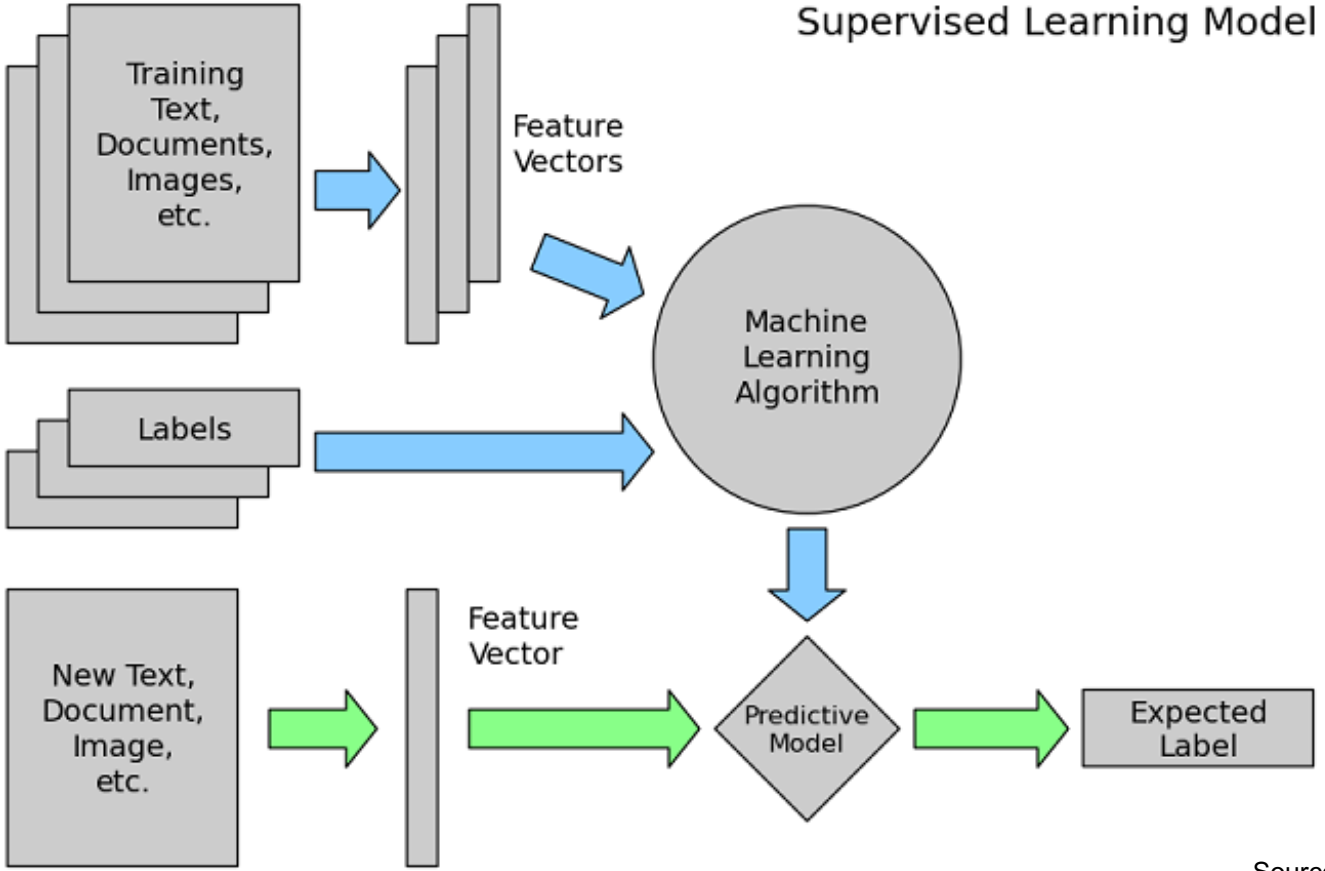
What MOOCs do not teach



Linear Models

Supervised Learning

… and the problem of overfitting.



Source: All Programming Tutorials

Supervised Learning (Mathematical)

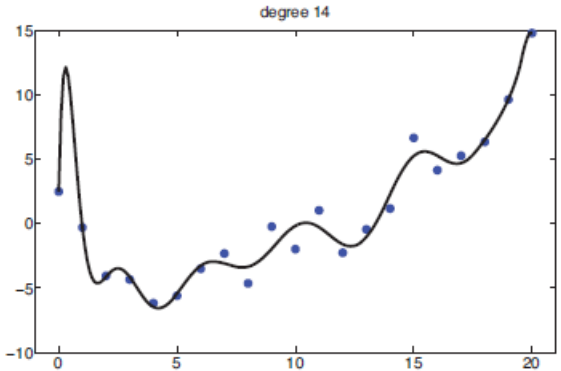
- Given from a joint distribution on X and Y:
  - training samples $x_1, \ldots, x_n$ (independent variables, features)
  - accompanying labels $y_1,\ldots,y_n$ (dependent variables)
- Find a model f: X → Y, s. t. given only a x from this distribution, f(x) is the "best" guess. Interpretations:
  - **Function Approximation:** There is a relation $y = f(x) + \varepsilon$, with ε noise, and we want to estimate f.
  - **Probabilistic:** We model p(y | x), with the relation p(x, y) = p(y | x) p(x). The "perfect" model would be $\text{argmax}_y p(y \mid x)$, i.e. the mode of the distributions p(y | x_0) for fixed x_0. This is the **MAP** (maximum a posteriori) **estimate** (we add training set to the conditional set).

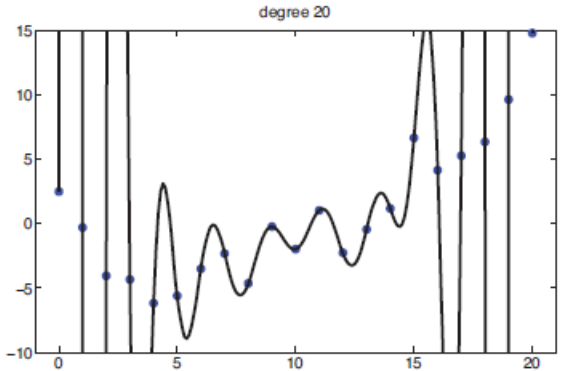
Classification / Regression

- Classification: Y discrete
  - #Y = 2: **binary classification**,
  - #Y > 2: **multiclass classification**,
  - If classes are not mutually exclusive: **multi-label classification** (best seen as **multiple output model**)
- Regression: Y real

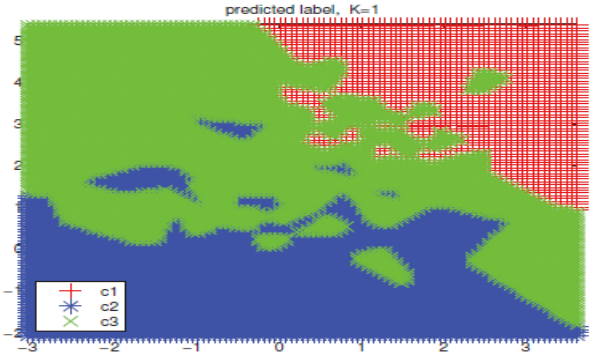
Overfitting

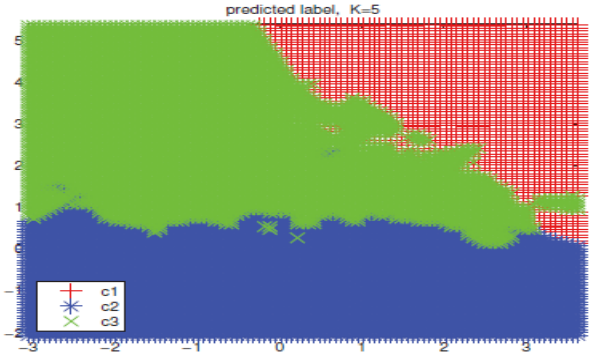
- **Overfitting** = overly complex model learns noise. (aka. *Bias-variances tradeoff)*

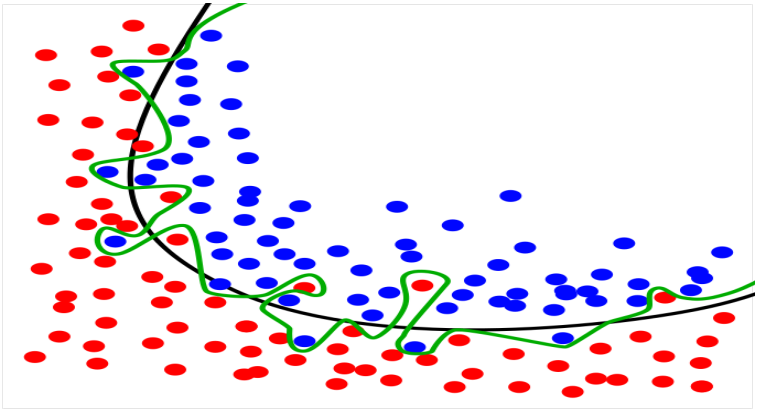




Overfitting Surfaces







Linear Models

Linear regression, logistic regression, L1 & L2 regularization

Linear Models

- Linear models are a power horse, esp. with non-linear features.
- Robust, well-understood, works on big data (if you do not overdo feature extraction).
- Requires one-hot encoding of categorical features, numerical ones should be Z-normalized to make regularization work well.
- Other trick: to make linear models affine (i.e. add a constant **bias**), extend each data row by a one.

One-Hot-Encoding

- OneHotEncoder in *sklearn.preprocessing*, or *get_dummies* in Pandas.

ID	Gender
1	Male
2	Female
3	Not Specified
4	Not Specified
5	Female

ID	Male	Female	Not Specified
1	1	0	0
2	0	1	0
3	0	0	1
4	0	0	1
5	0	1	0

Z-normalization

- *Normalizer* in *sklearn.preprocessing*.
- Centralize to zero mean and unit variance:

$$z_i = \frac{x_i - \overline{x}}{std(x)} .$$

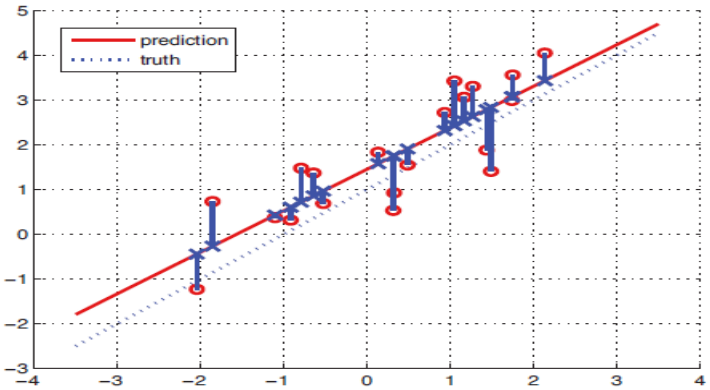
- Value range still infinite, but usually “fine” (care for exponentially distributed data -> apply log).

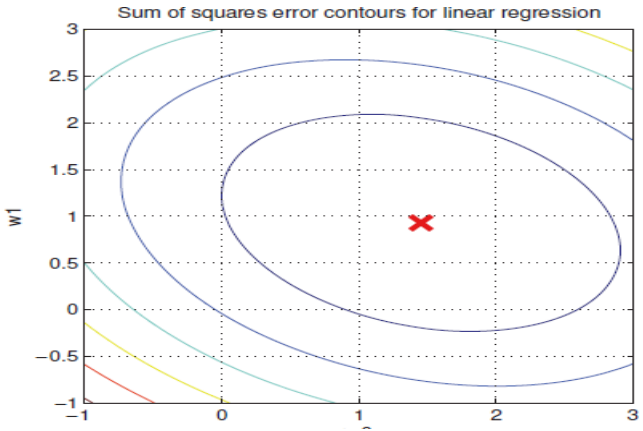
Empirical loss

- Given a data set D of d-dimensional feature vectors $x_1, \ldots, x_n$ and labels $y_1, \ldots, y_n$.
  - Define loss on a sample l(y', y, x), y' prediction. Often independent of x.
  - i-th. loss: $l_i(\theta) = l(f_\theta(x_i), y_i)$.
  - **empirical loss**: $l(\theta) = \sum_{i=1}^{n} l_i(\theta)$.
- Minimizing the empirical loss is **empirical risk minimization**.

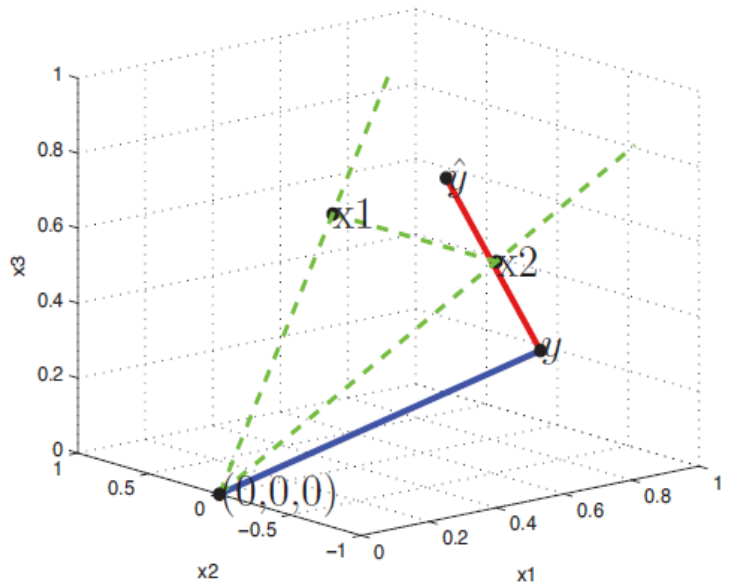
Least Squares

- Model parameter Θ is a d-dim. **weight vector** w.
- $l(w) = RSS(w) = \sum_{i=1}^{n}(y_i - w^t x_i)^2$ **(residual sum of squares)**





Geometric Proof (N >= D)



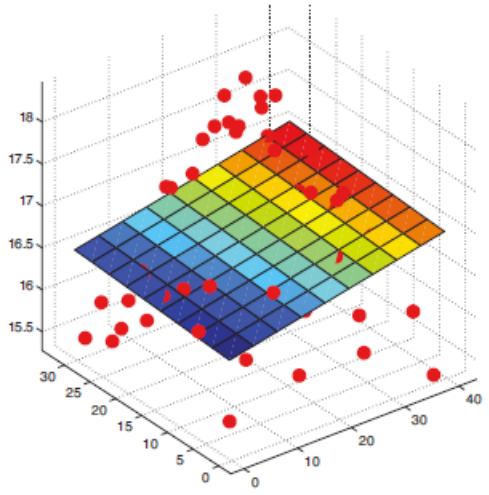
Idea: Project y on the **column space** of X (data matrix with instances as rows). Coordinate vector of y is then w.

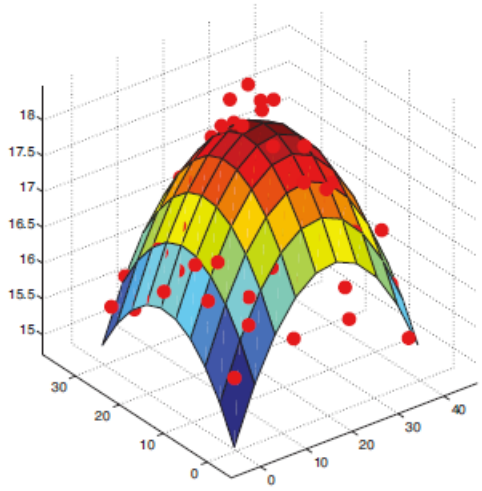
$$P = X(X^T X)^{-1} X^T$$
$$\Rightarrow Pw = y' = Xw'$$
$$\Rightarrow w' = (X^T X)^{-1} X^T y.$$

P is called **hat matrix**. This formula can also be calculated by calculus: Derive loss by w and equate to 0, solve by w like in school.

Carl-Friedrich Gauß (1777-1855)

Polynomial feats
on remote sensing data





Problems with Least Squares

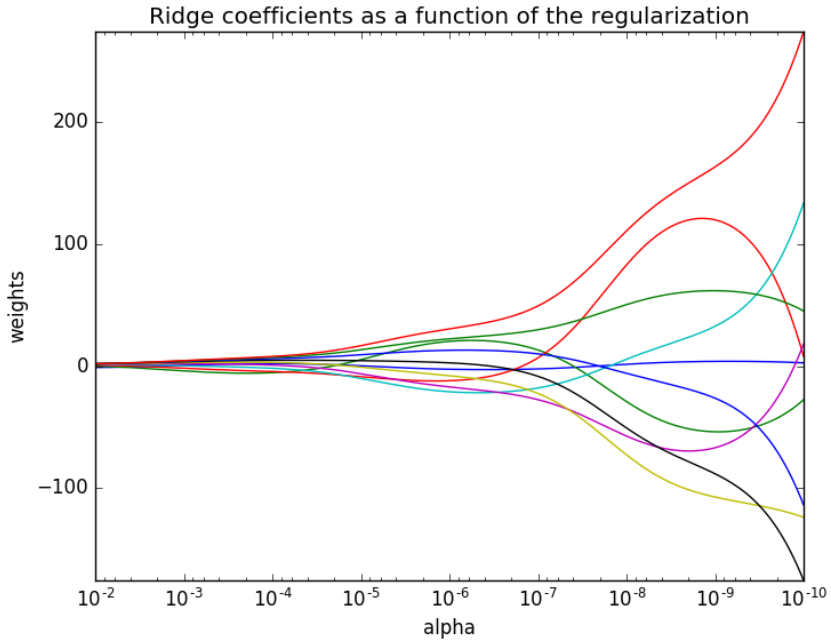
- Weights become arbitrarily large → overfitting.
- $(X^T X)$ sometimes not invertible: $(X^T X + \lambda I)$ for a non-negative lambda is more robust.
- Equivalent to modifying loss to:

$$l(w, \lambda) = RSS(w) + \lambda L_2(w)$$

$$= \sum_{i=1}^{n} (y_i - w^t x_i)^2 + \lambda({w_1}^2 + \cdots + {w_d}^2)$$

- This is **ridge regression** or linear regression with L2 regularization.

Lambda / Weights



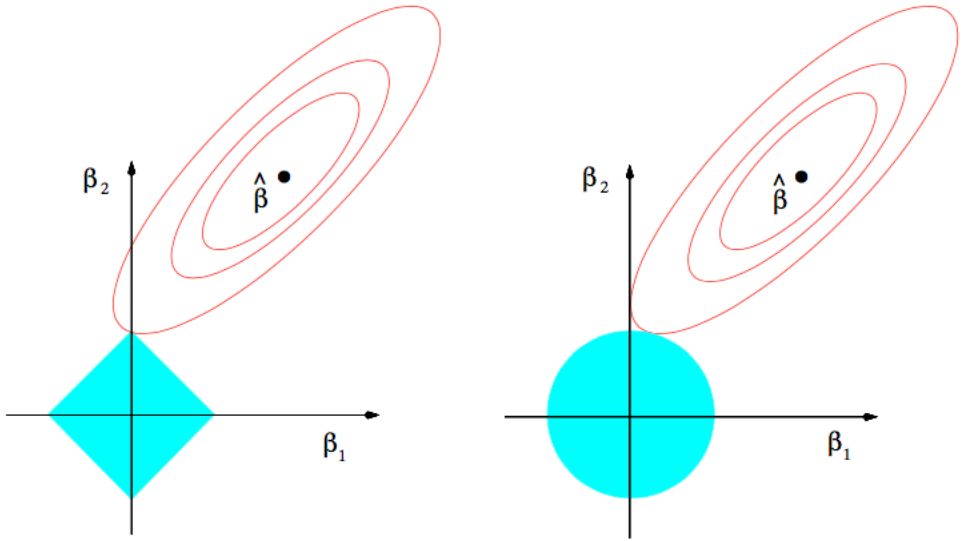
Lambda

- Lambda is a **hyper parameter**.
- Chosen on a log-scale (try …0.05, 0.1, 0.5, 1, 5, …).
- The smaller the lambda, the larger the weights can get and the model can become more complex.
- More data → smaller lambda.
- If you add more features → larger lambda. **But** that depends on the precise feature added and how it correlates to the target variable.

Other variants

- **Lasso**: $\lambda L_1(w) = \lambda(|w_1| + \cdots + |w_d|)$
  - Leads to **sparsity** of features (presses weights to 0).
- **Elastic net**: Combine both L1 and L2 on all weights.
  - better deals with correlated features,
  - harder to tune as a new hyper parameter is added.
- **Generalized Linear Models (GLMs)**

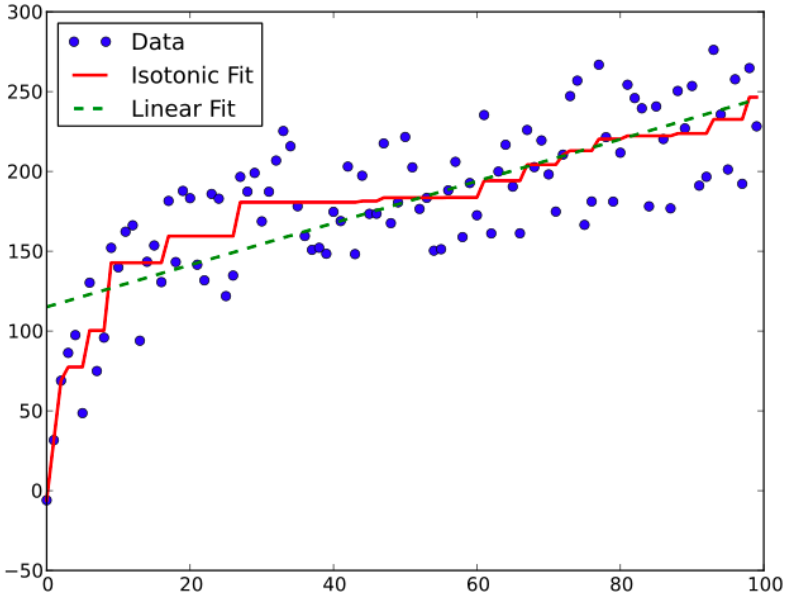
L1-Sparsity



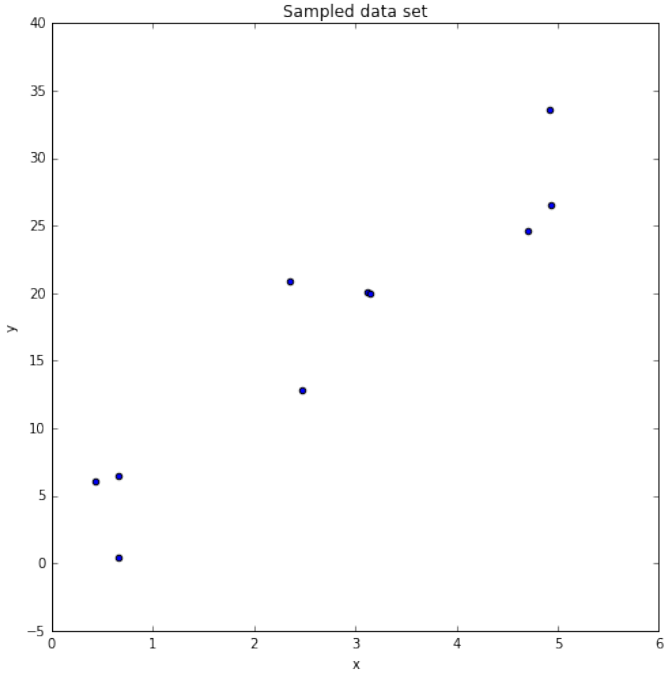
Special variants

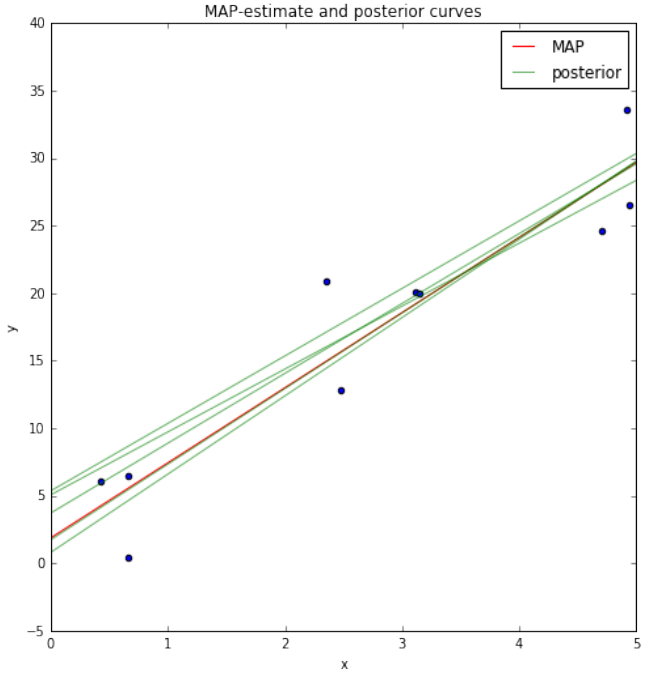
- **Robust regression**: More stable to outliers, rarely used as one has to solve a quadratic program (QP).
- **Bayesian Linear Regression**: Do not compute only one weight, but keep a distribution the weights!
- **Isotonic Regression**: Finds a non-decreasing piecewise linear curve to fit the model.

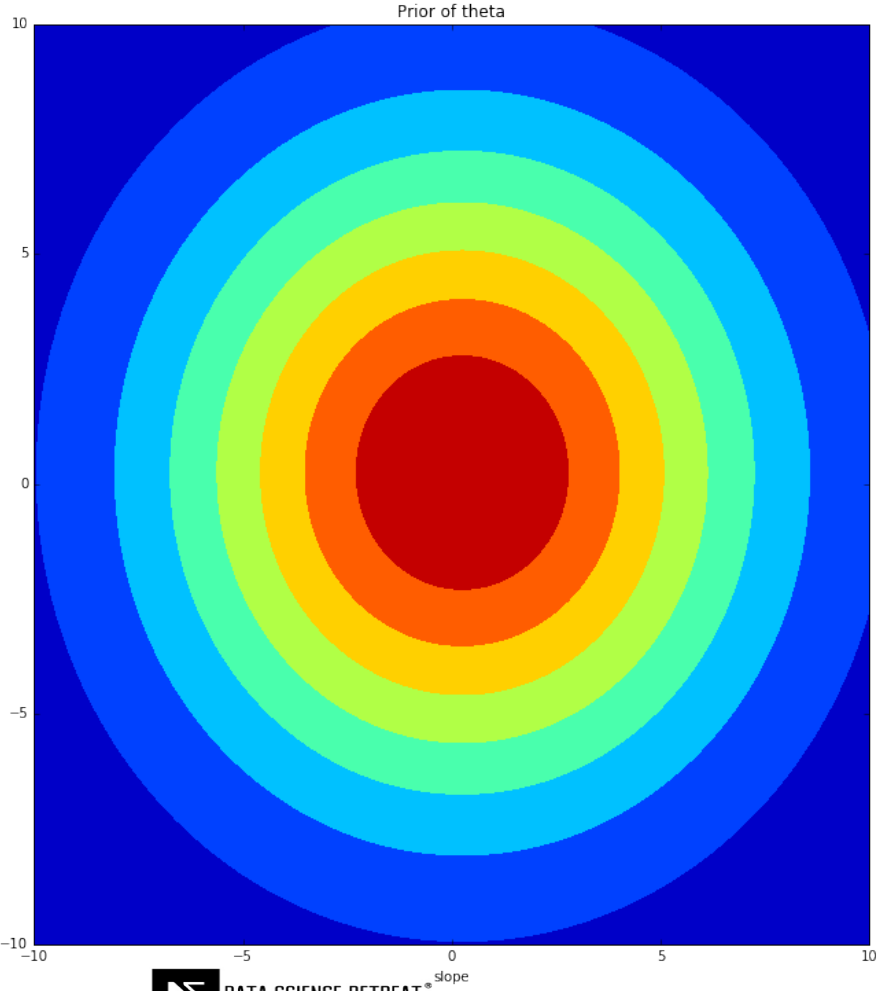
Isotonic Regression

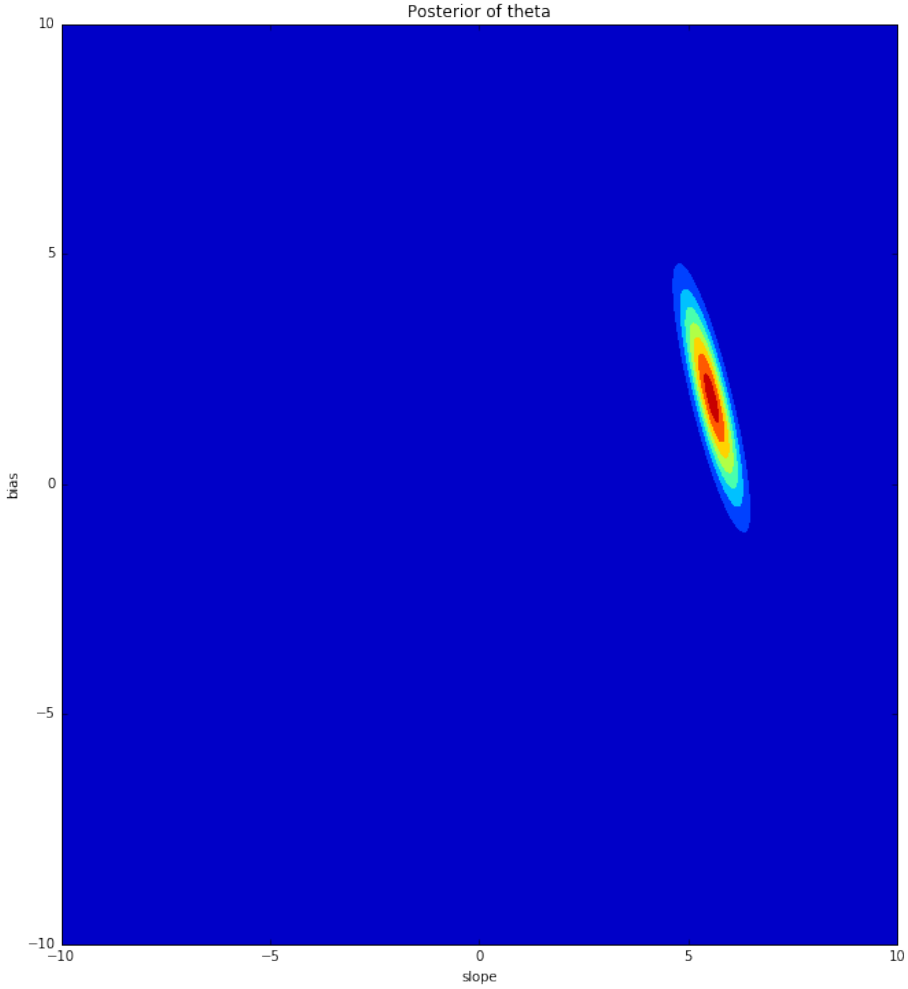


Outlook: Bayesian Linear Regression






Prior of theta
10
5
0
−5
−10
−10
−5
0
5
10
slope


Posterior of theta
10
5
0
−5
−10
bias
−10
−5
0
5
10
slope

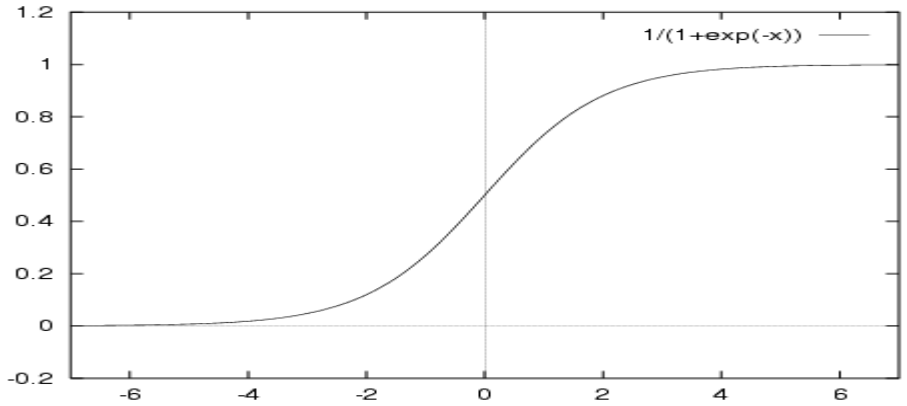
Linear Regression sklearn

```
from sklearn.linear_model
import Ridge # or least_squares, Lasso

l2_reg = Ridge(alpha=0.5) # lambda
l2.fit(X, y)
y_pred = l2.predict(X_train)

l2._coef # returns w
l2._intercept # returns constant
```

Logistic Regression

- Logistic Regression is simply linear regression + **squashing**, with the **sigmoid** function:

- $\sigma(h) = \frac{1}{1+ e^{-h}}, \; h = w^t x$



Logistic Regression II

- Outputs a probability in [0, 1] that outputs the likelihood of the label being 1: P(y = 1 | x, D)
  → binary classification problem.

$$logloss(w) = \sum_{i=1}^{n} \ln(1 + e^{-y_i(w^t x_i)})$$

- **multinomial logistic regression**: ($\mathbf{w}_i$ are model parameters)

$$P(y = c \mid x, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_C) = \frac{\exp(w_c^T x)}{\sum_{c'=1}^{C} \exp(w_{c'}^T x)}$$

  Alternative: one-vs-all approach.

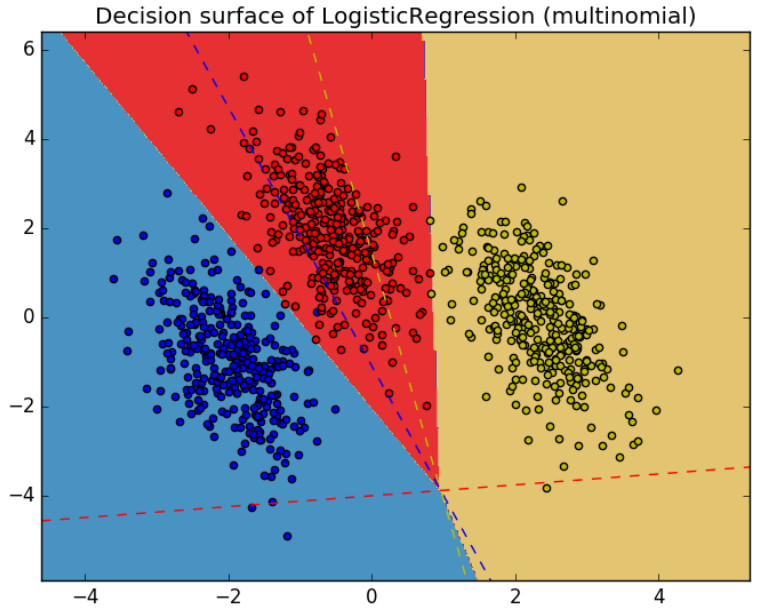
Logistic Regression sklearn

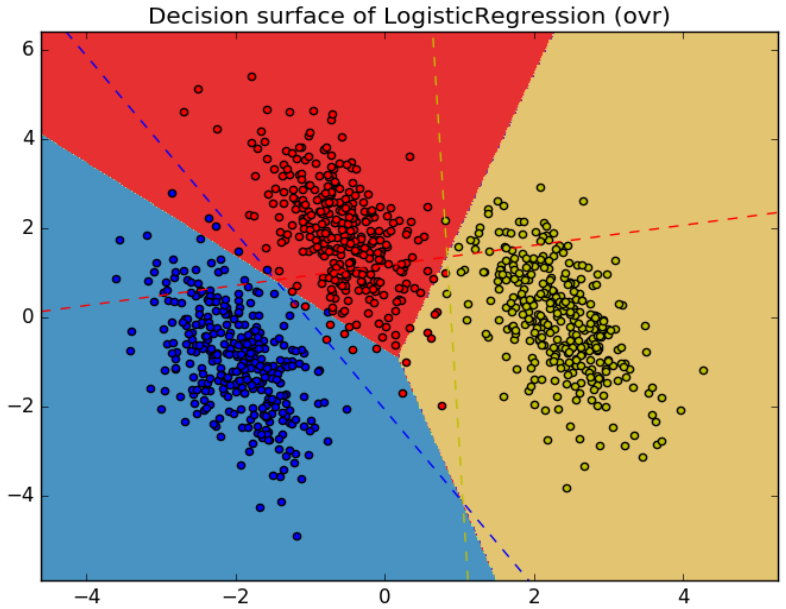
```
from sklearn.linear_model import
LogisticRegression

lr_clf = LogisticRegression(
penalty="l2", # or "l1"
C=1./lambda,  # capacity
fit_intercept=true, # add bias?
n_jobs=-1) # -1 = all cores

lr_clf.fit(X_train, y_train)
y_pred = lr_clf.predict_proba(X_test)
# or predict for labels

lr_clf.coef_ # the coefficients
```

Multiclass

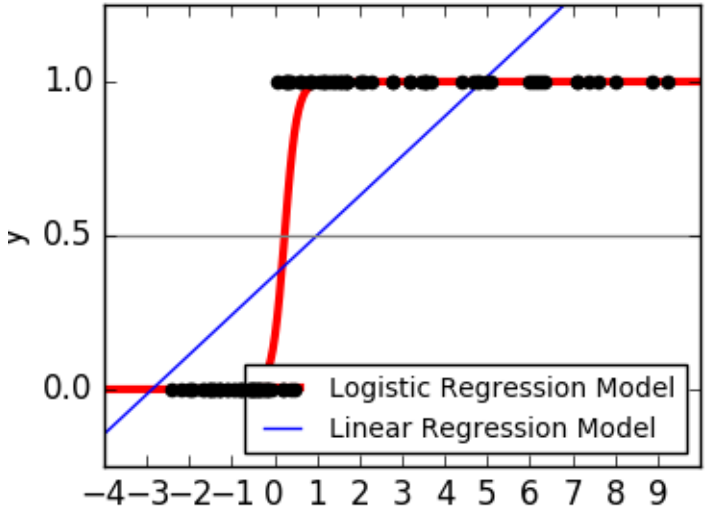
```
clf = LogisticRegression(
C=50. / train_samples,
multi_class='multinomial',
penalty='l1',
solver='saga')

# a bit annoying: not all combinations
# of penalty/solver work
# sage is really new and works with almost all
# variations

# Also take a look at SGDClassifier
# uses stochastic optimization instead of ERM
```

Multinomial vs One-vs-rest





Logistic Regression III



Model Evaluation

Outlook

- Understanding Model fitting vs selection vs evaluation:
  - Resampling: cross validation (CV) and nested CV,
  - Model selection criteria,
  - Overfitting, Over-/Underselection, Bias-variance tradeoff.
- Evaluation metrics in regression and classification:
  - ROC curves.

Goal of ML

- Model is supposed to learn from shown patterns to generalize from this data.
- How do we measure generalization performance of the model? Empirical risk minimization (ERM) framework.

” When you have two competing theories that make exactly the same predictions, the simpler one is the better.*"* --- ***Occam’s Razor***

Empirical Risk Minimization

- Two assumptions:
  - Data follows a distribution $p(x, y)$ on $X \times Y$.
  - Learner sees data set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$ of **independent** and **identically sampled** (from p) data (*IID assumption*).

- **The IID assumption is almost always broken in practice.**

Empirical Loss

- Given a loss function l the *empirical loss/risk is,*

$$R_D[f] = \sum_{n=1}^{N} l(f(x_n), y_n, x_n).$$

- This is a statistical estimator if you vary the selection of D.

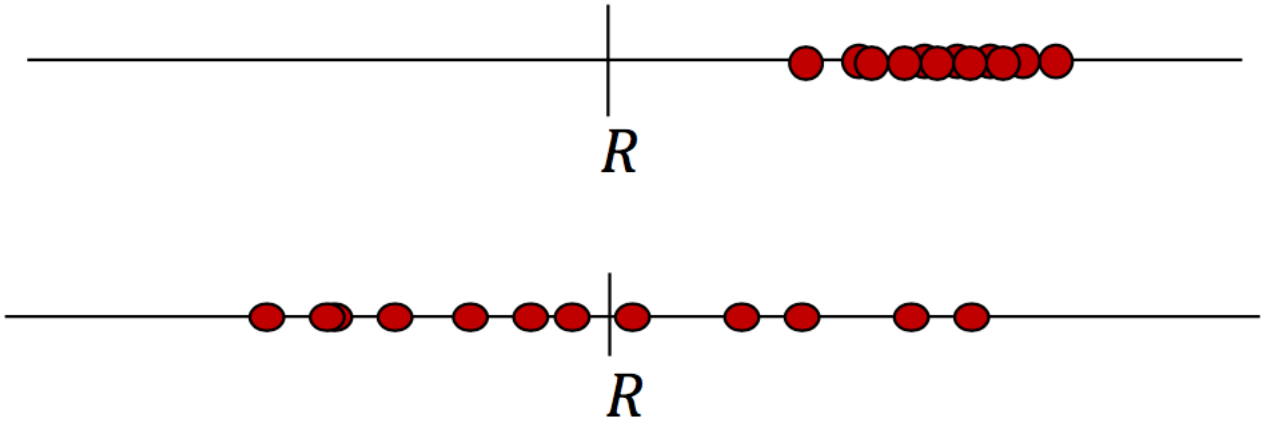
Empirical Risk Minimization II

- $R_D[f]$ is supposed to estimate the *generalization error/risk,*

$$R[f] = \int l(f(x), y, x) dp(x, y) \,.$$

- The larger $|D|$ the more accurate.
- $R_D[f]$ has a bias (distance to $\mathrm{R}[f]$) and a variance.

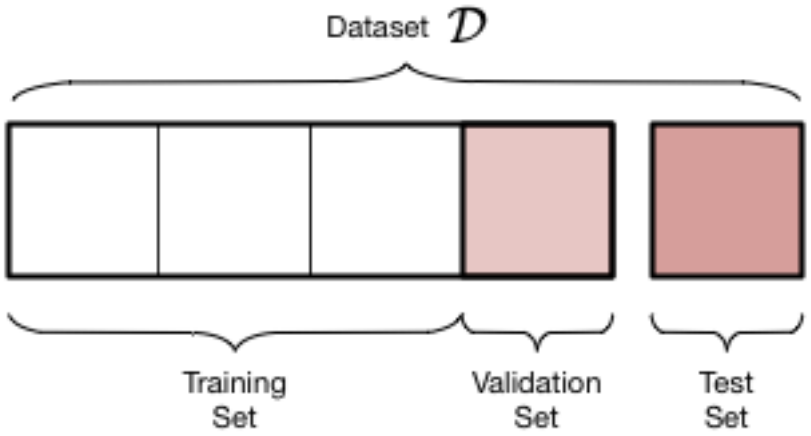
Bias / Variance



- **Model fitting:** finding the best model parameter:

$$\theta = argmin_{\theta} R_D[f_\theta]$$

- **Model selection:** find the best fitting model family / hyperparams.
- **Model evaluation:** estimate the generalization risk.



Journal of Machine Learning Research 11 (2010) 2079-2107 Submitted 10/09; Revised 3/10; Published 7/10

On Over-fitting in Model Selection and Subsequent Selection Bias in Performance Evaluation

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Editor: Isabelle Guyon

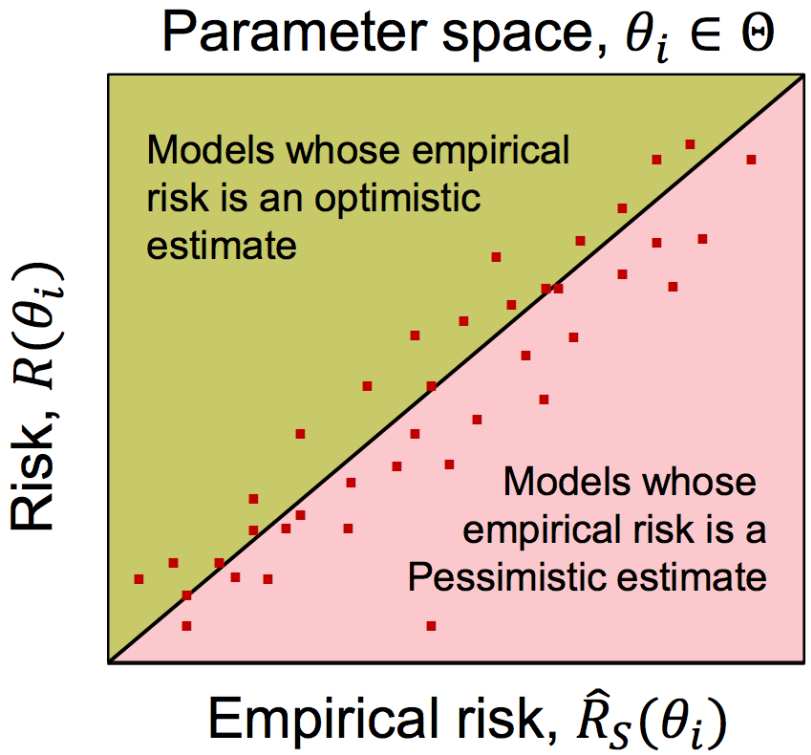
Abstract

Model selection strategies for machine learning algorithms typically involve the numerical optimisation of an appropriate model selection criterion, often based on an estimator of generalisation performance, such as k-fold cross-validation. The error of such an estimator can be broken down into bias and variance components. While unbiasedness is often cited as a beneficial quality of a model selection criterion, we demonstrate that a low variance is at least as important, as a non-negligible variance introduces the potential for over-fitting in model selection as well as in training the model. While this observation is in hindsight perhaps rather obvious, the degradation in performance due to over-fitting the model selection criterion can be surprisingly large, an observation that appears to have received little attention in the machine learning literature to date. In this paper, we

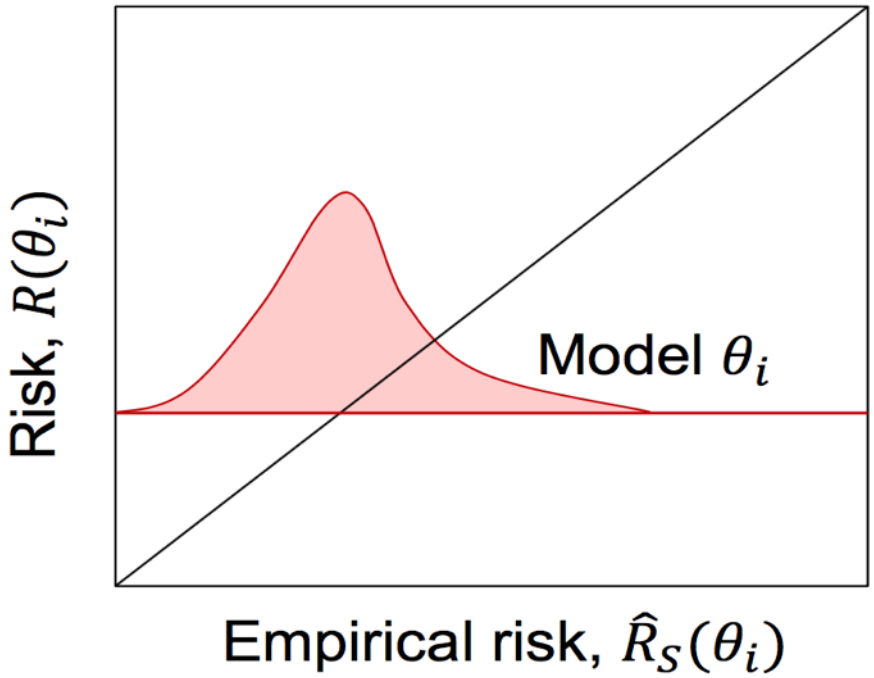
Prefer to call it “over-selection”

In “Learning with Kernels” from Smola & Schölkopf they name ex. 5.10. “overfitting on the test set”.

Paper: http://bit.ly/2gBIR1M



Source: University of Potsdam



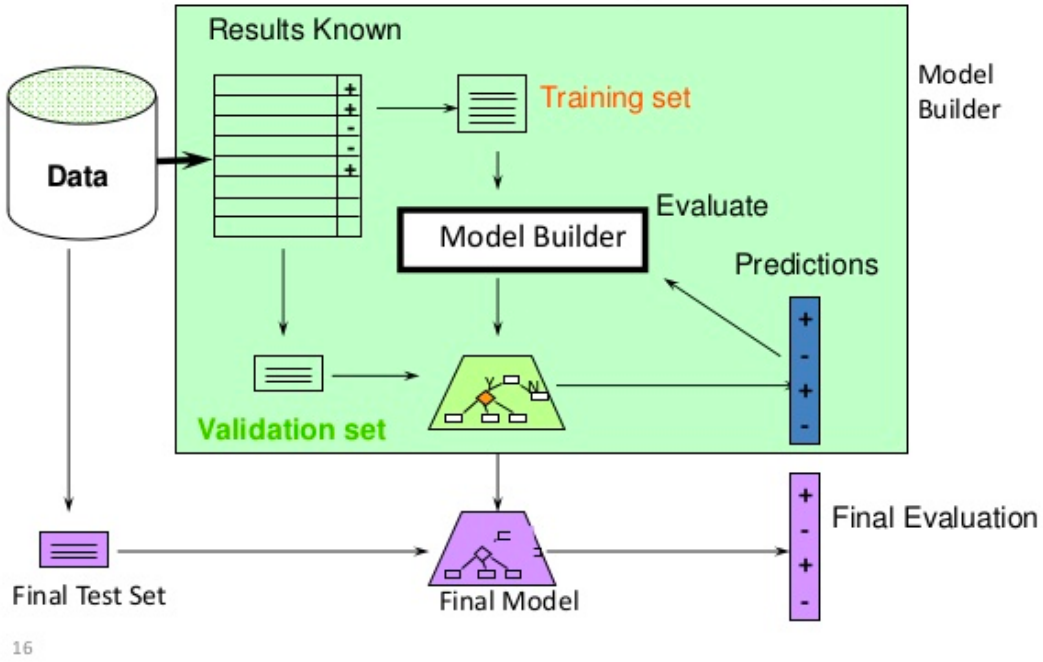
Source: University of Potsdam

Messing up your experiments

- Data split strategy is part of experiment.
- Mainly care for:
  - Class distribution
  - Problem domain relevant issues such as time

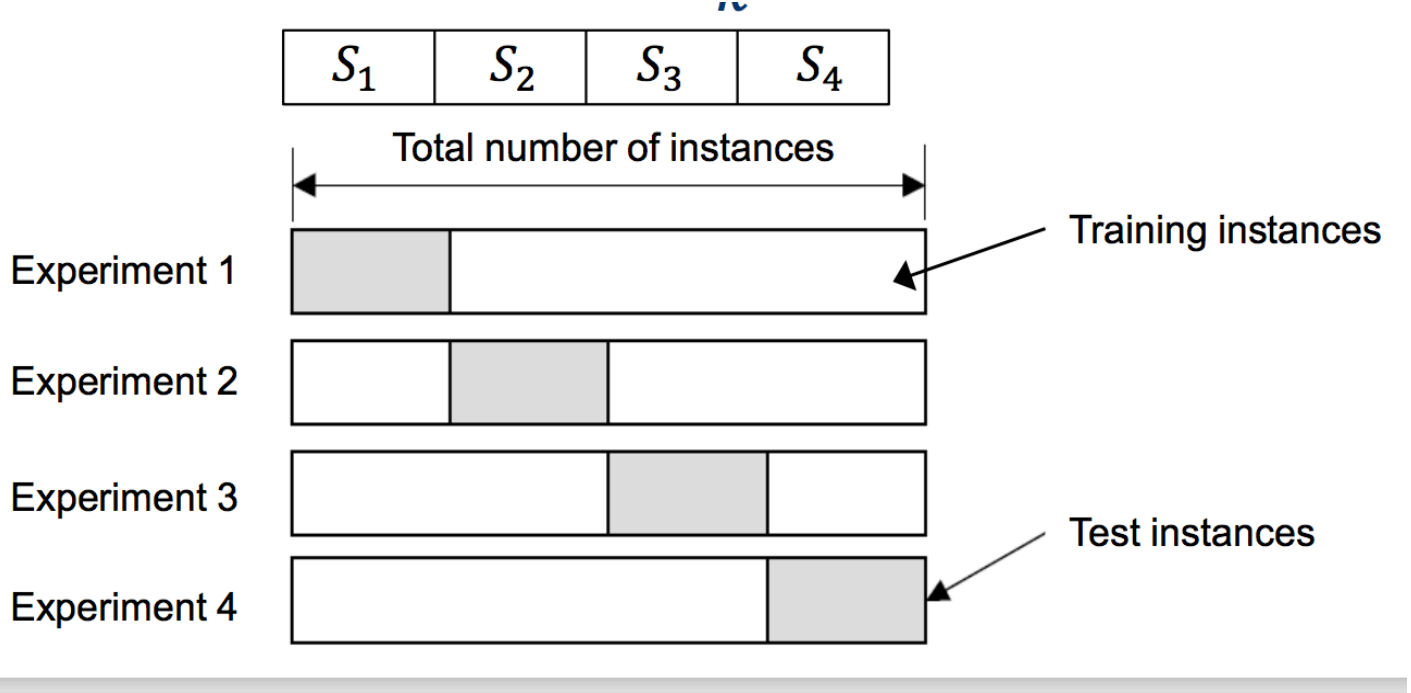
> *”Validation and Test sets should model nature and nature is not accommodating."* --- **Data Scientist’s Proverbs**

Classification:
Train, Validation, Test split

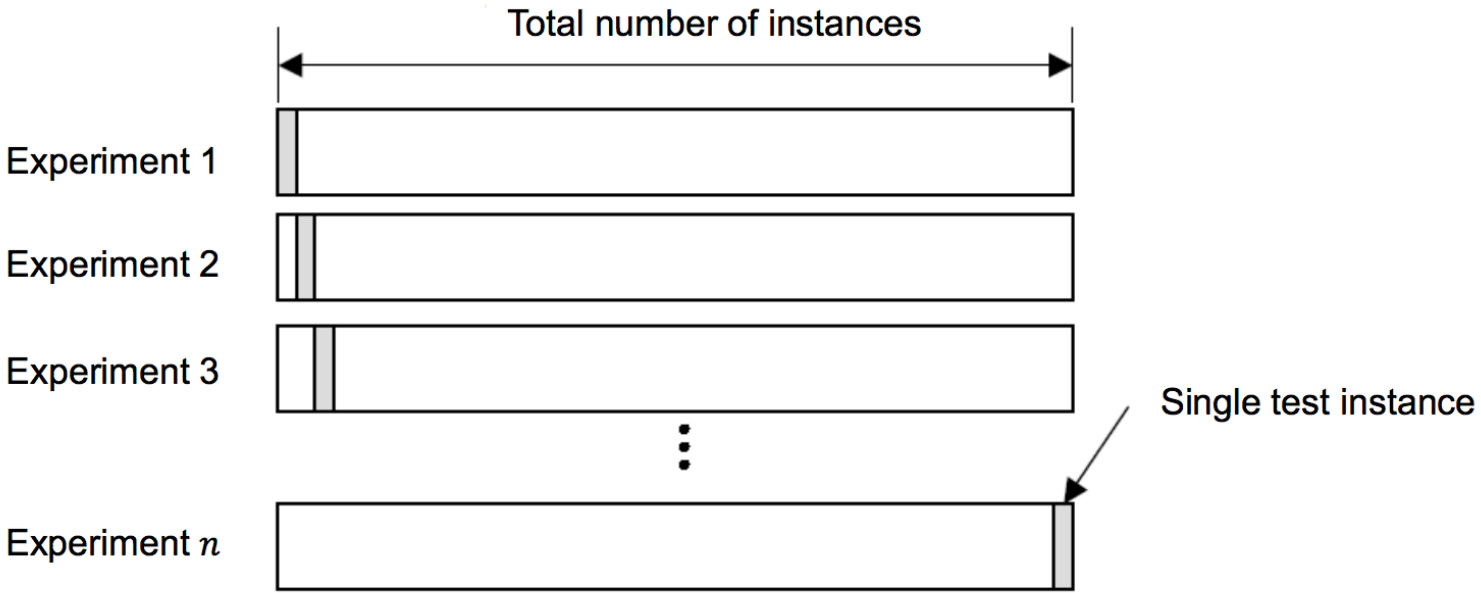


Source: http://bit.ly/2vDfoLp

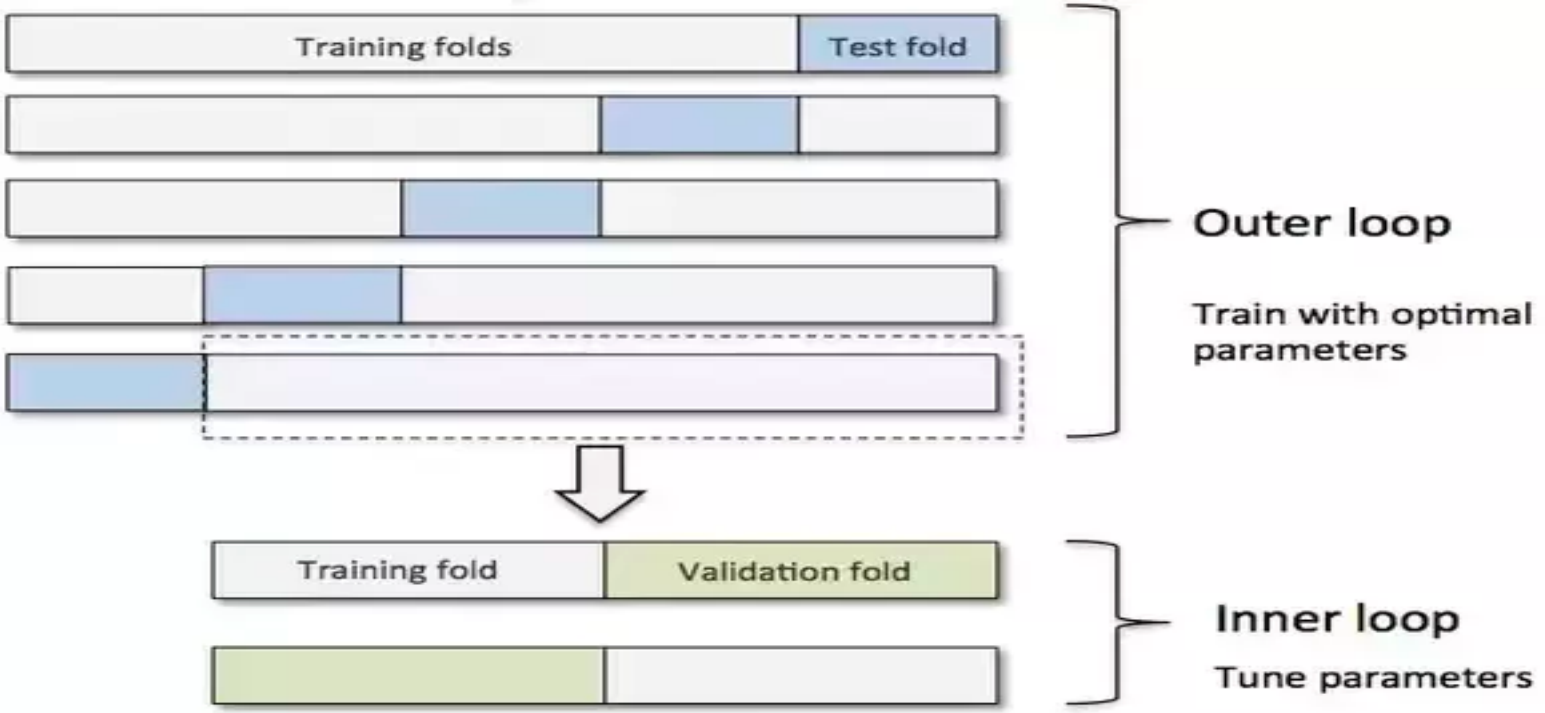
CV


S_1
S_2
S_3
S_4
Total number of instances
Training instances
Experiment 1
Experiment 2
Experiment 3
Test instances
Experiment 4

LOOCV


Total number of instances
Experiment 1
Experiment 2
Experiment 3
Experiment n
Single test instance

Nested CV



From Quora: http://bit.ly/2wvz2aZ

```
from sklearn.model_selection import cross_val_score
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import ShuffleSplit
from sklearn.model_selection import GridSearchCV

base_clf = LogisticRegression(C=1, solver="saga", multi_class="multinomial")

param = {
    "C": [0.03, 0.01, 0.1, 1, 10, 100, 1000],
    "penalty": ("l1", "l2")
}


clf = GridSearchCV(base_clf, param, scoring="accuracy", cv=ShuffleSplit(3),
verbose=1)
scores = cross_val_score(clf, X, y, scoring="accuracy", cv=ShuffleSplit(5), n_jobs=-
1, verbose=1)


print("%.4f (±%.4f)" % (np.mean(scores), np.std(scores)))
```

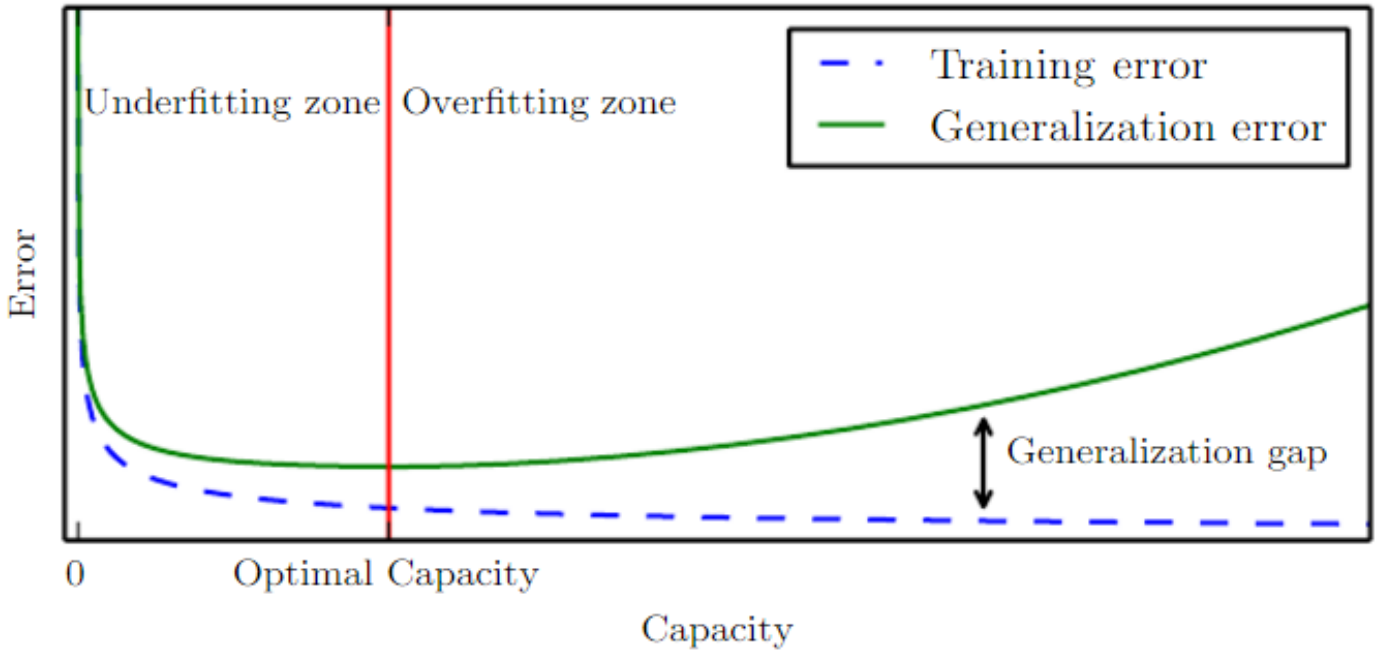
Alternative – Central Limit Theorem

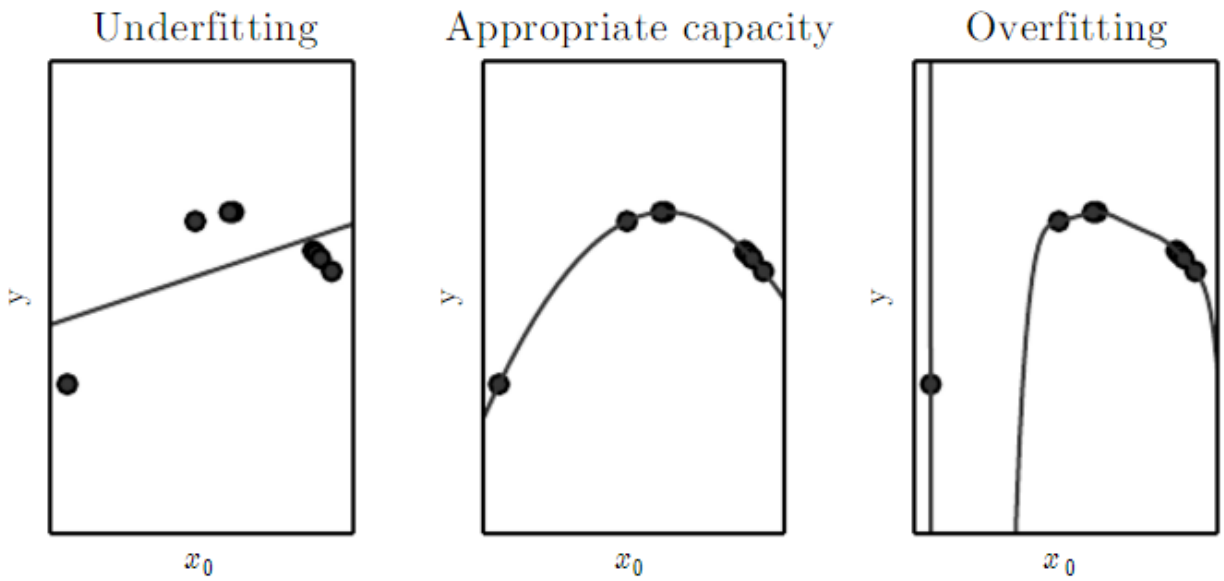
- Given test size of n elements the confidence interval for the estimate e is

$$e \pm z \sqrt{\frac{1}{n} e(1-e)}$$

  where z is set to the $1 - \frac{\alpha}{2}$ quantile of the normal distribution.

- Example: want 95% CI, n = 20, accuracy = 85% => e = 0.85, α = 0.05 => z = 1.96 => CI = $0.85 \pm 1.96 \sqrt{\frac{1}{20} 0.85(1-0.85)} = 0.85\% \pm 15.6\%$. For n = 100: $0.85\% \pm 7\%$.
- Models test process as binomial, then CLT.


Underfitting zone
Overfitting zone
Training error
Generalization error
Error
Generalization gap
0
Optimal Capacity
Capacity


Underfitting
Appropriate capacity
Overfitting
y
x_0

Evaluation Metrics

Regression

- Simple approach: compare errors (eg **RMSE)**
- Or R-squared (variance explained). If the models do not have the same complexity, then use adjusted R-squared
- There is no absolute standard for a "good" value of adjusted R-squared

		Condition (as determined by "Gold standard")	
	Total population	Condition positive	Condition negative
Test outcome	Test outcome positive	**True positive**	**False positive** (Type I error)
	Test outcome negative	**False negative** (Type II error)	**True negative**

https://en.wikipedia.org/wiki/Precision_and_recall

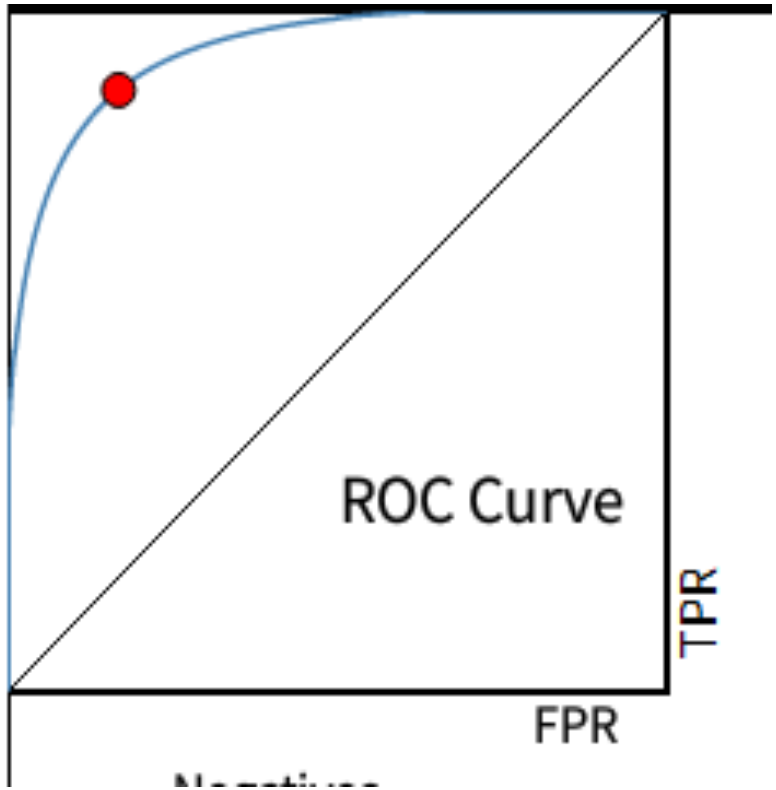
		Condition (as determined by "Gold standard")			
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	
Test outcome	Test outcome positive	**True positive**	**False positive** (Type I error)	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Test outcome positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Test outcome positive}}$
	Test outcome negative	**False negative** (Type II error)	**True negative**	False omission rate (FOR) = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Test outcome negative}}$	Negative predictive value (NPV) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Test outcome negative}}$
	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	True positive rate (TPR), Sensitivity, Recall = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) = $\frac{\text{LR+}}{\text{LR−}}$
		False negative rate (FNR), Miss rate = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) = $\frac{\text{FNR}}{\text{TNR}}$	

ROC curve

y-axis is true positive rate, and the *x*-axis is false positive rate

Interpretation:

Pick a random negative and a random positive example; The AUC gives you the probability that your classifier assigns a higher score to the positive example (ie, ranks the positive higher than the negative).



ROC curve

- The most common method for combining sensitivity and specificity into a single value uses the **receiver operating characteristic (ROC)** curve.

- The ROC curve is useful for determining alternate cutoffs for class probabilities

Precision and recall

- **Origins: information retrieval**
- **Precision** is the probability that a (randomly selected) retrieved document is relevant.

- **Recall** is the probability that a (randomly selected) relevant document is retrieved in a search.
- They are balanced: you can increase one at the cost of the other

		Condition (as determined by "Gold standard")			
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	
Test outcome	Test outcome positive	**True positive**	**False positive** (Type I error)	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Test outcome positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Test outcome positive}}$
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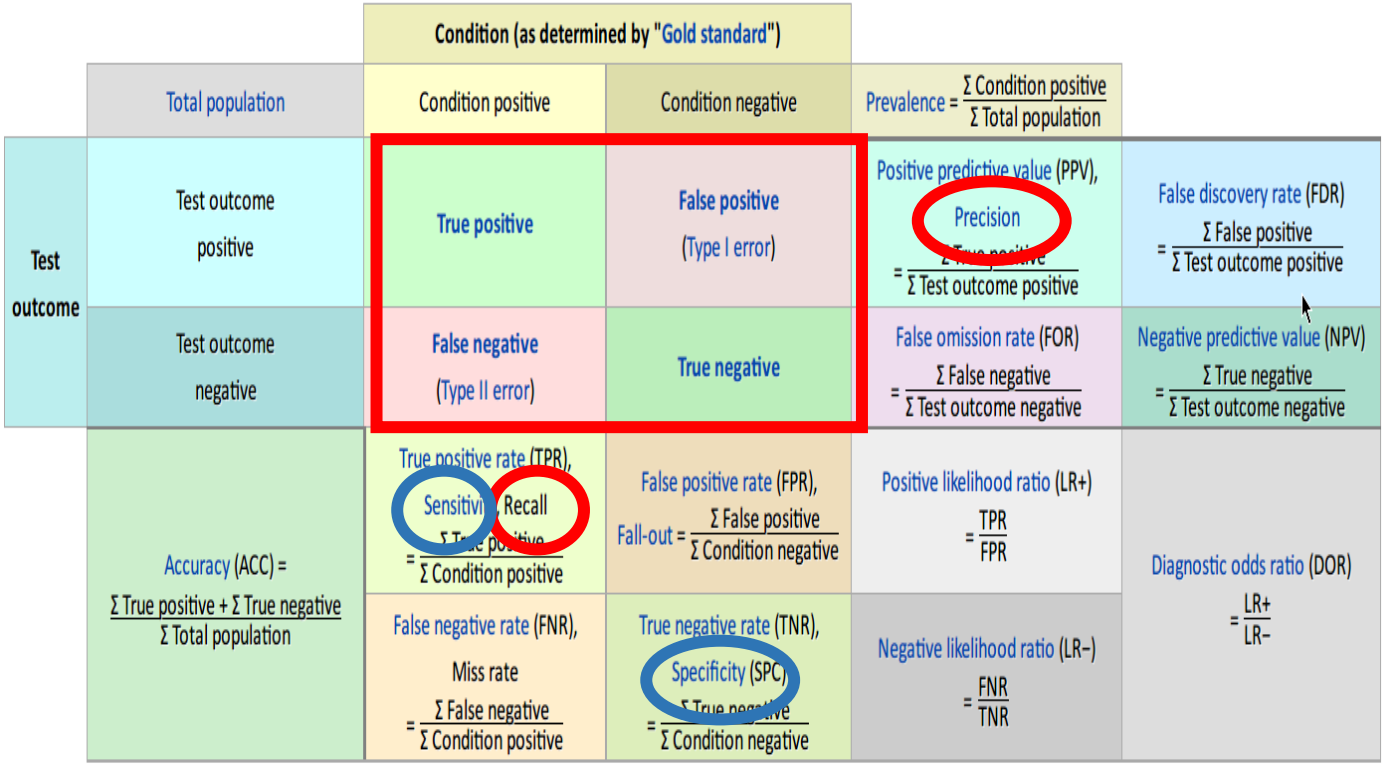
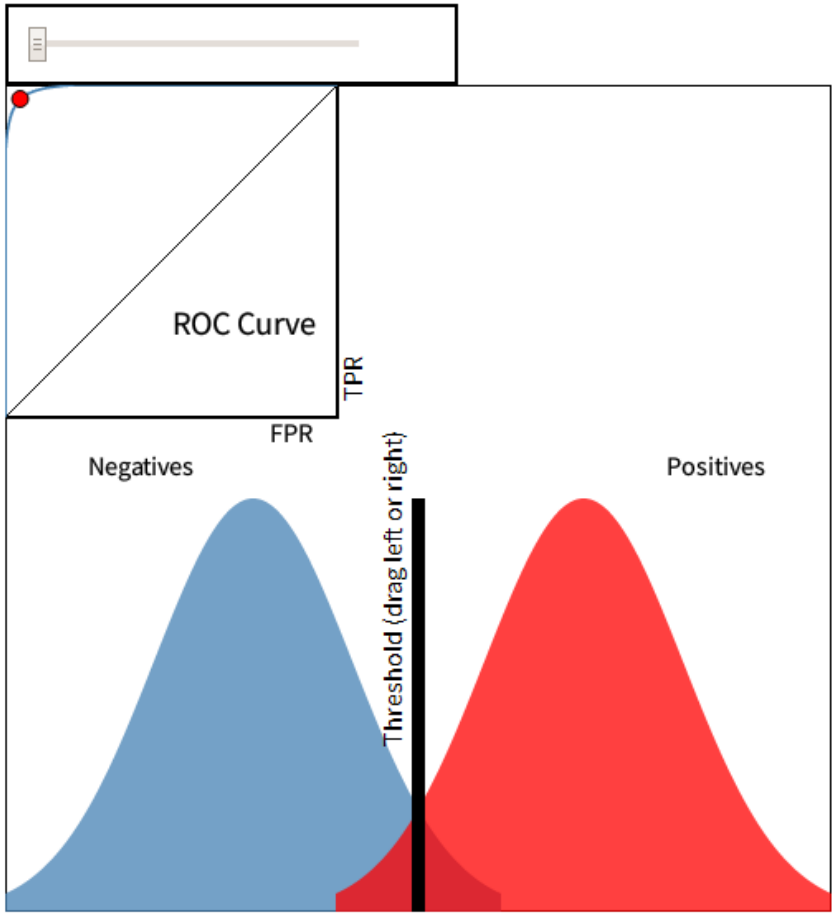
		False negative rate (FNR), Miss rate = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	True negative rate (TNR), Specificity (SPC) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) = $\frac{\text{FNR}}{\text{TNR}}$	


Condition (as determined by "Gold standard")
Total population
Condition positive
Condition negative
Prevalence = Σ Condition positive / Σ Total population
Test outcome
Test outcome positive
True positive
False positive (Type I error)
Positive predictive value (PPV), Precision = Σ True positive / Σ Test outcome positive
False discovery rate (FDR) = Σ False positive / Σ Test outcome positive
Test outcome negative
False negative (Type II error)
True negative
False omission rate (FOR) = Σ False negative / Σ Test outcome negative
Negative predictive value (NPV) = Σ True negative / Σ Test outcome negative
Accuracy (ACC) = Σ True positive + Σ True negative / Σ Total population
True positive rate (TPR), Sensitivity, Recall = Σ True positive / Σ Condition positive
False positive rate (FPR), Fall-out = Σ False positive / Σ Condition negative
Positive likelihood ratio (LR+) = TPR / FPR
Diagnostic odds ratio (DOR) = LR+ / LR−
False negative rate (FNR), Miss rate = Σ False negative / Σ Condition positive
True negative rate (TNR), Specificity (SPC) = Σ True negative / Σ Condition negative
Negative likelihood ratio (LR−) = FNR / TNR

ROC curve



- http://www.navan.name/roc/

Picking a good performance metrics is still a open question

The paper Facing Imbalanced Data Recommendations for the Use of Performance Metrics found that "while ROC was unaffected by skew, the precision-recall curves suggest that ROC may mask poor performance in some cases."

Picking a good performance metrics is still a open question, but in publications, competitions etc ROC is a safe bet.

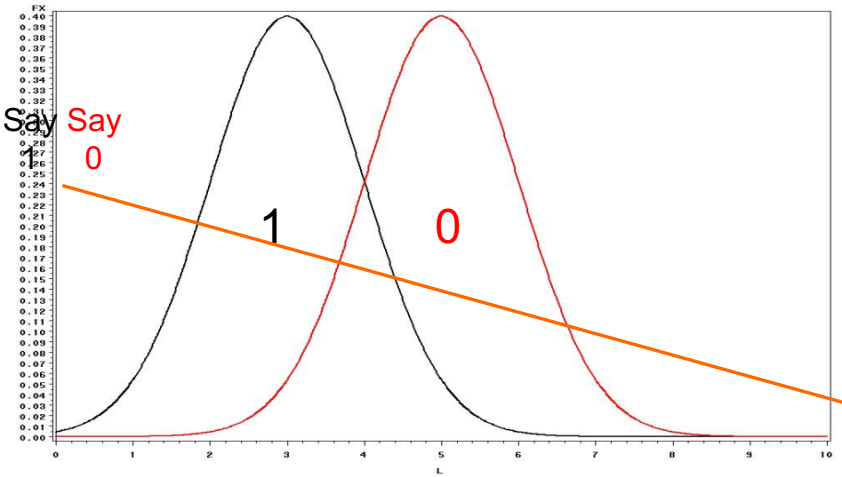
Always check what your problem needs first

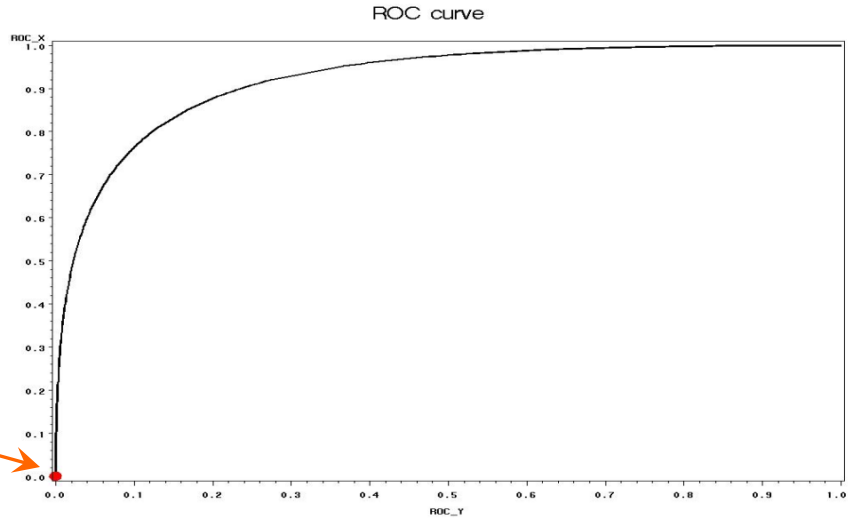
All in all, things to keep in mind

- The measure you optimize to makes a difference
- The measure you report makes a difference
- Use measure appropriate for problem/community
- Accuracy often is not sufficient/appropriate;
- ROC is gaining popularity in the ML community
- Only accuracy generalizes to >2 classes!

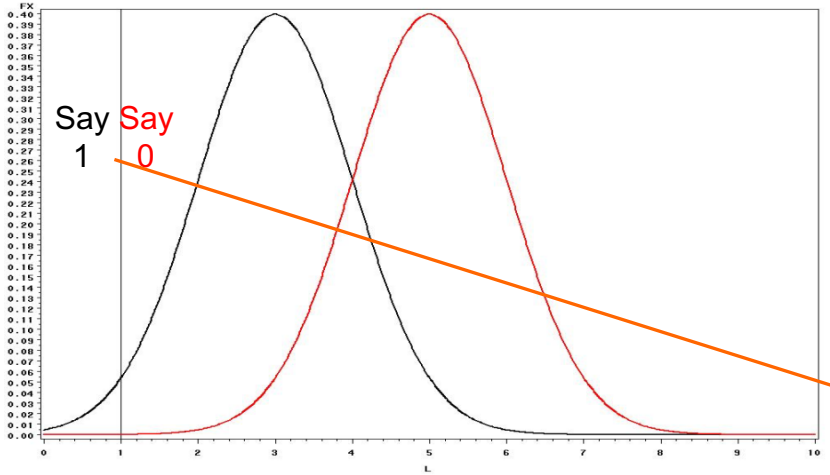
ROC Curve Demo

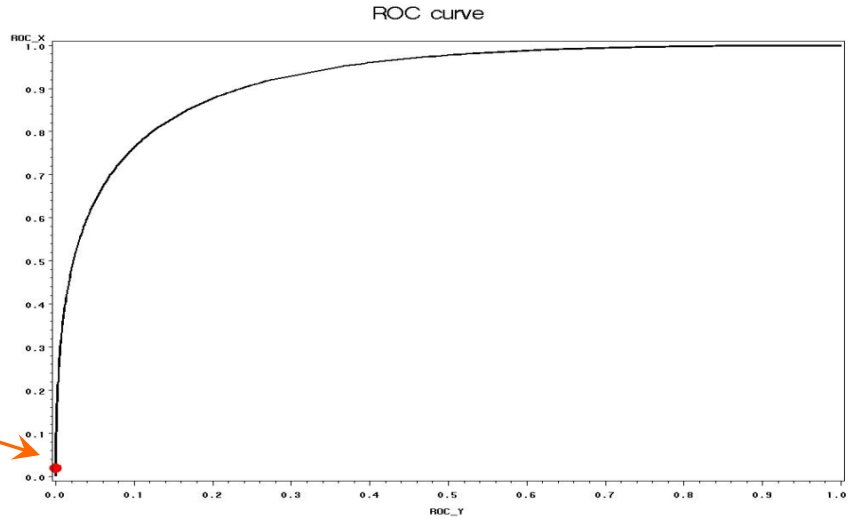
From Dave Dickey, used with permission

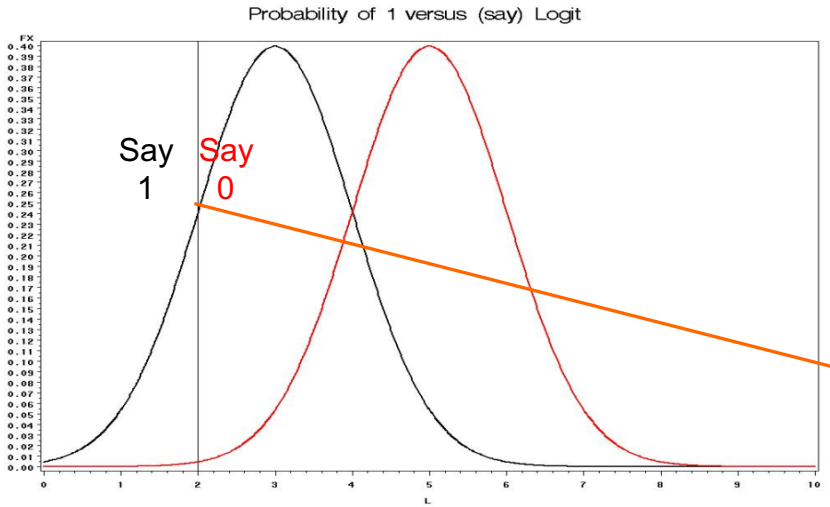

Probability of 1 versus (say) Logit
FX
L
Say 1
Say 0
1
0

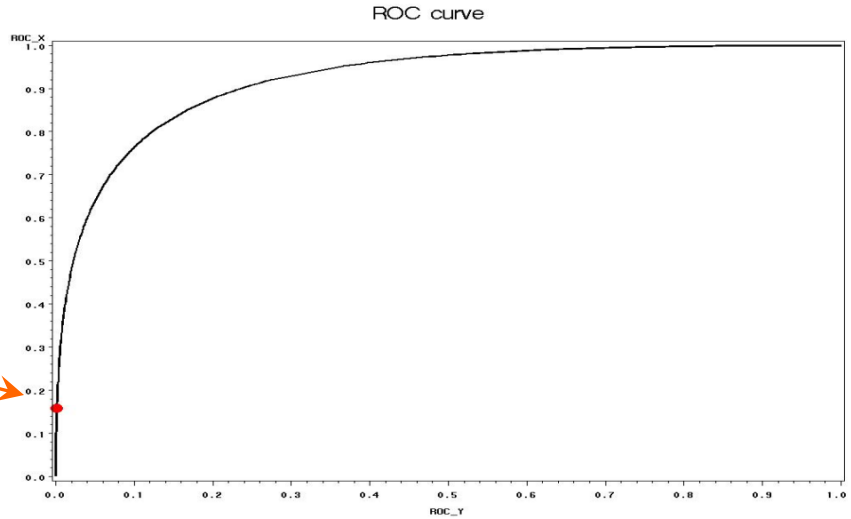

ROC curve
ROC_X
ROC_Y

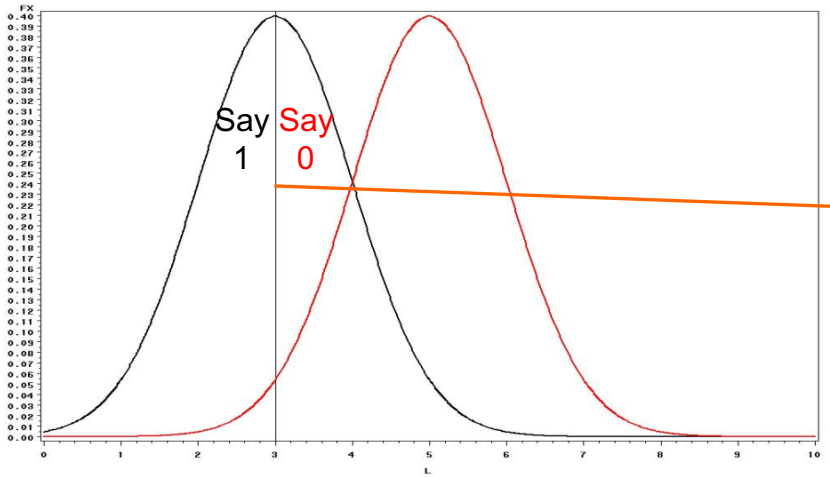
%0s

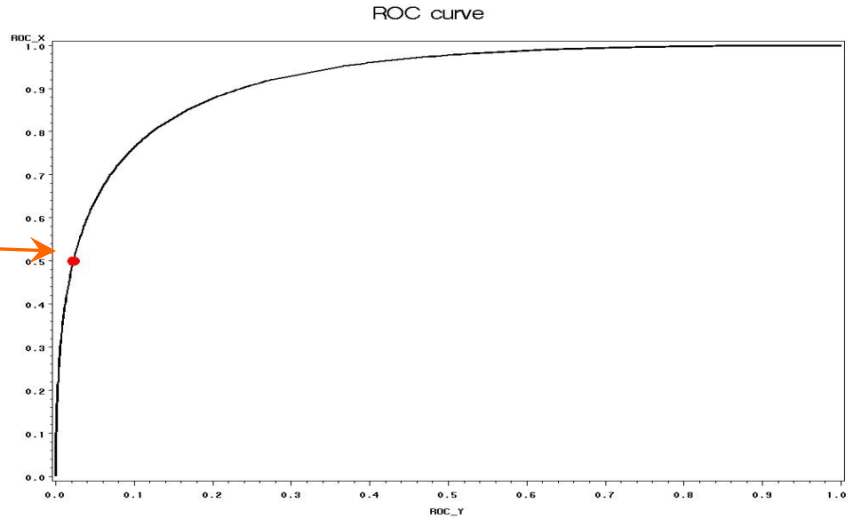

Probability of 1 versus (say) Logit
FX
L
Say 1
Say 0

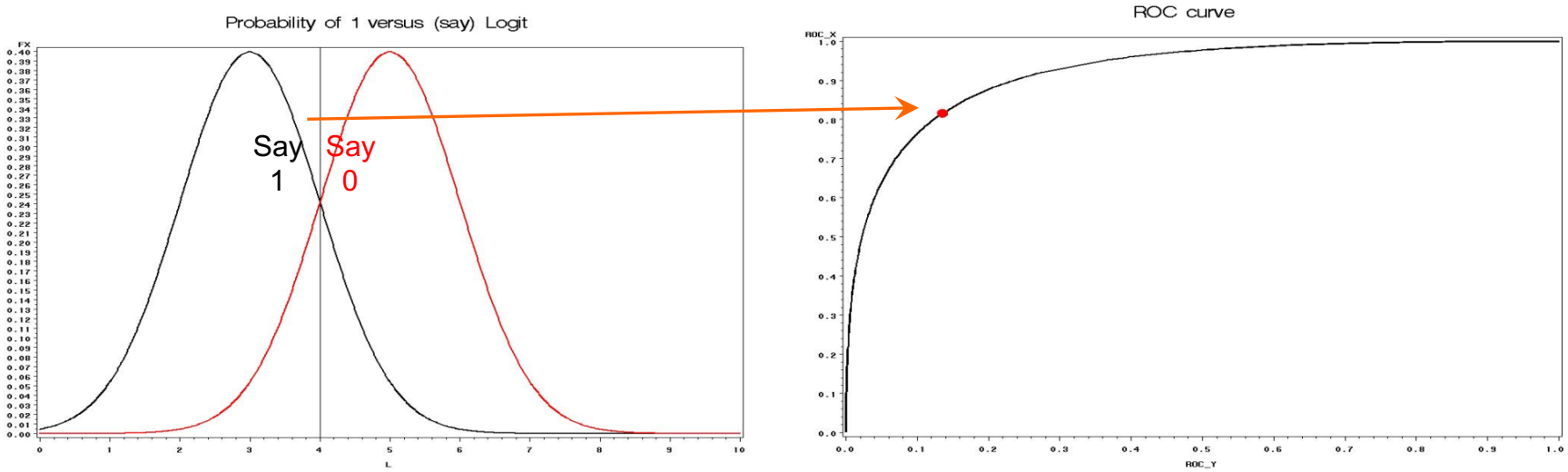

ROC curve
ROC_X
ROC_Y

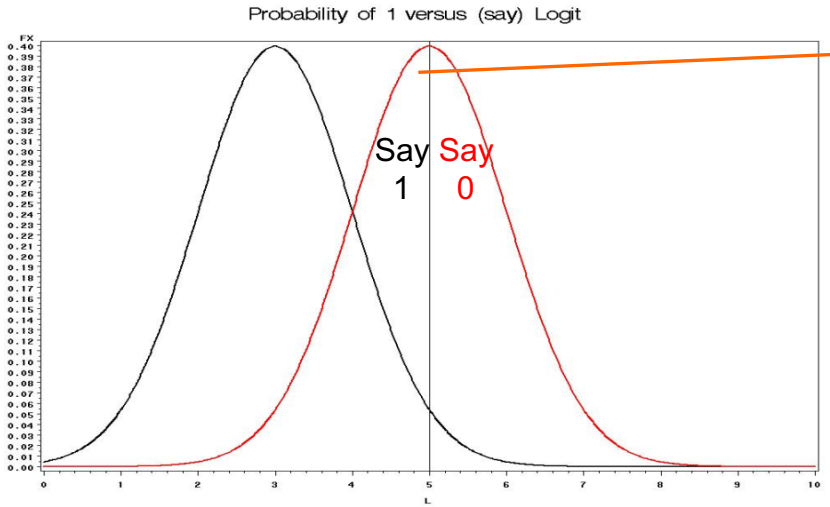

Probability of 1 versus (say) Logit
FX
L
Say
1
Say
0

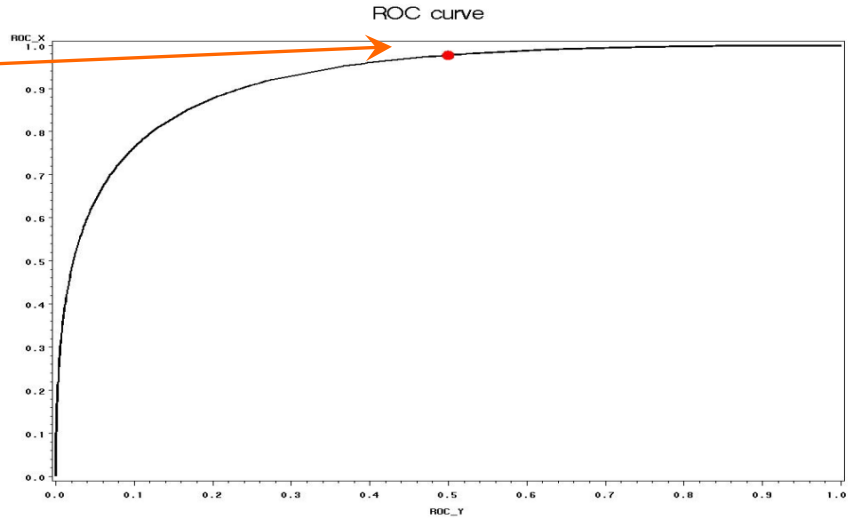

ROC curve
ROC_X
ROC_Y

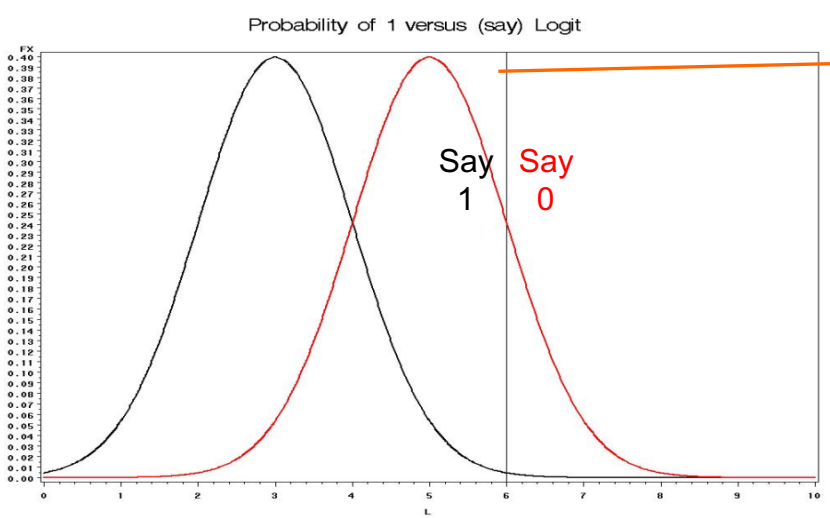

Probability of 1 versus (say) Logit
FX
L
Say 1
Say 0

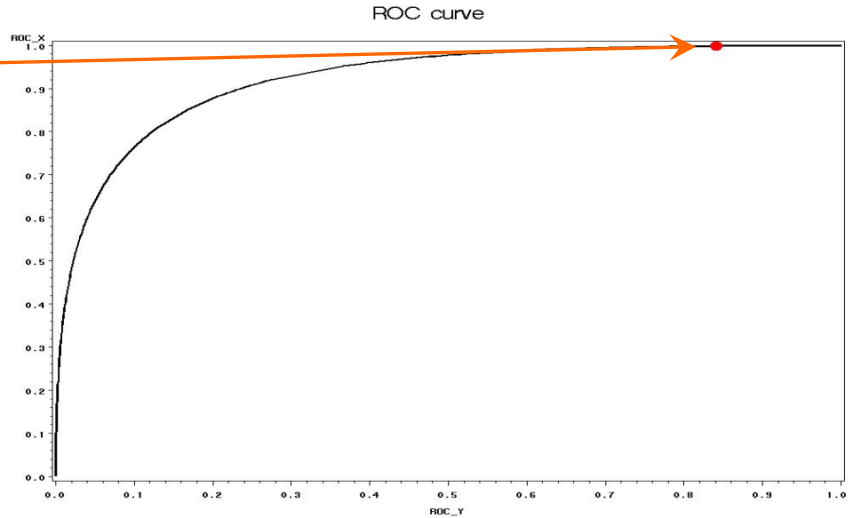

ROC curve
ROC_X
ROC_Y

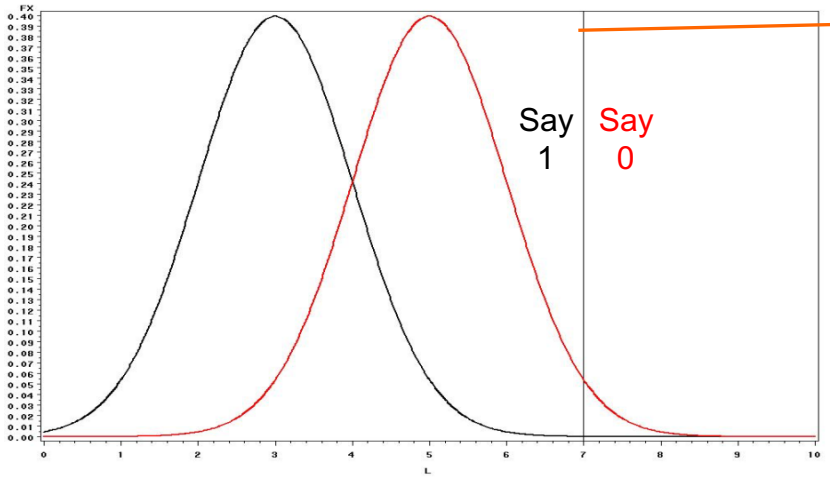

Probability of 1 versus (say) Logit
FX
L
Say
1
Say
0
ROC curve
ROC_X
ROC_Y

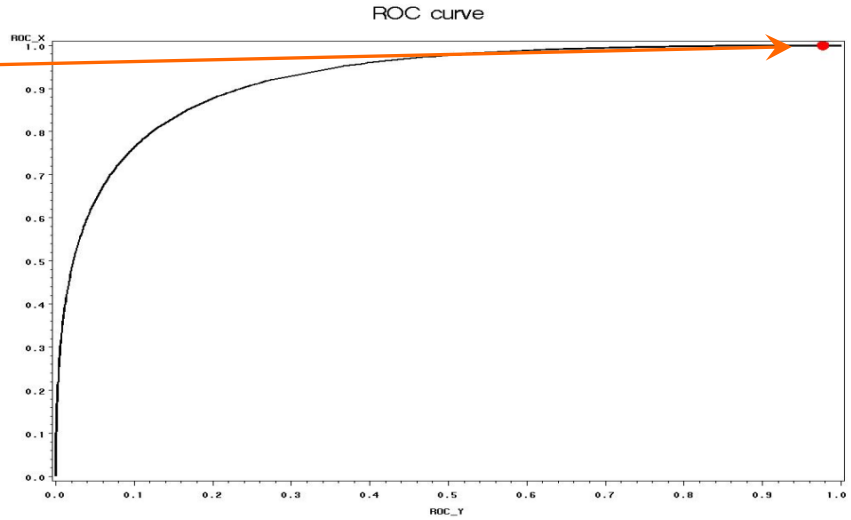

Probability of 1 versus (say) Logit
FX
L
Say 1
Say 0


ROC curve
ROC_X
ROC_Y


Probability of 1 versus (say) Logit
FX
L
Say
1
Say
0


ROC curve
ROC_X
ROC_Y


Probability of 1 versus (say) Logit
FX
L
Say
1
Say
0


ROC curve
ROC_X
ROC_Y

Example 2

	0	1
X=10	2	18
X=13	8	12
X=16	15	5

Say 1
Say 0

1 -
specificity

Example 2

	0	1
X=10	2	18
	8	12
X=13	15	5
X=16		

Say 1
Say 0

(2/25, 18/35)→

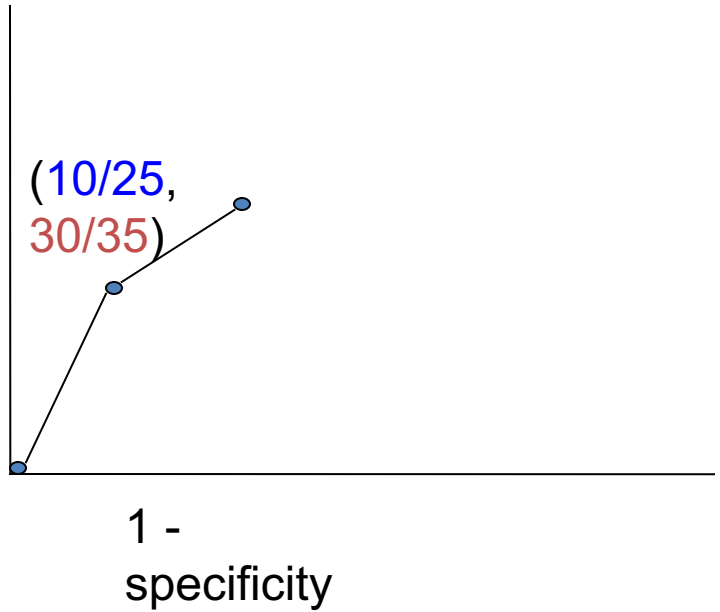
1 - specificity

Example 2

	0	1
X=10	2	18
	8	12
X=13	15	5
X=16		

Say 1
Say 0

(2/25, 18/35)→

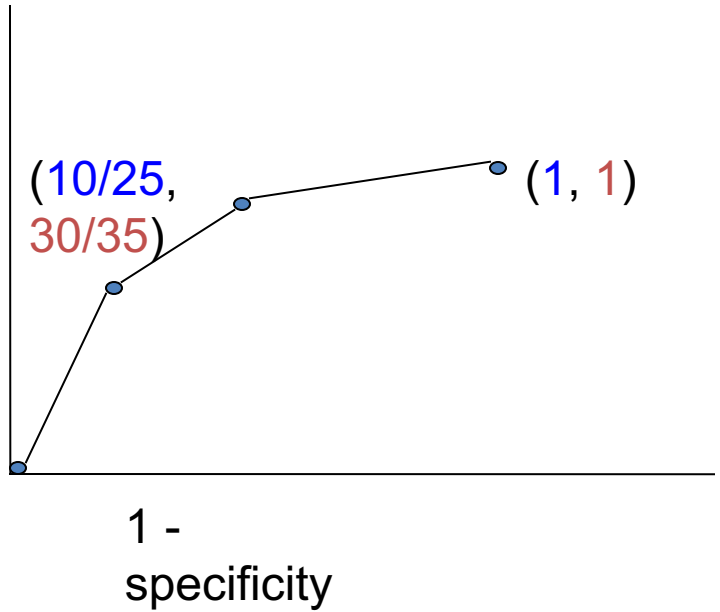


Example 2

	0	1
X=10	2	18
X=13	8	12
X=16	15	5

Say 1
Say 0

(2/25, 18/35)→

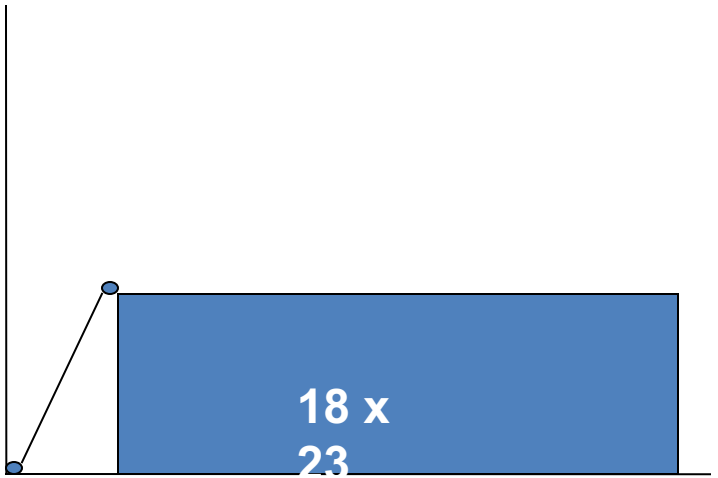


Example 2

	0	1
X=10	2 Tie	18
	8 Tie	12
X=13	15	5
X=16		

Say 1

Say 0



Example 2

	0	1
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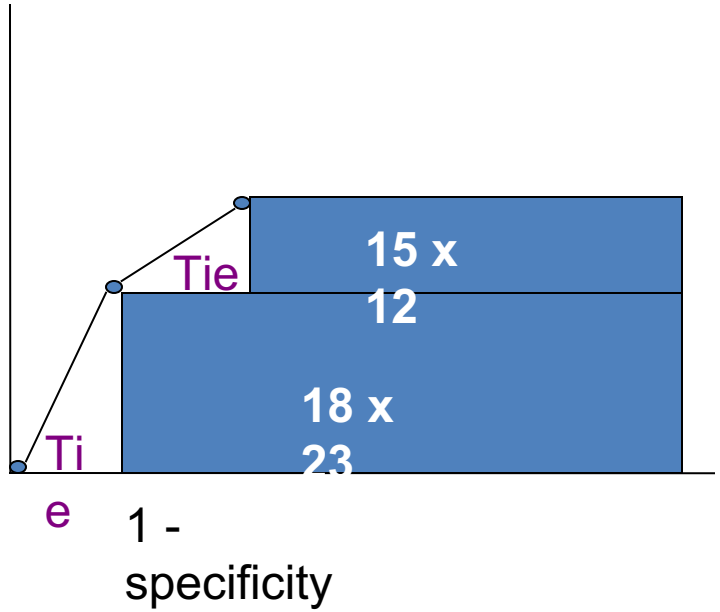
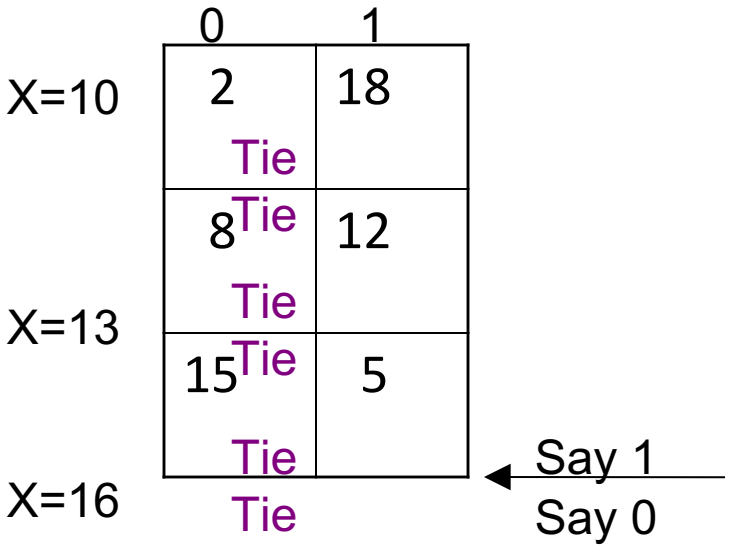
X=13	8 Tie Tie	12
X=16	15 Tie	5

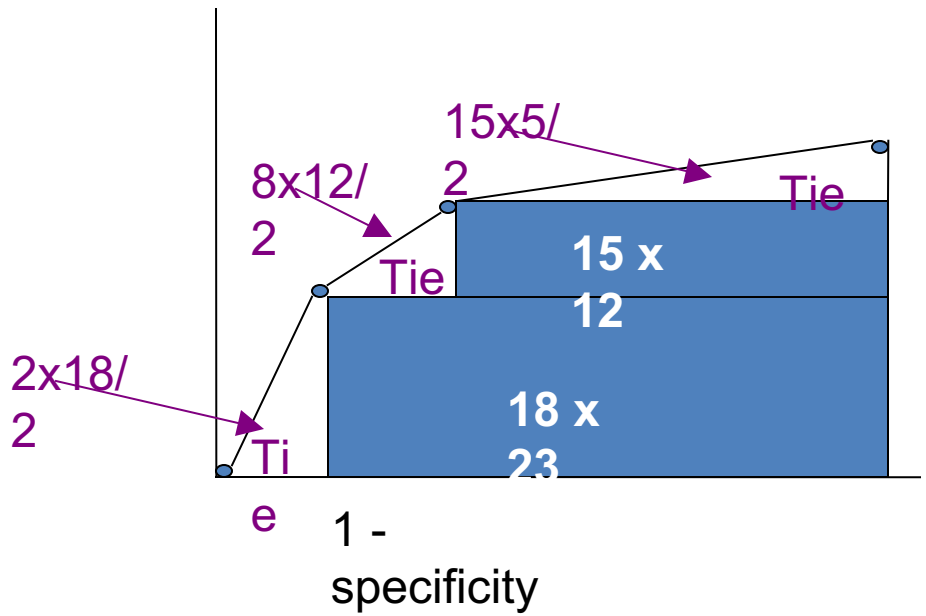
Say 1

Say 0



Example 2





AUC Area Under Curve = concordant pair plus ½ ties (proportions)

Pairs: 25x35=875 with 0 paired with 1.

Proportion Concordant:

(18x23+12x15)/(25x35)=(18/25)x(23/35)+(12/25)x(15/35)

½ Proportion Ties ½(2x18 + 8x12 + 15x5)/(25x35)