Introduction to Data Mining

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What is data mining?

Definition

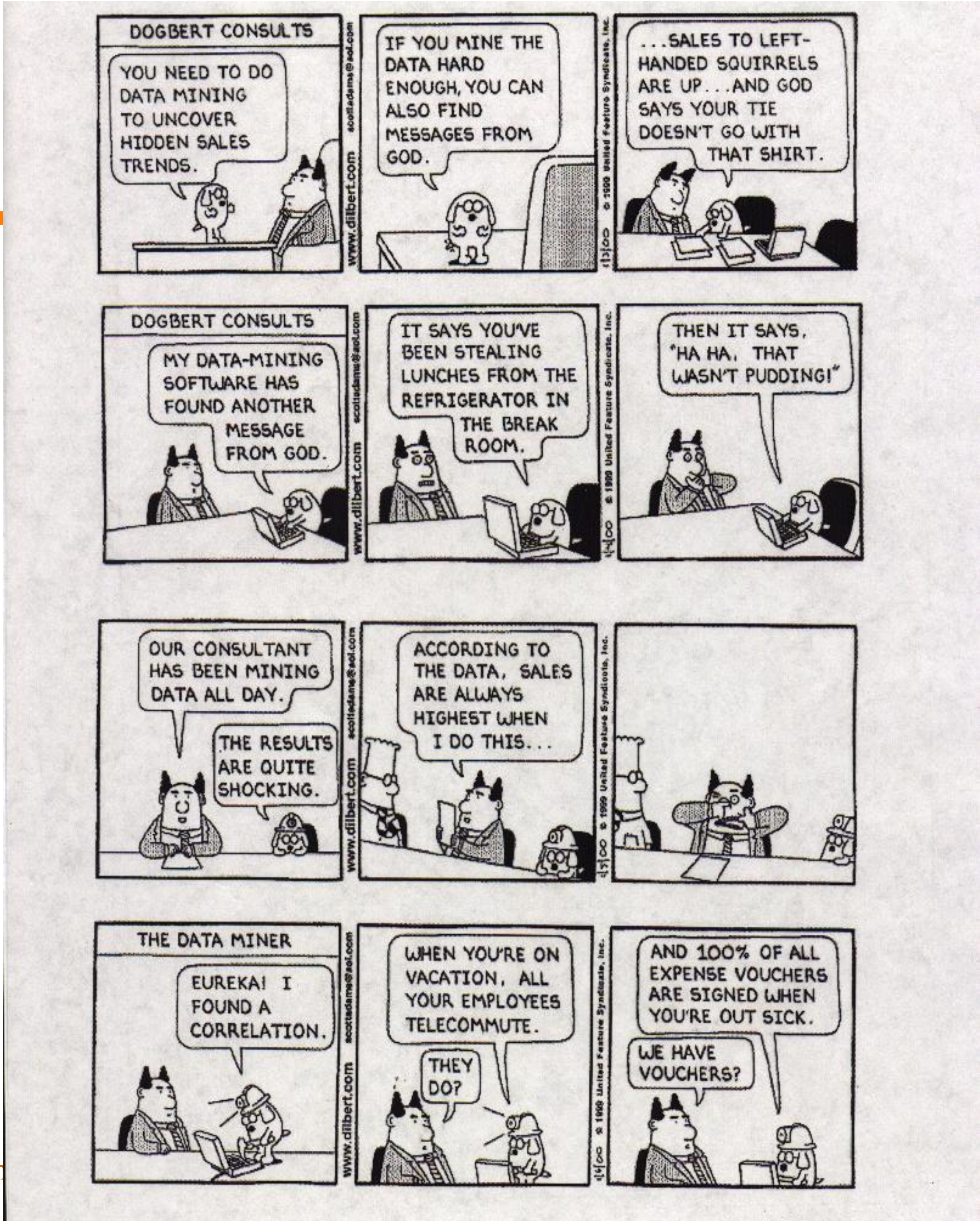
*"Knowledge Discovery in Databases (KDD) is the non-trivial process of identifying valid, novel, potentially useful, and ultimately understandable **patterns** in data."* (stored in databases, data warehouses, WWW and other large repositories)

(Fayyad, Piatetsky-Shapiro and Smyth, 96)

Patterns: associations, groupings, trends, anomalies,..

-"data mining" a misnomer!!

<u>Related Industry Terms</u>**: "business intelligence", "predictive modeling" and "data analytics"**


DOGBERT CONSULTS
YOU NEED TO DO DATA MINING TO UNCOVER HIDDEN SALES TRENDS.
IF YOU MINE THE DATA HARD ENOUGH, YOU CAN ALSO FIND MESSAGES FROM GOD.
...SALES TO LEFT-HANDED SQUIRRELS ARE UP...AND GOD SAYS YOUR TIE DOESN'T GO WITH THAT SHIRT.
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DOGBERT CONSULTS
MY DATA-MINING SOFTWARE HAS FOUND ANOTHER MESSAGE FROM GOD.
IT SAYS YOU'VE BEEN STEALING LUNCHES FROM THE REFRIGERATOR IN THE BREAK ROOM.
THEN IT SAYS, "HA HA. THAT WASN'T PUDDING!"
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OUR CONSULTANT HAS BEEN MINING DATA ALL DAY.
THE RESULTS ARE QUITE SHOCKING.
ACCORDING TO THE DATA, SALES ARE ALWAYS HIGHEST WHEN I DO THIS...
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THE DATA MINER
EUREKA! I FOUND A CORRELATION.
WHEN YOU'RE ON VACATION, ALL YOUR EMPLOYEES TELECOMMUTE.
THEY DO?
AND 100% OF ALL EXPENSE VOUCHERS ARE SIGNED WHEN YOU'RE OUT SICK.
WE HAVE VOUCHERS?
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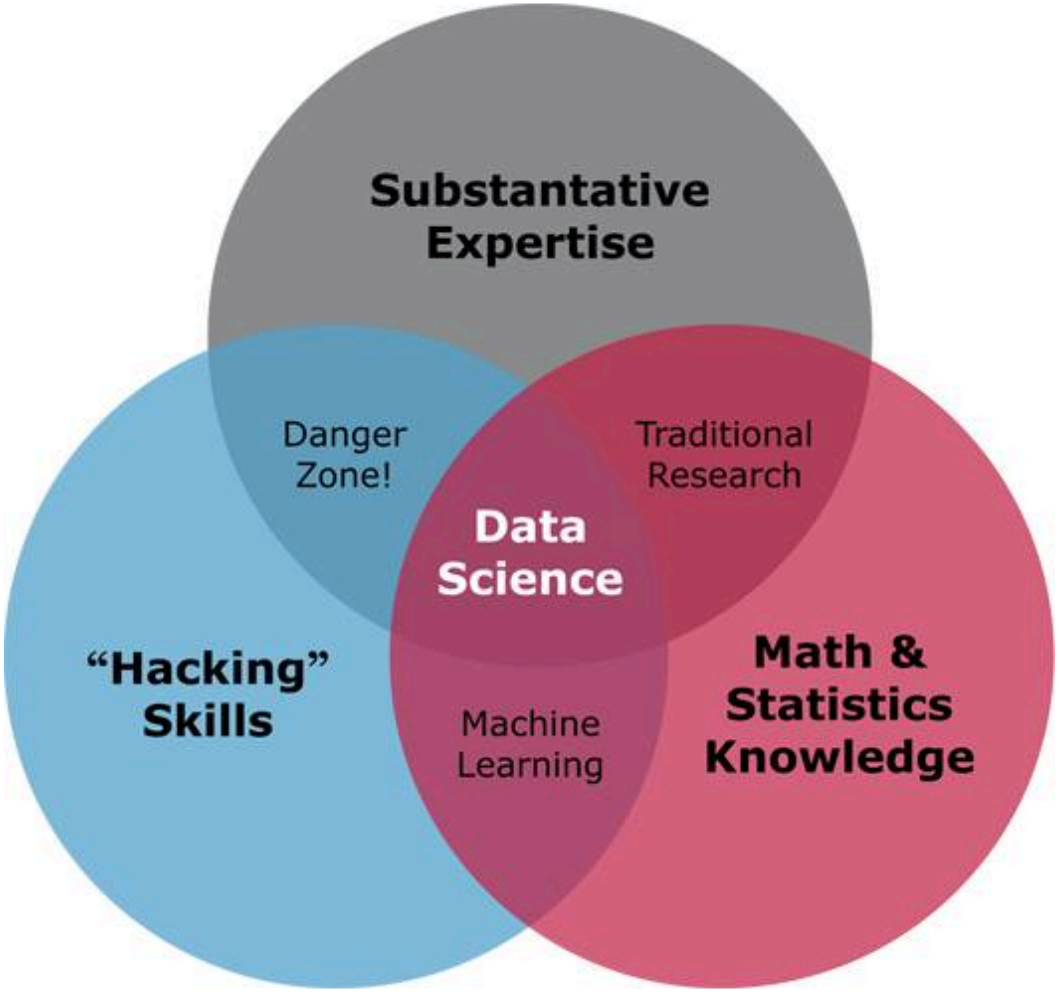
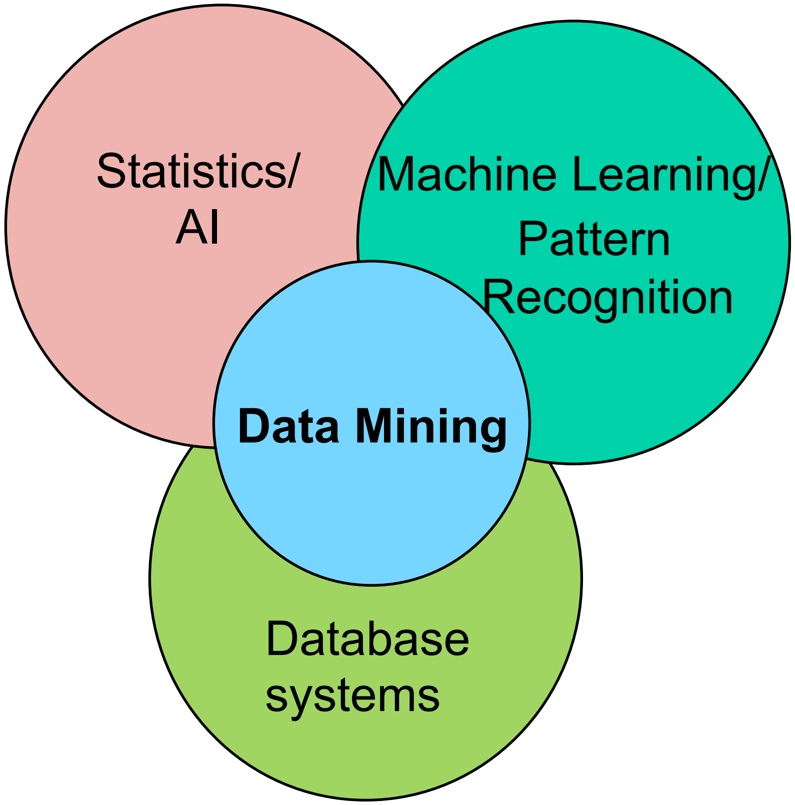
“Data Science”



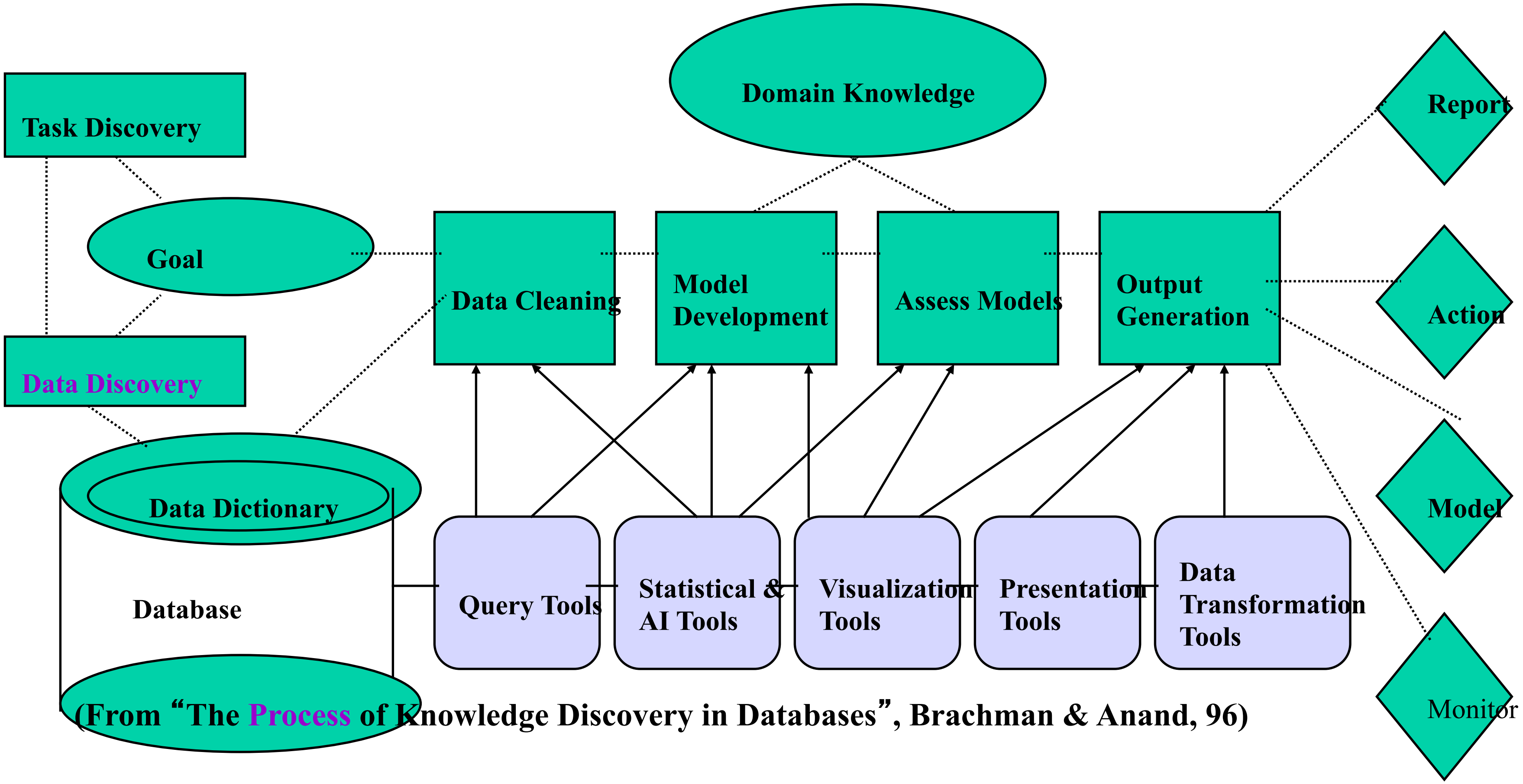
Skills Needed

- **Data Mining is multi-disciplinary**
  - machine learning/pattern recognition
  - Statistics
  - Databases and data warehouses
  - Business considerations
  - Visualization
  - Parallel/Distributed Processing (for BIGDATA)
  - …



(Inter-disciplinary) Process of Data Mining

Collect ***Prepare*** ***Analyze*** ***Consume***



(From "The Process of Knowledge Discovery in Databases", Brachman & Anand, 96)

Iterative Process at multiple levels

Data Driven Modeling Approaches and Goals

- **Seek (aggregate) models**
  - (quick) large scale summary of data
    - E.g. characterize dominant customer types

- **Seek (local) patterns**
  - Characterise a small portion of data
    e.g. "rare patterns": fraud or intrusion detection

- Goals:
  - **Description:** Find human-interpretable patterns that describe the data.
  - **Prediction:** Use some variables to predict unknown or future values of other variables.
  - Prescription: (tough!!)

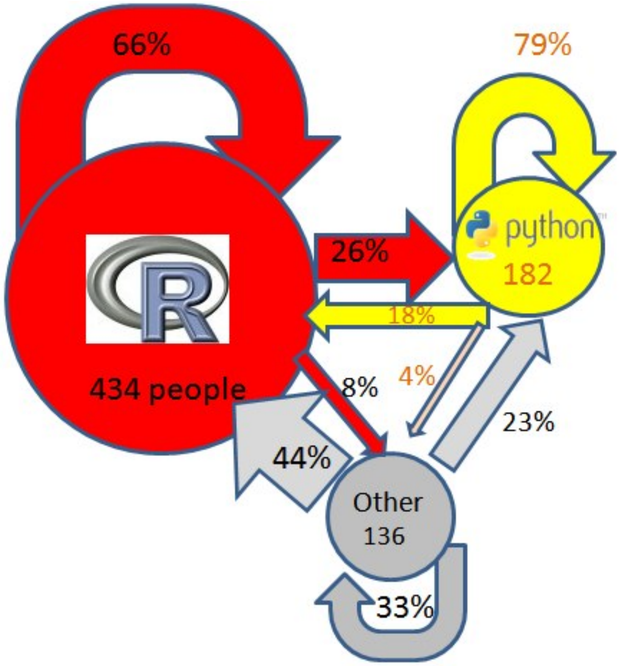
Analysis is often **retrospective.**

Texts

- **Basic**
  - **KJ:** Kjell and Johnson. Applied Predictive Modeling, Springer 2013.
  - http://appliedpredictivemodeling.com/
  - **JW: ISLR:** elementary stats with R
  - http://www-bcf.usc.edu/~gareth/ISL/ISLR%20First%20Printing.pdf
- **More Advanced**
  - **B: Bishop, Pattern Recognition and Machine Learning (more mathematical, Bayesian)** **http://www.rmki.kfki.hu/~banmi/elte/Bishop%20-%20Pattern%20Recognition%20and%20Machine%20Learning.pdf**
  - **HTF:** Hastie/Tibshirani/Friedman **(stats)**
  - **http://www-stat.stanford.edu/~tibs/ElemStatLearn/**
- **Other general references:**
  - **KM:** Kevin Murphy, MIT Press, 2013.
  - **TSK:** Tan/Steinbach/Kumar **(algorithms; broad)**
    - Book supplements, including sample chapters 4,6 and 8 found at:
    - http://www-users.cs.umn.edu/~kumar/dmbook/index.php

Languages and Software

- Stats oriented: R, Python (with packages)
  - Commercial: SAS, IBM SPSS,..
  - Open: GUI oriented: Knime, RapidMiner
- General purpose (Java for text analysis)
- Distributed/bigdata
  - Hadoop/Spark/MapReduce/PigLatin
  - HIVE (SQL like for Hadoop)
  - Various NoSQL



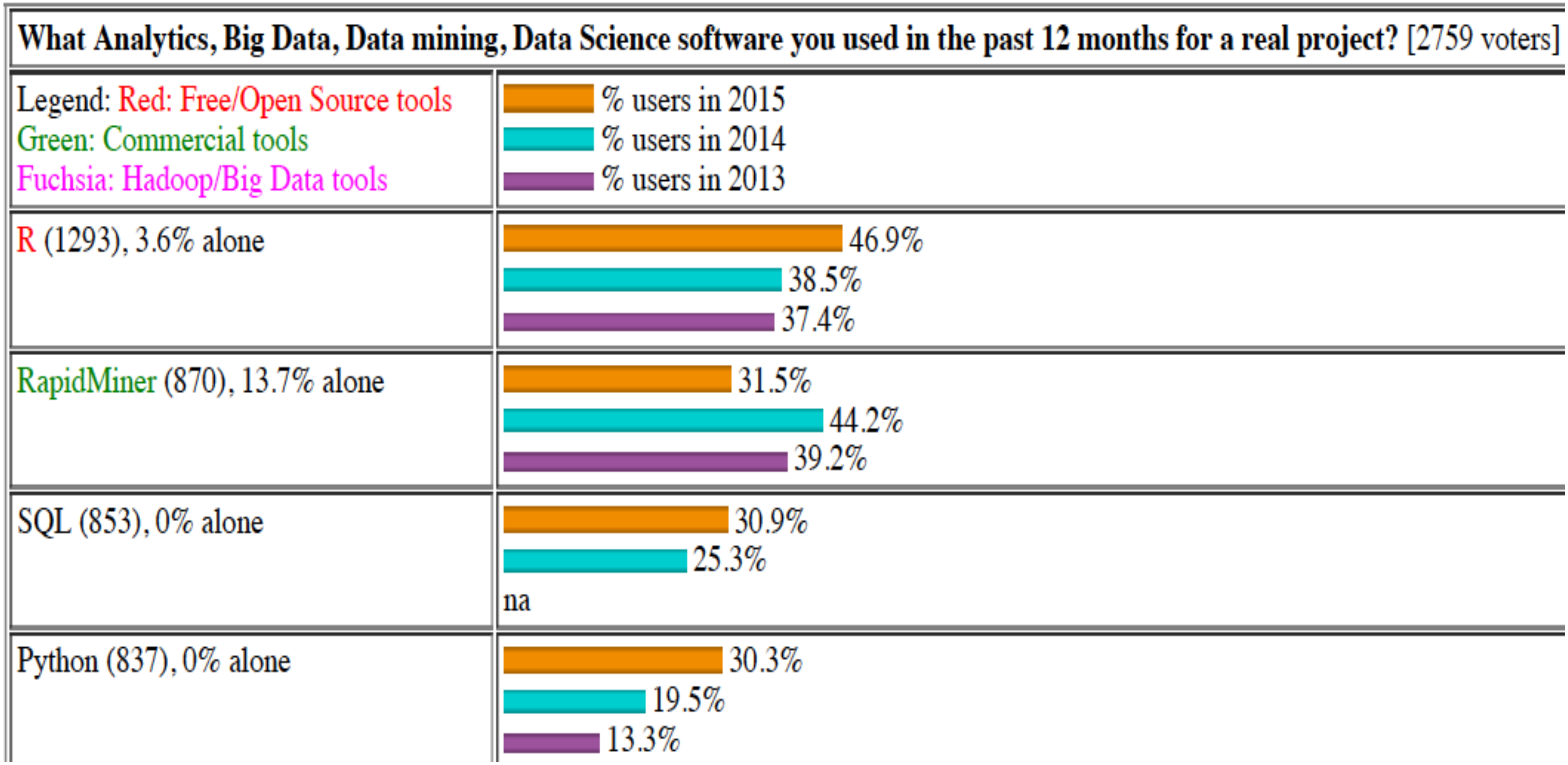
From KDNuggets Poll, 12/13
http://www.kdnuggets.com/2013/12/poll-results-r-leading-python-gaining.html

R or Python? See

- http://www.kdnuggets.com/2015/05/r-vs-python-data-science.html
- http://blog.udacity.com/2015/01/python-vs-r-learn-first.html

KDD Nuggets Survey May 2015

- http://www.kdnuggets.com/2015/05/poll-r-rapidminer-python-big-data-spark.html



What Analytics, Big Data, Data mining, Data Science software you used in the past 12 months for a real project? [2759 voters]

Legend: Red: Free/Open Source tools Green: Commercial tools Fuchsia: Hadoop/Big Data tools	🟧 % users in 2015 🟦 % users in 2014 🟪 % users in 2013
R (1293), 3.6% alone	46.9% 38.5% 37.4%
RapidMiner (870), 13.7% alone	31.5% 44.2% 39.2%
SQL (853), 0% alone	30.9% 25.3% na
Python (837), 0% alone	30.3% 19.5% 13.3%

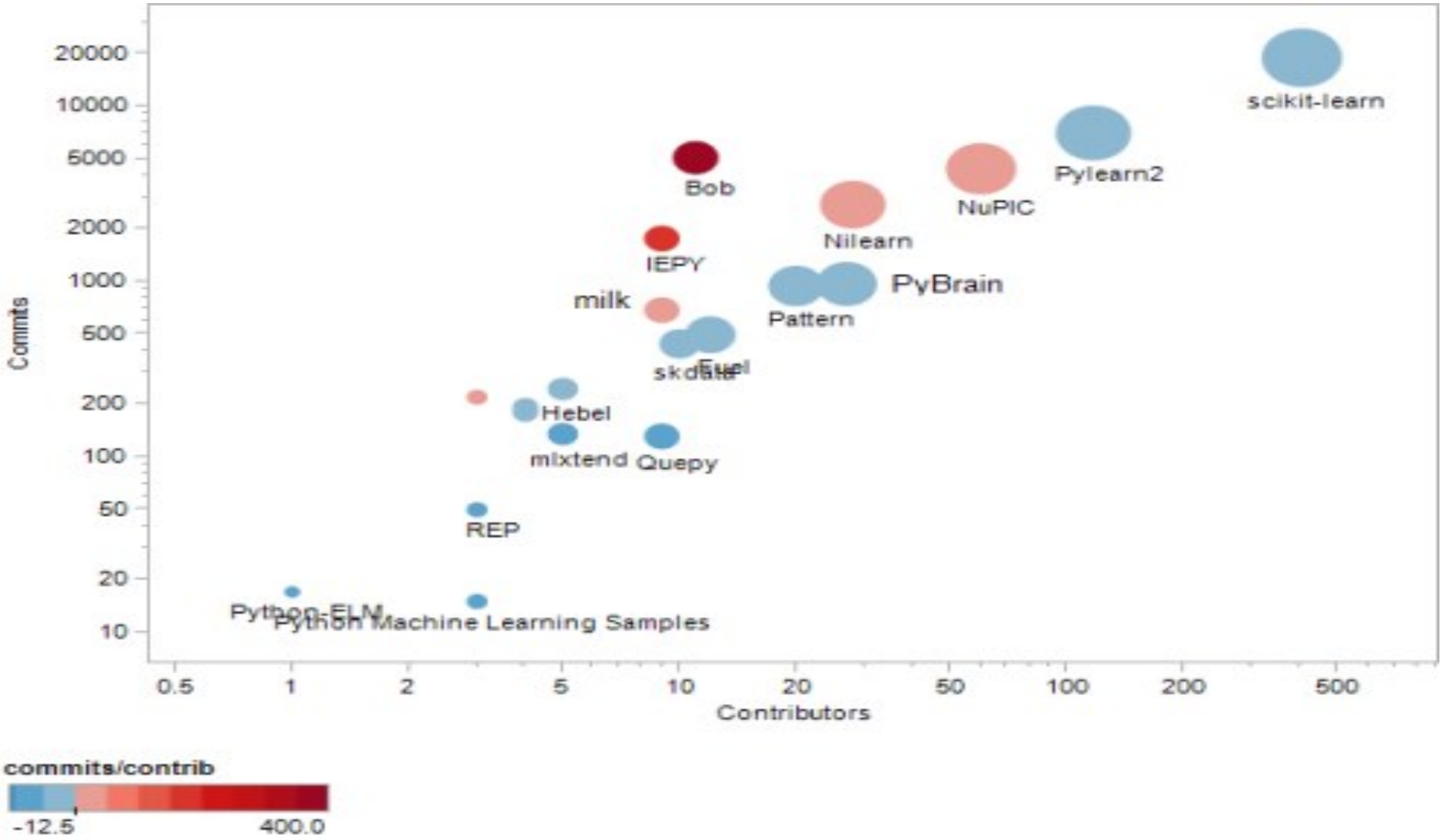
Cheat Sheets

- http://www.kdnuggets.com/2015/07/good-data-science-machine-learning-cheat-sheets.html

- Inter-operability
  – http://www.kdnuggets.com/2015/10/integrating-python-r-executing-part2.html

Top 20 Python Machine Learning Open Source Projects (on Github)

- http://www.kdnuggets.com/2015/06/top-20-python-machine-learning-open-source-projects.html



Types of Modeling

Consider a large collection of fruits

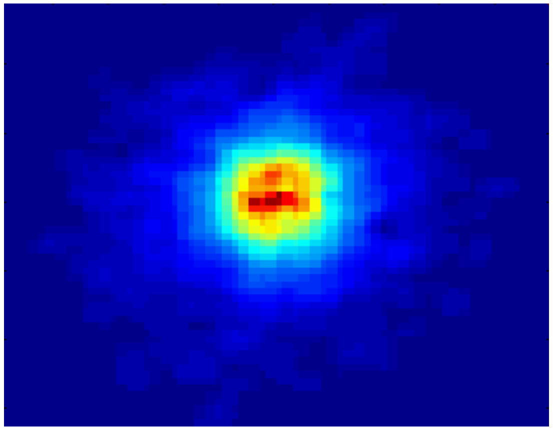
- How to characterize each fruit? (weight, volume, …..)
  - How many "attributes" to use?

- **Regression**: predicting weight based on other attributes….
- **Classification:** predicting what type of fruit is it? (class hierarchy!)
- **Ranking and Recommendations**
- **Clustering (grouping):** how many different types of fruits are there?
- **Anomaly detection**
- **Sequence analysis**
- **…..**
- **Topics not new, but some data mining concerns/aspects are…**
- Predictive Modeling: Developing mathematical models that make accurate predictions

Classifying Galaxies

Courtesy: http://aps.umn.edu

Early



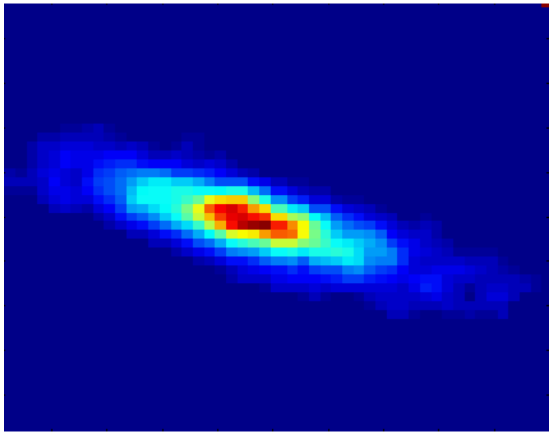
Class:

- **Stages of Formation**

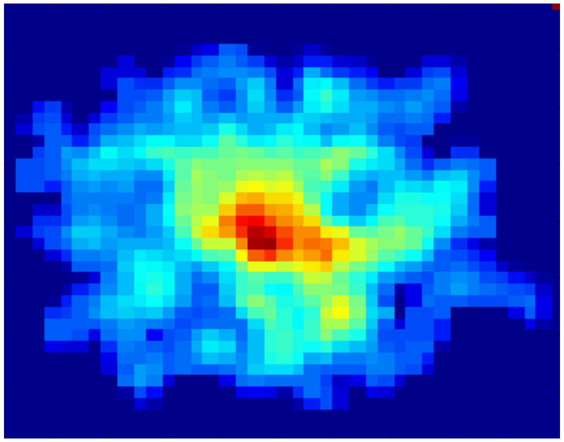
Attributes:

- **Image features,**
- **Characteristics of light waves received, etc.**

Intermediate



Late



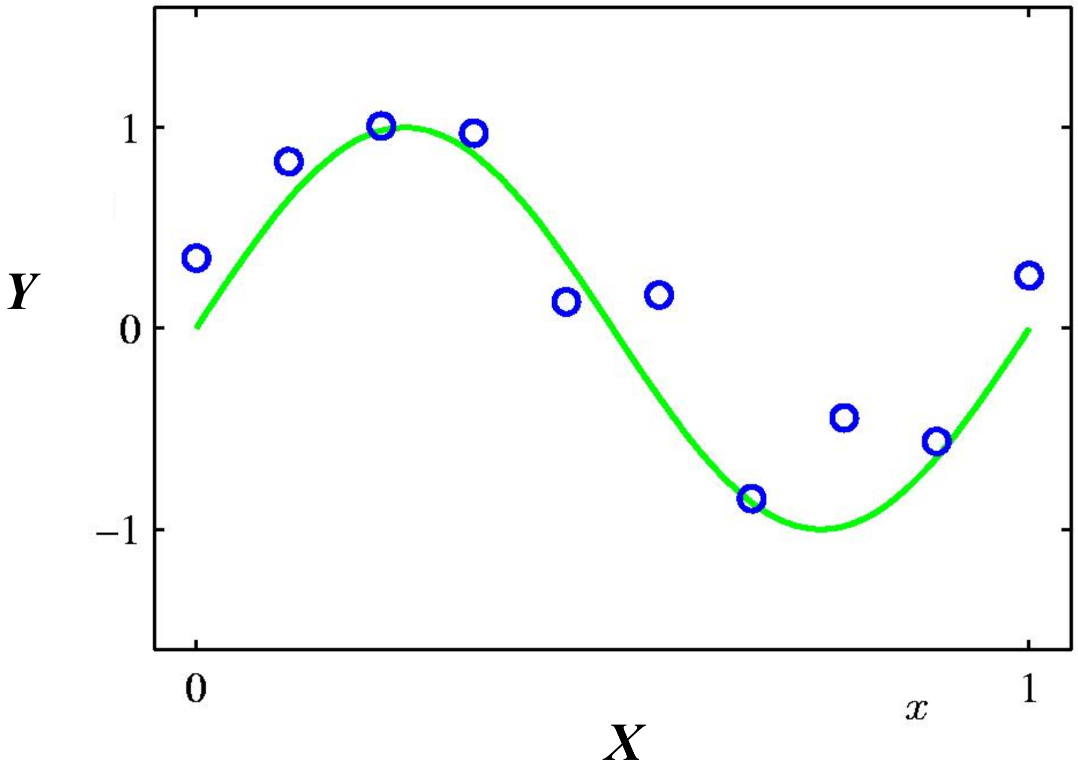
Data Size:

- **72 million stars, 20 million galaxies**
- **Object Catalog: 9 GB**
- **Image Database: 150 GB**

Regression: Curve Fitting

- **E.g. using polynomials:**

$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$



Jargon

- "**x**": independent variable(s) / predictors/input /features/ attributes
- "**y**": dependent variable(s) / target / output /

- Record: instance/ data-point /object
  - Contains **x**, may contain **y** (training data)

  - Classification: **y** =?
  - Regression: **y** =?

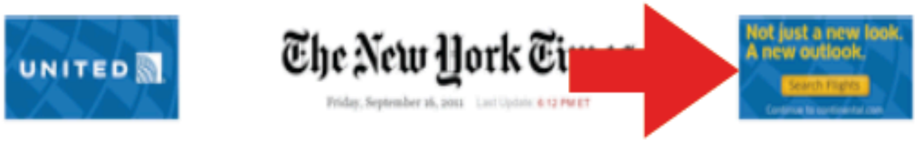
  - Common issues: model validity and fit, curse of dimensionality,…

Degrees of Supervision in Learning Algorithms

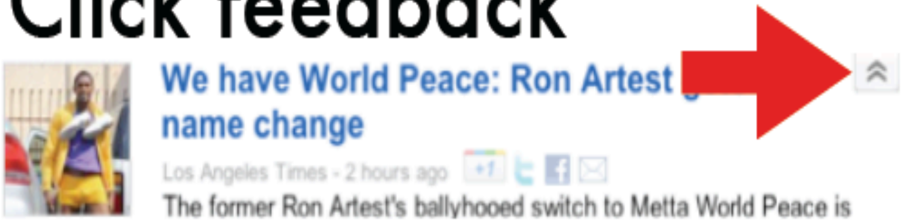
- 1. Unsupervised (clustering)
- 2. Semi-supervised
- 3. Noisy or implicit labels (examples to the right)
- 4. "Ground truth" – actual value of output known for some data

- Internet scale analytics relies a lot on 1-3:

- Ads



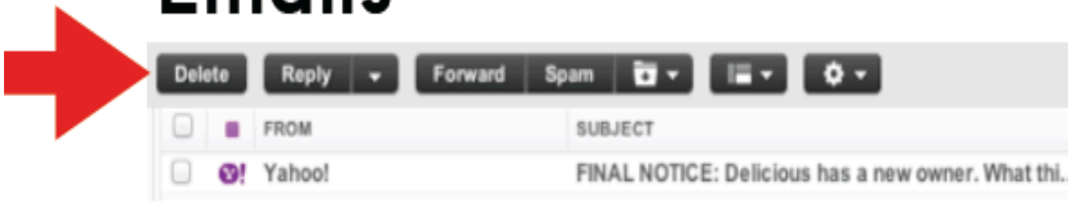
- Click feedback


We have World Peace: Ron Artest name change

Los Angeles Times - 2 hours ago

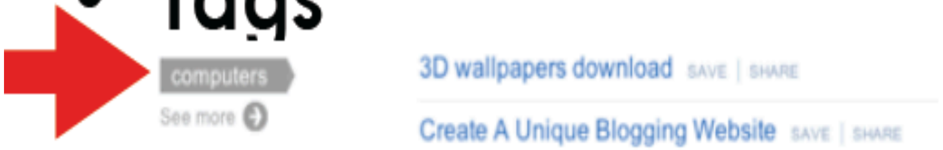
The former Ron Artest's ballyhooed switch to Metta World Peace is

- Emails



	FROM	SUBJECT
□	Yahoo!	FINAL NOTICE: Delicious has a new owner. What thi..

- Tags



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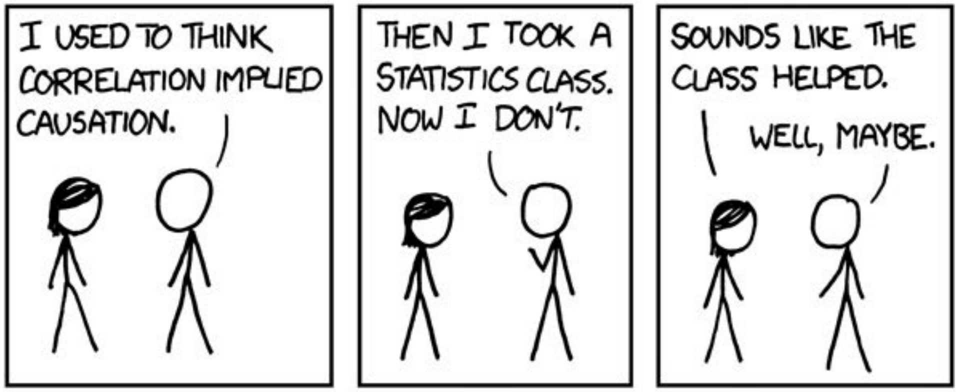
Course Goals

- study different predictive models for a given task
  - Properties, pros and cons
  - Evaluation metrics
  - Build predictive models in R and Python
- Process-oriented viewpoint
- Introduction to issues of scale and real data considerations
- Reason about data analysis and the "results" obtained
  - People who listen to smooth jazz and eat at Red Lobster voted for Obama and those who are big fans of college football and eat at Olive Garden voted for Romney (CNN-HN, 11/2012)


I USED TO THINK CORRELATION IMPLIED CAUSATION.
THEN I TOOK A STATISTICS CLASS. NOW I DON'T.
SOUNDS LIKE THE CLASS HELPED.
WELL, MAYBE.

XKCD

No Free Lunch (NFL)

- No universally best model; so understand tradeoffs.
- Table from HTF

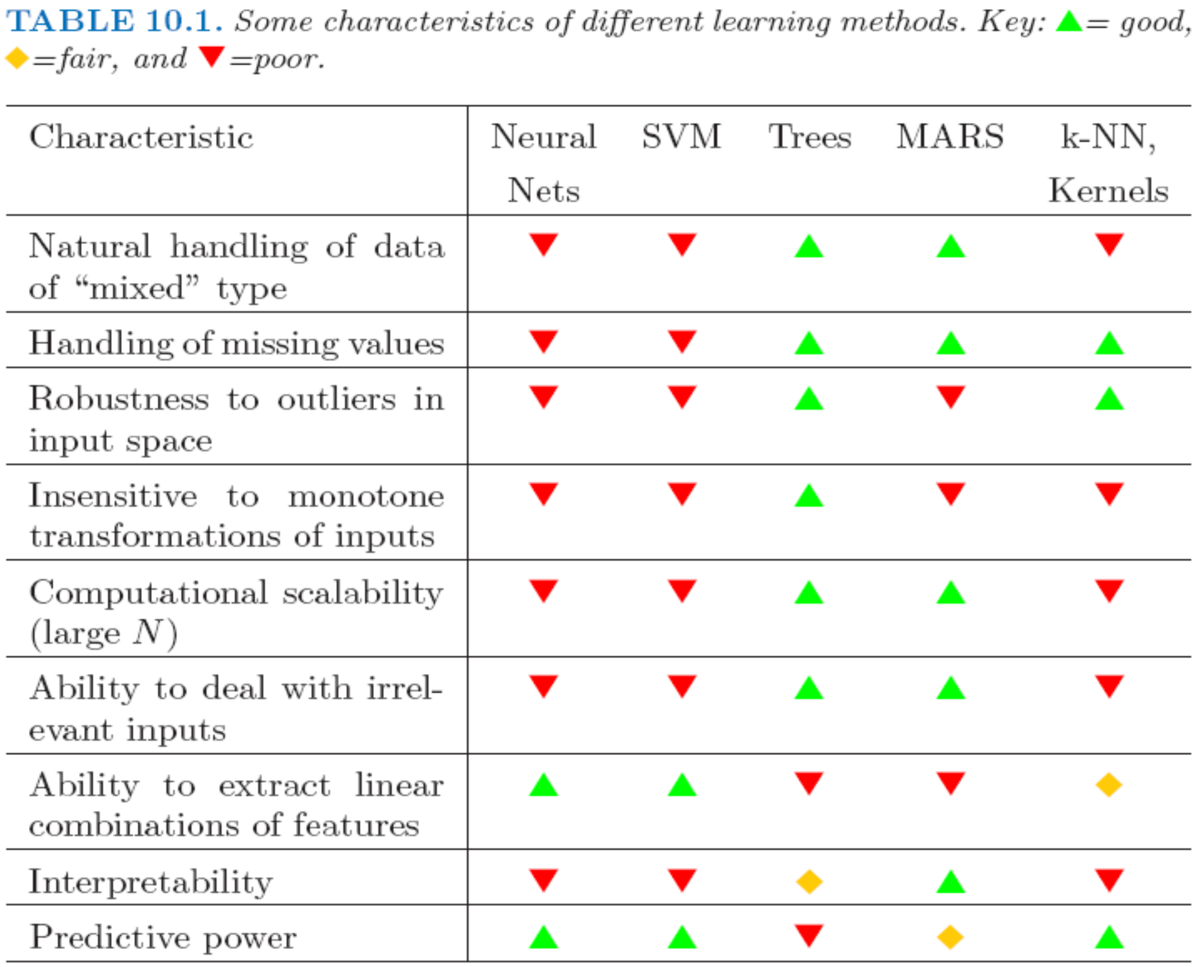


TABLE 10.1. *Some characteristics of different learning methods. Key:* ▲*= good,* ◆*=fair, and* ▼*=poor.*

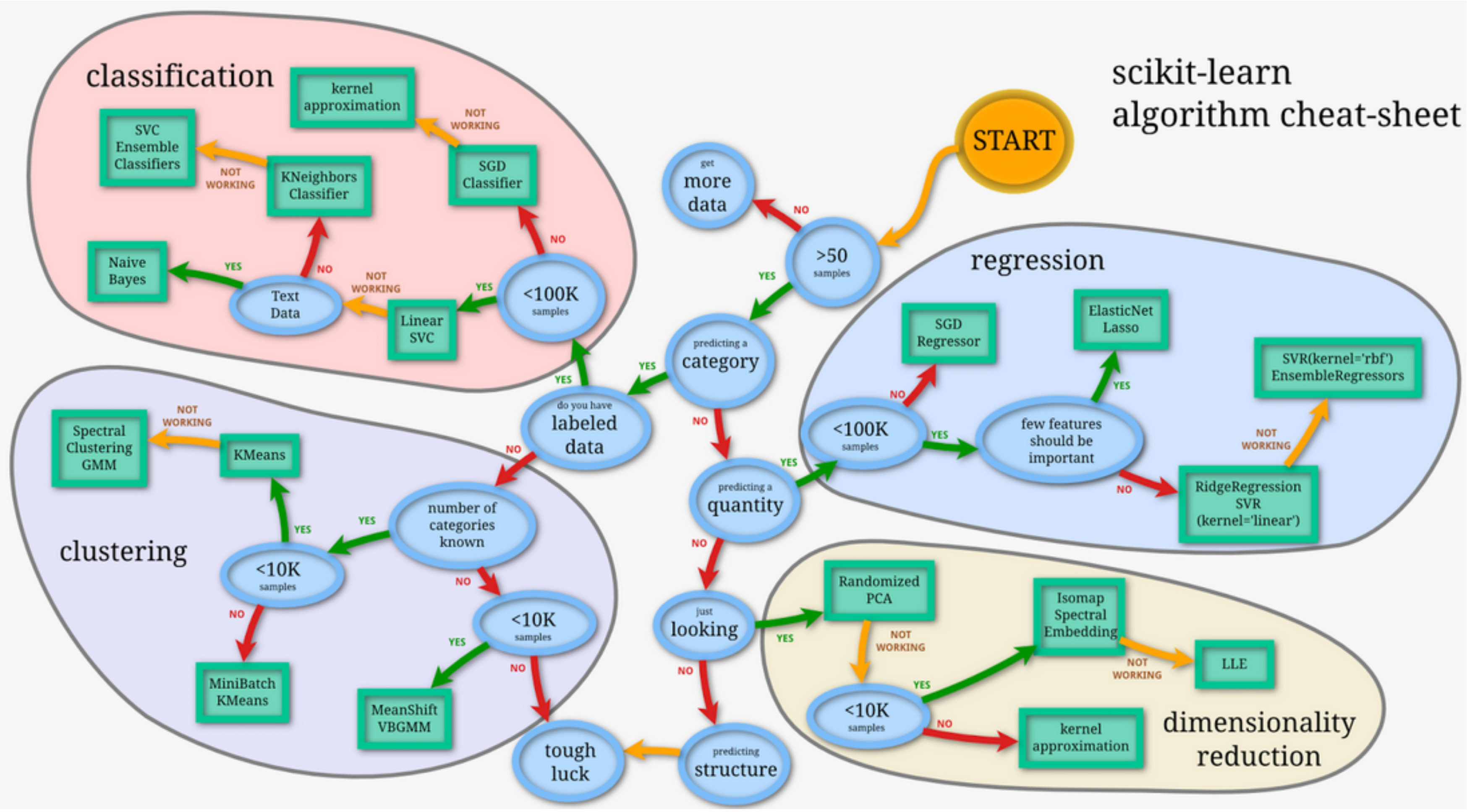
Characteristic	Neural Nets	SVM	Trees	MARS	k-NN, Kernels
Natural handling of data of "mixed" type	▼	▼	▲	▲	▼
Handling of missing values	▼	▼	▲	▲	▲
Robustness to outliers in input space	▼	▼	▲	▼	▲
Insensitive to monotone transformations of inputs	▼	▼	▲	▼	▼
Computational scalability (large N)	▼	▼	▲	▲	▼
Ability to deal with irrelevant inputs	▼	▼	▲	▲	▼
Ability to extract linear combinations of features	▲	▲	▼	▼	◆
Interpretability	▼	▼	◆	▲	▼
Predictive power	▲	▲	▼	◆	▲

It Depends

- “all models are wrong, but some are useful”
  - George Box, 1987

- All statistical models make assumptions
  - (Lets pretend…)
  - Given the situations, some assumptions are plausible, others are not

Cheat Sheets



Local vs Global Models (from HTF Ch. 2)

- K-nearest neighbor (KNN)

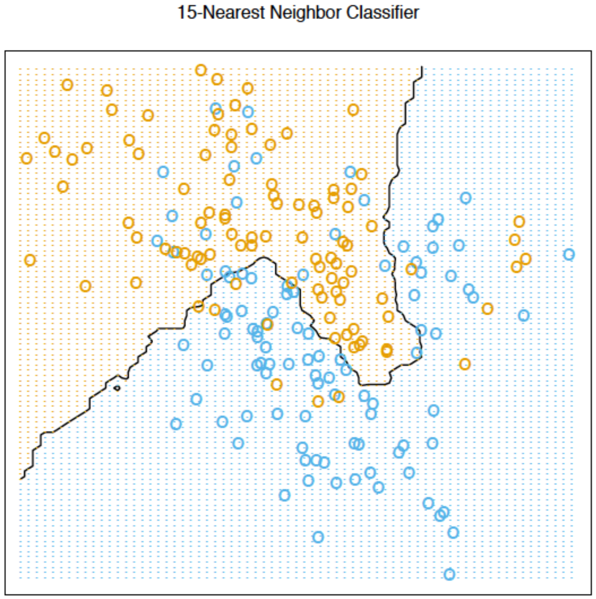


FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$) *and then fit by 15-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the 15-nearest neighbors.*

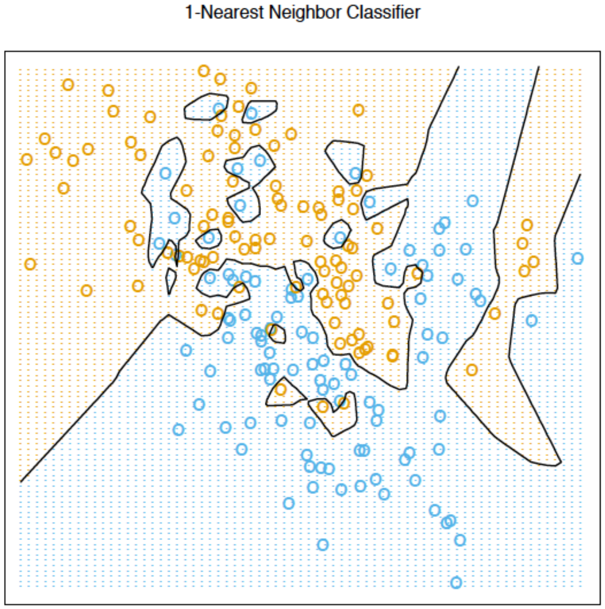


FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$), *and then predicted by 1-nearest-neighbor classification.*

KNN vs Linear Regression

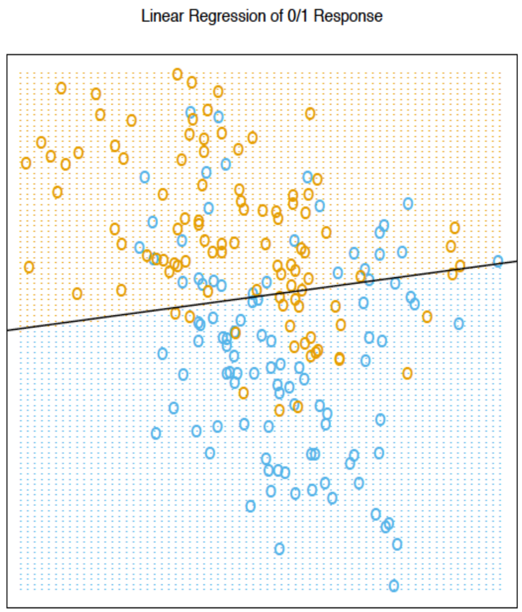


FIGURE 2.1. *A classification example in two dimensions. The classes are coded as a binary variable (*BLUE *$= 0$,* ORANGE *$= 1$), and then fit by linear regression. The line is the decision boundary defined by $x^T\hat{\beta} = 0.5$. The orange shaded region denotes that part of input space classified as* ORANGE*, while the blue region is classified as* BLUE.

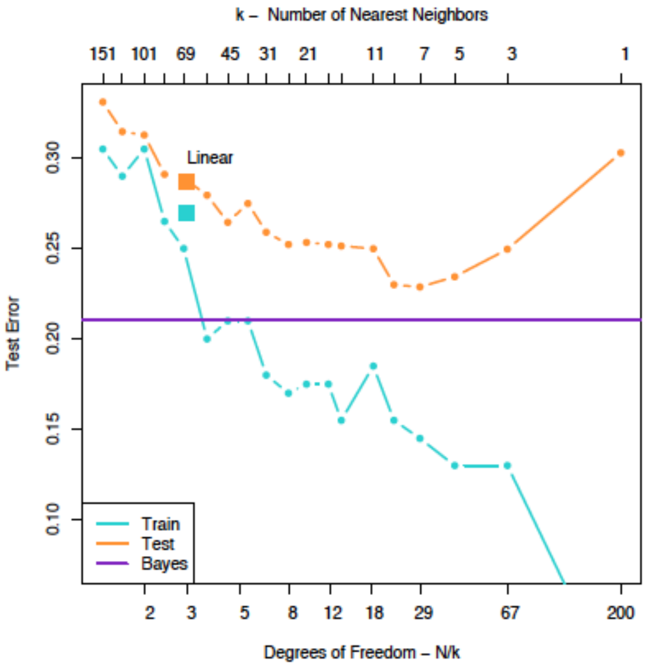


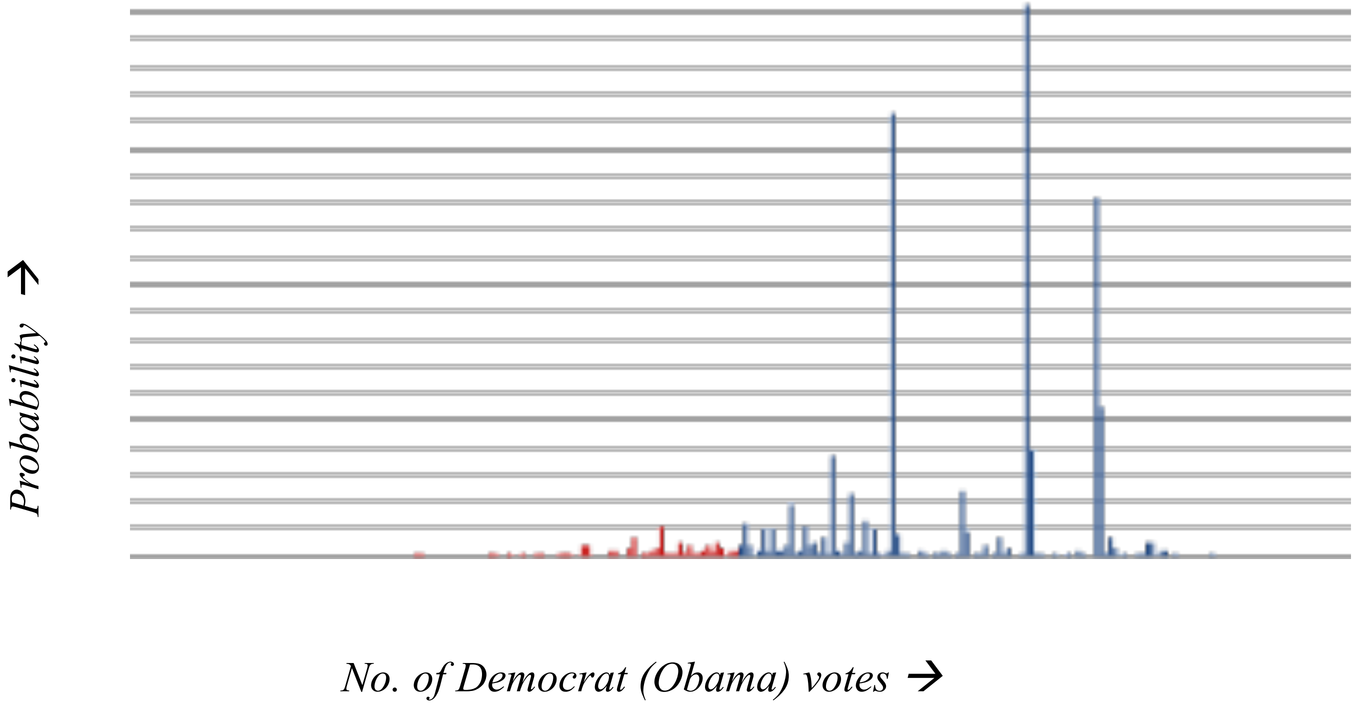
FIGURE 2.4. *Misclassification curves for the simulation example used in Figures 2.1, 2.2 and 2.3. A single training sample of size 200 was used, and a test sample of size 10,000. The orange curves are test and the blue are training error for k-nearest-neighbor classification. The results for linear regression are the bigger orange and blue squares at three degrees of freedom. The purple line is the optimal Bayes error rate.*

Towards Good Predictive Models

- Use data driven models to complement domain expertise and intuition (see quotes in KJ 1.2)
  - Understand problem context
  - Get relevant data
  - Use versatile toolbox and select appropriately
    - Prediction vs. interpretation tradeoff
    - Tailor to data properties
      - » But do not overfit
  - Convey results effectively

Nate Silver's 2012 model

- Uncertainly is everywhere
  - even in the "perfect" model
  - (used weighted ensemble)

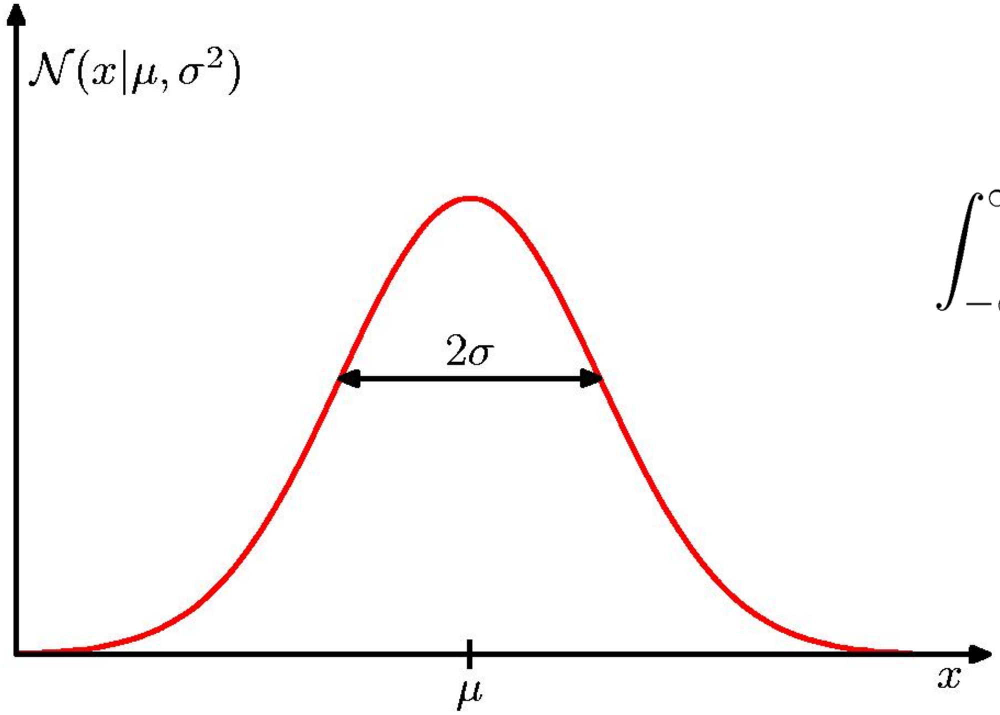


Probability Recap

- Basic Concepts:
  - Joint distribution
  - Marginal distribution
  - Conditional distribution
  - Variance and covariance

The Gaussian Distribution

$$\mathcal{N}\left(x|\mu,\sigma^2\right) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu,\sigma^2\right)\,\mathrm{d}x = 1$$

Gaussian Mean and Variance

$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x \, \mathrm{d}x = \mu$$

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x^2 \, \mathrm{d}x = \mu^2 + \sigma^2$$

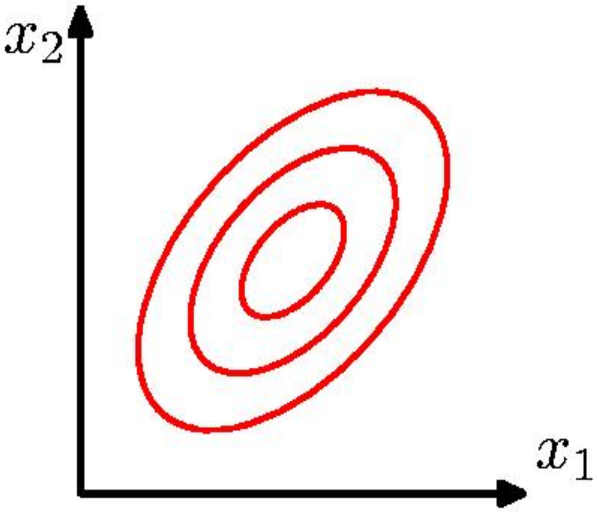
$$\operatorname{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$

The Multivariate Gaussian (in D dimensions)

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

Vector Mean

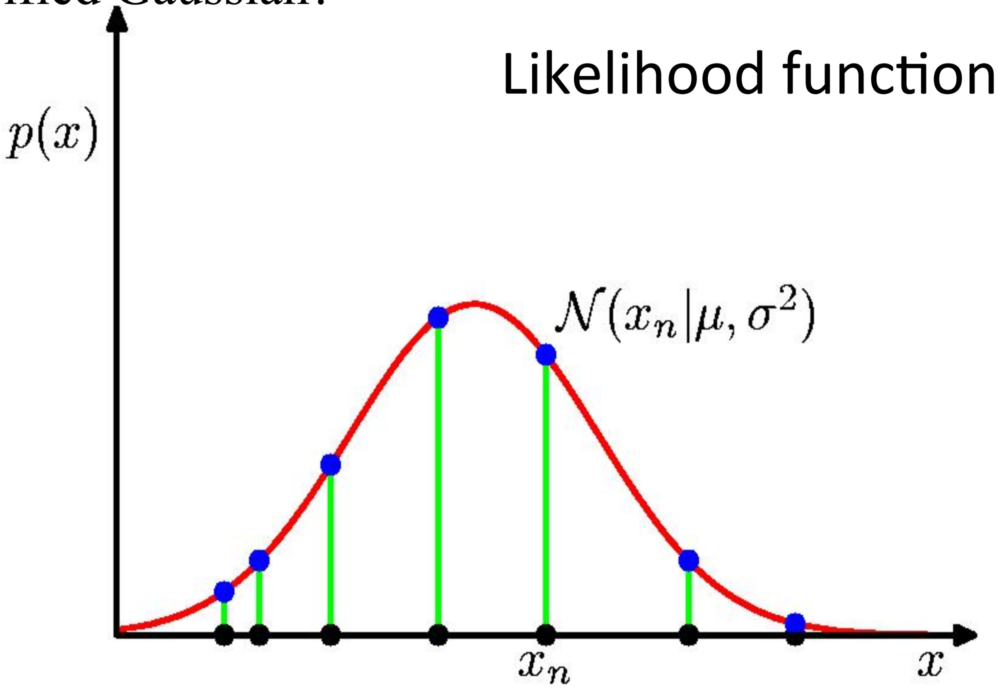
D-by-D Covariance Matrix



Marginals and *conditionals* of multivariate Gaussians?

Gaussian Parameter Estimation

- What is the probability that a datset **x** with $\mathcal{N}$i.i.d. points was obtained by a specified Gaussian?



Likelihood function

$$p(\mathbf{x}|\mu,\sigma^2) = \prod_{n=1}^{N} \mathcal{N}\left(x_n|\mu,\sigma^2\right)$$

Maximum (Log) Likelihood or M(L)L

- **Selects the Gaussian that most likely produced the given dataset x.**
- **Log Likelihood =**
- $$\ln p\left(\mathbf{x}|\mu,\sigma^2\right) = -\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu)^2 - \frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi)$$

(Note: for fixed σ, "cost" is sum/mean squared error)

- **Maximized when**

$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}x_n$$

$$\sigma^2_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}(x_n-\mu_{\mathrm{ML}})^2$$

Are ML estimates *biased*?

Curse of Dimensionality

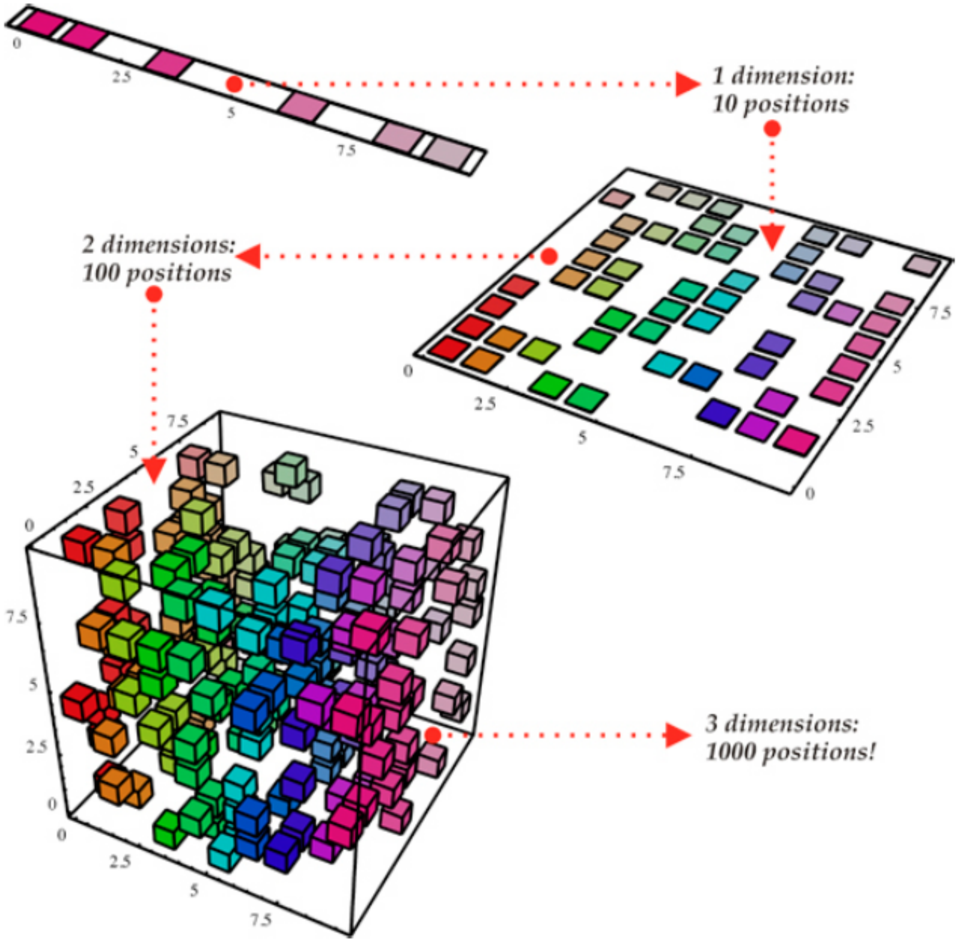
See HTF pp 22-26.

- Exponential growth of # of cells with # of dimensions, p
  - implications

- Where is probability mass concentrated in "hyper"cubes/spheres, as p gets large?

- What happens to inter-point distances for randomly scattered points in high-p?

Visualizing the Curse



1 dimension:
10 positions

2 dimensions:
100 positions

3 dimensions:
1000 positions!

Extras

A Brief History of Data Mining Society

- 1989 IJCAI Workshop on Knowledge Discovery in Databases
  - Knowledge Discovery in Databases (G. Piatetsky-Shapiro and W. Frawley, 1991)
- 1991-1994 Workshops on Knowledge Discovery in Databases
  - Advances in Knowledge Discovery and Data Mining (U. Fayyad, G. Piatetsky-Shapiro, P. Smyth, and R. Uthurusamy, 1996)
- 1995-1998 International Conferences on Knowledge Discovery in Databases and Data Mining (KDD' 95-98)
  - Journal of Data Mining and Knowledge Discovery (1997)
- ACM SIGKDD conferences since 1998 and SIGKDD Explorations
- More conferences on data mining
  - PAKDD (1997), PKDD (1997), SIAM-Data Mining (2001), (IEEE) ICDM (2001), etc.
- ACM Transactions on KDD started in 2007

Conferences and Journals on Data Mining

- KDD Conferences
  - ACM SIGKDD Int. Conf. on Knowledge Discovery in Databases and Data Mining (KDD)
  - SIAM Data Mining Conf. (SDM)
  - (IEEE) Int. Conf. on Data Mining (ICDM)
  - Conf. on Principles and practices of Knowledge Discovery and Data Mining (PKDD)
  - Pacific-Asia Conf. on Knowledge Discovery and Data Mining (PAKDD)
  - Predictive Analytic World (PAW)

    industry focussed.
- Other related conferences
  - ACM SIGMOD
  - VLDB
  - (IEEE) ICDE
  - WWW, SIGIR
  - ICML, CVPR, NIPS
- Journals
  - Data Mining and Knowledge Discovery (DAMI or DMKD)
  - IEEE Trans. On Knowledge and Data Eng. (TKDE)
  - KDD Explorations
  - ACM Trans. on KDD

Where to Find References?

DBLP, CiteSeer, Google Scholar

- Data mining and KDD (SIGKDD: CDROM)
  - Conferences: ACM-SIGKDD, IEEE-ICDM, SIAM-DM, PKDD, PAKDD, etc.
  - Journal: Data Mining and Knowledge Discovery, KDD Explorations, ACM TKDD (new)
- Database systems (SIGMOD: ACM SIGMOD Anthology—CD ROM)
  - Conferences: ACM-SIGMOD, ACM-PODS, VLDB, IEEE-ICDE, EDBT, ICDT, DASFAA
  - Journals: IEEE-TKDE, ACM-TODS/TOIS, JIIS, J. ACM, VLDB J., Info. Sys., etc.
- AI & Machine Learning
  - Conferences: Machine learning (ML), AAAI, IJCAI, COLT (Learning Theory), CVPR, NIPS, etc.
  - Journals: JMLR, Machine Learning, Artificial Intelligence, Knowledge and Information Systems, IEEE-PAMI, etc.
- Web and IR
  - Conferences: SIGIR, WWW, CIKM, etc.
  - Journals: WWW: Internet and Web Information Systems,
- Statistics
  - Conferences: Joint Stat. Meeting, etc.
  - Journals: Annals of statistics, etc.
- Visualization
  - Conference proceedings: CHI, ACM-SIGGraph, etc.
  - Journals: IEEE Trans. visualization and computer graphics, etc.

Data Mining Group at the University of Texas

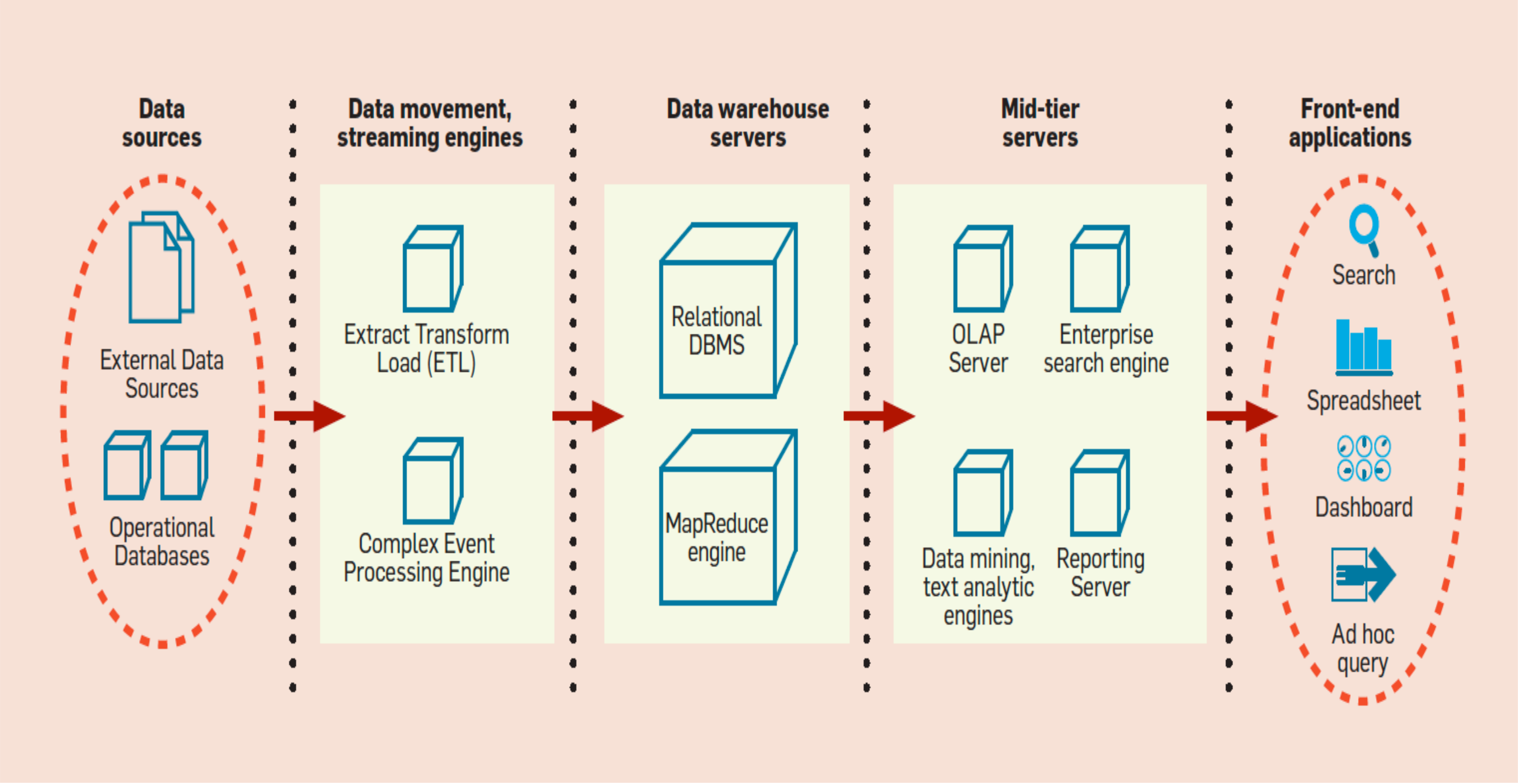
- Joydeep Ghosh (ECE):
  - web mining; adaptive systems; image/signals; system integration
- Raymond Mooney (CS):
  - Machine learning; natural language processing
- ML Theory Oriented: Sujay Sanghavi (ECE) sparsity); Caramanis (ECE) optimization; P. Ravikumar (CS) graphical models/stats;
- Applied Statisticians (McCombs)
- Inderjit Dhillon (CS) – linear algebra; Ed Marcotte (Biochem) – bioinformatics ; Mia Markey (Biomed); Kristen Grauman (CS) – computer vision; Maytal T. (marketing); Matt Lease (I-school) text; Jason Baldridge (linguistics)…

  - NEW: Division of Statistics and Scientific Computation http://ssc.utexas.edu/
  - **McCombs: Masters in Business Analytics**

PM vs. Business Intelligence (BI)

- From Chaudhuri et al, “An Overview of BI Technology”, CACM Aug 2011, pp. 88

Figure 1. Typical business intelligence architecture.


Data sources
External Data Sources
Operational Databases
Data movement, streaming engines
Extract Transform Load (ETL)
Complex Event Processing Engine
Data warehouse servers
Relational DBMS
MapReduce engine
Mid-tier servers
OLAP Server
Enterprise search engine
Data mining, text analytic engines
Reporting Server
Front-end applications
Search
Spreadsheet
Dashboard
Ad hoc query