Data Mining

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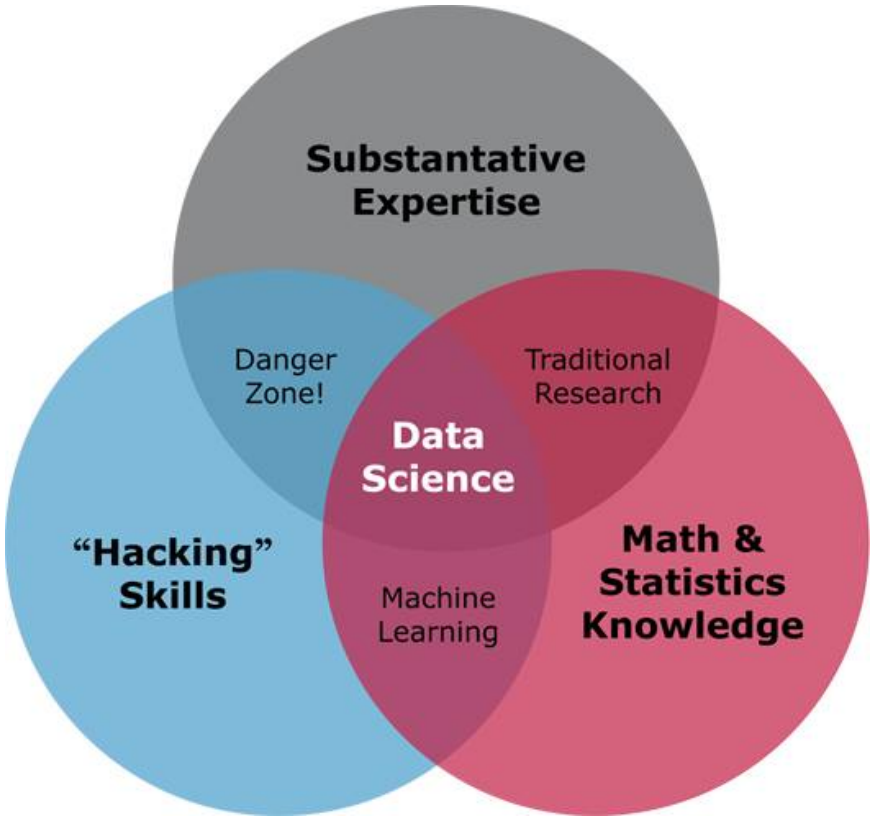
Data “Science”

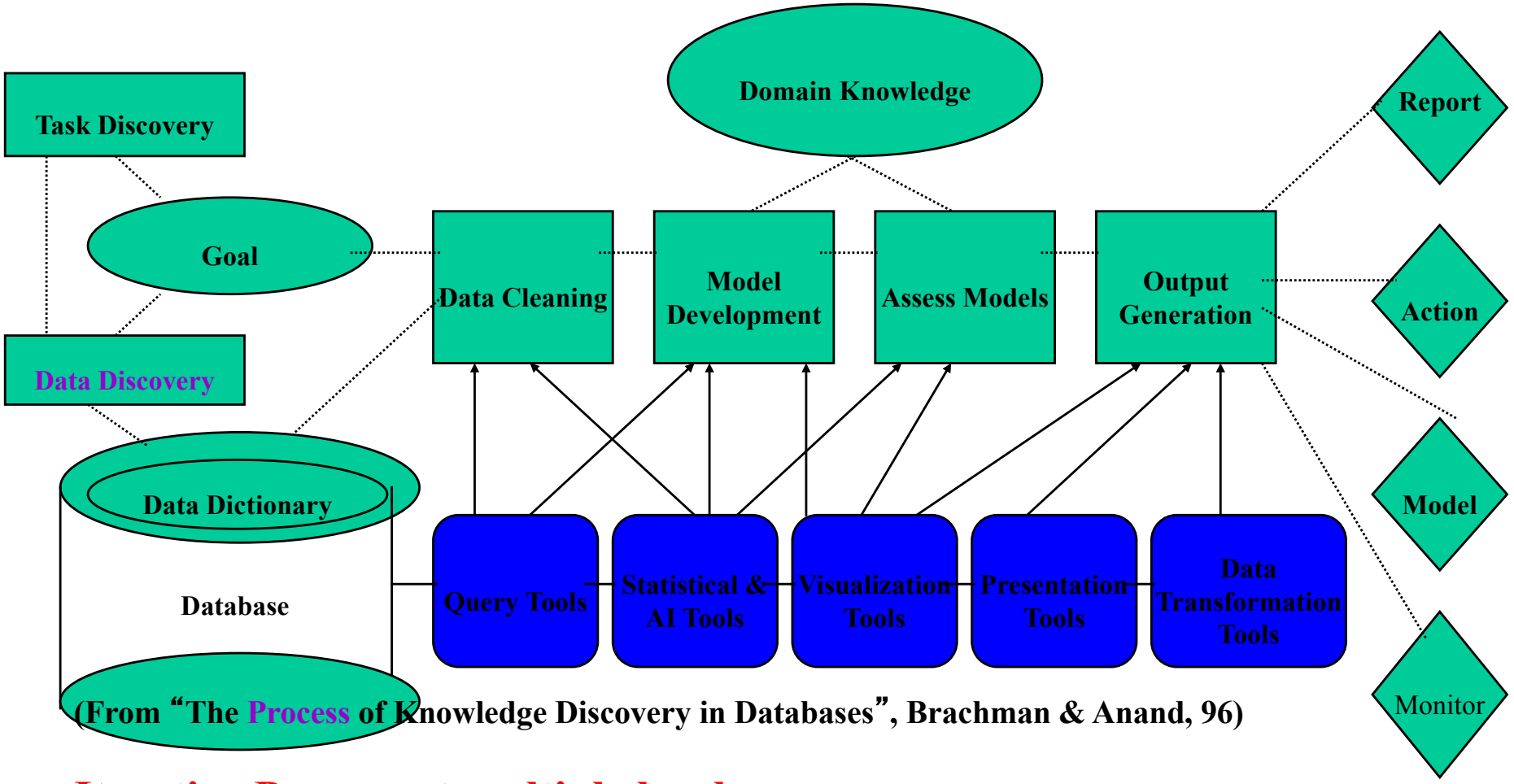


- *Business Problem → Data Science sub-problems*
- *Additional AI modalities*
- *Enterprise Delivery Platform*
- *U/I and U/X*

https://cyborgus.com/2017/03/13/think-like-data-scientist/

(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.**

Backup 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/**

Languages and Software

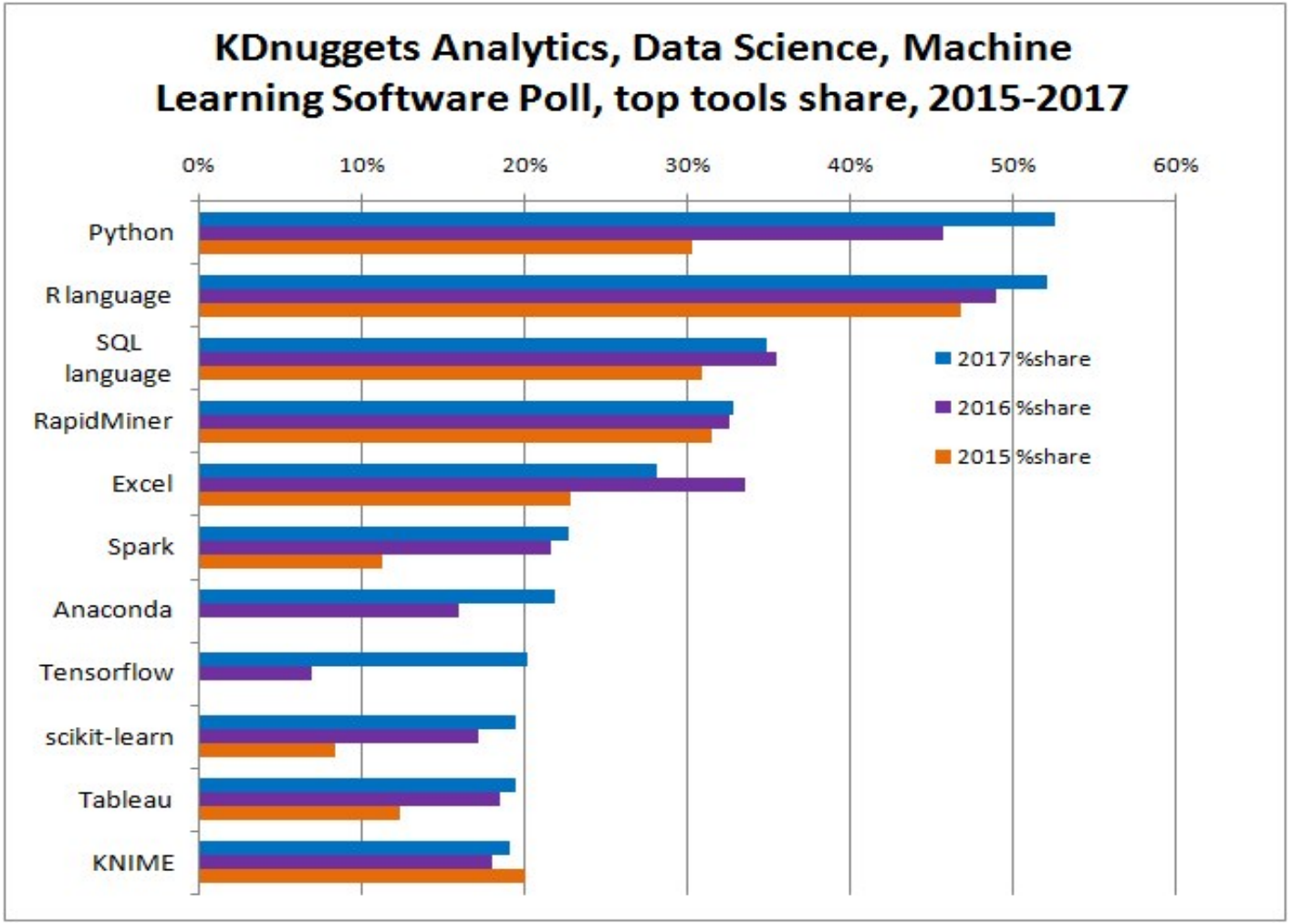
- Stats oriented: R, Python (with packages)
  - Commercial: SAS, IBM SPSS,..
  - Open: GUI oriented: Knime, RapidMiner
- General purpose (Java for text analysis)
- Distributed/bigdata
  - Hadoop/Spark/MapReduce/PigLatin
  - HIVE (SQL like for Hadoop)
  - Various NoSQL

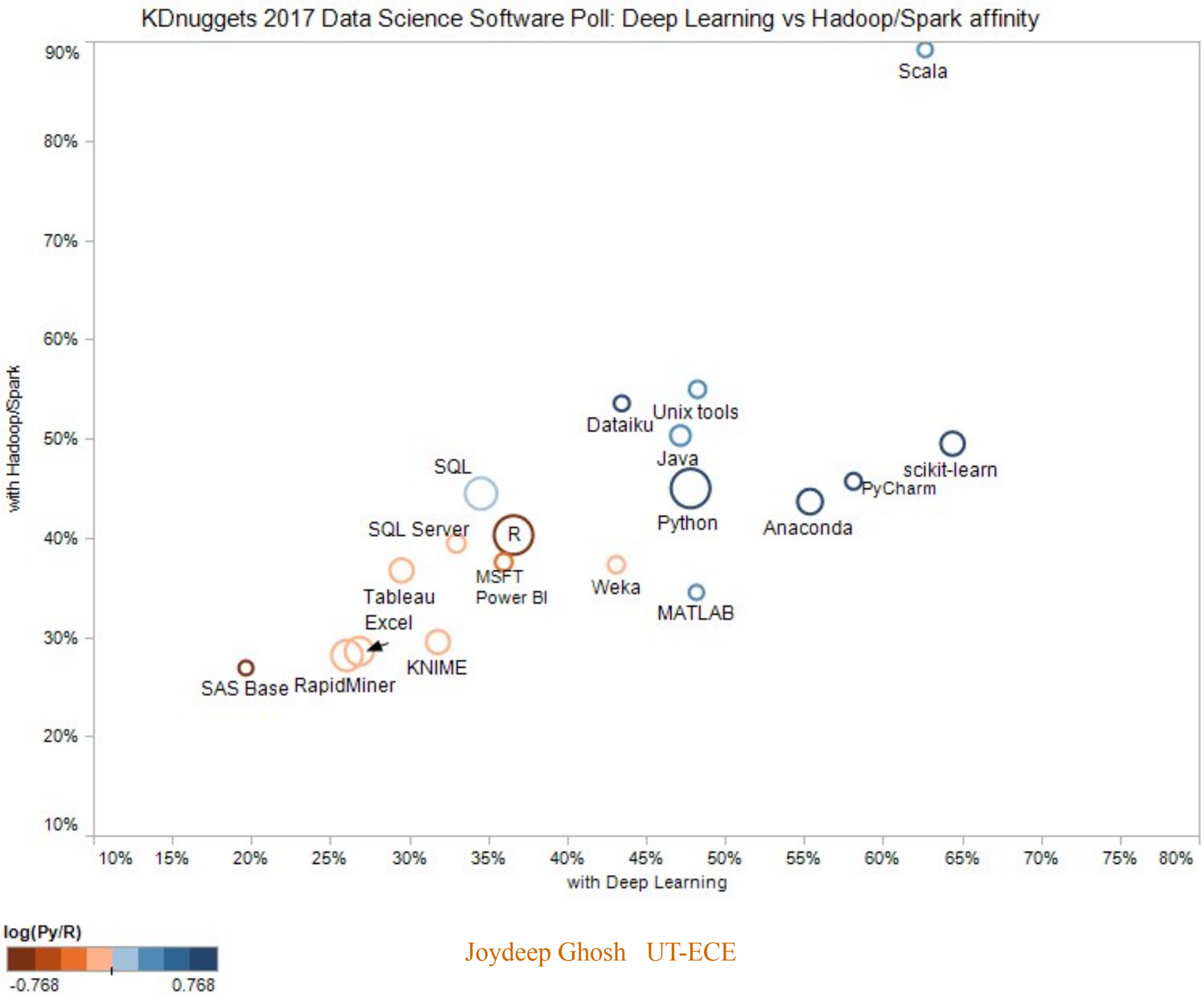
See: How Did Python Become A Data Science Powerhouse?

https://www.youtube.com/watch?v=9by46AAqz70

KDD Nuggets Survey May 2017

- http://www.kdnuggets.com/2017/05/poll-analytics-data-science-machine-learning-software-leaders.html
- Also see http://www.kdnuggets.com/2017/08/python-overtakes-r-leader-analytics-data-science.html




KDnuggets 2017 Data Science Software Poll: Deep Learning vs Hadoop/Spark affinity
with Hadoop/Spark
with Deep Learning
90%
80%
70%
60%
50%
40%
30%
20%
10%
10%
15%
20%
25%
30%
35%
40%
45%
50%
55%
60%
65%
70%
75%
80%
Scala
Dataiku
Unix tools
Java
SQL
scikit-learn
PyCharm
Python
Anaconda
SQL Server
R
MSFT
Power BI
Weka
Tableau
MATLAB
Excel
KNIME
SAS Base
RapidMiner
log(Py/R)
-0.768
0.768

R vs. Python

R or Python? See

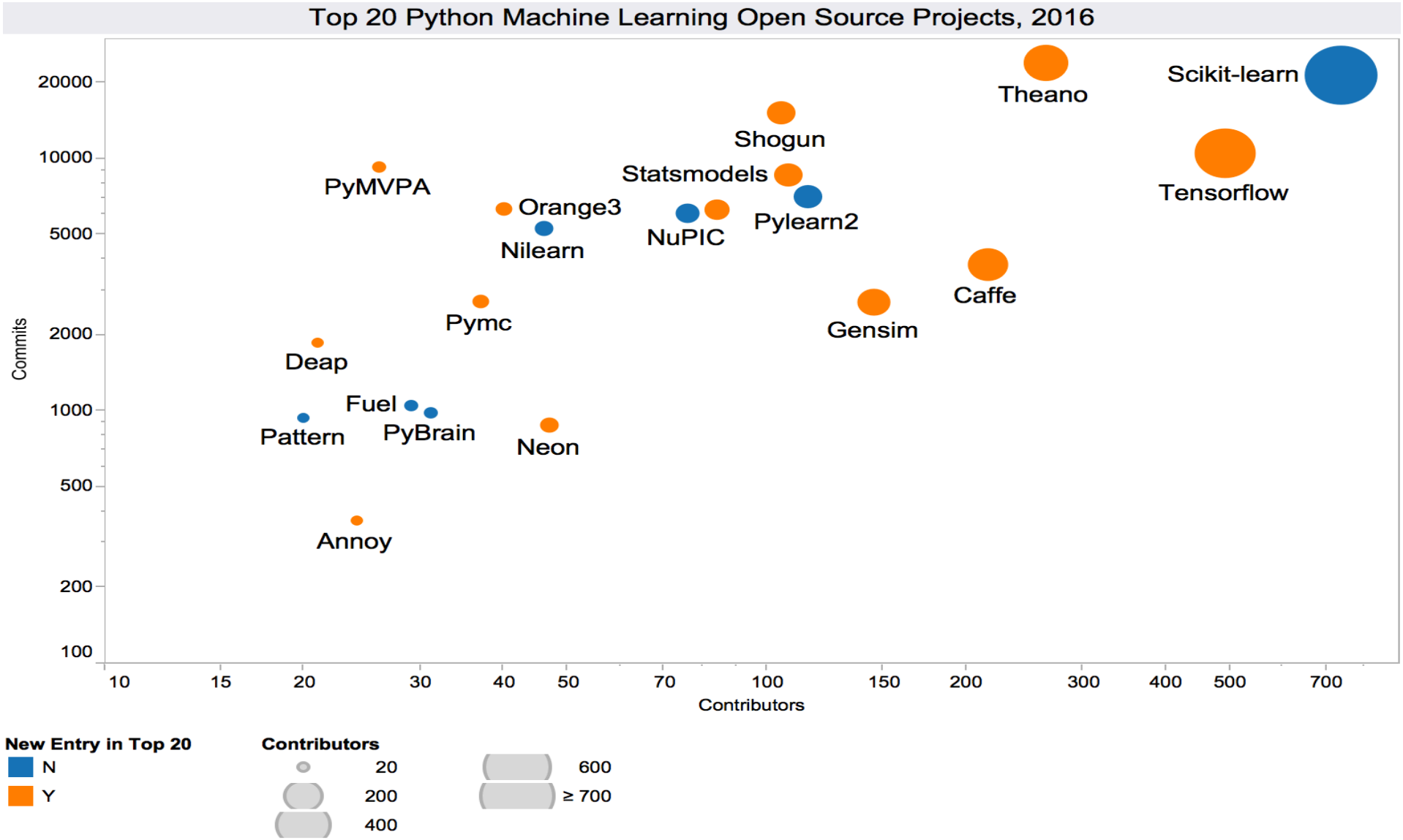
–http://www.kdnuggets.com/2017/07/6-reasons-python-suddenly-super-popular.html

- 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/2016/11/top-20-python-machine-learning-open-source-updated.html



Types of Modeling

Consider a large collection of fruits

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

- **Regression**: predicting shelf life 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**
- **Causality: what causes the fruit to rot?**
- **…..**
- **Topics not new, but some data mining concerns/aspects are…**
- Predictive Modeling: Developing mathematical models that make accurate predictions
- Prescriptive Analytics

Jargon

- "**x**": independent variable(s) / predictors/input /features/ attributes
- "**y**" or "t": 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,…

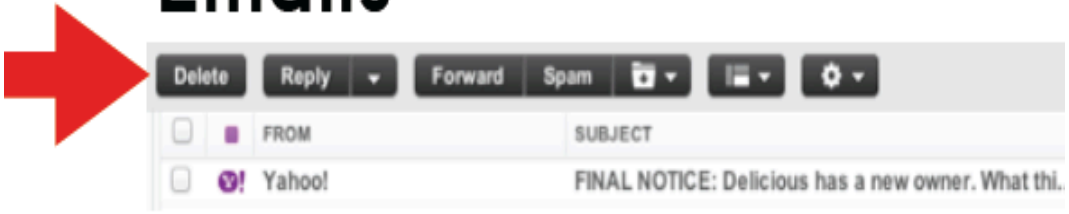
  -

50 shades of supervision

- Ads

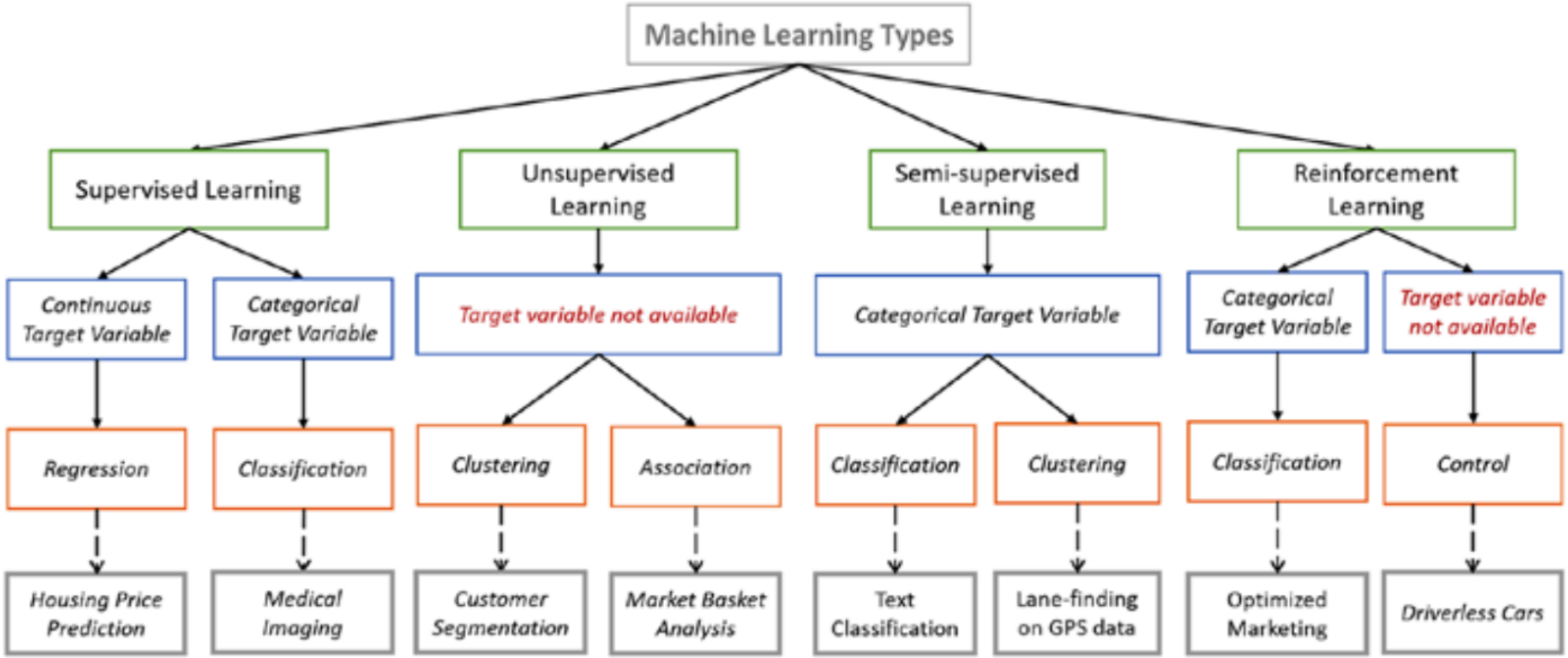
- Click feedback

- Emails



- Tags

- Ads on website
- Spam
- Product recommendations
  - Tinder
- Domain expert feedback on clusters produced



Cold Start Problem: Mismatch → Online learning methods

Course Goals

- study different predictive models for a given task
  - Properties, pros and cons
  - Evaluation metrics
    - Business relevance
  - Build predictive models in Python
- Process-oriented viewpoint
- Introduction to issues of scale and real data considerations

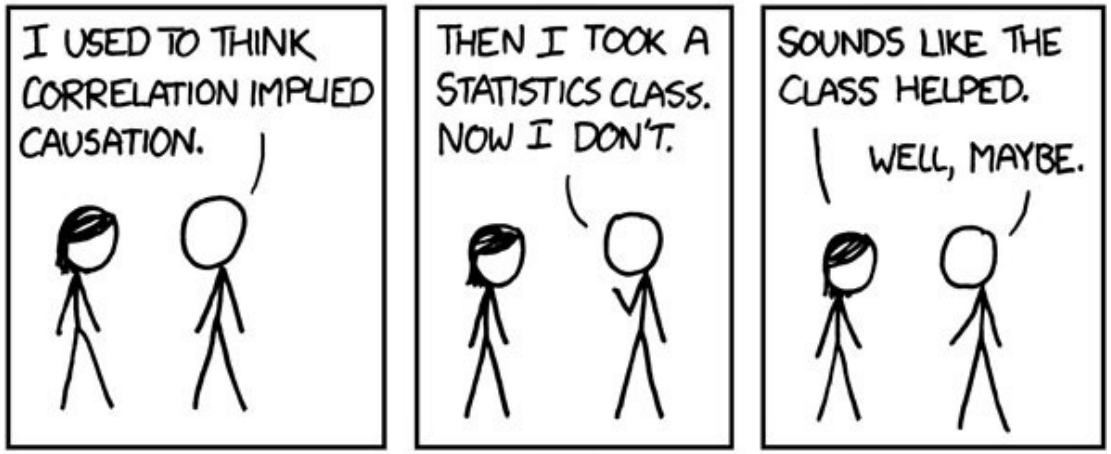
Broader Goals

Reason about data analysis and the "results" obtained

•- "Mr. Trump won 76% of Cracker Barrel counties and 22% of Whole Food counties"

- Economist, Jan 28th, 2017, quoting the Cook Political Report
- (compares 54% gap vs. 31 for Bush 2000 and 43 for Obama 2008)

•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)



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"

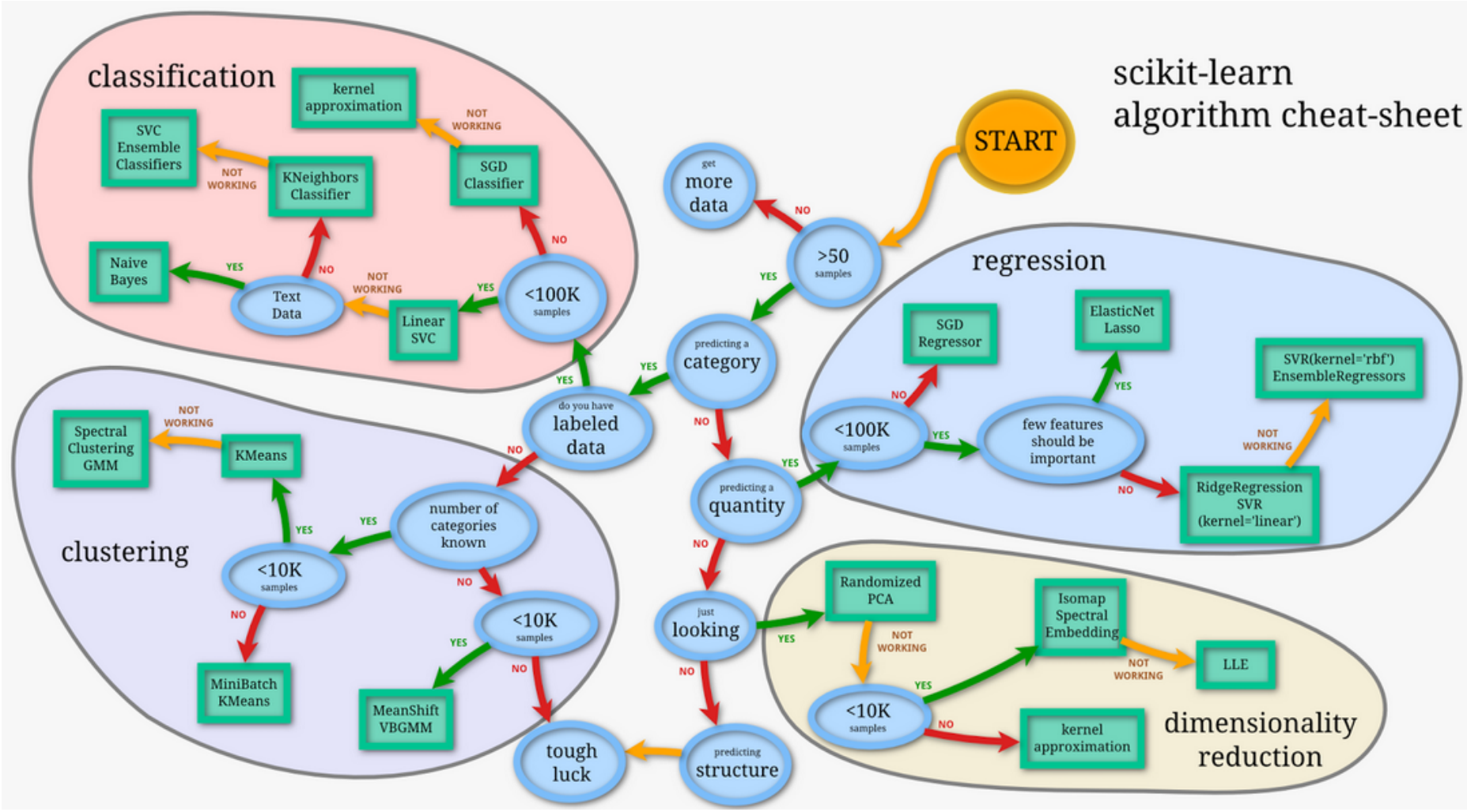
- George Box, 1987

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

Visualize: http://setosa.io/ev/ordinary-least-squares-regression/

Cheat Sheets (Python, R, SQL, ML,..)

Cheat Sheets: http://www.kdnuggets.com/2016/12/data-science-machine-learning-cheat-sheets-updated.html



Local vs Global Models (from HTF Ch. 2)

- K-nearest neighbor (KNN)

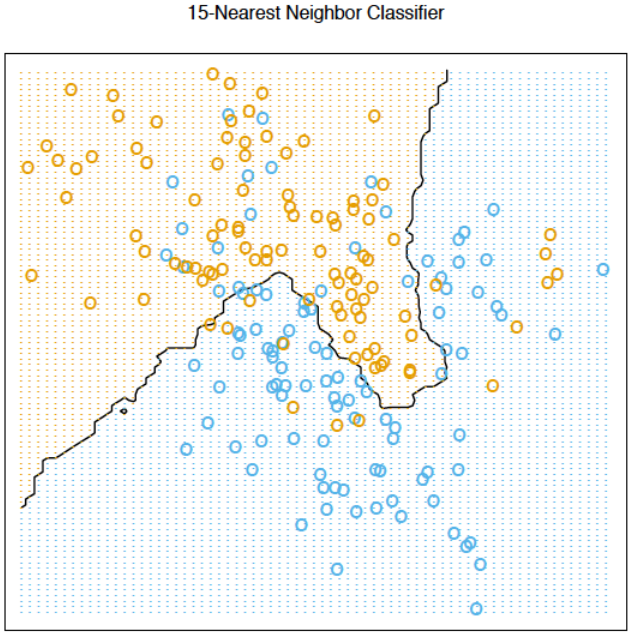


FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$) *and then fit by 15-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the 15-nearest neighbors.*

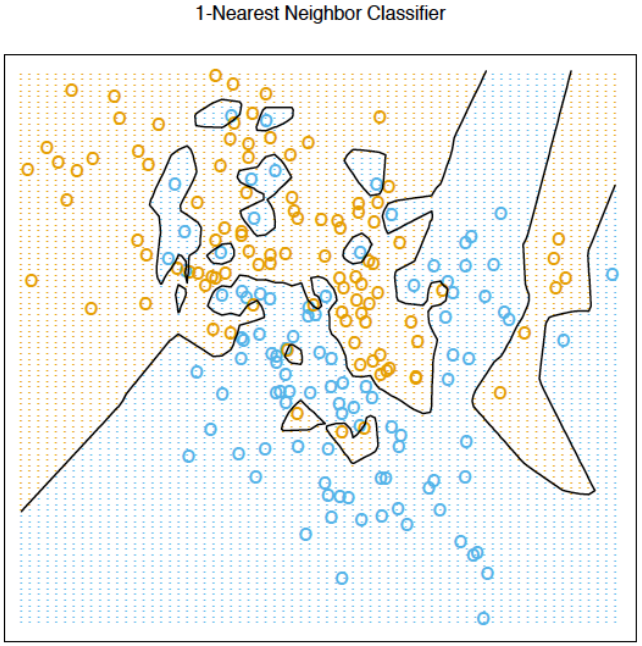


FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$), *and then predicted by 1-nearest-neighbor classification.*

KNN vs Linear Regression

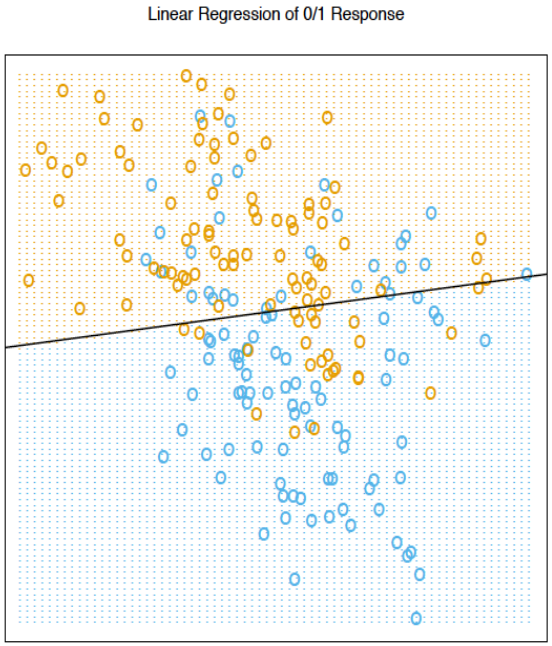


FIGURE 2.1. *A classification example in two dimensions. The classes are coded as a binary variable (BLUE = 0, ORANGE = 1), and then fit by linear regression. The line is the decision boundary defined by $x^T\hat{\beta} = 0.5$. The orange shaded region denotes that part of input space classified as ORANGE,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

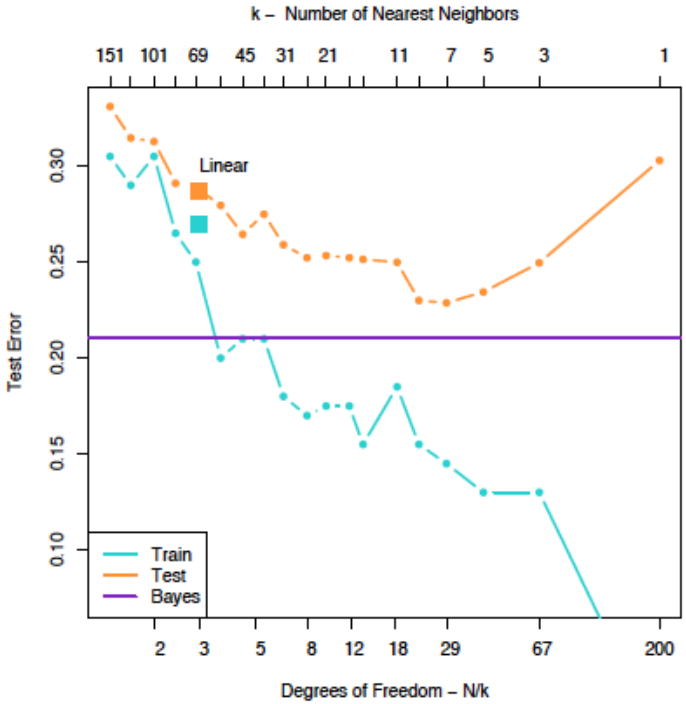


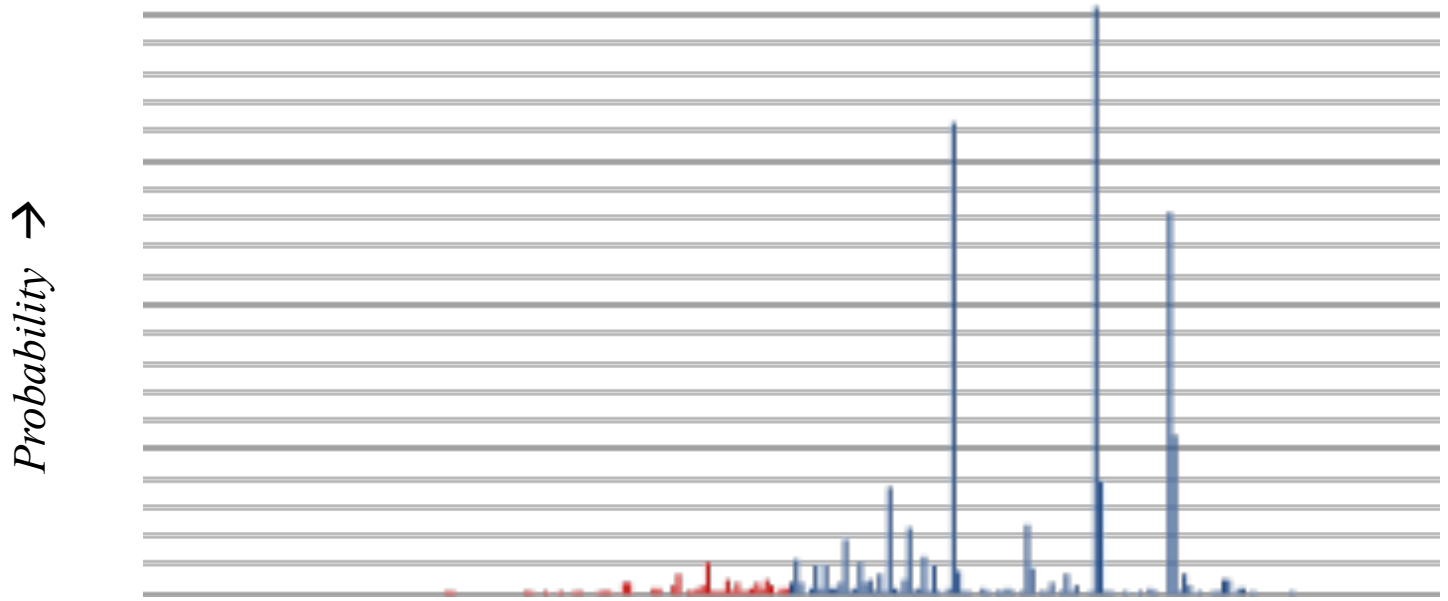
FIGURE 2.4. *Misclassification curves for the simulation example used in Figures 2.1, 2.2 and 2.3. A single training sample of size 200 was used, and a test sample of size 10,000. The orange curves are test and the blue are training error for k-nearest-neighbor classification. The results for linear 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)



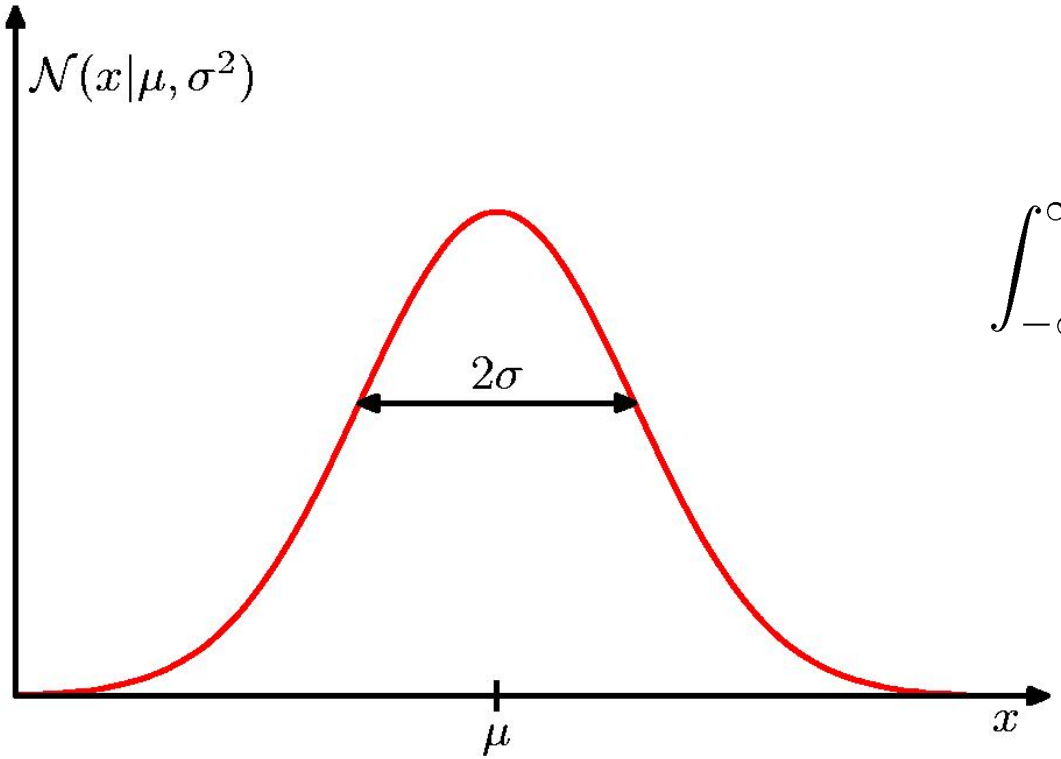
Probability Recap

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

Visualize: http://setosa.io/ev/conditional-probability/

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

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

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

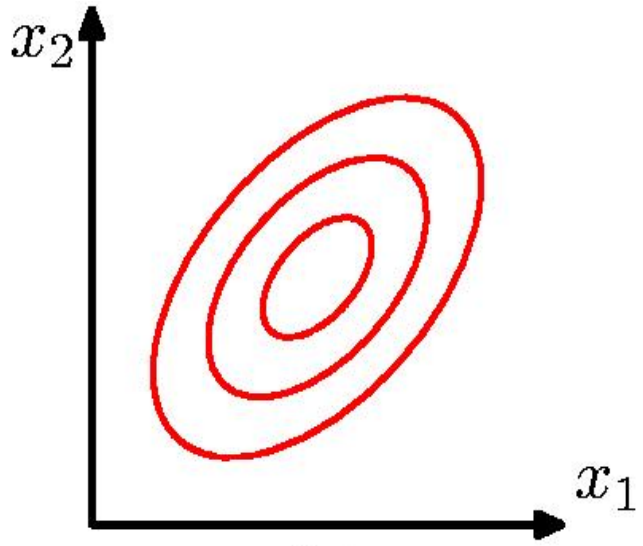
$$\mathrm{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$

Denotes the "expectation" operator

The Multivariate Gaussian (in D dimensions)

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

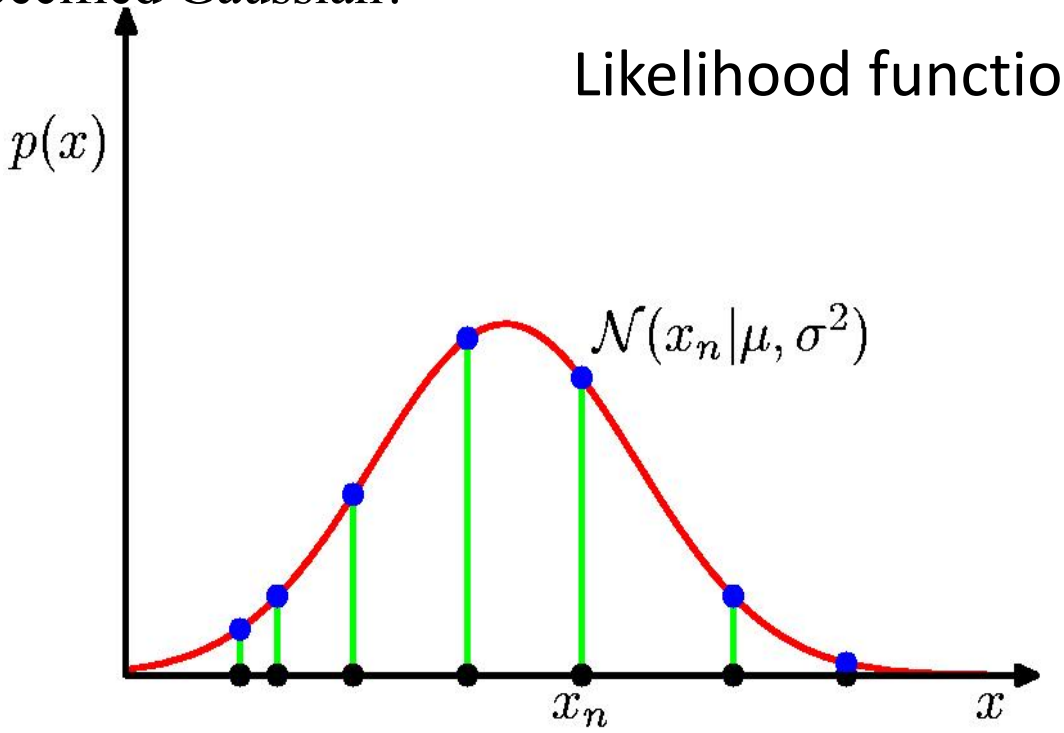
Vector Mean *D-by-D Covariance Matrix* *Determinant of the covariance matrix*



Marginals and *conditionals* of multivariate Gaussians?

Gaussian Parameter Estimation

- What is the probability that a datset X with N i.i.d. points was obtained from a specified Gaussian?



Likelihood of observing the given set of points X

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

Maximum (Log) Likelihood

- **Selects the Gaussian that most likely produced the given dataset x.**

$$\textit{Log Likelihood} = -\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu)^2 - \frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi)$$

(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*?

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?

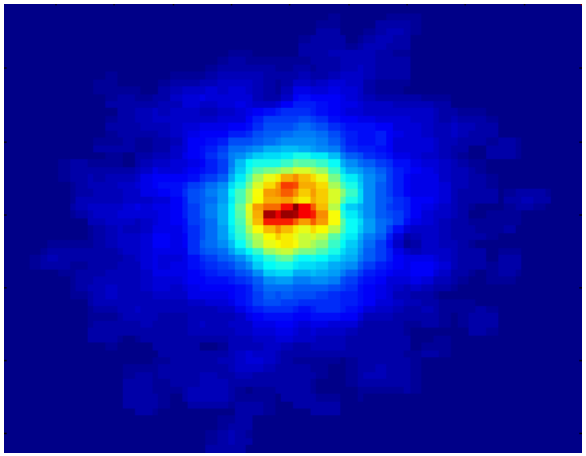
DBLP, CiteSeer, Google Scholar

- 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.

Classifying Galaxies

Courtesy: http://aps.umn.edu

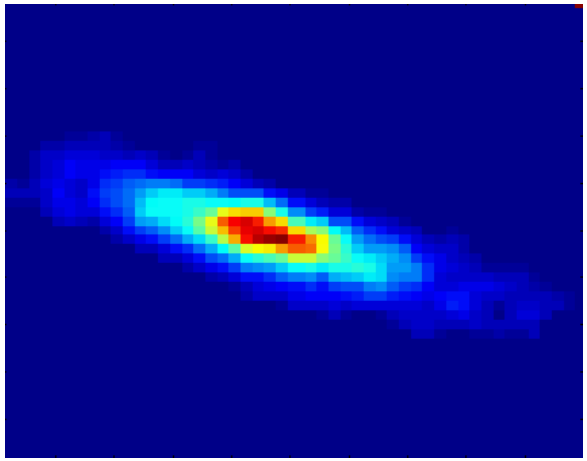
Early



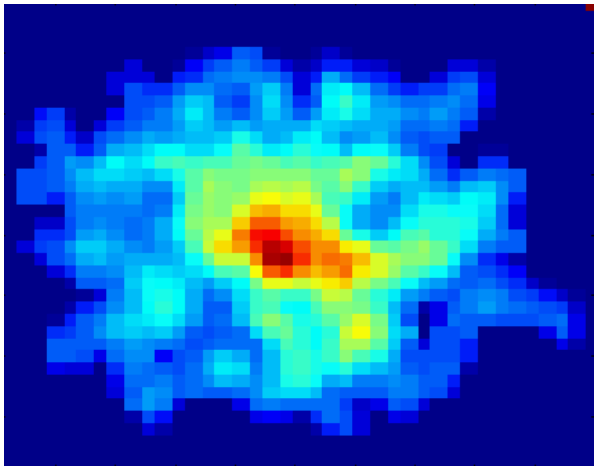
Class:
- **Stages of Formation**

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

Intermediate



Late

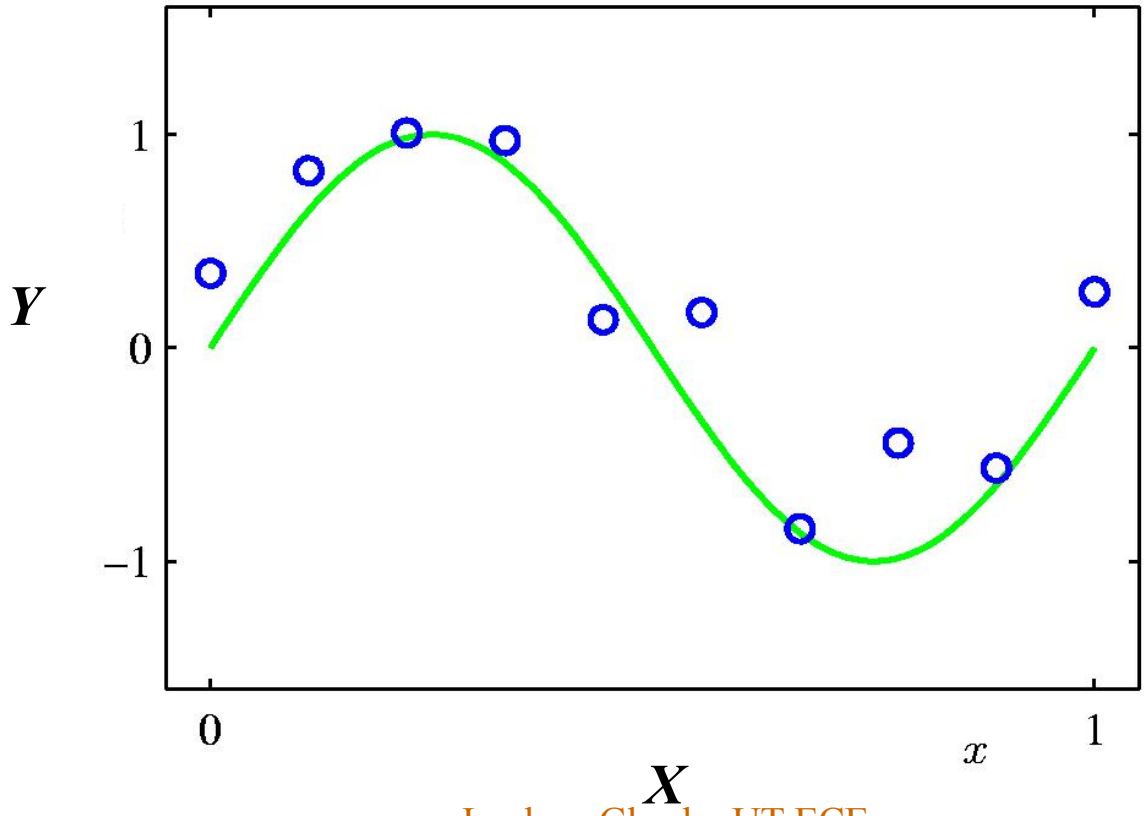


Data Size:
- **72 million stars, 20 million galaxies**
- **Object Catalog: 9 GB**
- **Image Database: 150 GB**

Regression: Curve Fitting

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

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



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.