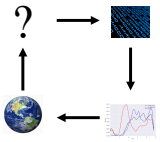
Data Science 100
Review

Problem formulation, experimental design, Clustering, LS, and linear models

Slides by Bin Yu (some from Joe Gonzalez)

binyu@stat.berkeley.edu



Data analytics cycle through PQR+S

- **P**opulation
- **Q**uestion
- **R**epresentative data collection (data neutral from the ethics angle)
- **+… Prediction, inference, … Least Squares, Linear Models, Clustering (K-means, EM, Hierarchical)…**
- **S**crutiny

P. "Population" of interest

- Population is the relevant group of people (objects, units) that the data-driven answer to the question will be applied to
- Example: all patients who need a kidney transplant on May 1, 2017 (is this enough a description to define "P"?)

Q ? Question, question, question

- Can we predict acute kidney rejection ahead of time? -- clearly a prediction question
- What are the important predictors for the acute rejection? -- an inference question since we need to address the uncertainty in the data

Predictors in the organ transplant project (dim=49)

- 43 genes are identified by the Sarwal Group at UCSF and collaborators (underlying kSORT, a blood test, to predict a rejection three months earlier than an invasive biopsy)
- Recipient age, race and gender
- Donor age
- Donor/recipient gender match
- Donor status (living or deceased)

Data collection experimental design principle

- **R**epresentativeness: data are similar to population in key aspects of interest
- **R-** through randomization
  - Simple Random Sampling (randomized experiment vs. observational study)
  - Confounding factors (in both randomized and obs. studies)
  - Association is not causation in general esp. in obs. studies

Understanding data before modeling

- Visualization of raw data if possible
- **Clustering** and then visualization
  -- the clusters in low-dim (after PCA say)
  -- look at the clusters, separately
- Try different clustering methods and compare results
- **Scrutiny**

Clustering is a form of information reduction/organization

- To store in human finite memory (or computer's finite memory) and facilitate understanding

- To communicate between people (or processors) for more effective understanding between people and collective decisions

Effective decision-making is impossible based on raw big data

Three clustering methods

- **K-means**
- **Hierarchical clustering:**
- EM: basic ideas (e.g. complete and incomplete data concepts)

K-means, given the number K of clusters

- Algorithm: alternating minimization between finding centers and partitions
- Starting values: random data points
- Selection of K: search for elbow in loss function, CV, Silhouette (graphic)
- Remarks:
  - K-means is sensitive to outliers if we use squared Euclidean distance
  - It converges to a local minimum of the loss function: good idea to start from multiple starting values and compare loss function values to find the best.

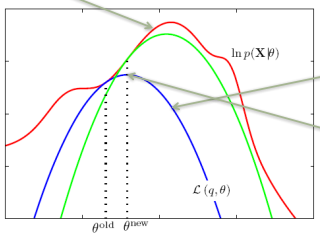
EM for model based clustering

- Applications: speech recognition with the hidden Markov Models (HMMs)
- Given iid data, no closed form for maximum likelihood.
- Numerical optimization routines can be used or the EM algorithm can be used.

The EM (Expectation-Maximization) algorithm is an iterative algorithm as gradient descent, however, the E- and M-steps have statistical meanings. The EM framework utilizes some missing data notation.

The EM algorithm is effective, when the maximum likelihood (M-step) is easy to solve with complete data (the missing data plus the observed data), and when the missing data is easy to impute (E-step). Modern generalizations of EM use approximations of various forms in the M- and E- steps.

EM (Dempster et al , 1977) to maximize the red curve – log likelihood function



At a current estimate point,

- E-step
makes a (lower bound blue) curve (in a systematic way) on the log likelihood function
- M-step
maximizes the blue curve for the next estimate
- now on the green curve
- ..

EM for two component Gaussian mixture

Data: incomplete **iid** data $X_1, ..., X_n$ without the labels

- Start with initial estimates of the 5 parameters
- Iterate between the E- and M-steps from previous slide until convergence: estimate the missing labels to impute the complete data; do maximum likelihood to estimate the parameters using the imputed complete data.
- It is guaranteed to converge to a local maximum of the likelihood function of the observed or incomplete data $X_1, ..., X_n$

Hierarchical clustering

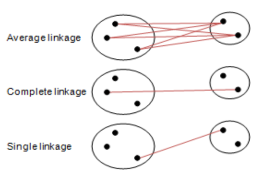
For a hierarchical clustering algorithm, we need

- A. a distance or dissimilarity measure between any two points.
- B. a rule to calculate the distances/dissimilarities between disjoint clusters of objects.

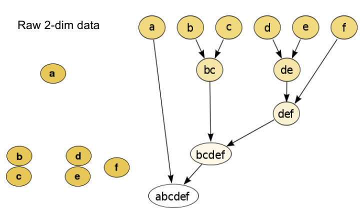
This between cluster distance can generally be calculated directly from the distances of the various elements involved in the clustering.

Three B. rules

- **Average linkage**: average dissimilarities between two clusters
- **Complete-linkage:** farthest points between the two clusters
- **Single-linkage:** smallest dissimilarity between the two clusters



Wiki example

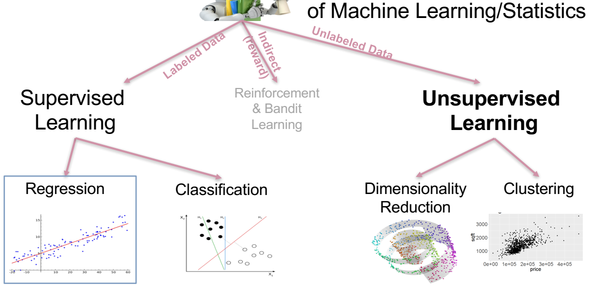


1. Take the two most similar
2. points and merge them into a new (super) point – we now have n-1 points

B-rule allows us to have a dissimilarity measure for the n-1 points

3. Continue until all points are grouped.

Taxonomy- hierarchical clustering- of Machine Learning/Statistics



LS: Least Squares as a fitting or prediction method

- Represent data $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ as:

Covariate (Design) Matrix

Response Vector

$$X = \underbrace{\begin{pmatrix} — & x_1 & — \\ — & x_2 & — \\ & \cdots & \\ — & x_n & — \end{pmatrix}}_{p} \in \mathbb{R}^{np} \qquad Y = \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{1} \in \mathbb{R}^n$$

(n rows in each)

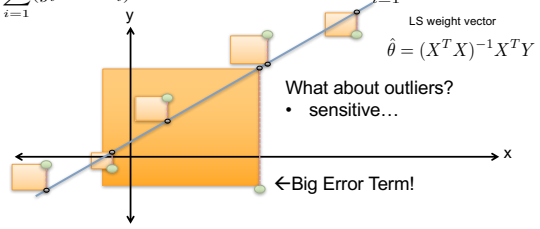
Least Squares (LS) predictor: $\hat{\theta}^T x$

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - \theta^T x_i)^2$$

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^p} \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta^T x_i)^2$$

LS weight vector

$$\hat{\theta} = (X^T X)^{-1} X^T Y$$



What about outliers?
- sensitive…

←Big Error Term!

Basic understanding of LS estimator derivation

- Taking derivatives of the loss function and setting them to zero
- Basic matrix manipulations at the HW problem levels

e.g. Residuals

$$e_i = y_i - \hat{\theta}^T x_i$$

$$e = Y - \hat{Y}$$

where $\hat{Y} = X\hat{\theta} = X(X^T X)^{-1} X^T Y$

Model assumption checking

- Residual plots (e against predictors, against fitted value) (
- Checking constant variance
- Checking dependence between the noise term and predictors

Normal (Gaussian) Linear Regression Model – idealized but useful

All models are wrong, but some are useful – George Box

Vector of Parameters; Vector of Features

Real Valued Observations: $y_i = \theta^T x_i + \epsilon_i$ Real Value Noise

Linear Combination of Covariates: $\sum_{j=1}^{p} \theta_j x_{ij}$

$\theta, x \in \mathbb{R}^p$

ϵ are independent, and independent of X, and with dist. $N(0, \sigma^2)$

$\epsilon = (\epsilon_1, ..., \epsilon_n)^T$

Maximum likelihood Est. under the Normal Linear Regression Model is the same as LS

- Since $y_i \sim N(\theta^T x_i, \sigma^2)$ and they are indep, the likelihood function is

$$\prod_{i=1}^{n}\{\frac{1}{\sqrt{2\pi}\sigma}\exp\left[-(y_i - \theta^T x_i)^2/(2\sigma^2)\right]\}$$

- The log likelihood function is

$$-\frac{n}{2}\log(2\pi\sigma^2) - \sum_{i=1}^{n}(y_i - \theta^T x_i)^2/(2\sigma^2)$$

- Maximizing the above for θ is the same as minimizing the squared sum term or LS regardless of the value of variance σ^2

Estimating variance σ^2

- The maximum likelihood estimator (MLE) of σ^2 is

$$\hat{\sigma}_1^2 = \sum_{i=1}^{n}(y_i - \hat{\theta}^T x_i)^2/n$$

where $\hat{\theta} = (X^T X)^{-1} X^T Y$ is the MLE or LS (or OLS) estimator of θ
OLS= Ordinary Least Squares (a statistics term)

- In fact, we always use another variance estimator

$$\hat{\sigma}^2 = \sum_{i=1}^{n}(y_i - \hat{\theta}^T x_i)^2/(n-p)$$

Linear Regression Model – idealized but useful

All models are wrong, but some are useful – George Box

Vector of Parameters; Vector of Features

Real Valued Observations $y_i = \theta^T x_i + \epsilon_i$ Real Value Noise

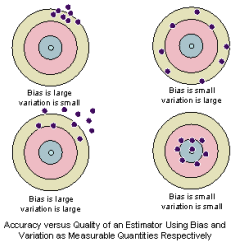
Linear Combination of Covariates $\sum_{j=1}^{p} \theta_j x_{ij}$ $\quad \theta, x \in \mathbb{R}^p$

ϵ are independent, and independent of X, and with mean 0 and var. σ^2

$\epsilon = (\epsilon_1, ..., \epsilon_n)^T$ (ϵ 's distribution's tail is not too heavy)

Good properties of estimators: unbiasedness under linear model

- $\hat{\sigma}^2$ is an unbiased estimator of σ^2
- $\hat{\theta}$ is an unbiased estimator of θ



Accuracy versus Quality of an Estimator Using Bias and Variation as Measurable Quantities Respectively

Facts under Linear Regression Model

- LS estimator is still unbiased and so is $\hat{\sigma}^2$
- When **n is large**, LS estimator has an **approximate normal distribution**

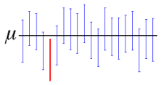
$$N(\theta, \sigma^2 (X^T X)^{-1})$$

provided that $X^T X/n$ **is approximately a positive definite matrix.**

We can plug in $\hat{\sigma}^2$ **for data-driven confidence intervals**

What does a 95% confidence interval for θ_1 mean?

- Given 100 (**oracle**) sets of n random samples (or 100 replicates) following the Linear Regression Model, we get 100 confidence interval for θ_1 using approximate normality, about 95 of them should cover the true θ_1 in the model.



For one data set in practice, one can also use bootstrap for confidence interval construction of θ_1

- We need 100 or more bootstrap replicates from the data set to do the job
- use approximate normality or $N(\theta, \hat{\sigma}^2 (X^T X)^{-1})$

Hypothesis testing

- Null hypothesis H_0 : slope θ_1 =0
- Alternative hypothesis H_1: $\theta_1 \neq 0$ (or $\theta_1 > 0$)

Remarks:

- Rationale: null hypothesis is favored unless there is strong evidence to refute it. Hence **accepting the null is not the same as proving null**.
- With one toss of a coin, the null ("coin is fair") will be always accepted, which is apparently no proof that the coin is fair.

Testing hypothesis via confidence interval construction

- Use a 95% confidence interval construction to test the null:

  if the interval contains the 0, the null is accepted;
  otherwise rejected – all at level 5%

Two confidence interval constructions

- (Full-blown) Bootstrap
- (Approximate) normality

Scrutiny – vetting or validation

- Stability over perturbed data and methods (e.g. do different clustering methods give similar clusters? If not, which to take? Domain knowledge can help prioritize or believe only the stable clusters)
- Residual analysis for LS and linear models
- Domain matter interpretation (e.g. do the important predictors make sense medically?)
- Prediction on new patients: does it work better than old prediction method
- Down-stream impacts (e.g. If they develop new matching policy based on the important predictors found, does the rejection rate go down?)

Extra slide: terms used in hypothesis testing

- Type I error = Probability that the null rejected when that null is true
- Type II error = Probability that the alternative is rejected when it is true
- Power = 1- Type II error = Prob. that the alternative is corrected accepted

In medical sciences (these terms below sound better or more positive)

- Sensitivity = 1- Type II error = Power
- Specificity (or selectivity) = 1- Type I error
- Setting type I error at 5% -- statistically significant
- Setting type I error at 1% -- highly statistically significant

- Thank you for being a wonderful class – I had fun co-teaching it…
- Good luck with your finals