Introduction to STA721

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Introduction to STA721

- Course: Theory and Application of linear models from both a frequentist (classical) and Bayesian perspective
- Prerequisites: linear algebra and a mathematical statistics course covering likelihoods and distribution theory (normal, t, F, chi-square, gamma distributions)
- Introduce R programming as needed in the lab
- Introduce Bayesian methods, but assume that you are co-registered in 702 or have taken it previously
- more info on Course website https://sta721-F24.github.io/website/
  - schedule and slides, HW, etc
  - critical dates (Midterms and Finals)
  - office hours
- Canvas for grades, email, announcements

Please let me know if there are broken links for slides, etc!

Notation

- scalors are a (italics or math italics)
- vectors are in bold lower case, $\mathbf{a}$, with the exception of random variables
- all vectors are column vectors

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

- $\mathbf{1}_n$ is a $n \times 1$ vector of all ones
- inner product $\langle \mathbf{a}, \mathbf{a} \rangle = \mathbf{a}^T \mathbf{a} = \|\mathbf{a}\|^2 = \sum_{i=1}^n a_i^2$; $\langle \mathbf{a}, \mathbf{b} \rangle = \mathbf{a}^T \mathbf{b}$
- length or norm of $\mathbf{a}$ is $\|\mathbf{a}\|$

Matrices

- Matrices are represented in bold $\mathbf{A} = (a_{ij})$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix}$$

- identity matrix $\mathbf{I}_n$ square matrix with diagonal elements 1 and off diagonal 0
- trace: if $\mathbf{A}$ is $n \times m$ tr$(\mathbf{A}) = \sum_i^{\max n,m} a_{ii}$
- determinant: for $\mathbf{A}$ is $n \times n$ then the determinant is $\det(A)$
- inverse: if $\mathbf{A}$ is nonsingular $\mathbf{A} > 0$, then its inverse is $\mathbf{A}^{-1}$

Statistical Models

Ohm's Law: Y is voltage across a resistor of r ohms and X is the amperes of the current through the resistor (in theory)

$$Y = rX$$

- Simple linear regression for observational data

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i \text{ for } i = 1, \ldots, n$$

- Rewrite in vectors:

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \beta_0 + \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \beta_1 + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

Nonlinear Models

Gravitational Law: $F = \alpha/d^{\beta}$ where d is distance between 2 objects and F is the force of gravity between them

- log transformations

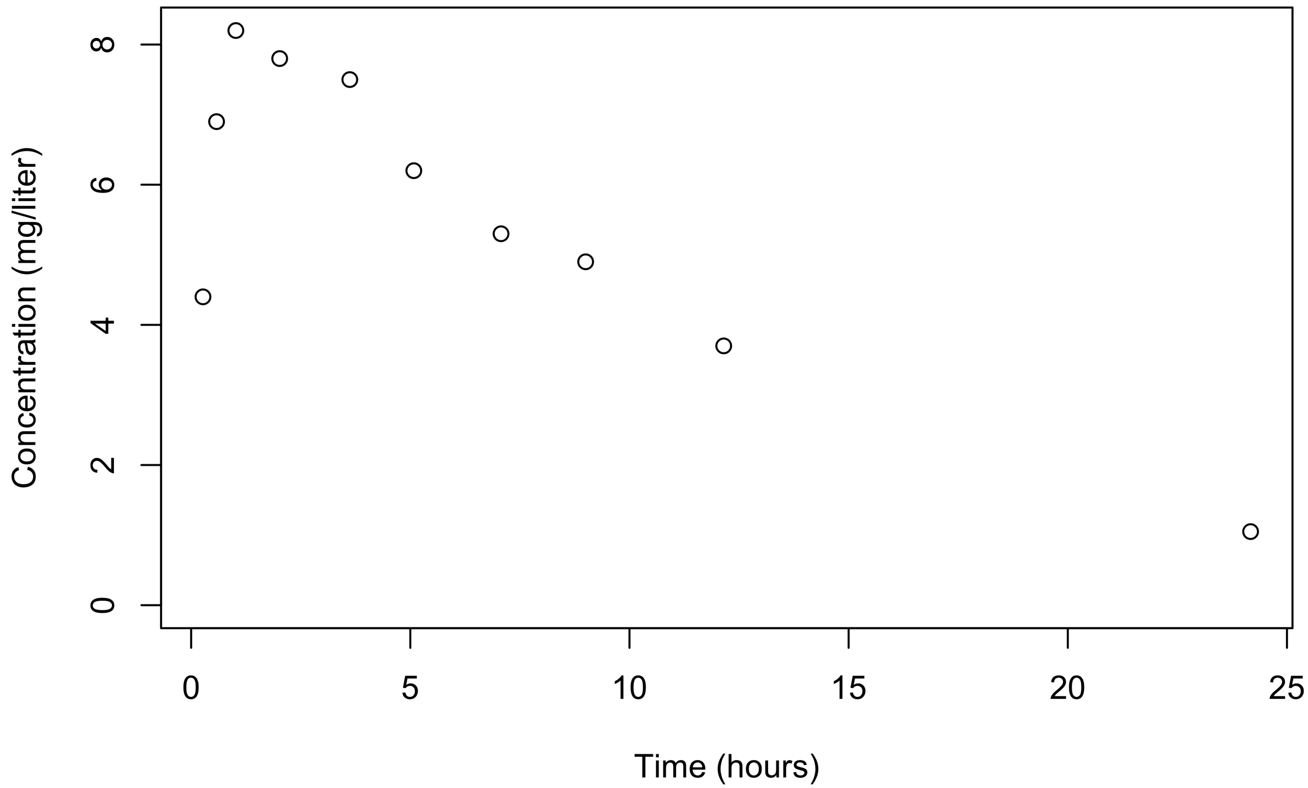
$$\log(F) = \log(\alpha) - \beta \log(d)$$

- compare to noisy experimental data $Y_i = \log(F_i)$ observed at $x_i = \log(d_i)$
- write $\mathbf{X} = [\mathbf{1}_n \, \mathbf{x}]$
- $\boldsymbol{\beta} = (\log(\alpha), -\beta)^T$
- model with additive error on log scale $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$
- test if $\beta = 2$
- error assumptions?

Intrinsically Nonlinear Models

Regression function may be an intrinsically nonlinear function of t_i (time) and parameters $\boldsymbol{\theta}$

$$Y_i = f(t_i, \boldsymbol{\theta}) + \epsilon_i$$


Concentration (mg/liter)
0
2
4
6
8
0
5
10
15
20
25
Time (hours)

Quadratic Linear Regression

Taylor's Theorem:

$$f(t_i, \boldsymbol{\theta}) = f(t_0, \boldsymbol{\theta}) + (t_i - t_0) f'(t_0, \boldsymbol{\theta}) + (t_i - t_0)^2 \frac{f''(t_0, \boldsymbol{\theta})}{2} + R(t_i, \boldsymbol{\theta})$$

$$Y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i \text{ for } i = 1, \ldots, n$$

Rewrite in vectors:

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \\ 1 & x_n & x_n^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

Quadratic in x, but linear in β's - how do we know this model is adequate?

Kernel Regression (NonParametric)

$$y_i = \beta_0 + \sum_{j=1}^{J} \beta_j e^{-\lambda(x_i - k_j)^d} + \epsilon_i \text{ for } i = 1, \ldots, n$$

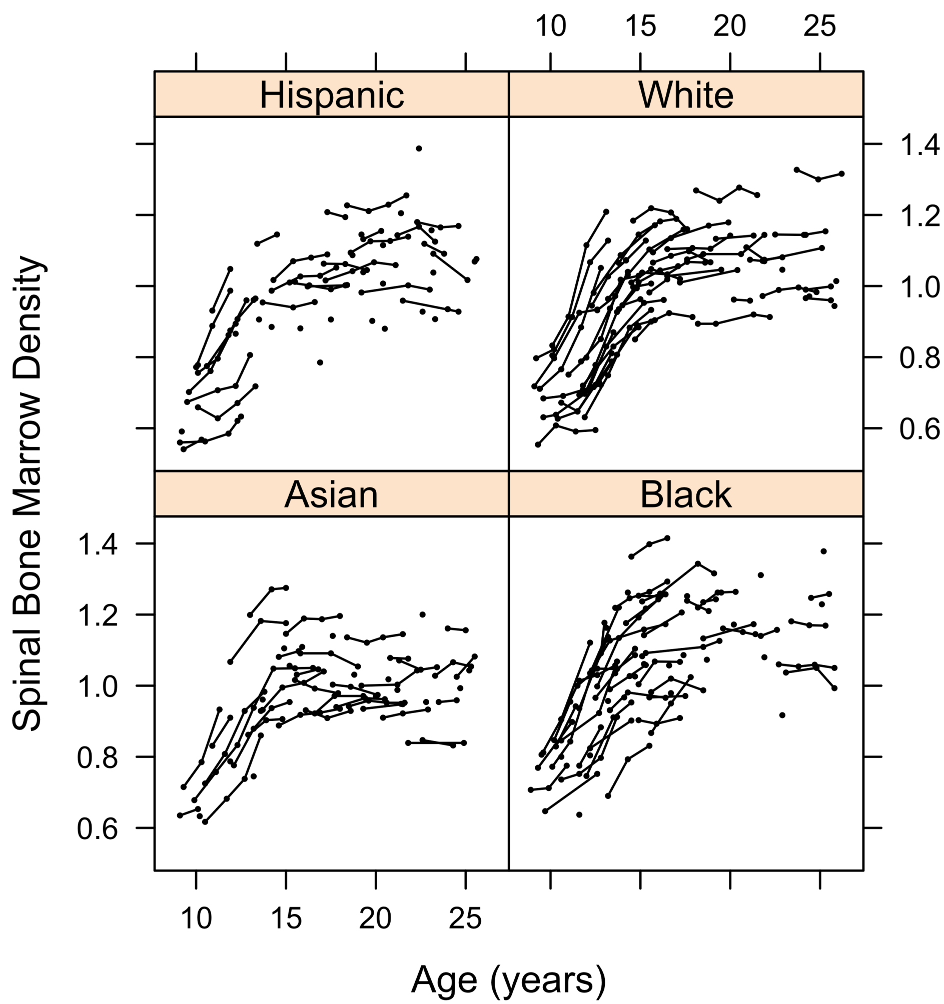
where k_j are kernel locations and λ is a smoothing parameter

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & e^{-\lambda(x_1 - k_1)^d} & \ldots & e^{-\lambda(x_1 - k_J)^d} \\ \vdots & \vdots & & \vdots \\ 1 & e^{-\lambda(x_n - k_1)^d} & \ldots & e^{-\lambda(x_n - k_J)^d} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_J \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

- Linear in β given λ and $k_1, \ldots k_J$
- Learn $\lambda, k_1, \ldots k_J$ and J

Hierarchical Models



- each line represent individual sample trajectories
- correlation between an individual's measurements
- similarities within groups
- differences among groups?
- allow individual regressions for each individual ?
- add more structure?

Linear Regression Models

Response Y_i and p predictors $x_{i1}, x_{i2}, \dots x_ip$

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots \beta_p x_{ip} + \epsilon_i$$

- Design matrix

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & \dots & x_{1p} \\ 1 & x_{21} & \dots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & \dots & x_{np} \end{bmatrix} = \begin{bmatrix} 1 & \mathbf{x}_1^T \\ \vdots & \vdots \\ 1 & \mathbf{x}_n^T \end{bmatrix} = [\mathbf{1}_n \quad \mathbf{X}_1 \quad \mathbf{X}_2 \cdots \mathbf{X}_p]$$

- matrix version

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \epsilon$$

what should go into $\mathbf{X}$ and do we need all columns of $\mathbf{X}$ for inference about $\mathbf{Y}$?

Linear Model

- $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$
- $\mathbf{Y}$ $(n \times 1)$ vector of random response (observe $\mathbf{y}$); $\mathbf{Y}, \mathbf{y} \in \mathbb{R}^n$
- $\mathbf{X}$ $(n \times p)$ design matrix (observe)
- $\boldsymbol{\beta}$ $(p \times 1)$ vector of coefficients (unknown)
- $\boldsymbol{\epsilon}$ $(n \times 1)$ vector of "errors" (unobservable)

Goals:

- What goes into $\mathbf{X}$? (model building, model selection - post-selection inference?)
- What if multiple models are "good"? (model averaging or ensembles)
- What about the future? (Prediction)
- Uncertainty Quantification - assumptions about $\boldsymbol{\epsilon}$

All models are wrong, but some may be useful (George Box)

Ordinary Least Squares

Goal: Find the best fitting "line" or "hyper-plane" that minimizes

$$\sum_i (Y_i - \mathbf{x}_i^T \boldsymbol{\beta})^2 = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) = \|\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}\|^2$$

- Optimization problem - seek $\boldsymbol{\beta} \ni \mathbf{X}\boldsymbol{\beta}$ is close to $\mathbf{Y}$ in squared error
- May over-fit $\Rightarrow$ add other criteria that provide a penalty **Penalized Least Squares**
- Robustness to extreme points $\Rightarrow$ replace quadratic loss with other functions
- no notion of uncertainty of estimates
- no structure of problem (repeated measures on individual, randomization restrictions, etc)

Need Distribution Assumptions of $\mathbf{Y}$ (or $\boldsymbol{\epsilon}$) for testing and uncertainty measures $\Rightarrow$ Likelihood and Bayesian inference

Random Vectors

- Let $Y_1, \ldots Y_n$ be random variables in $\mathbb{R}$ Then

$$\mathbf{Y} \equiv \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix}$$

  is a random vector in $\mathbb{R}^n$

- Expectations of random vectors are defined element-wise:

$$\mathsf{E}[\mathbf{Y}] \equiv \mathsf{E} \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix} \equiv \begin{bmatrix} \mathsf{E}[Y_1] \\ \vdots \\ \mathsf{E}[Y_n] \end{bmatrix} = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_n \end{bmatrix} \equiv \boldsymbol{\mu} \in \mathbb{R}^n$$

  where mean or expected value $\mathsf{E}[Y_i] = \mu_i$

Model Space

We will work with inner product spaces: a vector spaces, say $\mathbb{R}^n$ equipped with an inner product $\langle \mathbf{x}, \mathbf{y} \rangle \equiv \mathbf{x}^T \mathbf{y}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$

▼ **Definition:** Subspace

A set $\boldsymbol{\mathcal{M}}$ is a subspace of $\mathbb{R}^n$ if is a subset of $\mathbb{R}^n$ and also a vector space.

That is, if $\mathbf{x}_1 \in \boldsymbol{\mathcal{M}}$ and $\mathbf{x}_2 \in \boldsymbol{\mathcal{M}}$, then $b_1 \mathbf{x}_1 + b_2 \mathbf{x}_2 \in \boldsymbol{\mathcal{M}}$ for all $b_1, b_2 \in \mathbb{R}$

▼ **Definition:** Column Space

The column space of $\mathbf{X}$ is $C(\mathbf{X}) = \mathbf{X}\boldsymbol{\beta}$ for $\boldsymbol{\beta} \in \mathbb{R}^p$

If $\mathbf{X}$ is full column rank, then the columns of $\mathbf{X}$ form a basis for $C(\mathbf{X})$ and $C(\mathbf{X})$ is a p-dimensional subspace of $\mathbb{R}^n$

If we have just a single model matrix $\mathbf{X}$, then the subspace $\boldsymbol{\mathcal{M}}$ is the *model space*.

Philosophy

- for many problems frequentist and Bayesian methods will give similar answers (more a matter of taste in interpretation)
    - For small problems, Bayesian methods allow us to incorporate prior information which provides better calibrated answers
    - for problems with complex designs and/or missing data Bayesian methods are often easier to implement (do not need to rely on asymptotics)
- For problems involving hypothesis testing or model selection frequentist and Bayesian methods can be strikingly different.
- Frequentist methods often faster (particularly with “big data”) so great for exploratory analysis and for building a “data-sense”
- Bayesian methods sit on top of Frequentist Likelihood
- Goemetric perspective important in both!

Important to understand advantages and problems of each perspective!