## Lecture 1: Likelihoods and linear models

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[Go through syllabus]

## How do we estimate things?

- 1. Specify a model
  - Function generating predictions
- 2. Identify plausible values for any unknown parameters
  - Maximize probability of observations given function
- 3. Assess uncertainty
  - Explore function around plausible values

## Introduction to functions

$$\mathbf{y} = f(\mathbf{x})$$

- If y is a vector, then it's a "multivariate" function
- I'll assume that x is usually a vector

- We will work with derivatives:
  - 1<sup>st</sup> derivatives:

$$\frac{d}{dx}f(x)$$

– 2<sup>nd</sup> derivatives:

$$\frac{d}{dx_2}\frac{d}{dx_1}f(x_1,x_2)$$

#### A note on notation:

- Italic: a scalar (or function)
- Bold lowercase: a vector
- Bold uppercase: a matrix

- I'll try to be clear about probabilities
  - Uppercase and not bold: random variable
  - tilde (~): distributions
    - e.g.,  $c \sim \text{Normal}(\mu, \sigma^2)$

#### **Definitions**

- Probability
  - Usage: The probability of the data given fixed values for parameters
    - $Pr(y|\theta)$
    - y = data
    - $\theta$  = parameters
- Likelihood
  - Usage: The likelihood of the parameters given fixed values of data
    - $L(\mathbf{\theta}; \mathbf{y})$
  - Likelihood is only defined up to a constant of integration:
    - $Pr(\mathbf{y}|\mathbf{\theta}) = c \times L(\mathbf{\theta}; \mathbf{y})$

## Laws of probability

1. Axiom of conditional probability

$$Pr(X,Y) = Pr(Y|X) Pr(X)$$

- Often easier to specify conditional probabilities than joint probabilities
- 2. Definition of independent events

$$Pr(Y) = Pr(Y|X)$$
  
 $Pr(X) = Pr(X|Y)$ 

- Necessary to simplify computation of probabilities
- 3. Law of total probability

$$\Pr(X) = \int \Pr(X, Y) dY$$

Used when justifying hierarchical models

## Specify a linear model

Step 1 – Specify a linear predictor for response variable

$$y_i^* = \mathbf{x}_i \mathbf{b} = \sum_{j=1}^{n_j} x_{i,j} b_j$$

- where x<sub>i</sub> is a row of a predictor matrix X
- **b** is a vector of parameters

 Step 2 – Specify a probability distribution for your response variable

$$y_i \sim \text{Normal}(y_i^*, \sigma^2)$$

Maximum likelihood estimation (MLE)

$$\widehat{\boldsymbol{\theta}} = \operatorname{argmax}_{\boldsymbol{\theta}}(L(\boldsymbol{\theta}; \mathbf{y}))$$

- Where  $\widehat{m{\theta}}$  is the MLE estimate of parameters
- Where  $\arg\max_{\boldsymbol{\theta}}(L(\boldsymbol{\theta};\mathbf{y}))$  is the maximum value for  $L(\boldsymbol{\theta};\mathbf{y})$  that can be achieved for any value of  $\boldsymbol{\theta}$
- argmax is done using maximization algorithms

#### Imagine we have two observations

Axiom of conditional probability

$$Pr(y_1, y_2|\boldsymbol{\theta}) = Pr(y_2|y_1, \boldsymbol{\theta}) Pr(y_1|\boldsymbol{\theta})$$

Usually we specify that each datum is independent

$$Pr(y_1, y_2|\boldsymbol{\theta}) = Pr(y_2|\boldsymbol{\theta}) Pr(y_1|\boldsymbol{\theta})$$

Therefore:

$$L(\mathbf{\theta}; \mathbf{y}) = L(\mathbf{\theta}; y_2) L(\mathbf{\theta}; y_1) \propto \Pr(y_2 | \mathbf{\theta}) \Pr(y_1 | \mathbf{\theta})$$

And taking logs

$$\log(L(\mathbf{\theta}; \mathbf{y})) = \log(L(\mathbf{\theta}; y_2)) + \log(L(\mathbf{\theta}; y_1))$$

And generalizing to more than two observations

$$\log(L(\mathbf{\theta}; \mathbf{y})) = \sum_{i=1}^{n_i} \log(L(\mathbf{\theta}; y_i))$$

therefore

$$\widehat{\boldsymbol{\theta}} = \operatorname{argmax}_{\boldsymbol{\theta}} \left( \sum_{i=1}^{n_i} \log(L(\boldsymbol{\theta}; y_i)) \right)$$

$$\widehat{\boldsymbol{\theta}} = \operatorname{argmax}_{\boldsymbol{\theta}}(\log(L(\boldsymbol{\theta}; \mathbf{y})))$$

Where  $p(y|\theta) = L(\theta; y)$  is your specified probability distribution

- 1. Consistency (correct model)
- 2. Consistency (incorrect model)
- 3. Asymptotic normality

## 1. Consistency

Assume there's a true "data-generating process" (DGP)

$$Pr(y_i|\boldsymbol{\theta}_{true}) \sim f(y_i|\boldsymbol{\theta}_{true})$$

– You've specified some probability model  $p(y_i|\theta)$  and estimated  $\theta$  using your specified model

$$\widehat{\mathbf{\theta}} = \operatorname{argmax}_{\mathbf{\theta}} (L(\mathbf{\theta}; \mathbf{y}))$$

Assume that your model "includes" the true DGP

$$f(\cdot) \in p(\cdot)$$

Then as you collect more data

As 
$$n \to \infty$$
, then  $\widehat{\boldsymbol{\theta}} \to \boldsymbol{\theta}_{\text{true}}$ 

#### 2. Consistency (incorrect model)

Assume there's a true "data-generating process" (DGP)

$$\Pr(y_i|\boldsymbol{\theta}_{\text{true}}) \sim f(y_i|\boldsymbol{\theta}_{\text{true}})$$

– You've specified some probability model  $p(y_i|\mathbf{\theta})$  and estimated  $\mathbf{\theta}$  using your specified model

$$\widehat{\boldsymbol{\theta}} = \operatorname{argmax}_{\boldsymbol{\theta}} (L(\boldsymbol{\theta}; \mathbf{y}))$$

Assume there's an optimal estimator

$$\mathbf{\theta}_{optimal} = \operatorname{argmin}_{\mathbf{\theta}} (\mathbb{E}(D_{KL}(p(y^*|\mathbf{\theta}) \to f(y^*|\mathbf{\theta}_0))))$$

where  $D_{KL}(p(y^*|\mathbf{\theta}) \to f(y^*|\mathbf{\theta}_0))$  is the information lost when predicting new data  $y^*$  and approximating f as function p. This can be calculated as:

$$\theta_{optimal} = \operatorname{argmin}_{\boldsymbol{\theta}} \left( \int \log \left( \frac{f(\boldsymbol{\theta}_{\text{true}})}{p(\boldsymbol{\theta})} \right) f(\boldsymbol{\theta}_{\text{true}}) dy_i \right)$$

Then as you collect more data

As 
$$n \to \infty$$
, then  $\widehat{m{ heta}} \to m{ heta}_{optimal}$ 

### 3. Asymptotic normality

Assume there's an optimal estimator

$$\mathbf{\theta}_{optimal} = \operatorname{argmin}_{\mathbf{\theta}} \left( \int \log \left( \frac{f(\mathbf{\theta}_{true})}{p(\mathbf{\theta})} \right) f(\mathbf{\theta}_{true}) dy_i \right)$$

– You've specified some probability model  $p(y_i|\theta)$  and estimated  $\theta$  using your specified model

$$\widehat{\mathbf{\theta}} = \operatorname{argmax}_{\mathbf{\theta}} (L(\mathbf{\theta}; \mathbf{y}))$$

- As sample sizes get big  $(n \to \infty)$ , if you replicate an estimator:

$$\widehat{\boldsymbol{\theta}} \sim \text{MVN}(\boldsymbol{\theta}_{optimal}, \boldsymbol{\Sigma})$$

where  $\Sigma$  decreases with increasing n

## **Implications**

- If you have a simulation design...
  - ... and the model used to simulate data is identical to the model used to estimate parameters
    - Estimated parameters will be perfect with large sample sizes
    - Total error will go to zero with large sample sizes
  - ... and your estimation model doesn't match the simulation model
    - Estimated parameters will converge on values with large sample sizes
    - Total error will decrease to an asymptote

# Example #1 – What is the mean density of canary rockfish in the California Current?

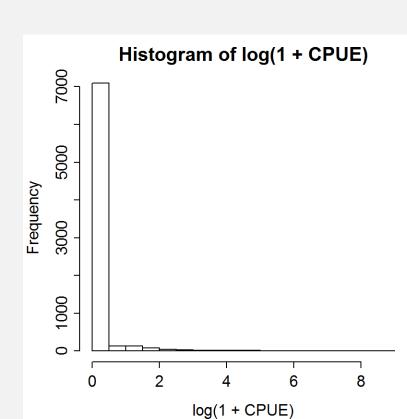
Define linear predictor matrix

$$x_i = 1$$

– i.e.,

$$X = 1$$

We call X an intercept matrix



- Approach 1 Use existing R functions
  - Step 1 Find function
    - For linear model, use Im in the base package
  - Step 2 Apply function
    - Usually easy in R
  - Step 3 Extract information from object
    - Often hard
    - Sometimes use *summary* or *attributes* commands

- Approach 1
  - [See R code]

- Approach 2 Build your own code
  - Step 1 make function for log-likelihood
  - Step 2 use nonlinear minimizer to find maximum likelihood estimate
  - Step 3 estimate standard errors

- How to estimate standard errors?
  - Estimate the "Hessian" at the MLE

$$H(\mathbf{\theta}; \mathbf{y}) = \begin{bmatrix} \frac{\partial^2 \ln L(\mathbf{\theta}; \mathbf{y})}{\partial \theta_1^2} & \frac{\partial^2 \ln L(\mathbf{\theta}; \mathbf{y})}{\partial \theta_1 \partial \theta_2} \\ \frac{\partial^2 \ln L(\mathbf{\theta}; \mathbf{y})}{\partial \theta_1 \delta \theta_2} & \frac{\partial^2 \ln L(\mathbf{\theta}; \mathbf{y})}{\partial \theta_2^2} \end{bmatrix}$$

Calculate its inverse

$$\widehat{Var}(\mathbf{\theta}; \mathbf{y}) = \mathbf{H}^{-1}$$

Extract element and take square root

$$\widehat{SE}(\theta_1; \mathbf{y}) = \sqrt{\widehat{Var}(\mathbf{\theta}; \mathbf{y})_{1,1}}$$

- Approach 2
  - [See R code]

- Approach 3 Use TMB
  - Step 1 Define TMB template file
    - Uses C++ code
  - Step 2 Define inputs for TMB
    - List of "tagged" (named) elements for data and starting parameters
  - Step 3 Run optimizer in R
    - Nonlinear optimizers using gradients
  - Step 4 Check model diagnostics

## TMB overview

CppAD (external C++ package)

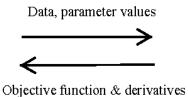
- derivative calculations



#### Native TMB

R controlling session (\*.R file)

- data pre-processing, call nlminb(), plot result



C++ objective function
(\*.cpp file)

evaluate objective
 function and its derivatives



R packages, C++ code



Eigen (external C++ package)

- matrix library

- Approach 3
  - [See R code]

## How to know you understand a model?

- 1. Make predictions about behavior, and double check predictions
- 2. Simulation experiments

### Next step:

- Add covariates (pass and latitude)
- Prediction: Adding fixed effects will always decrease the residual variance in a linear model

## Testing prediction: effect of adding linear predictors

- [See R code]
- Was the prediction supported?