Lecture 1: Likelihoods and linear models

March 29, 2016

[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 here generally work with differentiable functions

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} = \lim_{h \to 0} \frac{f(x) - f(x-h)}{h}$$

– For concepts, we only really need to know 2nd order differentiation. Useful reminder that order of multivariate derivative doesn't matter:

$$\frac{d}{dx_2}\frac{d}{dx_1} f = \frac{d}{dx_1}\frac{d}{dx_2} f$$

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
  - Script: 2D function:
    - e.g., $\mathcal{D}(s)$ for density at location $s = (x, y)^{\mathrm{T}}$
  - Script: operators
    - e.g., $\mathbb{E}$ and $\mathbb{V}$ for expectation and variance of a function)
  - tilde (~): distributions
    - e.g., $c \sim \mathrm{Normal}(\mu, \sigma^2)$

Definitions

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

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

$$\Pr(X) = \int \Pr(X,Y)\mathrm{d}Y$$

   – Used when justifying hierarchical models

Specify a linear model

- Step 1 – Specify a linear predictor for response variable

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

  - where $\mathbf{x}_\mathrm{i}$ is a row of a predictor matrix **X**
  - **b** is a vector of parameters

- Step 2 – Specify a probability distribution for your response variable

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

- Maximum likelihood estimation (MLE)

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

  - Where $\hat{\boldsymbol{\theta}}$ is the MLE estimate of parameters
  - Where $\operatorname{argmax}_{\boldsymbol{\theta}}(L(\boldsymbol{\theta}; \mathbf{y}))$ 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 (not interesting)

- Usually we specify that each datum is independent

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

therefore

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

Why use maximum likelihood estimation?

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

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

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

Why use maximum likelihood estimation?

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

$$\Pr(y_i|\boldsymbol{\theta}_0) \sim f(y_i|\boldsymbol{\theta}_0)$$

   - Assume that your model "includes" the true DGP

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

   - Then as you collect more data

$$\text{As } n \to \infty, \hat{\boldsymbol{\theta}} \to \boldsymbol{\theta}_0$$

Why use maximum likelihood estimation?

2. Consistency (incorrect model)
   - Assume there's a true "data-generating process" (DGP)

$$\Pr(y_i|\boldsymbol{\theta}_0) \sim f(y_i|\boldsymbol{\theta}_0)$$

   - Assume there's an optimal estimator

$$\boldsymbol{\theta}_{optimal} = \text{argmin}_{\boldsymbol{\theta}}\left(\mathbb{E}(D_{KL}(p(\mathbf{y}|\boldsymbol{\theta}) \to f(\boldsymbol{\theta}_0)))\right)$$

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

$$\boldsymbol{\theta}_{optimal} = \text{argmin}_{\boldsymbol{\theta}}\left(\int \log\left(\frac{f(\boldsymbol{\theta}_0)}{p(D|\boldsymbol{\theta})}\right) f(\boldsymbol{\theta}_0) dy_i\right)$$

   - Then as you collect more data

As $n \to \infty, \hat{\boldsymbol{\theta}} \to \boldsymbol{\theta}_{optimal}$

Why use maximum likelihood estimation?

3. Asymptotic normality

– Assume there's an optimal estimator

$$\boldsymbol{\theta}_{optimal} = \text{argmin}_{\boldsymbol{\theta}} \left(\int \log \left(\frac{f(\boldsymbol{\theta}_0)}{p(D|\boldsymbol{\theta})} \right) f(\boldsymbol{\theta}_0) dy_i \right)$$

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

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

where $\boldsymbol{\Sigma}$ 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?

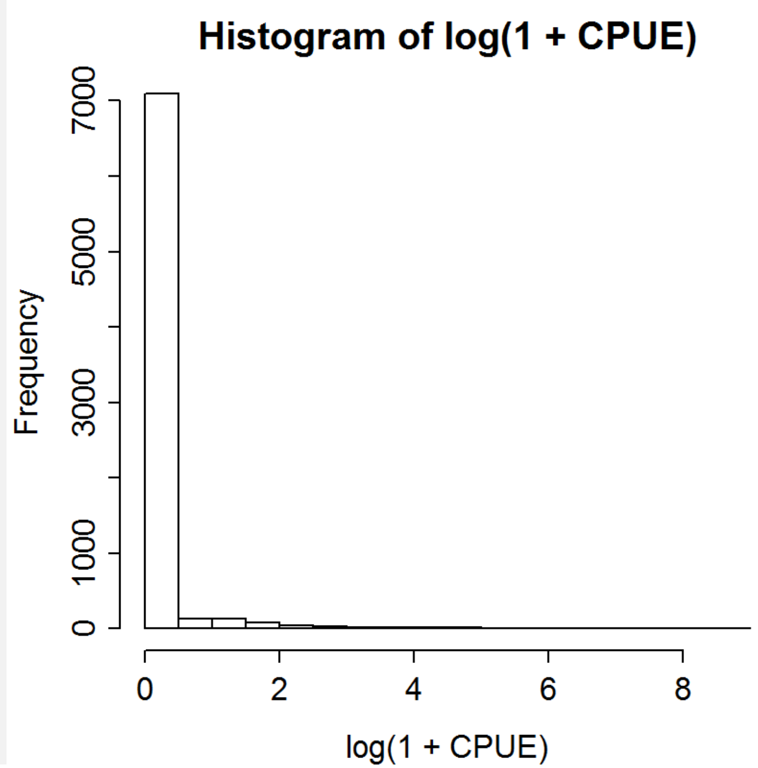
- Define linear predictor matrix

$$x_i = 1$$

  – i.e.,

$$\mathbf{X} = \mathbf{1}$$

  – We call **X** an intercept matrix



- Approach 1 – Use existing R functions
  - Step 1 – Find function
    - For linear model, use *lm* 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

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

  - Calculate its inverse

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

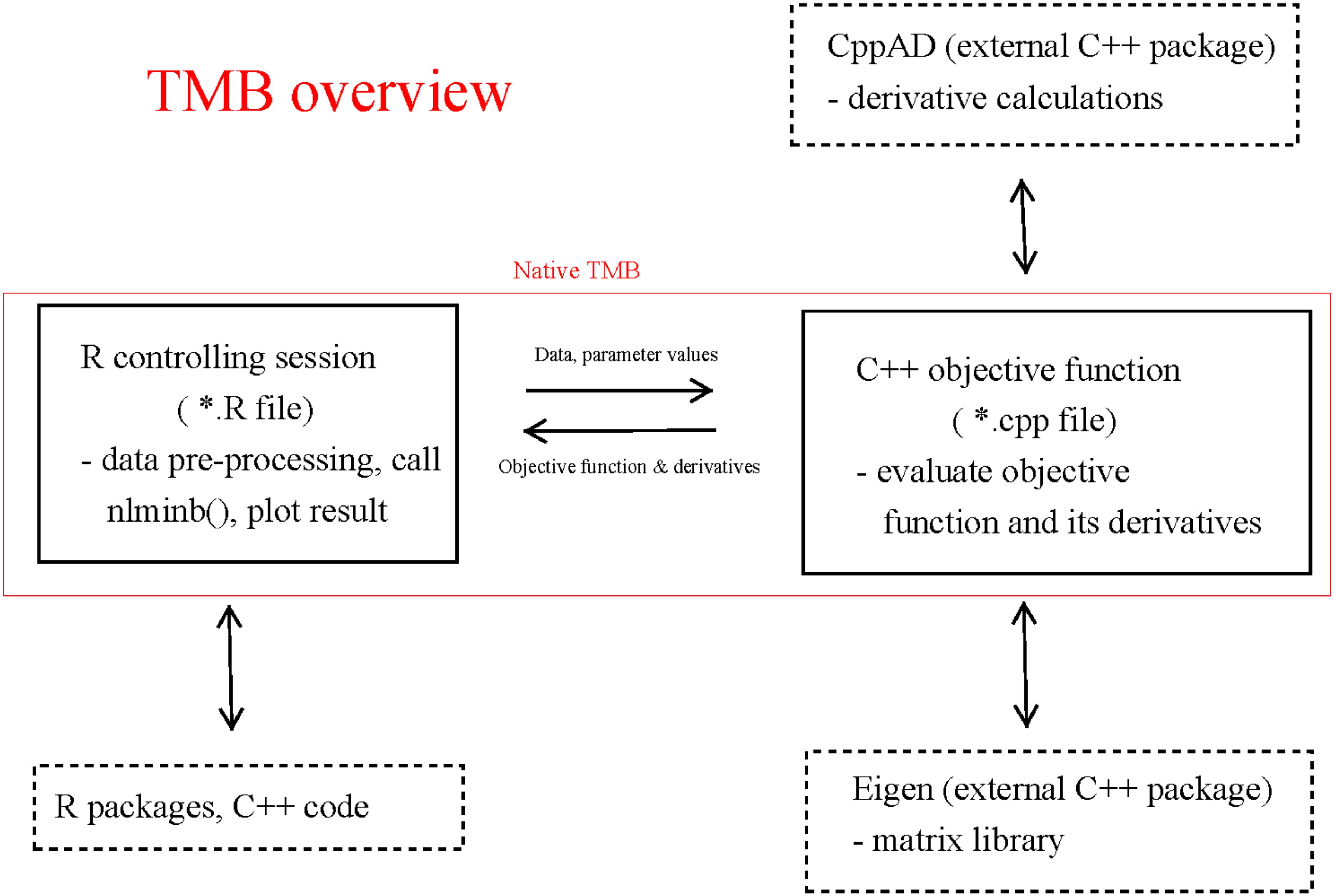
  - Extract element and take square root

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

- 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 paramesters
  - Step 3 – Run optimizer in R
    - Nonlinear optimizers using gradients
  - Step 4 – Check model diagnostics

TMB overview



- 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?