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:
  - 1st derivatives:

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

  - 2nd derivatives:

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

* Taylor series
* Local maximum vs minimum
* Getting standard errors

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*
    - $\Pr(\mathbf{y}|\boldsymbol{\theta})$
    - $\mathbf{y}$ = 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

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

Can always factor a joint probability into probability of one and conditional probability of others

   – 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 $\mathbf{X}$
  - $\mathbf{b}$ 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)

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

  - Where $\hat{\boldsymbol{\theta}}$ is the MLE estimate of parameters
  - Where $\mathrm{argmax}_{\boldsymbol{\theta}}(L(\boldsymbol{\theta}; \mathbf{y}))$ 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

Why maximum likelihood?
* invariant to transformations
* consistent (approaches true value with increased sample size)

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:

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

- And taking logs

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

And generalizing to more than two observations

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

therefore

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

Why use maximum likelihood estimation?

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

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)
     $$\Pr(y_i|\boldsymbol{\theta}_{\text{true}}) \sim f(y_i|\boldsymbol{\theta}_{\text{true}})$$
   - You've specified some probability model $p(y_i|\boldsymbol{\theta})$ and estimated $\boldsymbol{\theta}$ using your specified model
     $$\widehat{\boldsymbol{\theta}} = \text{argmax}_{\theta}\big(L(\boldsymbol{\theta};\mathbf{y})\big)$$
   - Assume that your model "includes" the true DGP
     $$f(\cdot) \in p(\cdot)$$
   - Then as you collect more data
     $$\text{As } n \to \infty, \text{ then } \widehat{\boldsymbol{\theta}} \to \boldsymbol{\theta}_{\text{true}}$$

Why use maximum likelihood estimation?

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 $p(y_i|\boldsymbol{\theta})$ and estimated $\boldsymbol{\theta}$ using your specified model

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

– Assume there's an optimal estimator

$$\boldsymbol{\theta}_{optimal} = \text{argmin}_{\boldsymbol{\theta}}\Big(\mathbb{E}\big(D_{KL}(p(y^*|\boldsymbol{\theta}) \rightarrow f(y^*|\boldsymbol{\theta}_0))\big)\Big)$$

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

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

– Then as you collect more data

As $n \rightarrow \infty$, then $\widehat{\boldsymbol{\theta}} \rightarrow \boldsymbol{\theta}_{optimal}$

Why use maximum likelihood estimation?

3. Asymptotic normality
   - Assume there's an optimal estimator

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

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

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

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

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

where $\boldsymbol{\Sigma}$ decreases with increasing *n*

Can estimate the covariance using the second derivative of the likelihood function

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?

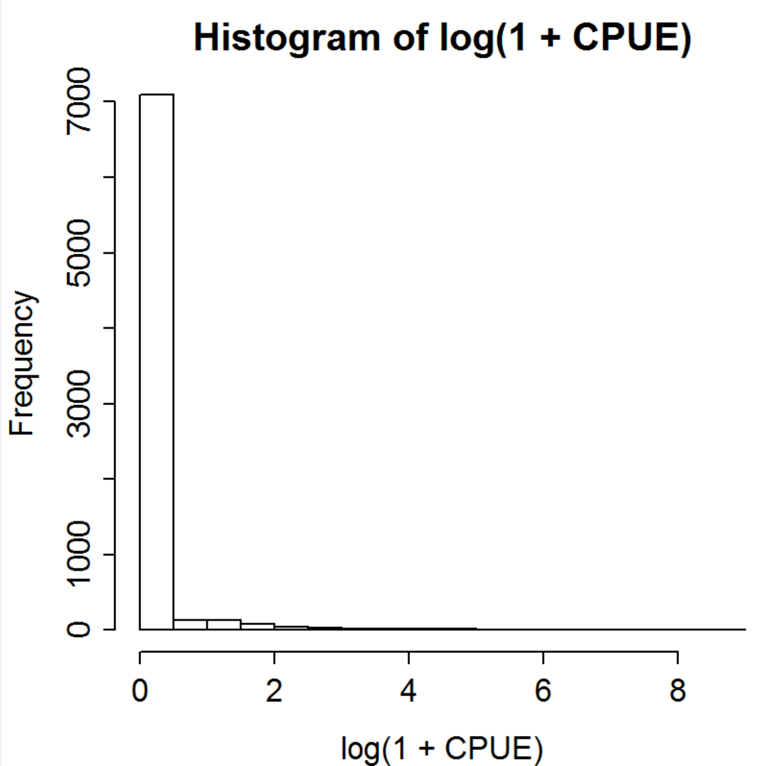
- Define linear predictor matrix

$$x_i = 1$$

  - 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

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

  - Calculate its inverse

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

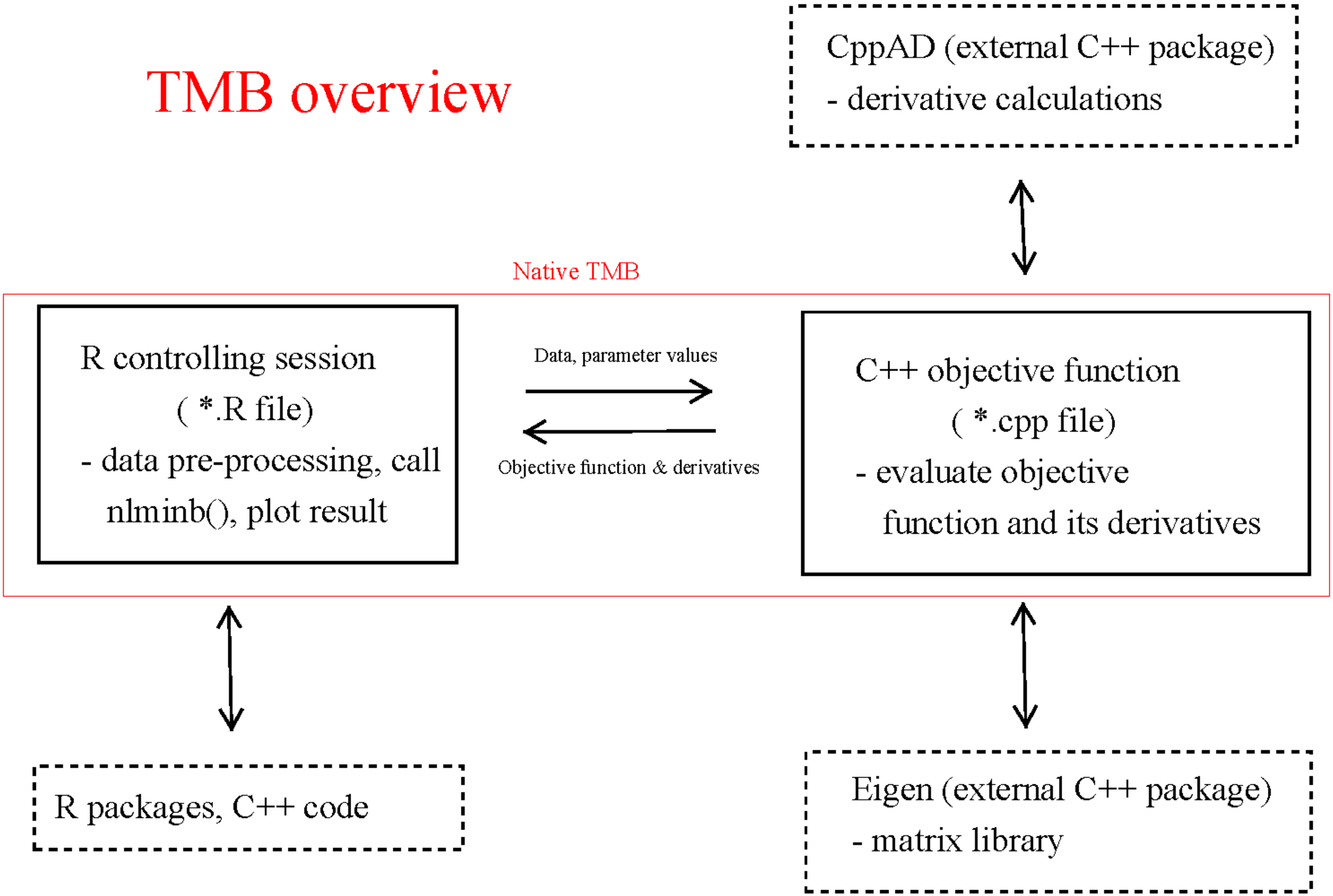
  - Extract element and take square root

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

- 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?