CSSS/POLS 510 Maximum Likelihood Estimation: Lab 4

Heteroskedastic Normal & Logit model

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Mid-quarter Evaluation

Your feedback is valuable: Evaluation URL

Agenda

1. Heteroskedastic Normal Example: Simulation
2. Logit model: Voting example
3. Homework: Recap HW2, Question HW3

1. Heteroskedastic Normal Example

- Steps
  - The full `R` code can be found here from Chris' website

    2.1 Generate Data

    2.2 Fit OLS - `lm()`

    2.3 Fit MLE - `optim()`

    2.4 Calculate quantities of interest
    - Use `predict()`
    - Use simulation

1.1 Recap

```r
rm(list=ls())          # Clear memory
set.seed(123456)       # For reproducible random numbers
library(MASS)          # Load packages
library(simcf)
library(tidyverse)

n <- 1500              # Generate 1500 observations

w0 <- rep(1, n)        # Create the constant
w1 <- runif(n)         # Create two covariates
w2 <- runif(n)

x <- cbind(w0, w1, w2)         # Create a matrix of the covariates
z <- x                         # i.e., same covariates affect mu and sigma

beta <- c(0, 5, 15) # Set a parameter vector for the mean
                    # One for constant, one for covariate 1,
                    # one for covariate 2.

gamma <- c(1, 0, 3) # Set a parameter vector for the variance
                    # Gamma estimate for covariate 2 is set to be 3,
                    # whic creates heteroskedasticity
```

1.1 Recap

```r
mu <- x %*% beta                # Create systemtic component for the mean

sigma2 <- exp(z %*% gamma)      # Create systematic component for the variance
                                # Since ith row of sigma2 = exp(1 + 0 + w2_i * 3)
                                # i.e., it is a function of w2 (heteroskedastic)

y <- rnorm(n = n,               # Create the outcome variable
           mean = mu,           # Think about the stochastic component!
           sd = sqrt(sigma2)
           )

data <- cbind(y, w1, w2)        # Save the data to a data frame
data <- as.data.frame(data)
names(data) <- c("y", "w1", "w2")
```

1.1 Recap

```
ls.result <- lm(y ~ w1 + w2, data = data) # Fit a linear model
                                          # using simulated data

ls.aic <- AIC(ls.result) # Calculate and print the AIC
                         # i.e. Akaike Information Criterion
                         # to assess goodness of fit; lower AIC is better
```

1.1 Recap

```r
# A likelihood function for ML heteroskedastic Normal
llk.hetnormlin <- function(param, y, x, z) {
  x <- as.matrix(x)                          # x (some covariates) as a matrix
  z <- as.matrix(z)                          # z (some covariates) as a matrix
  os <- rep(1, nrow(x))                      # Set the intercept as 1 (constant)
  x <- cbind(os, x)                          # Add intercept to covariates x
  z <- cbind(os, z)                          # Add intercept to covariates z

  b <- param[1 : ncol(x)]                              # Parameters for x
  g <- param[(ncol(x) + 1) : (ncol(x) + ncol(z))] # Parameters for z

  xb <- x %*% b                              # Systematic components for mean
  s2 <- exp(z %*% g)                         # Systematic components for variance

  sum(0.5 * (log(s2) + (y - xb)^2 / s2)) # Likelihood we want to maximize
                                             # optim is a minimizer by default
                                             # To maximize lnL is to minimize -lnL
                                             # so the +/- signs are reversed
}
```

1.1 Recap

```r
# Create input matrices
xcovariates <- cbind(w1, w2)
zcovariates <- cbind(w1, w2)

# Initial guesses of beta0, beta1, ..., gamma0, gamma1, ...
# We need one entry per parameter, in order!
# Note: also include beta and gamma estiamtes for constants
stval <- c(0, 0, 0, 0, 0, 0)

# Run ML, and get the output we need
hetnorm.result <- optim(stval,            # Initial guesses
                        llk.hetnormlin,   # Likelihood function
                        method = "BFGS",  # Gradient method
                        hessian = TRUE,   # Return Hessian matrix
                        y = y,            # Outcome variable
                        x = xcovariates,  # Covariates x (w/o constant)
                        z = zcovariates   # Covariates z (w/o constant)
                        )
```

Note: By default, `optim()` performs a minimizing procedure. You can make optim a maximizer by adding `control = list(fnscale = -1)`

1.1 Recap

```r
pe <- hetnorm.result$par              # Point estimates
round(pe, 3)
```

```
## [1] -0.167  5.007 15.698  0.910  0.224  2.994
```

```r
vc <- solve(hetnorm.result$hessian) # Var-cov matrix (for computing s.e.)
round(vc, 5)
```

```
##          [,1]     [,2]     [,3]     [,4]     [,5]     [,6]
## [1,]  0.02909 -0.03265 -0.02810  0.00059 -0.00087 -0.00032
## [2,] -0.03265  0.06787 -0.00025 -0.00091  0.00099  0.00084
## [3,] -0.02810 -0.00025  0.10331 -0.00056  0.00143 -0.00033
## [4,]  0.00059 -0.00091 -0.00056  0.00920 -0.00832 -0.00749
## [5,] -0.00087  0.00099  0.00143 -0.00832  0.01693 -0.00042
## [6,] -0.00032  0.00084 -0.00033 -0.00749 -0.00042  0.01568
```

```r
se <- sqrt(diag(vc))                  # To compute standard errors (s.e.)
                                      # take the diagonal of the Hessian;
                                      # then take square root
round(se, 3)
```

```
## [1] 0.171 0.261 0.321 0.096 0.130 0.125
```

1.1 Recap

```r
mle.result <- cbind(pe[1:3], se[1:3])          # Report ML results
colnames(mle.result) <- c("Estimate", "Std.Error")
rownames(mle.result) <- c("(Intercept)", "w1", "w2")
round(mle.result, 3)
```

```
##             Estimate Std.Error
## (Intercept)   -0.167     0.171
## w1             5.007     0.261
## w2            15.698     0.321
```

```r
round(coef(summary(ls.result))[, c(1, 2)], 3) # Compare with lm() results
```

```
##             Estimate Std. Error
## (Intercept)   -0.049      0.282
## w1             4.784      0.377
## w2            15.683      0.371
```

```r
ll <- -hetnorm.result$value                    # Report likelihood at maximum
                                               # No need to have negative sign
                                               # if optim is set as maximizer
ll
```

1.1 Recap

```
# AIC is 2 * number of parameters - 2 * ll (i.e. likelihood at maximum)
hetnorm.aic <- 2 * length(stval) - 2 * ll

# Compare AIC from ML and from lm(); lower is better
print(hetnorm.aic)
```

```
## [1] 5252.668
```

```
print(ls.aic)
```

```
## [1] 8545.903
```

1.2 Recap2: Predict QoI

Motivation: We want to study how the change in a particular explanatory variable affects the outcome variable, *all else being equal*

1.2 Recap2: Predict QoI

- Scenario 1: Vary covariate 1; hold covariate 2 constant

1. Create a data frame with a set of hypothetical scenarios for covariate 1, while keeping covariate 2 at its mean
   - What is the sensible range of some hypothetical scenarios for covariate 1? Consider the original range of `w1`.
2. Calculate the predicted values using the `predict()` function
   - Hint: you need at least the following arguments: `predict(object = ... , newdata = ... , interval = ... , level = ...)`
3. Plot the prediction intervals

1.2 Recap2: Predict QoI

4. Similarly, calculate the confidence intervals using the `predict()` function
5. Plot the confidence intervals; compare them with the predictive intervals

1.2 Recap2: Predict QoI

```r
# Set up
w1range <- seq(from = 0, to = 1, by = 0.05)    # Set up hypothetical values for w
w2mean <- mean(w2)                             # Set up mean for w2
xhypo <- crossing(w1 = w1range, w2 = w2mean)   # Create a new dataset using cross
# Calculate predicted values
simPI.w1 <- predict(ls.result,                  # A model object
                    newdata = xhypo,            # New dataset
                    interval = "prediction",    # What kind of intervals?
                    level = 0.95)               # What levels of confidence?
```

1.2 Recap2: Predict QoI

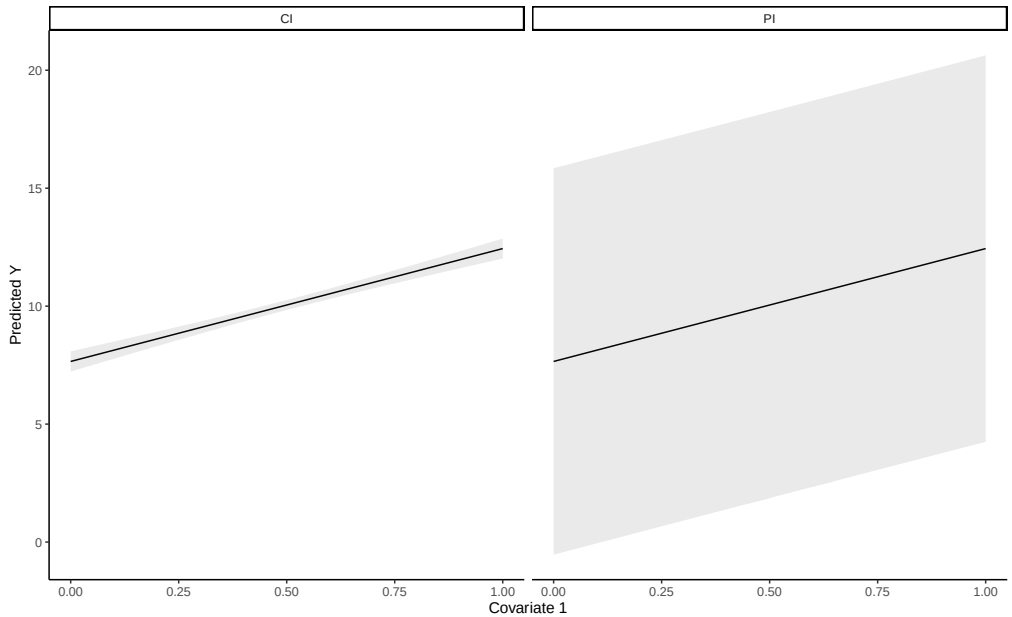
```r
simPI.w1 <- simPI.w1 %>%
  as_tibble() %>%          # Coerce it into a tibble
  bind_cols(w1 = w1range) # Combine hypo w1 with predicted y

# Calculate confidence intervals using predict()
simCI.w1 <- predict(ls.result,
                    newdata = xhypo,
                    interval = "confidence",
                    level = 0.95)
simCI.w1 <- simCI.w1 %>%
  as_tibble() %>%
  bind_cols(w1 = w1range)
```

1.2 Recap2: Predict QoI

```
# ggplot2
theme_set(theme_classic())
simALL.w1 <- bind_rows(
  simPI.w1 %>% mutate(type = "PI"),
  simCI.w1 %>% mutate(type = "CI")
  )
```

1.2 Recap2: Predict QoI

```r
# Plot confidence intervals and predictive intervals side by side
ggplot(simALL.w1, aes(x = w1, y = fit, ymax = upr, ymin = lwr)) +
  geom_line() +
  geom_ribbon(alpha = 0.1) +
  labs(y = "Predicted Y", x = "Covariate 1") +
  facet_grid(~ type)
```



1.2 Recap2: Predict QoI

Scenario 2: Vary covariate 2; hold covariate 1 constant

```
w2range <- seq(from = 0, to = 1, by = 0.05)    # Set up hypothetical values for w
w1mean <- mean(w1)                             # Set up mean for w2
xhypo <- crossing(w1 = w1mean,                # Create a new dataset
                  w2 = w2range)                  # crossing() is from tidyr packag
# Calculate predicted values
simPI.w2 <- predict(ls.result,                   # A model object
                    newdata = xhypo,             # New dataset
                    interval = "prediction",     # What kind of intervals?
                    level = 0.95)                # What levels of confidence?

simPI.w2 <- simPI.w2 %>%
  as_tibble() %>%
  bind_cols(w2 = w2range)
```

1.3 Simulating QoI using `simcf`

Motivation: Can we use simulation methods to produce the same prediction and confidence intervals? Recall the lecture: we can draw a bunch of $\tilde{\beta}$ from a multivariate normal distribution

Demonstration:

- Scenario 1: Vary covariate 1; hold covariate 2 constant

1. Create a data frame with a set of hypothetical scenarios for covariate 1 while keeping covariate 2 at its mean
2. Simulate the predicted values using `MASS` and `simcf`
3. Plot the results

1.3 Simulating QoI using `simcf`

In order to use `simcf` to generate quantities of interest, the following steps are needed:

1. Estimate: MLE $\hat{\beta}$ and its variance $\hat{V}(\hat{\beta})$
2. Simulate estimation uncertainty from a multivariate normal distribution:
   Draw $\tilde{\beta} \sim MVN\left[\hat{\beta}, \hat{V}(\hat{\beta})\right]$
3. Create hypothetical scenarios of your substantive interest:
   Choose valuese of X: X_c

1.3 Simulating QoI using `simcf`

4. Calculate expected values:
   $\tilde{\mu_c} = g(X_c, \tilde{\beta})$
5. Simulate fundamental uncertainty:
   $\tilde{y_c} \sim f(\tilde{\mu_c}, \tilde{\alpha})$
   or
6. Compute EVs, First Differences or Relative Risks
   EV: $\mathbb{E}(y|X_{c1})$
   FD: $\mathbb{E}(y|X_{c2}) - \mathbb{E}(y|X_{c1})$
   RR: $\frac{\mathbb{E}(y|X_{c2})}{\mathbb{E}(y|X_{c1})}$

1.3 Simulating QoI using `simcf`

In order to use `simcf` to generate quantities of interest, the following steps are needed:

1. Estimate: MLE $\hat{\beta}$ and its variance $\hat{V}(\hat{\beta})$
   → `optim()`, `glm()`
2. Simulate estimation uncertainty from a multivariate normal distribution:
   Draw $\tilde{\beta} \sim MVN\left[\hat{\beta}, \hat{V}(\hat{\beta})\right]$
   → `MASS::mvrnorm()`
3. Create hypothetical scenarios of your substantive interest:
   Choose valuese of X: X_c
   → `simcf::cfmake()`, `cfchange()` ...

1.3 Simulating QoI using `simcf`

4. Calculate expected values:
   $\tilde{\mu_c} = g(X_c, \tilde{\beta})$
5. Simulate fundamental uncertainty:
   $\tilde{y_c} \sim f(\tilde{\mu_c}, \tilde{\alpha})$
   → `simcf::hetnormsimpv()` ...
   or
6. Compute EVs, First Differences or Relative Risks
   EV: $\mathbb{E}(y|X_{c1})$
   → `simcf::logitsimev()` ...
   FD: $\mathbb{E}(y|X_{c2}) - \mathbb{E}(y|X_{c1})$
   → `simcf::logitsimfd()` ...
   RR: $\frac{\mathbb{E}(y|X_{c2})}{\mathbb{E}(y|X_{c1})}$
   → `simcf::logitsimrr()` ...

1.3 Simulating QoI using `simcf`

Recall our likelihood function is:

$$\mathrm{P}\left(\mathbf{y}|\boldsymbol{\mu},\boldsymbol{\sigma}^2\right) = \prod_{i=1}^{n} f_{\mathcal{N}}\left(y_i|\mu_i,\sigma_i^2\right) \quad \text{[Joint probability}$$

$$\mathrm{P}\left(\mathbf{y}|\boldsymbol{\mu},\boldsymbol{\sigma}^2\right) = \prod_{i=1}^{n} \left(2\pi\sigma_i^2\right)^{-1/2} \exp\left[\frac{-\left(y_i-\mu_i\right)^2}{2\sigma_i^2}\right] \quad \text{[Expressed in Normal distributio}$$

$$\log\mathcal{L}\left(\beta,\boldsymbol{\sigma}^2|\mathbf{y}\right) \propto -\frac{1}{2}\sum_{i=1}^{n}\log\sigma_i^2 - \frac{1}{2}\sum_{i=1}^{n}\frac{\left(y_i-\mathbf{x}_i\beta\right)^2}{\sigma_i^2} \quad \text{[Converted to log likelihood; simplif}$$

$$\log\mathcal{L}(\beta,\gamma|\mathbf{y}) \propto -\frac{1}{2}\sum_{i=1}^{n}\log\mathbf{z}_i\gamma - \frac{1}{2}\sum_{i=1}^{n}\frac{\left(y_i-\mathbf{x}_i\beta\right)^2}{\exp\left(\mathbf{z}_i\gamma\right)} \quad \text{[Substitute in systematic component}$$

1.3 Simulating QoI using `simcf`

```
# Draw parameters from the model predictive distribution
sims <- 10000
simparam <- mvrnorm(n = sims,
                    mu = pe,     # M.N.D. with population mean = pe (from ML);
                    Sigma = vc) # population var-covar matrix = vc (from ML)
head(simparam)                  # Inspect
```

```
##              [,1]     [,2]     [,3]      [,4]      [,5]     [,6]
## [1,]  0.24211743 4.253787 15.94193 0.8538881 0.1676888 3.187143
## [2,] -0.10028149 4.866367 15.88825 0.8131899 0.2369895 3.038976
## [3,] -0.15729804 4.813402 15.81664 0.9172401 0.3016272 2.864065
## [4,] -0.01521245 4.482252 16.12675 0.9590520 0.2337601 2.975280
## [5,]  0.10941227 4.821406 15.16535 0.9812625 0.2492318 2.763246
## [6,] -0.22838155 4.947090 15.62518 0.9596191 0.1447425 2.870572
```

1.3 Simulating QoI using `simcf` :S1

```r
# Separate into the simulated betas and simulated gammas
simbetas <- simparam[ , 1:(ncol(xcovariates) + 1)]
simgammas <- simparam[ , (ncol(simbetas) + 1):ncol(simparam)]

# Specify model formulas
varmodel <- (y ~ w1 + w2)

# Create hypothetical scenarios for covariate 1
w1range <- seq(from = 0, to = 1, by = 0.2)
```

1.3 Simulating QoI using `simcf` :S1

```
# Use 'cfMake' to create a baseline dataset
xhypo <- cfMake(varmodel,
                data,
                nscen = length(w1range))

xhypo
```

```
## $x
##           y        w1        w2
## 1 10.06525 0.5036167 0.4912698
## 2 10.06525 0.5036167 0.4912698
## 3 10.06525 0.5036167 0.4912698
## 4 10.06525 0.5036167 0.4912698
## 5 10.06525 0.5036167 0.4912698
## 6 10.06525 0.5036167 0.4912698
##
## $xpre
##           y        w1        w2
## 1 10.06525 0.5036167 0.4912698
## 2 10.06525 0.5036167 0.4912698
## 3 10.06525 0.5036167 0.4912698
## 4 10.06525 0.5036167 0.4912698
```

1.3 Simulating QoI using `simcf` :S1

```r
# Use 'cfChange' and loop function to loop through each hypothetical x values
for (i in 1:length(w1range)) {
  xhypo <- cfChange(xscen = xhypo,
                    covname = "w1",
                    x = w1range[i],
                    scen = i)
}

xhypo
```

```
## $x
##           y  w1        w2
## 1 10.06525 0.0 0.4912698
## 2 10.06525 0.2 0.4912698
## 3 10.06525 0.4 0.4912698
## 4 10.06525 0.6 0.4912698
## 5 10.06525 0.8 0.4912698
## 6 10.06525 1.0 0.4912698
##
## $xpre
##           y         w1        w2
## 1 10.06525 0.5036167 0.4912698
```

1.3 Simulating QoI using simcf :S1

```
# Repeat the same procedures for z
zhypo <- cfMake(varmodel, data, nscen = length(w1range))

for (i in 1:length(w1range)) {
  zhypo <- cfChange(zhypo, "w1", x = w1range[i], scen = i)
  }

zhypo
```

```
## $x
##           y  w1        w2
## 1 10.06525 0.0 0.4912698
## 2 10.06525 0.2 0.4912698
## 3 10.06525 0.4 0.4912698
## 4 10.06525 0.6 0.4912698
## 5 10.06525 0.8 0.4912698
## 6 10.06525 1.0 0.4912698
##
## $xpre
##           y         w1        w2
## 1 10.06525 0.5036167 0.4912698
## 2 10.06525 0.5036167 0.4912698
```

1.3 Simulating QoI using `simcf` :S1

```
# Simulate predictive intervals for heteroskedastic linear models
# 'hetnormsimpv()' is from simcf package
simRES.w1 <- hetnormsimpv(xhypo, simbetas,
                          zhypo, simgammas,
                          ci = 0.95,
                          constant = 1,
                          varconstant = 1)

simRES.w1
```

```
## $pe
## [1]  7.515323  8.566149  9.575781 10.579808 11.552741 12.524484
##
## $lower
##          [,1]
## low 0.8847932
## low 1.9381952
## low 2.8502531
## low 3.5495829
## low 4.5126707
## low 5.3290850
##
```

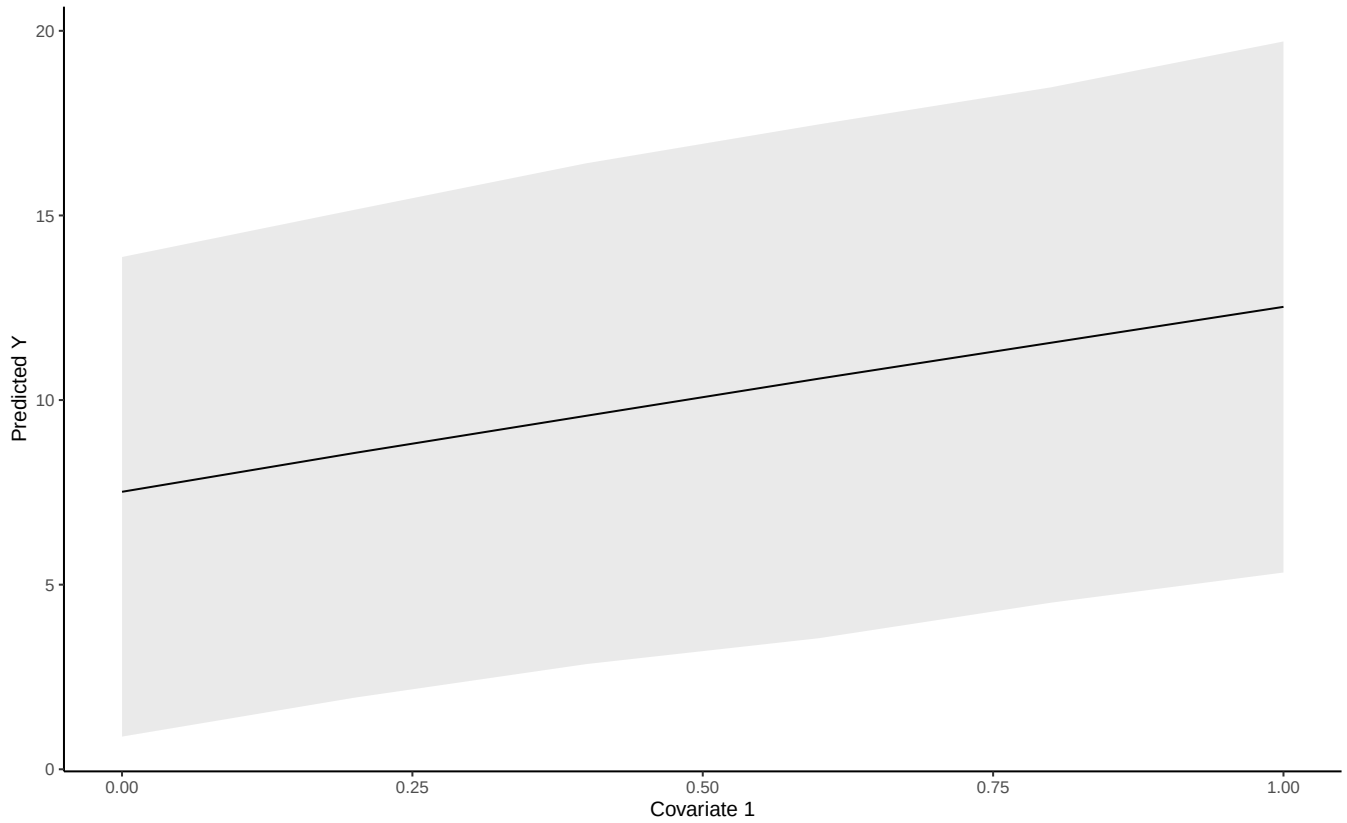
1.3 Simulating QoI using `simcf` :S1

```
simRES.w1 <- simRES.w1 %>%
  bind_rows() %>%          # Collaspe the list into d.f.
  bind_cols(w1 = w1range) # Combine with hypo. w1 values

simRES.w1                  # Inspect
```

```
## # A tibble: 6 x 4
##       pe lower[,1] upper[,1]    w1
## * <dbl>     <dbl>     <dbl> <dbl>
## 1  7.52     0.885      13.9   0
## 2  8.57     1.94       15.2   0.2
## 3  9.58     2.85       16.4   0.4
## 4 10.6      3.55       17.5   0.6
## 5 11.6      4.51       18.5   0.8
## 6 12.5      5.33       19.7   1
```

1.3 Simulating QoI using `simcf` :S1

```
# ggplot2
ggplot(simRES.w1, aes(x = w1, y = pe, ymax = upper, ymin = lower)) +
  geom_line() +
  geom_ribbon(alpha = 0.1) +
  labs(y = "Predicted Y", x = "Covariate 1")
```



1.3 Simulating QoI using `simcf` :S2

Scenario 2: Vary covariate 2; hold covariate 1 constant

1. Create a data frame with a set of hypothetical scenarios for covariate 2 while keeping covariate 1 at its mean
2. Simulate the predicted values using `MASS` and `simcf`
3. Plot the results

1.3 Simulating QoI using `simcf` :S2

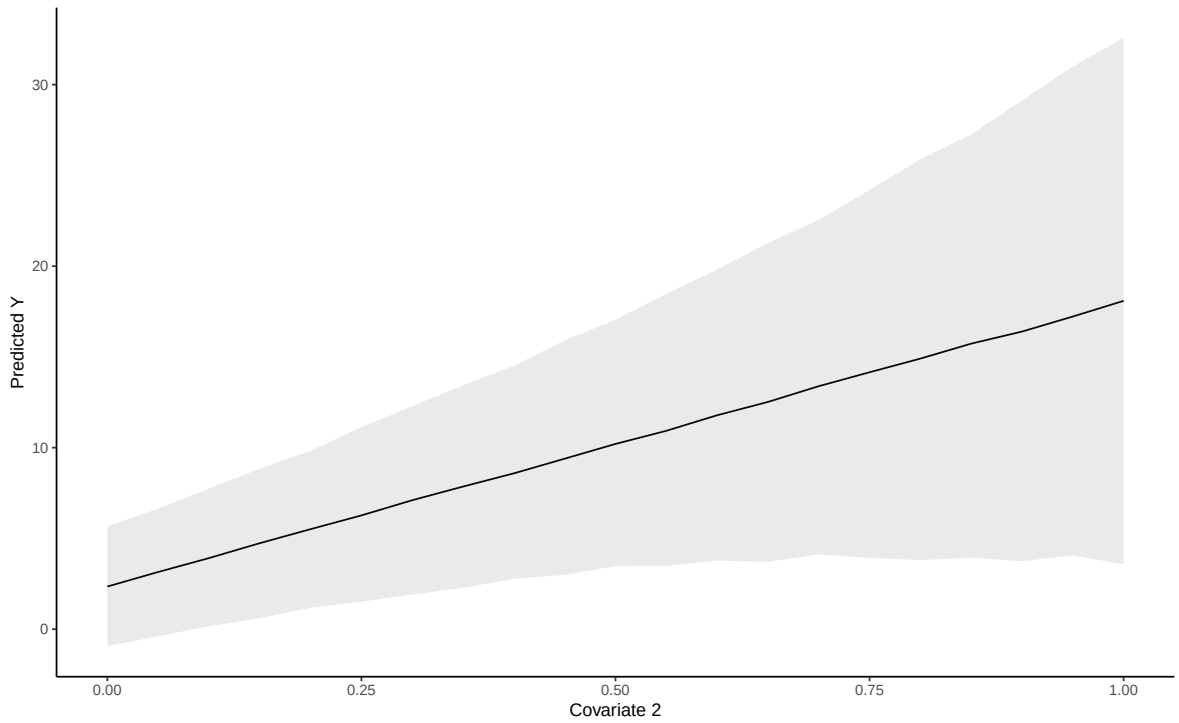
```
# Create hypothetical scenarios for w2
w2range <- seq(0, 1, by = 0.05)

xhypo <- cfMake(varmodel, data, nscen = length(w2range))

for (i in 1:length(w2range)) {
  xhypo <- cfChange(xhypo, "w2", x = w2range[i], scen = i)
}

zhypo <- cfMake(varmodel, data, nscen = length(w2range))

for (i in 1:length(w2range)) {
  zhypo <- cfChange(zhypo, "w2", x = w2range[i], scen = i)
}
```

1.3 Simulating QoI using `simcf` :S2

```
# Simulate the predicted Y's and PI's
simRES.w2 <- hetnormsimpv(xhypo, simbetas,
                          zhypo, simgammas,
                          ci = 0.95,
                          constant = 1,
                          varconstant = 1)

simRES.w2 <- simRES.w2 %>%
  bind_rows() %>%
  bind_cols(w2 = w2range)
```

1.3 Simulating QoI using `simcf` :S2

```
# Plot the predictive intervals for hypothetical w2
ggplot(simRES.w2, aes(x = w2, y = pe, ymax = upper, ymin = lower)) +
  geom_line() +
  geom_ribbon(alpha = 0.1) +
  labs(y = "Predicted Y", x = "Covariate 2")
```



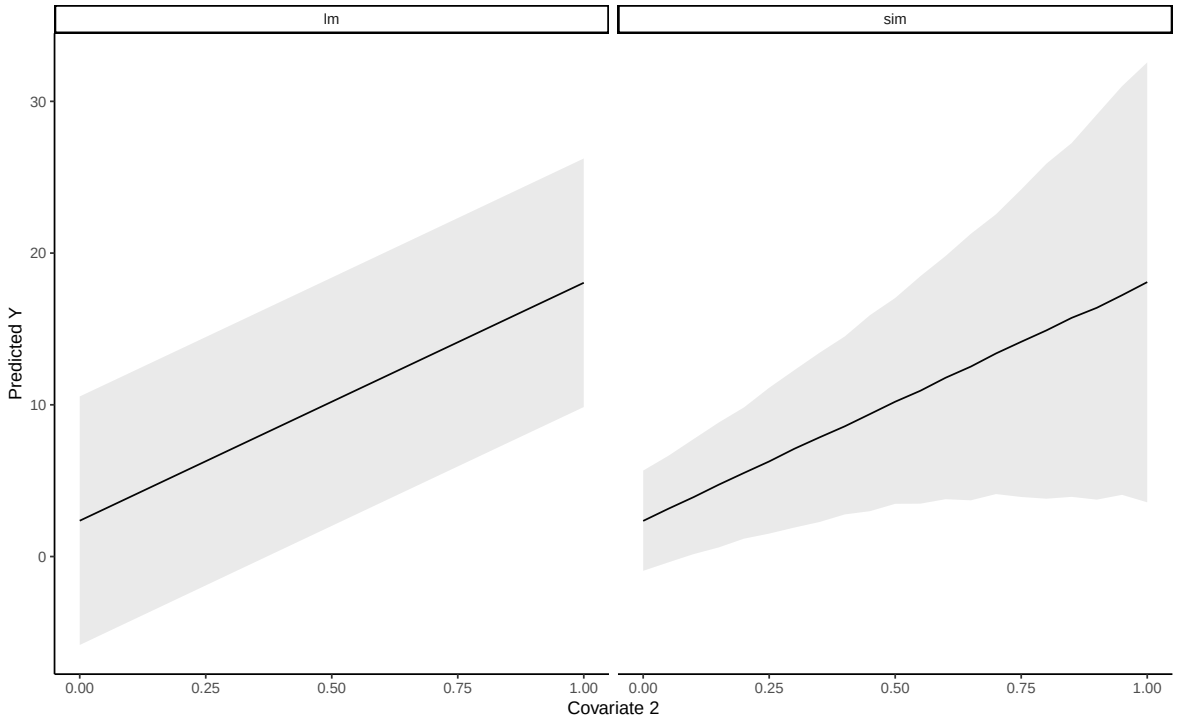
Can we compare them with the prediction intervals generated by `predict()`?

1.3 Simulating QoI using `simcf` :S2

```
# Combine two dataframes
simPI.w2 <- simPI.w2 %>%
  rename(pe = fit, lower = lwr, upper = upr)

simALL.w2 <- bind_rows(
  simRES.w2 %>% mutate(method = "sim"),
  simPI.w2 %>% mutate(method = "lm")
)
```

1.3 Simulating QoI using `simcf` :S2

```
# Plot the predictive intervals for hypothetical w2
ggplot(simALL.w2, aes(x = w2, y = pe, ymax = upper, ymin = lower)) +
  geom_line() +
  geom_ribbon(alpha = 0.1) +
  labs(y = "Predicted Y", x = "Covariate 2") +
  facet_grid(~ method)
```



2 Logit model: Voting example

Let's open `RStudio` and [**nesLogitPlot.r**]

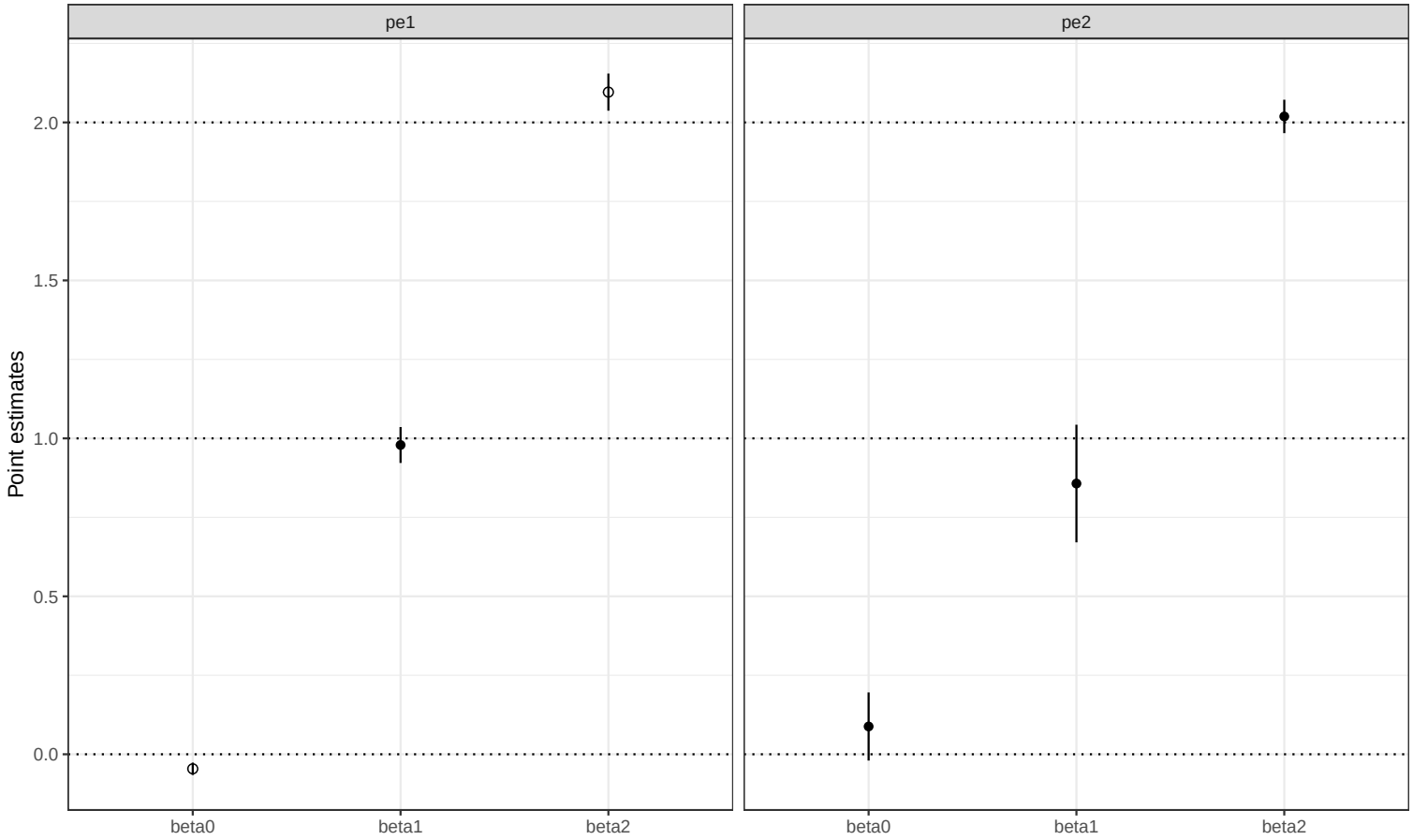
3. Homework: Recap HW2

Problem2: Which one do you have more confidence?

beta	pe1	se1	pe2	se2
beta0	-0.046	0.01	0.088	0.055
beta1	0.979	0.029	0.857	0.095
beta2	2.096	0.03	2.019	0.027

3. Homework: Recap HW2

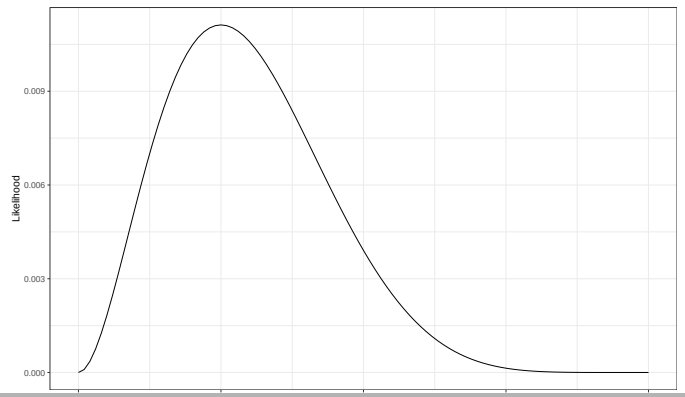
How about this?



3. Homework: Recap HW2

Lazy coder

```
y <- c(1, 0, 0, 1, 0, 0, 0, 0)

fun1 <- function(pi){
  (log(pi)*sum(y) + log(1-pi)*sum(1-y)) %>% exp()
}

ggplot(data = data.frame(x = 0), mapping = aes(x = x))+
  stat_function(fun = fun1)+
  xlim(0,1)+
  labs(x = "pi",
       y = "Likelihood")+
  theme_bw()
```



3. Homework: Question HW3

- One common problem when knitting: the math mode environment doesn't like white space or empty line + Try `\begin{alinged}` instead of `\begin{split}` + `R Markdown` guide is here
- Email subject: **MLE510HW3**
- File name: **MLE510HW3KenyaAmano**
- Your feedback is valuable: Evaluation URL