Bayesian linear regression

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Outline

- Linear regression
    - Classical regression
    - Default Bayesian regression
    - Conjugate subjective Bayesian regression
- Simulating from the posterior
    - Inference on functions of parameters
    - Posterior for optimum of a quadratic

Linear Regression

Basic idea

- understand the relationship between response y and explanatory variables $x = (x_1, \ldots, x_k)$
- based on data from experimental units index by i.

If we assume

- linearity, independence, normality, and constant variance,

then we have

$$y_i \stackrel{ind}{\sim} N(\beta_1 x_{i1} + \cdots + \beta_k x_{ik}, \sigma^2)$$

where $x_{i1} = 1$ if we want to include an intercept. In matrix notation, we have

$$y \sim N(X\beta, \sigma^2 \mathrm{I})$$

where $y = (y_1, \ldots, y_n)'$, $\beta = (\beta_1, \ldots, \beta_k)'$, and X is $n \times k$ with each row being $x_i = (x_{i1}, \ldots, x_{ik})$.

Classical regression

How do you find confidence intervals for β?

What is the MLE for β?

$$\hat{\beta} = \hat{\beta}_{MLE} = (X'X)^{-1}X'y$$

What is the sampling distribution for $\hat{\beta}$?

$$\hat{\beta} \sim t_{n-k}(\beta, s^2(X'X)^{-1})$$

where $s^2 = SSE/[n-k]$ and $SSE = (Y - X\hat{\beta})'(Y - X\hat{\beta})$.

What is the sampling distribution for s^2?

$$\frac{[n-k]s^2}{\sigma^2} \sim \chi^2_{n-k} \implies 1/s^2 \sim \text{Inv-}\chi^2(n-k, \sigma^2)$$

Default Bayesian regression

Assume the standard noninformative prior

$$p(\beta, \sigma^2) \propto 1/\sigma^2$$

then the posterior is

$$\begin{array}{rl} p(\beta, \sigma^2|y) & = p(\beta|\sigma^2, y)p(\sigma^2|y) \\ \beta|\sigma^2, y & \sim N(\hat{\beta}, \sigma^2 V_\beta) \\ \sigma^2|y & \sim \text{Inv-}\chi^2(n-k, s^2) \\ \beta|y & \sim t_{n-k}(\hat{\beta}, s^2 V_\beta) \end{array}$$

$$\begin{array}{rl} \hat{\beta} & = (X'X)^{-1}X'y \\ V_\beta & = (X'X)^{-1} \\ s^2 & = \frac{1}{n-k}(y - X\hat{\beta})'(y - X\hat{\beta}) \end{array}$$

The posterior is proper if $n > k$ and $\text{rank}(X) = k$.

Comparison to classical regression

For the regression coefficients, in a default Bayesian regression, we have

$$\beta|y \sim t_{n-k}(\hat{\beta}, s^2(X'X)^{-1}),$$

and in classical regression analysis, we have

$$\hat{\beta} \sim t_{n-k}(\beta, s^2(X'X)^{-1}).$$

For the error variance, in a default Bayesian regression, we have

$$\sigma^2|y \sim \text{Inv-}\chi^2(n-k, s^2)$$

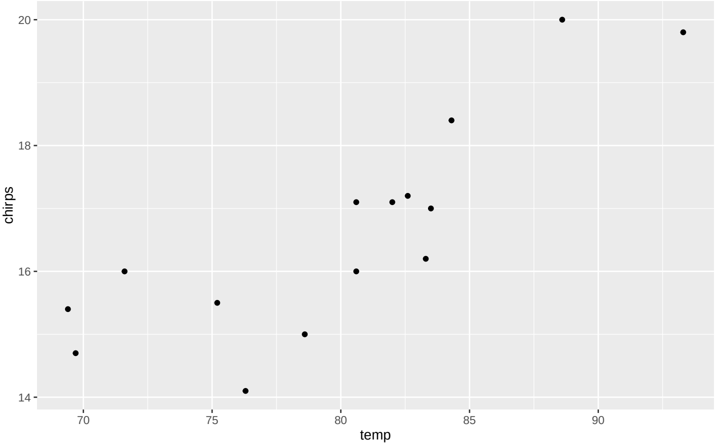
and in classical regression analysis, we have

$$1/s^2 \sim \text{Inv-}\chi^2(n-k, \sigma^2).$$

In the Bayesian statements, β is random and Y is fixed while in the classical statements, Y is random and β is fixed.

Cricket chirps

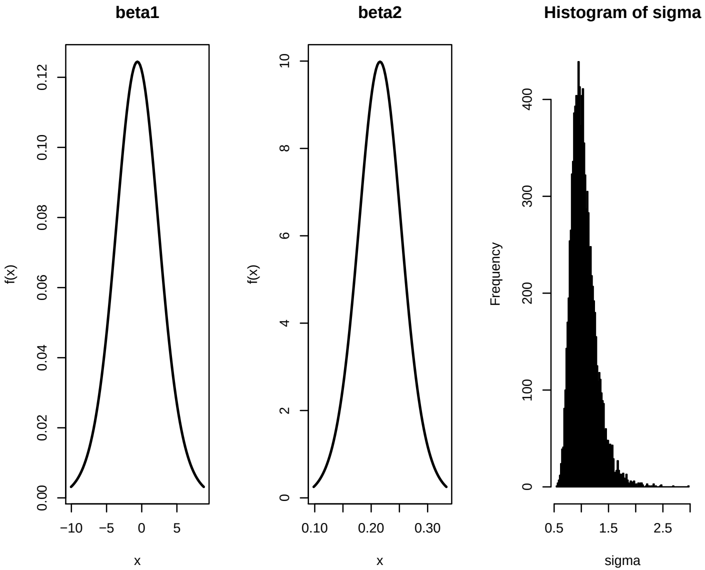
As an example, consider the relationship between the number of cricket chirps (in 15 seconds) and temperature (in Fahrenheit). From example in `LearnBayes::blinreg`.



Default Bayesian regression

```
summary(m <- lm(chirps~temp))


Call:
lm(formula = chirps ~ temp)

Residuals:
     Min       1Q   Median       3Q      Max 
-1.74107 -0.58123  0.02956  0.58250  1.50608 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) -0.61521    3.14434  -0.196 0.847903    
temp         0.21568    0.03919   5.504 0.000102 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.9849 on 13 degrees of freedom
Multiple R-squared:  0.6997, Adjusted R-squared:  0.6766 
F-statistic: 30.29 on 1 and 13 DF,  p-value: 0.0001015


confint(m) # Credible intervals


                 2.5 %    97.5 %
(Intercept) -7.4081577 6.1777286
temp         0.1310169 0.3003406
```

Default Bayesian regression - Full posteriors



Fully conjugate subjective Bayesian inference

If we assume the following normal-gamma prior,

$$\beta|\sigma^2 \sim N(m_0, \sigma^2 C_0) \qquad \sigma^2 \sim \text{Inv-}\chi^2(v_0, s_0^2)$$

then the posterior is

$$\beta|\sigma^2, y \sim N(m_n, \sigma^2 C_n) \qquad \sigma^2|y \sim \text{Inv-}\chi^2(v_n, s_n^2)$$

with

$$\begin{aligned} m_n &= m_0 + C_0 X'(X C_0 X' + \mathrm{I})^{-1}(y - X m_0) \\ C_n &= C_0 - C_0 X'(X C_0 X' + \mathrm{I})^{-1} X C_0 \\ v_n &= v_0 + n \\ v_n s_n^2 &= v_0 s_0^2 + (y - X m_0)'(X C_0 X' + \mathrm{I})^{-1}(y - X m_0) \end{aligned}$$

Information about chirps per 15 seconds

Let

- Y_i is the average number of chirps per 15 seconds and
- X_i is the temperature in Fahrenheit.

And we assume

$$Y_i \stackrel{ind}{\sim} N(\beta_0 + \beta_1 X_i, \sigma^2)$$

then

- β_0 is the expected number of chirps at 0 degrees Fahrenheit
- β_1 is the expected increase in number of chirps (per 15 seconds) for each degree increase in Fahrenheit.

Based on prior experience the prior $\beta_1 \sim N(0, 1)$ might be reasonable.

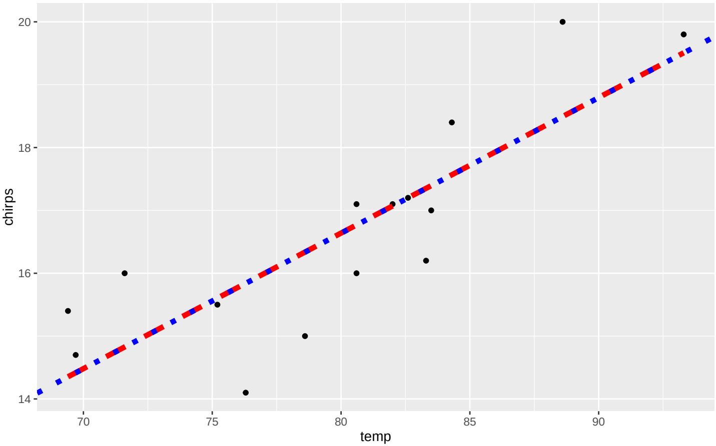
Subjective Bayesian regression

```
m = arm::bayesglm(chirps~temp,
                  prior.mean=0,  # E[\beta_1]
                  prior.scale=1, # V[\beta_1]
                  prior.df=Inf)  # normal prior
summary(m)



Call:
arm::bayesglm(formula = chirps ~ temp, prior.mean = 0, prior.scale = 1,
    prior.df = Inf)

Deviance Residuals:
     Min        1Q    Median        3Q       Max
-1.73940  -0.57939   0.03139   0.58435   1.50809

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.61478    3.14415  -0.196 0.847999
temp         0.21565    0.03919   5.503 0.000102 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for gaussian family taken to be 0.9700575)

    Null deviance: 41.993  on 14  degrees of freedom
Residual deviance: 12.611  on 13  degrees of freedom
AIC: 45.966

Number of Fisher Scoring iterations: 11
```

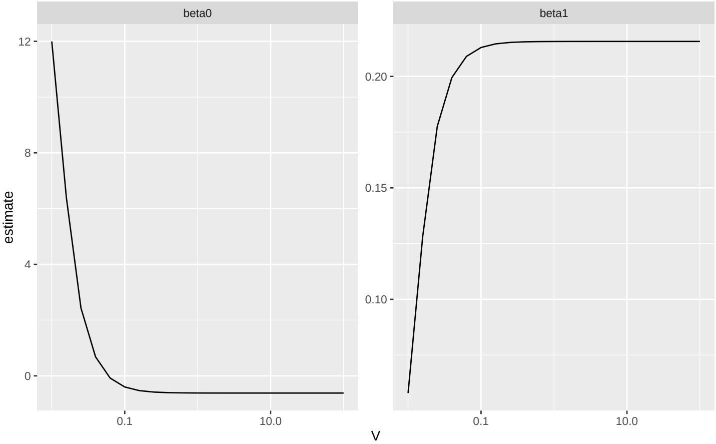
Subjective vs Default

```
# Subjective analysis
m$coefficients

(Intercept)        temp
 -0.6147847   0.2156511

confint(m)

                2.5 %    97.5 %
(Intercept) -6.7780731 5.5476365
temp         0.1388701 0.2924879

# compared to default analysis
tmp = lm(chirps~temp)
tmp$coefficients

(Intercept)        temp
 -0.6152146   0.2156787

confint(tmp)

                2.5 %    97.5 %
(Intercept) -7.4081577 6.1777286
temp         0.1310169 0.3003406
```

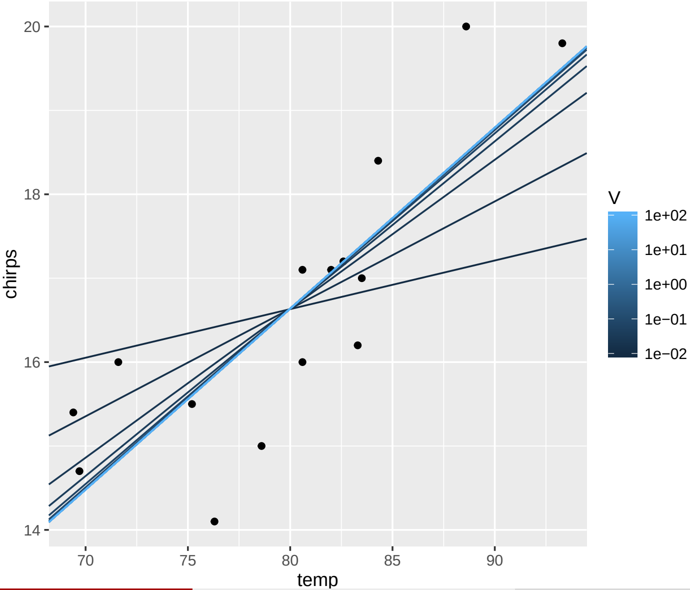
Subjective vs Default



Shrinkage (as $V[\beta_1]$ gets smaller)



Shrinkage (as $V[\beta_1]$ gets smaller)



Simulating from the posterior

Although the full posterior for β and σ^2 is available, the decomposition

$$p(\beta, \sigma^2|y) = p(\beta|\sigma^2, y)p(\sigma^2|y)$$

suggests an approach to simulating from the posterior via

1. $(\sigma^2)^{(j)} \sim \text{Inv-}\chi^2(n-k, s^2)$ and
2. $\beta^{(j)} \sim N(\hat{\beta}, (\sigma^2)^{(j)} V_\beta)$.

This also provides an approach to obtaining posteriors for any function $\gamma = f(\beta, \sigma^2)$ of the parameters via

$$\begin{array}{rl} p(\gamma|y) & = \int\int p(\gamma|\beta, \sigma^2, y)p(\beta|\sigma^2, y)p(\sigma^2|y)d\beta d\sigma^2 \\ & = \int\int p(\gamma|\beta, \sigma^2)p(\beta|\sigma^2, y)p(\sigma^2|y)d\beta d\sigma^2 \\ & = \int\int \delta(\gamma - f(\beta, \sigma^2))p(\beta|\sigma^2, y)p(\sigma^2|y)d\beta d\sigma^2 \end{array}$$

by adding the step

3. $\gamma^{(j)} = f(\beta^{(j)}, (\sigma^2)^{(j)})$.

Computation

For numerical stability and efficiency, the QR decomposition can be used to calculate posterior quantities.

Definition

For an $n \times k$ matrix X, a QR decomposition is $X = QR$ for an $n \times k$ matrix Q with orthonormal columns and a $k \times k$ upper triangular matrix R.

The quantities of interest are

$$\begin{aligned} V_\beta &= (X'X)^{-1} = ([QR]'QR)^{-1} = (R'Q'QR)^{-1} = (R'R)^{-1} \\ &= R^{-1}[R']^{-1} \end{aligned}$$

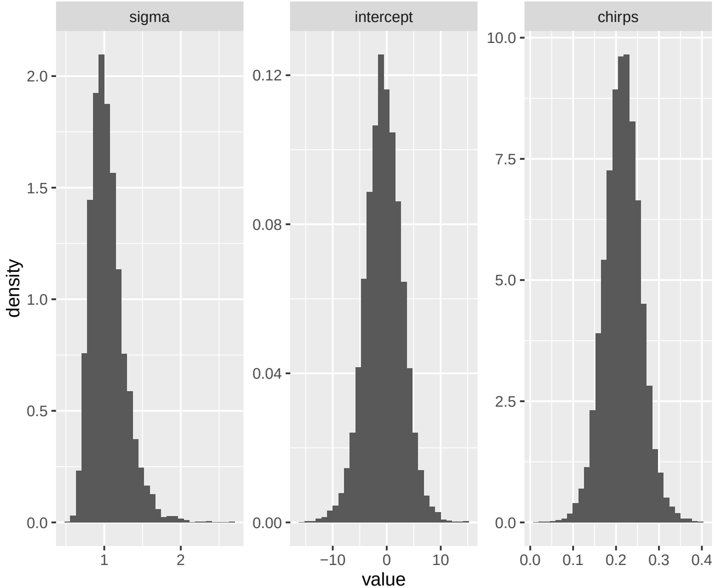
$$\begin{aligned} \hat\beta &= (X'X)^{-1}X'y = R^{-1}[R']^{-1}R'Q'y = R^{-1}Q'y \\ R\hat\beta &= Q'y \end{aligned}$$

The last equation is useful because R is upper triangular and therefore the system of linear equations can be solved without requiring the inverse of R.

Cricket chirps

```
library(MASS)
X = cbind(1,temp)
n = nrow(X)
k = ncol(X)
y = matrix(chirps,n,1)

qr = qr(X); Q = qr.Q(qr); R = qr.R(qr)
stopifnot(all.equal(X, Q%*%R),
          all.equal(rep(1,k), colSums(Q^2)),
          all.equal(diag(nrow=k), t(Q)%*%Q))

# Check for posterior propriety
stopifnot(n>k,qr$rank==k)

# Calculate posterior hyperparameters
Rinv = solve(qr.R(qr))
vbeta = Rinv%*%t(Rinv)
betahat = qr.solve(qr,y)
df = n-k
e = qr.resid(qr,y)
s2 = sum(e^2)/df

# Simulate from the posterior
n.sims = 10000
sigma = sqrt(1/rgamma(n.sims, df/2, df*s2/2))
beta = matrix(betahat, n.sims, k, byrow=T) + sigma * mvrnorm(n.sims, rep(0,k), vbeta)
```

Cricket chirps

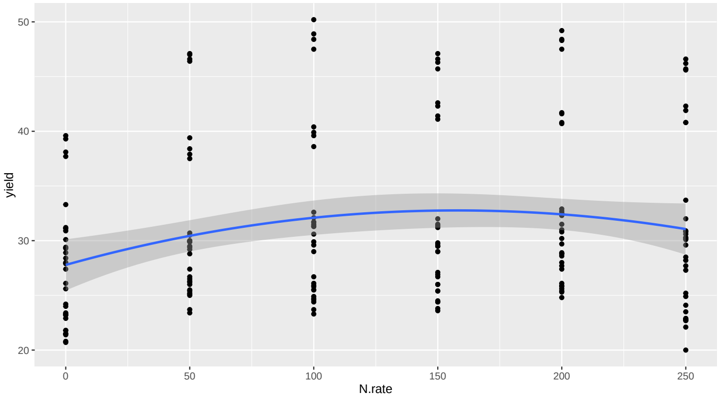


Monte Carlo error

```
# sigma^2
sqrt(df*s2/qchisq(c(.975,.025),df)) # Exact

[1] 0.7140166 1.5867368

quantile(sigma,c(.025,.975)) # MC

     2.5%     97.5%
0.7147342 1.5801627

# beta
confint(lm(chirps~temp)) # Exact

                 2.5 %    97.5 %
(Intercept) -7.4081577 6.1777286
temp         0.1310169 0.3003406

t(apply(beta, 2, quantile, probs=c(.025,.975))) # MC

           2.5%     97.5%
     -7.4576088 6.1585177
temp  0.1309921 0.3010475
```

Posterior for global maximum

Consider this potato yield data set



with a goal of estimating the optimal nitrogen rate.

Posterior for global maximum

Let

- Y_i be the potato yield and
- X_i be the nitrogen rate.

We assume the model

$$Y_i \stackrel{ind}{\sim} N(\beta_0 + \beta_1 X_i + \beta_2 X_i^2, \sigma^2)$$

Assuming this quadratic curve is correct, the maximum occurs at $\gamma = -\beta_1/[2\beta_2]$.

```
m = LearnBayes::blinreg(d$yield, cbind(1,d$N.rate, d$N.rate^2), 1e4)
beta1 = m$beta[,2]; beta2 = m$beta[,3]; gamma = -beta1/(2*beta2)
quantile(gamma, c(.025,.5,.975))
```

```
    2.5%      50%    97.5%
123.6191 157.2890 281.5544
```

This does not require any data asymptotics or approximations, e.g. delta method.

Summary

- Model: $y \sim N(X\beta, \sigma^2 \mathrm{I})$
- Default Bayesian analysis corresponds exactly to classical regression analysis

$$p(\beta, \sigma^2) \propto 1/\sigma^2 \implies$$

$$\beta|\sigma^2, y \sim N(\hat{\beta}, \sigma^2[X'X]^{-1}), \sigma^2|y \sim \text{Inv-}\chi^2(n-k, s^2)$$

- Conjugate subjective Bayesian analysis:

$$\beta|\sigma^2 \sim N(m_0, \sigma^2 C_0), \sigma^2 \sim \text{Inv-}\chi^2(v_0, s_0^2) \implies$$

$$\beta|\sigma^2, y \sim N(m_n, \sigma^2 C_n), \sigma^2|y \sim \text{Inv-}\chi^2(v_n, s_n^2)$$

- Obtain functions of parameters and their uncertainty by simulating the parameters from their joint posterior, calculating the function, and taking posterior quantiles.