Statictical Modeling and Advanced Regression Analyses

R Tutorials

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1 Software

We use the statistical software environment *R* (R Core Team, 2024), and R add-on packages *ggplot2* (Wickham, 2016).

This document is produced using *Quarto* (Allaire et al., 2024).

1.1 Organize R Session

```
rm(list = ls())
library("ggplot2")
```

2 Linear Regression Model

2.1 Data Simulation

Data are simulated according to the equations given in the lecture slides¹:

¹For two covariates x_1 and x_2 .

```
 df mu \leftarrow beta_0 + beta_x_1 * df x_1 + beta_x_2 * df x_2 \\ df + rnorm(n = N, mean = 0, sd = sigma)
```

2.1.1 Visualisations

```
ggplot(data = df, aes(x = x_1, y = x_2)) +
geom_point()
```

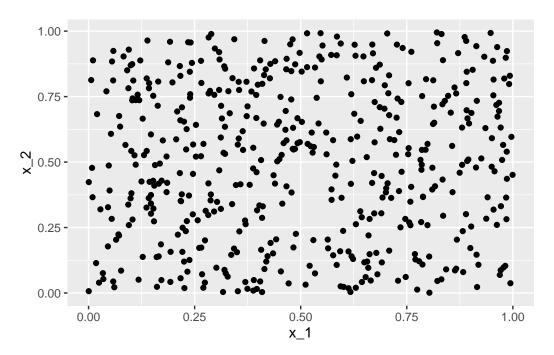


Figure 1: Scatterplot of the two simulated covariates x_1 and x_2 - each from the uniform distribution between 0 and 1.

```
ggplot(data = df, aes(x = x_1, y = mu, color = x_2)) +
  geom_point()
```

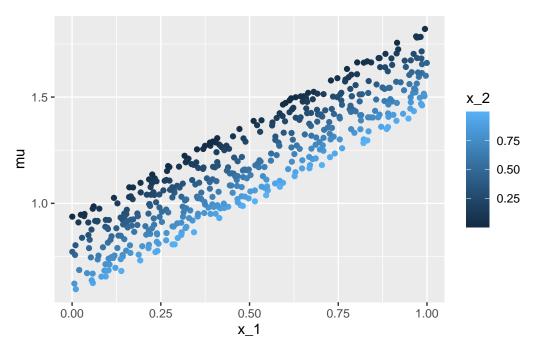


Figure 2: Scatterplot of covariate x_1 with response y - each individual observation is coloured according to the second covariate x_2 .

```
ggplot(data = df, aes(x = x_2, y = mu, color = x_1)) +
  geom_point()
```

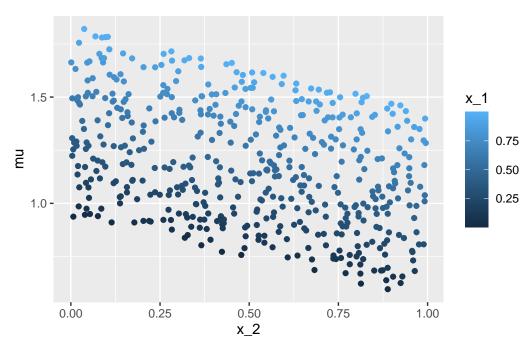


Figure 3: Scatterplot of covariate x_2 with response y - each individual observation is coloured according to the first covariate x_1 .

```
ggplot(data = df, aes(x = x_1, y = x_2, color = mu)) +
  geom_point()
```

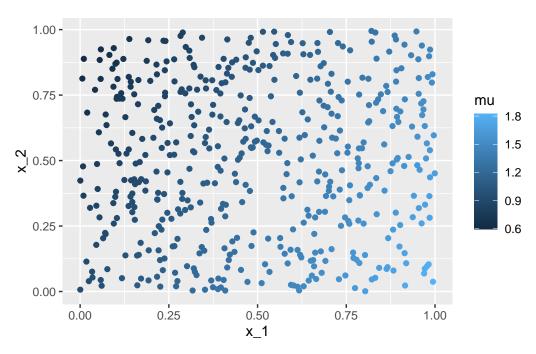


Figure 4: Scatterplot of the two simulated covariates x_1 and x_2 - each individual observation is coloured according to the underlying true conditional expectation mu.

```
ggplot(data = df, aes(x = x_1, y = x_2, color = y)) +
  geom_point()
```

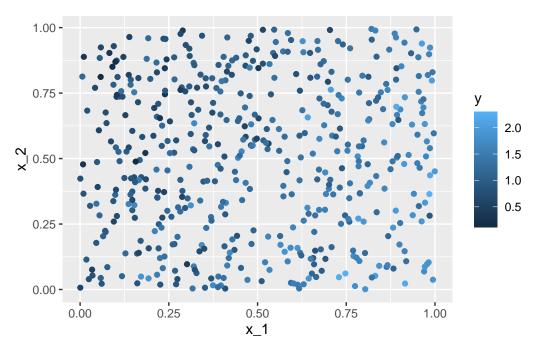


Figure 5: Scatterplot of the two simulated covariates x_1 and x_2 - each individual observation is coloured according to the response y.

2.2 Modeling

The basic R command for (frequentist) estimation of the parameters of a linear regression model is a call to the function 1m:

```
Call: lm(formula = y \sim x_1 + x_2, data = df)
```

Residuals:

```
Min 1Q Median 3Q Max -0.82082 -0.19805 0.00329 0.19051 0.81138
```

Coefficients:

```
Estimate Std. Error t value Pr(>|t|)

(Intercept) 0.91291 0.03448 26.476 < 2e-16 ***

x_1 0.91533 0.04668 19.610 < 2e-16 ***

x_2 -0.36218 0.04566 -7.933 1.43e-14 ***
```

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.2963 on 497 degrees of freedom Multiple R-squared: 0.4674, Adjusted R-squared: 0.4652 F-statistic: 218 on 2 and 497 DF, p-value: < 2.2e-16

2.2.1 Visualisations

```
nd <- data.frame(x_1 = seq(0, 1, by = .1), x_2 = .5)
nd$mu <- predict(m, newdata = nd)
ggplot(data = df, aes(x = x_1, y = mu, color = x_2)) + geom_point() + geom_line(data = nd, aes(x = x_1, y = mu, color = x_2))
```

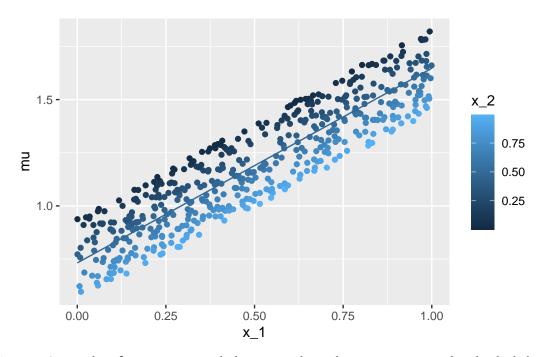


Figure 6: Scatterplot of covariate x_1 with the true conditional expectation mu - each individual observation is coloured according to the second covariate x_2 . The line gives the point estimation for the conditional expectation with the second covariate x_2 fixed to 0.5.

```
geom_point() +
geom_line(data = nd, aes(x = x_1, y = mu, color = x_2, group = x_2))
```

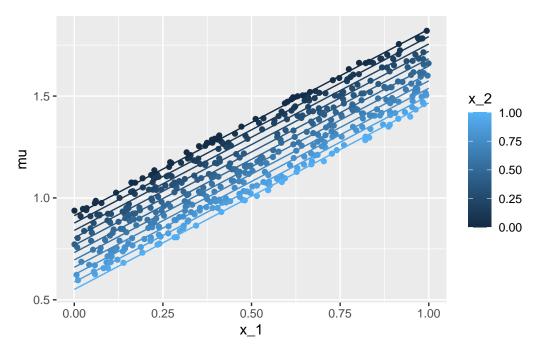


Figure 7: Scatterplot of covariate x_1 with the true conditional expectation mu - each individual observation is coloured according to the second covariate x_2 . The lines give the point estimation for the conditional expectation with the second covariate x_2 taking on values between 0 and 1 (at steps of 0.1).

2.3 Add-Ons

2.3.1 Add-On Linear Model: A) Stancode

2.3.1.1 Stan Users Guide

Probabilistic Programming Languages such as *Stan* (Carpenter et al., 2017) allow to plug together the single parts of a statistical regression model²:

The following Stan-code is published here in the Stan users guide:

```
data {
  int<lower=0> N;
  vector[N] x;
```

²Which is actually pretty 'readable' if you get used to the structure for a simple model such the linear regression model.

```
vector[N] y;
}
parameters {
  real alpha;
  real beta;
  real<lower=0> sigma;
}
model {
  y ~ normal(alpha + beta * x, sigma);
}
```

2.3.1.2 Stancode generated by calling brms::brm

The R add-on package *brms* (Bürkner, 2017, 2018) allows to implent advanced regression models without being an expert in 'Stan-programming'.

Here is the Stan-code that is implemented by 'brms' for our linear regression model example:

```
brms::make_stancode(brms::bf(y ~ x_1 + x_2, center = F), data = df)
// generated with brms 2.21.0
functions {
}
data {
  int<lower=1> N; // total number of observations
  vector[N] Y; // response variable
  int<lower=1> K; // number of population-level effects
 matrix[N, K] X; // population-level design matrix
  int prior_only; // should the likelihood be ignored?
}
transformed data {
}
parameters {
  vector[K] b; // regression coefficients
  real<lower=0> sigma; // dispersion parameter
transformed parameters {
  real lprior = 0; // prior contributions to the log posterior
  lprior += student_t_lpdf(sigma | 3, 0, 2.5)
    - 1 * student_t_lccdf(0 | 3, 0, 2.5);
}
model {
  // likelihood including constants
```

```
if (!prior_only) {
   target += normal_id_glm_lpdf(Y | X, 0, b, sigma);
}
// priors including constants
target += lprior;
}
generated quantities {
}
```

2.3.2 Add-On Linear Model: B) Posterior predictive check: an introduction 'by hand'

Having an 1m object already, it is rather straightforward to get posterior samples by using function sim from the *arm* (Gelman & Su, 2024) package:

```
library("arm")
S \leftarrow sim(m)
str(S)
Formal class 'sim' [package "arm"] with 2 slots
  ..@ coef : num [1:100, 1:3] 0.882 1.014 0.904 0.978 0.958 ...
  ...- attr(*, "dimnames")=List of 2
  .. .. ..$ : NULL
  .....$ : chr [1:3] "(Intercept)" "x_1" "x_2"
  ..@ sigma: num [1:100] 0.323 0.303 0.292 0.309 0.29 ...
S <- cbind(S@coef, 'sigma' = S@sigma)
head(S)
     (Intercept)
                       x_1
                                  x_2
                                          sigma
[1,]
       0.8816414 0.9245094 -0.3362733 0.3227662
       1.0139849 0.7317948 -0.3398411 0.3033703
[2,]
[3,]
      0.9037042 0.9155575 -0.3506924 0.2922883
[4,]
      0.9776909 0.8392790 -0.3845609 0.3090220
[5,]
       0.9579213 0.8977625 -0.4284596 0.2900632
[6,]
       0.9549211 0.8478278 -0.3937226 0.3094227
```

Predict the response for the covariate data as provided by the original data-frame df - here only by using the first posterior sample:

geom_histogram(alpha = .5, position = "identity")

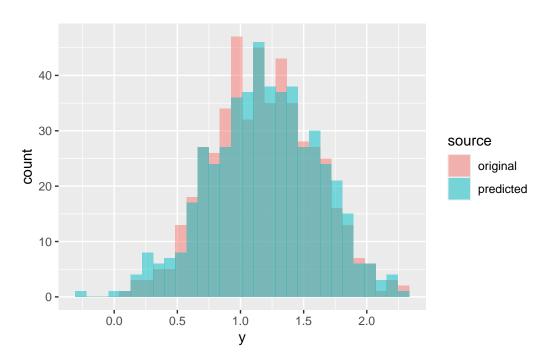


Figure 8: Histogram of the original and the posterior predicted response sample.

Now let's repeat the same for 9 different posterior samples:

```
data.frame(y = y_s, source = "predicted", s = s))
}
ggplot(data = pp, aes(x = y, fill = source)) +
  geom_histogram(alpha = .5, position = "identity") +
  facet_wrap(~ s)
```

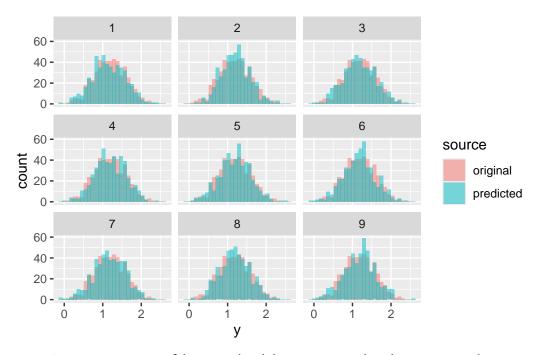


Figure 9: Histogram of the original and the posterior predicted response sample.

```
ggplot(data = pp, aes(x = y, fill = source)) +
  geom_density(alpha = .5, position = "identity") +
  facet_wrap(~ s)
```

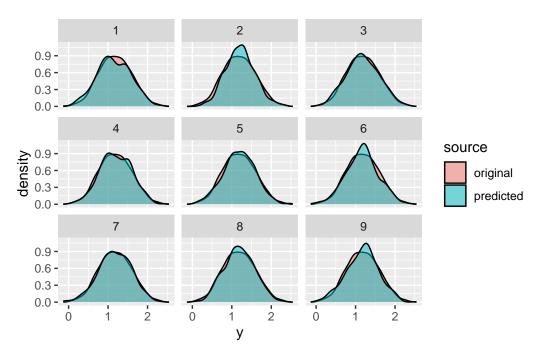


Figure 10: The same as in Figure 9, but now using kernel density visualisations.

```
ggplot(data = pp, aes(x = y, colour = source)) +
  stat_ecdf() +
  facet_wrap(~ s)
```

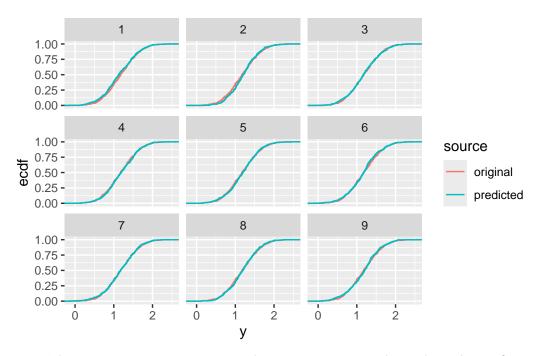


Figure 11: The same as in Figure 9 or Figure 10, but now using empirical cumulative density function visualisations.

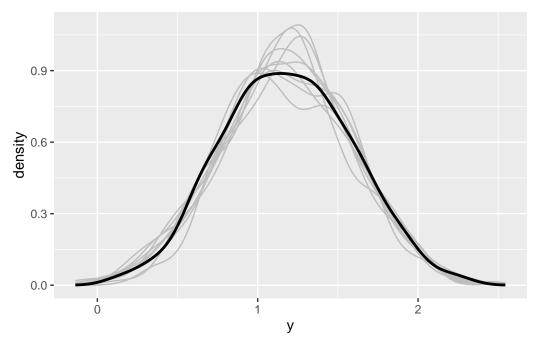


Figure 12: The same as in Figure 12, but now within one plotting window: This visualisation is what brms::pp_check will produce if applied on a brm object.

3 Binary Regression Model

```
rm(list = ls())
library("ggplot2")
library("plyr")
```

3.1 Data Simulation

Data are simulated similarly as for the linear model:

3.1.1 Visualisations

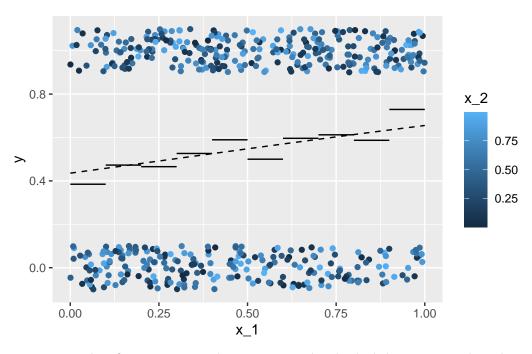


Figure 13: Scatterplot of covariate x_1 with response y - each individual observation is coloured according to the second covariate x_2, and additionally 'jittered' in vertical direction.

3.2 Modeling

The basic R command for (frequentist) estimation of the parameters of a binary regression model is a call to the function glm with family argument binomial:

```
m \leftarrow glm(y \sim x_1 + x_2, data = df,
        family = binomial(link = 'logit'))
summary(m)
Call:
glm(formula = y ~ x_1 + x_2, family = binomial(link = "logit"),
    data = df
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.2908 0.2358 -1.233 0.217531
             1.1598
x 1
                        0.3248 3.570 0.000356 ***
            -0.1713
                        0.3138 -0.546 0.585034
x_2
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
```

Null deviance: 688.53 on 499 degrees of freedom Residual deviance: 675.30 on 497 degrees of freedom

AIC: 681.3

Number of Fisher Scoring iterations: 4

3.2.1 Visualisations

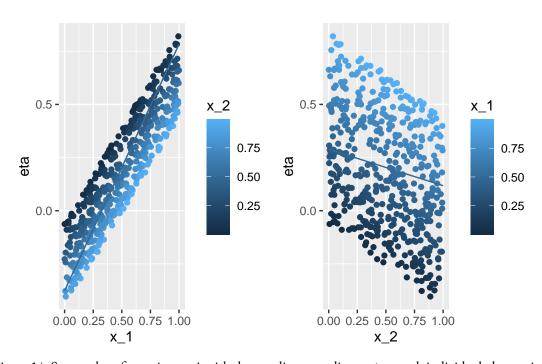


Figure 14: Scatterplot of covariate x_1 with the true linear predictor eta - each individual observation is coloured according to the second covariate x_2 . The line gives the point estimation for the conditional expectation with the second covariate x_2 fixed to 0.5.

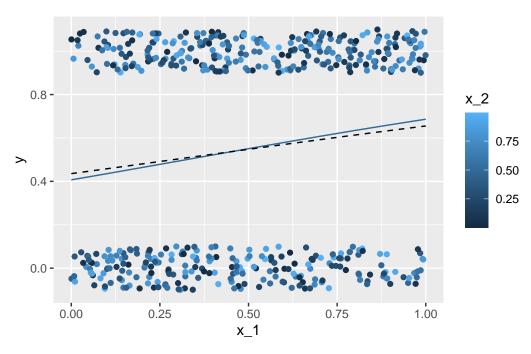


Figure 15: Scatterplot of covariate x_1 with the true conditional expectation p - each individual observation is coloured according to the second covariate x_2. The line gives the point estimation for the conditional expectation with the second covariate x_2 fixed to 0.5.

3.2.2 Estimated Expected Value

We can apply the Bernstein-von Mises theorem to estimate the *expected value*:

- **Fit the model**: Obtain the maximum likelihood estimate for the model's coefficients (coef) along with their variance-covariance matrix (vcov).
- **Simulate coefficients**: Perform an 'informal' Bayesian posterior simulation using the multivariate normal distribution, based on the *Bernstein-von Mises theorem*.
- **Convert simulated coefficients**: Apply an appropriate transformation to the simulated coefficients to compute the *simulated quantity of interest*. This quantity typically depends on the values of all explanatory variables, and researchers may:
 - Focus on a specific observation (usually an 'average'), or
 - Average across all sample observations.

In both cases, the applied transformation incorporates the researcher's specific choice.

```
library("MASS")
coef(m)
(Intercept)
                    x 1
 -0.2907775
             1.1597730 -0.1713224
vcov(m)
            (Intercept)
                                 x_1
(Intercept) 0.05560471 -0.048970067 -0.047028038
            -0.04897007 0.105509175 -0.004560743
x_1
            -0.04702804 -0.004560743 0.098439583
x_2
set.seed(0)
B <- mvrnorm(n = 100, mu = coef(m), Sigma = vcov(m))
head(B)
     (Intercept)
                       x_1
[1,] -0.08125910 0.6544775 -0.2581602
[2,] -0.40299145 1.3779659 -0.3263178
[3,] 0.09915843 1.0089580 -0.5398310
[4,] 0.03289839 0.8600445 -0.3880109
[5,] -0.12814786 1.3256621 -0.5036957
[6,] -0.55953065 1.4562644 0.3176658
```

```
nd \leftarrow expand.grid('x_1' = nd$x_1,
                   'x_2' = nd$x_2,
                   's' = 1:nrow(B)
head(nd)
  x_1 x_2 s
1 0.0 0.5 1
2 0.1 0.5 1
3 0.2 0.5 1
4 0.3 0.5 1
5 0.4 0.5 1
6 0.5 0.5 1
nd$p \leftarrow plogis(B[nd$s, 1] + B[nd$s, 2] * nd$x_1 +
                 B[nd\$s, 3] * nd\$x_2)
dd <- ddply(nd, c('x_1'), summarise,</pre>
            p_{mean} = mean(p),
            p_lwr_95 = quantile(p, prob = .025),
            p_upr_95 = quantile(p, prob = .975),
            p_lwr_9 = quantile(p, prob = .05),
            p_upr_9 = quantile(p, prob = .95),
            p_lwr_75 = quantile(p, prob = .125),
            p_upr_75 = quantile(p, prob = .875))
set.seed(0)
ggplot(data = df, aes(x = x_1)) +
  geom_jitter(aes(y = y, color = x_2), width = 0, height = .1) +
  geom_ribbon(data = dd, aes(x = x_1, ymin = p_lwr_95,
                              ymax = p_upr_95), alpha = .4) +
  geom_ribbon(data = dd, aes(x = x_1, ymin = p_lwr_9,
                              ymax = p_upr_9), alpha = .4) +
  geom_ribbon(data = dd, aes(x = x_1, ymin = p_lwr_75,
                              ymax = p_upr_75, alpha = .4) +
  geom_line(data = dd, aes(y = p_mean))
```

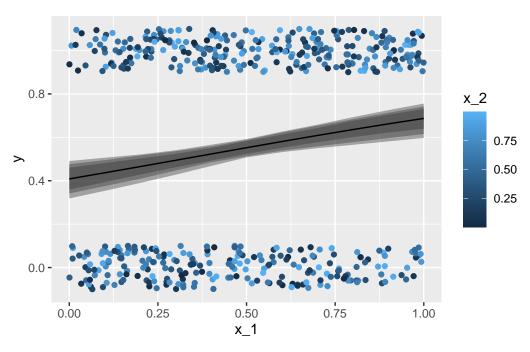


Figure 16: Scatterplot of covariate x_1 with the true conditional expectation mu - each individual observation is coloured according to the second covariate x_2 . The line gives the point estimation for the conditional expectation with the second covariate x_2 fixed to 0.5.

4 Poisson Regression Model

```
rm(list = ls())
library("ggplot2")
```

4.1 Data Simulation

Data are simulated similarly as for the linear model:

4.1.1 Visualisations

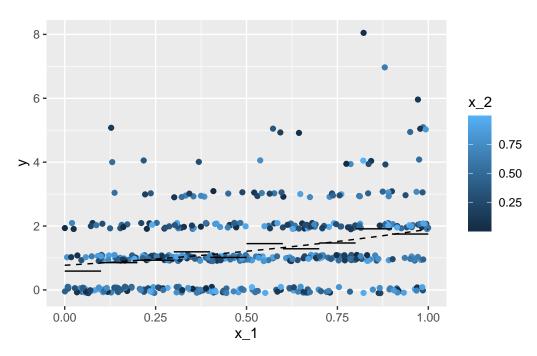


Figure 17: Scatterplot of covariate x_1 with response y - each individual observation is coloured according to the second covariate x_2.

4.2 Modeling

The basic R command for (frequentist) estimation of the parameters of a binary regression model is a call to the function glm with family argument poisson(link = 'log'):

```
m \leftarrow glm(y \sim x_1 + x_2, data = df, family = poisson(link = 'log')) summary(m)
```

```
Call:
glm(formula = y \sim x_1 + x_2, family = poisson(link = "log"),
   data = df
Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.09637 0.11000 -0.876
                                           0.381
                        0.14351 7.354 1.93e-13 ***
x_1
            1.05534
x_2
            -0.54067
                        0.13875 -3.897 9.74e-05 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for poisson family taken to be 1)
   Null deviance: 619.76 on 499 degrees of freedom
Residual deviance: 551.67 on 497 degrees of freedom
AIC: 1395.1
Number of Fisher Scoring iterations: 5
4.2.1 Estimated Expected Value
Let's again apply the Bernstein-von Mises theorem
library("MASS")
coef(m)
(Intercept)
                    x_1
-0.09636825 1.05534471 -0.54067416
vcov(m)
             (Intercept)
                                   x_1
(Intercept) 0.012100215 -0.0115419704 -0.0083283575
            -0.011541970 0.0205956476 -0.0008112633
x_1
           -0.008328358 -0.0008112633 0.0192505213
x_2
set.seed(0)
B <- mvrnorm(n = 100, mu = coef(m), Sigma = vcov(m))
head(B)
```

```
(Intercept)
                        x_1
[1,] 0.05743986 0.8596548 -0.5240625
[2,] -0.10120645 1.1692825 -0.5989887
[3,] 0.01910641 0.9263818 -0.7232511
[4,] 0.02386701 0.8912981 -0.6321912
[5,] -0.06117581 1.0833727 -0.7137618
[6,] -0.30539283 1.1687677 -0.3825595
nd \leftarrow expand.grid('x_1' = seq(0, 1, by = .1),
                   'x_2' = .5,
                   's' = 1:nrow(B)
head(nd)
  x_1 x_2 s
1 0.0 0.5 1
2 0.1 0.5 1
3 0.2 0.5 1
4 0.3 0.5 1
5 0.4 0.5 1
6 0.5 0.5 1
nd$mu \leftarrow exp(B[nd$s, 1] +
                B[nd\$s, 2] * nd\$x_1 +
                B[nd\$s, 3] * nd\$x_2)
dd <- ddply(nd, c('x_1'), summarise,</pre>
            mu_mean = mean(mu),
            mu_lwr_95 = quantile(mu, prob = .025),
            mu_upr_95 = quantile(mu, prob = .975),
            mu_lwr_9 = quantile(mu, prob = .05),
            mu_upr_9 = quantile(mu, prob = .95),
            mu_lwr_75 = quantile(mu, prob = .125),
            mu_upr_75 = quantile(mu, prob = .875))
df_p_B \leftarrow data.frame('x_1' = seq(0, 1, by = .01),
                      'mu' = \exp(\operatorname{coef}(m)[1] +
                                  coef(m)[2] * seq(0, 1, by = .01) +
                                  coef(m)[3] * .5))
set.seed(0)
ggplot(data = df, aes(x = x_1)) +
  geom_jitter(aes(y = y, color = x_2), width = 0, height = .1) +
  geom_ribbon(data = dd, aes(x = x_1, ymin = mu_lwr_95,
                              ymax = mu_upr_95), alpha = .4) +
  geom_ribbon(data = dd, aes(x = x_1, ymin = mu_lwr_9,
                              ymax = mu_upr_9), alpha = .4) +
```

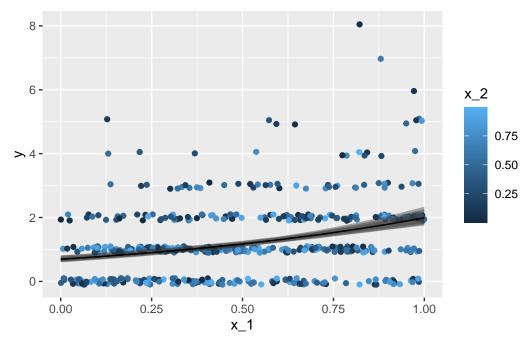


Figure 18: Scatterplot of covariate x_1 with the response observations y - each individual observation is coloured according to the second covariate x_2 . The line gives the point estimation for the conditional expectation with the second covariate x_2 fixed to 0.5, the coloured intervals give point-wise central 75%, 90%, and 95% credible intervals for the conditional expectation.

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