

Don't Feel Guilty About Selecting Variables

John Mount

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Introduction

Feature selection or feature pruning is the removal of some proposed columns or potential explanatory variables from a model. It can be an important step in data science, where many available data columns are not in fact pre-screened as suitable for a given project. In fact one could say that what a statistician calls an explanatory variable has already been filtered for problem appropriateness, so you sometimes don't see variable selection in statistics because we are often starting statistical stories after the variable qualification chapter!

We recommend incorporating mild feature pruning into your machine learning and modeling workflows. It is empirically known that feature selection can help (for example [here](#) and [here](#)). It is also known one can introduce problems if feature selection is done improperly (for example Freedman's paradox. The issues are avoidable, by using out of sample methods, cross methods, or differential privacy). We have also always felt a bit exposed in this, as feature selection *seems* unjustified in standard explanations of regression. One *feels* that if a coefficient were meant to be zero, the fitting procedure would have set it to zero. Under this misapprehension, stepping in and removing some variables *feels* unjustified.

Regardless of intuition or feelings, it is a fair question: is variable selection a natural justifiable part of modeling? Or is it something that is already done (therefore redundant). Or is it something that is not done for important reasons (such as avoiding damaging bias)?

In this note we will show that feature selection *is* in fact an obvious justified step when using a sufficiently sophisticated model of regression. This note is long, as it defines so many tiny elementary steps. However this note ends with a big point: variable selection *is* justified. It naturally appears in the right variation of Bayesian Regression. You *should* select variables, using your preferred methodology. And you *shouldn't* feel bad about selecting variables.

Bayesian Regression in Action

To work towards variable selection/pruning, let's work a specific Bayesian Regression example in **R**. We are going to use the direct generative method described in the last section instead of a package such as **rstan** or **lme4**. This is because:

- We want to follow the exact didactic path above, in anticipation of adding variable selection.
- **rstan** doesn't allow direct unobserved discrete parameters (a tool we will find convenient for variable selection).
- We can get away with the direct method because our problem is low dimensional.

First we prepare our R environment.

```
library(wrapr)
library(ggplot2)
source('fns.R')
```

```
set.seed(2020)

cl <- parallel::makeCluster(parallel::detectCores())
```

Now we define our functions. The first generates our proposed parameters `beta_0` and `beta_1`. The idea is: since the vector parameters were generated according to the normal distribution, picking one of them uniformly from the stored `data.frame` is also normally distributed.

```
generate_params <- function(
  ..., # force arguments to bind by name
  n_sample = 100000,
  prior_mean_beta_0 = 0,
  prior_sd_beta_0 = 1,
  prior_mean_beta_1 = 0,
  prior_sd_beta_1 = 1,
  prior_explanatory_prob = 0.5) {
  stop_if_dot_args(
    substitute(list(...)),
    "generate_params")
  params <- data.frame(
    explanatory = rbinom(
      n = n_sample,
      size = 1, prob =
        prior_explanatory_prob),
    beta_0 = rnorm(
      n = n_sample,
      mean = prior_mean_beta_0,
      sd = prior_sd_beta_0),
    beta_1 = rnorm(
      n = n_sample,
      mean = prior_mean_beta_1,
      sd = prior_sd_beta_1),
    prior_weight = 1/n_sample
  )
  return(params)
}
```

`explanatory` is a random variable that is always 0 or 1. We will use it later to perform variable selection. For now it is not used.

Now we define functions to compute $P[\text{data} \mid \text{parameters}]$. We want to know $P[\text{parameters} \mid \text{data}]$, but we know with our above derivation if we can estimate $P[\text{data} \mid \text{parameters}]$, then using Bayes' Law we can get the desired $P[\text{data} \mid \text{parameters}]$.

```
# per setting parameter calculation function
mk_fun_p_data_given_params <- function(params, data, sd_noise) {
  force(params)
  force(data)
  force(sd_noise)
  function(i) {
    pi <- params[i, , drop = FALSE]
    ei <- data$y - (pi$beta_1 * data$x + pi$beta_0)
    sum(dnorm(ei, mean=0, sd = sd_noise, log = TRUE))
  }
}
```

`mk_fun_p_data_given_params` realizes the following probability model: parameters are plausible if `data$y - (pi$beta_1 * data$x + pi$beta_0)` is small. All of the definitions and math are to justify this block of code. `mk_fun_p_data_given_params` embodies the generative model illustrated in the following dependency diagram. The only important bit is the statement `ei <- data$y - (pi$beta_1 * data$x + pi$beta_0)`.

With this model defined we can run some experiments.

Experiment 1: Standard Bayesian Inference with `beta_1` explanatory.

We can now run our first experiment.

First we generate our observed data `d$x` and `d$y`.

```
n_example <- 100
actual_b1 <- 0.7
actual_b0 <- 0.3

d <- data.frame(x = rnorm(n_example))
d$y <- actual_b1 * d$x + actual_b0 + rnorm(nrow(d), mean = 0, sd = 1)
```

Notice `d$y` is $0.7 * d$x + 0.3$ with mean zero standard deviation one noise. A good fitting procedure should recover the coefficients `beta_0 = 0.3` and `beta_1 = 0.7`.

Our Bayesian fitting procedure is as follows.

First: propose many possible values of the fit coefficients `beta_0`, `beta_1`, each with probability according to the assumed prior distributions.

```
params <- generate_params()
```

Second: compute the posterior plausibility of all of the coefficient proposals with respect to the observed data. This is just us using Bayes' Law to criticize all of the proposed coefficient combinations. The least criticized is considered the best.

```
params$posterior_weight <- p_data_given_params(
  params = params,
  data = d,
  fn_factory = mk_fun_p_data_given_params)
```

This sampling or inference process can be summarized with the following diagram.

In Bayesian methods: having access to a description of or samples from the posterior distribution is pretty much the same as inferring the parameters or solving the problem. This may seem alien or weird; but it is why we consider the problem solved if we can get an estimate or approximation of the posterior distribution.

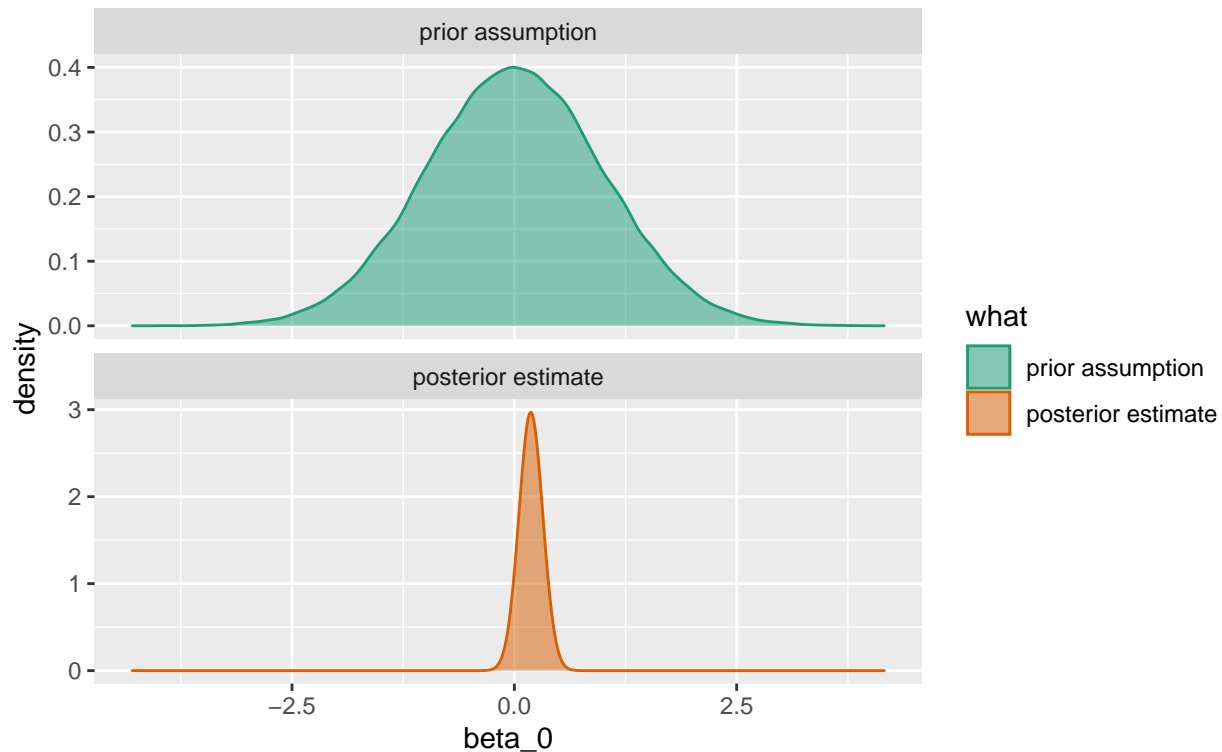
And we now have our coefficient estimates.

For `beta_0` we have:

```
plot_parameter(
  params, 'beta_0',
  subtitle = 'regular model, beta_1 explanatory')
```

prior and posterior estimates for beta_0

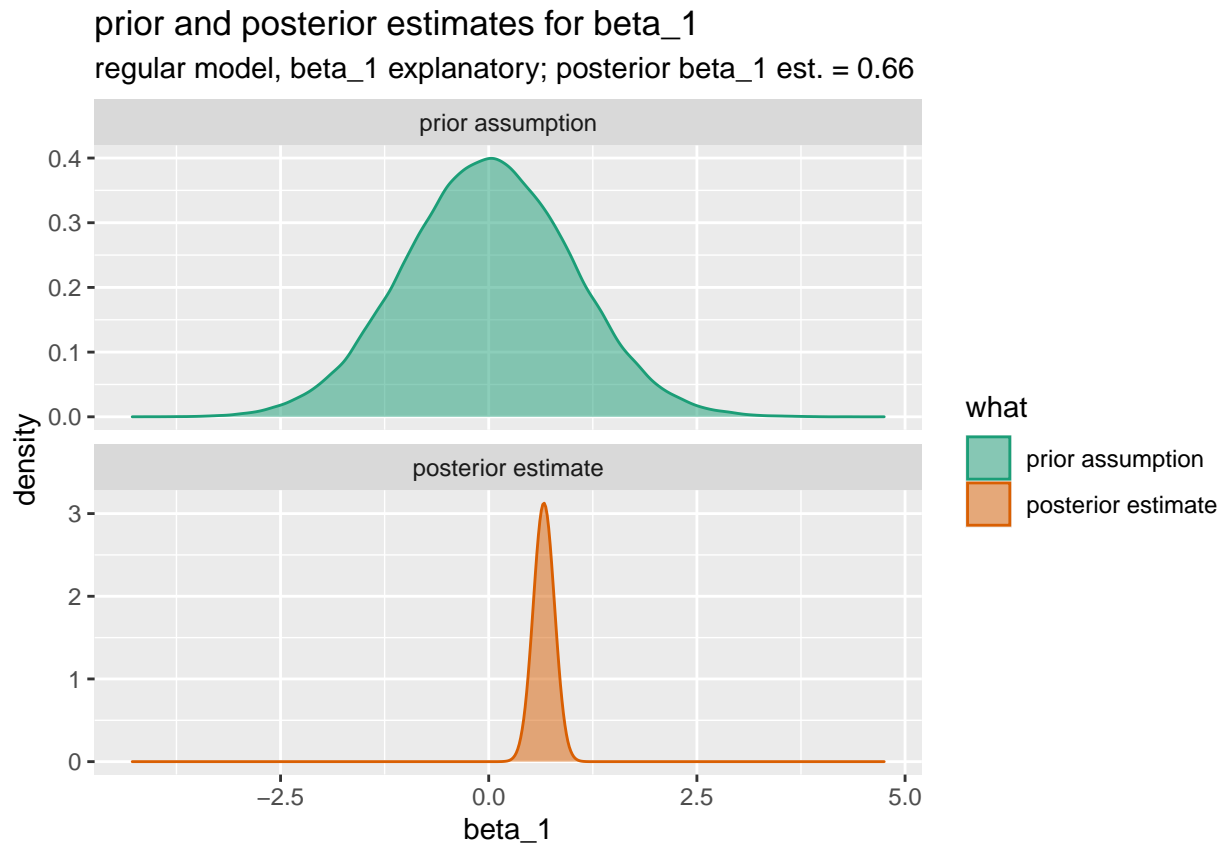
regular model, beta_1 explanatory; posterior beta_0 est. = 0.19



The above plot is two facets or panels. In each facet the x-axis is possible values for the unknown parameter **beta_0**. The height is the density for each value of the unknown parameters. The area under the curve is 1. So the amount of area above any interval of x-values is the probability of observing the parameter in that interval. The top facet is the assumed distribution of the **beta_0** before looking at the data, or “the prior”. This ideally is just the unit normal we plugged into the model as a modeling assumption. The variation is: we are using only a finite sample. The bottom facet is the estimated distribution of **beta_0** after looking at the data, or the “posterior”. Parameters that the observed data is inconsistent with are greatly punished. As we can see the posterior distribution is concentrated not too far from the true value used to generate the data. The model has roughly inferred the coefficients or parameters from the data, even though these are not directly observed.

And for **beta_1** we have:

```
plot_parameter(  
  params, 'beta_1',  
  subtitle = 'regular model, beta_1 explanatory')
```



Notice the posterior distributions are peaked near the unknown true values of the coefficients. The distribution of the estimates represents the remaining uncertainty in the estimate given the prior assumptions and amount of data. If we had more data, these distributions would tighten up considerably.

Experiment 2: Standard Bayesian Inference with beta_1 not explanatory.

Let's try the Bayesian fitting again. However this time let's not have a β_1 be an influence in the observed d .

```
n_example <- 100
actual_b0 <- 0.3

d <- data.frame(x = rnorm(n_example))
d$y <- actual_b0 + rnorm(nrow(d), mean = 0, sd = 1)
```

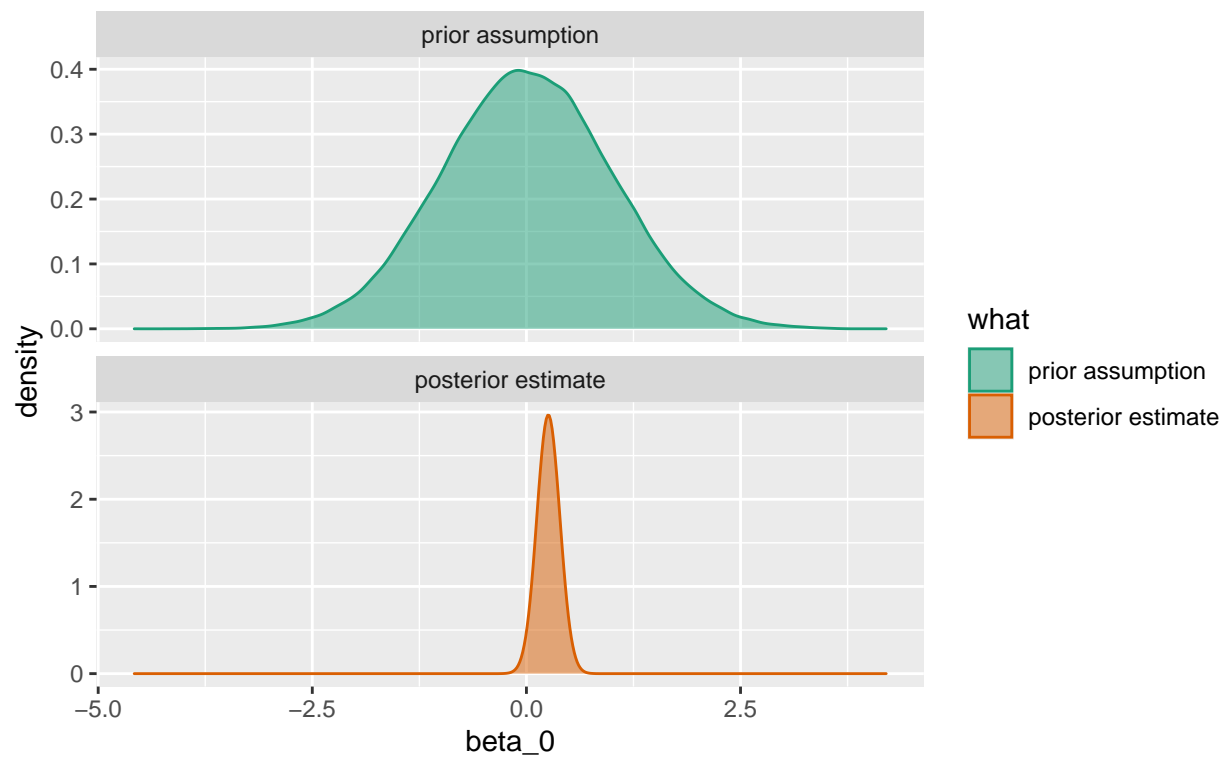
Notice this time we did not include β_1 in how the data was generated. β_1 is still a proposed modeling parameter, so it is up to the inference method to figure out the true relation is zero.

```
params <- generate_params()
params$posterior_weight <- p_data_given_params(
  params = params,
  data = d,
  fn_factory = mk_fun_p_data_given_params)

plot_parameter(
  params, 'beta_0',
  subtitle = 'regular model, beta_1 not explanatory')
```

prior and posterior estimates for beta_0

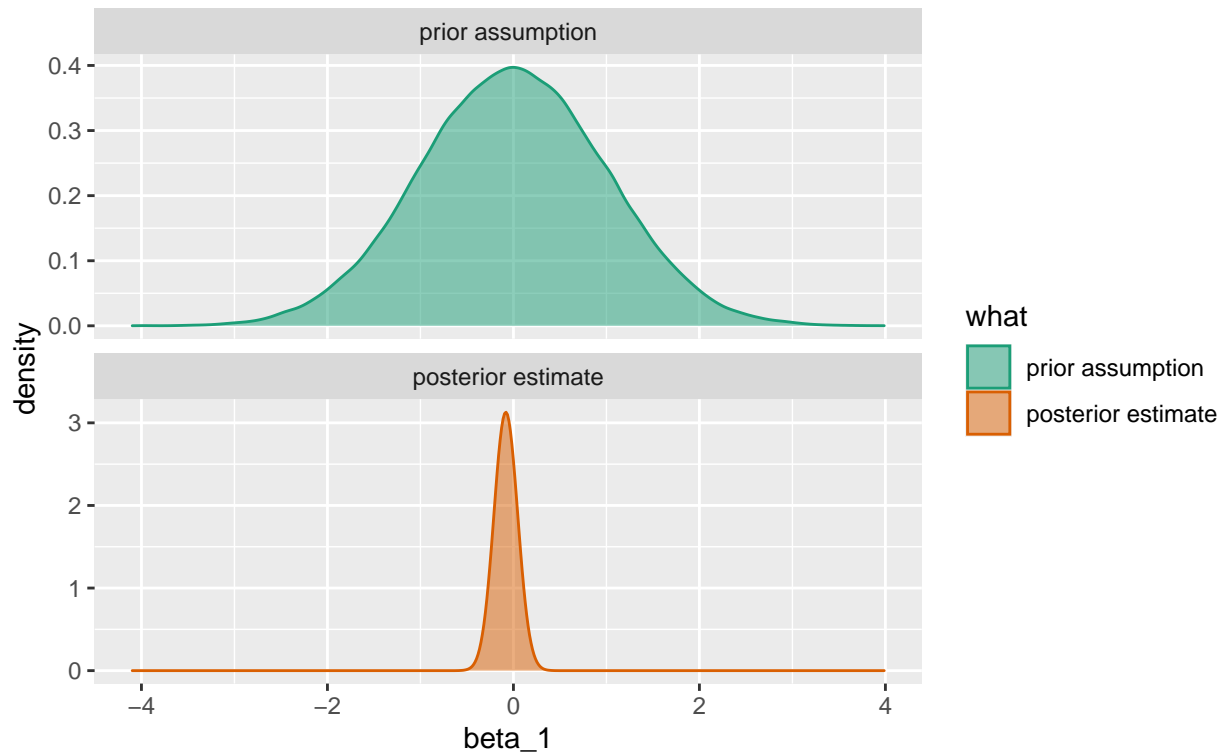
regular model, beta_1 not explanatory; posterior beta_0 est. = 0.26



```
plot_parameter(  
  params, 'beta_1',  
  subtitle = 'regular model, beta_1 not explanatory')
```

prior and posterior estimates for beta_1

regular model, beta_1 not explanatory; posterior beta_1 est. = -0.081



And here is where treatments of regression usually stop. The inference correctly worked out that **beta_1** is not likely to be any large value.

Our issue is: the model *almost never* says **beta_1** = 0! It gets values close to the right answer, but it can not in fact write down the correct answer. That is it can't reliably set **beta_1** = 0 indicating the variable **x** was thought to be irrelevant or non-explanatory. This modeling procedure in fact can not truly fit the above situation, as the above situation requires variable selection. We gave the model a column that wasn't involved in the outcome, and instead of inferring the column was not involved it says the involvement is likely small.

Let's draw few examples according to the posterior weighting, giving us access to the posterior distribution. We might use any one of them as "point estimate" of the inference or fitting.

```
row_ids <- sample.int(
  length(params$posterior_weight),
  size = 5, replace = TRUE,
  prob = params$posterior_weight)

params[row_ids, qc(beta_0, beta_1)] %>%
  knitr::kable(.)
```

	beta_0	beta_1
84667	0.1422966	-0.1079590
15939	0.4923473	0.0052186
8325	0.3605787	0.0875147
24078	0.1459436	-0.2729991
23807	0.2355377	-0.2087532

Usually we see `beta_1` not exactly equal to zero. That isn't what we want.

Now, standard frequentist fitting (such as `lm`) does use distributional assumptions on the residuals to tag the non-explanatory coefficient as non-significant. This isn't all the way to variable pruning, but it is sometimes used as a pruning signal in methods such as step-wise regression.

Let's take a look at that.

```
model <- lm(y ~ x, data = d)
summary(model)

##
## Call:
## lm(formula = y ~ x, data = d)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -2.16998 -0.54309 -0.08189  0.62498  2.10476
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  0.25703     0.08486   3.029  0.00314 **
## x           -0.07844     0.07588  -1.034  0.30379
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.8412 on 98 degrees of freedom
## Multiple R-squared:  0.01079,    Adjusted R-squared:  0.0006931
## F-statistic: 1.069 on 1 and 98 DF,  p-value: 0.3038
```

A non-negligible “ $\text{Pr}(>|t|)$ ” on the coefficient for `x` is the warning that `x` may not be truly explanatory. The reported standard errors take a role analogous to the posterior distributions we plotted earlier. (Note bene: Bayesian credible intervals and frequentist confidence intervals represent different kinds of uncertainty, so they are not in fact measuring the same thing.)

Bayesian Variable Selection

We have shown the common fallacy, and we can now show a solution: variable selection.

First we adjust our `P[data | parameters]` function to include a new unobserved parameter called `explanatory`. `explanatory` is always zero or one. The change in code is: we now compute the residual or error as `data$y - (pi$explanatory * pi$beta_1 * data$x + pi$beta_0)`. The idea is if `explanatory` is 1 our `P[data | parameters]` function works as before. However when `explanatory` is 0 the error model changes to `data$y - pi$beta_0`. `explanatory == 0` stomps out the `pi$beta_1 * data$x` term.

We arbitrarily start `explanatory` with a simple prior: it is 0 half of the time and 1 half of the time. We hope after inference it has a posterior distribution that is nearly always 1 (indicating the data is more plausible when `beta_1` is not zero, and `x` is in fact an explanatory variable) or nearly always 0 (indicating that the data is more plausible when `beta_0` is zero, and `x` is not in fact an explanatory variable). Note this prior is actually easy to get right: just put in what fraction of the variables you tried on similar previous problems turned out to be useful as the prior estimate on acceptance rate. However, with enough data we are not sensitive to initial settings away from zero and one.

We define a new unscaled log-probability of error calculation: `mk_fun_p_data_given_params_with_conditional`.

```
# per setting parameter calculation function with explanatory 0/1 parameter
mk_fun_p_data_given_params_with_conditional <- function(params, data, sd_noise) {
```



```

force(params)
force(data)
force(sd_noise)
function(i) {
  pi <- params[i, , drop = FALSE]
  ei <- data$y - (pi$explanatory * pi$beta_1 * data$x + pi$beta_0)
  sum(dnorm(ei, mean=0, sd = sd_noise, log = TRUE))
}
}

```

Essentially `pi$explanatory * pi$beta_1` is a “zero inflated” parameter. (Note: traditionally in zero inflated models observable outcomes, rather than unobservable parameters are zero inflated.) Our new model is more powerful, as it can now put an atomic (non-negligible) mass exactly on zero.

This new code instantiates the critique implied by the following graphical model.

Again, the only important line of code is the `ei <- data$y - (pi$explanatory * pi$beta_1 * data$x + pi$beta_0)` statement. All other code is just in service of this model specifying line.

Let’s see how these are different using this model for inference on the same data.

Experiment 3: Conditional Bayesian Inference with `beta_1` not explanatory.

Let’s re-run our example where `x` is not explanatory and we should infer `beta_1 = 0`. For our software this is the same as inferring `explanatory * beta_1 = 0` or `explanatory = 0`.

We set up the data and observed relation of `y` to `x`.

```

n_example <- 100
actual_b0 <- 0.3

d <- data.frame(x = rnorm(n_example))
d$y <- actual_b0 + dnorm(nrow(d), mean = 0, sd = 1)

params <- generate_params()
params$posterior_weight <- p_data_given_params(
  params = params,
  data = d,
  fn_factory = mk_fun_p_data_given_params_with_conditional)

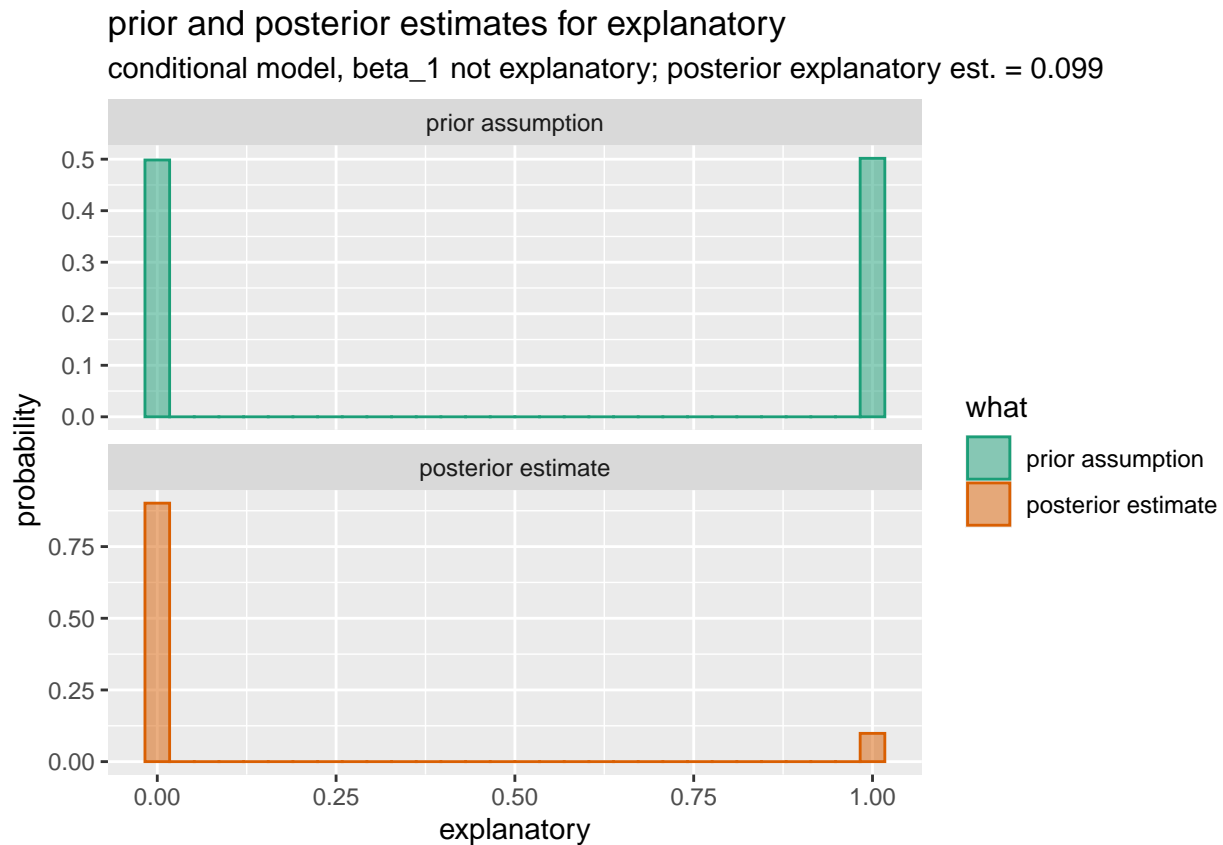
```

And we plot what we came for: the prior and posterior distributions of the `explanatory` parameter.

```

plot_parameter(
  params, 'explanatory',
  subtitle = 'conditional model, beta_1 not explanatory',
  use_hist = TRUE)

```



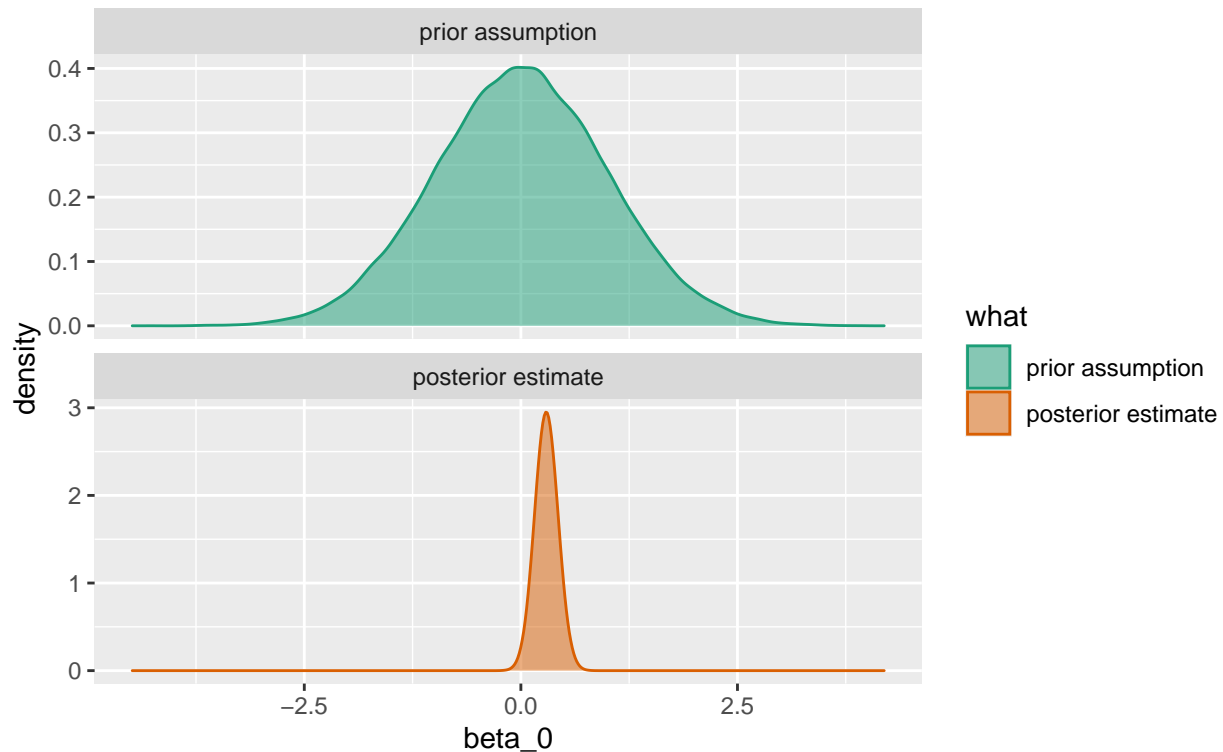
It worked! The model says the data is more consistent with x not being a variable. Note: this is not a frequentist setup, so we have not done something silly or impossible such as “accepting the null hypothesis.” Strictly we have only said: the data is plausible under the assumption that x is not an explanatory variable.

We can of course also plot the inferred distributions of the remaining variables.

```
plot_parameter(  
  params, 'beta_0',  
  subtitle = 'conditional model, beta_1 not explanatory')
```

prior and posterior estimates for beta_0

conditional model, beta_1 not explanatory; posterior beta_0 est. = 0.29

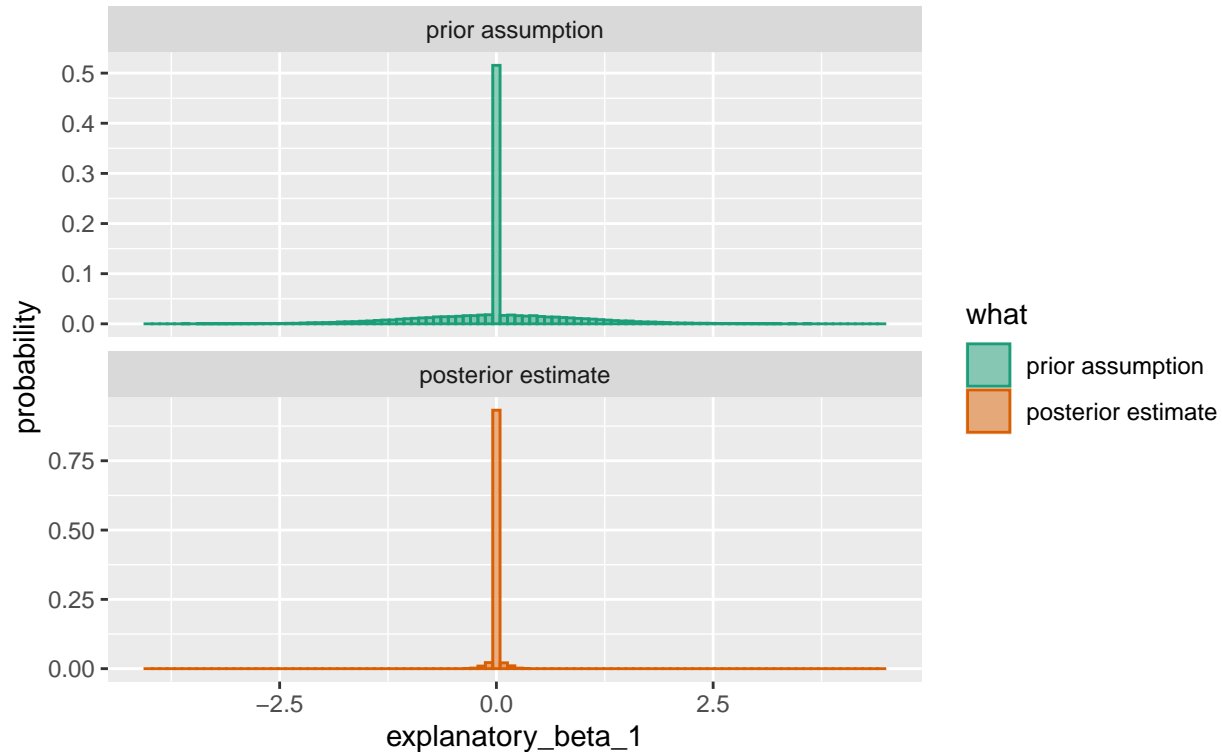


Keep in mind that β_1 isn't as interesting in this model formulation as $\text{explanatory} * \beta_1$, so the distribution of β_1 isn't as important as the distribution of $\text{explanatory} \beta_1$.

```
params$explanatory_beta_1 <- params$explanatory * params$beta_1
plot_parameter(
  params, 'explanatory_beta_1',
  subtitle = 'conditional model, beta_1 not explanatory',
  use_hist = TRUE,
  bins = 100)
```

prior and posterior estimates for explanatory_beta_1

conditional model, beta_1 not explanatory; posterior explanatory_beta_1 est. = $-4.2e-04$



Let's draw few examples according to the posterior weighting. We might use any one of them as “point estimate” of the inference or fitting.

```
row_ids <- sample.int(
  length(params$posterior_weight),
  size = 5, replace = TRUE,
  prob = params$posterior_weight)

params[row_ids, qc(beta_0, explanatory, explanatory_beta_1)] %>%
  knitr::kable()
```

	beta_0	explanatory	explanatory_beta_1
89730	0.3502084	0	0
1623	0.2772984	0	0
38785	0.2637149	0	0
72876	0.2267579	0	0
51349	0.4321816	0	0

Usually we see `explanatory_beta_1` exactly equal to zero. That is correct.

Experiment 4: Conditional Bayesian Inference with beta_1 explanatory.

We saw in the last experiment that if we started with a some mass of the distribution of `explanatory * beta_1` at zero, then after inference for a non-explanatory variable a lot of mass of `explanatory * beta_1` is at zero.

We need to see if a variable is in fact explanatory that we see both `explanatory` move its distribution to 1 and for `explanatory * beta_1` to move to the right value.

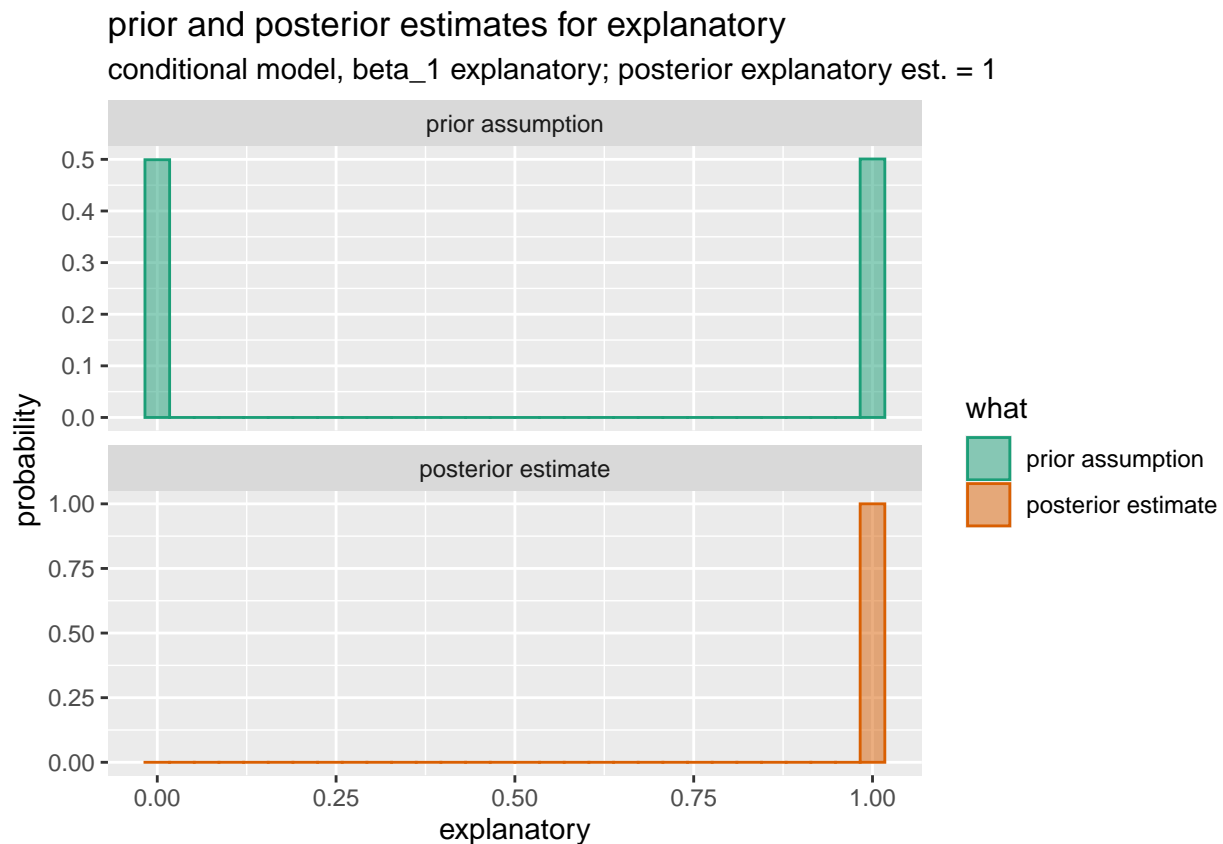
Let's try that experiment.

```
n_example <- 100
actual_b1 <- 0.7
actual_b0 <- 0.3

d <- data.frame(x = rnorm(n_example))
d$y <- actual_b1 * d$x + actual_b0 + rnorm(nrow(d), mean = 0, sd = 1)

params <- generate_params()
params$posterior_weight <- p_data_given_params(
  params = params,
  data = d,
  fn_factory = mk_fun_p_data_given_params_with_conditional)

plot_parameter(
  params, 'explanatory',
  subtitle = 'conditional model, beta_1 explanatory',
  use_hist = TRUE)
```



This looks good, in this case the posterior distribution for `explanatory` is more concentrated towards 1, indicating the data has evidence for using the associated variable `x`.

Let's look out our main (composite) parameter of interest `explanatory * beta_1`.

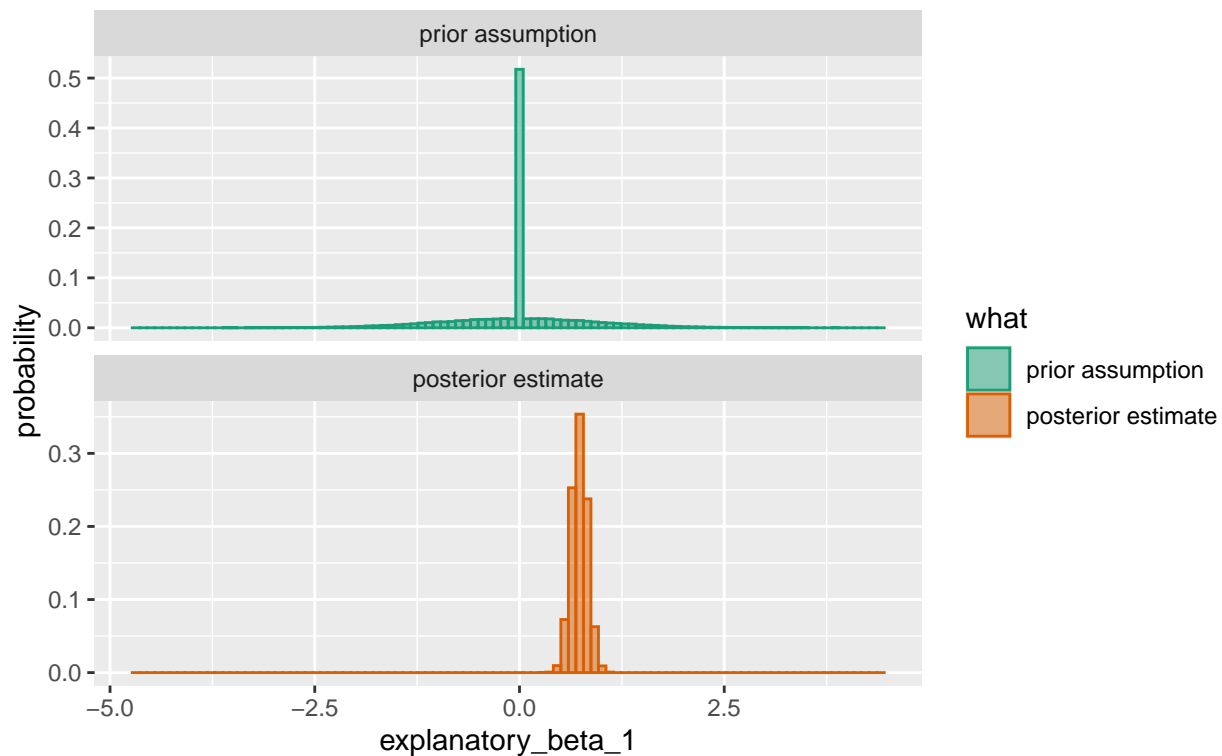
```

params$explanatory_beta_1 <- params$explanatory * params$beta_1
plot_parameter(
  params, 'explanatory_beta_1',
  subtitle = 'conditional model, beta_1 explanatory',
  use_hist = TRUE,
  bins = 100)

```

prior and posterior estimates for explanatory_beta_1

conditional model, beta_1 explanatory; posterior explanatory_beta_1 est. = 0.73



The joint estimate of `explanatory * beta_1` is similar to the unobserved true model that generated the observed data (`d$y <- actual_b1 * d$x + actual_b0 + rnorm(nrow(d), mean = 0, sd = 1)`).

The procedure worked. The inference recovered the parameters that generated the data. This is going to be a small measure less statistically efficient than a standard regression, as the inference was forced to consider cases we know not to be the case. But the procedure seems sound.

```

#cleanup
parallel::stopCluster(c1)

```

Conclusion

Variable selection falls out naturally from the right sort of Bayesian model. If a column is not explanatory, correct fitting procedures can have a high probability of exactly excluding it. If you are using columns that are not all strenuously pre-vetted for your problem you should probably introduce some variable selection to your data science or machine learning workflow. Identifying that a column may have no effect is not the same as saying a column has at most a small effect. Though thinking in terms of mere averages or point estimates sometimes is not rich enough to distinguish these two concepts.

Appendices

Regression

Regression is the modeling of a numeric outcome or dependent variable as a noisy function of one or more explanatory variables. A simple example would be a linear regression of the form:

$$y \sim \beta_0 + \beta_1 x + \text{error}$$

That is: x and y are observed vectors of numeric values. *error* is an *unobserved* numeric vector. We usually insist on some distributional assumptions such as *error* being mean-zero, identically and normally distributed values. β_0 and β_1 are the scalar model parameters to be estimated.

In this context, variable selection would be to consider whether a model of the simpler form $y \sim \beta_0 + \text{error}$ might be more appropriate than one of the form $y \sim \beta_0 + \beta_1 x + \text{error}$. A good discussion on what the assumptions of linear regression are can be found here (the point being: the assumptions are not always what people remember them to be).

Least Squares

The usual least-squares solution is to pick β_0, β_1 that minimize:

$$\|y - \beta_0 + \beta_1 x\|_2^2$$

(This is just the squared 2-norm, or the sum of squares of the error or residuals.)

Least squares is commonly thought of as a frequentist method, and requires few distributional assumptions on the x, y, β_0 , and β_1 beyond independence of examples. There are some distributional assumptions on *error* (such as being mean-zero and possibly normally distributed), but these are mostly used in regression diagnostics such as significances estimates and confidence intervals.

In least-squares regression, variable selection has to be done on held-out test data or through cross-validation methods. This is because in the least-squares formulation we have an overly aggressive empirical loss criteria: having the model match the data before us.

This “training data”-only criteria is what generates the fitting fallacy we are interested in. It appears to imply: “if β_1 should be zero, the fitting procedure would have already told us so.” And the “would have already told us so” is where we might have some discomfort in explicitly removing a proposed explanatory variable from a model (forcing the corresponding β to zero).

Our goal is to demonstrate there are natural fitting procedures that imply variable selection. Variable or feature selection is built into some inference procedures, and can be beneficial when added to procedures that do not incorporate feature selection. In particular using an “out of training data procedure” (held out test data, or cross-methods) can improve least squares fitting performance on new data, as the least squares procedure does not itself incorporate sufficiently strong feature selection.

Bayesian Regression

There are Bayesian forms of regression. These require detailed distributional assumptions on the errors and parameters called priors. In a Bayesian regression don’t so much point-estimate the parameters, but build up the posterior distribution of what are the likely values of the parameters given the priors and data.

Probabilities and Densities/Likelihoods

We assume we have access to several probability density functions. A probability density function can be written as $f(X = v)$ where X is the name of a random variable of interest (or a description of a distribution), and v is a numeric value. A given $f(X = v)$ is a map from numeric values v to new non-negative numeric values. The X is just the name of the density as a random variable or is a distribution specification.

Densities are designed so we can integrate them to read off probabilities as follows:

$$P[a \leq X \leq b] = \int_{v=a}^b f(X = v) dv$$

The above is read as: the probability that the random variable X is between a and b is $P[a \leq X \leq b]$. This value can be calculated by integrating the density $f(X = v)$ for v in the range a to b . We will commonly write $P[A]$ where A is an event of the form $a \leq X \leq b$. The notation $P[A|B]$ is read as “probability of A being true, given B is known to be true” and can be seen to be $P[A \text{ and } B]/P[B]$ when $P[B]$ is non-zero. Note $P[A|B]$ can be sensible even when $P[B]$ is zero, we just need to derive $P[A|B]$ in a different manner in this case.

Bayes’ Law

Our big inference tool is: Bayes’ Law. This is:

$$P[A|B] = \frac{P[B|A]P[A]}{P[B]}$$

(when all of the above quantities are non-zero).

The idea is: B is what we observe (example: the data x and y) and A is what we are interested in (the unobserved coefficients β_0 and β_1). We want to calculate $P[A|B]$. To do this we assume a plausible value for $P[A]$ (the “prior”, getting this exactly right is not important, as this term eventually gets swamped out by other terms), and calculate $P[B|A]$ (which can be easier for us to do than calculating $P[A|B]$ directly). We almost never estimate $P[B]$, but instead “sum it out” using the law of total probability.

To use Bayes’ Law we assume A_1, A_2, \dots, A_k are disjoint and every possible A -event (or at least a very close approximation). That is A_i being true implies A_j false for all $i \neq j$ and $\sum_i P[A_i] = 1$.

Under these assumptions we have:

$$P[B] = \sum_i P[B|A_i]P[A_i]$$

so

$$P[A|B] = \frac{P[B|A]P[A]}{\sum_i P[B|A_i]P[A_i]}$$

This is just a long winded way of saying: to apply Bayes’ Law use:

$$P[A|B] = \frac{P[B|A]P[A]}{Z}$$

where Z is an unknown to be solved for. Then pick Z so that all of your estimates $P[A_i|B]$ sum to one. That is pick Z so:

$$\sum_i \frac{P[B|A_i]P[A_i]}{Z} = 1$$

We will use Bayes' Law both for probabilities, as we showed above, and for densities (which work much the same for this application, with the exception that the Z term is found by integration instead of summation).

Densities of interest

The densities we commonly see in regression are non-atomic: they assign zero to all probabilities of the form $P[a \leq X \leq a]$. In other words, the probability mass on any single point is always zero. Our densities are also proper normalized densities that have $\int_{v=-\infty}^{\infty} f(X = v)dv = 1$. Such non-atomic distributions are typically expanded as:

$$P[a \leq X \leq a] = \int_{x=a}^b f(X = x)dx$$

The expression $f(X = x)$ is read as "the probability *density* assigned to seeing the random variable X take the specified value x . It can be confusing, we usually have $P[X = x] = 0$ and the associated $f(X = x) > 0$.

The density functions we are interested in are:

- $f(\beta_0 = v)$, the prior belief of the likelihood of β_0 having the value v .
- $f(\beta_1 = v)$, the prior belief of the likely-hood of β_1 having the value v .
- $f(error = v)$, the prior belief of the likely-hood of *error* having the value v .

To perform a Bayesian regression we must assume we have at least plausible guesses at all of these prior density functions. Our results become less dependent on these exact values as we have more data (longer vectors x and y). So not having the exact right values for these prior densities is not a blocker.

Typically we will use a convenient normal prior for all of these densities (for more technical work it could in fact be t-distributions, or variations on gamma-distributions). For example we could, for the sake of convenience, just assume all of these densities are normal distributions with mean-zero and standard-deviation one. That is, we assume (without worrying about justification):

- $f(\beta_0 = v) = \exp(-\frac{1}{2}v^2)/\sqrt{2\pi}$
- $f(\beta_1 = v) = \exp(-\frac{1}{2}v^2)/\sqrt{2\pi}$
- $f(error = v) = \exp(-\frac{1}{2}v^2)/\sqrt{2\pi}$

and that all of these quantities are independent of each other (and also independent of the data x).

Finally, Bayesian Regression

Bayesian regression is applying Bayes' Law to our regression problem. Informally we want to know $P[\beta_0, \beta_1 | x, y]$. That is we want to know for any β_0 and β_1 how likely or plausible they are given our observed data x, y . We introduce random variables X and Y that our observed data x and y are specific realizations of.

Formally we want to know $f(\beta_0 = v_0, \beta_1 = v_1 | X = x, Y = y)$. We've introduced proposed values v_0 and v_1 to not be confused with the random variables β_0 and β_1 . Bayes' Law applied to our densities of interest gives us:

$$f(\beta_0 = v_0, \beta_1 = v_1 | X = x, Y = y) = \frac{f(Y = y | \beta_0 = v_0, \beta_1 = v_1, X = x)f(\beta_0 = v_0, \beta_1 = v_1 | X = x)}{f(Y = y | X = x)}$$

(this is just Bayes' Law in a universe where $X = x$ is always known). We need our additional independence assumption that $f(\beta_0 = v_0, \beta_1 = v_1 | X = x) = f(\beta_0 = v_0, \beta_1 = v_1)$. I.e. the unknown parameters β_0, β_1 are independent of X , or at least our weak assumed estimate of β_0, β_1 is independent of X .

So for this method, we are assuming:

$$f(\beta_0 = v_0, \beta_1 = v_1 | X = x, Y = y) = \frac{f(Y = y | \beta_0 = v_0, \beta_1 = v_1, X = x) f(\beta_0 = v_0, \beta_1 = v_1)}{f(Y = y | X = x)}$$

We in fact know $f(Y = y | \beta_0 = v_0, \beta_1 = v_1, X = x)$. It is equal to $f(\text{error} = y - (v_0 + v_1 x) | \beta_0 = v_0, \beta_1 = v_1, X = x)$. And this in turn equals (due to our distributional assumptions) $\exp(-\frac{1}{2} \|y - (v_0 + v_1 x)\|_2^2) / \sqrt{2\pi}$.

So our density estimate is:

$$f(\beta_0 = v_0, \beta_1 = v_1 | X = x, Y = y) = \frac{\exp(-\frac{1}{2} \|y - (v_0 + v_1 x)\|_2^2) f(\beta_0 = v_0, \beta_1 = v_1)}{\sqrt{2\pi} f(Y = y | X = x)}$$

Or:

$$f(\beta_0 = v_0, \beta_1 = v_1 | X = x, Y = y) = \frac{\exp(-\frac{1}{2} \|y - (v_0 + v_1 x)\|_2^2) f(\beta_0 = v_0, \beta_1 = v_1)}{Z}$$

where Z is a quantity we will solve for later (the $\sqrt{2\pi}$ and $f(Y = y | X = x)$ are hidden in this Z).

In a formal setting we would solve for Z by integrating out v_0 and v_1 , as we know the total integral should equal 1.

What we are going to do in practice is the following.

We generate a large finite collection of values $v_0[i], v_1[i]$ distributed according to the density $f(\beta_0 = v_0, \beta_1 = v_1)$, We then pick Z so that

$$\sum_i \frac{\exp(-\frac{1}{2} \|y - (v_0[i] + v_1[i]x)\|_2^2)}{Z} = 1$$

Once we have Z we define:

$$\text{posterior_weight}[i] = \frac{\exp(-\frac{1}{2} \|y - (v_0[i] + v_1[i]x)\|_2^2)}{Z}$$

is our new weighting of the data.

The point is: we generated $v_0[i], v_1[i]$ by drawing from the distribution density $f(\beta_0 = v_0, \beta_1 = v_1)$. So drawing an index i with uniform odds gives us a discrete approximation of the distribution $f(\beta_0 = v_0, \beta_1 = v_1)$. So if we instead draw index i with probability proportional to $\text{posterior_weight}[i]$ then this new re-sample is a discrete approximation to a distribution with density proportional to:

$$\exp(-\frac{1}{2} \|y - (v_0[i] + v_1[i]x)\|_2^2) f(\beta_0 = v_0, \beta_1 = v_1)$$

So re-drawing a sample with odds proportional to posterior_weight behaves exactly like the desired posterior distribution. For any statistical method that takes weights, we can pass the posterior_weight values in and avoid the second resampling.

Remembering Bayes' Law

An important mental trick is: never try to remember Bayes' Law. Instead remember the smaller expression

$$P[A|B] = P[A \text{ and } B]/P[B]$$

From this one quickly gets:

$$P[A \text{ and } B] = P[A|B]P[B]$$

And by symmetry:

$$P[B \text{ and } A] = P[B|A]P[A]$$

As $P[A \text{ and } B] = P[B \text{ and } A]$ we can equate that last two expressions to get:

$$P[A|B]P[B] = P[B|A]P[A]$$

And we have recovered Bayes' Law.

Links

- PDF render of full article with appendices
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