Solving the model representation problem with `broom`

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Who am I?

Statistical models

The model representation problem

The `broom` package

Use cases

Open Questions & Hot Takes

`tidymodels`

These slides are available online!

https://tinyurl.com/broom-talk-sgsa

Who am I?

About Me

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- Current maintainer of the `broom` package
- Active on #rstats Twitter and Github

Statistical models

What is a model?

Let x be values that live in some space $\mathcal{X}$, and let y be observations of interest that live in some space $\mathcal{Y}$. A **statistical model** is a *set* of probability distributions $\mathcal{P}(y|x)$ indexed by parameters $\theta \in \Theta$[1].

[1] In some cases we treat θ as itself random, which means that our model is a class of probability distributions $\mathcal{P}(y, \theta|x)$.

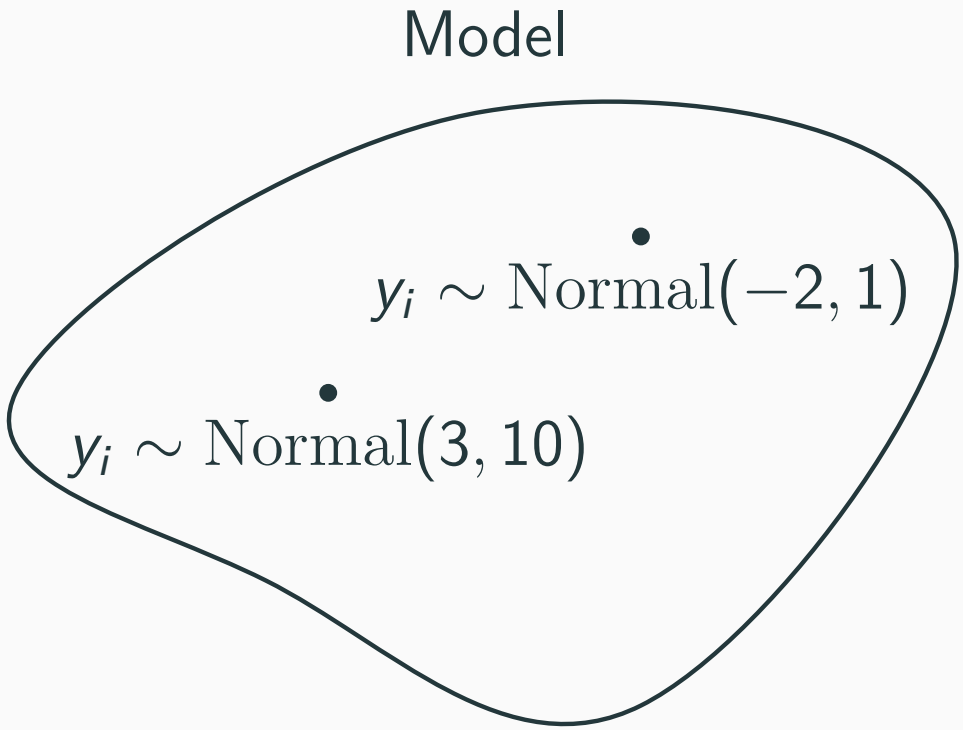
Example: the normal model

$$y_i \overset{\text{iid}}{\sim} \text{Normal}(\mu, \sigma^2)$$

Here $\theta = (\mu, \sigma^2)$ and the parameter space is $\mathbb{R} \times \mathbb{R}^+$.

Visualizing the normal model

Again: a model is a *set*.



We call a single element of a model a **fit**. The distribution with $\mu = -2, \sigma^2 = 1$ is a fit, for example.

Another (parametric) example: the linear model

Given response y and predictor variables x_1 and x_2, the linear model looks like:

$$y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \varepsilon_i \qquad \varepsilon_i \overset{\text{iid}}{\sim} \text{Normal}(0, \sigma^2)$$

This model says that y is i.i.d with a mean that depends on x and $\vec{\beta}$, and with fixed variance σ^2.

Estimation

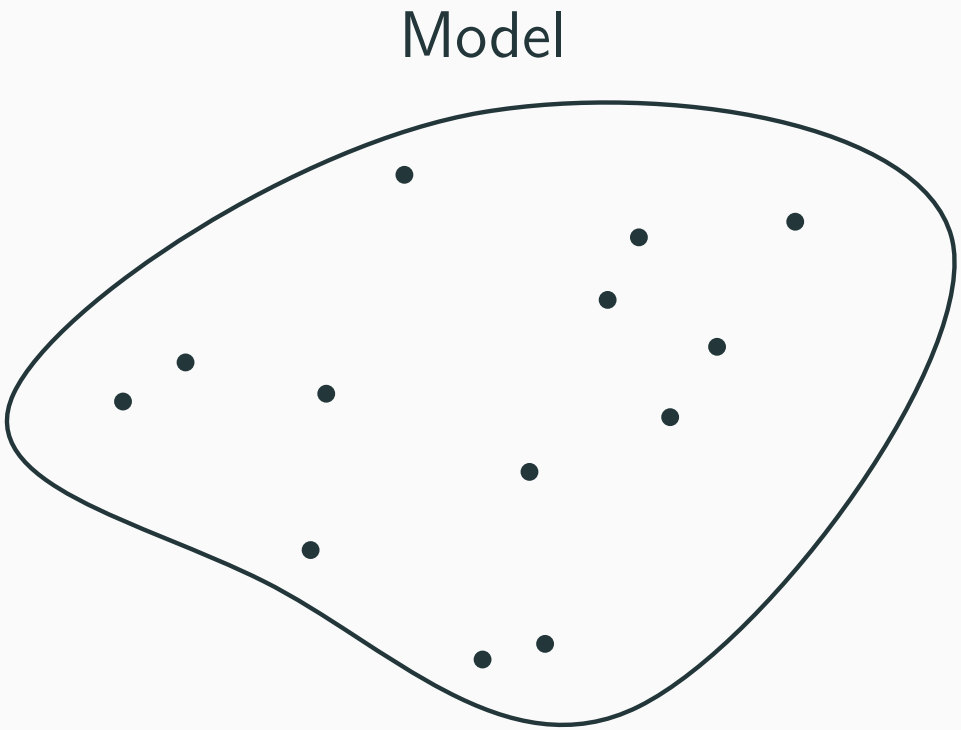
An **estimator** is a way to calculate the parameters of a model from data[2]. They are many estimators for any given model, and which one we think is best depends on how we define "agrees best with the data."

[2] This is equivalent to selecting the best fit!

Some estimators for the normal model

- $\hat{\mu} = 1 \qquad \hat{\sigma}^2 = 10$
- $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$
- $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$

Visualizing estimation



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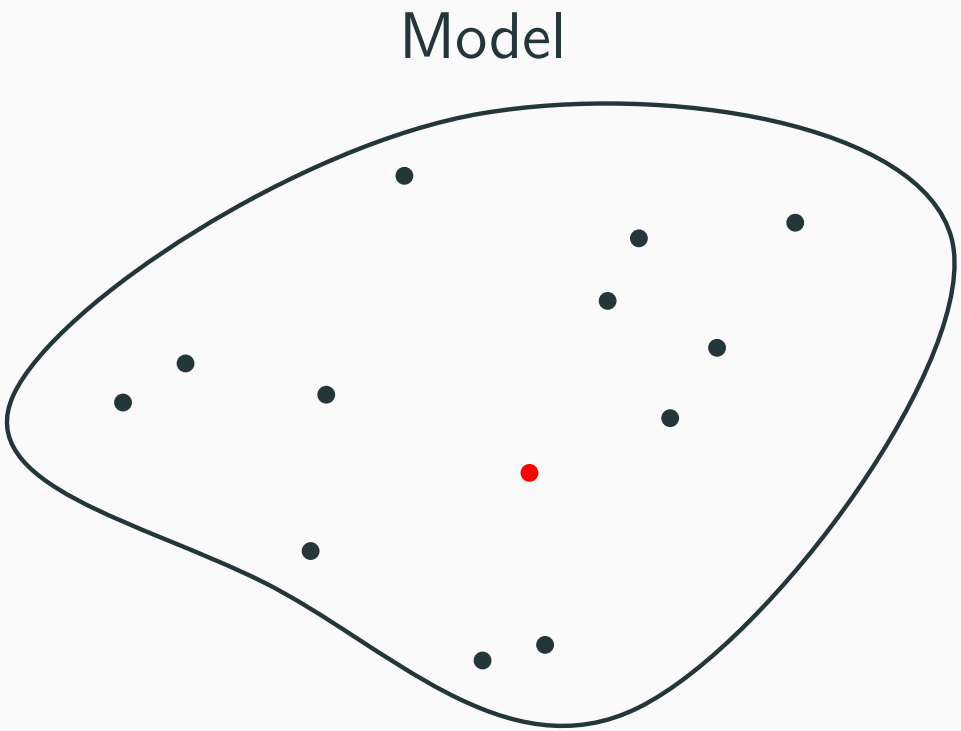
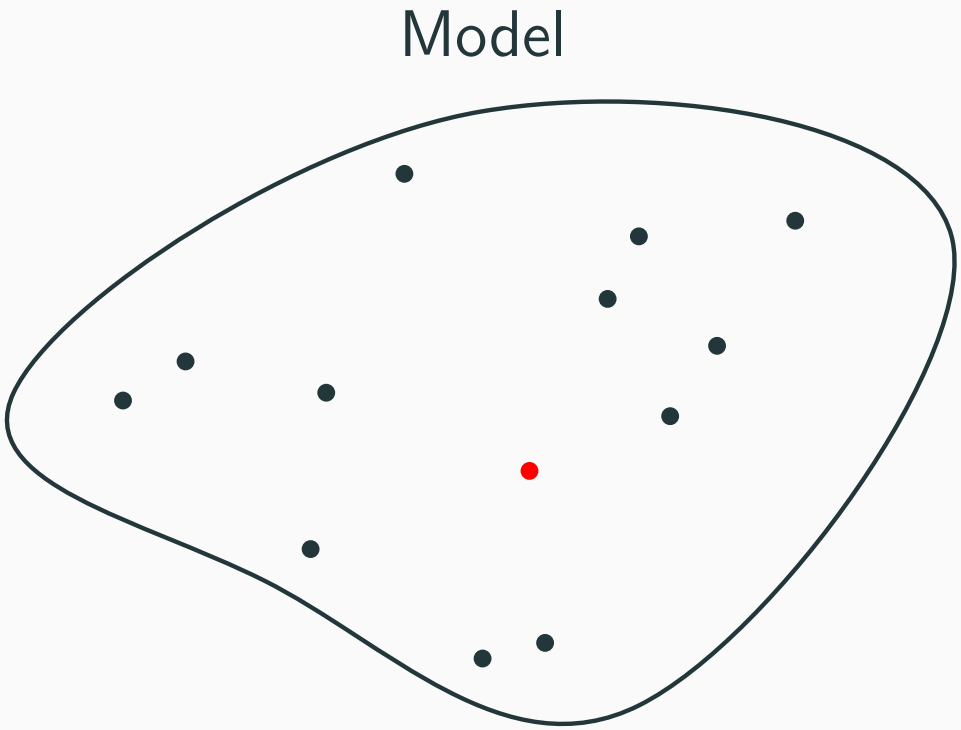
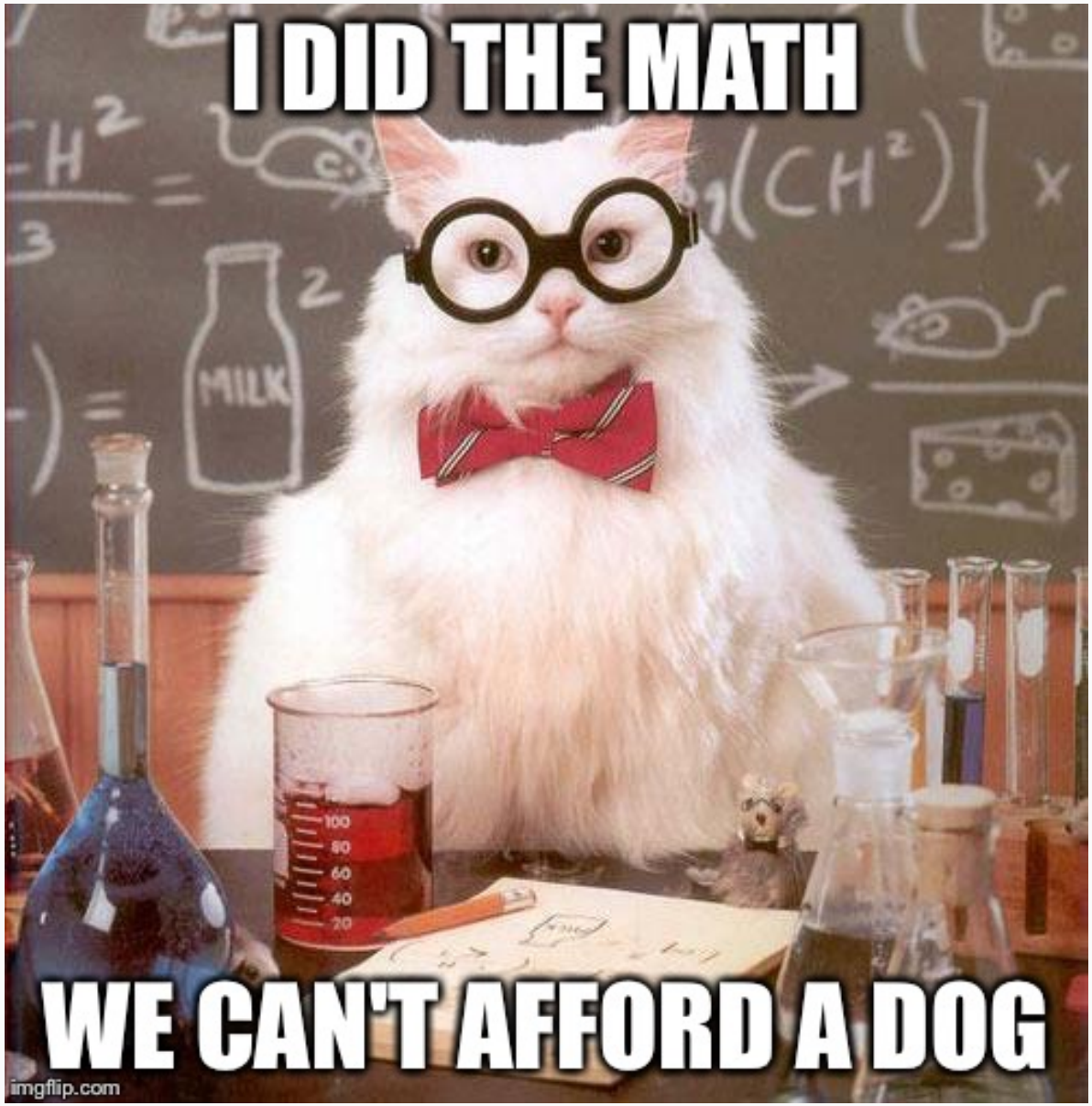


Estimates found!



Best fit: $y_i \sim \mathrm{Normal}(-2, 1)$. Finally we can do inference!

Do all the inference



Some intuition about models, estimators and fits

A **model** corresponds to a set of possible truths about the world. A **fit** is a single truth about the world. An **estimator** is a way to choose the truth most suggested by the data from a set of many possible truths.

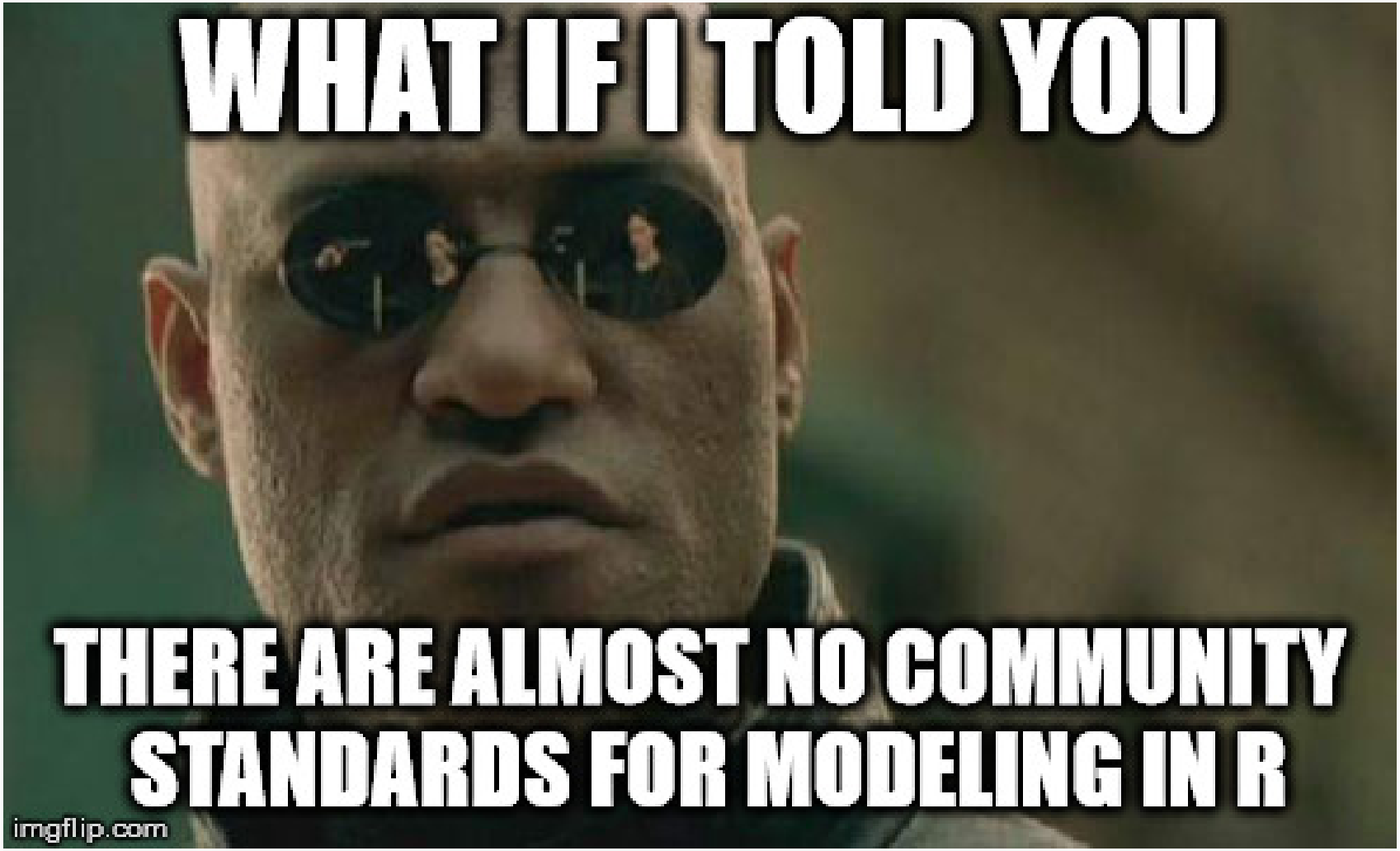
The model representation problem

Representing a fit in mathematical terms

Hopefully it feels natural to describe models mathematically

- Normal model: $y_i \sim \mathrm{Normal}(\mu, \sigma^2)$
  - Fit from normal model: $y_i \sim \mathrm{Normal}(-2, 1)$
  - Can also identify fits by parameter vectors: $\theta = (-2, 1)$
  - Estimators for normal model:
  - $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$
- Key: shared notation and community standards

How does R represent models, estimators and fits?

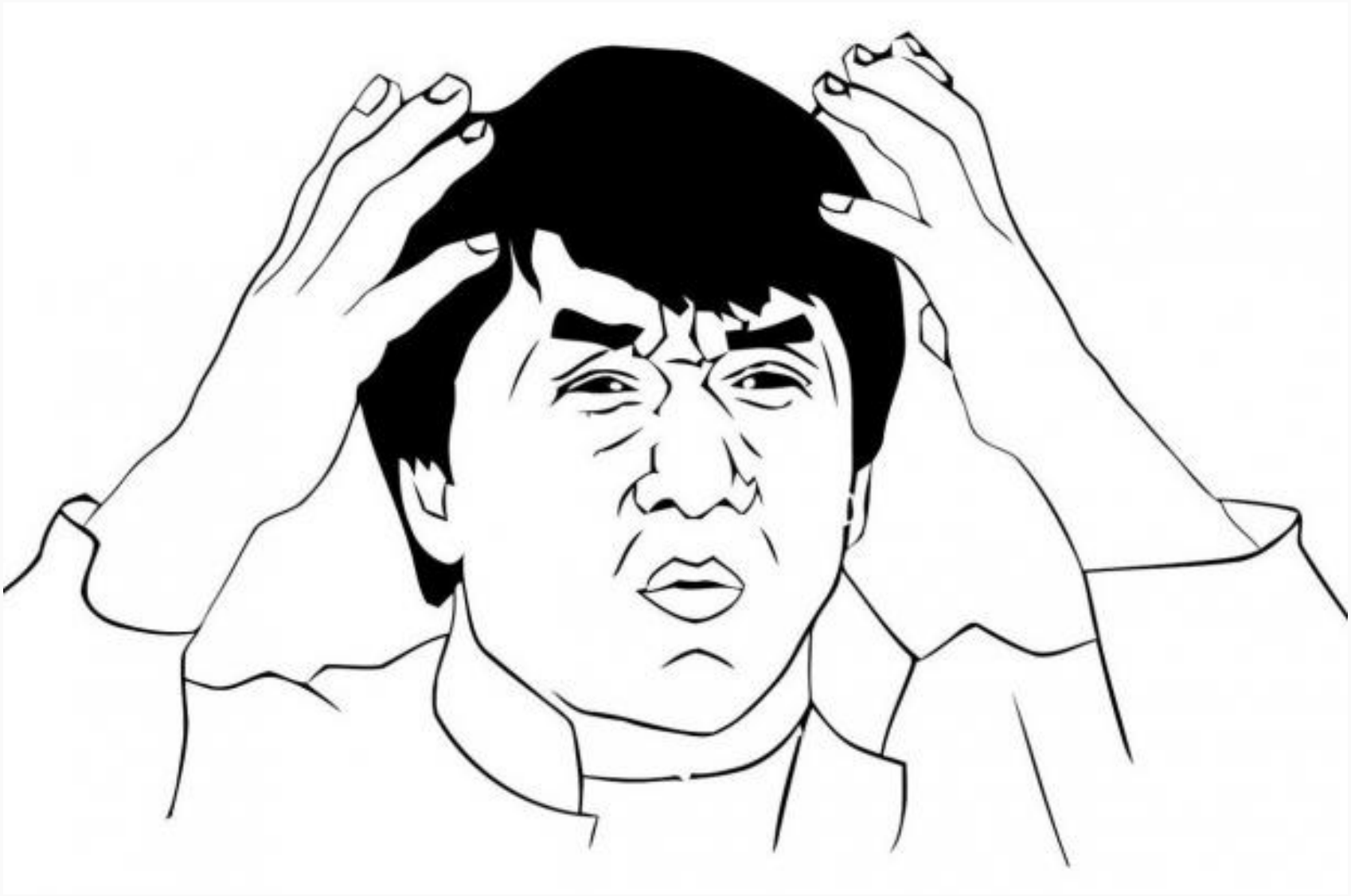


A taste of the pain

Suppose you want class probabilities from a fit called `obj`:

Object	Code
`lda`	`predict(obj)`
`glm`	`predict(obj, type = "response")`
`gbm`	`predict(obj, type = "response", n.trees)`
`mda`	`predict(obj, type = "posterior")`
`rpart`	`predict(obj, type = "prob")`
`Weka`	`predict(obj, type = "probability")`
`logitboost`	`predict(obj, type = "raw", nIter)`
`pamr.train`	`pamr.predict(obj, type = "posterior")`

How am I supposed to keep track of all this!?



The model representation problem

We have no shared framework or understanding of how to represent statistical models, estimation methods and fits with R objects.

Aside

- People who write and share code to enable data analysis are awesome
- This isn't anyone's fault
- Trying to get things done can still be frustrating

The `broom` package

The scene

Say we:

1. pick a model,
2. pick an estimator for that model, and then
3. get an R object `fit` using that estimator.

- The `fit` object is different for every model.
- The `fit` object could be great to work with, or awful.

`broom` provides a standard way to represent fits

`broom` treats fits as having three parts:

1. A table of information about fit parameters
2. A table of information about each observation used to estimate the fit
3. A table of overall goodness-of-fit measures

- Each of table reported as a tidy `tibble`.
- Together these constitute a *tidy representation* of a fit.

Aside: What is a `tibble`

A `tibble` is a more consistent `data.frame`. `tibbles` are used widely throughout the `tidyverse`.

```
library(tibble)
```

```
tibble(x = 1:2, y = 3:4)
```

```
## # A tibble: 2 x 2
##       x     y
##   <int> <int>
## 1     1     3
## 2     2     4
```

Aside: What does it mean to be tidy?

I highly recommend reading Hadley Wickham's Tidy Data paper! The short version: a **tidy dataset** is one where:

1. Each variable forms a column.
2. Each observation forms a row.
3. Differents kinds of data live in different tables.

The `broom` generics

So how do we turn fits into tidy tibbles?

- `tidy()` summarizes information about fit components
- `glance()` reports information about the entire fit
- `augment()` adds information about observations to a dataset

Continuing with the normal model example

```r
# simulate Normal(-2, 1) data
x <- rnorm(5000, -2, 1)

# create a fit object using
# MLE estimator and normal model
normal_fit <- MASS::fitdistr(
  x,
  dnorm,  # use the normal model!
  start = list(mean = 0, sd = 1)
)
```

What is normal_fit?

```
str(normal_fit)
## List of 5
##  $ estimate: Named num [1:2] -2.03 1.01
##   ..- attr(*, "names")= chr [1:2] "mean" "sd"
##  $ sd      : Named num [1:2] 0.0143 0.0101
##   ..- attr(*, "names")= chr [1:2] "mean" "sd"
##  $ vcov    : num [1:2, 1:2] 2.06e-04 -4.62e-13 -4.
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : chr [1:2] "mean" "sd"
##   .. ..$ : chr [1:2] "mean" "sd"
##  $ loglik  : num -7165
##  $ n       : int 5000
##  - attr(*, "class")= chr "fitdistr"
```

What is the tidy representation of `normal_fit`?

```
library(tidyverse)
library(broom)

tidy(normal_fit)
## # A tibble: 2 x 3
##   term  estimate std.error
##   <chr>    <dbl>     <dbl>
## 1 mean     -2.03    0.0143
## 2 sd        1.01    0.0101
```

What is the tidy representation of `normal_fit`?

```
glance(normal_fit)
## # A tibble: 1 x 4
##       n logLik    AIC    BIC
##   <int>  <dbl>  <dbl>  <dbl>
## 1  5000 -7165. 14334. 14347.
```

There's no `augment()` method defined for univariate distributions at the moment.

Another example: the linear model

```r
# create a fit object using the
# OLS estimator for the linear model
ols_fit <- lm(hp ~ mpg + cyl, mtcars)

# try the following for yourself:

str(ols_fit)
```

The tidy representation of `lm` objects

```
tidy(ols_fit)
## # A tibble: 3 x 5
##   term         estimate std.error statistic p.value
##   <chr>           <dbl>     <dbl>     <dbl>   <dbl>
## 1 (Intercept)    54.1      86.1       0.628 0.535
## 2 mpg            -2.77      2.18     -1.27  0.213
## 3 cyl            24.0       7.35      3.26  0.00281
```

The tidy representation of `lm` objects

```
glance(ols_fit)[, 1:5]
## # A tibble: 1 x 5
##   r.squared adj.r.squared sigma statistic       p.v
##       <dbl>         <dbl> <dbl>     <dbl>      <
## 1     0.709         0.689  38.2      35.4 0.000000
```

The tidy representation of `lm` objects

```
augment(ols_fit)[, 1:7]
## # A tibble: 32 x 7
##    .rownames          hp   mpg   cyl .fitted .se.fit
##    <chr>           <dbl> <dbl> <dbl>   <dbl>   <dbl>
## 1 Mazda RX4          110  21       6   140.     6.84
## 2 Mazda RX4 Wag      110  21       6   140.     6.84
## 3 Datsun 710          93  22.8     4    86.7   13.3
## # ... with 29 more rows
```

Notes about the tidy representation

- Always get a tibble back
- Column names in returned tibbles are consistent
- Some information in the original R object is lost

Use cases

Report model coefficients with `tidy()`

```
kable2 <- function(data)
knitr::kable(mutate_if(data, is.numeric, round, 2))

tidy(ols_fit) %>%
kable2()
```

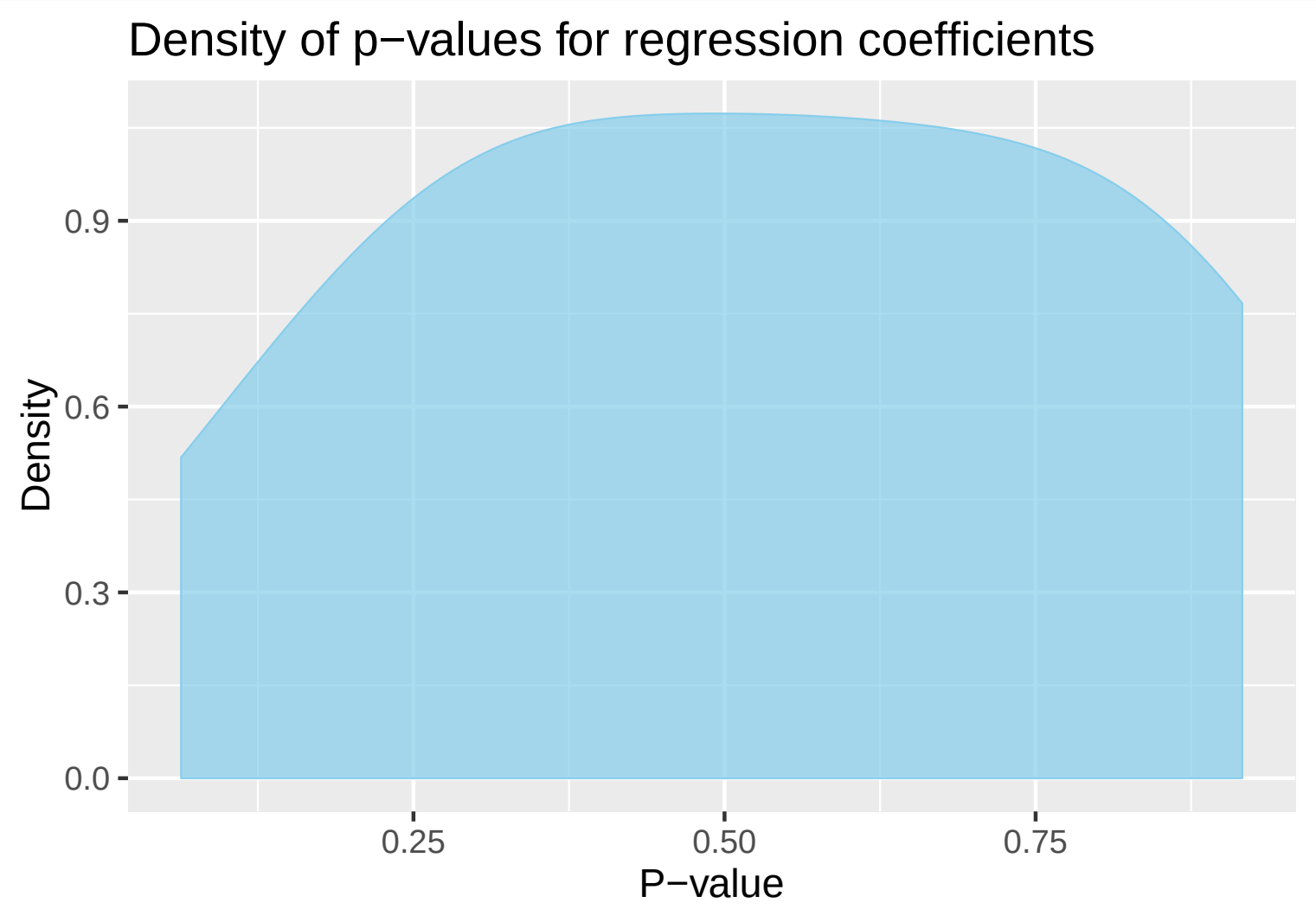
term	estimate	std.error	statistic	p.value
(Intercept)	54.07	86.09	0.63	0.53
mpg	-2.77	2.18	-1.27	0.21
cyl	23.98	7.35	3.26	0.00

Plot histograms/densities of p-values

```r
fit <- lm(mpg ~ ., mtcars)
td <- tidy(fit)

p <- ggplot(td, aes(p.value)) +
  geom_density(
    fill = "skyblue", color = "skyblue", alpha = 0.7
  ) +
  labs(
    title = "Density of p-values for regression coeffic
    x = "P-value",
    y = "Density"
  )
```

Plot histograms/densities of p-values



Comparing models by goodness of fit measures

```
fits <- list(
  fit1 = lm(hp ~ cyl, mtcars),
  fit2 = lm(hp ~ cyl + mpg, mtcars),
  fit3 = lm(hp ~ ., mtcars)
)

gof <- map_df(fits, glance, .id = "model") %>%
  arrange(AIC)
```

Comparing models by goodness of fit measures

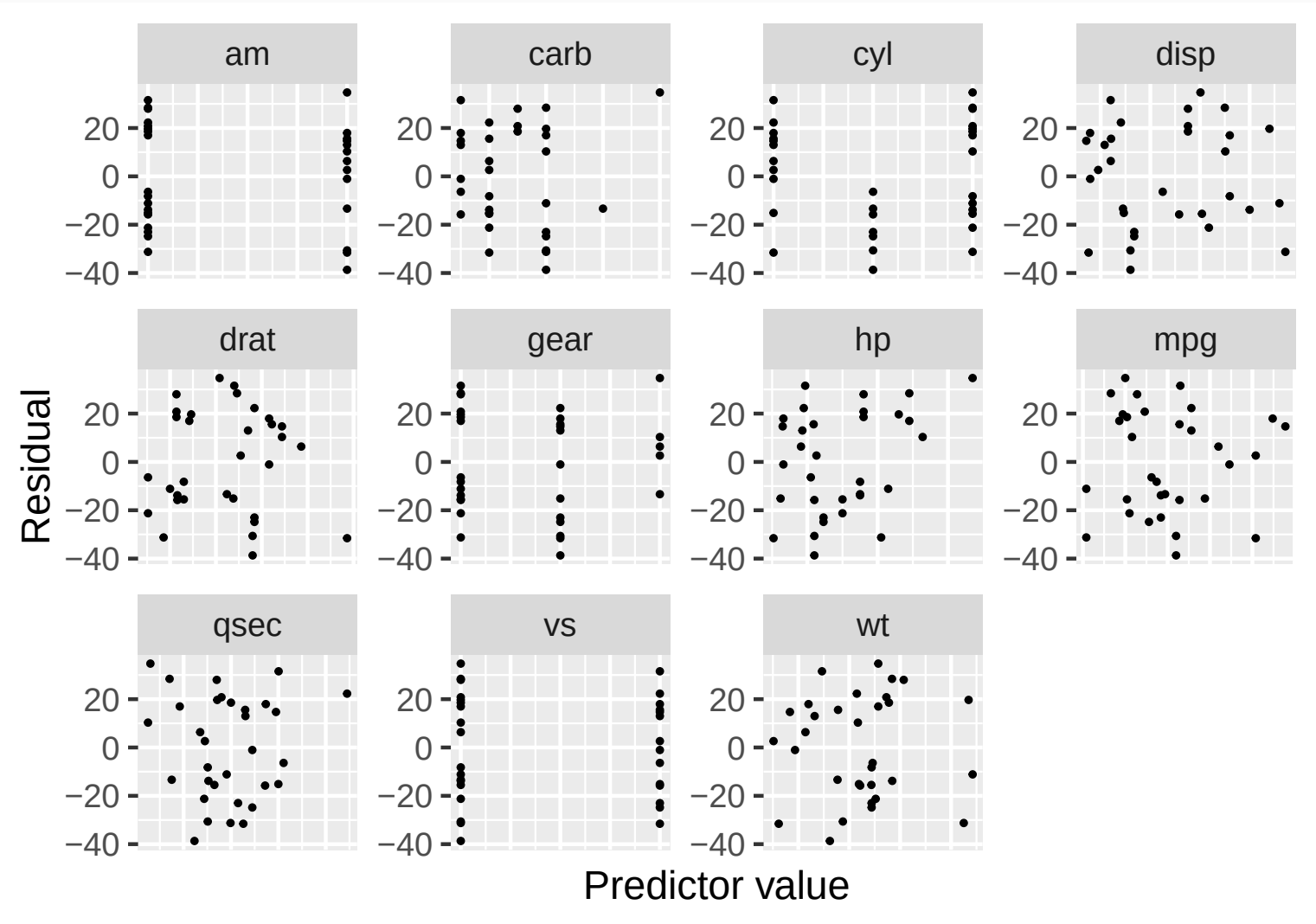
```
select(gof, -c(2:7))
## # A tibble: 3 x 6
##   model logLik   AIC   BIC deviance df.residual
##   <chr>  <dbl> <dbl> <dbl>    <dbl>       <int>
## 1 fit3   -143.  310.  327.   14165.          21
## 2 fit1   -161.  329.  333.   44743.          30
## 3 fit2   -160.  329.  335.   42369.          29
```

Inspecting residuals from multiple linear regression

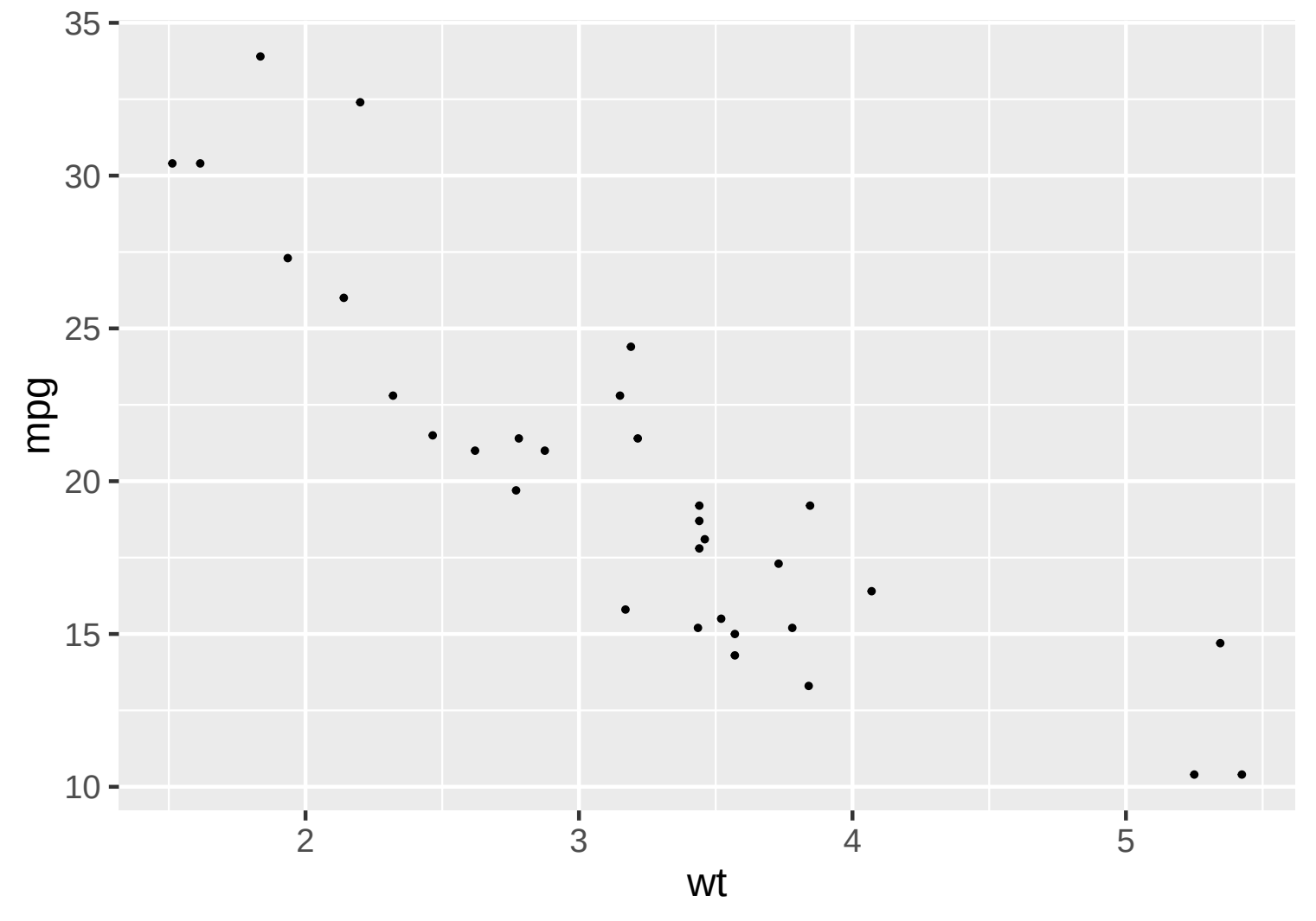
```
fit <- lm(hp ~ ., mtcars)
au <- broom::augment(fit)

p <- au %>%
  gather(x, val, -contains(".")) %>%
  ggplot(aes(val, .resid)) +
  geom_point() +
  facet_wrap(~x, scales = "free") +
  labs(x = "Predictor value", y = "Residual") +
  theme(axis.text.x = element_blank(),
        axis.ticks.x = element_blank())
```

Inspecting residuals from multiple linear regression



Bootstrapping



Bootstrapping

Consider a model:

$$\texttt{mpg} = \frac{k}{\texttt{wt}} + b + \varepsilon, \quad \varepsilon \sim \text{Normal}(0, \sigma^2)$$

Suppose we want to know the sampling distributions of k and b via bootstrapping

Bootstrapping

```
library(rsample)

boots <- bootstraps(mtcars, times = 100)
boots
## # Bootstrap sampling
## # A tibble: 100 x 2
##   splits          id
##   <list>          <chr>
## 1 <split [32/10]> Bootstrap001
## 2 <split [32/7]>  Bootstrap002
## 3 <split [32/13]> Bootstrap003
## # ... with 97 more rows
```

Bootstrapping

```
fit_nls_on_bootstrap <- function(split) {
  nls(
    mpg ~ k / wt + b,
    analysis(split),
    start = list(k = 1, b = 0)
  )
}
```

Bootstrapping

```
boot_fits <- boots %>%
  mutate(fit = map(splits, fit_nls_on_bootstrap),
         coef_info = map(fit, tidy))

boot_fits
## # Bootstrap sampling
## # A tibble: 100 x 4
##   splits          id           fit        coef_info
## * <list>          <chr>        <list>     <list>
## 1 <split [32/10]> Bootstrap001 <S3: nls> <tibble [
## 2 <split [32/7]>  Bootstrap002 <S3: nls> <tibble [
## 3 <split [32/13]> Bootstrap003 <S3: nls> <tibble [
## # ... with 97 more rows
```

Bootstrapping

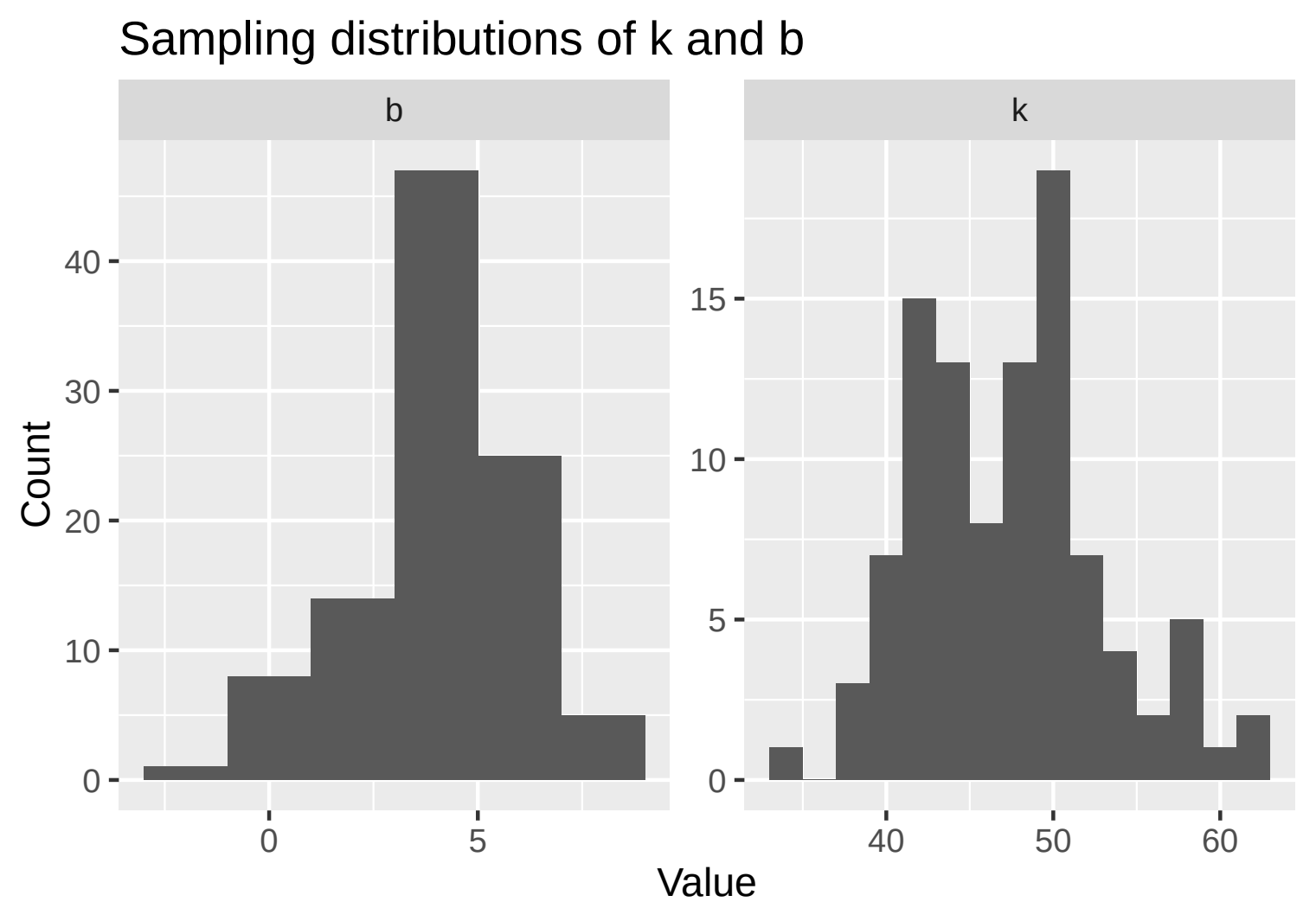
```
boot_coefs <- boot_fits %>%
  unnest(coef_info)

boot_coefs
## # A tibble: 200 x 6
##    id           term  estimate std.error statistic
##    <chr>        <chr>    <dbl>     <dbl>     <dbl>
## 1 Bootstrap001 k         41.8      4.05      10.3
## 2 Bootstrap001 b          5.96     1.64       3.64
## 3 Bootstrap002 k         50.6      3.96      12.8
## # ... with 197 more rows
```

Bootstrapping

```r
p <- ggplot(boot_coefs, aes(estimate)) +
  geom_histogram(binwidth = 2) +
  facet_wrap(~ term, scales = "free") +
  labs(
    title = "Sampling distributions of k and b",
    y = "Count",
    x = "Value"
  )
```

Bootstrapping

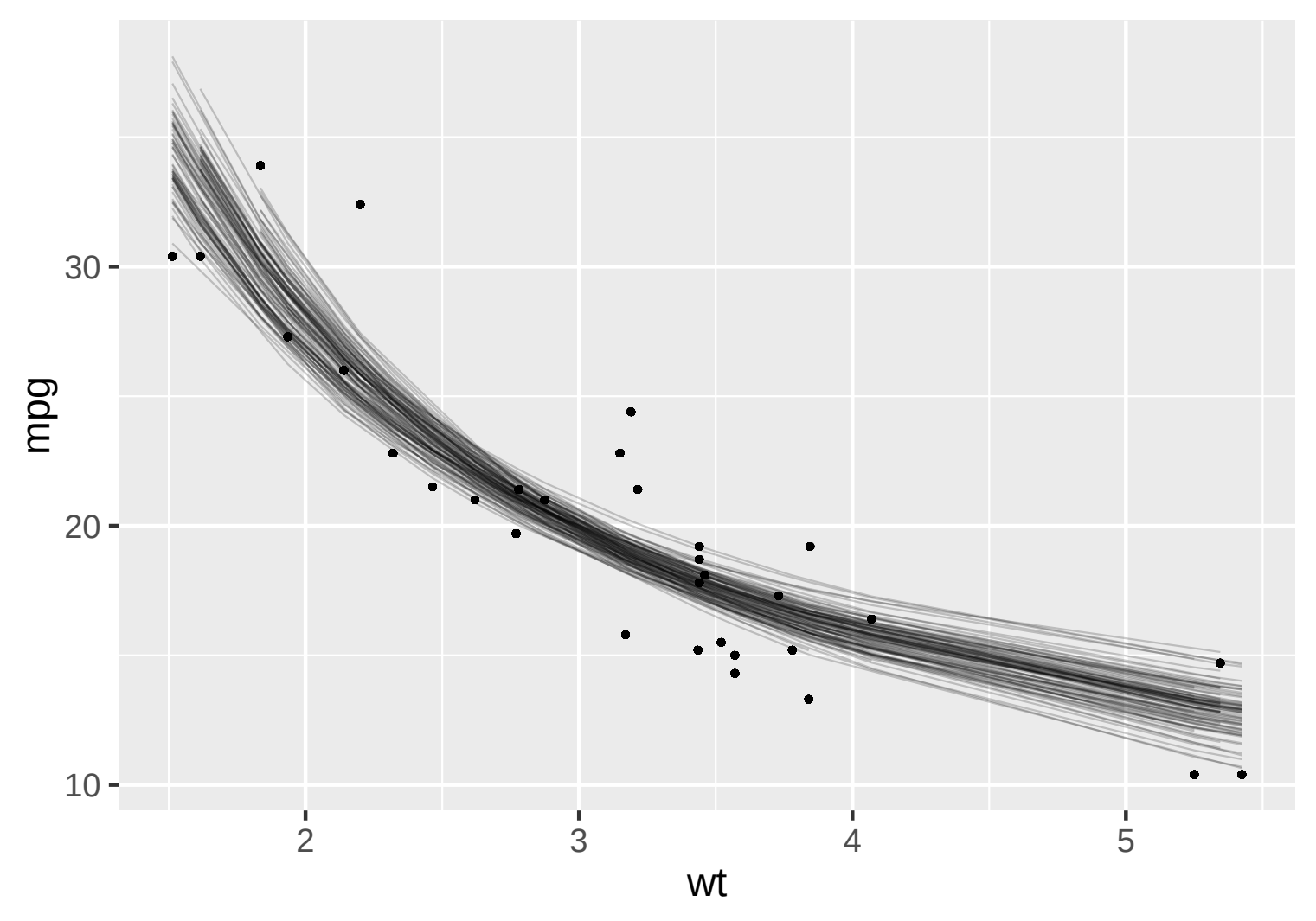


Bootstrapping

```
boot_aug <- boot_fits %>%
  mutate(augmented = map(fit, augment)) %>%
  unnest(augmented)

p <- ggplot(boot_aug, aes(wt, mpg)) +
  geom_point() +
  geom_line(aes(y = .fitted, group = id), alpha = 0.2)
```

Bootstrapping



General strategy

`broom` provides tidying methods for 100+ classes!

1. Put fits in a list, or a list-column of a `tibble`
2. Use `purrr::map()` to apply `tidy()`, `glance()` or `augment()` to each fit
3. Use `tidyverse` tools to manipulate and visualize resulting data!

Open Questions & Hot Takes

How should we represent the following objects?

Sets of fits are particularly interesting to think about:

- Path algorithms (i.e. LASSO fits)

Are there different types of sets of fits?

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  - Can do inference from the entire LASSO path

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Sets of fits are particularly interesting to think about:

- Path algorithms (i.e. LASSO fits)
  - Can do inference from a single fit
  - Can do inference from the entire LASSO path
- Ensembles (i.e. random forests)

Are there different types of sets of fits?

Generics should operate on *fits*, not models

Consider the following methods, all for the linear model:

- `plot_lasso_path()` for OLS vs LASSO fits
- `coef_standard_errors()` for OLS vs LASSO fits
- `interpret_coefficients()` for OLS vs GEE fits

What operations should we be able to perform?

Things pretty much everybody agrees on:

- `fit(model, estimator, data)`

Actions that are begging for S3 generics:

If you have thoughts about these, please talk to me!

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- Model visualization
- ...

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tidymodels

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- best practices for developing modeling packages

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- `recipes`: data pre-processing

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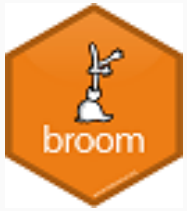
A general attempt to make modeling in R more consistent and tidy. Lots of big projects. Highlights:

- best practices for developing modeling packages
- `parnsip`: standardized modeling interfaces (now on CRAN!!)
- `recipes`: data pre-processing
- `rsample`: infrastructure for resampling

Questions?

Read about the recent `broom` release on the tidyverse blog.



https://broom.tidyverse.org

https://github.com/tidymodels/broom/

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