Model Fitting

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Fitting Models

How do you fit a linear model in R?

How many different ways can you think of?

- `lm` for linear model
- `glm` for generalized linear model (e.g. logistic regression)
- `glmnet` for regularized regression
- `keras` for regression using TensorFlow
- `stan` for Bayesian regression
- `spark` for large data sets

To specify a model using parsnip

- Choose a model
- Specify an engine
- Set the mode
- **fit** the model

To specify a model using parsnip

```
1 library(tidymodels)
2 linear_reg()
```

```
#> Linear Regression Model Specification (regression)
#>
#> Computational engine: lm
```

To specify a model using parsnip

```
linear_reg() %>%
  set_engine("glmnet")
```

```
#> Linear Regression Model Specification (regression)
#>
#> Computational engine: glmnet
```

To specify a model using parsnip

```
linear_reg() %>%
  set_engine("stan")
```

```
#> Linear Regression Model Specification (regression)
#>
#> Computational engine: stan
```

To specify a model using parsnip

```
1 decision_tree()
```

```
#> Decision Tree Model Specification (unknown mode)
#>
#> Computational engine: rpart
```

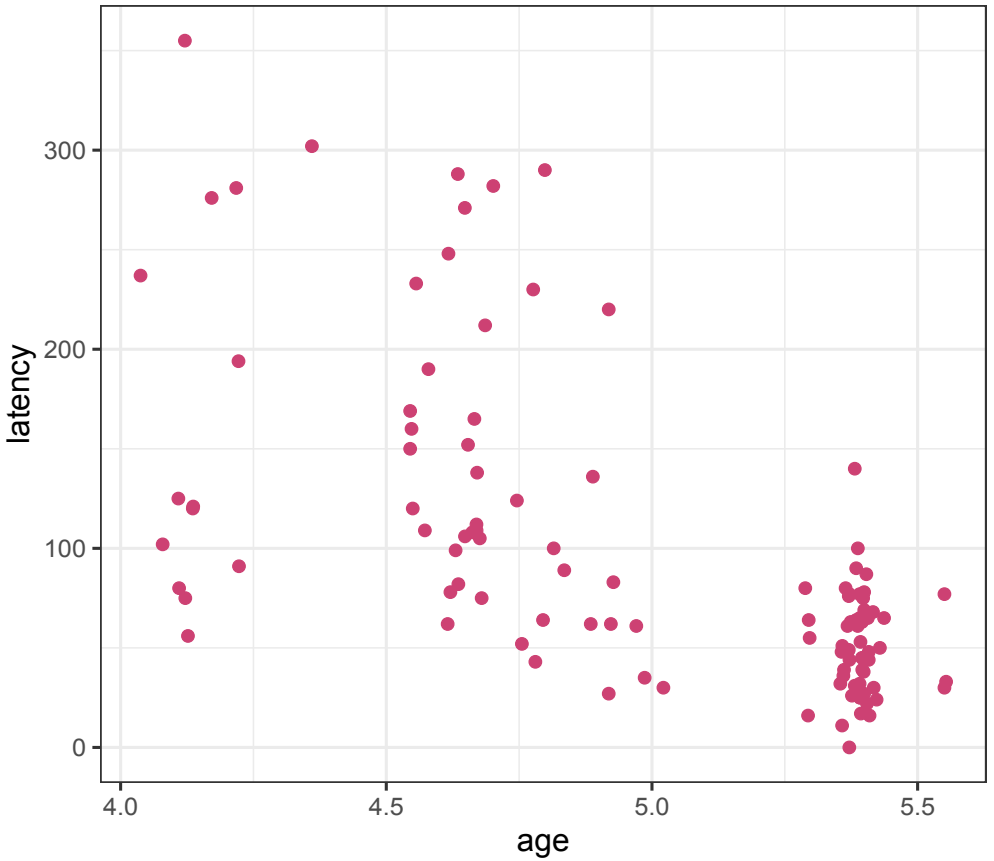
To specify a model using parsnip

```
decision_tree() %>%
  set_mode("regression")
```

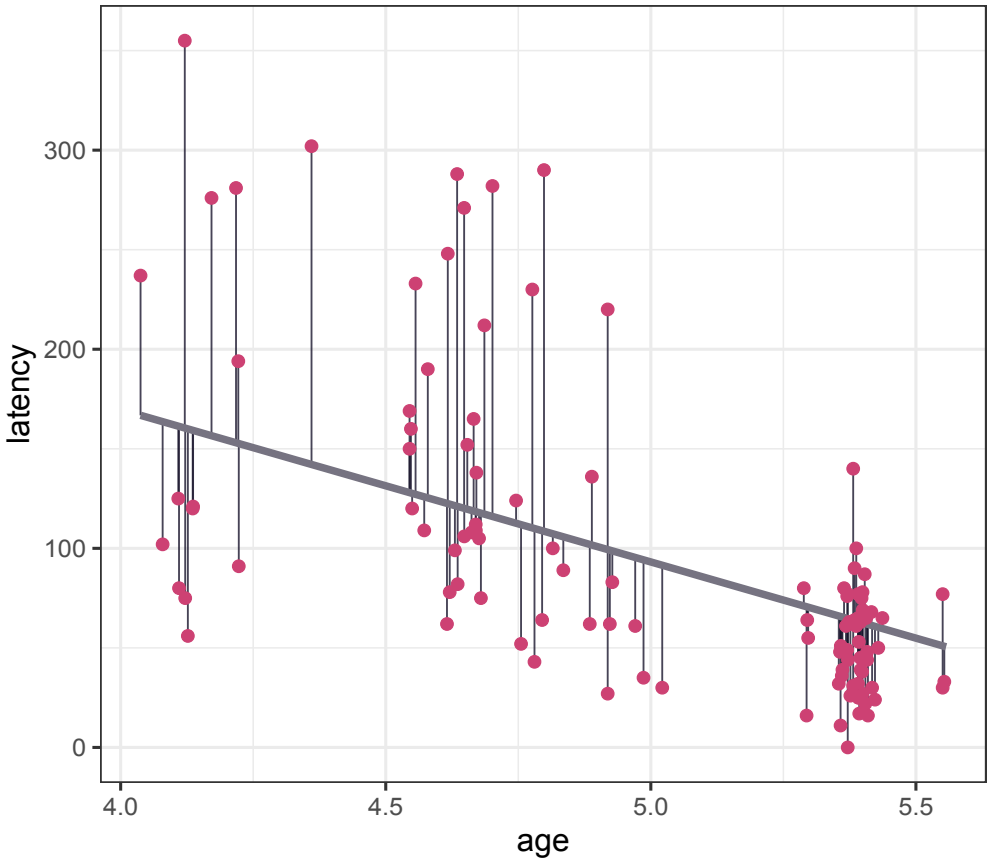
```
#> Decision Tree Model Specification (regression)
#>
#> Computational engine: rpart
```

All available models are listed at https://www.tidymodels.org/find/p

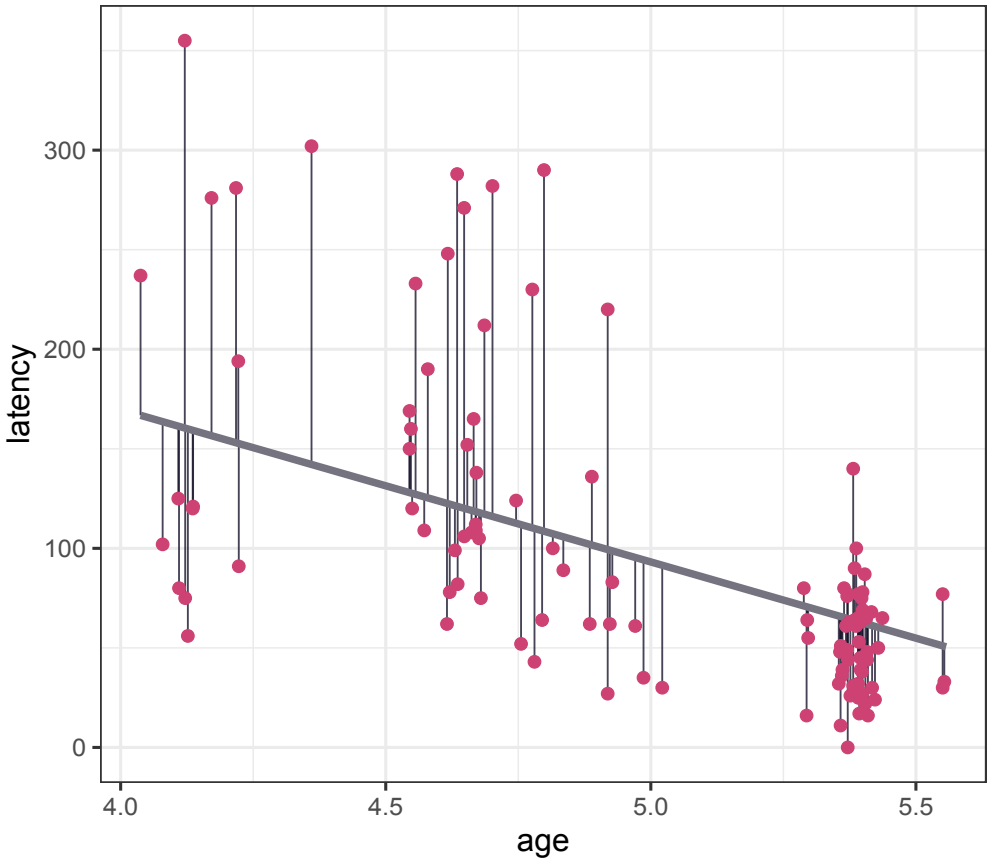
Linear regression



Linear regression



Linear regression



- Outcome modeled as linear combination of predictors:

$$\text{latency} = \beta_0 + \beta_1 \cdot \text{age} +$$

- Find a line that minimizes the mean squared error (MSE)

Comparing base R vs tidymodels

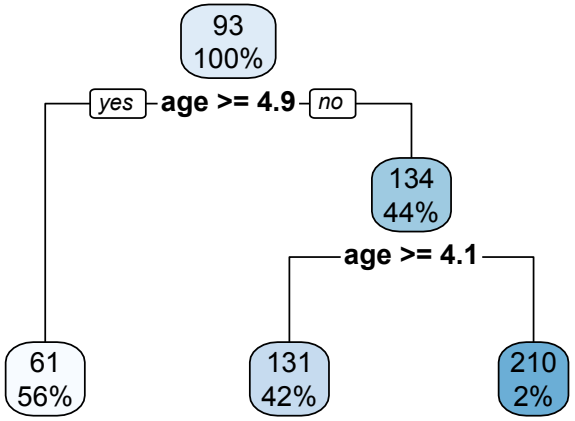
```
lm(latency ~ age, data = frog_train) %>%
  broom::tidy()
```

```
#> # A tibble: 2 × 5
#>   term        estimate std.error statistic  p.value
#>   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
#> 1 (Intercept)    476.      31.9       14.9 2.76e-41
#> 2 age            -76.5      6.34     -12.1 2.98e-29
```

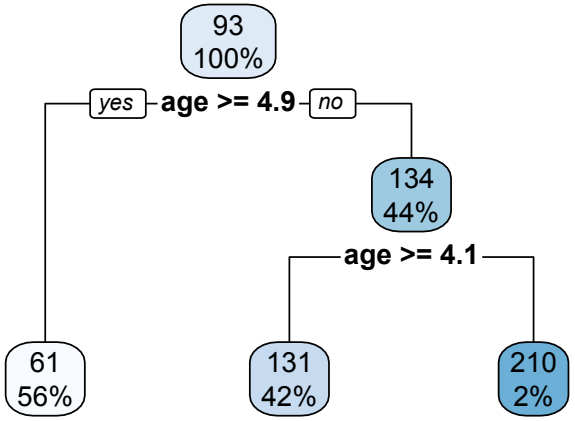
```
linear_reg() %>%
  set_engine('lm') %>%
  set_mode('regression') %>%
  fit(latency ~ age, data = frog_train) %>%
  broom::tidy()
```

```
#> # A tibble: 2 × 5
#>   term        estimate std.error statistic  p.value
#>   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
#> 1 (Intercept)    476.      31.9       14.9 2.76e-41
#> 2 age            -76.5      6.34     -12.1 2.98e-29
```

Decision trees

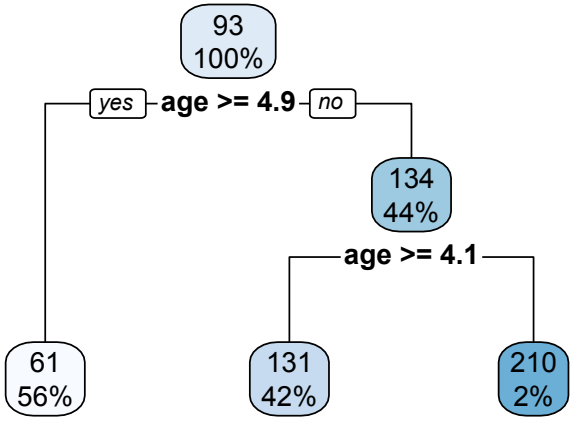


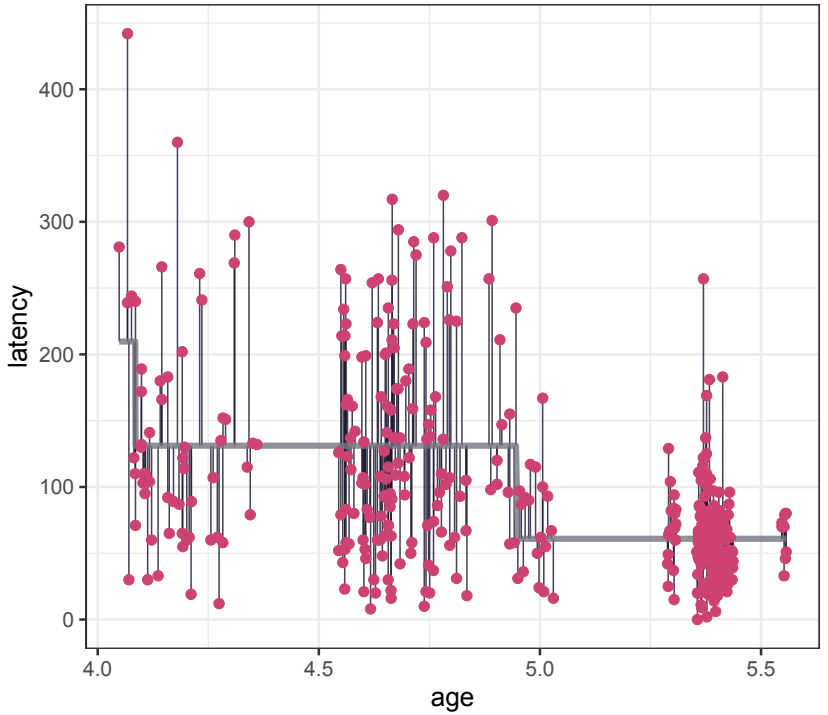
Decision trees



- Series of splits or if/then statements based on predictors
- First the tree *grows* until some condition is met (maximum depth, no more data)
- Then the tree is *pruned* to reduce its complexity

Decision trees





Comparing base R vs tidymodels

```
rpart(latency ~ age,
      data=frog_train,
      control=rpart.control(cp=0.015))
```

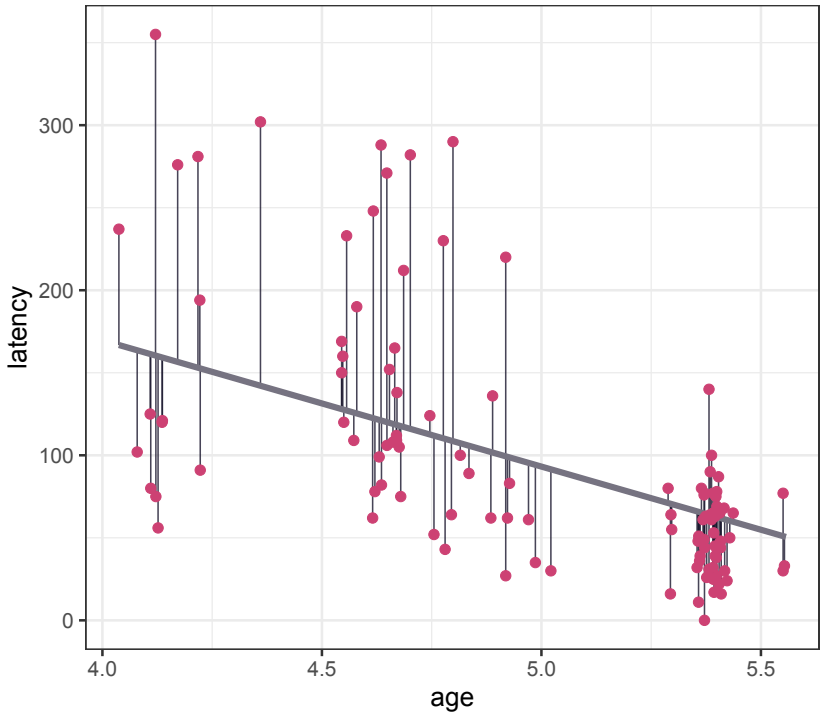
```
#> n= 456
#>
#> node), split, n, deviance, yval
#>       * denotes terminal node
#>
#> 1) root 456 2197966.0  92.90351
#>   2) age>=4.947975 256  252347.4  60.89844 *
#>   3) age< 4.947975 200 1347741.0 133.87000
#>     6) age>=4.085127 193 1195008.0 131.11920 *
#>     7) age< 4.085127 7  111005.4 209.71430 *
```

```
decision_tree(cost_complexity = 0.015) %>%
  set_engine('rpart') %>%
  set_mode('regression') %>%
  fit(latency ~ age, data = frog_train)
```

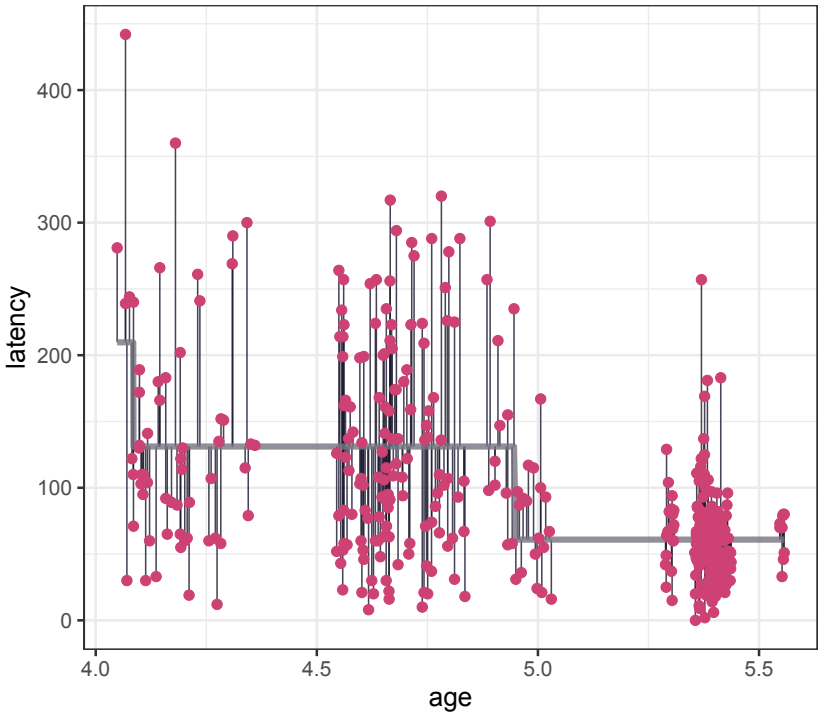
```
#> parsnip model object
#>
#> n= 456
#>
#> node), split, n, deviance, yval
#>       * denotes terminal node
#>
#> 1) root 456 2197966.0  92.90351
#>   2) age>=4.947975 256  252347.4  60.89844 *
#>   3) age< 4.947975 200 1347741.0 133.87000
#>     6) age>=4.085127 193 1195008.0 131.11920 *
#>     7) age< 4.085127 7  111005.4 209.71430 *
```

All models are wrong, but some are useful!

Linear regression

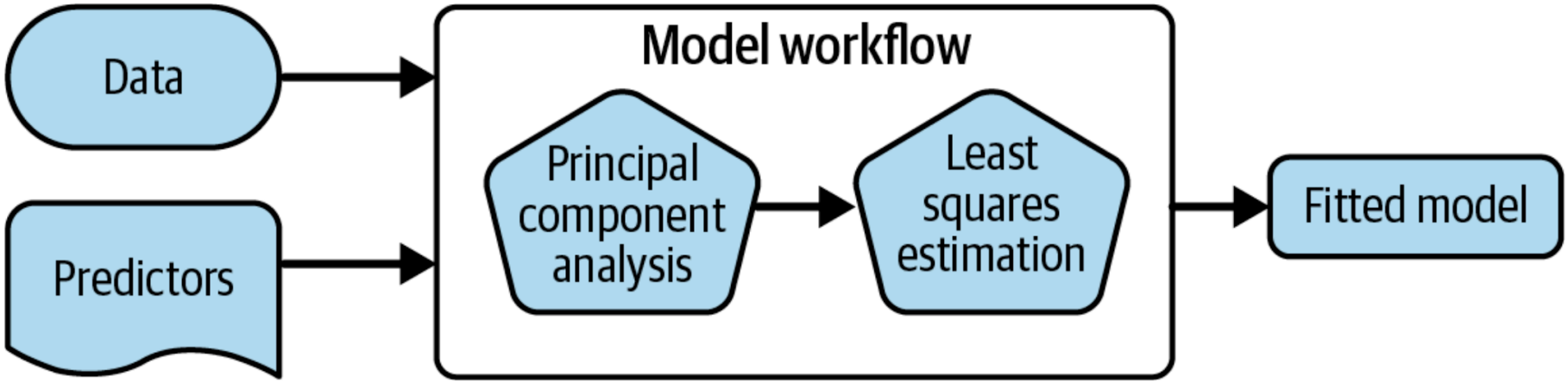


Decision trees

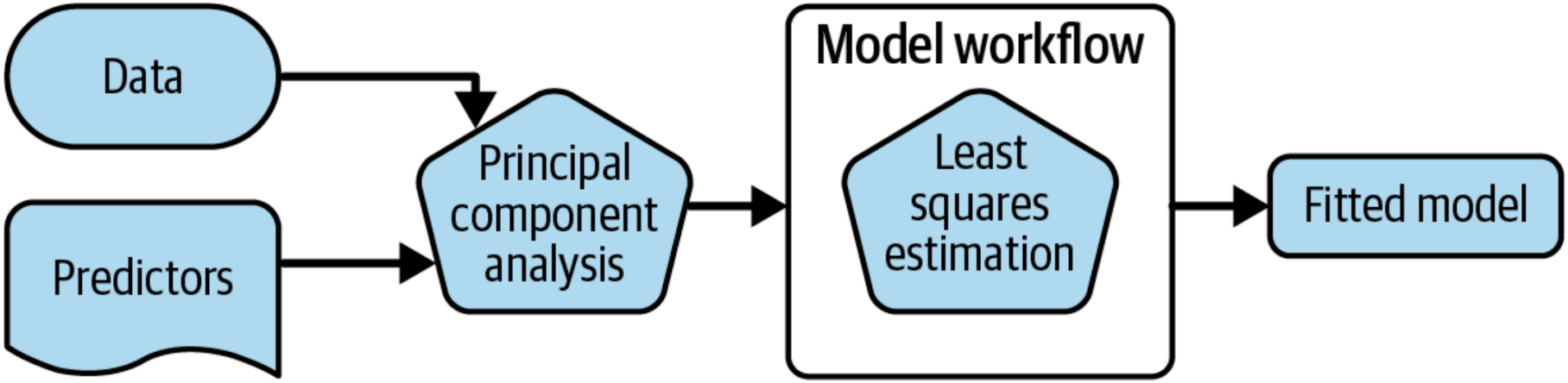


A model workflow

Workflows bind preprocessors and models



What is wrong with this?



Why a `workflow()`?

- Workflows handle new data better than base R tools in terms of new factor levels
- You can use other preprocessors besides formulas (more on feature engineering tomorrow!)
- They can help organize your work when working with multiple models
- Most importantly, a workflow captures the entire modeling process: `fit()` and `predict()` apply to the preprocessing steps in addition to the actual model fit

A model workflow

```
tree_spec <-
  decision_tree() %>%
  set_mode("regression")

tree_spec %>%
  fit(latency ~ ., data = frog_train)
```

```
#> parsnip model object
#>
#> n= 456
#>
#> node), split, n, deviance, yval
#>       * denotes terminal node
#>
#>  1) root 456 2197966.00  92.90351
#>    2) age>=4.947975 256  252347.40  60.89844
#>      4) treatment=control 131   91424.06  48.42748 *
#>      5) treatment=gentamicin 125  119197.90  73.96800 *
#>    3) age< 4.947975 200 1347741.00 133.87000
#>      6) treatment=control 140  986790.70 118.25710
#>       12) reflex=mid,full 129  754363.70 111.56590 *
#>       13) reflex=low 11  158918.20 196.72730 *
#>      7) treatment=gentamicin 60  247194.60 170.30000
#>       14) age< 4.664439 30  102190.20 147.83330
#>         28) age>=4.566638 22   53953.86 129.77270 *
#>         29) age< 4.566638 8   21326.00 197.50000 *
#>       15) age>=4.664439 30  114719.40 192.76670 *
```

A model workflow

```
tree_spec <-
  decision_tree() %>%
  set_mode("regression")

workflow() %>%
  add_formula(latency ~ .) %>%
  add_model(tree_spec) %>%
  fit(data = frog_train)
```

```
#> == Workflow [trained] ==========================================
#> Preprocessor: Formula
#> Model: decision_tree()
#>
#> -- Preprocessor ----------------------------------------------
#> latency ~ .
#>
#> -- Model ----------------------------------------------------
#> n= 456
#>
#> node), split, n, deviance, yval
#>       * denotes terminal node
#>
#>  1) root 456 2197966.00  92.90351
#>    2) age>=4.947975 256  252347.40  60.89844
#>      4) treatment=control 131   91424.06  48.42748 *
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#>      7) treatment=gentamicin 60  247194.60 170.30000
#>       14) age< 4.664439 30  102190.20 147.83330
```

A model workflow

```
tree_spec <-
  decision_tree() %>%
  set_mode("regression")

workflow(latency ~ ., tree_spec) %>%
  fit(data = frog_train)
```

```
#> == Workflow [trained] ==========================================
#> Preprocessor: Formula
#> Model: decision_tree()
#>
#> -- Preprocessor ----------------------------------------------------
#> latency ~ .
#>
#> -- Model ----------------------------------------------------------
#> n= 456
#>
#> node), split, n, deviance, yval
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#>       14) age< 4.664439 30  102190.20 147.83330
```

Predict with your model

How do you use your new `tree_fit` model?

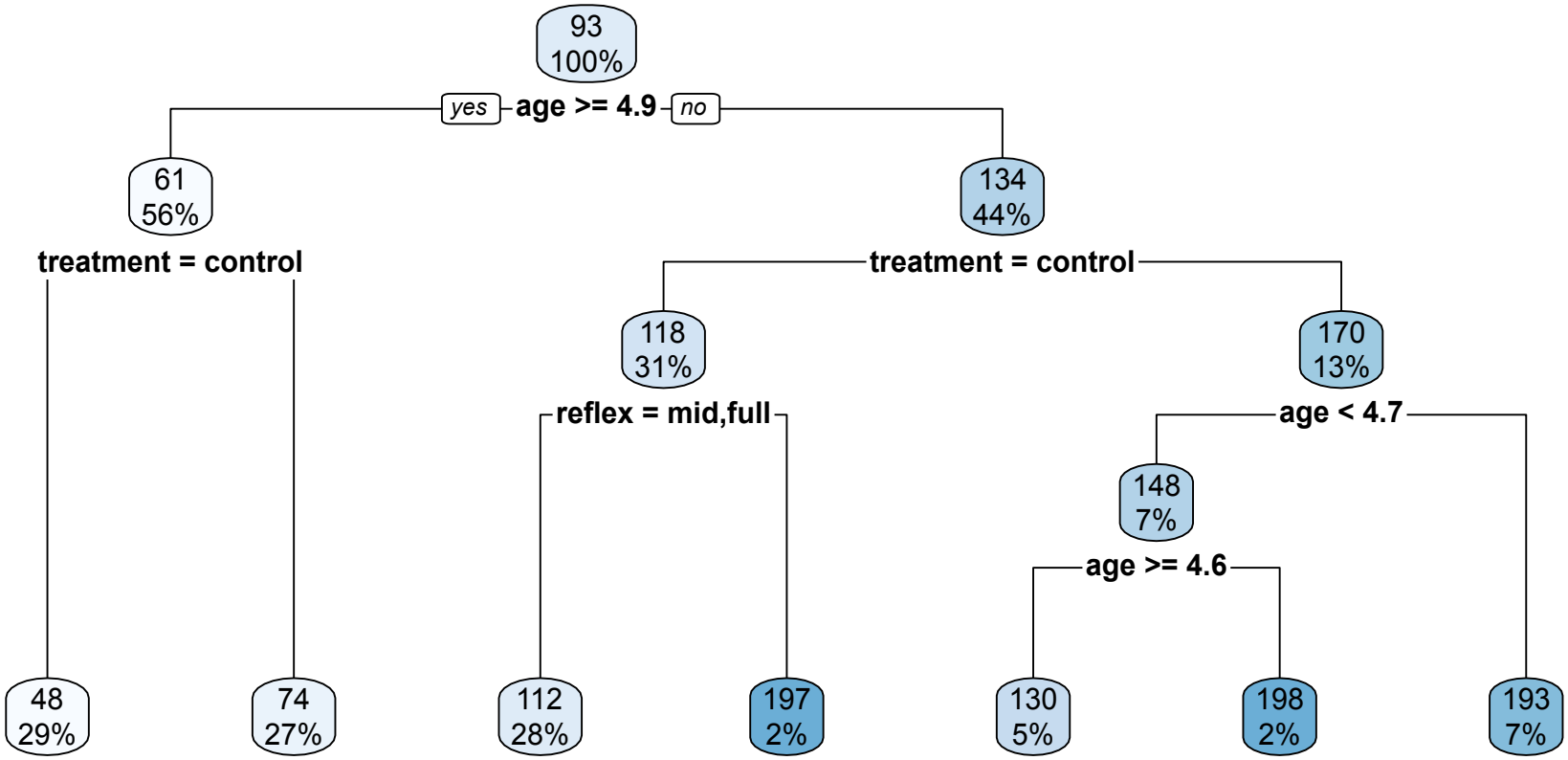
```
tree_spec <-
  decision_tree() %>%
  set_mode("regression")

tree_fit <-
  workflow(latency ~ ., tree_spec) %>%
  fit(data = frog_train)
```

The tidymodels prediction guarantee!

- The predictions will always be inside a **tibble**
- The column names and types are **unsurprising** and **predictable**
- The number of rows in `new_data` and the output **are the same**

Understand your model

How do you **understand** your new `tree_fit` model?



Understand your model

How do you **understand** your new `tree_fit` model?

```
library(rpart.plot)
tree_fit %>%
  extract_fit_engine() %>%
  rpart.plot(roundint = FALSE)
```

You can `extract_*()` several components of your fitted workflow.

Understand your model

How do you **understand** your new `tree_fit` model?

You can use your fitted workflow for model and/or prediction explanations:

- overall variable importance, such as with the vip package
- flexible model explainers, such as with the DALEXtra package

Learn more at https://www.tmwr.org/explain.html