13 Grid search

In Chapter 12 we demonstrated how users can mark or tag arguments in preprocessing recipes and/or model specifications for optimization using the `tune()` function. Once we know what to optimize, it's time to address the question of how to optimize the parameters. This chapter describes **grid search** methods that specify the possible values of the parameters *a priori*. (Chapter 14 will continue the discussion by describing iterative search methods.)

Let's start by describing two main approaches for assembling a grid.

13.1 REGULAR AND NON-REGULAR GRIDS

There are two main types of grids. The first is a regular grid where each parameter has a corresponding set of possible values. A regular grid combines these factorially, i.e., by using all combinations of the sets. Alternatively, a non-regular grid is one where the parameter combinations are not formed from a small set of points.

Before considering each type, let's consider an example model: the multilayer perceptron model (a.k.a. single layer artificial neural network). The parameters marked for tuning are:

- the number of hidden units,
- the number of fitting epochs/iterations in model training, and
- the amount of weight decay penalization.

> Historically, the number of epochs was determined by early stopping; a separate validation set determined the length of training based on the error rate, since re-predicting the training set led to overfitting. In our case, the use of a weight decay penalty should prohibit overfitting, and there is little harm in tuning the penalty and the number of epochs.

Using **parsnip**, the specification for a classification model fit using the **nnet** package is:

```
library(tidymodels)
tidymodels_prefer()

mlp_spec <-
  mlp(hidden_units = tune(), penalty = tune(), epochs = tune()) %>%
  set_engine("nnet", trace = 0) %>%
  set_mode("classification")
```

The argument `trace = 0` prevents extra logging of the training process. As shown in Section 12.5, the `parameters()` function can extract the set of arguments with unknown values and sets their **dials** objects:

```
mlp_param <- parameters(mlp_spec)
mlp_param %>% pull_dials_object("hidden_units")
#> # Hidden Units (quantitative)
#> Range: [1, 10]
mlp_param %>% pull_dials_object("penalty")
#> Amount of Regularization (quantitative)
#> Transformer:  log-10
#> Range (transformed scale): [-10, 0]
mlp_param %>% pull_dials_object("epochs")
#> # Epochs (quantitative)
#> Range: [10, 1000]
```

This output indicates that the parameter objects are complete and prints their default ranges. These values will be used to demonstrate how to create different types of parameter grids.

REGULAR GRIDS

Regular grids are combinations of separate sets of parameter values. First, the user creates a distinct set of values for each parameter. The number of possible values need not be the same for each parameter. The **tidyr** function `crossing()` is one way to create a regular grid:

```
crossing(
  hidden_units = 1:3,
  penalty = c(0.0, 0.1),
  epochs = c(100, 200)
)
#> # A tibble: 12 × 3
#>   hidden_units penalty epochs
#>          <int>   <dbl>  <dbl>
#> 1            1     0      100
#> 2            1     0      200
#> 3            1     0.1    100
#> 4            1     0.1    200
#> 5            2     0      100
#> 6            2     0      200
#> # … with 6 more rows
```

The parameter object knows the ranges of the parameters. The **dials** package contains a set of `grid_*()` functions that take the parameter object as input to produce different types of grids. For example:

```
grid_regular(mlp_param, levels = 2)
#> # A tibble: 8 × 3
#>   hidden_units      penalty epochs
#>          <int>        <dbl>  <int>
#> 1            1 0.0000000001     10
#> 2           10 0.0000000001     10
#> 3            1 1                10
#> 4           10 1                10
#> 5            1 0.0000000001   1000
#> 6           10 0.0000000001   1000
#> # … with 2 more rows
```

The `levels` argument is the number of levels *per parameter* to create. It can also take a named vector of values:

```
mlp_param %>%
  grid_regular(levels = c(hidden_units = 3, penalty = 2, epochs = 2))
#> # A tibble: 12 × 3
#>   hidden_units      penalty epochs
#>          <int>        <dbl>  <int>
#> 1            1 0.0000000001     10
#> 2            5 0.0000000001     10
#> 3           10 0.0000000001     10
#> 4            1 1                10
#> 5            5 1                10
#> 6           10 1                10
#> # … with 6 more rows
```

There are techniques for creating regular grids that do not use all possible values of each parameter set. These *fractional factorial designs* (Box, Hunter, and Hunter 2005) could also be used. To learn more, consult the CRAN Task View for experimental design[18].

> Regular grids can be computationally expensive to use, especially when there are a medium-to-large number of tuning parameters. This is true for many models but not all. As discussed in Section 13.5 below, there are many models whose tuning time *decreases* with a regular grid!

One advantage to using a regular grid is that the relationships and patterns between the tuning parameters and the model metrics are easily understood. The factorial nature of these designs allows for examination of each parameter separately with little confounding between parameters.

IRREGULAR GRIDS

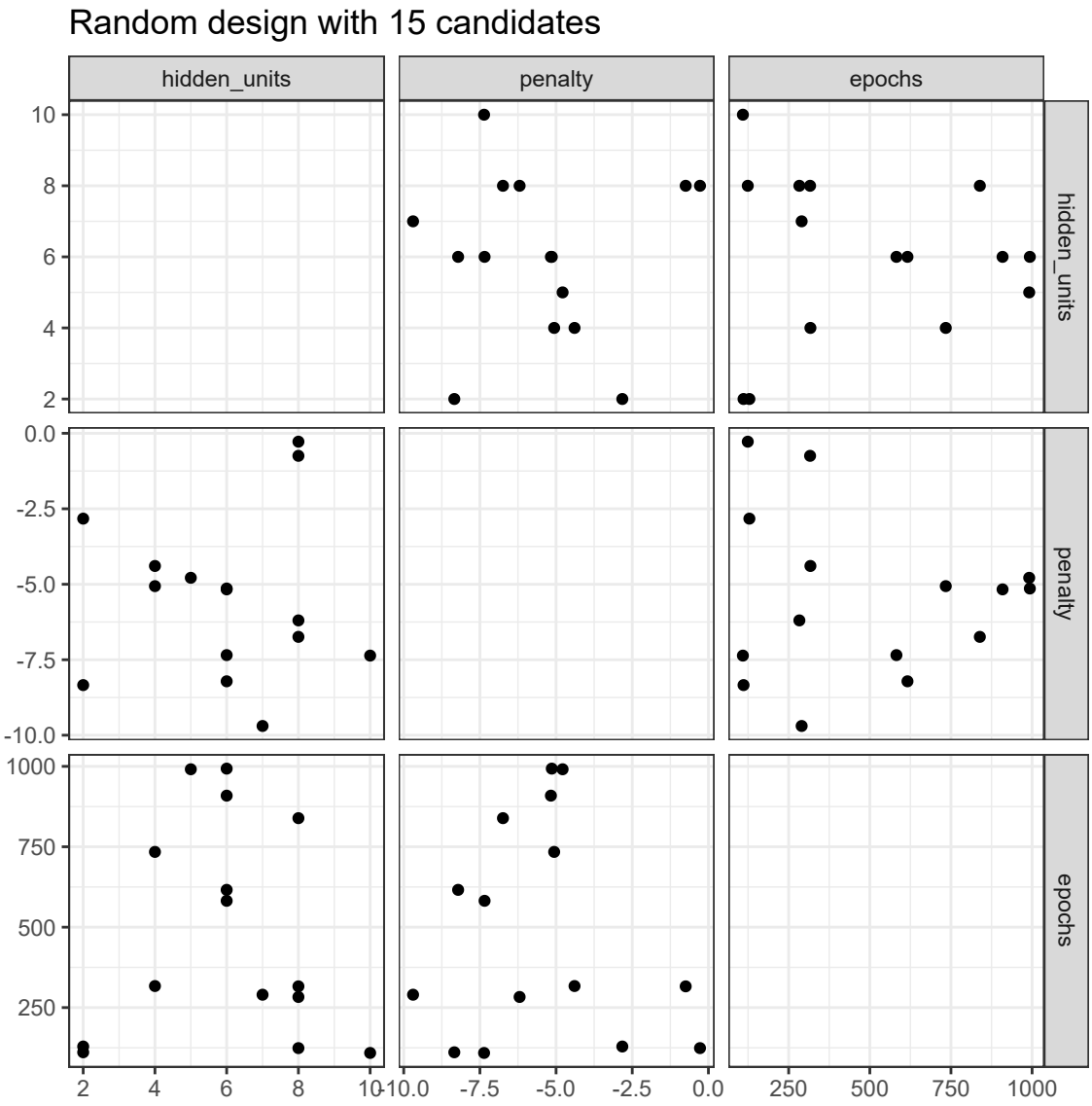
There are several options for creating non-regular grids. The first is to use random sampling across the range of parameters. The `grid_random()` function generates independent uniform random numbers across the parameter ranges. If the parameter object has an associated transformation (such as we have for `penalty`), the random numbers are generated on the transformed scale. For example:

```
set.seed(10)
mlp_param %>%
  grid_random(size = 1000) %>% # 'size' is the number of combinations
  summary()
#>   hidden_units      penalty           epochs
#>  Min.   : 1.00   Min.   :0.0000   Min.   :  10
#>  1st Qu.: 3.00   1st Qu.:0.0000   1st Qu.: 259
#>  Median : 6.00   Median :0.0000   Median : 480
#>  Mean   : 5.58   Mean   :0.0432   Mean   : 496
#>  3rd Qu.: 8.00   3rd Qu.:0.0050   3rd Qu.: 738
#>  Max.   :10.00   Max.   :0.9932   Max.   :1000
```

For `penalty`, the random numbers are uniform on the log (base 10) scale but the values in the grid are in the natural units.

The issue with random grids is that, with small-to-medium grids, random values can result in overlapping parameter combinations. Also, the random grid needs to cover the whole parameter space but the likelihood of good coverage increases with the number of grid values. Even for a sample of 15 candidate points, this plot shows some overlap between points for our example multilayer perceptron:

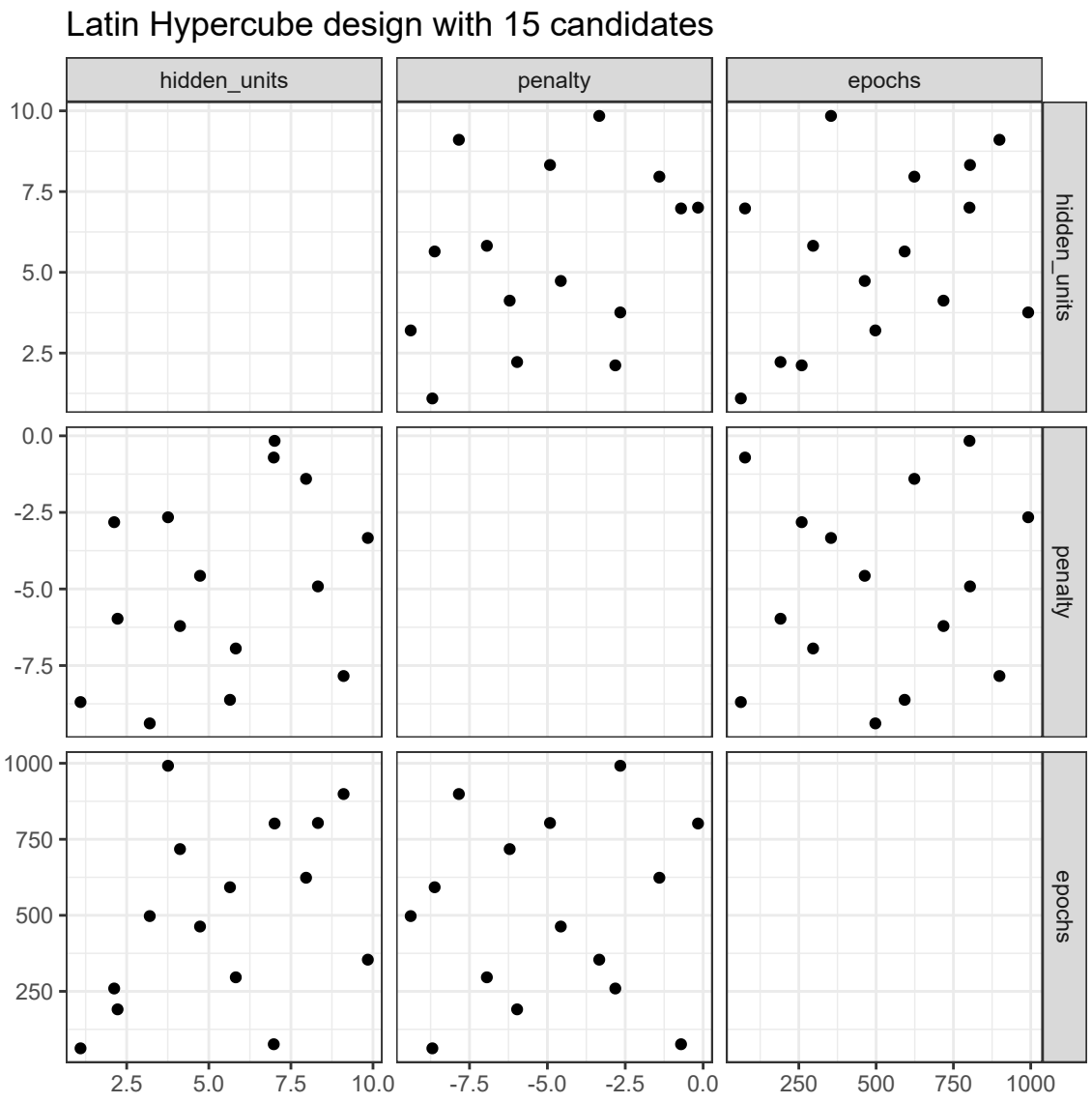
```
library(ggforce)
set.seed(200)
mlp_param %>%
  # The 'original = FALSE' option keeps penalty in log10 units
  grid_random(size = 15, original = FALSE) %>%
  ggplot(aes(x = .panel_x, y = .panel_y)) +
  geom_point() +
  geom_blank() +
  facet_matrix(vars(hidden_units, penalty, epochs), layer.diag = 2) +
  labs(title = "Random design with 15 candidates")
```



A much better approach is to use a set of experimental designs called *space-filling designs*. While different design methods have slightly different goals, they generally find a configuration of points that cover the parameter space with the smallest chance of overlapping or redundant values. Examples of such designs are Latin hypercubes (McKay, Beckman, and Conover 1979), maximum entropy designs (Shewry and Wynn 1987), maximum projection designs (Joseph, Gul, and Ba 2015), and others. See Santner et al. (2003) for an overview.

The **dials** package contains functions for Latin hypercube and maximum entropy designs. As with `grid_random()`, the primary inputs are the number of parameter combinations and a parameter object. Let's compare a random design with a Latin hypercube design for 15 candidate parameter values:

```
set.seed(200)
mlp_param %>%
  grid_latin_hypercube(size = 15, original = FALSE) %>%
  ggplot(aes(x = .panel_x, y = .panel_y)) +
  geom_point() +
  geom_blank() +
  facet_matrix(vars(hidden_units, penalty, epochs), layer.diag = 2) +
  labs(title = "Latin Hypercube design with 15 candidates")
```



While not perfect, this design spaces the points further away from one another.

Space-filling designs can be very effective at representing the parameter space. The default design used by the **tune** package is the maximum entropy design. These tend to produce grids that cover the candidate space well and drastically increase the chances of finding good results.

13.2 EVALUATING THE GRID

To choose the best tuning parameter combination, each candidate set is assessed using data that were not used to train that model. Resampling methods or a single validation set work well for this purpose. The process (and syntax) closely resembles the approach in Section 10.3 that used the `fit_resamples()` function from the **tune** package.

After resampling, the user selects the most appropriate candidate parameter set. It might make sense to choose the empirically best parameter combination or bias the choice towards other aspects of the model fit, such as simplicity.

We use a classification data set to demonstrate model tuning in this and the next chapter. The data come from Hill et al. (2007), who developed an automated microscopy laboratory tool for cancer research. The data consists of 56 imaging measurements on 2019 human breast cancer cells. These predictors represent shape and intensity characteristics of different parts of the cells (e.g., the nucleus, the cell boundary, etc.). There is a high degree of correlation between the predictors. For example, there are several different predictors that measure the size and shape of the nucleus and cell boundary. Also, individually, many predictors have skewed distributions.

Each cell belongs to one of two classes. Since this is part of an automated lab test, the focus was on prediction capability rather than inference.

The data are included in the **modeldata** package. Let's remove one column not needed for analysis (`case`).

```
library(tidymodels)
data(cells)
cells <- cells %>% select(-case)
```

Given the dimensions of the data, we can compute performance metrics using 10-fold cross-validation.

```
set.seed(33)
cell_folds <- vfold_cv(cells)
```

Because of the high degree of correlation between predictors, it makes sense to use PCA feature extraction to decorrelate the predictors. The following recipe contains steps to transform the predictors to increase symmetry, normalize them to be on the same scale, then conduct feature extraction. The number of PCA components to retain is also tuned, along with the model parameters.

> While the resulting PCA components are technically on the same scale, the lower-rank components tend to have a wider range than the higher-rank components. For this reason, we normalize again to coerce the predictors to have the same mean and variance.

Many of the predictors have skewed distributions. Since PCA is variance based, extreme values can have a detrimental effect on these calculations. To counter this, a recipe step estimates a Yeo-Johnson transformation for each predictor (Yeo and Johnson 2000). While originally intended as a transformation of the *outcome*, it can also be used to estimate transformations that encourage more symmetric distributions. This step occurs in the recipe just prior to the initial normalization.

```
mlp_rec <-
  recipe(class ~ ., data = cells) %>%
  step_YeoJohnson(all_numeric_predictors()) %>%
  step_normalize(all_numeric_predictors()) %>%
  step_pca(all_numeric_predictors(), num_comp = tune()) %>%
  step_normalize(all_numeric_predictors())

mlp_wflow <-
  workflow() %>%
  add_model(mlp_spec) %>%
  add_recipe(mlp_rec)
```

Let's create a parameter object to adjust a few of the default ranges. We can change the number of epochs to have a smaller range (50 to 200 epochs). Also, the default range for `num_comp()` defaults to a very narrow range (one to four components); we can increase the range to 40 components and set the minimum value to zero.

> In `step_pca()`, using zero PCA components is a shortcut to *skip* the feature extraction. In this way, the original predictors can be directly compared to the results that include PCA components.

```
mlp_param <-
  mlp_wflow %>%
  parameters() %>%
  update(
    epochs = epochs(c(50, 200)),
    num_comp = num_comp(c(0, 40))
  )
```

The `tune_grid()` function is the primary function for conducting grid search. Its functionality is very similar to `fit_resamples()` from Section 10.3, although it has additional arguments related to the grid:

- `grid` : An integer or data frame. When an integer is used, the function creates a space-filling design with `grid` number of candidate parameter combinations. If specific parameter combinations exist, the `grid` parameter is used to pass them to the function.

- `param_info` : An *optional* argument for defining the parameter ranges. The argument is most useful when `grid` is an integer.

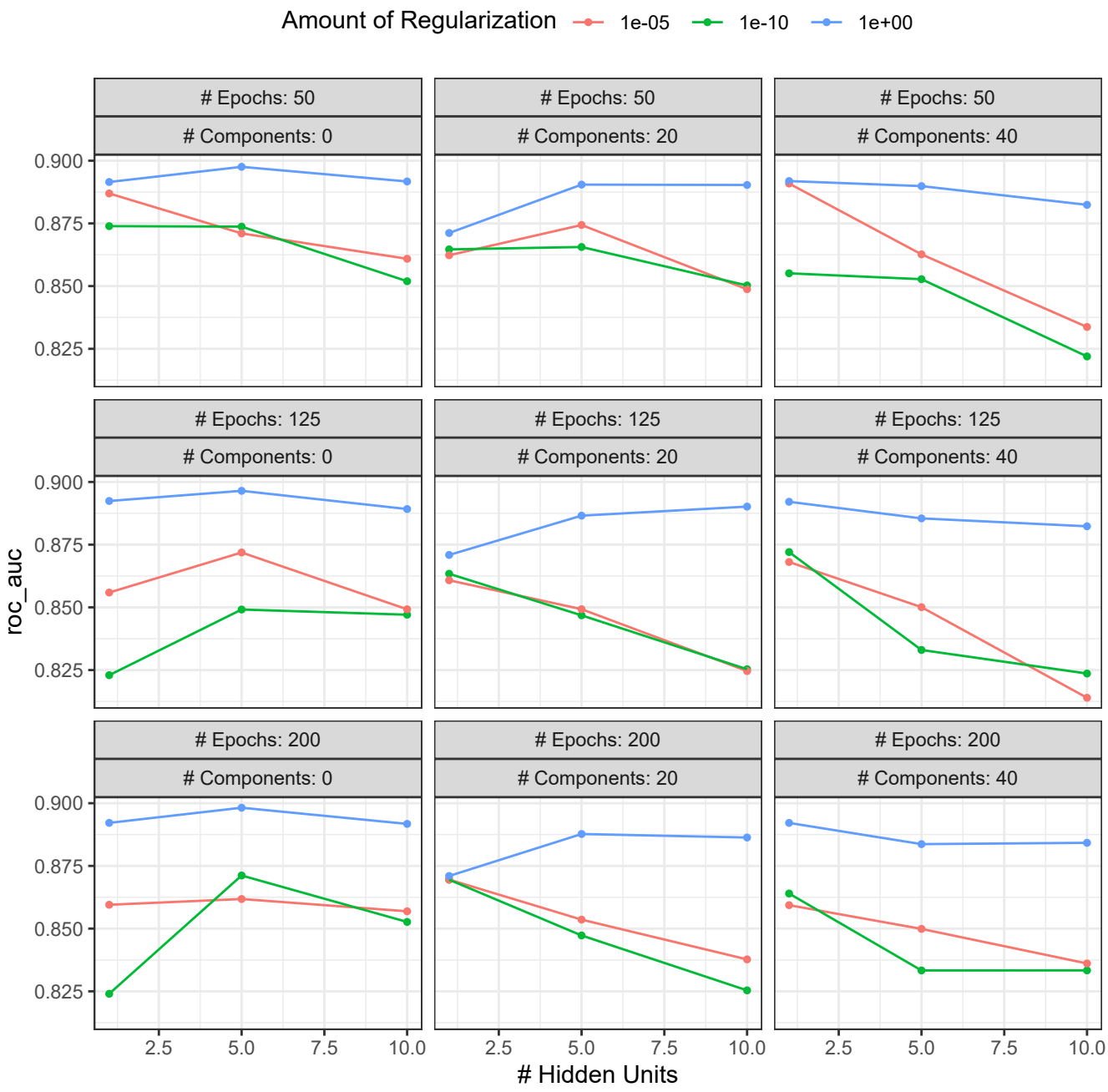
Otherwise, the interface to `tune_grid()` is the same as `fit_resamples()` . The first argument is either a model specification or workflow. When a model is given, the second argument can be either a recipe or formula. The other required argument is an **rsample** resampling object (such as `cell_folds`). The call below also passes a metric set so that the area under the ROC curve is measured during resampling.

To start, let's evaluate a regular grid with three levels across the resamples:

```
roc_res <- metric_set(roc_auc)
set.seed(99)
mlp_reg_tune <-
  mlp_wflow %>%
  tune_grid(
    cell_folds,
    grid = mlp_param %>% grid_regular(levels = 3),
    metrics = roc_res
  )
mlp_reg_tune
#> # Tuning results
#> # 10-fold cross-validation
#> # A tibble: 10 × 4
#>   splits             id     .metrics          .notes
#>   <list>             <chr>  <list>            <list>
#> 1 <split [1817/202]> Fold01 <tibble [81 × 8]> <tibble [0 × 1]>
#> 2 <split [1817/202]> Fold02 <tibble [81 × 8]> <tibble [0 × 1]>
#> 3 <split [1817/202]> Fold03 <tibble [81 × 8]> <tibble [0 × 1]>
#> 4 <split [1817/202]> Fold04 <tibble [81 × 8]> <tibble [0 × 1]>
#> 5 <split [1817/202]> Fold05 <tibble [81 × 8]> <tibble [0 × 1]>
#> 6 <split [1817/202]> Fold06 <tibble [81 × 8]> <tibble [0 × 1]>
#> # … with 4 more rows
```

There are high-level convenience functions to understand the results. First, the `autoplot()` method for regular grids shows the performance profiles across tuning parameters:

```
autoplot(mlp_reg_tune) + theme(legend.position = "top")
```



For these data, the amount of penalization has the largest impact on the area under the ROC curve. The number of epochs doesn't appear to have a pronounced effect on performance. The change in the number of hidden units appears to matter most when the amount of regularization is low (and harms performance). There are several parameter configurations that have roughly equivalent performance, as seen using the function `show_best()` :

```
show_best(mlp_reg_tune) %>% select(-.estimator)
#> # A tibble: 5 × 9
#>   hidden_units penalty epochs num_comp .metric  mean     n std_err .config
#>          <int>   <dbl>  <int>    <int> <chr>   <dbl> <int>   <dbl> <chr>
#> 1            5       1    200        0 roc_auc 0.898    10 0.00697 Preprocessor1_Mo…
#> 2            5       1     50        0 roc_auc 0.898    10 0.00720 Preprocessor1_Mo…
#> 3            5       1    125        0 roc_auc 0.896    10 0.00625 Preprocessor1_Mo…
#> 4            1       1    125        0 roc_auc 0.892    10 0.00693 Preprocessor1_Mo…
#> 5            1       1    200        0 roc_auc 0.892    10 0.00695 Preprocessor1_Mo…
```

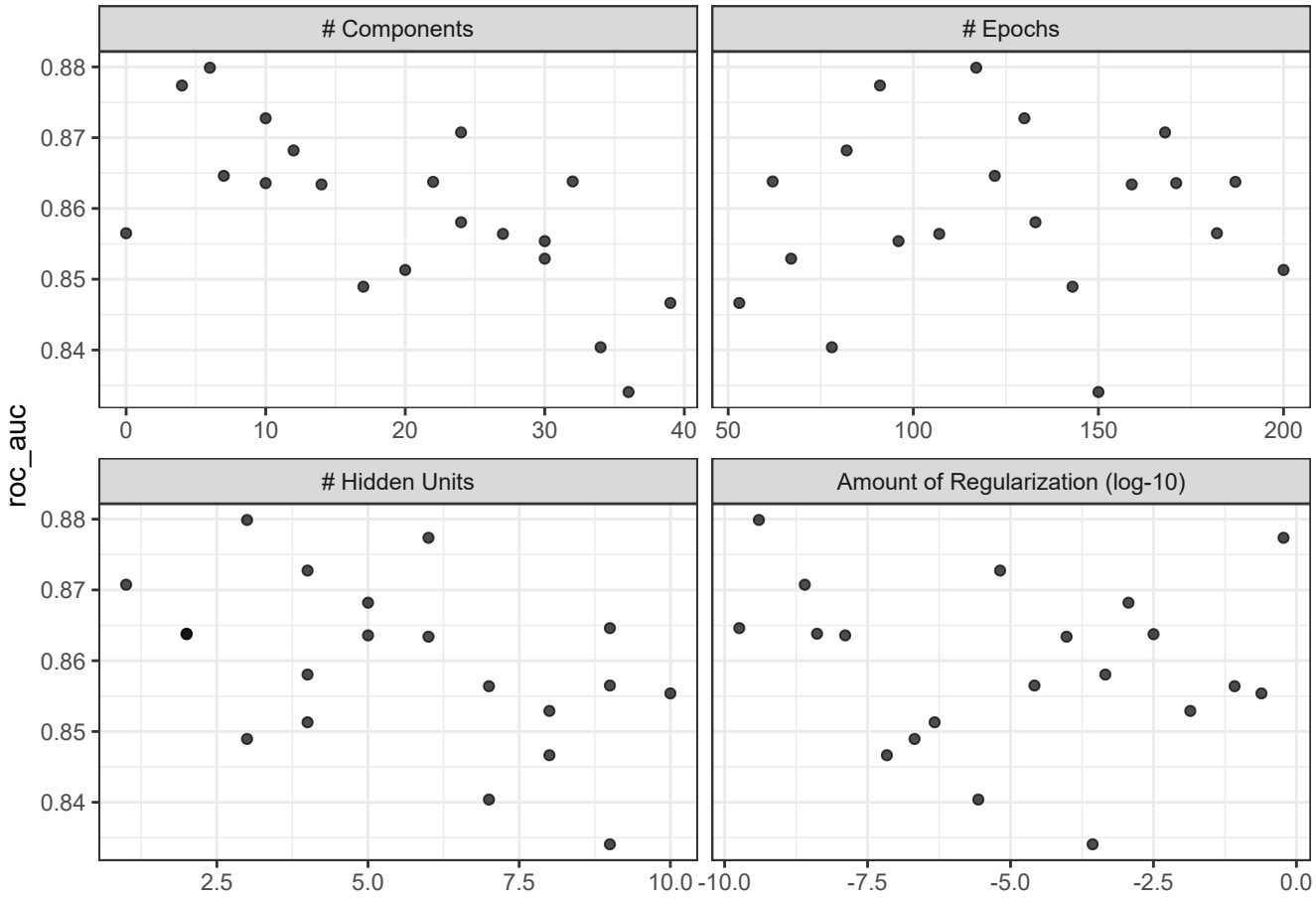
Based on these results, it would make sense to conduct another run of grid search with larger values of the weight decay penalty.

To use a space-filling design, either the `grid` argument can be given an integer or one of the `grid_*()` functions can produce a data frame. To evaluate the same range using a maximum entropy design with 20 candidate values:

```
set.seed(99)
mlp_sfd_tune <-
  mlp_wflow %>%
  tune_grid(
    cell_folds,
    grid = 20,
    # Pass in the parameter object to use the appropriate range:
    param_info = mlp_param,
    metrics = roc_res
  )
mlp_sfd_tune
#> # Tuning results
#> # 10-fold cross-validation
#> # A tibble: 10 × 4
#>   splits             id     .metrics          .notes
#>   <list>             <chr>  <list>            <list>
#> 1 <split [1817/202]> Fold01 <tibble [20 × 8]> <tibble [0 × 1]>
#> 2 <split [1817/202]> Fold02 <tibble [20 × 8]> <tibble [0 × 1]>
#> 3 <split [1817/202]> Fold03 <tibble [20 × 8]> <tibble [0 × 1]>
#> 4 <split [1817/202]> Fold04 <tibble [20 × 8]> <tibble [0 × 1]>
#> 5 <split [1817/202]> Fold05 <tibble [20 × 8]> <tibble [0 × 1]>
#> 6 <split [1817/202]> Fold06 <tibble [20 × 8]> <tibble [0 × 1]>
#> # … with 4 more rows
```

The `autoplot()` method will also work with these designs, although the format of the results will be different:

```
autoplot(mlp_sfd_tune)
```



This *marginal effects plot* shows the relationship of each parameter with the performance metric.

> Care should be taken when examining this plot; since a regular grid is not used, the values of the other tuning parameters can affect each panel.

The penalty parameter appears to result in better performance with *smaller* amounts of weight decay. This is the opposite of the results from the regular grid. Since each point in each panel is shared with the other three tuning parameters, the trends in one panel can be affected by the others. Using a regular grid, each point in each panel is equally averaged over the other parameters. For this reason, the effect of each parameter is better isolated with regular grids.

As with the regular grid, `show_best()` can report on the numerically best results:

```
show_best(mlp_sfd_tune) %>% select(-.estimator)
#> # A tibble: 5 × 9
#>   hidden_units  penalty epochs num_comp .metric  mean     n std_err .config
#>          <int>    <dbl>  <int>    <int> <chr>   <dbl> <int>   <dbl> <chr>
#> 1            3 3.98e-10    117        6 roc_auc 0.880    10 0.00840 Preprocessor13_…
#> 2            6 5.95e- 1     91        4 roc_auc 0.877    10 0.00938 Preprocessor16_…
#> 3            4 6.57e- 6    130       10 roc_auc 0.873    10 0.00539 Preprocessor09_…
#> 4            1 2.52e- 9    168       24 roc_auc 0.871    10 0.00676 Preprocessor12_…
#> 5            5 1.16e- 3     82       12 roc_auc 0.868    10 0.00728 Preprocessor14_…
```

Generally, it is a good idea to evaluate the models over multiple metrics so that different aspects of the model fit are taken into account. Also, it often makes sense to choose a slightly suboptimal parameter combination that is associated with a simpler model. For this model, simplicity corresponds to larger penalty values and/or fewer hidden units.

As with the results from `fit_resamples()`, there is usually no value in retaining the intermediary model fits across the resamples and tuning parameters. However, as before, the `extract` option to `control_grid()` allows the retention of the fitted models and/or recipes. Also, setting the `save_pred` option to `TRUE` retains the assessment set predictions and these can be accessed using `collect_predictions()`.

13.3 FINALIZING THE MODEL

If one of the sets of possible model parameters found via `show_best()` were an attractive final option for these data, we might wish to evaluate how well it does on the test set. However, the results of `tune_grid()` only provide the substrate to choose appropriate tuning parameters. The function *does not fit* a final model.

To do this, a final set of parameter values must be determined. There are two methods to do so:

- manually pick values that appear appropriate or
- use a `select_*()` function.

For example, `select_best()` will choose the parameters with the numerically best results:

```
select_best(mlp_reg_tune, metric = "roc_auc")
#> # A tibble: 1 × 5
#>   hidden_units penalty epochs num_comp .config
#>          <int>   <dbl>  <int>    <int> <chr>
#> 1            5       1    200        0 Preprocessor1_Model26
```

Looking at the results for the regular grid plot, a model with a single hidden unit trained for 125 epochs on the original predictors with a large amount of penalization has performance competitive with this option, and is simpler. This is basically penalized logistic regression! To manually specify these parameters, we can create a tibble with these values and then use a *finalization* function to splice the values back into the workflow:

```
logistic_param <-
  tibble(
    num_comp = 0,
    epochs = 125,
    hidden_units = 1,
    penalty = 1
  )

final_mlp_wflow <-
  mlp_wflow %>%
  finalize_workflow(logistic_param)
final_mlp_wflow
#> == Workflow ====================================================================
#> Preprocessor: Recipe
#> Model: mlp()
#>
#> -- Preprocessor ----------------------------------------------------------------
#> 4 Recipe Steps
#>
#> • step_YeoJohnson()
#> • step_normalize()
#> • step_pca()
#> • step_normalize()
#>
#> -- Model ----------------------------------------------------------------------
#> Single Layer Neural Network Specification (classification)
#>
#> Main Arguments:
#>   hidden_units = 1
#>   penalty = 1
#>   epochs = 125
#>
#> Engine-Specific Arguments:
#>   trace = 0
```

```
#>
#> Computational engine: nnet
```

No more values of `tune()` are included in this finalized workflow. Now the model can be fit to the *entire training set*:

```
final_mlp_fit <-
  final_mlp_wflow %>%
  fit(cells)
```

This object can now be used to make future predictions on new data.

If you did not use a workflow, finalization of a model and/or recipe is done using `finalize_model()` and `finalize_recipe()`.

13.4 TOOLS FOR CREATING TUNING SPECIFICATIONS

The **usemodels** package can take a data frame and model formula, then write out R code for tuning the model. The code also creates an appropriate recipe whose steps depend on the requested model as well as the predictor data.

For example, for the Ames data, `xgboost` modeling code could be created with:

```
library(usemodels)

use_xgboost(Sale_Price ~ Neighborhood + Gr_Liv_Area + Year_Built + Bldg_Type +
              Latitude + Longitude,
            data = ames_train,
            # Add comments explaining some of the code:
            verbose = TRUE)
```

The results are this code:

```
xgboost_recipe <-
  recipe(formula = Sale_Price ~ Neighborhood + Gr_Liv_Area + Year_Built + Bldg_Type +
    Latitude + Longitude, data = ames_train) %>%
  step_novel(all_nominal_predictors()) %>%
  ## This model requires the predictors to be numeric. The most common
  ## method to convert qualitative predictors to numeric is to create
  ## binary indicator variables (aka dummy variables) from these
  ## predictors. However, for this model, binary indicator variables can be
  ## made for each of the levels of the factors (known as 'one-hot
  ## encoding').
  step_dummy(all_nominal_predictors(), one_hot = TRUE) %>%
  step_zv(all_predictors())

xgboost_spec <-
  boost_tree(trees = tune(), min_n = tune(), tree_depth = tune(), learn_rate = tune(),
    loss_reduction = tune(), sample_size = tune()) %>%
  set_mode("regression") %>%
  set_engine("xgboost")

xgboost_workflow <-
  workflow() %>%
  add_recipe(xgboost_recipe) %>%
  add_model(xgboost_spec)

set.seed(69305)
xgboost_tune <-
  tune_grid(xgboost_workflow,
            resamples = stop("add your rsample object"),
            grid = stop("add number of candidate points"))
```

This code is, based on what **usemodels** understands about the data, the minimal preprocessing required. For other models, operations like `step_normalize()` are added to fulfill the basic needs of the model. Notice that it is our responsibility, as the modeling practitioner, to choose what

`resamples` to use for tuning, as well as what kind of `grid`.

> The **usemodels** package can also be used to create model fitting code with no tuning by setting the argument `tune = FALSE`.

13.5 TOOLS FOR EFFICIENT GRID SEARCH

A few different tricks and optimizations are possible to make grid search more computationally efficient. This section describes several techniques.

13.5.1 SUBMODEL OPTIMIZATION

There are types of models where, from a single model fit, multiple tuning parameters can be evaluated without refitting.

For example, partial least squares (PLS) is a supervised version of principal component analysis (Geladi and Kowalski 1986). It creates components that maximize the variation in the predictors (like PCA) but simultaneously tries to maximize the correlation between these predictors and the outcome. One tuning parameter is the number of PLS components to retain. Suppose that a data set with 100 predictors is fit using PLS. The number of possible components to retain can range from one to fifty. However, in many implementations, a single model fit can compute predicted values across many values of `num_comp`. As a result, a PLS model created with 100 components can also make predictions for any `num_comp <= 100`. This saves time since, instead of creating redundant model fits, a single fit can be used to evaluate many *submodels*.

While not all models can exploit this feature, many broadly used ones do:

- Boosting models can typically make predictions across multiple values for the number of boosting iterations.
- Regularization methods, such as the **glmnet** model, can make simultaneous predictions across the amount of regularization used to fit the model.

- Multivariate adaptive regression splines (MARS) adds a set of nonlinear features to linear regression models (Friedman 1991). The number of terms to retain is a tuning parameter and it is computationally fast to make predictions across many values of this parameter from a single model fit.

The **tune** package automatically applies this type of optimization whenever an applicable model is tuned.

For example, if a boosted C5.0 classification model (Kuhn and Johnson 2013) was fit to the cell data, we can tune the number of boosting iterations (`trees`). With all other parameters set at their default values, we can evaluate iterations from 1 to 100 on the same resamples as used previously:

```
c5_spec <-
  boost_tree(trees = tune()) %>%
  set_engine("C5.0") %>%
  set_mode("classification")

set.seed(2)
c5_spec %>%
  tune_grid(
    class ~ .,
    resamples = cell_folds,
    grid = data.frame(trees = 1:100),
    metrics = roc_res
  )
```

Without the submodel optimization, the call to `tune_grid()` used 62.2 minutes to resample 100 submodels. With the optimization, the same call took 100 *seconds* (a speedup of 37-fold). The reduced time is the difference in `tune_grid()` fitting 1000 models versus 10 models.

> Even though we fit the model with and without the submodel prediction trick, this optimization is *automatically* applied by **parsnip**.

13.5.2 PARALLEL PROCESSING

As previously mentioned in Section 10.4, parallel processing is an effective method for decreasing execution time when resampling models. This advantage conveys to model tuning via grid search, although there are additional considerations.

Let's consider two different parallel processing schemes.

When tuning models via grid search, there are two distinct loops: one over resamples and another over the unique tuning parameter combinations. Representing this process with pseudocode:

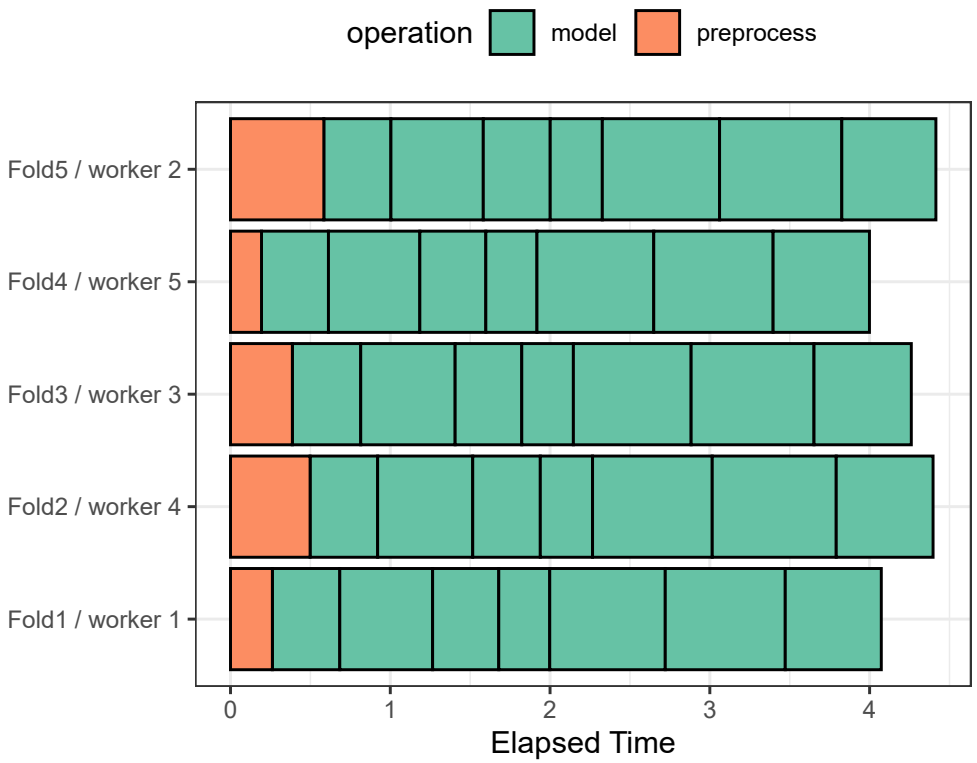
```
1 for (rs in resamples) {
2   # Create analysis and assessment sets
3   # Preprocess data (e.g. formula or recipe)
4   for (mod in configurations) {
5     # Fit model {mod} to the {rs} analysis set
6     # Predict the {rs} assessment set
7   }
8 }
```

By default, the **tune** package only parallelizes over resamples (line 1 above), as opposed to the two loops at lines 1 *and* 4.

This is the optimal scenario when the preprocessing method is expensive. However, there are two potential downsides to this approach:

- It limits the achievable speed-ups when the preprocessing is not expensive.
- The number of parallel workers is limited by the number of resamples. For example, with 10-fold cross-validation you can only use 10 parallel workers even when the computer has more than 10 cores.

To illustrate how the parallel processing works, we'll use a case where there are 7 model tuning parameter values, with 5-fold cross-validation. This visualization shows how the tasks are allocated to the worker processes:



Note that each fold is assigned to its own worker process and, since only model parameters are being tuned, the preprocessing is conducted once per fold/worker. If fewer than 5 worker processes were used, some workers would receive multiple folds.

In the control functions for the `tune_*()` functions, the argument `parallel_over` controls how the process is executed. To use the approach shown above, the argument is `parallel_over = "resamples"` .

Instead of parallel processing the resamples, an alternate scheme combines the loops over resamples and models into a single loop. The pseudocode for this approach is:

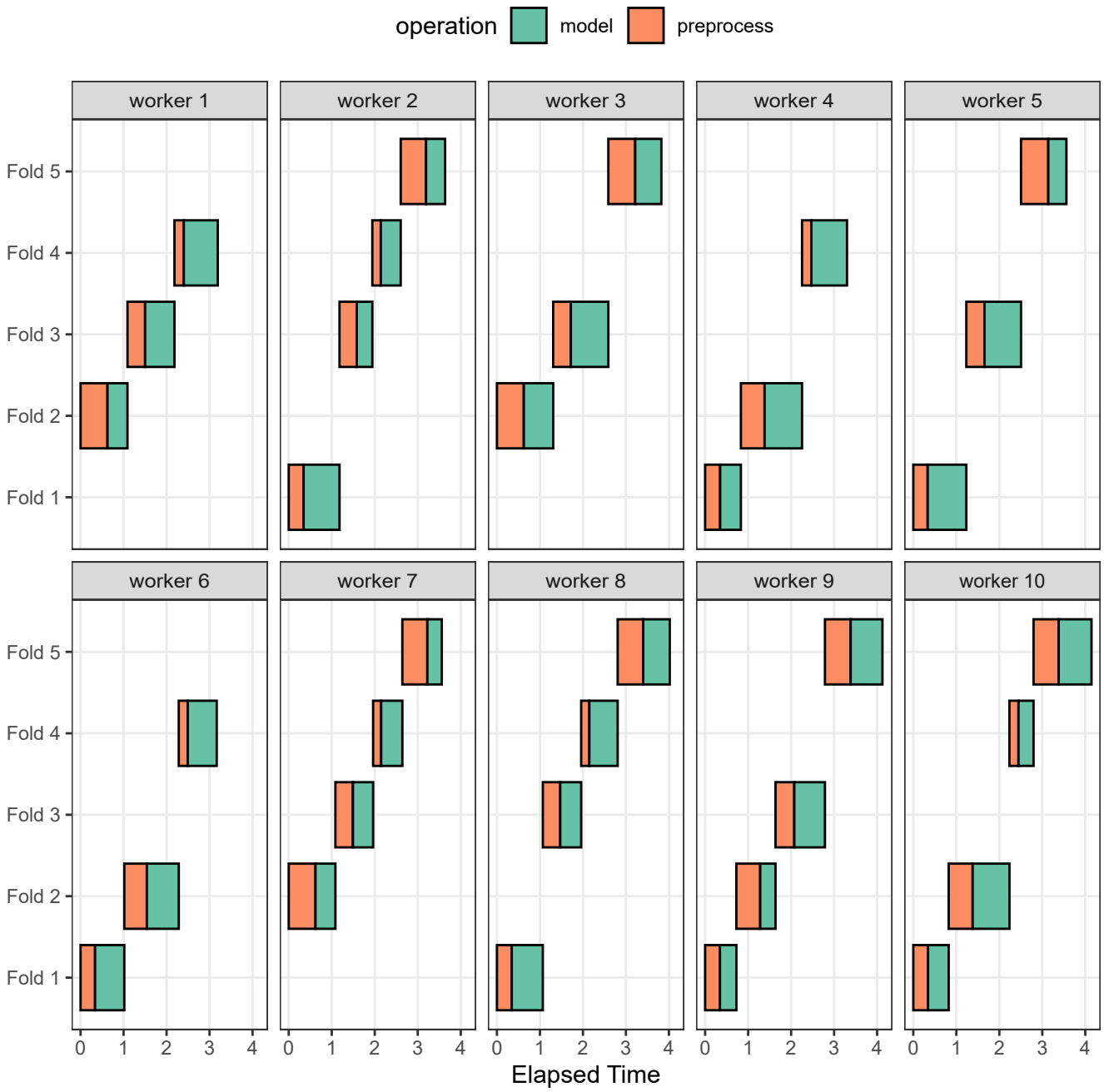
```
all_tasks <- crossing(resamples, configurations)

for (iter in all_tasks) {
  # Create analysis and assessment sets for {iter}
  # Preprocess data (e.g. formula or recipe)
  # Fit model {iter} to the {iter} analysis set
  # Predict the {iter} assessment set
}
```

In this case, parallelization now occurs at line 11. For example, if we use 5-fold cross-validation with M tuning parameter values, the loop is executed over $5 \times M$ iterations. This increases the number of potential workers that can be used. However, the work in lines 12-13 (related to data preprocessing) is *repeated* multiple times. If those steps are expensive, this approach will be inefficient.

In tidymodels, validation sets are treated as a single resample. In these cases, this parallelization scheme would be best.

To illustrate the delegation of tasks to the workers in this scheme, the same example is used but with 10 workers:



Here, each worker process handles multiple folds and the preprocessing is needlessly repeated. For example, for the first fold, the preprocessing was computed 7 times instead of once.

For this scheme, the control function argument is `parallel_over = "everything"` .

13.5.3 BENCHMARKING BOOSTED TREES

As an example, a boosted tree with the **xgboost** engine was tuned for a data set of 4,000 samples, using 5-fold cross-validation and 10 candidate models. These data required some baseline preprocessing that did not require any estimation. The preprocessing was handled three different

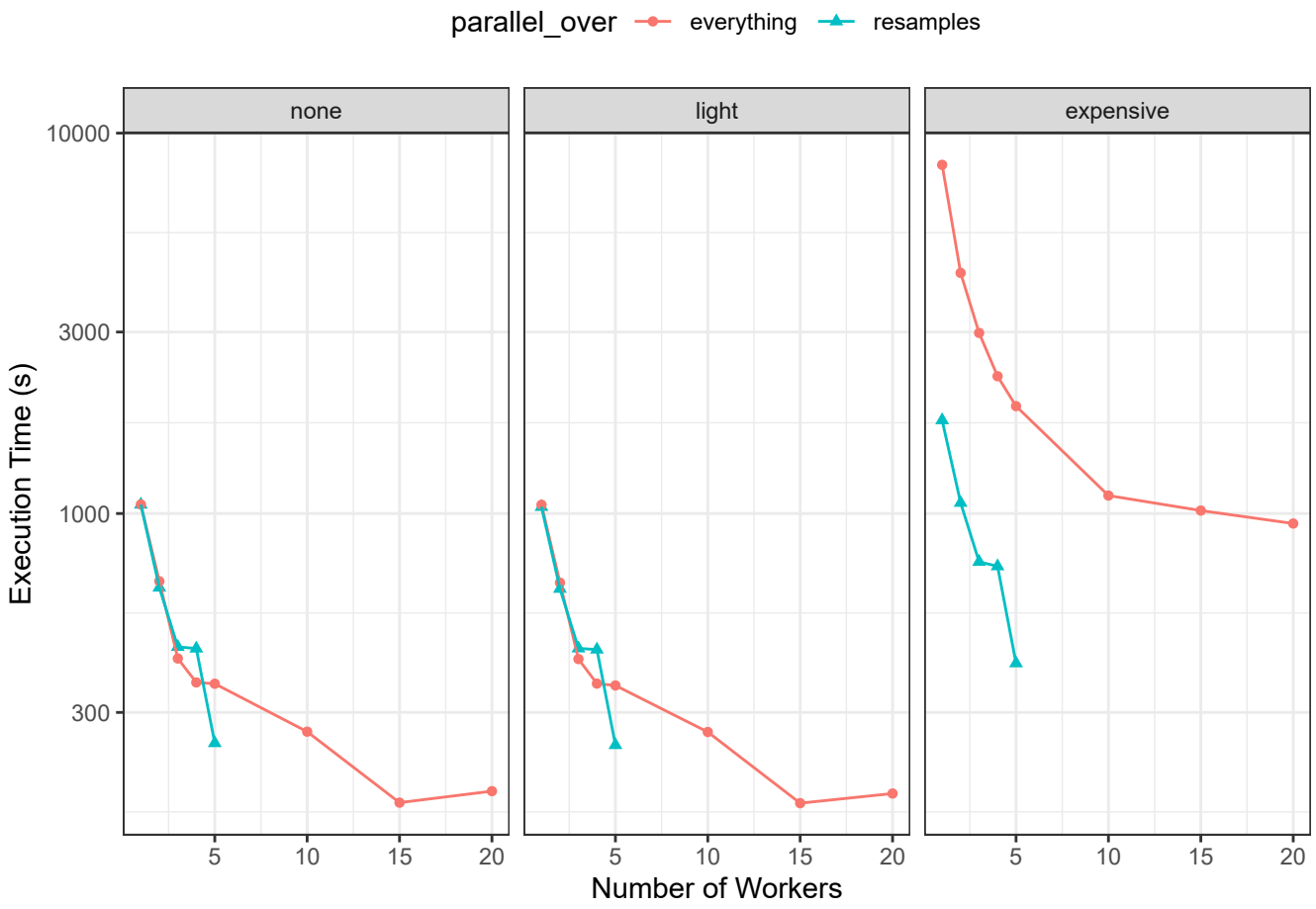
ways:

1. Preprocess the data prior to modeling using a **dplyr** pipeline (labeled as "none" in the plots below).
2. Conduct the same preprocessing via a recipe (shown as "light" preprocessing).
3. With a recipe, add an additional step that has a high computational cost (labeled as "expensive").

The first and second preprocessing options are designed for comparison, to measure the computational cost of the recipe in the second option. The third option measures the cost of performing redundant computations with `parallel_over = "everything"` .

We evaluated this process using variable numbers of worker processes and using the two `parallel_over` options, on a computer with 10 physical cores and 20 virtual cores (via hyper-threading).

First, let's consider the raw execution times:



Since there were only five resamples, the number of cores used when `parallel_over = "resamples"` is limited to five.

Comparing the curves in the first two panels for “none” and “light”:

- There is little difference in the execution times between the panels. This indicates, for these data, there is no real computational penalty for doing the preprocessing steps in a recipe.
- There is some benefit for using `parallel_over = "everything"` with many cores. However, as shown in the figure, the majority of the benefit of parallel processing occurs in the first five workers.

With the expensive preprocessing step, there is a considerable difference in execution times. Using `parallel_over = "everything"` is problematic since, even using all cores, it never achieves the execution time that `parallel_over = "resamples"` attains with just five cores. This is because the costly preprocessing step is unnecessarily repeated in the computational scheme.

We can also view these data in terms of speed-ups:

The best speed-ups, for these data, occur when `parallel_over = "resamples"` and when the computations are expensive. However, in the latter case, remember that the previous analysis indicates that the overall model fits are slower.

What is the benefit of using the submodel optimization method *in conjunction* with parallel processing? The C5.0 classification model shown in Section 13.5.1 was also run in parallel with ten workers. The parallel computations took 13.3 seconds for a speed-up of 7.5-fold (both runs used the submodel optimization trick). Between the submodel optimization trick and parallel processing, there was a **total speed-up of 282-fold** over the most basic grid search code.

> Overall, note that the increased computational savings will vary from model-to-model and are also affected by the size of the grid, the number of resamples, etc. A very computationally efficient model may not benefit as much from parallel processing.

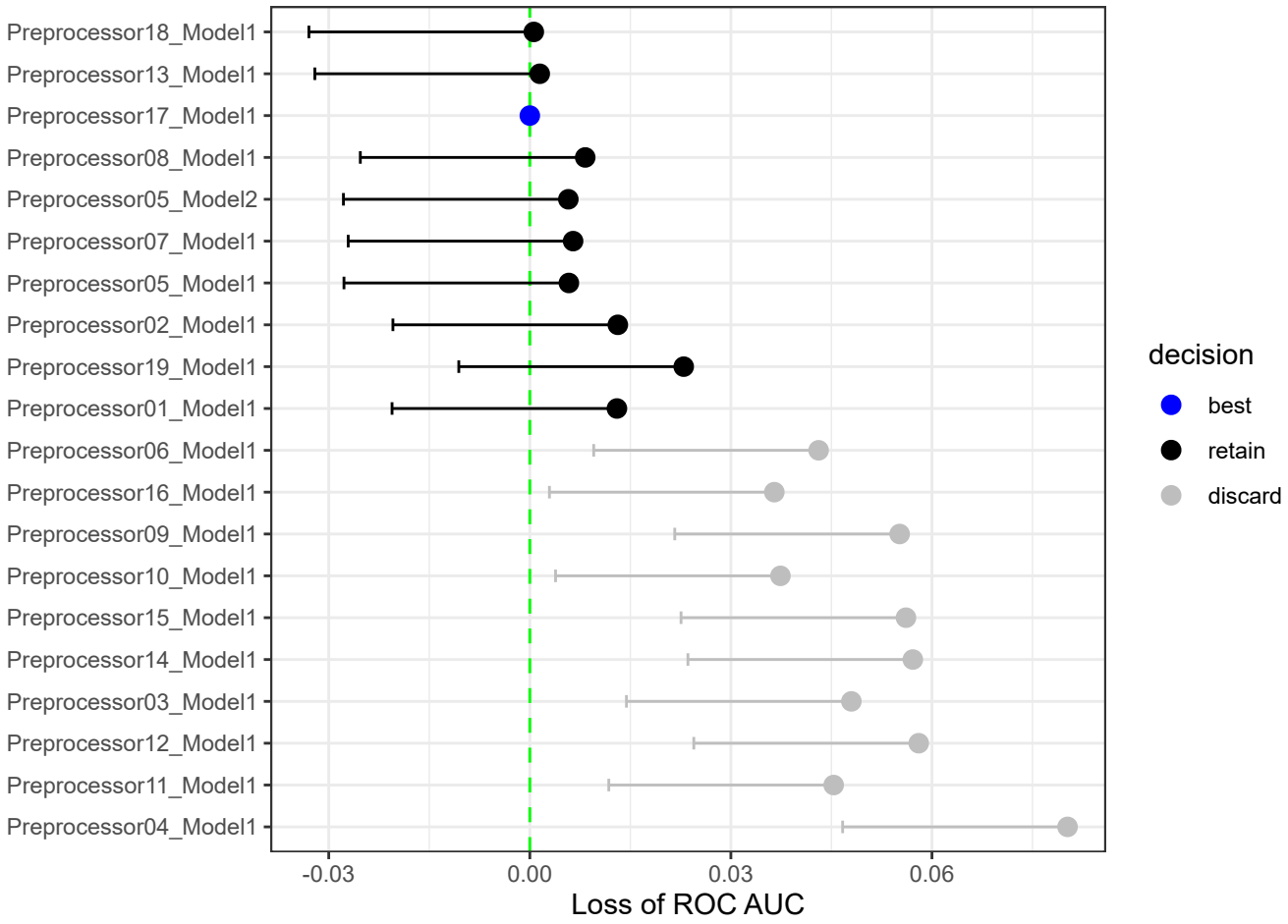
13.5.4 RACING METHODS

One issue with grid search is that all models need to be fit across all resamples before any tuning parameters can be evaluated. It would be helpful if instead, at some point during tuning, an interim analysis could be conducted to eliminate any truly awful parameter candidates. This would be akin to *futility analysis* in clinical trials. If a new drug is performing excessively poorly (or well), it is potentially unethical to wait until the trial finishes to make a decision.

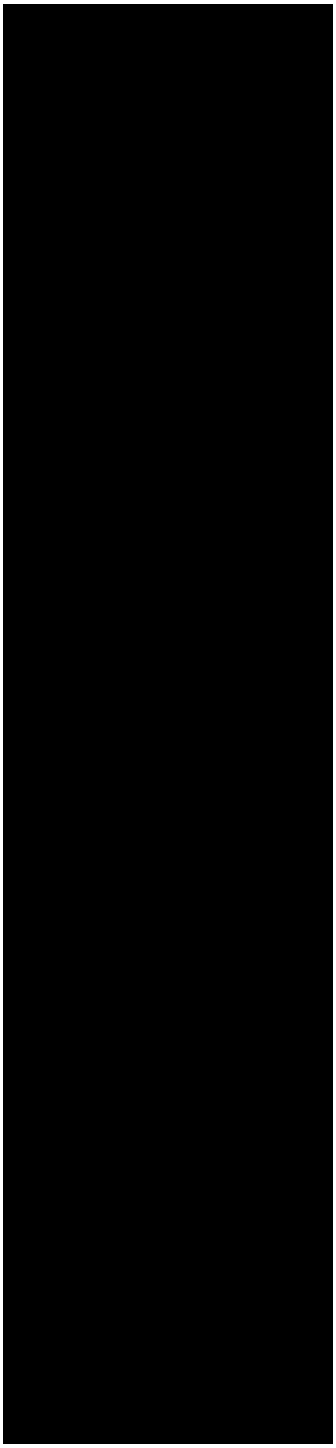
In machine learning, the set of techniques called *racing methods* provide a similar function (Maron and Moore 1994). Here, the tuning process evaluates all models on an initial subset of resamples. Based on their current performance metrics, some parameter sets are not considered in subsequent resamples.

As an example, in the multilayer perceptron tuning process with a regular grid explored in this chapter, what would the results look like after only the first three folds? Using techniques similar to those shown in Chapter 11, we can fit a model where the outcome is the resampled area under the ROC curve and the predictor is an indicator for the parameter combination. The model takes the

resample-to-resample effect into account and produces point and interval estimates for each parameter setting. The results of the model are one-sided 95% confidence intervals that measure the loss of the ROC value relative to the currently best performing parameters:



Any parameter set whose confidence interval includes zero would lack evidence that its performance is not statistically different from the best results. We retain 10 settings; these are resampled more. The remaining 10 submodels are no longer considered.



0:00 / 0:30

The process continues for each resample; after the next set of performance metrics, a new model is fit to these statistics, and more submodels are potentially discarded. See Kuhn (2014) for more details on the computational aspects of this approach.

> Racing methods can be more efficient than basic grid search as long as the interim analysis is fast and some parameter settings have poor performance. It also is most helpful when the model does *not* have the ability to exploit submodel predictions.

The **finetune** package contains functions for racing. The `tune_race_anova()` function conducts an Analysis of Variance (ANOVA) model to test for statistical significance of the different model configurations. The syntax to reproduce the filtering shown above is

```
library(finetune)

set.seed(99)
mlp_sfd_race <-
  mlp_wflow %>%
  tune_race_anova(
    cell_folds,
    grid = 20,
    param_info = mlp_param,
    metrics = roc_res,
    control = control_race(verbose_elim = TRUE)
  )
```

The arguments mirror those of `tune_grid()`. The function `control_race()` has options for the elimination procedure.

As shown in the animation above, there were 2 tuning parameter combinations under consideration once the full set of resamples were evaluated. `show_best()` returns the best models (ranked by performance) but only returns the configurations that were never eliminated:

```
show_best(mlp_sfd_race, n = 10)
#> # A tibble: 2 × 10
#>   hidden_units penalty epochs num_comp .metric .estimator  mean     n std_err
#>          <int>   <dbl>  <int>    <int> <chr>   <chr>      <dbl> <int>   <dbl>
#> 1            5   0.467     60       25 roc_auc binary     0.888    10 0.00708
#> 2            2   0.198    190        4 roc_auc binary     0.878    10 0.00878
#> # … with 1 more variable: .config <chr>
```

There are other interim analysis techniques for discarding settings. For example, Krueger, Panknin, and Braun (2015) use traditional sequential analysis methods whereas Kuhn (2014) treats the data as a sports competition and uses the Bradley-Terry model (Bradley and Terry 1952) to measure the winning ability of parameter settings.

13.6 CHAPTER SUMMARY

This chapter discussed the two main classes of grids (regular and non-regular) that can be used for model tuning and demonstrated how to construct these grids, either manually or using the family of `grid_*()` functions. The `tune_grid()` function can evaluate these candidate sets of model parameters using resampling. The chapter also showed how to finalize a model, recipe, or workflow to update the parameter values for the final fit. Grid search can be computationally expensive, but thoughtful choices in the experimental design of such searches can make them tractable.

The data analysis code that will be reused in the next chapter is:

```
library(tidymodels)

data(cells)
cells <- cells %>% select(-case)

set.seed(33)
cell_folds <- vfold_cv(cells)

roc_res <- metric_set(roc_auc)
```

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