caret Package
Cheat Sheet

Specifying the Model

Possible syntaxes for specifying the variables in the model:

```
train(y ~ x1 + x2, data = dat, ...)
train(x = predictor_df, y = outcome_vector, ...)
train(recipe_object, data = dat, ...)
```

- `rfe`, `sbf`, `gafs`, and `safs` only have the `x/y` interface.
- The `train` formula method will **always** create dummy variables.
- The `x/y` interface to `train` will not create dummy variables (but the underlying model function might).

Remember to:

- Have column names in your data.
- Use factors for a classification outcome (not 0/1 or integers).
- Have valid R names for class levels (not “0"/"1")
- Set the random number seed prior to calling `train` repeatedly to get the same resamples across calls.
- Use the `train` option `na.action = na.pass` if you will being imputing missing data. Also, use this option when predicting new data containing missing values.

To pass options to the underlying model function, you can pass them to `train` via *the ellipses*:

```
train(y ~ ., data = dat, method = "rf",
      # options to `randomForest`:
      importance = TRUE)
```

Parallel Processing

The `foreach` package is used to run models in parallel. The `train` code does not change but a “`do`” package must be called first.

```
# on MacOS or Linux
library(doMC)
registerDoMC(cores=4)
```

```
# on Windows
library(doParallel)
cl <- makeCluster(2)
registerDoParallel(cl)
```

The function `parallel::detectCores` can help too.

Preprocessing

Transformations, filters, and other operations can be applied to the *predictors* with the `preProc` option.

```
train(, preProc = c("method1", "method2"), ...)
```

Methods include:

- `"center"`, `"scale"`, and `"range"` to normalize predictors.
- `"BoxCox"`, `"YeoJohnson"`, or `"expoTrans"` to transform predictors.
- `"knnImpute"`, `"bagImpute"`, or `"medianImpute"` to impute.
- `"corr"`, `"nzv"`, `"zv"`, and `"conditionalX"` to filter.
- `"pca"`, `"ica"`, or `"spatialSign"` to transform groups.

`train` determines the order of operations; the order that the methods are declared does not matter.

The `recipes` package has a more extensive list of preprocessing operations.

Adding Options

Many `train` options can be specified using the `trainControl` function:

```
train(y ~ ., data = dat, method = "cubist",
      trControl = trainControl(<options>))
```

Resampling Options

`trainControl` is used to choose a resampling method:

```
trainControl(method = <method>, <options>)
```

Methods and options are:

- `"cv"` for K-fold cross-validation (`number` sets the # folds).
- `"repeatedcv"` for repeated cross-validation (`repeats` for # repeats).
- `"boot"` for bootstrap (`number` sets the iterations).
- `"LGOCV"` for leave-group-out (`number` and `p` are options).
- `"LOO"` for leave-one-out cross-validation.
- `"oob"` for out-of-bag resampling (only for some models).
- `"timeslice"` for time-series data (options are `initialWindow`, `horizon`, `fixedWindow`, and `skip`).

Performance Metrics

To choose how to summarize a model, the `trainControl` function is used again.

```
trainControl(summaryFunction = <R function>,
             classProbs = <logical>)
```

Custom R functions can be used but `caret` includes several: `defaultSummary` (for accuracy, RMSE, etc), `twoClassSummary` (for ROC curves), and `prSummary` (for information retrieval). For the last two functions, the option `classProbs` must be set to TRUE.

Grid Search

To let `train` determine the values of the tuning parameter(s), the `tuneLength` option controls how many values **per tuning** parameter to evaluate.

Alternatively, specific values of the tuning parameters can be declared using the `tuneGrid` argument:

```
grid <- expand.grid(alpha = c(0.1, 0.5, 0.9),
                    lambda = c(0.001, 0.01))

train(x = x, y = y, method = "glmnet",
      preProc = c("center", "scale"),
      tuneGrid = grid)
```

Random Search

For tuning, `train` can also generate random tuning parameter combinations over a wide range. `tuneLength` controls the total number of combinations to evaluate. To use random search:

```
trainControl(search = "random")
```

Subsampling

With a large class imbalance, `train` can subsample the data to balance the classes them prior to model fitting.

```
trainControl(sampling = "down")
```

Other values are `"up"`, `"smote"`, or `"rose"`. The latter two may require additional package installs.

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