



Instead of a transformer, you can specify the string "drop" if you want the columns to be dropped. Or you can specify "pass through" if you want the columns to be left untouched. By default, the remaining columns (i.e., the ones that were not listed) will be dropped, but you can set the remainder hyperparameter to any transformer (or to "passthrough") if you want these columns to be handled differently.

If you are using Scikit-Learn 0.19 or earlier, you can use a third-party library such as `sklearn-pandas`, or roll out your own custom transformer to get the same functionality as the `ColumnTransformer`. Alternatively, you can use the `FeatureUnion` class which can also apply different transformers and concatenate their outputs, but you cannot specify different columns for each transformer, they all apply to the whole data. It is possible to work around this limitation using a custom transformer for column selection (see the Jupyter notebook for an example).

## Select and Train a Model

At last! You framed the problem, you got the data and explored it, you sampled a training set and a test set, and you wrote transformation pipelines to clean up and prepare your data for Machine Learning algorithms automatically. You are now ready to select and train a Machine Learning model.

### Training and Evaluating on the Training Set

The good news is that thanks to all these previous steps, things are now going to be much simpler than you might think. Let's first train a Linear Regression model, like we did in the previous chapter:

```
from sklearn.linear_model import LinearRegression

lin_reg = LinearRegression()
lin_reg.fit(housing_prepared, housing_labels)
```

Done! You now have a working Linear Regression model. Let's try it out on a few instances from the training set:

```
>>> some_data = housing.iloc[:5]
>>> some_labels = housing_labels.iloc[:5]
>>> some_data_prepared = full_pipeline.transform(some_data)
>>> print("Predictions:", lin_reg.predict(some_data_prepared))
Predictions: [ 210644.6045  317768.8069  210956.4333  59218.9888  189747.5584]
>>> print("Labels:", list(some_labels))
Labels: [286600.0, 340600.0, 196900.0, 46300.0, 254500.0]
```

It works, although the predictions are not exactly accurate (e.g., the first prediction is off by close to 40%!). Let's measure this regression model's RMSE on the whole training set using Scikit-Learn's `mean_squared_error` function:

```
>>> from sklearn.metrics import mean_squared_error
>>> housing_predictions = lin_reg.predict(housing_prepared)
>>> lin_mse = mean_squared_error(housing_labels, housing_predictions)
>>> lin_rmse = np.sqrt(lin_mse)
>>> lin_rmse
68628.19819848922
```

Okay, this is better than nothing but clearly not a great score: most districts' median\_housing\_values range between \$120,000 and \$265,000, so a typical prediction error of \$68,628 is not very satisfying. This is an example of a model underfitting the training data. When this happens it can mean that the features do not provide enough information to make good predictions, or that the model is not powerful enough. As we saw in the previous chapter, the main ways to fix underfitting are to select a more powerful model, to feed the training algorithm with better features, or to reduce the constraints on the model. This model is not regularized, so this rules out the last option. You could try to add more features (e.g., the log of the population), but first let's try a more complex model to see how it does.

Let's train a `DecisionTreeRegressor`. This is a powerful model, capable of finding complex nonlinear relationships in the data (Decision Trees are presented in more detail in [Chapter 6](#)). The code should look familiar by now:

```
from sklearn.tree import DecisionTreeRegressor

tree_reg = DecisionTreeRegressor()
tree_reg.fit(housing_prepared, housing_labels)
```

Now that the model is trained, let's evaluate it on the training set:

```
>>> housing_predictions = tree_reg.predict(housing_prepared)
>>> tree_mse = mean_squared_error(housing_labels, housing_predictions)
>>> tree_rmse = np.sqrt(tree_mse)
>>> tree_rmse
0.0
```

Wait, what!? No error at all? Could this model really be absolutely perfect? Of course, it is much more likely that the model has badly overfit the data. How can you be sure? As we saw earlier, you don't want to touch the test set until you are ready to launch a model you are confident about, so you need to use part of the training set for training, and part for model validation.

## Better Evaluation Using Cross-Validation

One way to evaluate the Decision Tree model would be to use the `train_test_split` function to split the training set into a smaller training set and a validation set, then

train your models against the smaller training set and evaluate them against the validation set. It's a bit of work, but nothing too difficult and it would work fairly well.

A great alternative is to use Scikit-Learn's *K-fold cross-validation* feature. The following code randomly splits the training set into 10 distinct subsets called *folds*, then it trains and evaluates the Decision Tree model 10 times, picking a different fold for evaluation every time and training on the other 9 folds. The result is an array containing the 10 evaluation scores:

```
from sklearn.model_selection import cross_val_score
scores = cross_val_score(tree_reg, housing_prepared, housing_labels,
                        scoring="neg_mean_squared_error", cv=10)
tree_rmse_scores = np.sqrt(-scores)
```



Scikit-Learn's cross-validation features expect a utility function (greater is better) rather than a cost function (lower is better), so the scoring function is actually the opposite of the MSE (i.e., a negative value), which is why the preceding code computes `-scores` before calculating the square root.

Let's look at the results:

```
>>> def display_scores(scores):
...     print("Scores:", scores)
...     print("Mean:", scores.mean())
...     print("Standard deviation:", scores.std())
...
>>> display_scores(tree_rmse_scores)
Scores: [70194.33680785 66855.16363941 72432.58244769 70758.73896782
 71115.88230639 75585.14172901 70262.86139133 70273.6325285
 75366.87952553 71231.65726027]
Mean: 71407.68766037929
Standard deviation: 2439.4345041191004
```

Now the Decision Tree doesn't look as good as it did earlier. In fact, it seems to perform worse than the Linear Regression model! Notice that cross-validation allows you to get not only an estimate of the performance of your model, but also a measure of how precise this estimate is (i.e., its standard deviation). The Decision Tree has a score of approximately 71,407, generally  $\pm 2,439$ . You would not have this information if you just used one validation set. But cross-validation comes at the cost of training the model several times, so it is not always possible.

Let's compute the same scores for the Linear Regression model just to be sure:

```
>>> lin_scores = cross_val_score(lin_reg, housing_prepared, housing_labels,
...                             scoring="neg_mean_squared_error", cv=10)
...
>>> lin_rmse_scores = np.sqrt(-lin_scores)
>>> display_scores(lin_rmse_scores)
```

```
Scores: [66782.73843989 66960.118071 70347.95244419 74739.57052552
68031.13388938 71193.84183426 64969.63056405 68281.61137997
71552.91566558 67665.10082067]
Mean: 69052.46136345083
Standard deviation: 2731.674001798348
```

That's right: the Decision Tree model is overfitting so badly that it performs worse than the Linear Regression model.

Let's try one last model now: the `RandomForestRegressor`. As we will see in [Chapter 7](#), Random Forests work by training many Decision Trees on random subsets of the features, then averaging out their predictions. Building a model on top of many other models is called *Ensemble Learning*, and it is often a great way to push ML algorithms even further. We will skip most of the code since it is essentially the same as for the other models:

```
>>> from sklearn.ensemble import RandomForestRegressor
>>> forest_reg = RandomForestRegressor()
>>> forest_reg.fit(housing_prepared, housing_labels)
>>> [...]
>>> forest_rmse
18603.515021376355
>>> display_scores(forest_rmse_scores)
Scores: [49519.80364233 47461.9115823 50029.02762854 52325.28068953
49308.39426421 53446.37892622 48634.8036574 47585.73832311
53490.10699751 50021.5852922 ]
Mean: 50182.303100336096
Standard deviation: 2097.0810550985693
```

Wow, this is much better: Random Forests look very promising. However, note that the score on the training set is still much lower than on the validation sets, meaning that the model is still overfitting the training set. Possible solutions for overfitting are to simplify the model, constrain it (i.e., regularize it), or get a lot more training data. However, before you dive much deeper in Random Forests, you should try out many other models from various categories of Machine Learning algorithms (several Support Vector Machines with different kernels, possibly a neural network, etc.), without spending too much time tweaking the hyperparameters. The goal is to shortlist a few (two to five) promising models.



You should save every model you experiment with, so you can come back easily to any model you want. Make sure you save both the hyperparameters and the trained parameters, as well as the cross-validation scores and perhaps the actual predictions as well. This will allow you to easily compare scores across model types, and compare the types of errors they make. You can easily save Scikit-Learn models by using Python's pickle module, or using `sklearn.externals.joblib`, which is more efficient at serializing large NumPy arrays:

```
from sklearn.externals import joblib

joblib.dump(my_model, "my_model.pkl")
# and later...
my_model_loaded = joblib.load("my_model.pkl")
```

## Fine-Tune Your Model

Let's assume that you now have a shortlist of promising models. You now need to fine-tune them. Let's look at a few ways you can do that.

### Grid Search

One way to do that would be to fiddle with the hyperparameters manually, until you find a great combination of hyperparameter values. This would be very tedious work, and you may not have time to explore many combinations.

Instead you should get Scikit-Learn's `GridSearchCV` to search for you. All you need to do is tell it which hyperparameters you want it to experiment with, and what values to try out, and it will evaluate all the possible combinations of hyperparameter values, using cross-validation. For example, the following code searches for the best combination of hyperparameter values for the `RandomForestRegressor`:

```
from sklearn.model_selection import GridSearchCV

param_grid = [
    {'n_estimators': [3, 10, 30], 'max_features': [2, 4, 6, 8]},
    {'bootstrap': [False], 'n_estimators': [3, 10], 'max_features': [2, 3, 4]},
]

forest_reg = RandomForestRegressor()

grid_search = GridSearchCV(forest_reg, param_grid, cv=5,
                           scoring='neg_mean_squared_error',
                           return_train_score=True)

grid_search.fit(housing_prepared, housing_labels)
```



When you have no idea what value a hyperparameter should have, a simple approach is to try out consecutive powers of 10 (or a smaller number if you want a more fine-grained search, as shown in this example with the `n_estimators` hyperparameter).

This `param_grid` tells Scikit-Learn to first evaluate all  $3 \times 4 = 12$  combinations of `n_estimators` and `max_features` hyperparameter values specified in the first dict (don't worry about what these hyperparameters mean for now; they will be explained in [Chapter 7](#)), then try all  $2 \times 3 = 6$  combinations of hyperparameter values in the second dict, but this time with the `bootstrap` hyperparameter set to `False` instead of `True` (which is the default value for this hyperparameter).

All in all, the grid search will explore  $12 + 6 = 18$  combinations of `RandomForestRegressor` hyperparameter values, and it will train each model five times (since we are using five-fold cross validation). In other words, all in all, there will be  $18 \times 5 = 90$  rounds of training! It may take quite a long time, but when it is done you can get the best combination of parameters like this:

```
>>> grid_search.best_params_  
{'max_features': 8, 'n_estimators': 30}
```



Since 8 and 30 are the maximum values that were evaluated, you should probably try searching again with higher values, since the score may continue to improve.

You can also get the best estimator directly:

```
>>> grid_search.best_estimator_  
RandomForestRegressor(bootstrap=True, criterion='mse', max_depth=None,  
                        max_features=8, max_leaf_nodes=None, min_impurity_decrease=0.0,  
                        min_impurity_split=None, min_samples_leaf=1,  
                        min_samples_split=2, min_weight_fraction_leaf=0.0,  
                        n_estimators=30, n_jobs=None, oob_score=False, random_state=None,  
                        verbose=0, warm_start=False)
```



If `GridSearchCV` is initialized with `refit=True` (which is the default), then once it finds the best estimator using cross-validation, it retrains it on the whole training set. This is usually a good idea since feeding it more data will likely improve its performance.

And of course the evaluation scores are also available:

```
>>> cvres = grid_search.cv_results_  
>>> for mean_score, params in zip(cvres["mean_test_score"], cvres["params"]):
```

```

...     print(np.sqrt(-mean_score), params)
...
63669.05791727153 {'max_features': 2, 'n_estimators': 3}
55627.16171305252 {'max_features': 2, 'n_estimators': 10}
53384.57867637289 {'max_features': 2, 'n_estimators': 30}
60965.99185930139 {'max_features': 4, 'n_estimators': 3}
52740.98248528835 {'max_features': 4, 'n_estimators': 10}
50377.344409590376 {'max_features': 4, 'n_estimators': 30}
58663.84733372485 {'max_features': 6, 'n_estimators': 3}
52006.15355973719 {'max_features': 6, 'n_estimators': 10}
50146.465964159885 {'max_features': 6, 'n_estimators': 30}
57869.25504027614 {'max_features': 8, 'n_estimators': 3}
51711.09443660957 {'max_features': 8, 'n_estimators': 10}
49682.25345942335 {'max_features': 8, 'n_estimators': 30}
62895.088889905004 {'bootstrap': False, 'max_features': 2, 'n_estimators': 3}
54658.14484390074 {'bootstrap': False, 'max_features': 2, 'n_estimators': 10}
59470.399594730654 {'bootstrap': False, 'max_features': 3, 'n_estimators': 3}
52725.01091081235 {'bootstrap': False, 'max_features': 3, 'n_estimators': 10}
57490.612956065226 {'bootstrap': False, 'max_features': 4, 'n_estimators': 3}
51009.51445842374 {'bootstrap': False, 'max_features': 4, 'n_estimators': 10}

```

In this example, we obtain the best solution by setting the `max_features` hyperparameter to 8, and the `n_estimators` hyperparameter to 30. The RMSE score for this combination is 49,682, which is slightly better than the score you got earlier using the default hyperparameter values (which was 50,182). Congratulations, you have successfully fine-tuned your best model!



Don't forget that you can treat some of the data preparation steps as hyperparameters. For example, the grid search will automatically find out whether or not to add a feature you were not sure about (e.g., using the `add_bedrooms_per_room` hyperparameter of your `CombinedAttributesAdder` transformer). It may similarly be used to automatically find the best way to handle outliers, missing features, feature selection, and more.

## Randomized Search

The grid search approach is fine when you are exploring relatively few combinations, like in the previous example, but when the hyperparameter *search space* is large, it is often preferable to use `RandomizedSearchCV` instead. This class can be used in much the same way as the `GridSearchCV` class, but instead of trying out all possible combinations, it evaluates a given number of random combinations by selecting a random value for each hyperparameter at every iteration. This approach has two main benefits:

- If you let the randomized search run for, say, 1,000 iterations, this approach will explore 1,000 different values for each hyperparameter (instead of just a few values per hyperparameter with the grid search approach).
- You have more control over the computing budget you want to allocate to hyperparameter search, simply by setting the number of iterations.

## Ensemble Methods

Another way to fine-tune your system is to try to combine the models that perform best. The group (or “ensemble”) will often perform better than the best individual model (just like Random Forests perform better than the individual Decision Trees they rely on), especially if the individual models make very different types of errors. We will cover this topic in more detail in [Chapter 7](#).

## Analyze the Best Models and Their Errors

You will often gain good insights on the problem by inspecting the best models. For example, the `RandomForestRegressor` can indicate the relative importance of each attribute for making accurate predictions:

```
>>> feature_importances = grid_search.best_estimator_.feature_importances_
>>> feature_importances
array([7.33442355e-02, 6.29090705e-02, 4.11437985e-02, 1.46726854e-02,
       1.41064835e-02, 1.48742809e-02, 1.42575993e-02, 3.66158981e-01,
       5.64191792e-02, 1.08792957e-01, 5.33510773e-02, 1.03114883e-02,
       1.64780994e-01, 6.02803867e-05, 1.96041560e-03, 2.85647464e-03])
```

Let’s display these importance scores next to their corresponding attribute names:

```
>>> extra_attribs = ["rooms_per_hhold", "pop_per_hhold", "bedrooms_per_room"]
>>> cat_encoder = full_pipeline.named_transformers_["cat"]
>>> cat_one_hot_attribs = list(cat_encoder.categories_[0])
>>> attributes = num_attribs + extra_attribs + cat_one_hot_attribs
>>> sorted(zip(feature_importances, attributes), reverse=True)
[(0.3661589806181342, 'median_income'),
 (0.1647809935615905, 'INLAND'),
 (0.10879295677551573, 'pop_per_hhold'),
 (0.07334423551601242, 'longitude'),
 (0.0629090704826203, 'latitude'),
 (0.05641917918195401, 'rooms_per_hhold'),
 (0.05335107734767581, 'bedrooms_per_room'),
 (0.041143798478729635, 'housing_median_age'),
 (0.014874280890402767, 'population'),
 (0.014672685420543237, 'total_rooms'),
 (0.014257599323407807, 'households'),
 (0.014106483453584102, 'total_bedrooms'),
 (0.010311488326303787, '<1H OCEAN'),
 (0.002856474637320158, 'NEAR OCEAN'),
```



```
(0.00196041559947807, 'NEAR BAY'),  
(6.028038672736599e-05, 'ISLAND')]
```

With this information, you may want to try dropping some of the less useful features (e.g., apparently only one `ocean_proximity` category is really useful, so you could try dropping the others).

You should also look at the specific errors that your system makes, then try to understand why it makes them and what could fix the problem (adding extra features or, on the contrary, getting rid of uninformative ones, cleaning up outliers, etc.).

## Evaluate Your System on the Test Set

After tweaking your models for a while, you eventually have a system that performs sufficiently well. Now is the time to evaluate the final model on the test set. There is nothing special about this process; just get the predictors and the labels from your test set, run your `full_pipeline` to transform the data (call `transform()`, *not* `fit_transform()`, you do not want to fit the test set!), and evaluate the final model on the test set:

```
final_model = grid_search.best_estimator_  
  
X_test = strat_test_set.drop("median_house_value", axis=1)  
y_test = strat_test_set["median_house_value"].copy()  
  
X_test_prepared = full_pipeline.transform(X_test)  
  
final_predictions = final_model.predict(X_test_prepared)  
  
final_mse = mean_squared_error(y_test, final_predictions)  
final_rmse = np.sqrt(final_mse) # => evaluates to 47,730.2
```

In some cases, such a point estimate of the generalization error will not be quite enough to convince you to launch: what if it is just 0.1% better than the model currently in production? You might want to have an idea of how precise this estimate is. For this, you can compute a 95% *confidence interval* for the generalization error using `scipy.stats.t.interval()`:

```
>>> from scipy import stats  
>>> confidence = 0.95  
>>> squared_errors = (final_predictions - y_test) ** 2  
>>> np.sqrt(stats.t.interval(confidence, len(squared_errors) - 1,  
...                           loc=squared_errors.mean(),  
...                           scale=stats.sem(squared_errors)))  
...  
array([45685.10470776, 49691.25001878])
```

The performance will usually be slightly worse than what you measured using cross-validation if you did a lot of hyperparameter tuning (because your system ends up fine-tuned to perform well on the validation data, and will likely not perform as well

on unknown datasets). It is not the case in this example, but when this happens you must resist the temptation to tweak the hyperparameters to make the numbers look good on the test set; the improvements would be unlikely to generalize to new data.

Now comes the project prelaunch phase: you need to present your solution (highlighting what you have learned, what worked and what did not, what assumptions were made, and what your system's limitations are), document everything, and create nice presentations with clear visualizations and easy-to-remember statements (e.g., “the median income is the number one predictor of housing prices”). In this California housing example, the final performance of the system is not better than the experts', but it may still be a good idea to launch it, especially if this frees up some time for the experts so they can work on more interesting and productive tasks.

## Launch, Monitor, and Maintain Your System

Perfect, you got approval to launch! You need to get your solution ready for production, in particular by plugging the production input data sources into your system and writing tests.

You also need to write monitoring code to check your system's live performance at regular intervals and trigger alerts when it drops. This is important to catch not only sudden breakage, but also performance degradation. This is quite common because models tend to “rot” as data evolves over time, unless the models are regularly trained on fresh data.

Evaluating your system's performance will require sampling the system's predictions and evaluating them. This will generally require a human analysis. These analysts may be field experts, or workers on a crowdsourcing platform (such as Amazon Mechanical Turk or CrowdFlower). Either way, you need to plug the human evaluation pipeline into your system.

You should also make sure you evaluate the system's input data quality. Sometimes performance will degrade slightly because of a poor quality signal (e.g., a malfunctioning sensor sending random values, or another team's output becoming stale), but it may take a while before your system's performance degrades enough to trigger an alert. If you monitor your system's inputs, you may catch this earlier. Monitoring the inputs is particularly important for online learning systems.

Finally, you will generally want to train your models on a regular basis using fresh data. You should automate this process as much as possible. If you don't, you are very likely to refresh your model only every six months (at best), and your system's performance may fluctuate severely over time. If your system is an online learning system, you should make sure you save snapshots of its state at regular intervals so you can easily roll back to a previously working state.