Advanced pandas

The preceding chapters have focused on introducing different types of data wrangling workflows and features of NumPy, pandas, and other libraries. Over time, pandas has developed a depth of features for power users. This chapter digs into a few more advanced feature areas to help you deepen your expertise as a pandas user.

12.1 Categorical Data

This section introduces the pandas Categorical type. I will show how you can achieve better performance and memory use in some pandas operations by using it. I also introduce some tools for using categorical data in statistics and machine learning applications.

Background and Motivation

Frequently, a column in a table may contain repeated instances of a smaller set of distinct values. We have already seen functions like unique and value_counts, which enable us to extract the distinct values from an array and compute their frequencies, respectively:

```
4  apple
5  orange
6  apple
7  apple
dtype: object

In [13]: pd.unique(values)
Out[13]: array(['apple', 'orange'], dtype=object)

In [14]: pd.value_counts(values)
Out[14]:
apple  6
orange  2
dtype: int64
```

Many data systems (for data warehousing, statistical computing, or other uses) have developed specialized approaches for representing data with repeated values for more efficient storage and computation. In data warehousing, a best practice is to use so-called *dimension tables* containing the distinct values and storing the primary observations as integer keys referencing the dimension table:

```
In [15]: values = pd.Series([0, 1, 0, 0] * 2)
In [16]: dim = pd.Series(['apple', 'orange'])
In [17]: values
Out[17]:
0
     0
1
     1
2
     0
3
     0
4
     0
5
    1
6
     0
dtype: int64
In [18]: dim
Out[18]:
      apple
     orange
dtype: object
```

We can use the take method to restore the original Series of strings:

```
In [19]: dim.take(values)
Out[19]:
0    apple
1    orange
0    apple
0    apple
0    apple
1    orange
```

```
0 apple
0 apple
dtype: object
```

This representation as integers is called the *categorical* or *dictionary-encoded* representation. The array of distinct values can be called the *categories*, *dictionary*, or *levels* of the data. In this book we will use the terms *categorical* and *categories*. The integer values that reference the categories are called the *category codes* or simply *codes*.

The categorical representation can yield significant performance improvements when you are doing analytics. You can also perform transformations on the categories while leaving the codes unmodified. Some example transformations that can be made at relatively low cost are:

- Renaming categories
- Appending a new category without changing the order or position of the existing categories

Categorical Type in pandas

pandas has a special Categorical type for holding data that uses the integer-based categorical representation or *encoding*. Let's consider the example Series from before:

```
In [20]: fruits = ['apple', 'orange', 'apple', 'apple'] * 2
In [21]: N = len(fruits)
In [22]: df = pd.DataFrame({'fruit': fruits,
                           'basket_id': np.arange(N),
                           'count': np.random.randint(3, 15, size=N),
   . . . . :
                           'weight': np.random.uniform(0, 4, size=N)},
   . . . . :
                          columns=['basket_id', 'fruit', 'count', 'weight'])
   . . . . :
In [23]: df
Out[23]:
  basket id fruit count weight
              apple
                         5 3.858058
0
          0
1
          1 orange
                         8 2.612708
2
              apple
                        4 2.995627
3
          3 apple
                        7 2.614279
4
          4 apple
                        12 2.990859
5
          5 orange
                        8 3.845227
                        5 0.033553
6
          6
              apple
          7
              apple
                     4 0.425778
```

Here, df['fruit'] is an array of Python string objects. We can convert it to categorical by calling:

```
In [24]: fruit cat = df['fruit'].astype('category')
In [25]: fruit cat
Out[25]:
0
      apple
1
     orange
2
      apple
3
      apple
4
      apple
5
     orange
6
      apple
      apple
Name: fruit, dtype: category
Categories (2, object): [apple, orange]
```

The values for fruit cat are not a NumPy array, but an instance of pandas. Catego rical.

```
In [26]: c = fruit_cat.values
In [27]: type(c)
Out[27]: pandas.core.categorical.Categorical
```

The Categorical object has categories and codes attributes:

```
In [28]: c.categories
Out[28]: Index(['apple', 'orange'], dtype='object')
In [29]: c.codes
Out[29]: array([0, 1, 0, 0, 0, 1, 0, 0], dtype=int8)
```

You can convert a DataFrame column to categorical by assigning the converted result:

```
In [30]: df['fruit'] = df['fruit'].astype('category')
In [31]: df.fruit
Out[31]:
0
      apple
1
     orange
2
      apple
3
      apple
4
      apple
5
     orange
6
      apple
      apple
Name: fruit, dtype: category
Categories (2, object): [apple, orange]
```

You can also create pandas. Categorical directly from other types of Python sequences:

```
In [32]: my categories = pd.Categorical(['foo', 'bar', 'baz', 'foo', 'bar'])
In [33]: my_categories
```

```
Out[33]:
[foo, bar, baz, foo, bar]
Categories (3, object): [bar, baz, foo]
```

If you have obtained categorical encoded data from another source, you can use the alternative from_codes constructor:

```
In [34]: categories = ['foo', 'bar', 'baz']
In [35]: codes = [0, 1, 2, 0, 0, 1]
In [36]: my_cats_2 = pd.Categorical.from_codes(codes, categories)
In [37]: my_cats_2
Out[37]:
[foo, bar, baz, foo, foo, bar]
Categories (3, object): [foo, bar, baz]
```

Unless explicitly specified, categorical conversions assume no specific ordering of the categories. So the categories array may be in a different order depending on the ordering of the input data. When using from_codes or any of the other constructors, you can indicate that the categories have a meaningful ordering:

The output [foo < bar < baz] indicates that 'foo' precedes 'bar' in the ordering, and so on. An unordered categorical instance can be made ordered with as_ordered:

```
In [40]: my_cats_2.as_ordered()
Out[40]:
[foo, bar, baz, foo, foo, bar]
Categories (3, object): [foo < bar < baz]</pre>
```

As a last note, categorical data need not be strings, even though I have only showed string examples. A categorical array can consist of any immutable value types.

Computations with Categoricals

Using Categorical in pandas compared with the non-encoded version (like an array of strings) generally behaves the same way. Some parts of pandas, like the groupby function, perform better when working with categoricals. There are also some functions that can utilize the ordered flag.

Let's consider some random numeric data, and use the pandas.qcut binning function. This return pandas.Categorical; we used pandas.cut earlier in the book but glossed over the details of how categoricals work:

```
In [41]: np.random.seed(12345)
In [42]: draws = np.random.randn(1000)
In [43]: draws[:5]
Out[43]: array([-0.2047,  0.4789, -0.5194, -0.5557,  1.9658])
```

Let's compute a quartile binning of this data and extract some statistics:

```
In [44]: bins = pd.qcut(draws, 4)

In [45]: bins
Out[45]:
[(-0.684, -0.0101], (-0.0101, 0.63], (-0.684, -0.0101], (-0.684, -0.0101], (0.63, 3.928], ..., (-0.0101, 0.63], (-0.684, -0.0101], (-2.95, -0.684], (-0.0101, 0.63], (0.63, 3.928]]
Length: 1000
Categories (4, interval[float64]): [(-2.95, -0.684] < (-0.684, -0.0101] < (-0.0101, 0.63] </pre>
(0.63, 3.928]]
```

While useful, the exact sample quartiles may be less useful for producing a report than quartile names. We can achieve this with the labels argument to qcut:

```
In [46]: bins = pd.qcut(draws, 4, labels=['Q1', 'Q2', 'Q3', 'Q4'])
In [47]: bins
Out[47]:
[Q2, Q3, Q2, Q2, Q4, ..., Q3, Q2, Q1, Q3, Q4]
Length: 1000
Categories (4, object): [Q1 < Q2 < Q3 < Q4]
In [48]: bins.codes[:10]
Out[48]: array([1, 2, 1, 1, 3, 3, 2, 2, 3, 3], dtype=int8)</pre>
```

The labeled bins categorical does not contain information about the bin edges in the data, so we can use groupby to extract some summary statistics:

```
1 Q2 250 -0.683066 -0.010115
2 Q3 250 -0.010032 0.628894
3 Q4 250 0.634238 3.927528
```

The 'quartile' column in the result retains the original categorical information, including ordering, from bins:

```
In [52]: results['quartile']
Out[52]:
0    Q1
1    Q2
2    Q3
3    Q4
Name: quartile, dtype: category
Categories (4, object): [Q1 < Q2 < Q3 < Q4]</pre>
```

Better performance with categoricals

If you do a lot of analytics on a particular dataset, converting to categorical can yield substantial overall performance gains. A categorical version of a DataFrame column will often use significantly less memory, too. Let's consider some Series with 10 million elements and a small number of distinct categories:

```
In [53]: N = 10000000
In [54]: draws = pd.Series(np.random.randn(N))
In [55]: labels = pd.Series(['foo', 'bar', 'baz', 'qux'] * (N // 4))
```

Now we convert labels to categorical:

```
In [56]: categories = labels.astype('category')
```

Now we note that labels uses significantly more memory than categories:

```
In [57]: labels.memory_usage()
Out[57]: 80000080
In [58]: categories.memory_usage()
Out[58]: 10000272
```

The conversion to category is not free, of course, but it is a one-time cost:

```
In [59]: %time _ = labels.astype('category')
CPU times: user 490 ms, sys: 240 ms, total: 730 ms
Wall time: 726 ms
```

GroupBy operations can be significantly faster with categoricals because the underlying algorithms use the integer-based codes array instead of an array of strings.

Categorical Methods

Series containing categorical data have several special methods similar to the Series.str specialized string methods. This also provides convenient access to the categories and codes. Consider the Series:

```
In [60]: s = pd.Series(['a', 'b', 'c', 'd'] * 2)
In [61]: cat_s = s.astype('category')
In [62]: cat s
Out[62]:
0
     a
1
     h
2
     c
3
     d
4
5
     Ь
     c
7
     d
dtype: category
Categories (4, object): [a, b, c, d]
```

The special attribute cat provides access to categorical methods:

```
In [63]: cat_s.cat.codes
Out[63]:
0
     0
1
     1
2
     2
3
     3
4
     0
5
     1
     2
6
     3
dtype: int8
In [64]: cat s.cat.categories
Out[64]: Index(['a', 'b', 'c', 'd'], dtype='object')
```

Suppose that we know the actual set of categories for this data extends beyond the four values observed in the data. We can use the set_categories method to change them:

```
In [65]: actual_categories = ['a', 'b', 'c', 'd', 'e']
In [66]: cat_s2 = cat_s.cat.set_categories(actual_categories)
In [67]: cat_s2
Out[67]:
0     a
1     b
```

```
4 a
5 b
6 c
7 d
dtype: category
Categories (5, object): [a, b, c, d, e]
```

c

d

3

While it appears that the data is unchanged, the new categories will be reflected in operations that use them. For example, value_counts respects the categories, if present:

```
In [68]: cat_s.value_counts()
Out[68]:
Ч
     2
     2
h
     2
     2
dtype: int64
In [69]: cat_s2.value_counts()
Out[69]:
d
     2
     2
c
     2
h
     2
a
     0
dtype: int64
```

In large datasets, categoricals are often used as a convenient tool for memory savings and better performance. After you filter a large DataFrame or Series, many of the categories may not appear in the data. To help with this, we can use the remove_unused_categories method to trim unobserved categories:

```
In [70]: cat_s3 = cat_s[cat_s.isin(['a', 'b'])]
In [71]: cat_s3
Out[71]:
0
     b
1
dtype: category
Categories (4, object): [a, b, c, d]
In [72]: cat_s3.cat.remove_unused_categories()
Out[72]:
0
     a
1
     a
5
     Ь
```

```
dtype: category
Categories (2, object): [a, b]
```

See Table 12-1 for a listing of available categorical methods.

Table 12-1. Categorical methods for Series in pandas

Method	Description
add_categories	Append new (unused) categories at end of existing categories
as_ordered	Make categories ordered
as_unordered	Make categories unordered
remove_categories	Remove categories, setting any removed values to null
remove_unused_categories	Remove any category values which do not appear in the data
rename_categories	Replace categories with indicated set of new category names; cannot change the number of categories
reorder_categories	Behaves like rename_categories, but can also change the result to have ordered categories
set_categories	Replace the categories with the indicated set of new categories; can add or remove categories

Creating dummy variables for modeling

When you're using statistics or machine learning tools, you'll often transform categorical data into *dummy variables*, also known as *one-hot* encoding. This involves creating a DataFrame with a column for each distinct category; these columns contain 1s for occurrences of a given category and 0 otherwise.

Consider the previous example:

```
In [73]: cat_s = pd.Series(['a', 'b', 'c', 'd'] * 2, dtype='category')
```

As mentioned previously in Chapter 7, the pandas.get_dummies function converts this one-dimensional categorical data into a DataFrame containing the dummy variable:

12.2 Advanced GroupBy Use

While we've already discussed using the groupby method for Series and DataFrame in depth in Chapter 10, there are some additional techniques that you may find of use.

Group Transforms and "Unwrapped" GroupBys

In Chapter 10 we looked at the apply method in grouped operations for performing transformations. There is another built-in method called transform, which is similar to apply but imposes more constraints on the kind of function you can use:

- It can produce a scalar value to be broadcast to the shape of the group
- It can produce an object of the same shape as the input group
- It must not mutate its input

Let's consider a simple example for illustration:

```
In [75]: df = pd.DataFrame({'key': ['a', 'b', 'c'] * 4,
                             'value': np.arange(12.)})
   . . . . :
In [76]: df
Out[76]:
   kev value
0
          0.0
     a
1
     Ь
          1.0
2
     C
          2.0
3
          3.0
     a
4
    Ь
          4.0
5
    C
         5.0
          6.0
7
     Ь
          7.0
8
         8.0
     c
9
     а
         9.0
10
     b
         10.0
11
         11.0
```

Here are the group means by key:

```
In [77]: g = df.groupby('key').value
In [78]: g.mean()
Out[78]:
key
a     4.5
b     5.5
c     6.5
Name: value, dtype: float64
```

Suppose instead we wanted to produce a Series of the same shape as df['value'] but with values replaced by the average grouped by 'key'. We can pass the function lambda x: x.mean() to transform:

```
In [79]: g.transform(lambda x: x.mean())
Out[79]:
0
      4.5
      5.5
1
2
      6.5
3
      4.5
      5.5
4
5
      6.5
6
      4.5
7
      5.5
8
      6.5
9
      4.5
10
      5.5
      6.5
11
Name: value, dtype: float64
```

For built-in aggregation functions, we can pass a string alias as with the GroupBy agg method:

```
In [80]: g.transform('mean')
Out[80]:
0
      4.5
1
      5.5
2
      6.5
3
      4.5
4
      5.5
5
      6.5
      4.5
6
      5.5
7
      6.5
8
9
      4.5
      5.5
10
      6.5
11
Name: value, dtype: float64
```

Like apply, transform works with functions that return Series, but the result must be the same size as the input. For example, we can multiply each group by 2 using a lambda function:

```
In [81]: g.transform(lambda x: x * 2)
Out[81]:
0
       0.0
1
       2.0
2
       4.0
3
      6.0
4
      8.0
5
      10.0
6
      12.0
```

```
7 14.0
8 16.0
9 18.0
10 20.0
11 22.0
Name: value, dtype: float64
```

As a more complicated example, we can compute the ranks in descending order for each group:

```
In [82]: g.transform(lambda x: x.rank(ascending=False))
Out[82]:
     4.0
1
     4.0
2
     4.0
3
     3.0
4
     3.0
5
     3.0
6
     2.0
7
     2.0
     2.0
8
9
     1.0
     1.0
10
11
     1.0
Name: value, dtype: float64
```

Consider a group transformation function composed from simple aggregations:

```
def normalize(x):
    return (x - x.mean()) / x.std()
```

We can obtain equivalent results in this case either using transform or apply:

```
In [84]: g.transform(normalize)
Out[84]:
0 -1.161895
1
   -1.161895
2
   -1.161895
3
   -0.387298
4
   -0.387298
5
   -0.387298
6
    0.387298
7
    0.387298
    0.387298
8
9
     1.161895
10
     1.161895
     1.161895
Name: value, dtype: float64
In [85]: g.apply(normalize)
Out[85]:
0 -1.161895
    -1.161895
```

2

-1.161895

```
3
     -0.387298
4
     -0.387298
5
    -0.387298
     0.387298
7
     0.387298
8
     0.387298
9
      1.161895
10
      1.161895
11
      1.161895
Name: value, dtype: float64
```

Built-in aggregate functions like 'mean' or 'sum' are often much faster than a general apply function. These also have a "fast past" when used with transform. This allows us to perform a so-called *unwrapped* group operation:

```
In [86]: q.transform('mean')
Out[86]:
0
      4.5
1
      5.5
2
      6.5
3
      4.5
      5.5
5
      6.5
      4.5
6
7
      5.5
      6.5
      4.5
9
      5.5
10
      6.5
11
Name: value, dtype: float64
In [87]: normalized = (df['value'] - g.transform('mean')) / g.transform('std')
In [88]: normalized
Out[88]:
   -1.161895
1
    -1.161895
2
    -1.161895
3
    -0.387298
    -0.387298
5
    -0.387298
6
    0.387298
7
     0.387298
8
     0.387298
9
      1.161895
10
      1.161895
      1.161895
Name: value, dtype: float64
```

While an unwrapped group operation may involve multiple group aggregations, the overall benefit of vectorized operations often outweighs this.

Grouped Time Resampling

For time series data, the resample method is semantically a group operation based on a time intervalization. Here's a small example table:

```
In [89]: N = 15
In [90]: times = pd.date range('2017-05-20 00:00', freq='1min', periods=N)
In [91]: df = pd.DataFrame({'time': times,
                            'value': np.arange(N)})
   . . . . :
In [92]: df
Out[92]:
                 time value
0 2017-05-20 00:00:00
1 2017-05-20 00:01:00
2 2017-05-20 00:02:00
3 2017-05-20 00:03:00
                           3
4 2017-05-20 00:04:00
5 2017-05-20 00:05:00
6 2017-05-20 00:06:00
7 2017-05-20 00:07:00
                           7
8 2017-05-20 00:08:00
9 2017-05-20 00:09:00
                          9
10 2017-05-20 00:10:00
                          10
11 2017-05-20 00:11:00
                          11
12 2017-05-20 00:12:00
                          12
13 2017-05-20 00:13:00
                          13
14 2017-05-20 00:14:00
                      14
```

Here, we can index by 'time' and then resample:

Suppose that a DataFrame contains multiple time series, marked by an additional group key column:

```
2 c 2017-05-20 00:00:00 2.0

3 a 2017-05-20 00:01:00 3.0

4 b 2017-05-20 00:01:00 4.0

5 c 2017-05-20 00:01:00 5.0

6 a 2017-05-20 00:02:00 6.0
```

To do the same resampling for each value of 'key', we introduce the pandas. Time Grouper object:

```
In [96]: time_key = pd.TimeGrouper('5min')
```

We can then set the time index, group by 'key' and time_key, and aggregate:

```
In [97]: resampled = (df2.set index('time')
   . . . . :
                      .groupby(['key', time_key])
                      .sum())
   . . . . :
In [98]: resampled
Out[98]:
                        value
kev time
   2017-05-20 00:00:00
                         30.0
    2017-05-20 00:05:00
                        105.0
   2017-05-20 00:10:00
                        180.0
                        35.0
Ь
   2017-05-20 00:00:00
    2017-05-20 00:05:00
                        110.0
   2017-05-20 00:10:00
                        185.0
c
  2017-05-20 00:00:00
                        40.0
    2017-05-20 00:05:00 115.0
    2017-05-20 00:10:00 190.0
In [99]: resampled.reset index()
Out[99]:
 key
                    time value
   a 2017-05-20 00:00:00 30.0
1 a 2017-05-20 00:05:00 105.0
 a 2017-05-20 00:10:00 180.0
3 b 2017-05-20 00:00:00 35.0
4 b 2017-05-20 00:05:00 110.0
5 b 2017-05-20 00:10:00 185.0
6 c 2017-05-20 00:00:00 40.0
7 c 2017-05-20 00:05:00 115.0
   c 2017-05-20 00:10:00 190.0
```

One constraint with using TimeGrouper is that the time must be the index of the Series or DataFrame.

12.3 Techniques for Method Chaining

When applying a sequence of transformations to a dataset, you may find yourself creating numerous temporary variables that are never used in your analysis. Consider this example, for instance:

```
df = load_data()
df2 = df[df['col2'] < 0]
df2['col1_demeaned'] = df2['col1'] - df2['col1'].mean()
result = df2.groupby('key').col1_demeaned.std()</pre>
```

While we're not using any real data here, this example highlights some new methods. First, the DataFrame.assign method is a *functional* alternative to column assignments of the form df[k] = v. Rather than modifying the object in-place, it returns a new DataFrame with the indicated modifications. So these statements are equivalent:

```
# Usual non-functional way
df2 = df.copy()
df2['k'] = v
# Functional assign way
df2 = df.assign(k=v)
```

Assigning in-place may execute faster than using assign, but assign enables easier method chaining:

I used the outer parentheses to make it more convenient to add line breaks.

One thing to keep in mind when doing method chaining is that you may need to refer to temporary objects. In the preceding example, we cannot refer to the result of load_data until it has been assigned to the temporary variable df. To help with this, assign and many other pandas functions accept function-like arguments, also known as *callables*.

To show callables in action, consider a fragment of the example from before:

```
df = load_data()
df2 = df[df['col2'] < 0]</pre>
```

This can be rewritten as:

Here, the result of load_data is not assigned to a variable, so the function passed into [] is then *bound* to the object at that stage of the method chain.

We can continue, then, and write the entire sequence as a single chained expression:

Whether you prefer to write code in this style is a matter of taste, and splitting up the expression into multiple steps may make your code more readable.

The pipe Method

You can accomplish a lot with built-in pandas functions and the approaches to method chaining with callables that we just looked at. However, sometimes you need to use your own functions or functions from third-party libraries. This is where the pipe method comes in.

Consider a sequence of function calls:

```
a = f(df, arg1=v1)
b = g(a, v2, arg3=v3)
c = h(b, arg4=v4)
```

When using functions that accept and return Series or DataFrame objects, you can rewrite this using calls to pipe:

The statement f(df) and df.pipe(f) are equivalent, but pipe makes chained invocation easier.

A potentially useful pattern for pipe is to generalize sequences of operations into reusable functions. As an example, let's consider substracting group means from a column:

```
g = df.groupby(['key1', 'key2'])
df['col1'] = df['col1'] - g.transform('mean')
```

Suppose that you wanted to be able to demean more than one column and easily change the group keys. Additionally, you might want to perform this transformation in a method chain. Here is an example implementation:

```
def group_demean(df, by, cols):
    result = df.copy()
    g = df.groupby(by)
    for c in cols:
        result[c] = df[c] - g[c].transform('mean')
    return result
```

Then it is possible to write:

12.4 Conclusion

pandas, like many open source software projects, is still changing and acquiring new and improved functionality. As elsewhere in this book, the focus here has been on the most stable functionality that is less likely to change over the next several years.

To deepen your expertise as a pandas user, I encourage you to explore the documentation and read the release notes as the development team makes new open source releases. We also invite you to join in on pandas development: fixing bugs, building new features, and improving the documentation.