Bridging the pandas – scikit-learn dtype divide

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The Problem

Two Data Models

	Broadcast-ing	Vectorization	ufuncs	typed arrays	ND-arrays	Labels	Heterogeneous	Extension dtypes
scikit-learn / NumPy	✔	✔	✔	✔	✔			
Pandas	✔	✔	✔	✔		✔	✔	✔

Two Data Models

Claim: “Real world” data are

- Labeled
- Heterogenous
- Messy

The Data

```
In [1]: import numpy as np
   ...: import pandas as pd
   ...: import seaborn as sns
   ...:
   ...: tips = pd.read_csv('tips.csv')
   ...: tips.head()
   ...:
Out[1]:
   total_bill   tip     sex smoker  day    time  size
0       16.99  1.01  Female     No  Sun  Dinner     2
1       10.34  1.66    Male     No  Sun  Dinner     3
2       21.01  3.50    Male     No  Sun  Dinner     3
3       23.68  3.31    Male     No  Sun  Dinner     2
4       24.59  3.61  Female     No  Sun  Dinner     4
```

The Data

```
In [2]: tips.info()
Out[2]:
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 244 entries, 0 to 243
Data columns (total 7 columns):
total_bill    244 non-null float64
tip           244 non-null float64
sex           244 non-null object
smoker        244 non-null object
day           244 non-null object
time          244 non-null object
size          244 non-null int64
dtypes: float64(2), int64(1), object(4)
memory usage: 13.4+ KB
```

```
In [3]: X = tips.drop("tip", axis=1)
   ...: y = tips[“tip”]
```

The Stats

The Statistics: linear model

```
>>> model = LinearRegression()

>>> model.fit(X, y)
```

The Statistics: linear model

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>>> model.fit(X, y)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
  File "sklearn/linear_model/base.py", line 427, in fit
    y_numeric=True, multi_output=True)
  File "sklearn/utils/validation.py", line 510, in check_X_y
    ensure_min_features, warn_on_dtype, estimator)
  File "sklearn/utils/validation.py", line 393, in check_array
    array = array.astype(np.float64)
ValueError: could not convert string to float: 'Dinner'
```

The Statistics: linear model

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```

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$$\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T\boldsymbol{X}\right)^{-1}\boldsymbol{X}^T\boldsymbol{y}$$

Aside: R vs. Python

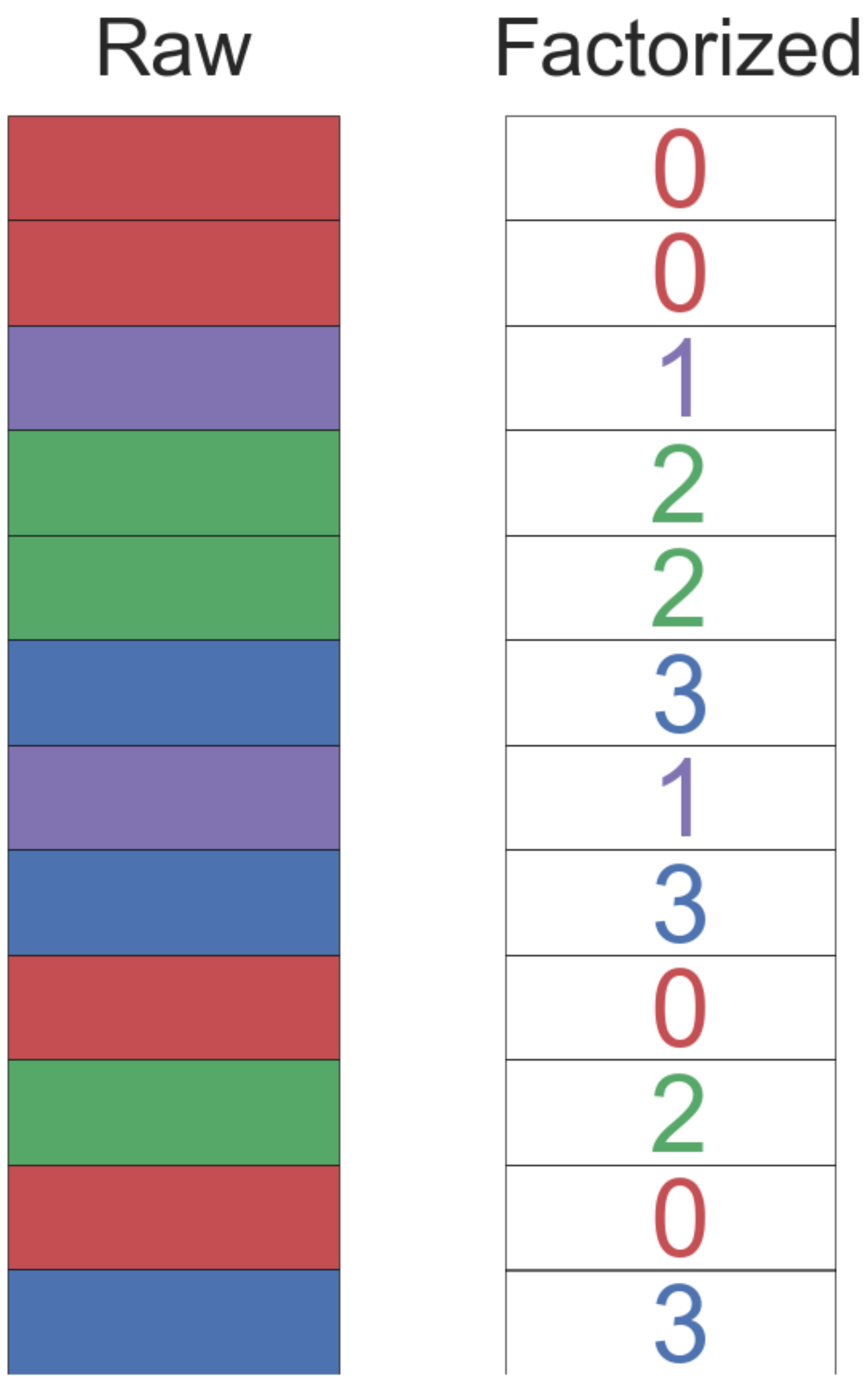
```
> lm(tip ~ ., tips)

Call:
lm(formula = tip ~ ., data = tips)

Coefficients:
(Intercept)   total_bill      sexMale    smokerYes       daySat       daySun
    0.80382      0.09449     -0.03244     -0.08641     -0.12146     -0.02548
    dayThur    timeLunch         size
   -0.16226      0.06813      0.17599
```

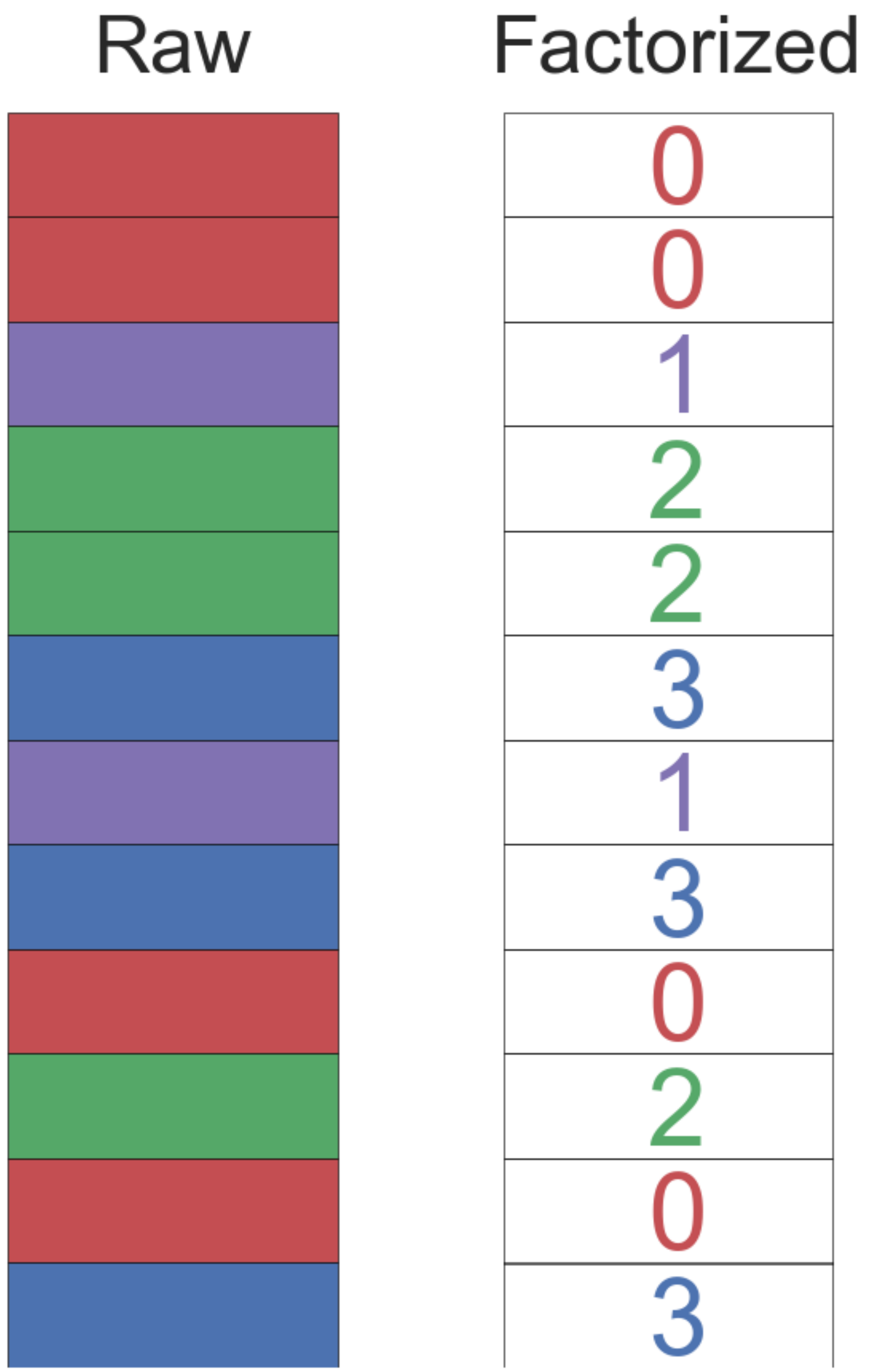
transformations

transformations: `pd.factorize`



transformations: `pd.factorize`

```
In [4]: codes, labels = pd.factorize(tips['day'])
   ...: codes
   ...:
Out[4]:
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       ...
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2])
```



transformations: `pd.factorize`

```
In [5]: X_factorized = X.copy()
   ...: columns = ['sex', 'smoker', 'day', 'time']
   ...: X_factorized[columns] = X[columns].apply(lambda x: pd.factorize(x)[0])
   ...:
   ...: lm = LinearRegression()
   ...: lm.fit(X_factorized, y)
   ...: lm.coef_
Out[5]:
array([ 0.09407595, -0.02921608, -0.08104051, -0.00783382,  0.00572054,
        0.17936677])
```

transformations: `pd.factorize`

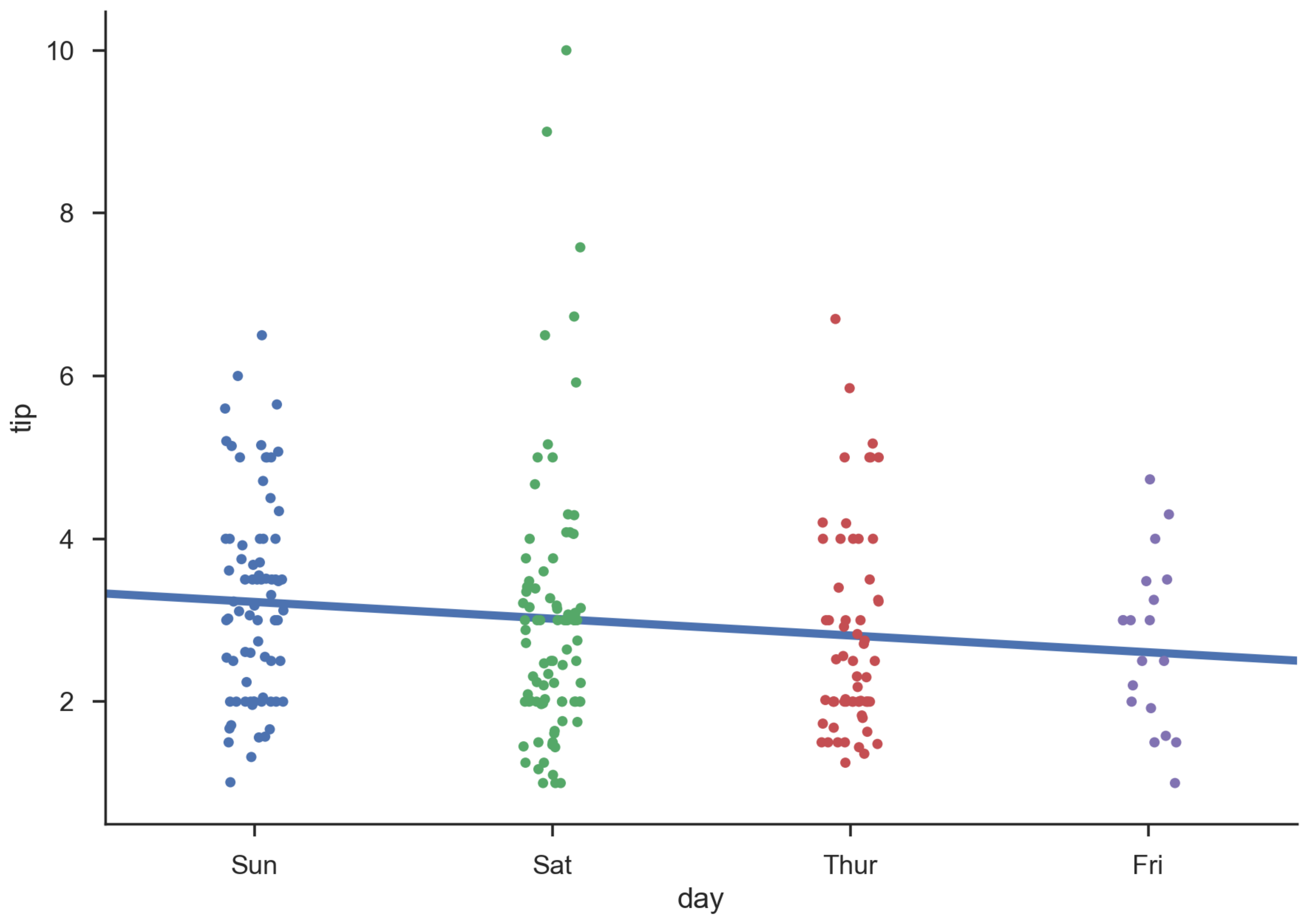
That "worked", but

- Ordering becomes important
- All categories are equally spaced
- All categories have equal effects*

$$\frac{\Delta \text{tip}}{\Delta(\text{Sun.} \to \text{Sat.})} = \frac{\Delta \text{tip}}{\Delta(\text{Thur.} \to \text{Fri.})}$$

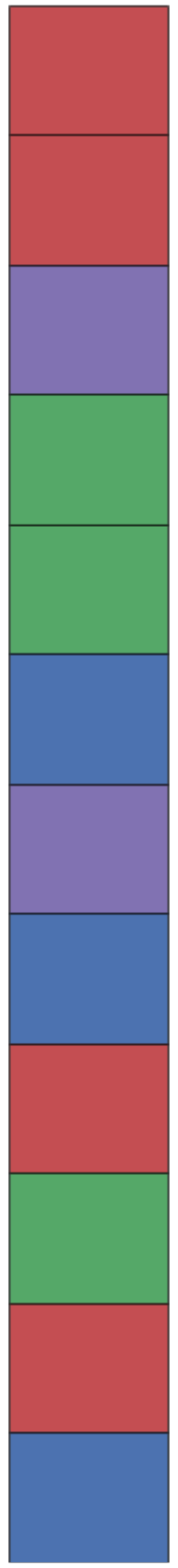
* for our linear model

transformations: `pd.factorize`



transformations: Dummy Encoding

Raw

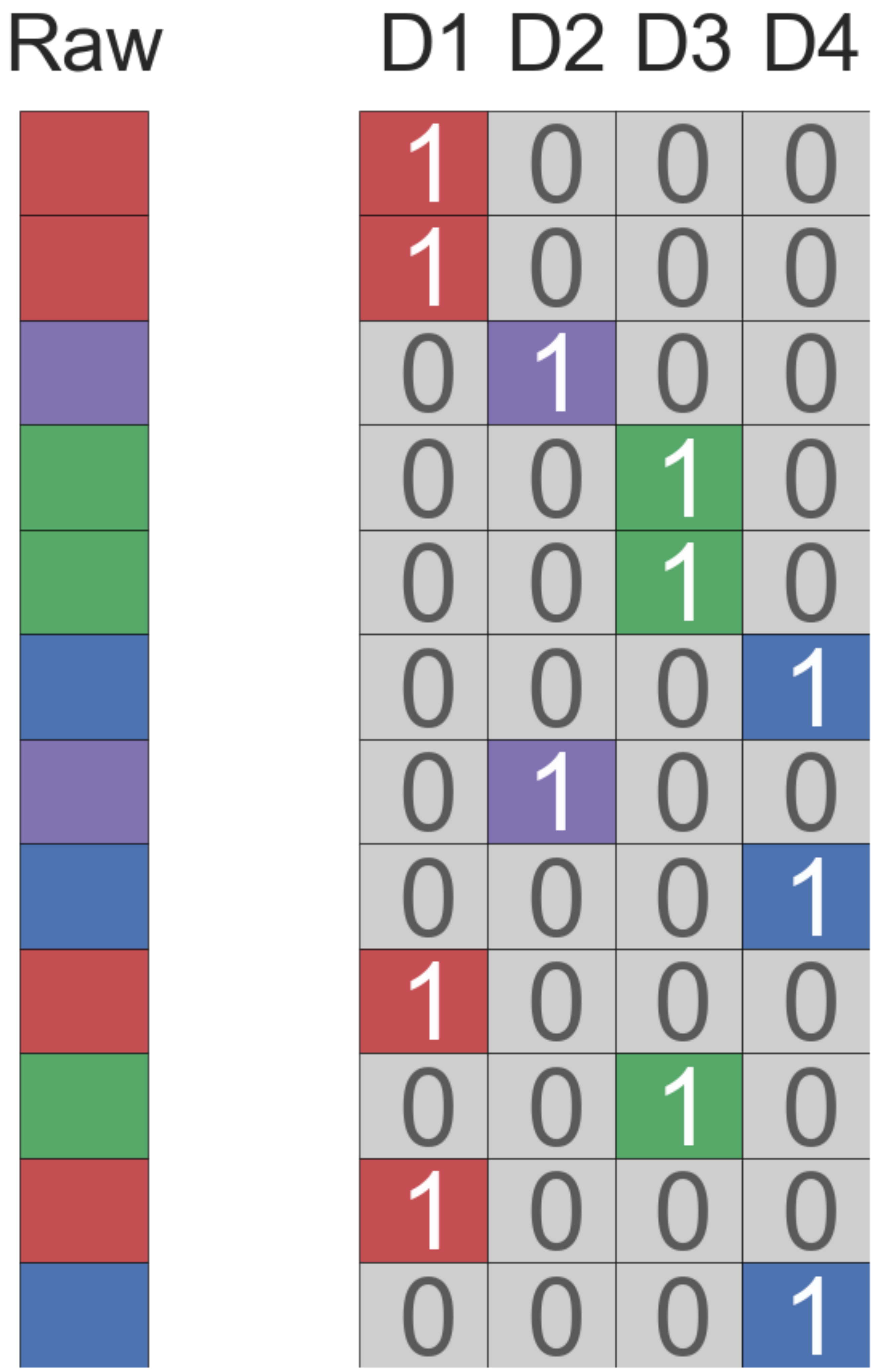


D1	D2	D3	D4
1	0	0	0
1	0	0	0
0	1	0	0
0	0	1	0
0	0	1	0
0	0	0	1
0	1	0	0
0	0	0	1
1	0	0	0
0	0	1	0
1	0	0	0
0	0	0	1

transformations: Dummy Encoding

```
In [6]: pd.get_dummies(df.day)
Out[6]:
     Fri  Sat  Sun  Thur
0    0.0  0.0  1.0   0.0
1    0.0  0.0  1.0   0.0
2    0.0  0.0  1.0   0.0
3    0.0  0.0  1.0   0.0
4    0.0  0.0  1.0   0.0
..   ...  ...  ...   ...
239  0.0  1.0  0.0   0.0
240  0.0  1.0  0.0   0.0
241  0.0  1.0  0.0   0.0
242  0.0  1.0  0.0   0.0
243  0.0  0.0  0.0   1.0

[244 rows x 4 columns]
```



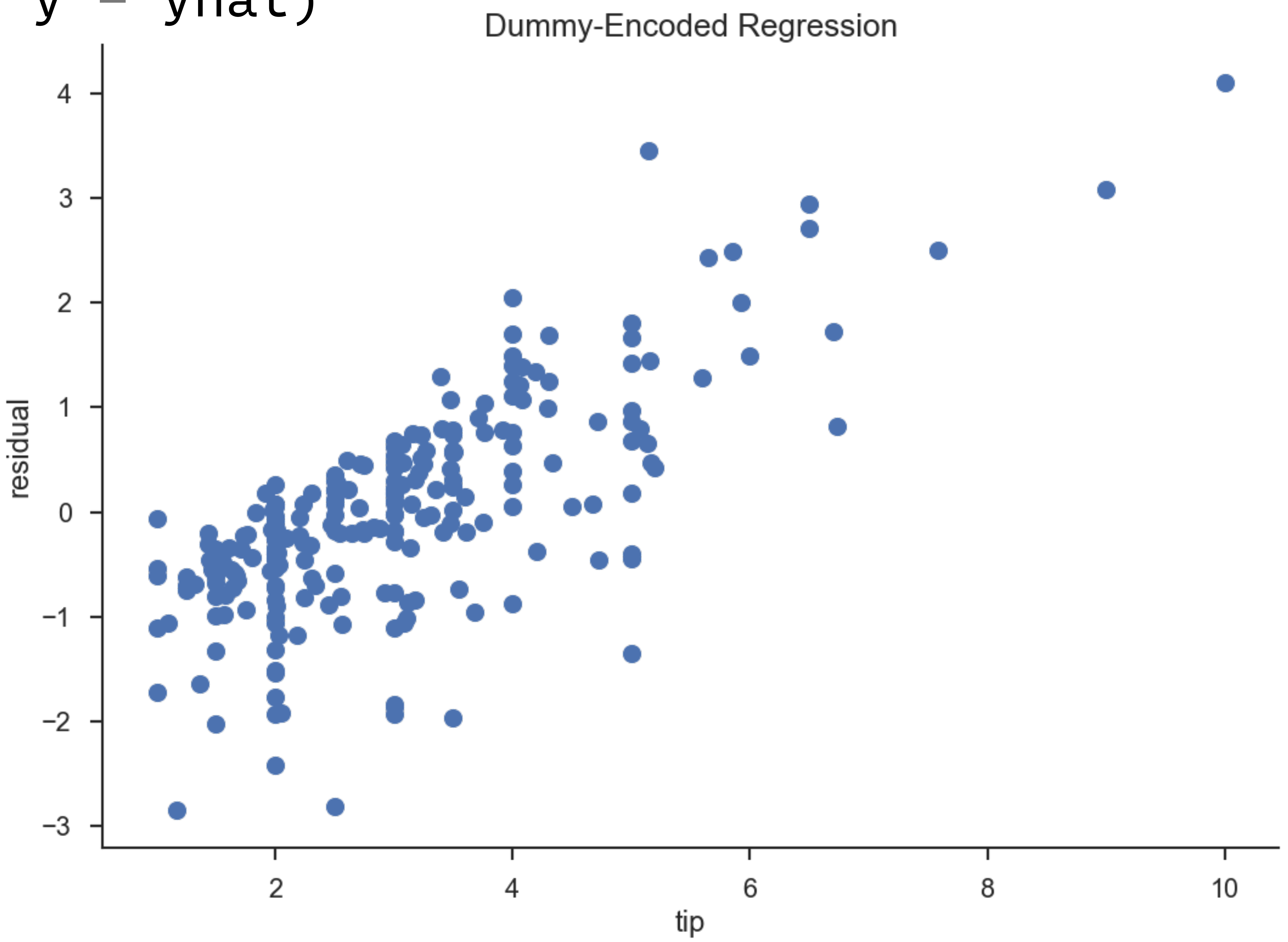
transformations: `pd.get_dummies`

```
In [7]: X_dummies = pd.get_dummies(X)
   ...: X_dummies.head()
Out[7]:
   total_bill  size  sex_Female  sex_Male  smoker_No  smoker_Yes  day_Fri  \
0       16.99     2         1.0       0.0        1.0         0.0      0.0
1       10.34     3         0.0       1.0        1.0         0.0      0.0
2       21.01     3         0.0       1.0        1.0         0.0      0.0
3       23.68     2         0.0       1.0        1.0         0.0      0.0
4       24.59     4         1.0       0.0        1.0         0.0      0.0

   day_Sat  day_Sun  day_Thur  time_Dinner  time_Lunch
0      0.0      1.0       0.0          1.0         0.0
1      0.0      1.0       0.0          1.0         0.0
2      0.0      1.0       0.0          1.0         0.0
3      0.0      1.0       0.0          1.0         0.0
4      0.0      1.0       0.0          1.0         0.0
```

transformations: `pd.get_dummies`

```
In [8]: from sklearn.linear_model import LinearRegression
   ...: lm = LinearRegression().fit(X_dummies, y)
   ...:
   ...: yhat = lm.predict(X_dummies)
   ...: plt.scatter(y, y - yhat)
```



DummyEncoder

`DummyEncoder`

The last solution is brittle

1. We can't easily go from dummies back to categoricals

2. Doesn't integrate with scikit-learn `Pipeline` objects.

3. If working with a larger dataset and `partial_fit`, codes could be missing from subsets of the data.

4. Memory inefficient if there are many records relative to distinct categories

DummyEncoder

Step 1: Categorize

```
In [9]: columns = ['sex', 'smoker', 'day', 'time']
   ...: tips[columns] = tips[columns].apply(lambda x: x.astype('category'))
   ...: tips.info()

In [9]: tips.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 244 entries, 0 to 243
Data columns (total 7 columns):
total_bill    244 non-null float64
tip           244 non-null float64
sex           244 non-null category
smoker        244 non-null category
day           244 non-null category
time          244 non-null category
size          244 non-null int64
dtypes: category(4), float64(2), int64(1)
memory usage: 6.8 KB
```

Stores values information in the type

- Categories
- Order

DummyEncoder

Step 2: Transformer

DummyEncoder

```python
import numpy as np
import pandas as pd
from sklearn.pipeline import TransformerMixin


class DummyEncoder(TransformerMixin):
    ...
```

DummyEncoder

```python
class DummyEncoder(TransformerMixin):

    def fit(self, X, y=None):
        self.index_ = X.index
        self.columns_ = X.columns
        self.cat_columns_ = X.select_dtypes(include=['category']).columns
        self.non_cat_columns_ = X.columns.drop(self.cat_columns_)

        self.cat_map_ = {col: X[col].cat for col in self.cat_columns_}

        left = len(self.non_cat_columns_)
        self.cat_blocks_ = {}
        for col in self.cat_columns_:
            right = left + len(X[col].cat.categories)
            self.cat_blocks_[col], left = slice(left, right), right
        return self
```

DummyEncoder

```python
class DummyEncoder(TransformerMixin):
    ...

    def transform(self, X, y=None):
        return np.asarray(pd.get_dummies(X))
```

DummyEncoder

```
class DummyEncoder(TransformerMixin):
    ...

    def inverse_transform(self, X):
        non_cat = pd.DataFrame(X[:, :len(self.non_cat_columns_)],
                               columns=self.non_cat_columns_)
        cats = []
        for col, cat in self.cat_map_.items():
            slice_ = self.cat_blocks_[col]
            codes = X[:, slice_].argmax(1)
            series = pd.Series(pd.Categorical.from_codes(
                codes, cat.categories, ordered=cat.ordered
            ), name=col)
            cats.append(series)
        df = pd.concat([non_cat] + cats, axis=1)[self.columns_]
        return df
```

DummyEncoder

```
In [14]: X = tips.drop('tip', axis=1)
    ...: y = tips['tip']
    ...:
    ...: pipe = make_pipeline(
    ...:     DummyEncoder(),
    ...:     LinearRegression()
    ...: )
    ...: pipe.fit(X, y)

Out[14]: Pipeline(
    steps=[('dummyencoder',
           <DummyEncoder object at 0x10992af60>),
          ('linearregression',
           LinearRegression(copy_X=True, fit_intercept=True,
                            n_jobs=1, normalize=False))])
```

Takeaway

Takeaway

- That particular transformer isn't the point
- Pandas is evolving further, more bridges needed
- Be comfortable writing the shims (or write a library to do it?)

Takeaway

https://mail.python.org/mailman/listinfo/pandas-dev

https://github.com/pydata/pandas