Introduction to Data Science using Python

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Day Two

Day 1	Day 2
Why Python for Data Science?	Data visualization
A Python Primer	Statistical modeling
Pandas for data munging	Machine learning

Topic	Notebook
Python primer	00_python_primer
Numpy and the data science stack (not covered)	01_python_tools_ds
Pandas for data munging	02_python_pandas
Data visualization	03_python_vis
Statistical modeling	04_python_stat
Machine learning	05_python_learning

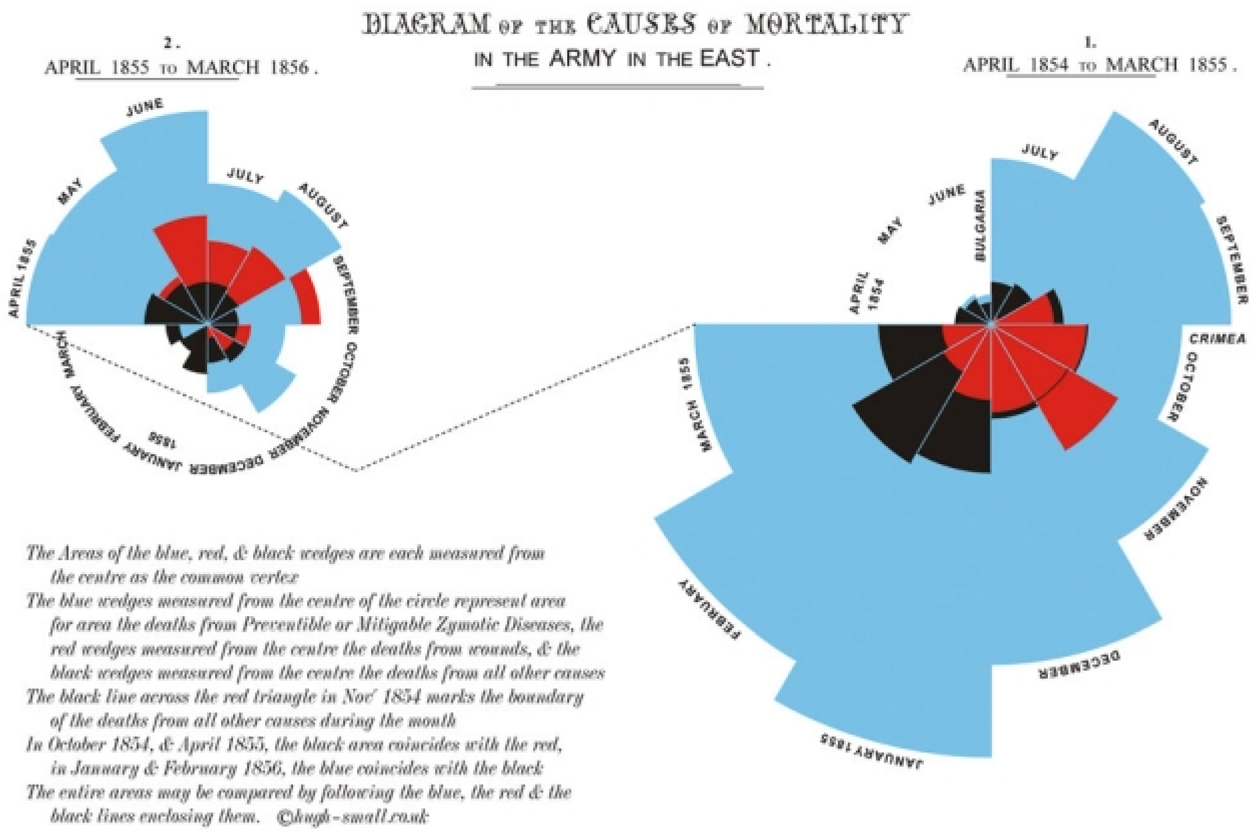
Data visualization

Data visualization is a basic task in data exploration and understanding.

Data visualization provides an opportunity to enhance communication of the story within the data.

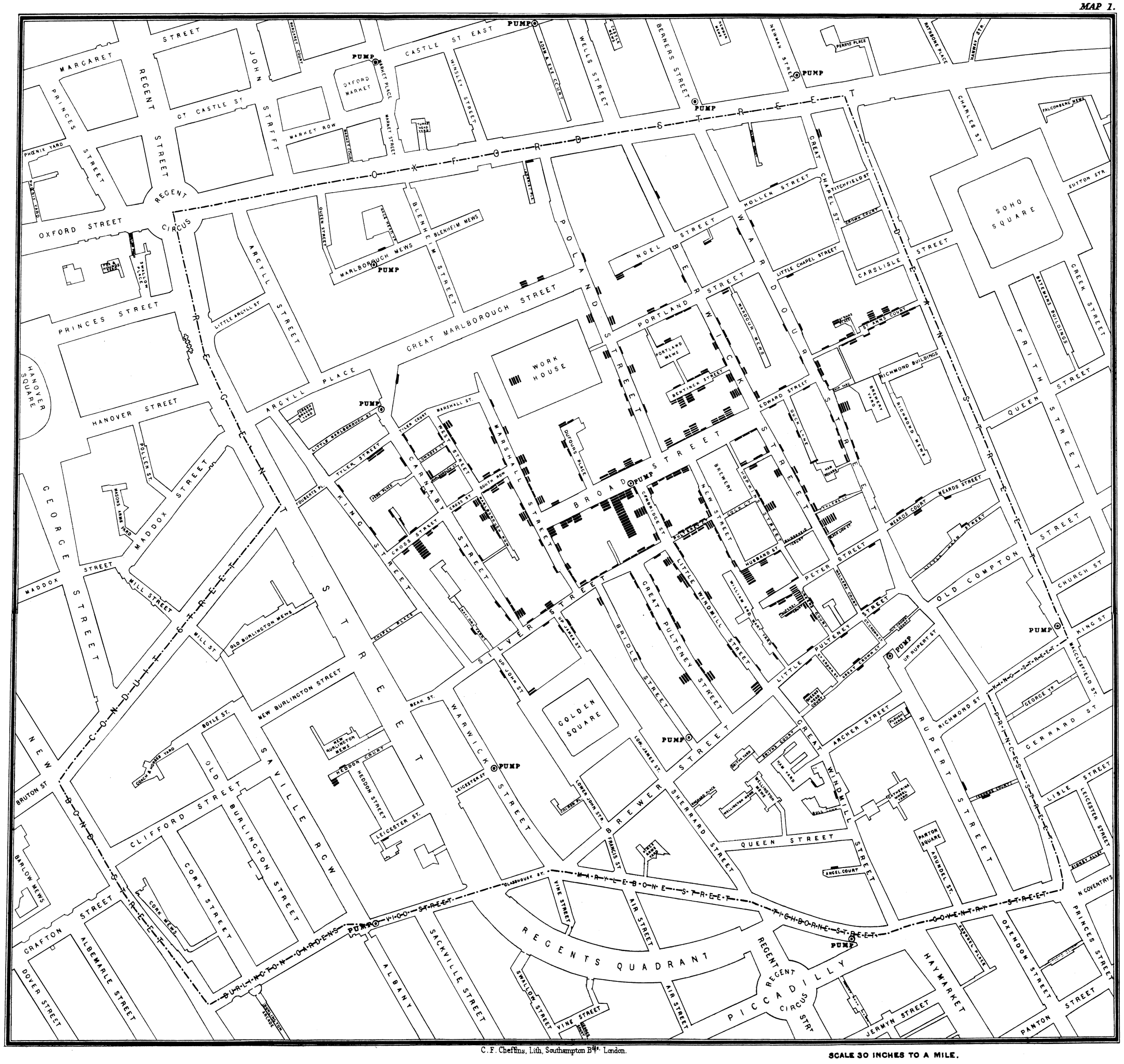
A visual representation of the data and our innate ability at pattern recognition can help reveal the complexities in a cognitively accessible way.

Florence Nightangle, Crimean War



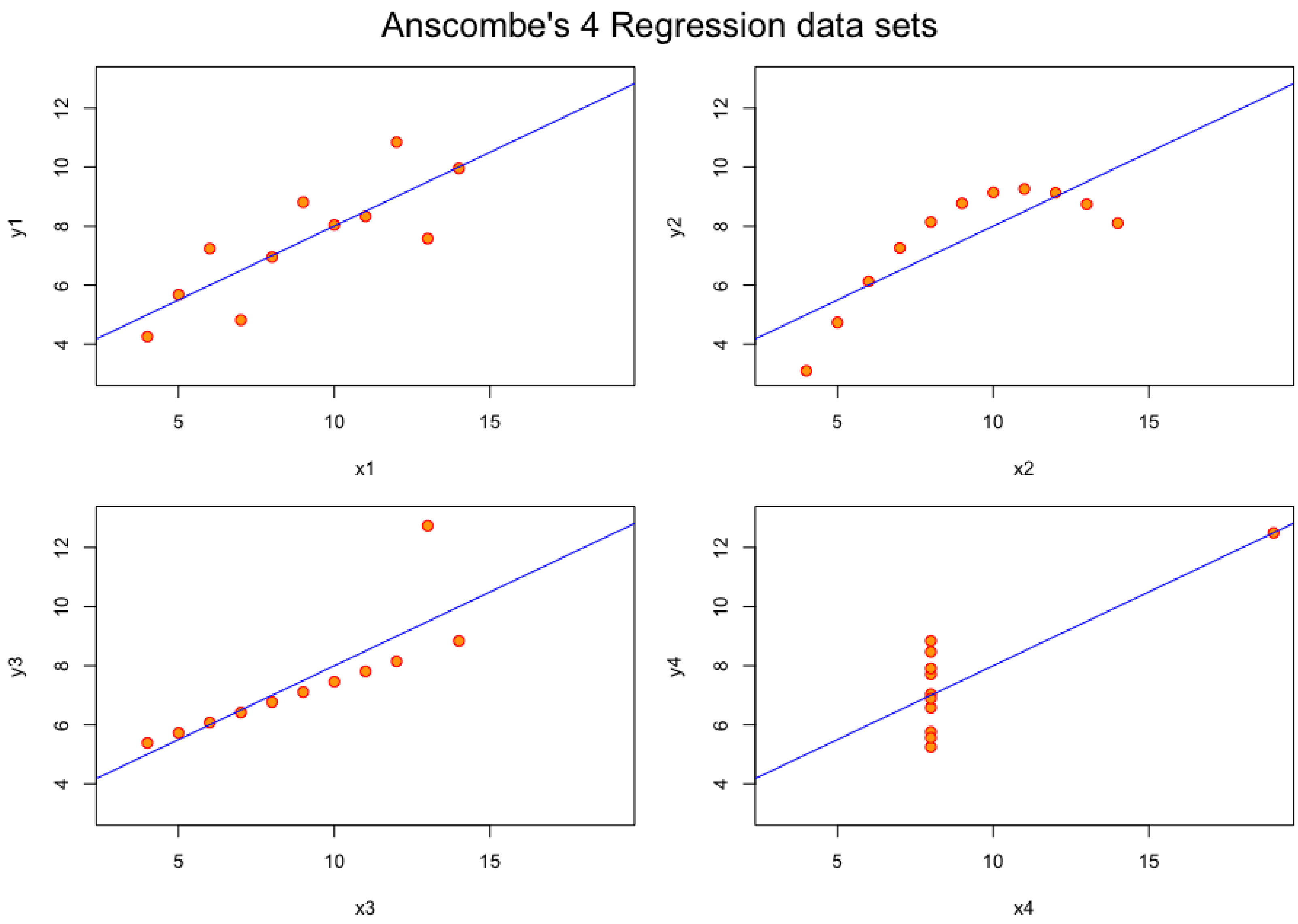
+ Plotting war dead in Crimean war + Developed "rose plot" + Made point that most deaths were due to sepsis in hospital

John Snow, 1854

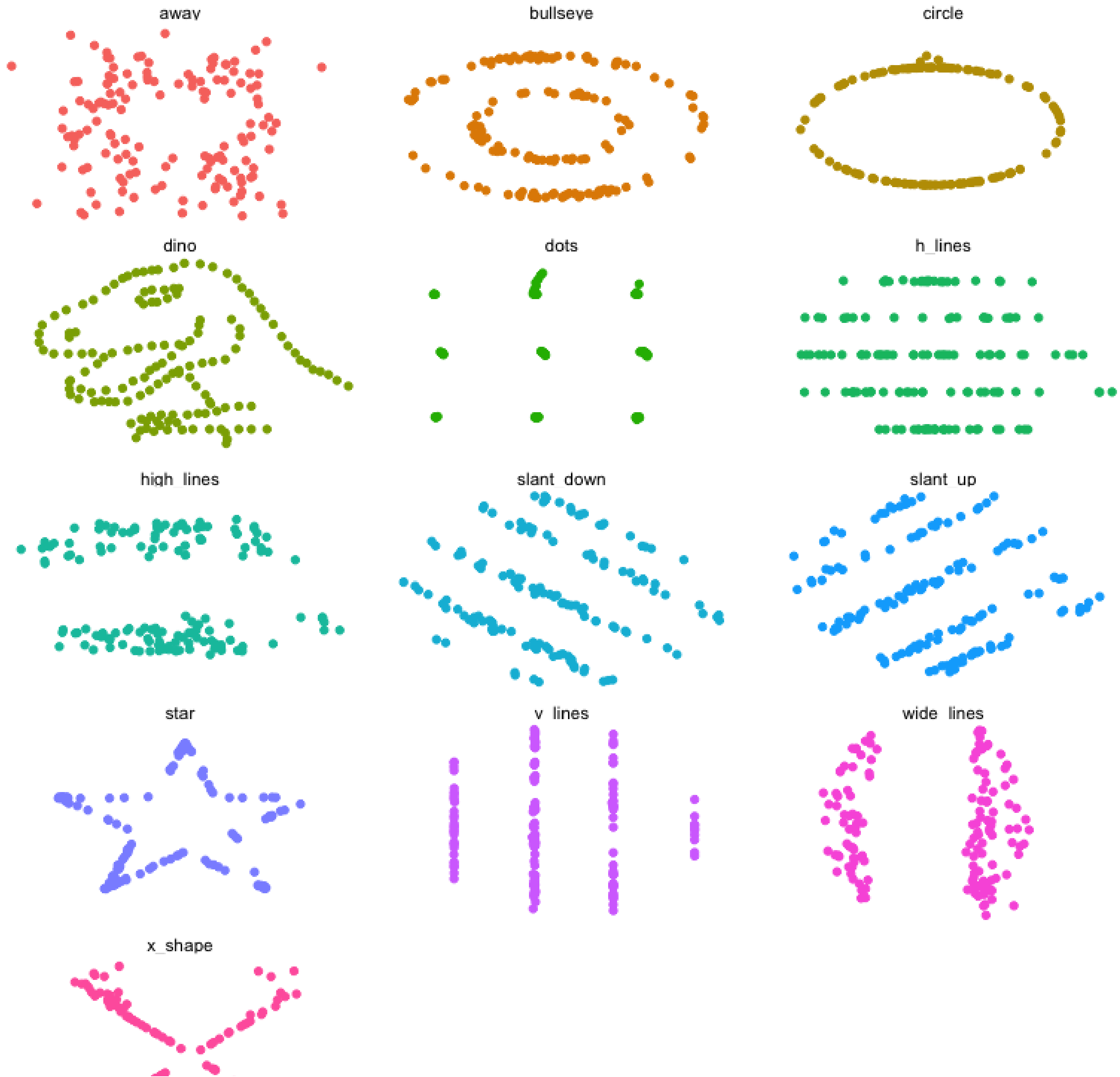


+ Cholera outbreak in London + Spatial mapping of households with cholera showed clustering + Helped identify wells that were contaminated

Why do we need visualization on top of analytics?



In both sets of plots, all the variables have the same means and variances and the same pairwise correlations


away
bullseye
circle
dino
dots
h_lines
high_lines
slant_down
slant_up
star
v_lines
wide_lines
x_shape

Strip plot	Boxplot	Violin plot

General concepts

Begin with the consumer in mind

- You have a deep understanding of the data you're presenting
- The person seeing the visualization **doesn't**
- Develop simpler visualizations first that are easier to explain

Tell a story

- Make sure the graphic is clear
- Make sure the main point you want to make "pops"

A matter of perception

- Color (including awareness of color deficiencies)
- Shape
- Fonts

Our starting point

We will start our journey today from the `pandas` `DataFrame`

- Rectangular set of data
- Different columns can be of different types

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- Rectangular set of data
- Different columns can be of different types

We will see different functions applied to `DataFrame` objects (on the right)

We will see different functions from different packages applied on `DataFrame` objects (on the left)

Python setup

In [4]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
```

Python setup

In [4]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
```

In [36]:

```
sns.set_context('notebook')
sns.set_style('white', {'font.family':'Futura', 'text.color':'1'})
```

Python setup

In [37]:

```
mtcars = pd.read_csv('data/mtcars.csv')

mtcars.head()
```

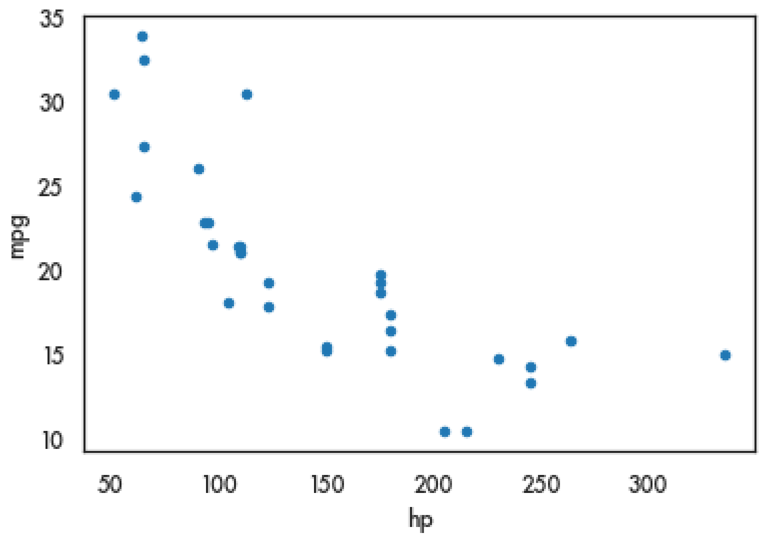
Out[37]:

	make	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
0	Mazda RX4	21.0	6	160.0	110	3.90	2.620	16.46	0	1	4	4
1	Mazda RX4 Wag	21.0	6	160.0	110	3.90	2.875	17.02	0	1	4	4
2	Datsun 710	22.8	4	108.0	93	3.85	2.320	18.61	1	1	4	1
3	Hornet 4 Drive	21.4	6	258.0	110	3.08	3.215	19.44	1	0	3	1
4	Hornet Sportabout	18.7	8	360.0	175	3.15	3.440	17.02	0	0	3	2

In [38]:

```
mtcars.plot(x = 'hp', y = 'mpg',
            kind = 'scatter')
```

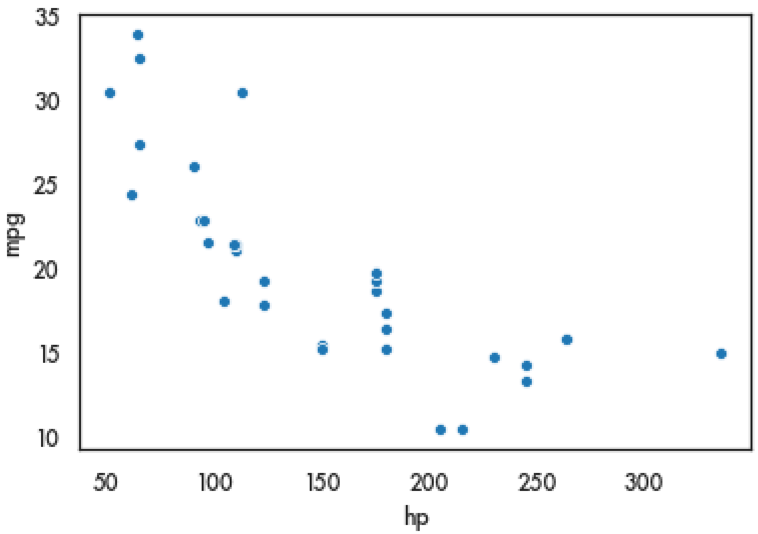
Out[38]: <matplotlib.axes._subplots.AxesSubplot at 0x12ea0ae20>



In [39]:

```
sns.scatterplot(data=mtcars,
                x = 'hp', y = 'mpg')
```

Out[39]: <matplotlib.axes._subplots.AxesSubplot at 0x12f753cd0>



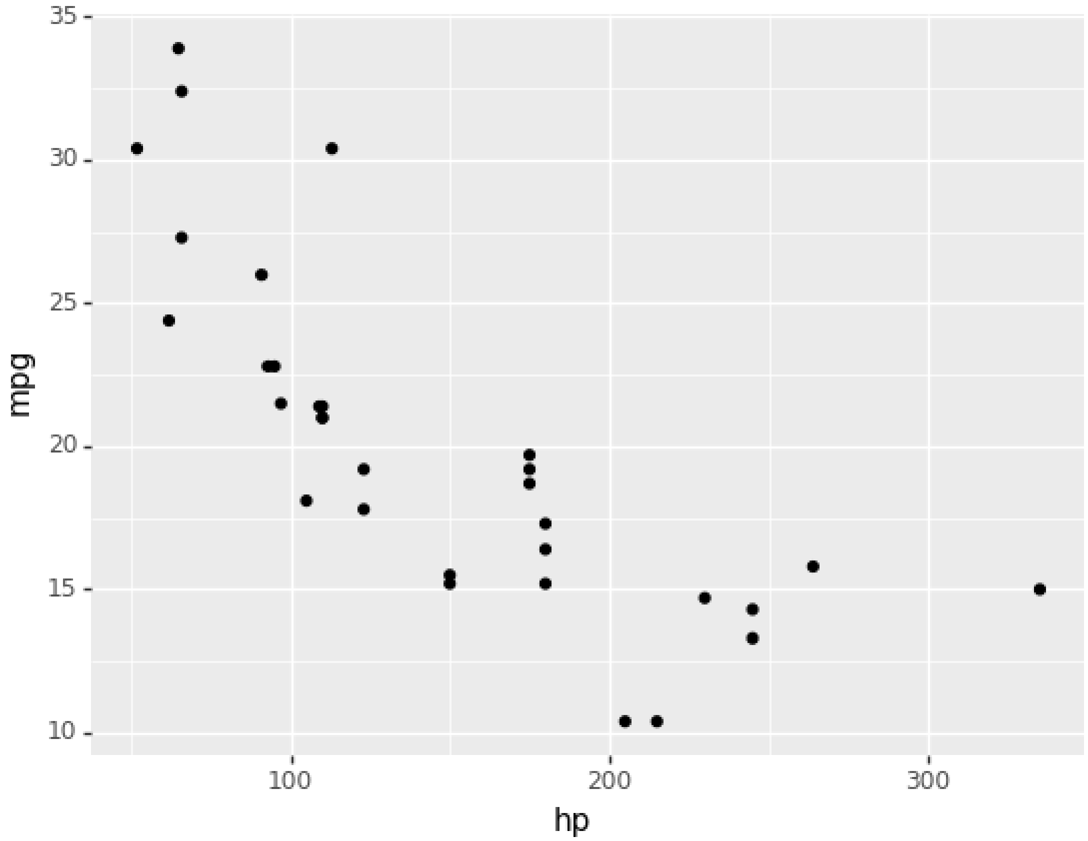
35
30
25
20
15
10
mpg
50
100
150
200
250
300
hp

A ggplot clone

In [40]:

```
from plotnine import *

(ggplot(mtcars) +
    aes(x = 'hp', y = 'mpg')+
    geom_point())
```



Out[40]:

```
<ggplot: (317677087)>
```

Some dynamic options

In [41]:

```
import plotly.express as px

fig = px.scatter(mtcars, x = 'hp', y = 'mpg')
fig.show()
```

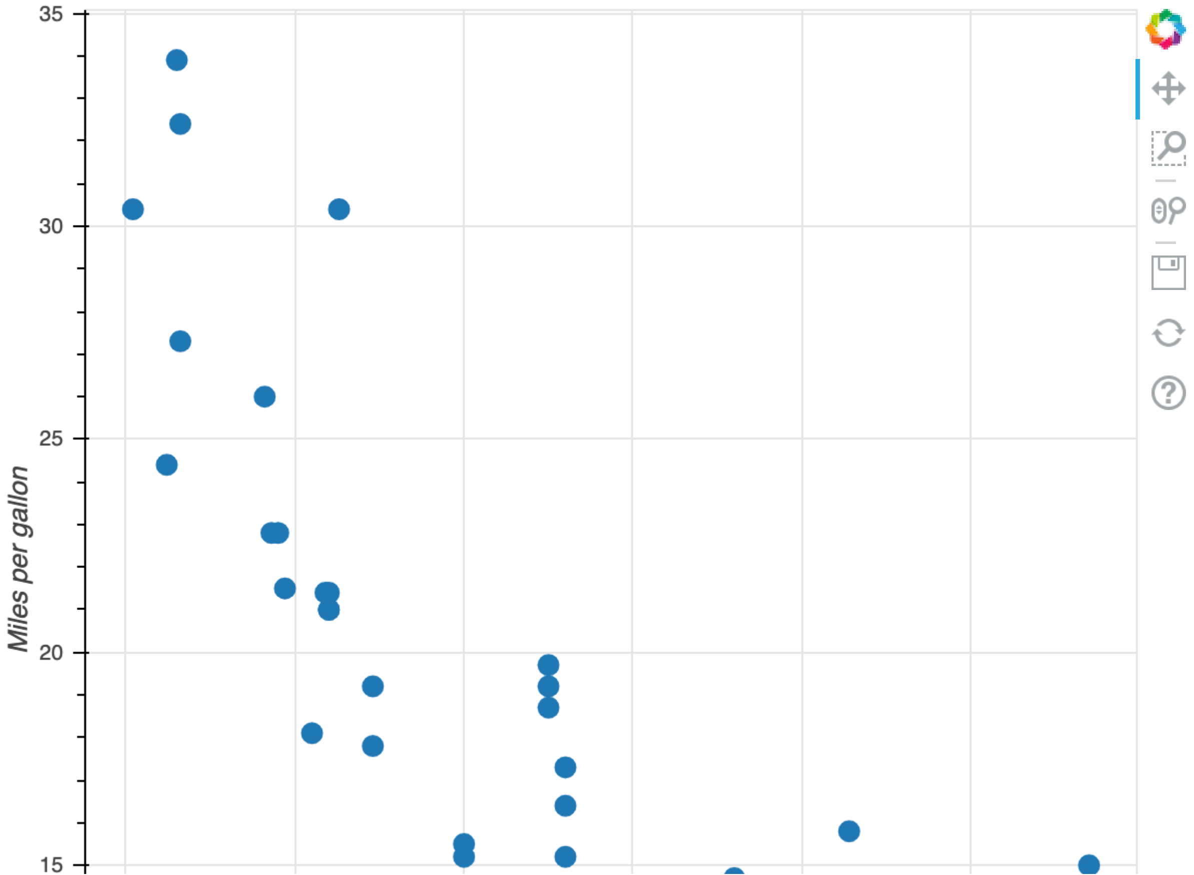
In [42]:

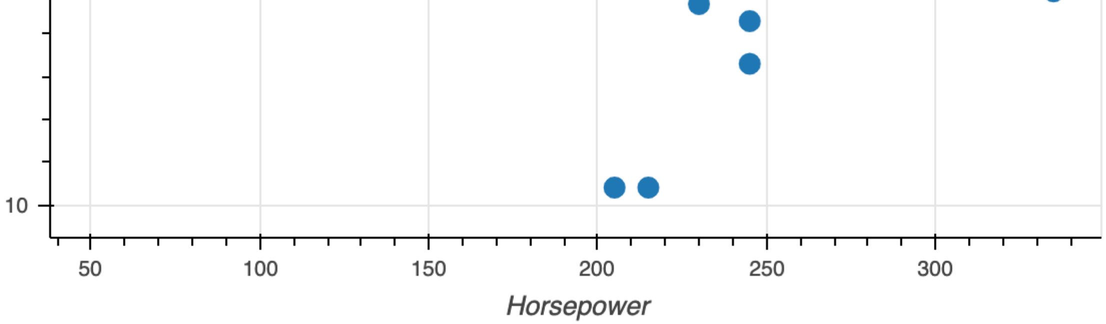
```
from bokeh.plotting import figure, output_file
from bokeh.io import output_notebook, show
output_notebook()
p = figure()
p.xaxis.axis_label = 'Horsepower'
p.yaxis.axis_label = 'Miles per gallon'

p.circle(mtcars['hp'], mtcars['mpg'], size=10);

show(p)
```

BokehJS 2.0.1 successfully loaded.



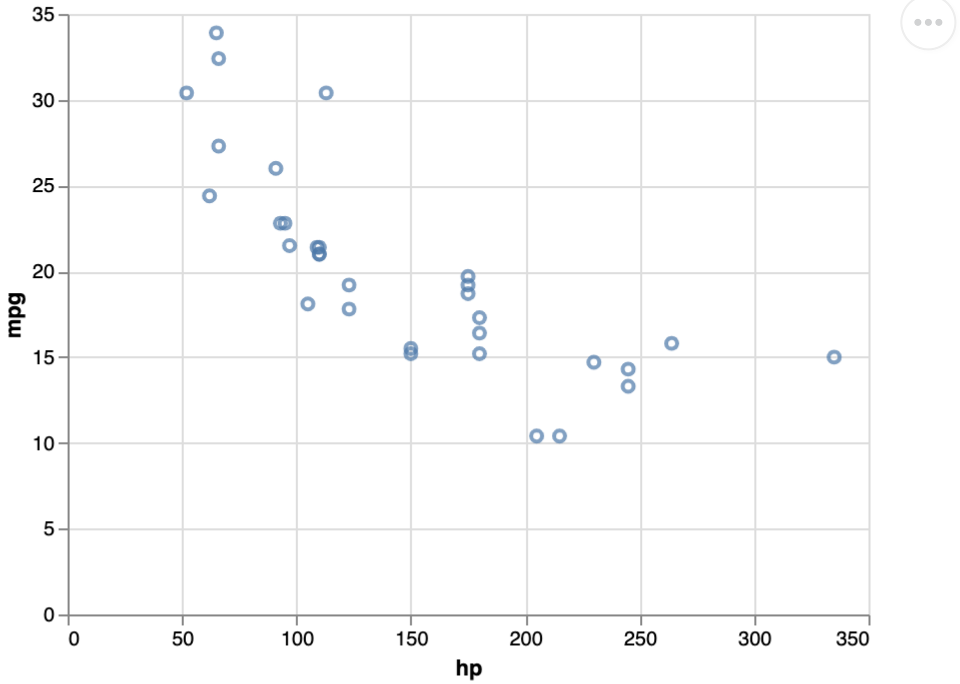

10
50
100
150
200
250
300
Horsepower

In [43]:

```python
import altair as alt

alt.Chart(mtcars).mark_point().encode(
    x='hp',
    y='mpg'
).interactive()
```

Out[43]:



Static plots

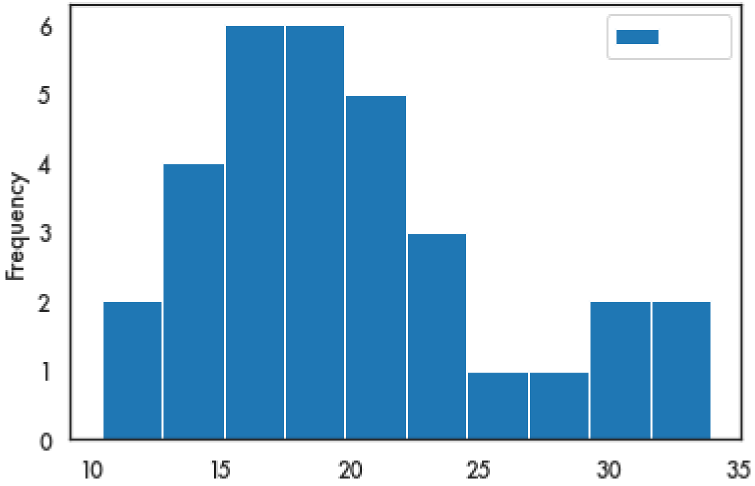
A pathway to learning (Chris Moffit)

1. Learn the basic matplotlib terminology, specifically what is a `Figure` and an `Axes` .
2. Always use the object-oriented interface. Get in the habit of using it from the start of your analysis. (*not really getting into this, but basically don't use the Matlab form that was originally used*)
3. Start your visualizations with basic pandas plotting.
4. Use seaborn for the more complex statistical visualizations.
5. Use matplotlib to customize the pandas or seaborn visualization.

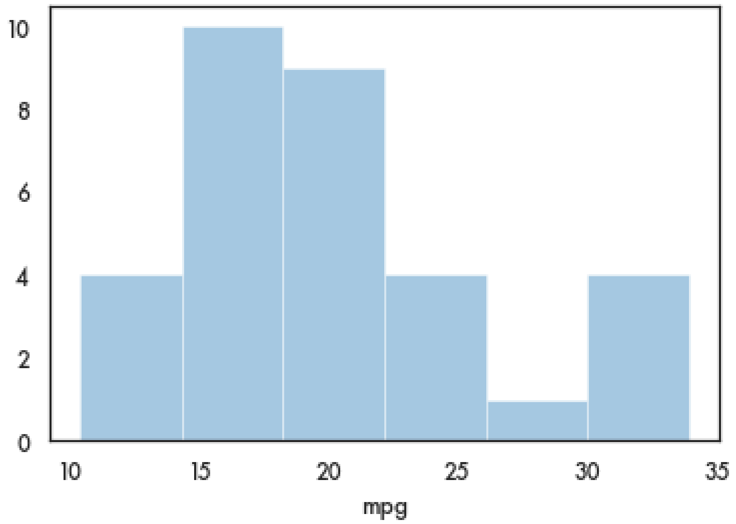
Histogram

In [44]:
```
#mtcars.plot.hist(y = 'mpg');
#mtcars['mpg'].plot(kind = 'hist')

mtcars.plot(y = 'mpg', kind = 'hist')
plt.show()
```



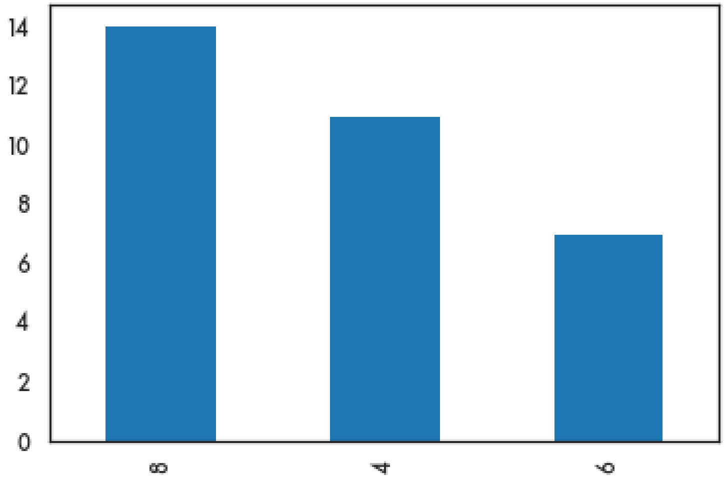
In [45]:
```
sns.distplot(mtcars.mpg, kde=False)
plt.show()
```


10
8
6
4
2
0
10
15
20
25
30
35
mpg

Bar plot

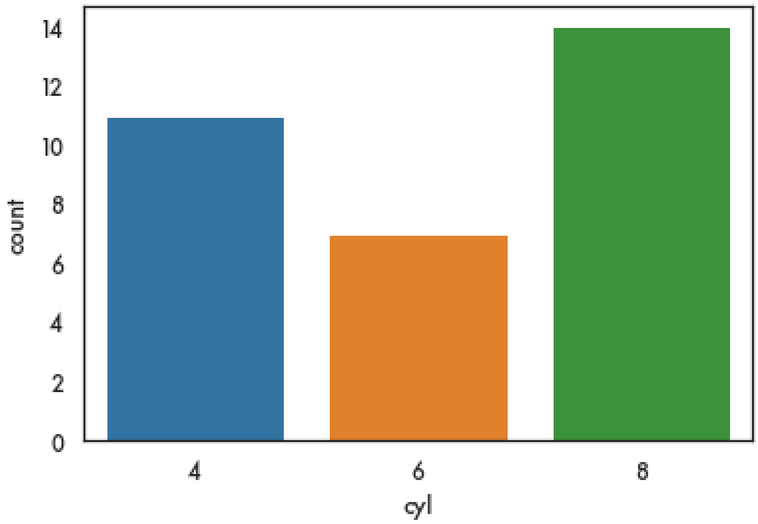
In [46]:

```
mtcars['cyl'].value_counts().plot.bar();
plt.show()
```



In [47]:

```
sns.countplot(data = mtcars, x = 'cyl');
plt.show()
```



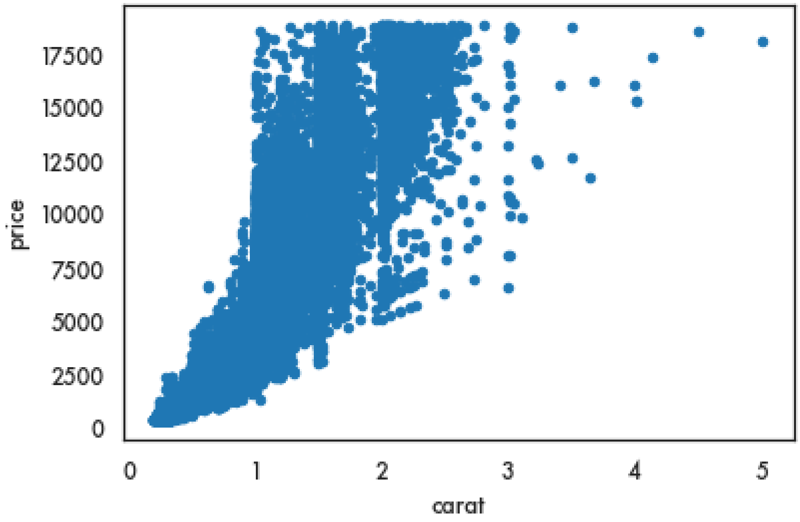
14
12
10
8
6
4
2
0
count
4
6
8
cyl

Scatter plot

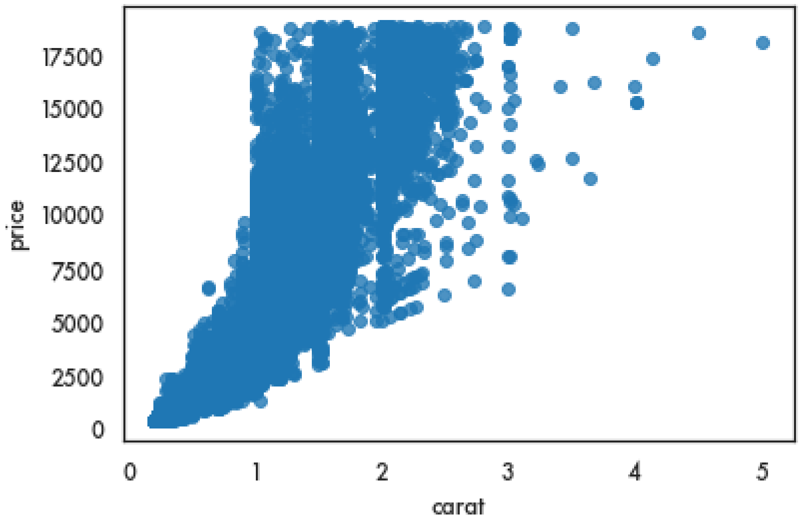
In [48]:
```
diamonds = pd.read_csv('data/diamonds.csv.gz')
```

In [49]:
```
diamonds.plot(x = 'carat', y = 'price',
              kind = 'scatter');

plt.show()
```



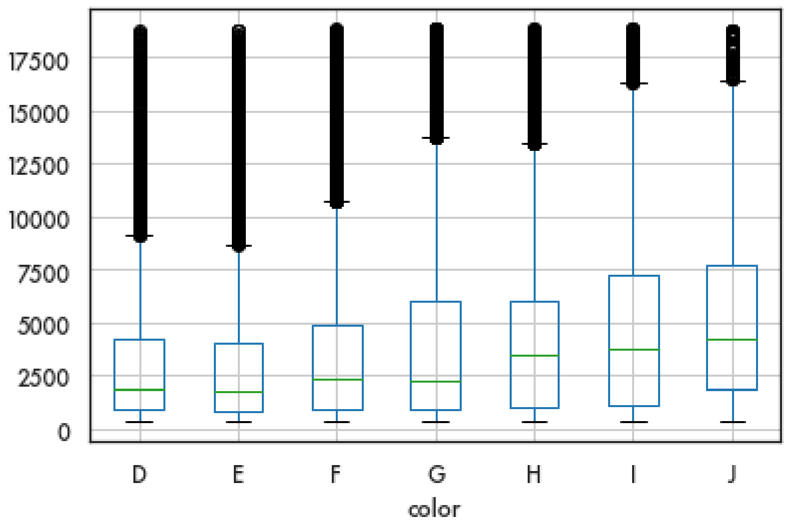
In [50]:
```
sns.regplot(data = diamonds,
            x = 'carat', y = 'price',
            fit_reg=False);
plt.show()
```



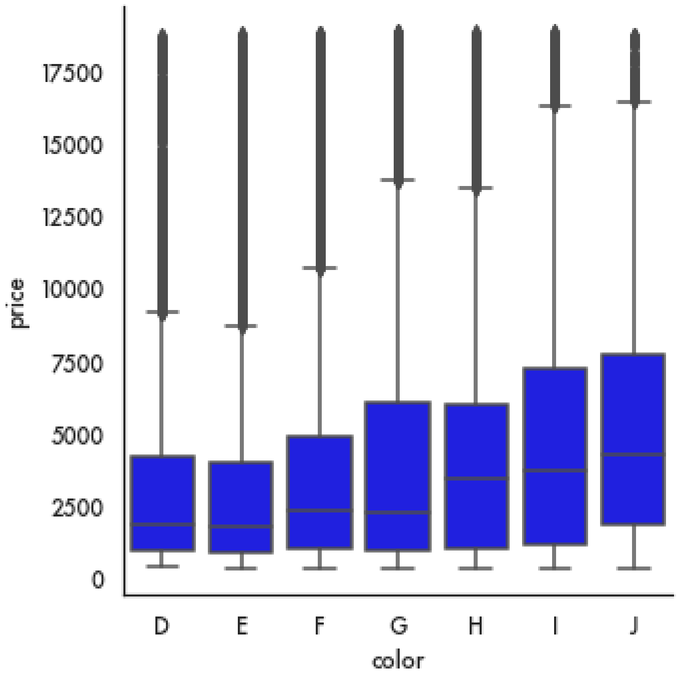
17500
15000
12500
10000
7500
5000
2500
0
price
0
1
2
3
4
5
carat

Box plot

In [51]:
```
diamonds.boxplot(column = 'price', by = 'color');
plt.show()
```

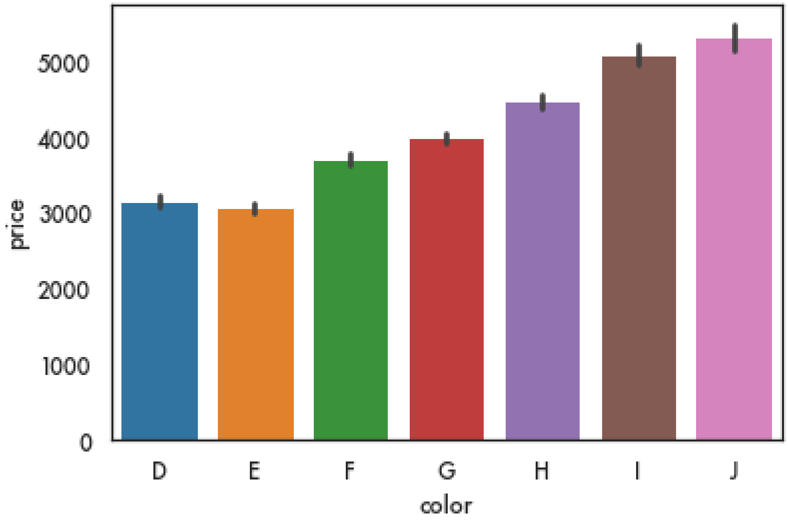


In [52]:
```
ordered_color = ['D','E','F','G','H','I','J']
sns.catplot(data = diamonds, x = 'color', y = 'price',
            order = ordered_color, color = 'blue', kind = 'box');
plt.show()
```


17500
15000
12500
10000
7500
5000
2500
0
price
D
E
F
G
H
I
J
color

Barplot (categorical vs continuous)

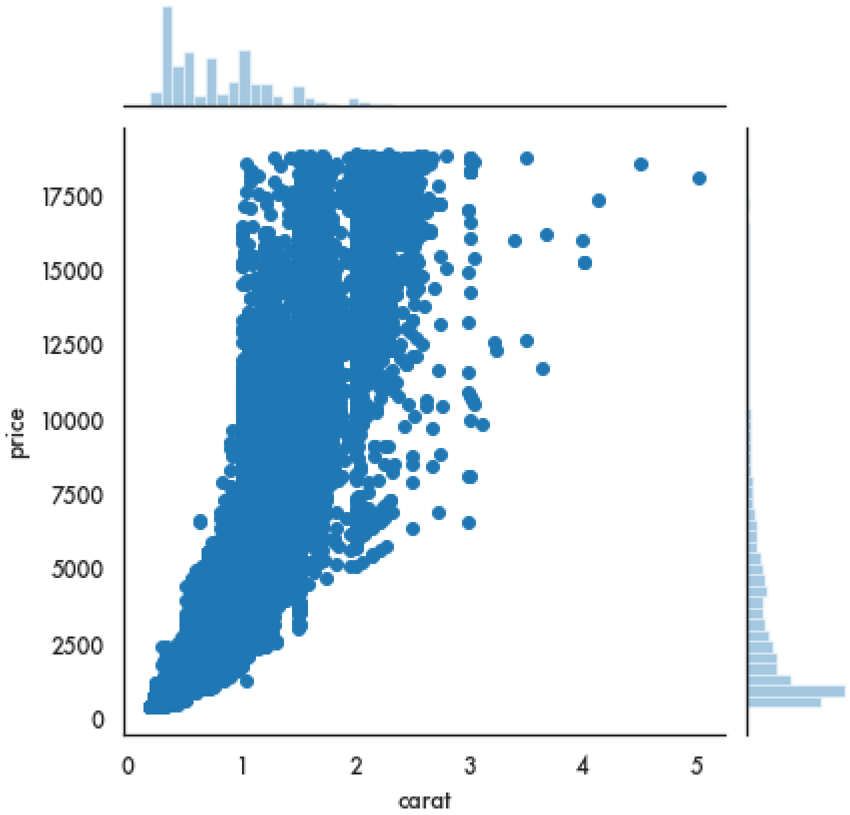
In [53]:
```
ordered_colors = ['D','E','F','G','H','I','J']
sns.barplot(data = diamonds, x = 'color', y = 'price', order = ordered_colors);
plt.show()
```



Joint plot

In [54]:

```
sns.jointplot(data = diamonds, x = 'carat', y = 'price');
plt.show()
```

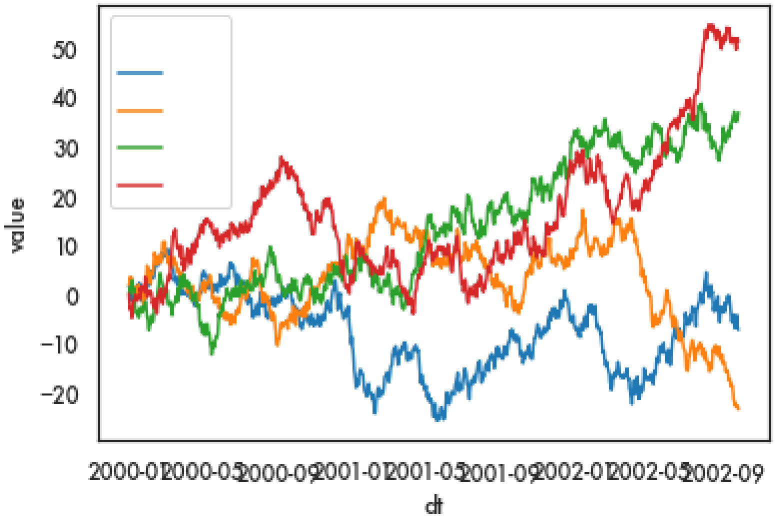


Facets and multiples

Line plots

In [55]:

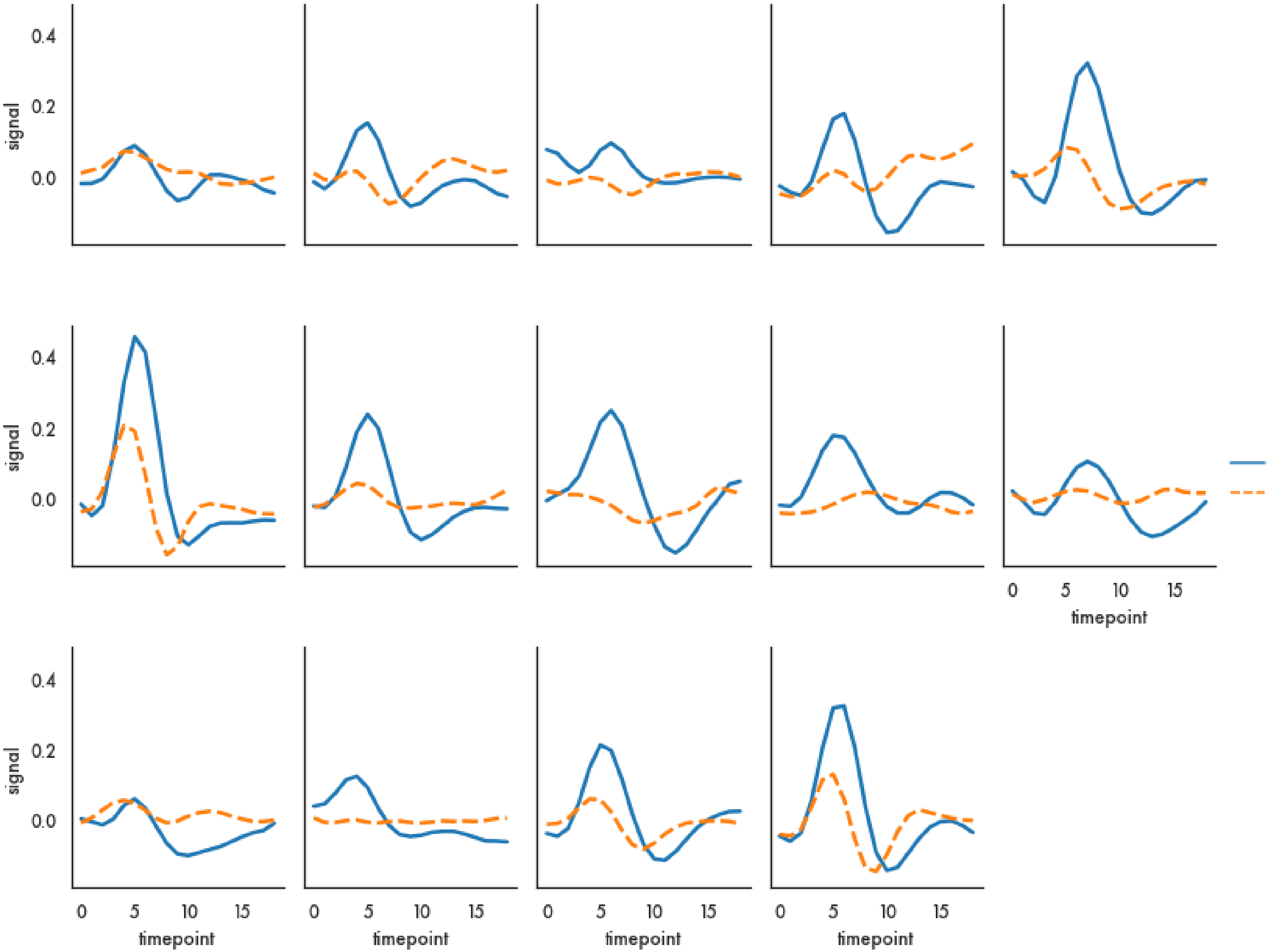
```
ts = pd.read_csv('data/ts.csv')
ts.dt = pd.to_datetime(ts.dt)
sns.lineplot(data = ts, x = 'dt', y = 'value', hue = 'kind');
plt.show()
```



Facets

In [56]:

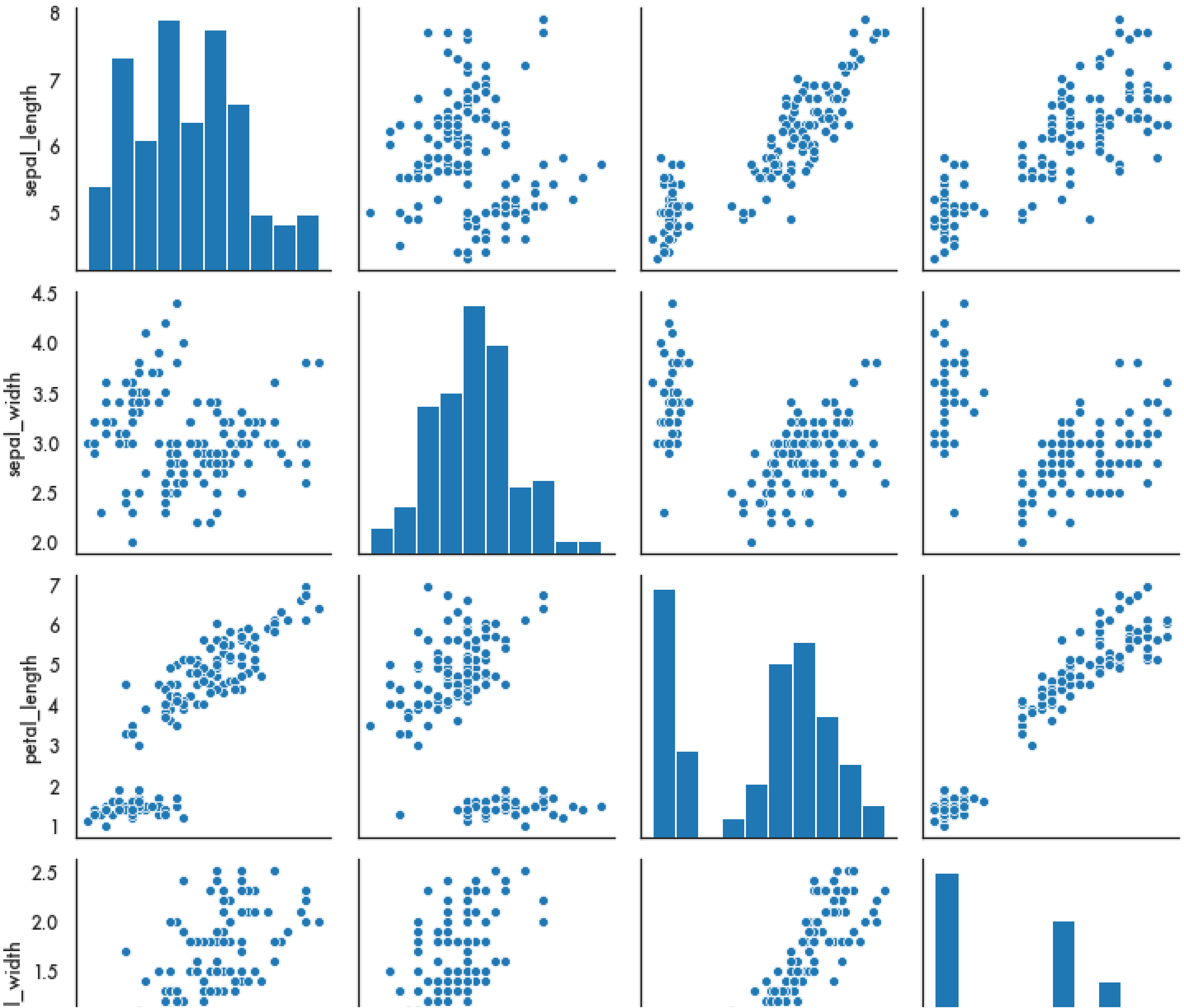
```
fmri = sns.load_dataset('fmri')
sns.relplot(x="timepoint", y="signal", hue="event", style="event",
            col="subject", col_wrap=5,
            height=3, aspect=.75, linewidth=2.5,
            kind="line", data=fmri.query("region == 'frontal'"));
```

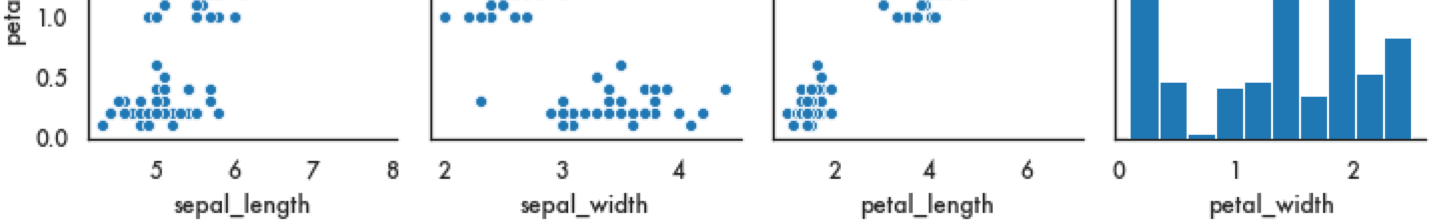

signal
0.4
0.2
0.0
timepoint
0
5
10
15

Pairs plot

In [58]:

```
iris = pd.read_csv('data/iris.csv')
sns.pairplot(data=iris);
```





peta
1.0
0.5
0.0
5
6
7
8
sepal_length
2
3
4
sepal_width
2
4
6
petal_length
0
1
2
petal_width

Statistical modeling

Descriptive statistics

- Several descriptive statistics are available through **numpy**, like `mean`, `std` (standard deviation), `median`, `value_counts` (frequency distribution)
- We take advantage of split-apply-combine to investigate and describe data

In [ ]:

```python
diamonds = pd.read_csv('data/diamonds.csv.gz')
```

In [62]:

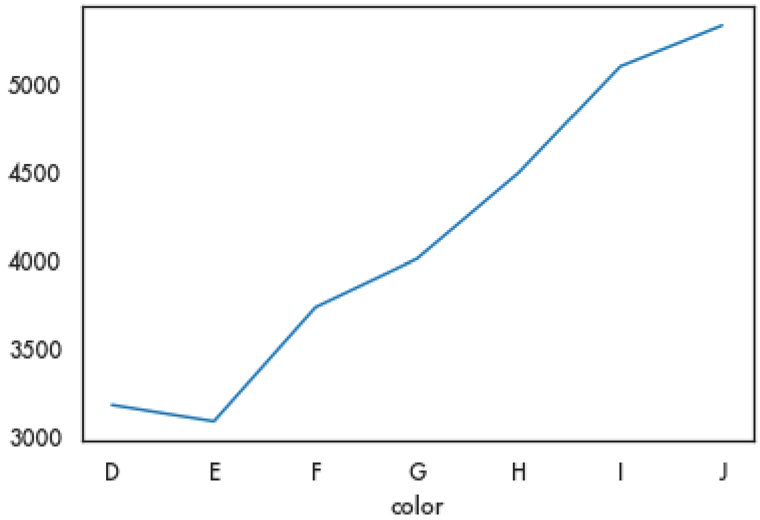
```python
(diamonds.groupby('color').price.
    agg([np.mean, np.median, np.std]))
```

Out[62]:

	mean	median	std
color			
D	3169.954096	1838.0	3356.590935
E	3076.752475	1739.0	3344.158685
F	3724.886397	2343.5	3784.992007
G	3999.135671	2242.0	4051.102846
H	4486.669196	3460.0	4215.944171
I	5091.874954	3730.0	4722.387604
J	5323.818020	4234.0	4438.187251

In [66]:

```python
(diamonds.groupby('color').price.
    mean().plot());
```


5000
4500
4000
3500
3000
D
E
F
G
H
I
J
color

Hypothesis tests

```
import scipy.stats
```

Function	Test
`ttest_1samp`	One-sample t-test
`ttest_ind`	Two-sample t-test
`ttest_rel`	Paired t-test
`wilcoxon`	Wilcoxon signed-rank test (nonparametric paired t-test)
`mannwhitneyu`	Wilcoxon rank-sum test (nonparametric 2-sample t-test)
`chi2_contingency`	Chi-square test for independence
`fisher_exact`	Fisher's exact test on a 2x2 contingency table
`f_oneway`	One-way ANOVA
`pearsonr`	Testing for correlation

```
import statsmodels.stats
```

Functions	Tests
`proportions_ztest`	Test for difference in proportions
`mcnemar`	McNemar's test
`sign_test`	Sign test
`multipletests`	p-value correction for multiple tests
`fdrcorrection`	p-value correction by FDR

In [68]:

```python
brca = pd.read_csv('data/brca.csv')
brca.columns = brca.columns.str.replace(' ', '_')
brca.head()
```

Out[68]:

	Unnamed:_0	Complete_TCGA_ID	Gender	Age_at_Initial_Pathologic_Diagnosis	ER_Status	PR_Status	HER2_Final_Status	Tum
0	0	TCGA-A2-A0CM	FEMALE	40	Negative	Negative	Negative	
1	1	TCGA-BH-A18Q	FEMALE	56	Negative	Negative	Negative	
2	2	TCGA-A7-A0CE	FEMALE	57	Negative	Negative	Negative	
3	3	TCGA-D8-A142	FEMALE	74	Negative	Negative	Negative	
4	4	TCGA-AO-A0J6	FEMALE	61	Negative	Negative	Negative	

5 rows × 12585 columns

In [71]:

```
import scipy as sc
import statsmodels as sm
test_probe = 'NP_001193600'

tst = sc.stats.ttest_ind(
    brca[brca.ER_Status=='Positive'][test_probe],
    brca[brca.ER_Status=='Negative'][test_probe],
    nan_policy = 'omit')
np.round(tst.pvalue, 3)
```

Out[71]:

```
0.277
```

In [73]:

```
tst = sc.stats.mannwhitneyu(
    brca[brca.ER_Status=='Positive'][test_probe],
    brca[brca.ER_Status=='Negative'][test_probe],
    alternative = 'two-sided')
np.round(tst.pvalue, 3)
```

Out[73]:

```
0.996
```

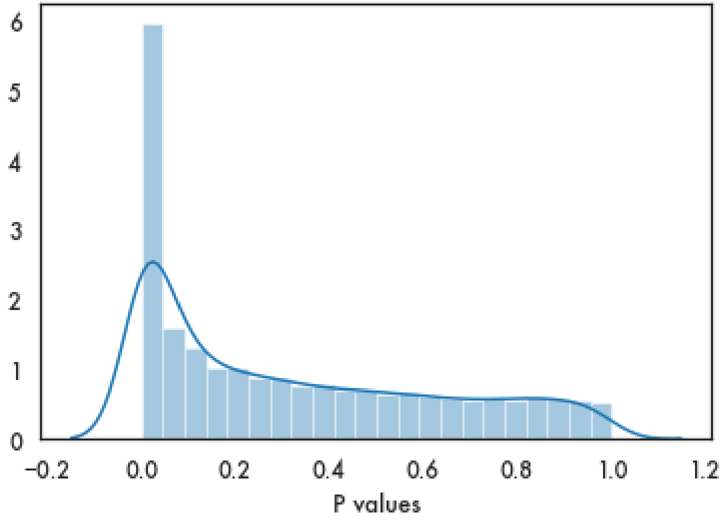
Multiple tests

In [75]:

```
expr_names = [u for u in list(brca.columns) if u.find('NP') > -1]
            # Find all column names with NP

exprs = brca[expr_names] # Extract the protein data

groups = np.where(brca.ER_Status=='Positive', 1, 0)
pvals_t = np.zeros(exprs.shape[1]) # initialize storage
for i in range(exprs.shape[1]):
    stat, pvals_t[i] = sc.stats.ttest_ind(exprs.iloc[groups==1, i],
                                          exprs.iloc[groups==0, i],
                                          nan_policy = 'omit')
sns.distplot(pvals_t);
plt.xlabel('P values');
```



Regression analysis

Setup

In [76]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import statsmodels.api as sm
import statsmodels.formula.api as smf # Use the formula interface to statsmodels
```

In [77]:

```
diamonds = sm.datasets.get_rdataset('diamonds','ggplot2').data
mod1 = smf.ols('price ~ np.log(carat) + clarity + depth + cut * color', data = diamonds)
mod1 = mod1.fit() # Actually do the fit
mod1.summary()
```

Out[77]:

OLS Regression Results

Dep. Variable:	price	**R-squared:**	0.786
Model:	OLS	**Adj. R-squared:**	0.786
Method:	Least Squares	**F-statistic:**	4598.
Date:	Thu, 04 Jun 2020	**Prob (F-statistic):**	0.00
Time:	11:35:16	**Log-Likelihood:**	-4.8222e+05
No. Observations:	53940	**AIC:**	9.645e+05
Df Residuals:	53896	**BIC:**	9.649e+05
Df Model:	43		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
Intercept	2745.0643	415.804	6.602	0.000	1930.085	3560.043
clarity[T.IF]	4916.7221	83.694	58.746	0.000	4752.681	5080.763
clarity[T.SI1]	2686.1493	71.397	37.623	0.000	2546.210	2826.088
clarity[T.SI2]	2060.8180	71.809	28.699	0.000	1920.072	2201.564
clarity[T.VS1]	3710.1759	72.891	50.900	0.000	3567.309	3853.043
clarity[T.VS2]	3438.3999	71.792	47.894	0.000	3297.687	3579.112
clarity[T.VVS1]	4540.1420	77.314	58.724	0.000	4388.606	4691.678
clarity[T.VVS2]	4343.0545	75.136	57.803	0.000	4195.788	4490.321
cut[T.Good]	708.5981	161.869	4.378	0.000	391.334	1025.862
cut[T.Ideal]	1198.2067	149.690	8.005	0.000	904.812	1491.601
cut[T.Premium]	1147.1417	152.896	7.503	0.000	847.464	1446.820
cut[T.Very Good]	1011.3463	152.977	6.611	0.000	711.510	1311.183
color[T.E]	-59.4094	190.227	-0.312	0.755	-432.256	313.437
color[T.F]	-86.0097	178.663	-0.481	0.630	-436.191	264.172
color[T.G]	-370.6455	178.642	-2.075	0.038	-720.784	-20.507
color[T.H]	-591.0922	179.786	-3.288	0.001	-943.474	-238.710
color[T.I]	-1030.7417	201.485	-5.116	0.000	-1425.655	-635.829
color[T.J]	-1210.6501	223.111	-5.426	0.000	-1647.949	-773.351

cut[T.Good]:color[T.E]	-30.3553	212.126	-0.143	0.886	-446.123	385.413
cut[T.Ideal]:color[T.E]	-211.3711	195.630	-1.080	0.280	-594.807	172.065
cut[T.Premium]:color[T.E]	-91.3261	199.440	-0.458	0.647	-482.230	299.578
cut[T.Very Good]:color[T.E]	-45.2968	199.656	-0.227	0.821	-436.625	346.031
cut[T.Good]:color[T.F]	-365.4060	202.035	-1.809	0.071	-761.397	30.585
cut[T.Ideal]:color[T.F]	-198.0428	184.498	-1.073	0.283	-559.661	163.575
cut[T.Premium]:color[T.F]	-322.8527	188.465	-1.713	0.087	-692.246	46.540
cut[T.Very Good]:color[T.F]	-186.0519	189.090	-0.984	0.325	-556.670	184.566
cut[T.Good]:color[T.G]	-93.0430	202.404	-0.460	0.646	-489.757	303.671
cut[T.Ideal]:color[T.G]	-65.8579	183.980	-0.358	0.720	-426.461	294.745
cut[T.Premium]:color[T.G]	35.4302	187.596	0.189	0.850	-332.260	403.121
cut[T.Very Good]:color[T.G]	-81.2595	188.786	-0.430	0.667	-451.282	288.764
cut[T.Good]:color[T.H]	137.0235	205.696	0.666	0.505	-266.142	540.189
cut[T.Ideal]:color[T.H]	-83.4763	186.060	-0.449	0.654	-448.155	281.202
cut[T.Premium]:color[T.H]	-44.4372	189.378	-0.235	0.814	-415.620	326.745
cut[T.Very Good]:color[T.H]	-43.2485	190.851	-0.227	0.821	-417.318	330.821
cut[T.Good]:color[T.I]	331.4048	228.614	1.450	0.147	-116.681	779.490
cut[T.Ideal]:color[T.I]	106.2368	208.391	0.510	0.610	-302.210	514.684
cut[T.Premium]:color[T.I]	357.1453	212.341	1.682	0.093	-59.045	773.335
cut[T.Very Good]:color[T.I]	149.1555	213.697	0.698	0.485	-269.693	568.004
cut[T.Good]:color[T.J]	-406.8484	256.938	-1.583	0.113	-910.448	96.752
cut[T.Ideal]:color[T.J]	-330.0602	234.063	-1.410	0.159	-788.826	128.706
cut[T.Premium]:color[T.J]	-156.8065	236.860	-0.662	0.508	-621.055	307.442
cut[T.Very Good]:color[T.J]	-381.5722	238.799	-1.598	0.110	-849.620	86.475
np.log(carat)	6630.7799	15.605	424.923	0.000	6600.195	6661.365
depth	-0.7353	5.961	-0.123	0.902	-12.418	10.948

Omnibus:	13993.592	**Durbin-Watson:**	0.134
Prob(Omnibus):	0.000	**Jarque-Bera (JB):**	34739.732
Skew:	1.432	**Prob(JB):**	0.00
Kurtosis:	5.693	**Cond. No.**	7.08e+03

Warnings:

[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 7.08e+03. This might indicate that there are
strong multicollinearity or other numerical problems.

```
mod1 = smf.glm(
    'price ~ np.log(carat) + clarity + depth + cut * color',
    data = diamonds)
```

This formula will read as

price depends on

- log(carat),
- clarity, depth, cut and color,
- and the interaction of cut and color".

```
mod1 = smf.glm(
    'price ~ np.log(carat) + clarity + depth + cut * color',
    data = diamonds)
```

color, clarity, and cut are all categorical variables.

They actually need to be expanded into dummy variables, so we will have one column for each category level, which is 1 when the diamond is of that category and 0 otherwise.

One less dummy than levels, since we keep a reference level

```
mod1 = smf.glm(
    'price ~ np.log(carat) + clarity + depth + cut * color',
    data = diamonds)
```

An intercept term is added

```
mod1 = smf.glm(
    'price ~ np.log(carat) + clarity + depth + cut * color',
    data = diamonds)
```

The variable `carat` is transformed using `np.log`, i.e. the natural logarithm available in the `numpy` package. Generally, any valid Python function can be used here, even ones you create.

```
mod1 = smf.glm(
    'price ~ np.log(carat) + clarity + depth + cut * color',
    data = diamonds)
```

Interactions are computed. The syntax `cut * color` is a shortcut for `cut + color + cut:color`, where the `:` denotes interaction.

```
mod2 = smf.ols(
    'price ~ np.log(carat) + clarity + depth +
     C(cut, Treatment("Ideal")) * color',
     data = diamonds).fit()
```

Here we specify that `cut` is a categorical variable, and we are using *treatment contrasts* with *Ideal* as the reference category

Logistic regression

In [78]:

```
titanic = sm.datasets.get_rdataset('Titanic','Stat2Data').data
titanic.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1313 entries, 0 to 1312
Data columns (total 6 columns):
 #   Column    Non-Null Count  Dtype  
---  ------    --------------  -----  
 0   Name      1313 non-null   object 
 1   PClass    1313 non-null   object 
 2   Age       756 non-null    float64
 3   Sex       1313 non-null   object 
 4   Survived  1313 non-null   int64  
 5   SexCode   1313 non-null   int64  
dtypes: float64(1), int64(2), object(3)
memory usage: 61.7+ KB
```

In [79]:

```python
mod_logistic = smf.glm('Survived ~ Age + Sex + PClass', data=titanic,
  family = sm.families.Binomial()).fit()
mod_logistic.summary()
```

Out[79]:

Generalized Linear Model Regression Results

Dep. Variable:	Survived	**No. Observations:**	756
Model:	GLM	**Df Residuals:**	751
Model Family:	Binomial	**Df Model:**	4
Link Function:	logit	**Scale:**	1.0000
Method:	IRLS	**Log-Likelihood:**	-347.57
Date:	Thu, 04 Jun 2020	**Deviance:**	695.14
Time:	11:44:14	**Pearson chi2:**	813.
No. Iterations:	5		
Covariance Type:	nonrobust		

	coef	std err	z	P>|z|	[0.025	0.975]
Intercept	1.8664	0.217	8.587	0.000	1.440	2.292
Sex[T.male]	-2.6314	0.202	-13.058	0.000	-3.026	-2.236
PClass[T.1st]	1.8933	0.208	9.119	0.000	1.486	2.300
PClass[T.2nd]	0.6013	0.148	4.052	0.000	0.310	0.892
PClass[T.3rd]	-0.6282	0.132	-4.754	0.000	-0.887	-0.369
Age	-0.0392	0.008	-5.144	0.000	-0.054	-0.024

To get odds ratios

```
In [81]: np.exp(mod_logistic.params.drop('Intercept'))

Out[81]: Sex[T.male]        0.071981
         PClass[T.1st]      6.640989
         PClass[T.2nd]      1.824486
         PClass[T.3rd]      0.533574
         Age                0.961581
         dtype: float64
```

Machine Learning

scikit-learn

scikit-learn (`sklearn`) is the main machine learning package in Python

1. `sklearn` requires that all inputs be numeric, and in fact, `numpy` arrays.
2. `sklearn` requires that all categorical variables by replaced by 0/1 dummy variables
3. `sklearn` requires us to separate the predictors from the outcome. We need to have one `X` matrix for the predictors and one `y` vector for the outcome.

1. First of all, we know that all `pandas` Series and DataFrame objects can be converted to `numpy` arrays using the `values` or `to_numpy` functions.
2. Second, we can easily extract a single variable from the data set using either the usual extracton methods or the `pop` function.
3. Third, `pandas` gives us a way to convert all categorical values to numeric dummy variables using the `get_dummies` function.

In [86]:

```python
import numpy as np
import pandas as pd
import sklearn
import statsmodels.api as sm
import matplotlib.pyplot as plt
import seaborn as sns

iris = sm.datasets.get_rdataset('iris').data
iris.head()
```

Out[86]:

	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa

Separate out outcome and predictors

In [87]:

```
y = iris['Species']
X = iris.drop('Species', axis = 1) # drops column, makes a copy
```

In [ ]:

```
# y = iris.pop('Species') # Now iris contains just the predictors
```

Transform `y` to be numeric

In [88]:
```
from sklearn.preprocessing import LabelEncoder
le = LabelEncoder()
y = le.fit_transform(y)
y
```

Out[88]:
```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 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, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

Transforming the predictors

The usual transformations that we need for heterogeneous predictors is to create *dummy variables* for the categorical predictors.

We don't directly have a formula interface in `sklearn`, but we can use tools from `pandas` and `patsy` to take care of this

In [89]:

```
diamonds = pd.read_csv('data/diamonds.csv.gz')

y = diamonds.pop('price').values
X = pd.get_dummies(diamonds)

# Alternatively
# import patsy
# f = '~ np.log(carat) + clarity + depth + cut * color'
# X = patsy.dmatrix(f, data=diamonds)
```

In [90]:

```
X.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 53940 entries, 0 to 53939
Data columns (total 26 columns):
 #   Column         Non-Null Count  Dtype  
---  ------         --------------  -----  
 0   carat          53940 non-null  float64
 1   depth          53940 non-null  float64
 2   table          53940 non-null  float64
 3   x              53940 non-null  float64
 4   y              53940 non-null  float64
 5   z              53940 non-null  float64
 6   cut_Fair       53940 non-null  uint8  
 7   cut_Good       53940 non-null  uint8  
 8   cut_Ideal      53940 non-null  uint8  
 9   cut_Premium    53940 non-null  uint8  
 10  cut_Very Good  53940 non-null  uint8  
 11  color_D        53940 non-null  uint8  
 12  color_E        53940 non-null  uint8  
 13  color_F        53940 non-null  uint8  
 14  color_G        53940 non-null  uint8  
 15  color_H        53940 non-null  uint8  
```

```
 16  color_I        53940 non-null  uint8
 17  color_J        53940 non-null  uint8
 18  clarity_I1     53940 non-null  uint8
 19  clarity_IF     53940 non-null  uint8
 20  clarity_SI1    53940 non-null  uint8
 21  clarity_SI2    53940 non-null  uint8
 22  clarity_VS1    53940 non-null  uint8
 23  clarity_VS2    53940 non-null  uint8
 24  clarity_VVS1   53940 non-null  uint8
 25  clarity_VVS2   53940 non-null  uint8
dtypes: float64(6), uint8(20)
memory usage: 3.5 MB
```

Supervised machine learning methods

ML method	Code to call it
Decision Tree	`sklearn.tree.DecisionTreeClassifier` , `sklearn.tree.DecisionTreeRegressor`
Random Forest	`sklearn.ensemble.RandomForestClassifier` , `sklearn.ensemble.RandomForestRegressor`
Linear Regression	`sklearn.linear_model.LinearRegression`
Logistic Regression	`sklearn.linear_model.LogisticRegression`
Support Vector Machines	`sklearn.svm.LinearSVC` , `sklearn.svm.LinearSVR`

The general method that the code will follow is :

```
from sklearn.... import Machine
machine = Machine(*parameters*)
machine.fit(X, y)
```

Split the data into a training set and a test set (80/20)

Model build on the training set **only**, and see predictive performance on the test set

In [93]:
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y , test_size = 0.2, random_state=
```

Initialize 2 models

In [94]:

```
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor


lm = LinearRegression()
dt = DecisionTreeRegressor()
```

Fit the models to the data

In [96]:

```
lm.fit(X_train, y_train)
dt.fit(X_train, y_train)
```

See how the models do on the training set (don't really do or report this)

In [98]:

```
from sklearn.metrics import  r2_score

print('Linear regression:', r2_score(y_train, lm.predict(X_train)))
print('Decision tree:', r2_score(y_train, dt.predict(X_train)))
```

```
Linear regression: 0.9202636015648039
Decision tree: 0.9999965428396391
```

See how the models do on the training set (don't really do or report this)

In [98]:
```python
from sklearn.metrics import  r2_score

print('Linear regression:', r2_score(y_train, lm.predict(X_train)))
print('Decision tree:', r2_score(y_train, dt.predict(X_train)))
```

```
Linear regression: 0.9202636015648039
Decision tree: 0.9999965428396391
```

We're almost certainly overfitting!!

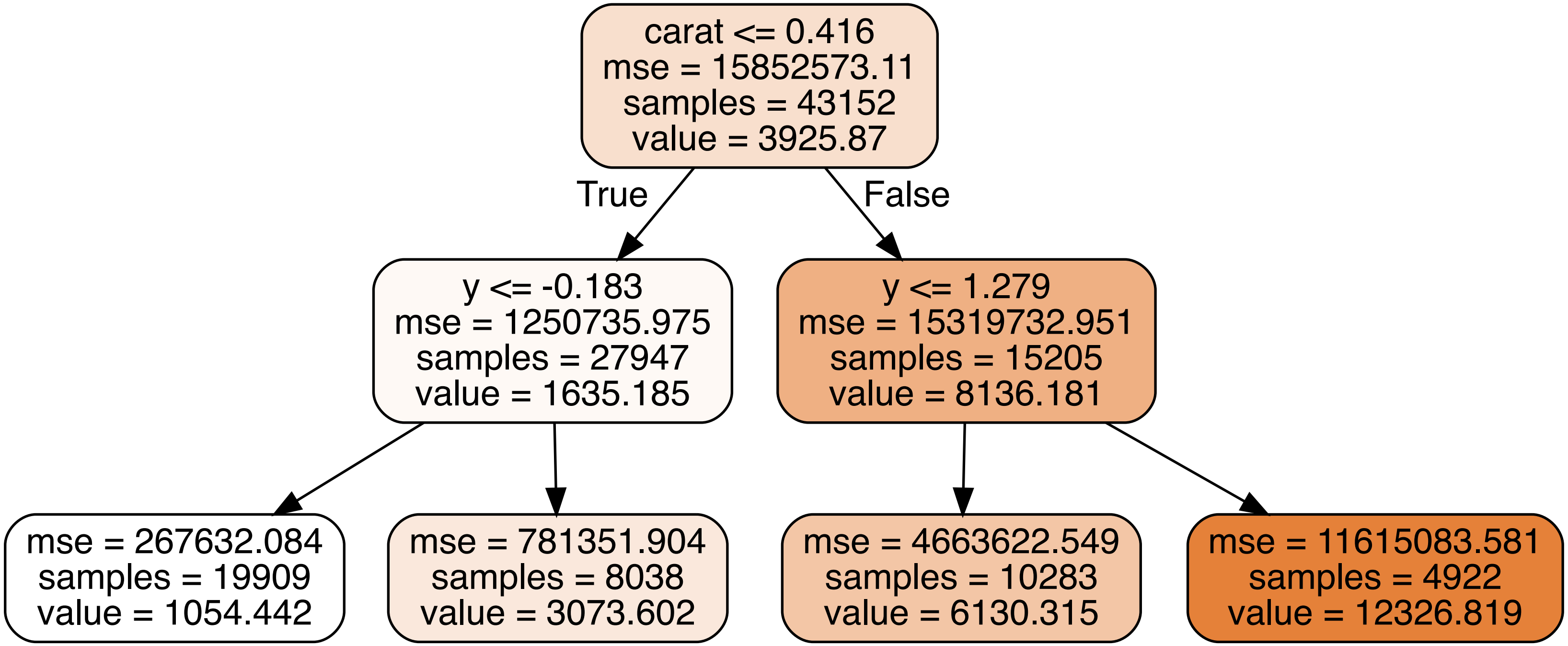
Visualizing a decision tree

In [100]:

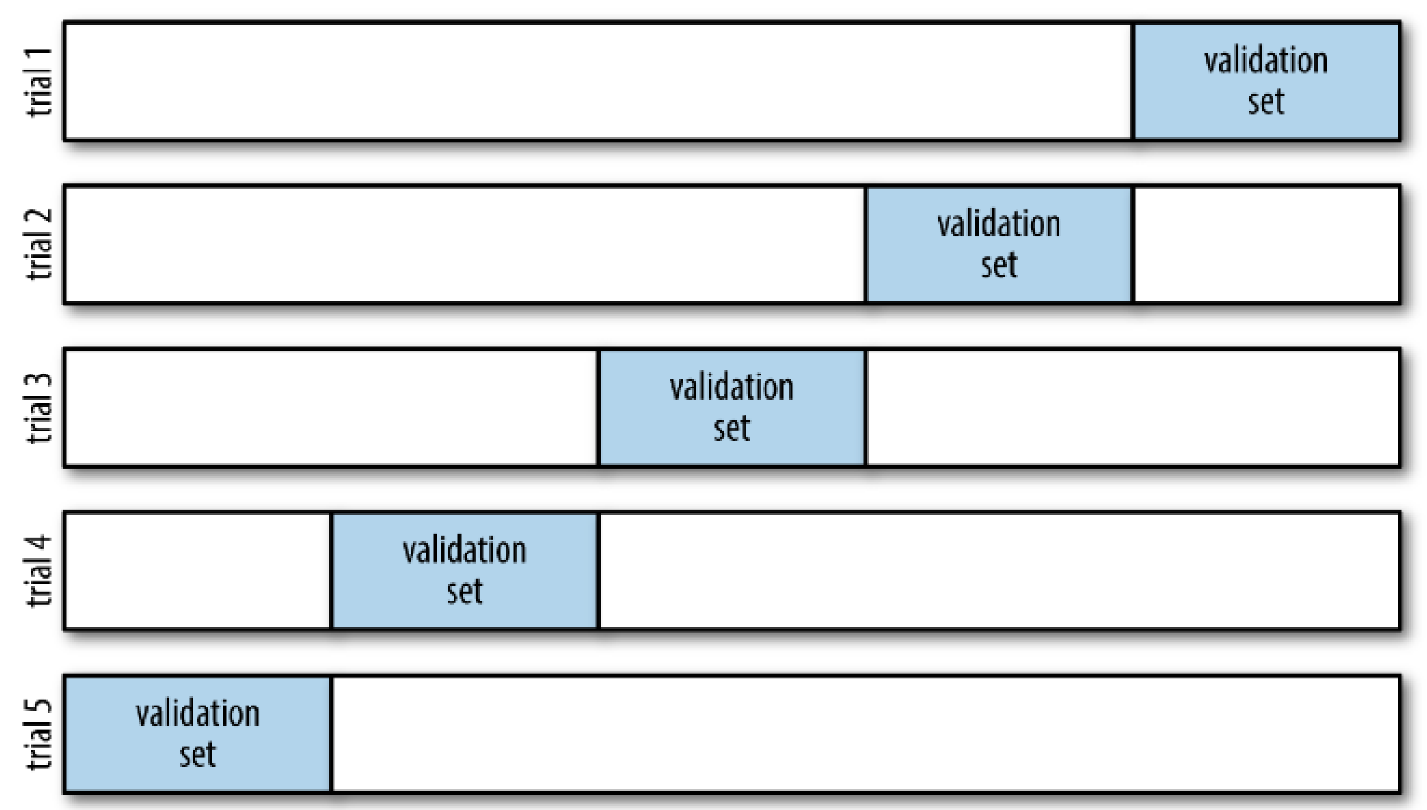
```
import graphviz
from sklearn import tree

dt = DecisionTreeRegressor(max_depth=2) # Limit to 2 layers
dt.fit(X_train, y_train)
dot_data = tree.export_graphviz(dt, out_file=None,
                                feature_names = X_train.columns,
                                filled=True, rounded=True)
graph = graphviz.Source(dot_data);
graph
```

Out[100]:



Cross-validaton



In [102]:

```python
from sklearn.model_selection import cross_val_score

cv_score = cross_val_score(dt, X_train, y_train, cv=5, scoring='r2')
print("CV average score =", np.round(np.mean(cv_score), 3))
```

```
CV average score = 0.829
```

Tuning models using cross-validation

In [103]:

```python
from sklearn.model_selection import GridSearchCV
import numpy.random as rnd
rnd.RandomState(39358)

param_grid = {'max_depth': [1,3,5,7, 10], 'min_samples_leaf': [1,5,10,20],
  'max_features' : ['auto','sqrt']}

clf = GridSearchCV(dt, param_grid, scoring = 'r2', cv = 5) # Tuning dt
clf.fit(X_train, y_train)

clf.best_estimator_
print(clf.best_score_)
```

```
0.9645325340549133
```

How does this model do on the test set?

In [104]:

```
p = clf.best_estimator_.predict(X_test)
r2_score(y_test, p)
```

Out[104]:

```
0.9657241131204777
```

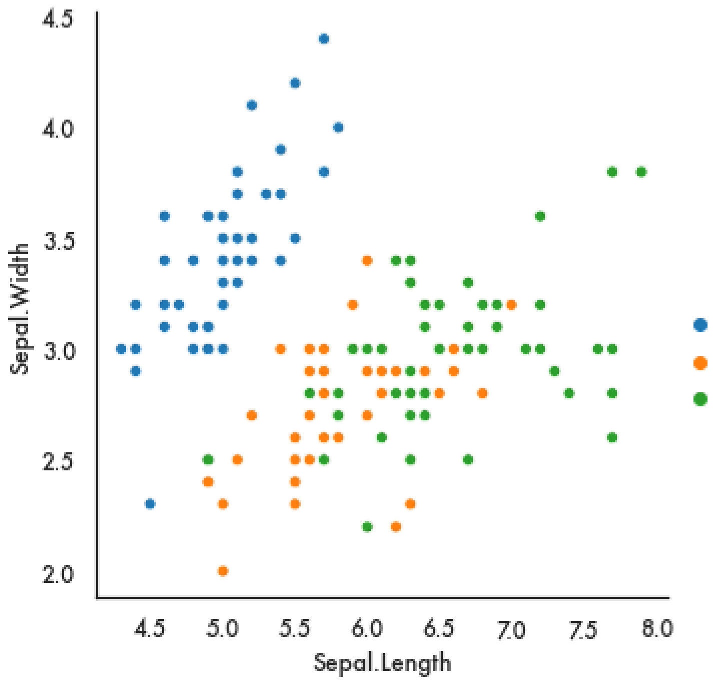
Unsupervised learning

Method name	Parameters	Scalability	Usecase	Geometry (metric used)
K-Means	number of clusters	Very large `n_samples`, medium `n_clusters` with MiniBatch code	General-purpose, even cluster size, flat geometry, not too many clusters	Distances between points
Affinity propagation	damping, sample preference	Not scalable with n_samples	Many clusters, uneven cluster size, non-flat geometry	Graph distance (e.g. nearest-neighbor graph)
Mean-shift	bandwidth	Not scalable with `n_samples`	Many clusters, uneven cluster size, non-flat geometry	Distances between points
Spectral clustering	number of clusters	Medium `n_samples`, small `n_clusters`	Few clusters, even cluster size, non-flat geometry	Graph distance (e.g. nearest-neighbor graph)
Ward hierarchical clustering	number of clusters or distance threshold	Large `n_samples` and `n_clusters`	Many clusters, possibly connectivity constraints	Distances between points
Agglomerative clustering	number of clusters or distance threshold, linkage type, distance	Large `n_samples` and `n_clusters`	Many clusters, possibly connectivity constraints, non Euclidean distances	Any pairwise distance
DBSCAN	neighborhood size	Very large `n_samples`, medium `n_clusters`	Non-flat geometry, uneven cluster sizes	Distances between nearest points
OPTICS	minimum cluster membership	Very large `n_samples`, large `n_clusters`	Non-flat geometry, uneven cluster sizes, variable cluster density	Distances between points
Gaussian mixtures	many	Not scalable	Flat geometry, good for density estimation	Mahalanobis distances to centers
Birch	branching factor, threshold, optional global clusterer.	Large `n_clusters` and `n_samples`	Large dataset, outlier removal, data reduction.	Euclidean distance between points

K-Means clustering

In [105]:

```
iris = sm.datasets.get_rdataset('iris').data
sns.relplot(data=iris, x = 'Sepal.Length',y = 'Sepal.Width', hue = 'Species');
```



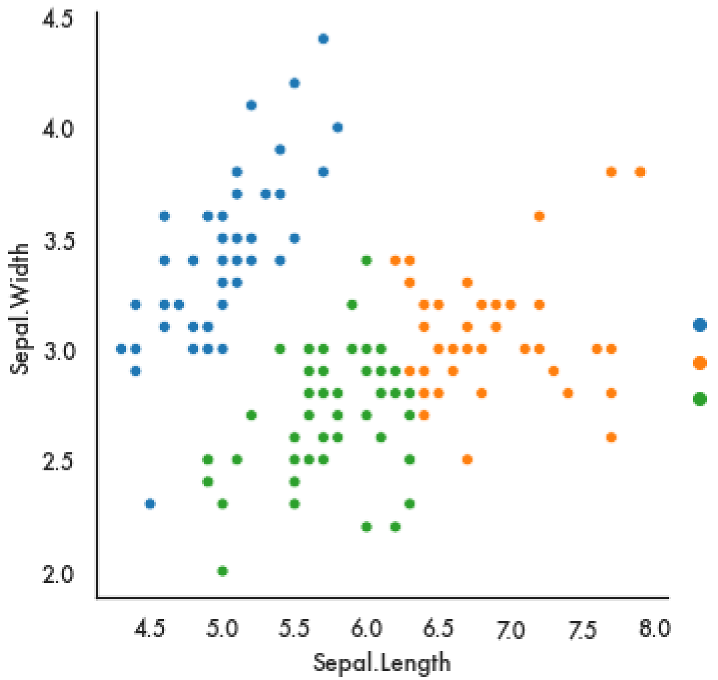
In [107]:

```python
from sklearn.cluster import KMeans, AgglomerativeClustering

km = KMeans(n_clusters = 3)
km.fit(iris[['Sepal.Length','Sepal.Width']]);

iris['km_labels'] = km.labels_
iris['km_labels'] = iris.km_labels.astype('category')

sns.relplot(data=iris, x = 'Sepal.Length', y = 'Sepal.Width',
            hue = 'km_labels');
```

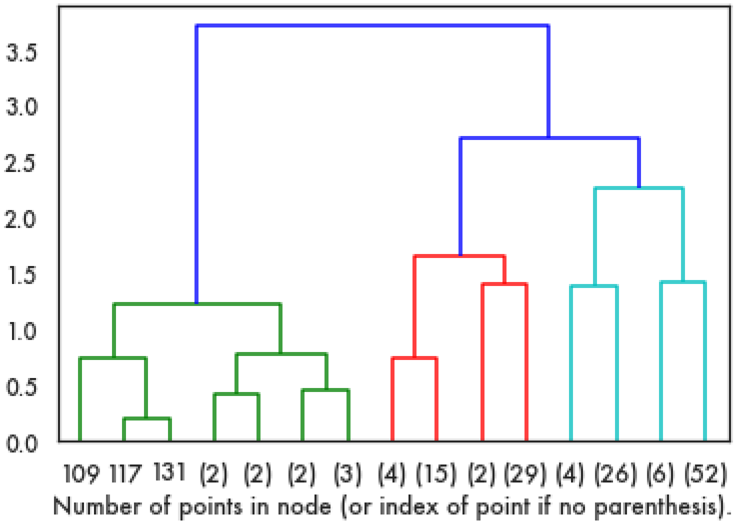


Agglomerative (hierarchical) clustering

In [110]:

```
hc = AgglomerativeClustering(distance_threshold=0, n_clusters=None,
                             linkage='complete')
hc.fit(iris[['Sepal.Length','Sepal.Width']])

plot_dendrogram(hc, truncate_mode='level', p=3)
plt.xlabel("Number of points in node (or index of point if no parenthesis).");
```



In [112]:

```
iris['hc_labels'] = pd.Series(hc.labels_).astype('category')

sns.relplot(data=iris, x = 'Sepal.Length', y= 'Sepal.Width',
            hue = 'hc_labels');
```