Linear regression: deep dive

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```
from sklearn import datasets
from sklearn import metrics
from sklearn import preprocessing
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split


import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import seaborn as sns
sns.set()

# for 3d interactive plots
from ipywidgets import interact, fixed
from mpl_toolkits import mplot3d

from IPython.core.interactiveshell import InteractiveShell
InteractiveShell.ast_node_interactivity = "all"
```

Data generated by a linear function

Suppose we have a process that generates data as

$$y_i = w_0 + w_1 x_{i,1} + \ldots + w_d x_{i,d} + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$.

Note: in this example, we use a “stochastic error” term. This is not to be confused with a residual term which can include systematic, non-random error.

- stochastic error: difference between observed value and “true” value. These random errors are independent, not systematic, and cannot be “learned” by any machine learning model.
- residual: difference between observed value and estimated value. These errors are typical *not* independent, and they can be systematic.

Here’s a function to generate this kind of data

```
def generate_linear_regression_data(n=100, d=1, coef=[5], intercept=1, sigma=0):
  x = np.random.randn(n,d)
  y = (np.dot(x, coef) + intercept).squeeze() + sigma * np.random.randn(n)
  return x, y
```

and some default values we’ll use:

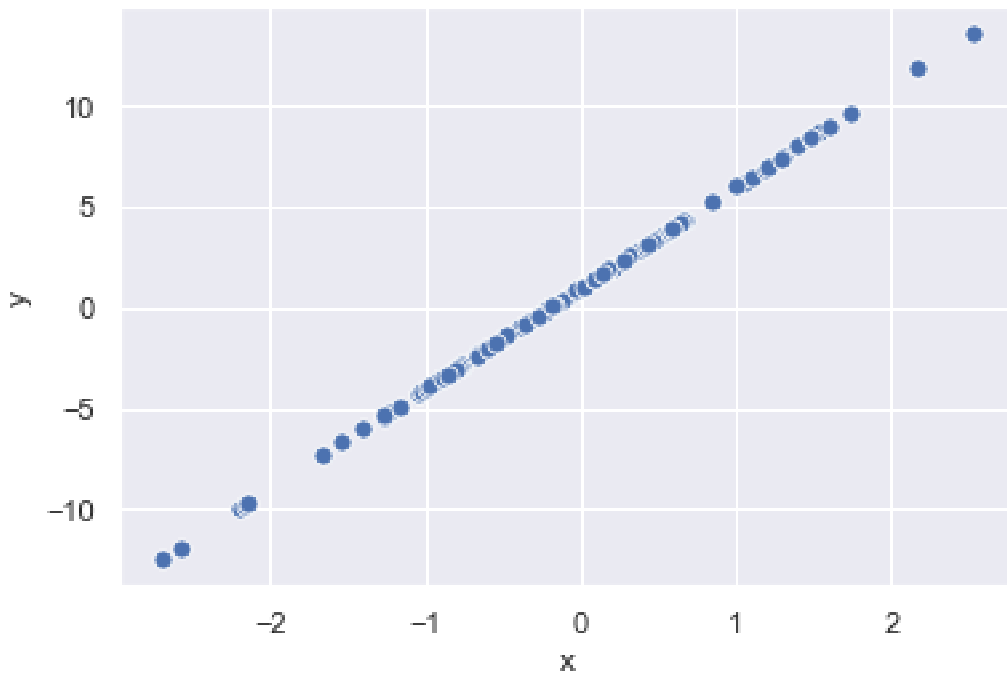
```
n_samples = 100
coef = [5]
intercept = 1
```

Simple linear regression

Generate some data

```
x_train, y_train = generate_linear_regression_data(n=n_samples, d=1, coef=coef,
    intercept=intercept)
x_test,  y_test  = generate_linear_regression_data(n=50, d=1, coef=coef, intercept=intercept)
```

```
sns.scatterplot(x=x_train.squeeze(), y=y_train, s=50);
plt.xlabel('x');
plt.ylabel('y');
```

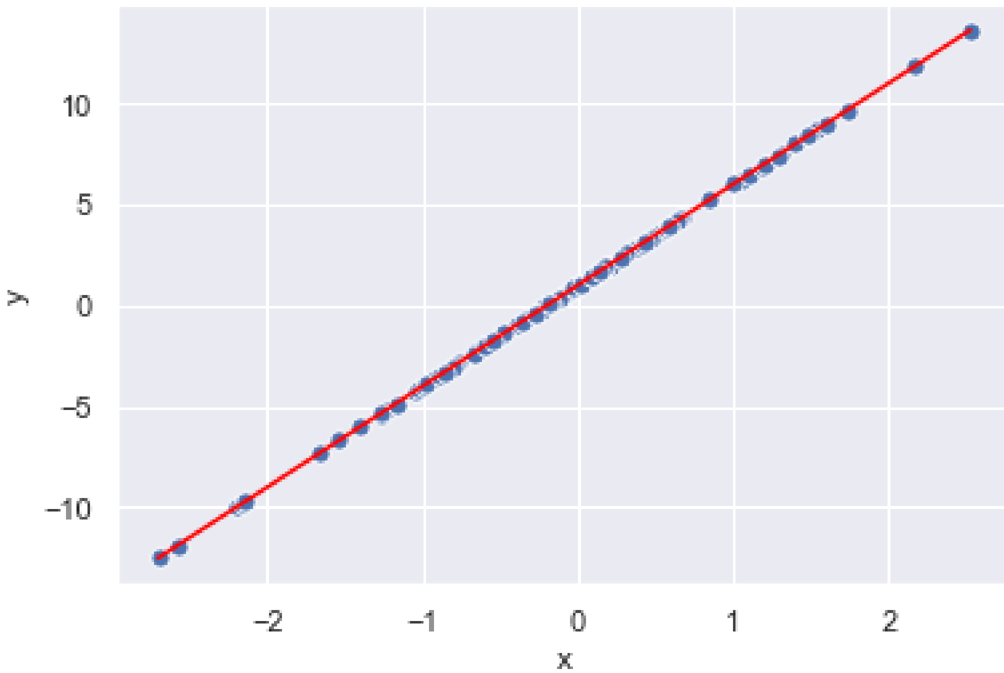


Fit a linear regression

```
reg_simple = LinearRegression().fit(x_train, y_train)
print("Intercept: " , reg_simple.intercept_)
print("Coefficient list: ", reg_simple.coef_)
```

```
Intercept:  0.9999999999999999
Coefficient list:  [5.]
```

```
x_line = [np.min(x_train), np.max(x_train)]
y_line = x_line*reg_simple.coef_ + reg_simple.intercept_

sns.scatterplot(x=x_train.squeeze(), y=y_train, s=50);
sns.lineplot(x=x_line, y=y_line, color='red');
plt.xlabel('x');
plt.ylabel('y');
```



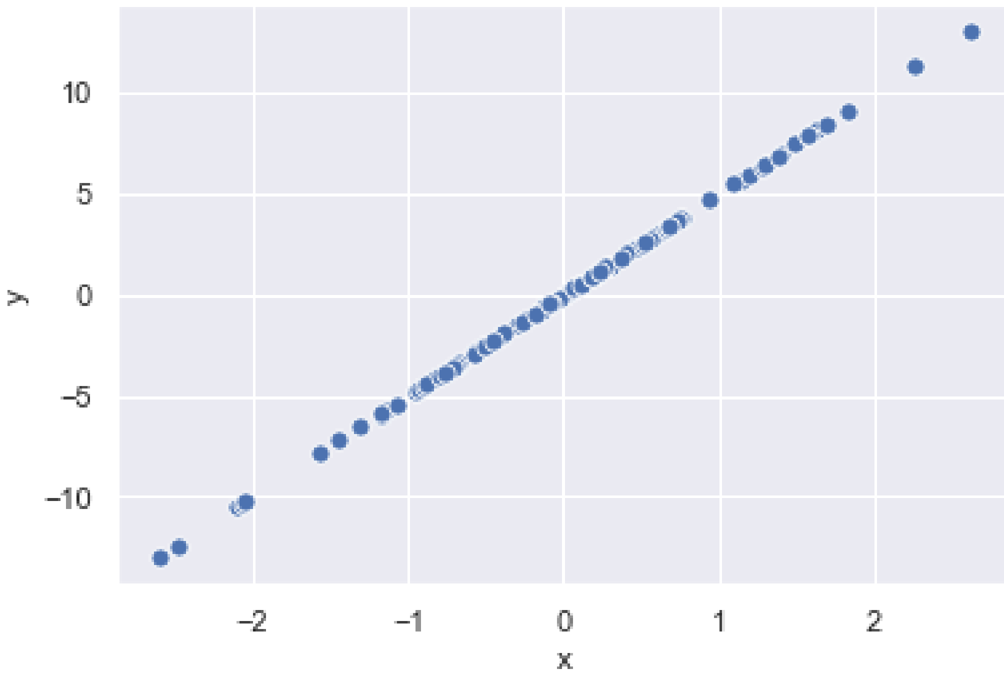

```
# Note: other ways to do the same thing...
# first, add a ones column to design matrix
x_tilde = np.hstack((np.ones((n_samples, 1)), x_train))

# using matrix operations to find w = (X^T X)^{-1} X^T y
print( (np.linalg.inv((x_tilde.T.dot(x_tilde))).dot(x_tilde.T)).dot(y_train) )

# using solve on normal equations: X^T X w = X^T y
# solve only works on matrix that is square and of full-rank
# see https://numpy.org/doc/stable/reference/generated/numpy.linalg.solve.html
print( np.linalg.solve(x_tilde.T.dot(x_tilde), x_tilde.T.dot(y_train)) )

# using the lstsq solver
# problem may be under-, well-, or over-determined
# see https://numpy.org/doc/stable/reference/generated/numpy.linalg.lstsq.html
print( np.linalg.lstsq(x_tilde,y_train,rcond=0)[0] )
```

```
[1. 5.]
[1. 5.]
[1. 5.]
```

The mean-removed equivalent

Quick digression - what if we don't want to bother with intercept?

```
x_train_mr = x_train - np.mean(x_train)
y_train_mr = y_train - np.mean(y_train)
sns.scatterplot(x=x_train_mr.squeeze(), y=y_train_mr, s=50);
plt.xlabel('x');
plt.ylabel('y');
```



Note that now the data is mean removed - zero mean in every dimension. (Removing the mean is also called *centering* the data.)

This time, the fitted linear regression has 0 intercept:

```
reg_mr = LinearRegression().fit(x_train_mr, y_train_mr)
print("Intercept: " , reg_mr.intercept_)
print("Coefficient list: ", reg_mr.coef_)
```

```
Intercept:  -4.996003610813204e-17
Coefficient list:  [5.]
```

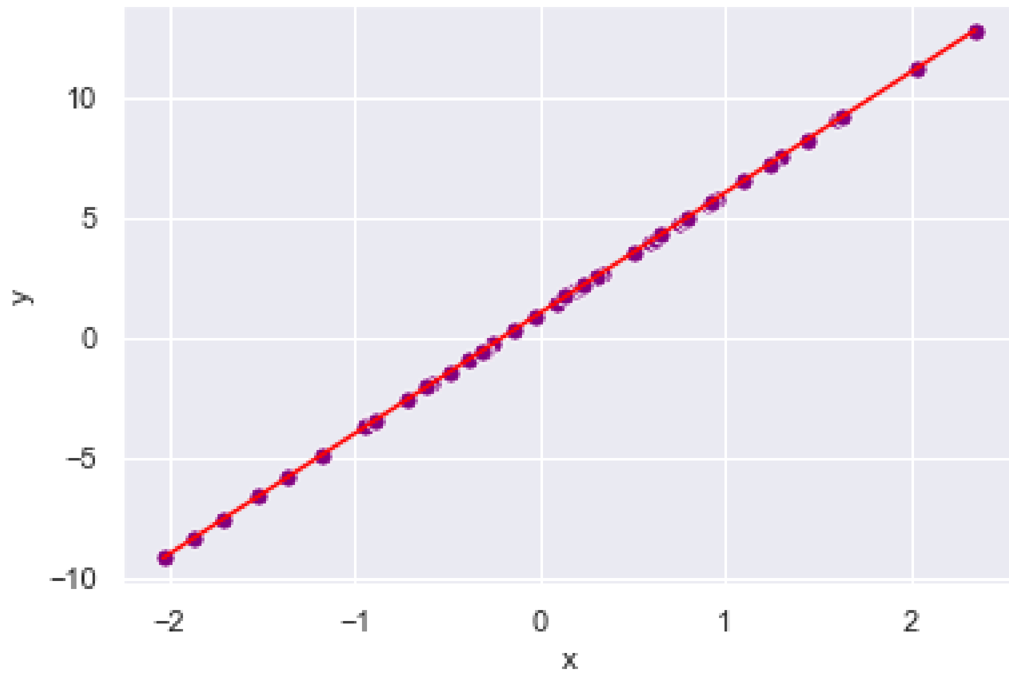
Predict some new points

OK, now we can predict some new points:

```
y_test_hat = reg_simple.intercept_ + np.dot(x_test,reg_simple.coef_)
```

```
x_line = [np.min(x_test), np.max(x_test)]
y_line = x_line*reg_simple.coef_ + reg_simple.intercept_
```

```
sns.lineplot(x=x_line, y=y_line, color='red');
sns.scatterplot(x=x_test.squeeze(), y=y_test_hat, s=50, color='purple');
plt.xlabel('x');
plt.ylabel('y');
```



Compute MSE

To evaluate the model, we will compute the MSE on the test data (not the data used to find the parameters).

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - (w_0 + w_1 x_i))^2$$

Use $\hat{y}_i = w_0 + w_1 x_i$, then

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

```
y_test_hat = reg_simple.intercept_ + np.dot(x_test,reg_simple.coef_)
mse_simple = 1.0/(len(y_test)) * np.sum((y_test - y_test_hat)**2)
mse_simple
```

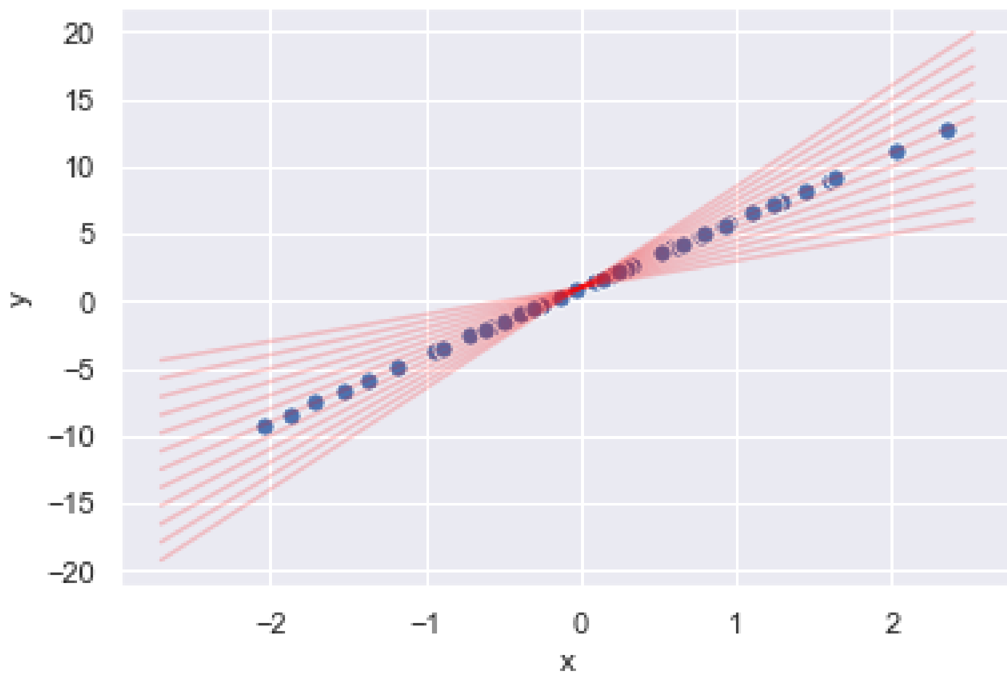
```
8.850033280448226e-32
```

```
# another way to do the same thing using sklearn
y_test_hat = reg_simple.predict(x_test)
metrics.mean_squared_error(y_test, y_test_hat)
```

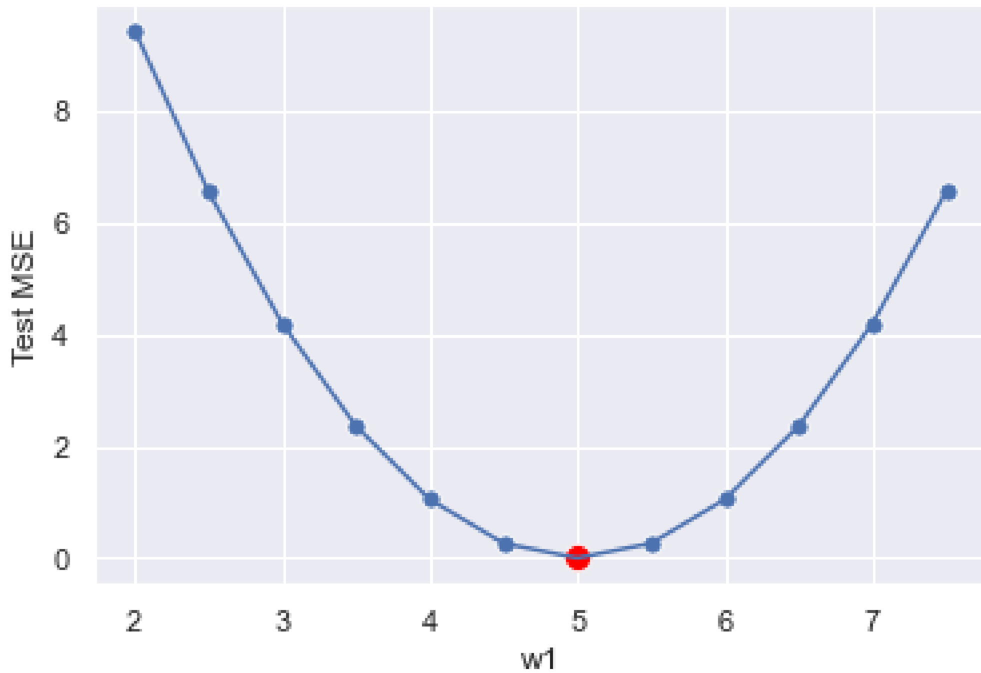
```
8.850033280448226e-32
```

Visualize MSE for different coefficients

```
p = sns.scatterplot(x=x_test.squeeze(), y=y_test_hat, s=50);
p = plt.xlabel('x')
p = plt.ylabel('y')

coefs = np.arange(2, 8, 0.5)
mses = np.zeros(len(coefs))

for idx, c in enumerate(coefs):
  y_test_hat_c = (reg_simple.intercept_ + np.dot(x_test,c)).squeeze()
  mses[idx] =  1.0/(len(y_test_hat_c)) * np.sum((y_test - y_test_hat_c)**2)
  x_line = [np.min(x_train), np.max(x_train)]
  y_line = [x_line[0]*c + reg_simple.intercept_, x_line[1]*c + intercept]
  p = sns.lineplot(x=x_line, y=y_line, color='red', alpha=0.2);
```




```
sns.lineplot(x=coefs, y=mses);
sns.scatterplot(x=coefs, y=mses, s=50);
sns.scatterplot(x=reg_simple.coef_, y=mse_simple, color='red', s=100);
p = plt.xlabel('w1');
p = plt.ylabel('Test MSE');
```



Variance, explained variance, R2

Quick reminder:

Mean of x and y:

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \quad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

Sample variance of x and y:

$$\sigma_x^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2, \quad \sigma_y^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$$

Sample covariance of x and y:

$$\sigma_{xy} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

```
var_y = 1.0/len(y_test) * np.sum((y_test - np.mean(y_test))**2)
var_y
```

```
25.834987181344587
```

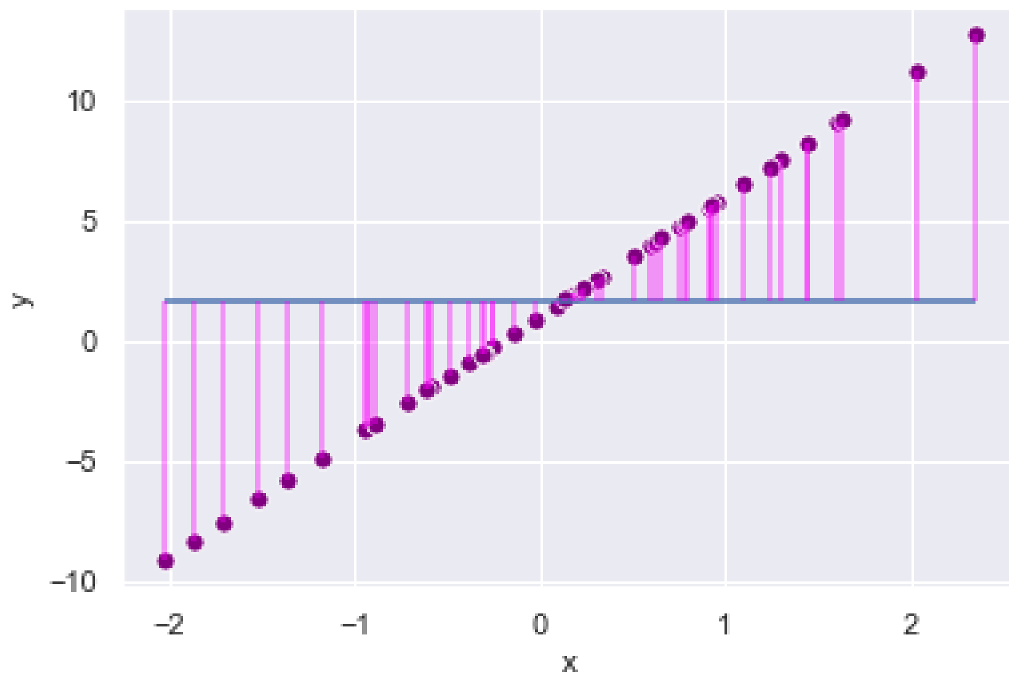
```
mean_y = np.mean(y_test)
mean_y
```

```
1.6180311111502985
```

The variance of y is the mean sum of the squares of the distances from each y_i to $\bar{y}$. These distances are illustrated here:

- the horizontal line shows $\bar{y}$
- each vertical line is a distance from a y_i to $\bar{y}$

```
plt.hlines(y=mean_y, xmin=np.min(x_test), xmax=np.max(x_test));
plt.vlines(x_test, ymin=mean_y, ymax=y_test, alpha=0.5, color='magenta');
sns.scatterplot(x=x_test.squeeze(), y=y_test, color='purple', s=50);
plt.xlabel('x');
plt.ylabel('y');
```

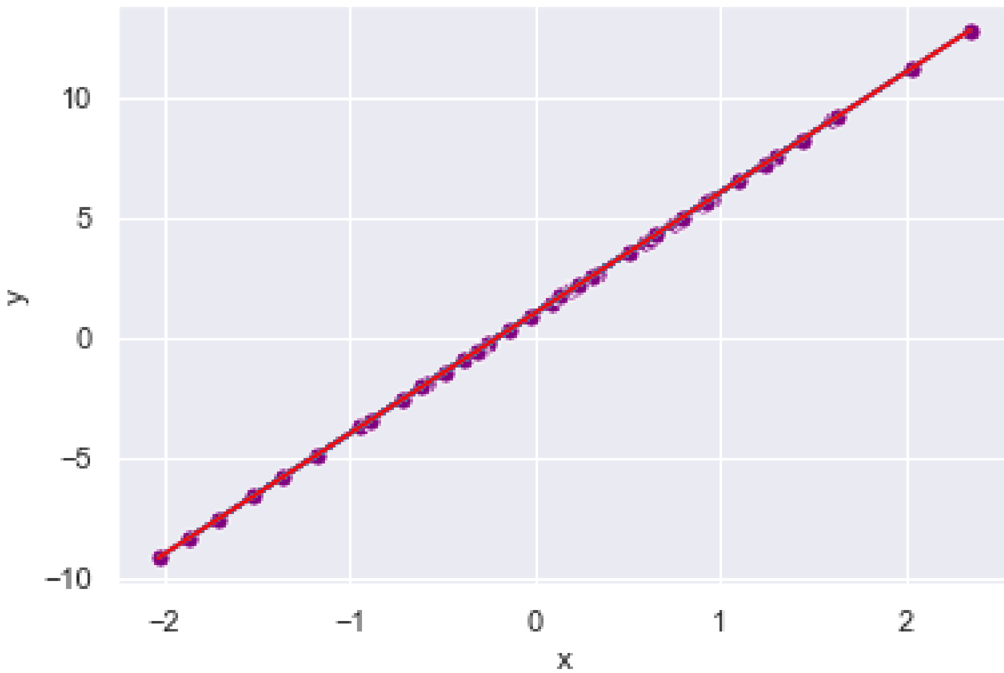


Now let's look at a similar kind of plot, but with distances to the regression line instead of the to mean line:

- In the previous plot, each vertical line was a $y_i - \bar{y}$
- In the following plot, each vertical line is a $y_i - \hat{y}_i$

(where $\hat{y}_i$ is the prediction of the linear regression for a given sample i)

```
plt.plot(x_test, y_test_hat);
plt.vlines(x_test, ymin=y_test, ymax=y_test_hat, color='magenta', alpha=0.5);
sns.scatterplot(x=x_test.squeeze(), y=y_test, color='purple', s=50);
x_line = [np.min(x_test), np.max(x_test)]
y_line = x_line*reg_simple.coef_ + reg_simple.intercept_
sns.lineplot(x=x_line, y=y_line, color='red');
plt.xlabel('x');
plt.ylabel('y');
```



These two plots together show how well the variance of y is "explained" by the linear regression model:

- The total variance of y is shown in the first plot, where each vertical line is $y_i - \bar{y}$
- The *unexplained* variance of y is shown in the second plot, where each vertical line is the error of the model, $y_i - \hat{y}_i$

In this example, *all* of the variance of y is "explained" by the linear regression.

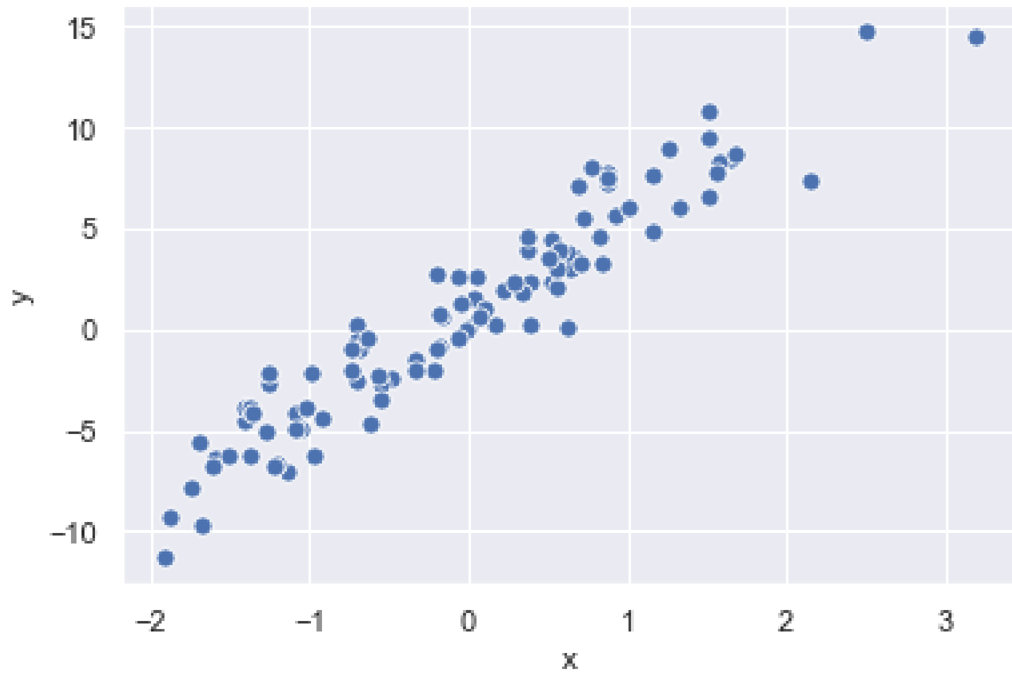
MSE for this example is 0, R2 is 1.

Simple linear regression with noise

Generate some data

```
x_train, y_train = generate_linear_regression_data(n=n_samples, d=1, coef=coef,
    intercept=intercept, sigma=2)
x_test,  y_test =  generate_linear_regression_data(n=50, d=1, coef=coef,
    intercept=intercept, sigma=2)
```

```
sns.scatterplot(x=x_train.squeeze(), y=y_train, s=50);
plt.xlabel('x');
plt.ylabel('y');
```

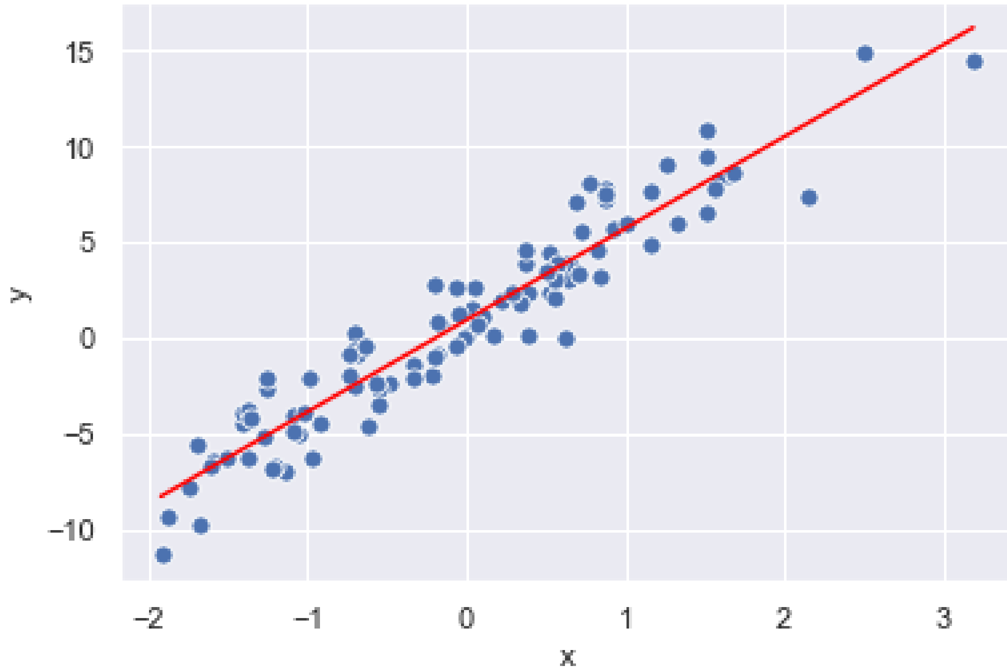


Fit a linear regression

```
reg_noisy = LinearRegression().fit(x_train, y_train)
print("Coefficient list: ", reg_noisy.coef_)
print("Intercept: " , reg_noisy.intercept_)
```

```
Coefficient list:  [4.78380532]
Intercept:  0.9284388724127042
```

```
x_line = [np.min(x_train), np.max(x_train)]
y_line = x_line*reg_noisy.coef_ + reg_noisy.intercept_

sns.scatterplot(x=x_train.squeeze(), y=y_train, s=50);
sns.lineplot(x=x_line, y=y_line, color='red');
plt.xlabel('x');
plt.ylabel('y');
```

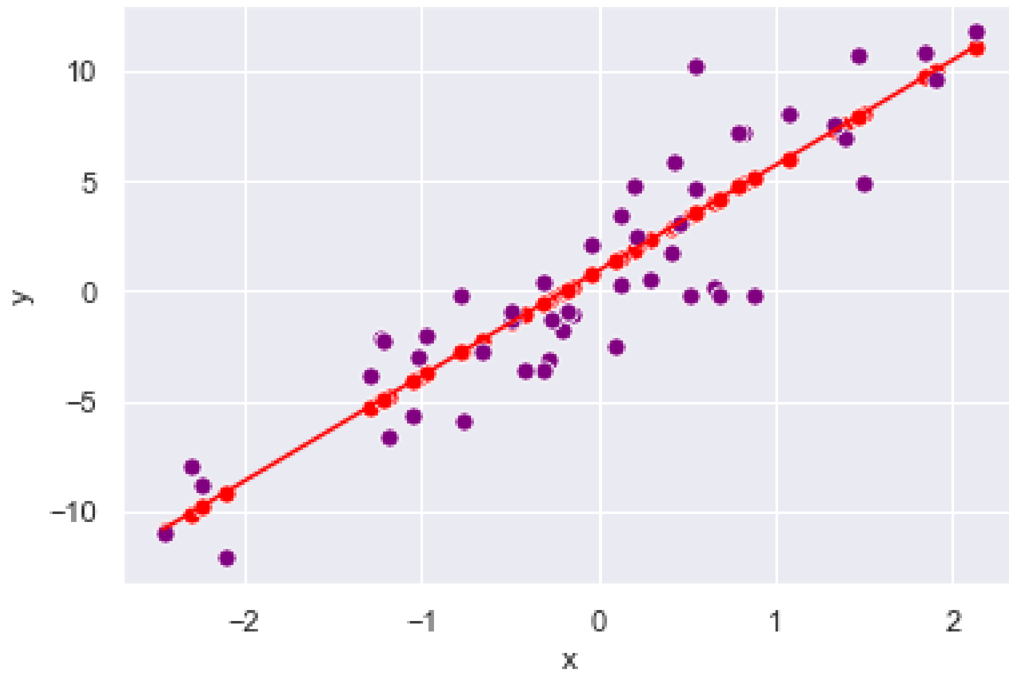


Predict some new points

```
y_test_hat = reg_noisy.intercept_ + np.dot(x_test,reg_noisy.coef_)
```

```
x_line = [np.min(x_test), np.max(x_test)]
y_line = x_line*reg_noisy.coef_ + reg_noisy.intercept_
```

```
sns.lineplot(x=x_line, y=y_line, color='red');
sns.scatterplot(x=x_test.squeeze(), y=y_test_hat, color='red', s=50);
sns.scatterplot(x=x_test.squeeze(), y=y_test, color='purple', s=50);
plt.xlabel('x');
plt.ylabel('y');
```



Compute MSE

```
y_test_hat = reg_noisy.intercept_ + np.dot(x_test,reg_noisy.coef_)
mse_noisy = 1.0/(len(y_test)) * np.sum((y_test - y_test_hat)**2)
mse_noisy
```

```
5.768555777022246
```

The MSE is higher than before!

Does this mean our estimate of w_0 and w_1 is not optimal?

Since we generated the data, we know the "true" coefficient value and we can see how much the MSE would be with the true coefficient values.

```
y_test_perfect_coef = intercept + np.dot(x_test,coef)

mse_perfect_coef = 1.0/(len(y_test_perfect_coef)) * np.sum((y_test_perfect_coef - y_test)**2)
mse_perfect_coef
```

```
5.868021561184981
```

Important: I thought we selected the coefficients that minimize MSE! But sometimes our linear regression doesn't select the "true" coefficients?

```
y_train_hat = reg_noisy.intercept_ + np.dot(x_train,reg_noisy.coef_)
mse_train_est = 1.0/(len(y_train)) * np.sum((y_train - y_train_hat)**2)
mse_train_est
```

```
2.5155527407109175
```

```python
y_train_perfect_coef = intercept + np.dot(x_train,coef)
mse_train_perfect = 1.0/(len(y_train_perfect_coef)) * np.sum((y_train_perfect_coef -
    y_train)**2)
mse_train_perfect
```

```
2.5720675581030883
```

The “correct” coefficients had slightly higher MSE on the training set than the fitted coefficients. We fit parameters so that they are optimal on the *training* set, then we use the test set to understand how the model will generalize to new, unseen data.

We saw that part of the MSE is due to noise in the data, and part is due to error in the parameter estimates.

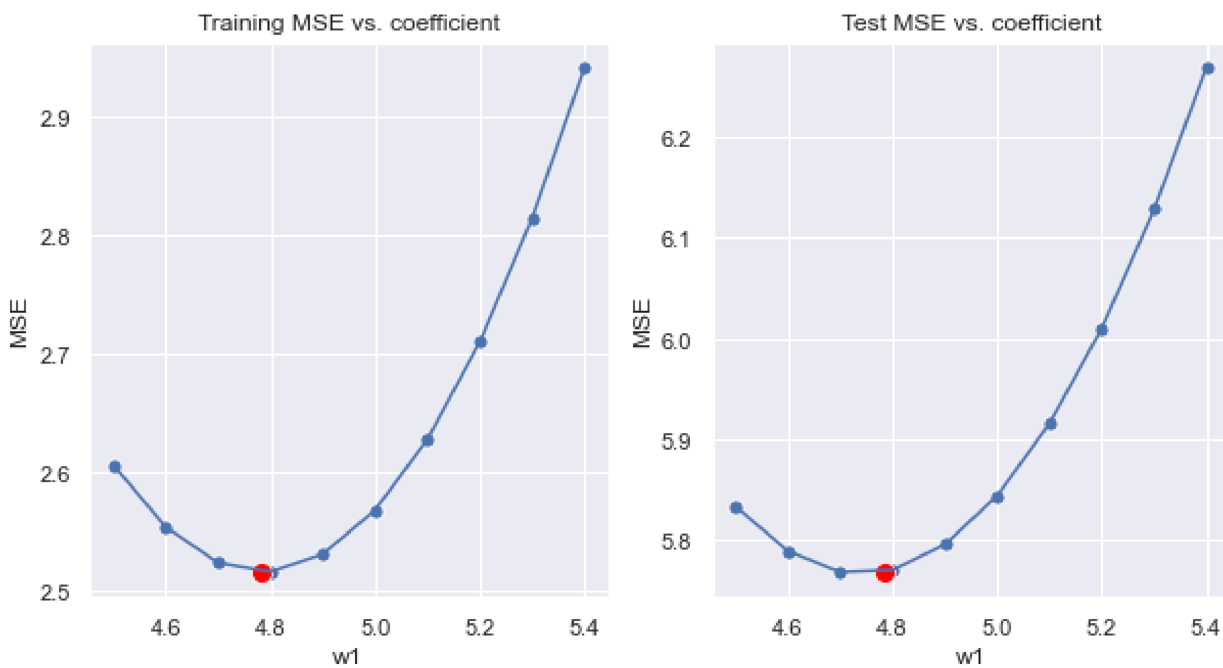
Soon - we will formalize this discussion of different sources of error:

- Error in parameter estimates
- “Noise” - any variation in data that is not a function of the X that we use as input to the model
- Other error - model (hypothesis class) not a good choice for the data, for example

Visualize MSE for different coefficients

```python
coefs = np.arange(4.5, 5.5, 0.1)
mses_test = np.zeros(len(coefs))
mses_train = np.zeros(len(coefs))

for idx, c in enumerate(coefs):
  y_test_hat_c = (reg_noisy.intercept_ + np.dot(x_test,c)).squeeze()
  mses_test[idx] =  1.0/(len(y_test_hat_c)) * np.sum((y_test - y_test_hat_c)**2)
  y_train_hat_c = (reg_noisy.intercept_ + np.dot(x_train,c)).squeeze()
  mses_train[idx] =  1.0/(len(y_train_hat_c)) * np.sum((y_train - y_train_hat_c)**2)
```

```python
plt.figure(figsize=(10,5))

plt.subplot(1,2,1)
sns.lineplot(x=coefs, y=mses_train)
sns.scatterplot(x=coefs, y=mses_train, s=50);
sns.scatterplot(x=reg_noisy.coef_, y=mse_train_est, color='red', s=100);
plt.title("Training MSE vs. coefficient");
plt.xlabel('w1');
plt.ylabel('MSE');

plt.subplot(1,2,2)
sns.lineplot(x=coefs, y=mses_test)
sns.scatterplot(x=coefs, y=mses_test, s=50);
sns.scatterplot(x=reg_noisy.coef_, y=mse_noisy, color='red', s=100);
plt.title("Test MSE vs. coefficient");
plt.xlabel('w1');
plt.ylabel('MSE');
```



In the plot on the left (for training MSE), the red dot (our coefficient estimate) should always have minimum MSE, because we select parameters to minimize MSE on the training set.

In the plot on the right (for test MSE), the red dot might not have the minimum MSE, because the best coefficient on the training set might not be the best coefficient on the test set. This gives us some idea of how our model will generalize to new, unseen data. We may suspect that if the coefficient estimate is not perfect for *this* test data, it might have some error on other new, unseen data, too.

If you re-run this notebook many times, you'll get a new random sample of training and test data each time. Sometimes, the "true" coefficients may have smaller MSE on the test set than the estimated coefficients. On other runs, the estimated coefficients might have smaller MSE on the test set.

Variance, explained variance, R2

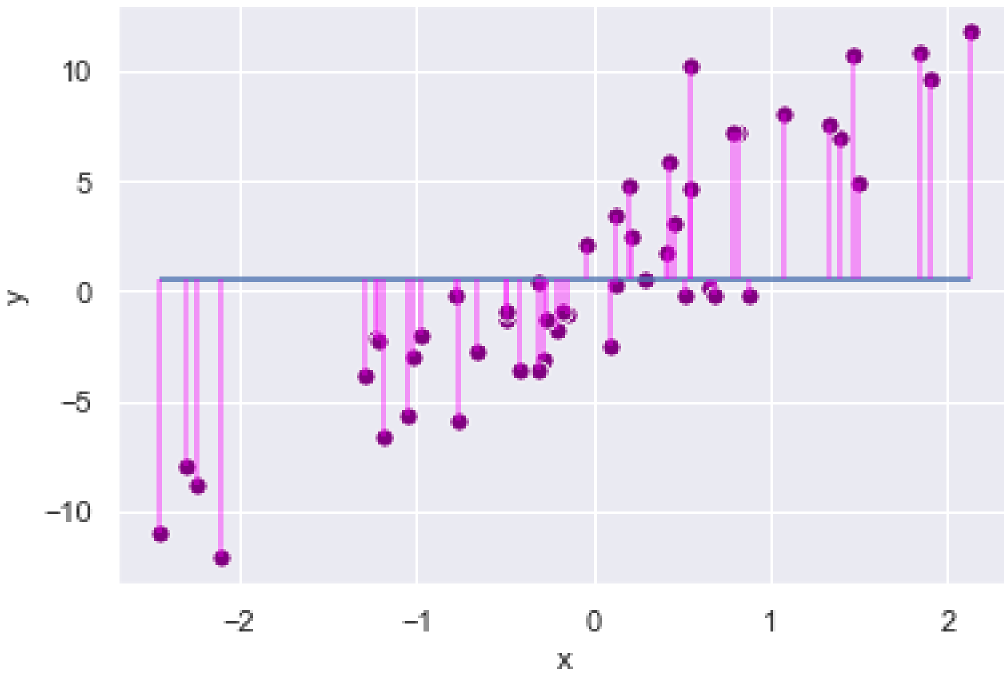
```
var_y = 1.0/len(y_test) * np.sum((y_test - np.mean(y_test))**2)
var_y
```

```
31.703055444579768
```

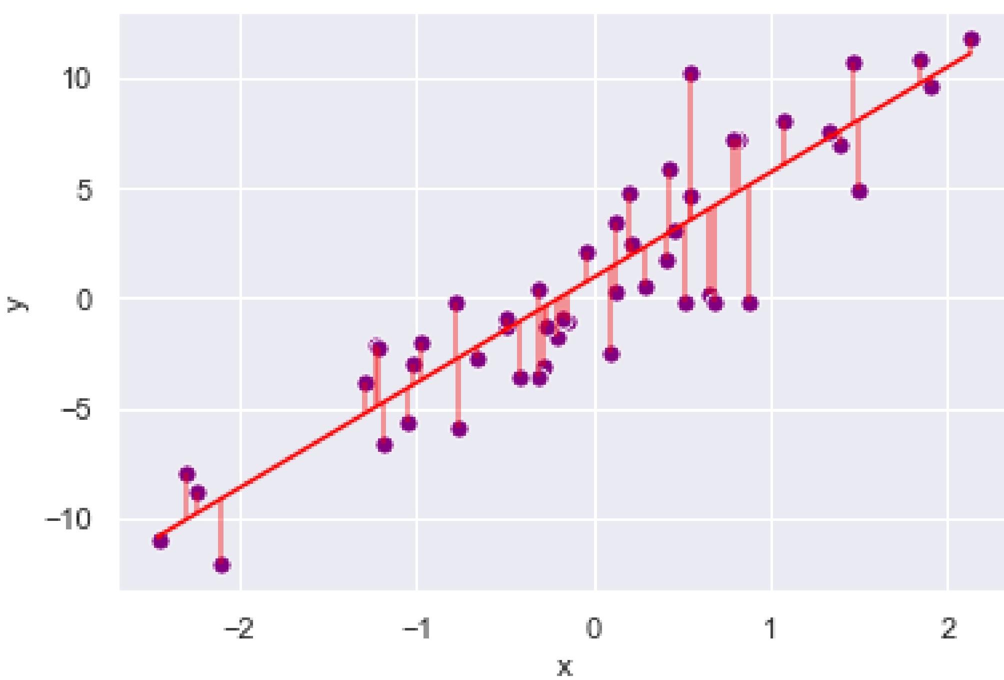
```
mean_y = np.mean(y_test)
mean_y
```

```
0.5974103400539256
```

```
x_line = [np.min(x_test), np.max(x_test)]
y_line = x_line*reg_noisy.coef_ + reg_noisy.intercept_
plt.hlines(mean_y, xmin=np.min(x_test), xmax=np.max(x_test));
plt.vlines(x_test, ymin=mean_y, ymax=y_test, color='magenta', alpha=0.5);
sns.scatterplot(x=x_test.squeeze(), y=y_test, color='purple', s=50);
plt.xlabel('x');
plt.ylabel('y');
```




```
plt.vlines(x_test, ymin=y_test, ymax=y_test_hat, color='red', alpha=0.5);
sns.scatterplot(x=x_test.squeeze(), y=y_test, color='purple', s=50);
x_line = [np.min(x_test), np.max(x_test)]
y_line = x_line*reg_noisy.coef_ + reg_noisy.intercept_
sns.lineplot(x=x_line, y=y_line, color='red');
plt.xlabel('x');
plt.ylabel('y');
```

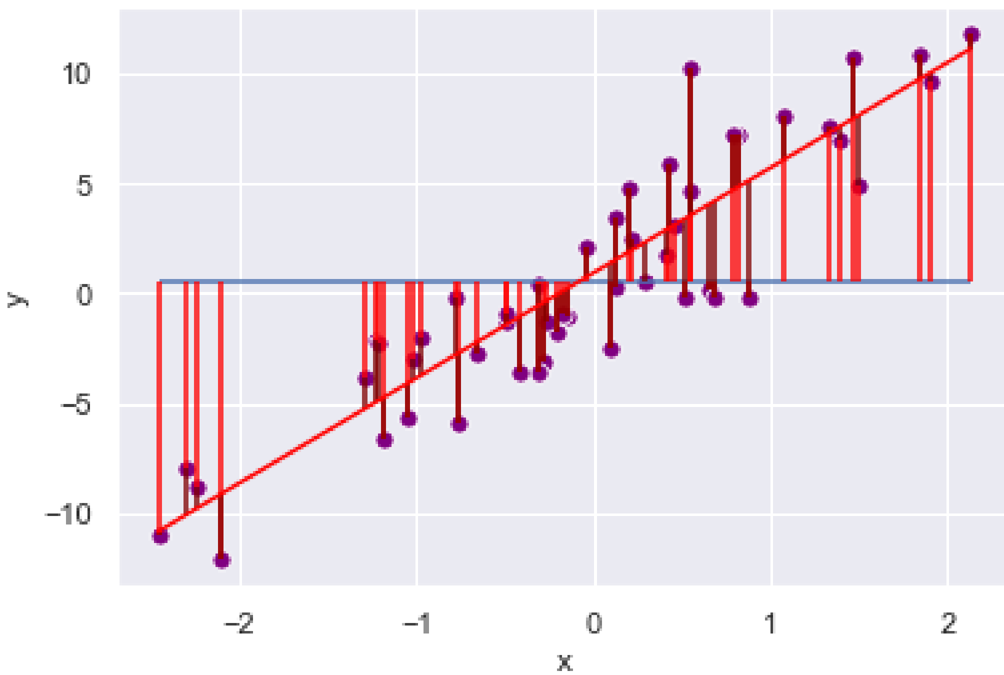


Remember:

- The total variance of y is shown in the first plot, where each vertical line is $y_i - \bar{y}$
- The *unexplained* variance of y is shown in the second plot, where each vertical line is the error of the model, $y_i - \hat{y}_i$

In the next plot, we'll combine them to get some intuition regarding the *fraction of unexplained variance*. The dark maroon part of each vertical bar is the *unexplained* part, while the red part is *explained* by the linear regression.

```
x_line = [np.min(x_test), np.max(x_test)]
y_line = x_line*reg_noisy.coef_ + reg_noisy.intercept_

plt.hlines(mean_y, xmin=np.min(x_test), xmax=np.max(x_test));
plt.vlines(x_test, ymin=mean_y, ymax=y_test, color='red');
plt.vlines(x_test, ymin=y_test, ymax=y_test_hat, color='maroon');
sns.scatterplot(x=x_test.squeeze(), y=y_test, color='purple', s=50);
sns.lineplot(x=x_line, y=y_line, color='red');
plt.xlabel('x');
plt.ylabel('y');
```



Fraction of variance unexplained is the ratio of the sum of squared distances from data to the regression line (sum of squared vertical distances in second plot), to the sum of squared distanced from data to the mean (sum of squared vertical distances in first plot):

$$\frac{MSE}{Var(y)} = \frac{Var(y - \hat{y})}{Var(y)} = \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

Alternative interpretation: imagine we would develop a very simple ML model, in which we always predict $\hat{y}_i = \bar{y}_i$. Then, we use this model as a basis for comparison for other, more sophisticated models. The ratio above is the ratio of error of the regression model, to the error of a "prediction by mean" model.

- If this quantity is less than 1, our model is better than "prediction by mean"
- If this quantity is greater than 1, our model is worse than "prediction by mean"

```
fvu = mse_noisy/var_y
fvu
```

```
0.18195583031756293
```

```
r2 = 1 - fvu
r2
```

```
0.8180441696824371
```

```
# another way to do the same thing...
metrics.r2_score(y_test, y_test_hat)
```

```
0.8180441696824371
```

What does a negative R2 mean, in terms of a comparison to "prediction by mean"?

Residual analysis

```
df = sns.load_dataset("anscombe")
df.groupby('dataset').agg({'x': ['count','mean', 'std'], 'y': ['count','mean', 'std']})
```

```
            x                    y
        count mean       std count      mean       std
dataset
I          11  9.0  3.316625    11  7.500909  2.031568
II         11  9.0  3.316625    11  7.500909  2.031657
III        11  9.0  3.316625    11  7.500000  2.030424
IV         11  9.0  3.316625    11  7.500909  2.030579
```

```
data_i   = df[df['dataset'].eq('I')]
data_ii  = df[df['dataset'].eq('II')]
data_iii = df[df['dataset'].eq('III')]
data_iv  = df[df['dataset'].eq('IV')]
```

```
reg_i   = LinearRegression().fit(data_i[['x']],   data_i['y'])
reg_ii  = LinearRegression().fit(data_ii[['x']],  data_ii['y'])
reg_iii = LinearRegression().fit(data_iii[['x']], data_iii['y'])
reg_iv  = LinearRegression().fit(data_iv[['x']],  data_iv['y'])
```

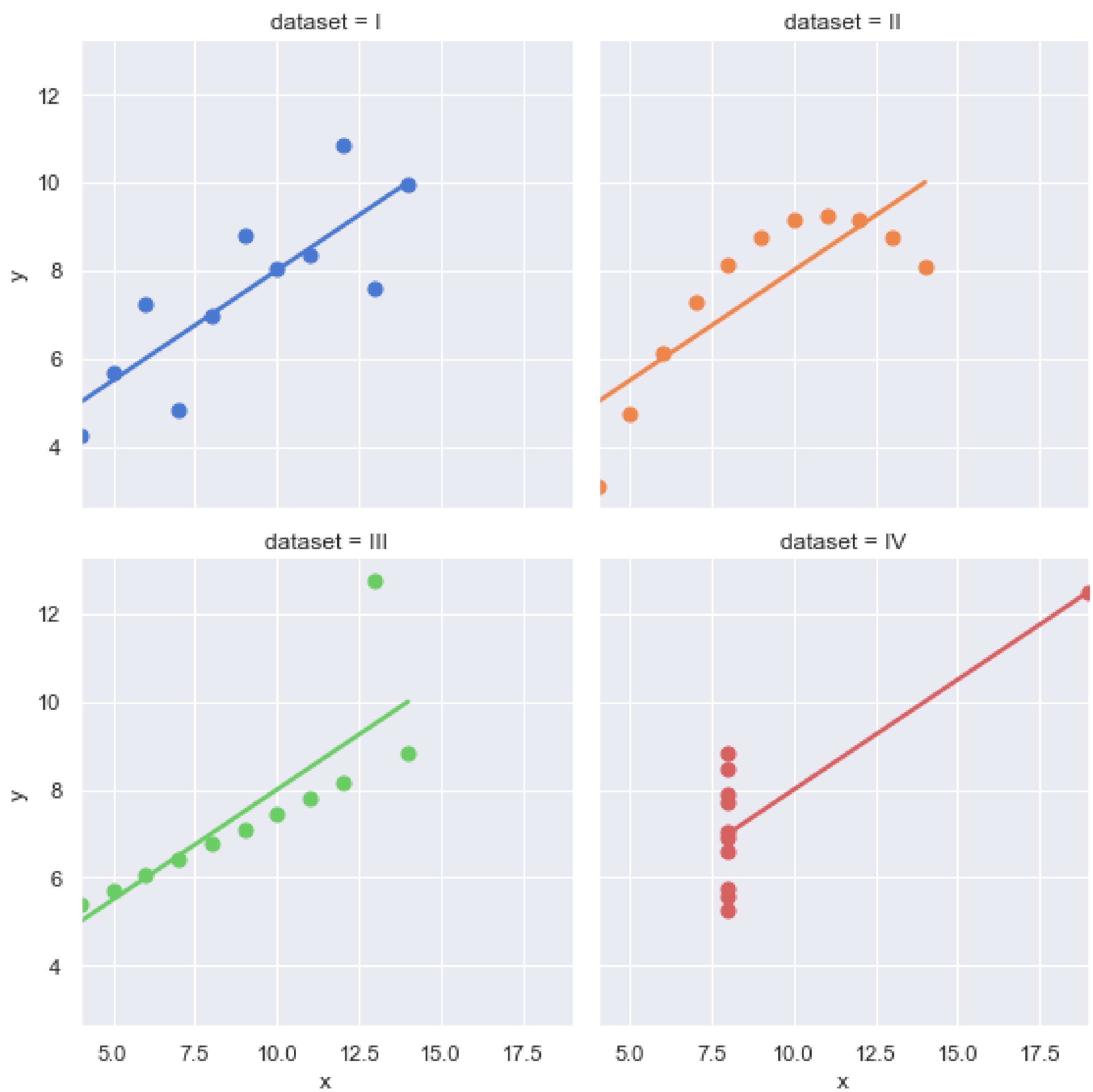
```
print("Dataset I:   ",   reg_i.coef_,   reg_i.intercept_)
print("Dataset II:  ",  reg_ii.coef_,  reg_ii.intercept_)
print("Dataset III: ", reg_iii.coef_, reg_iii.intercept_)
print("Dataset IV:  ",  reg_iv.coef_,  reg_iv.intercept_)
```

```
Dataset I:    [0.50009091] 3.0000909090909094
Dataset II:   [0.5] 3.000909090909089
Dataset III:  [0.49972727] 3.002454545454544
Dataset IV:   [0.49990909] 3.0017272727272726
```

```python
print("Dataset I:   ", metrics.r2_score(data_i['y'],  reg_i.predict(data_i[['x']])))
print("Dataset II:  ", metrics.r2_score(data_ii['y'], reg_ii.predict(data_ii[['x']])))
print("Dataset III: ", metrics.r2_score(data_iii['y'],reg_iii.predict(data_iii[['x']])))
print("Dataset IV:  ", metrics.r2_score(data_iv['y'], reg_iv.predict(data_iv[['x']])))
```

```
Dataset I:    0.6665424595087748
Dataset II:   0.6662420337274844
Dataset III:  0.6663240410665591
Dataset IV:   0.6667072568984653
```

```python
sns.lmplot(x="x", y="y", col="dataset", hue="dataset",
           data=df, col_wrap=2, ci=None, palette="muted", height=4,
           scatter_kws={"s": 50, "alpha": 1});
```



Does the linear model fit well?

- the linear model is a good fit for Dataset I
- Dataset II is clearly non-linear
- Dataset III has an outlier
- Dataset IV has a high leverage point

Easy to identify problems in 1D - what about in higher D?

- Plot $\hat{y}$ against y
- Plot residuals against $\hat{y}$
- Plot residuals against each x (including any x not in the model)
- Plot residuals against time (for time series data)

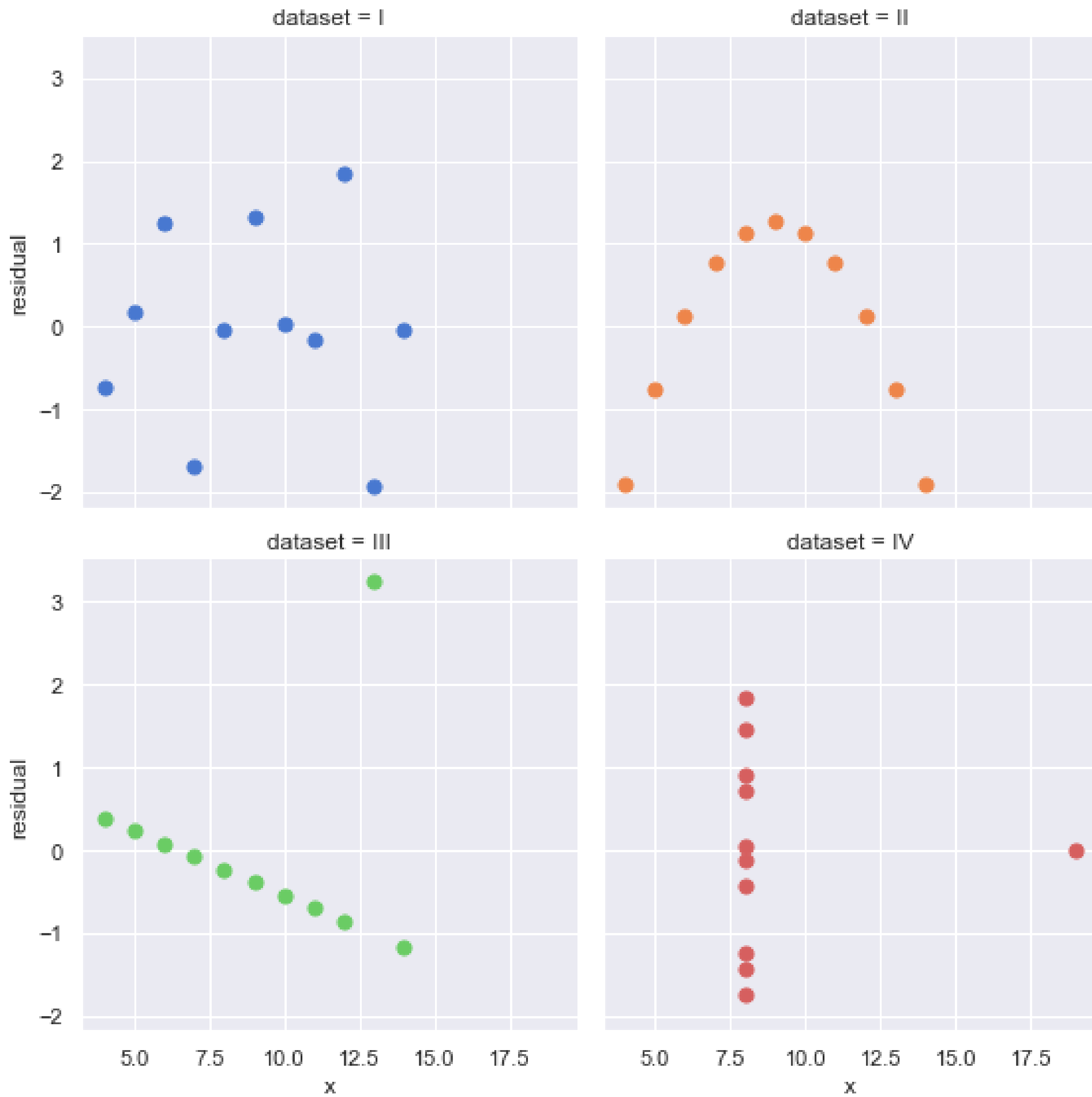
What should each of these plots look like if the regression is "good"?

```
data_i   = data_i.assign(   yhat = reg_i.predict(  data_i[['x']]) )
```

```
data_ii  = data_ii.assign(  yhat = reg_ii.predict( data_ii[['x']]) )
data_iii = data_iii.assign( yhat = reg_iii.predict( data_iii[['x']]) )
data_iv  = data_iv.assign(  yhat = reg_iv.predict(  data_iv[['x']]) )

data_i   = data_i.assign(   residual = data_i['y'] - data_i['yhat'] )
data_ii  = data_ii.assign(  residual = data_ii['y'] - data_ii['yhat'] )
data_iii = data_iii.assign( residual = data_iii['y'] - data_iii['yhat'] )
data_iv  = data_iv.assign(  residual = data_iv['y'] - data_iv['yhat'] )

data_all = pd.concat([data_i, data_ii, data_iii, data_iv])
data_all.head()
```

```
  dataset     x     y      yhat  residual
0       I  10.0  8.04  8.001000  0.039000
1       I   8.0  6.95  7.000818 -0.050818
2       I  13.0  7.58  9.501273 -1.921273
3       I   9.0  8.81  7.500909  1.309091
4       I  11.0  8.33  8.501091 -0.171091
```

```
sns.lmplot(x="x", y="residual", col="dataset", hue="dataset",
           data=data_all, col_wrap=2, ci=None, palette="muted", height=4,
           scatter_kws={"s": 50, "alpha": 1}, fit_reg=False);
```



Multiple linear regression

Generate some data

```
x_train, y_train = generate_linear_regression_data(n=n_samples, d=2, coef=[5,5],
    intercept=intercept)
x_test,  y_test  = generate_linear_regression_data(n=50, d=2, coef=[5,5],
    intercept=intercept)
```

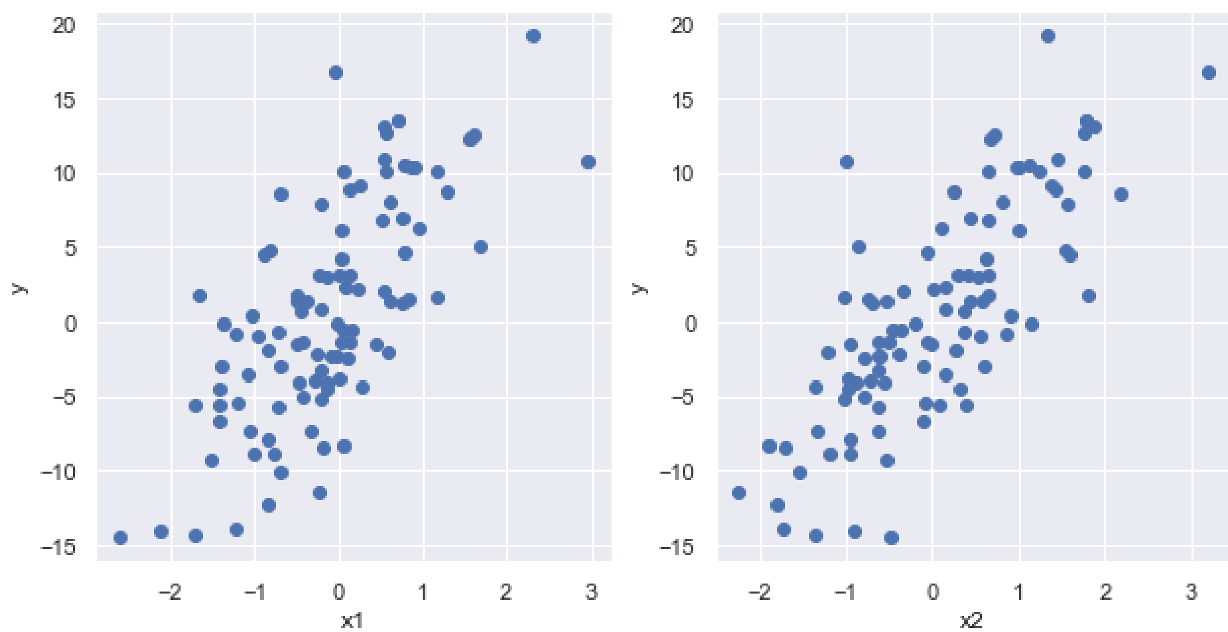
```
x_train.shape
```

```
(100, 2)
```

```
y_train.shape
```

```
(100,)
```

```
plt.figure(figsize=(10,5));
plt.subplot(1,2,1);
plt.scatter(x_train[:,0],  y_train);
plt.xlabel("x1");
plt.ylabel("y");
plt.subplot(1,2,2);
plt.scatter(x_train[:,1],  y_train);
plt.xlabel("x2");
plt.ylabel("y");
```



Recall that there is no stochastic noise in this data - so it fits a linear model perfectly. But it's more difficult to see that linear relationship in higher dimensions.

Fit a linear regression

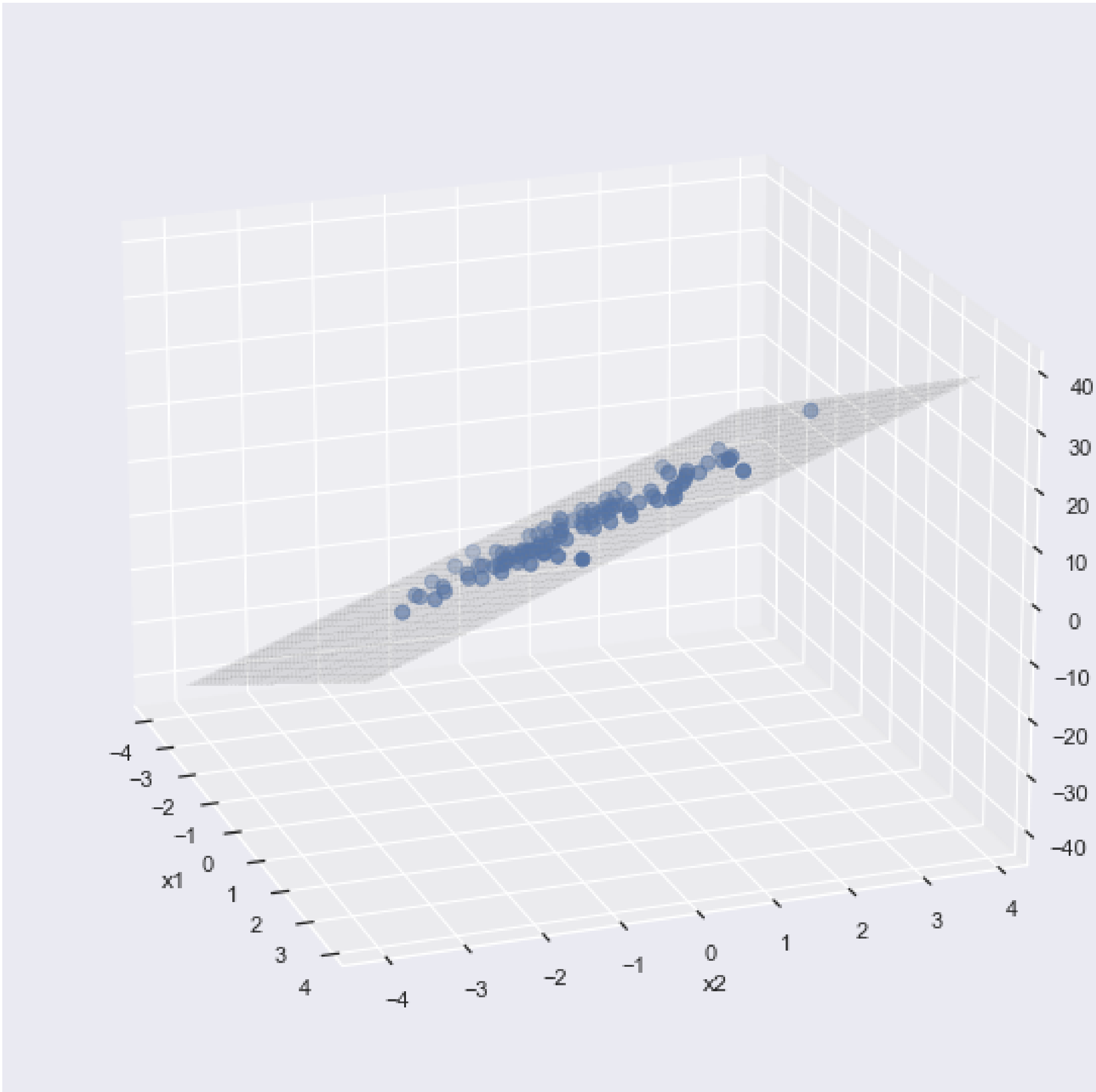
```
reg_multi = LinearRegression().fit(x_train, y_train)
print("Coefficient list: ", reg_multi.coef_)
print("Intercept: " , reg_multi.intercept_)
```

```
Coefficient list:  [5. 5.]
Intercept:  1.0
```

Plot hyperplane

```
def plot_3D(elev=20, azim=-20, X=x_train, y=y_train):
    plt.figure(figsize=(10,10))
```

```
    ax = plt.subplot(projection='3d')


    X1 = np.arange(-4, 4, 0.2)
    X2 = np.arange(-4, 4, 0.2)
    X1, X2 = np.meshgrid(X1, X2)
    Z = X1*reg_multi.coef_[0] + X2*reg_multi.coef_[1]

    # Plot the surface.
    ax.plot_surface(X1, X2, Z, alpha=0.1, color='gray',
                           linewidth=0, antialiased=False)
    ax.scatter3D(X[:, 0], X[:, 1], y, s=50)

    ax.view_init(elev=elev, azim=azim)
    ax.set_xlabel('x1')
    ax.set_ylabel('x2')
    ax.set_zlabel('y')

interact(plot_3D, elev=np.arange(-90,90,10), azim=np.arange(-90,90,10),
         X=fixed(x_train), y=fixed(y_train));
```

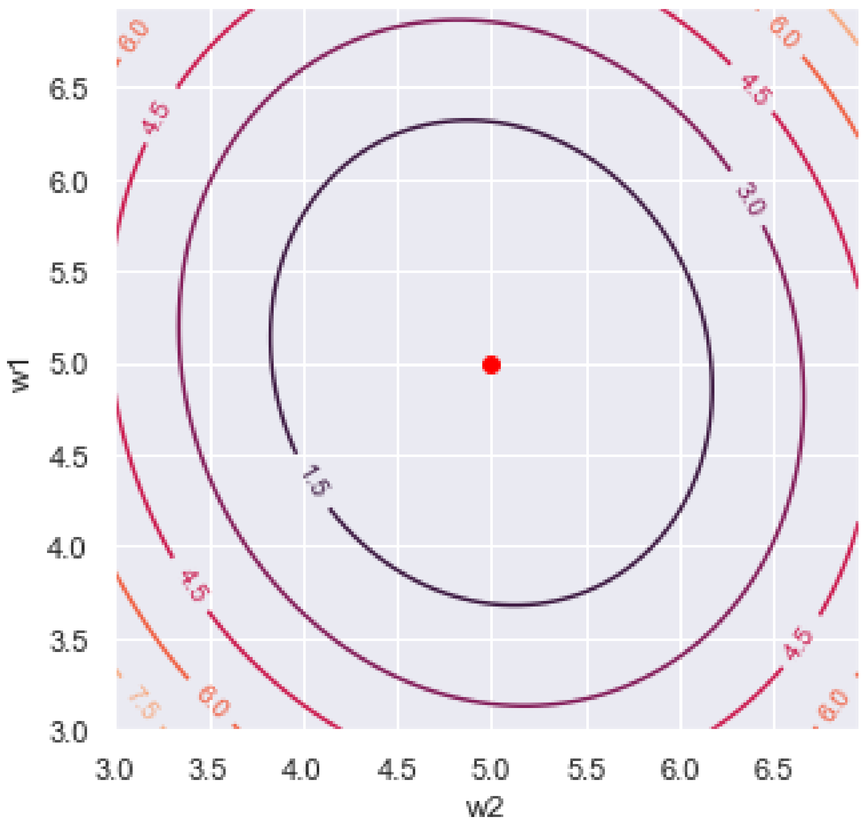


MSE contour

```
coefs = np.arange(3.0, 7.0, 0.05)
mses_train = np.zeros((len(coefs), len(coefs)))

for idx_1, c_1 in enumerate(coefs):
  for idx_2, c_2 in enumerate(coefs):
    y_train_hat_c = (reg_multi.intercept_ + np.dot(x_train,[c_1, c_2])).squeeze()
    mses_train[idx_1,idx_2] =  1.0/(len(y_train_hat_c)) * np.sum((y_train -
        y_train_hat_c)**2)
```

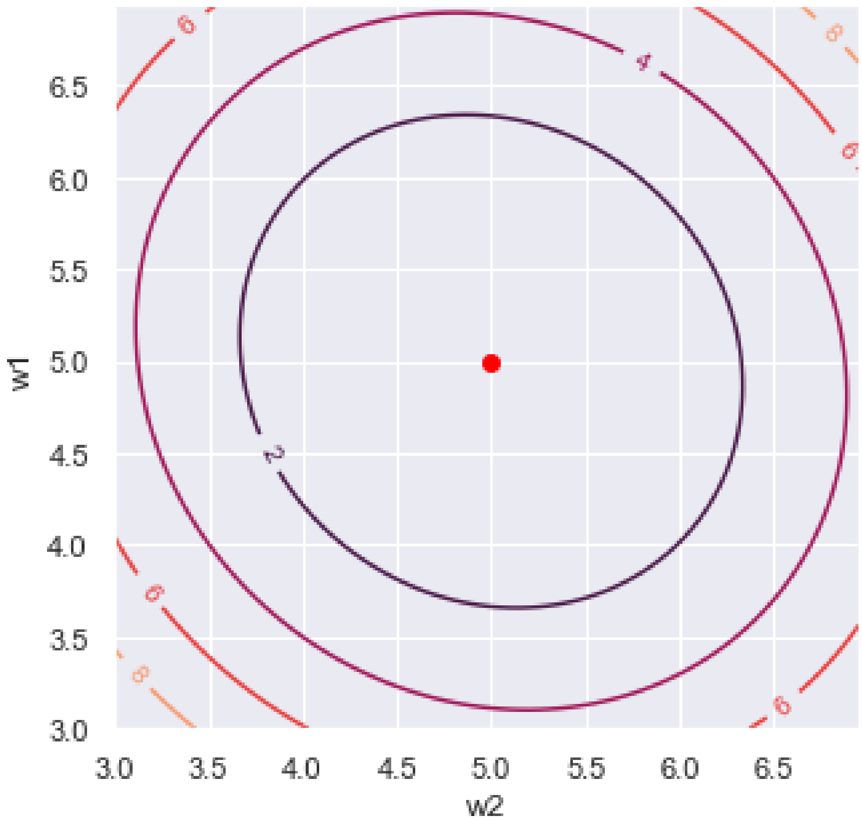
```
plt.figure(figsize=(5,5));
X1, X2 = np.meshgrid(coefs, coefs)
p = plt.scatter(x=reg_multi.coef_[1], y=reg_multi.coef_[0], c='red')
```

```
p = plt.contour(X1, X2, mses_train, levels=5);
plt.clabel(p, inline=1, fontsize=10);
plt.xlabel('w2');
plt.ylabel('w1');
```




```
coefs = np.arange(3.0, 7.0, 0.05)
mses_test = np.zeros((len(coefs), len(coefs)))

for idx_1, c_1 in enumerate(coefs):
  for idx_2, c_2 in enumerate(coefs):
    y_test_hat_c = (reg_multi.intercept_ + np.dot(x_test,[c_1, c_2])).squeeze()
    mses_test[idx_1,idx_2] =  1.0/(len(y_test_hat_c)) * np.sum((y_test - y_test_hat_c)**2)
```

```
plt.figure(figsize=(5,5));
X1, X2 = np.meshgrid(coefs, coefs)
p = plt.scatter(x=reg_multi.coef_[1], y=reg_multi.coef_[0], c='red')
p = plt.contour(X1, X2, mses_test, levels=5);
plt.clabel(p, inline=1, fontsize=10);
plt.xlabel('w2');
plt.ylabel('w1');
```

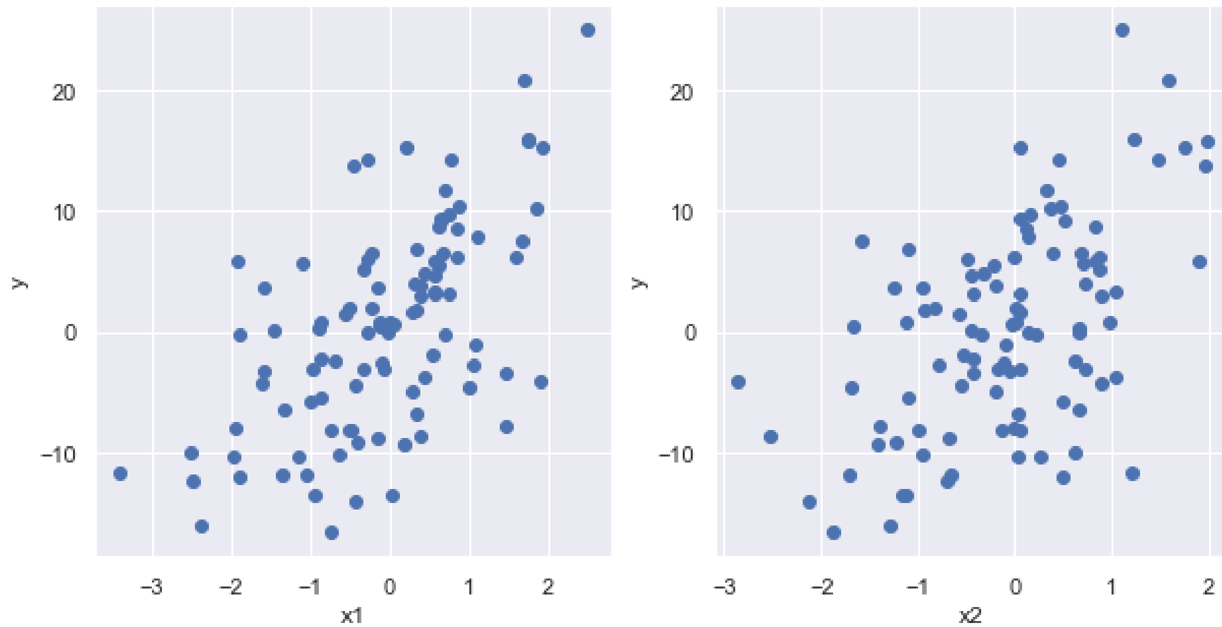


Multiple linear regression with noise

Generate some data

```
x_train, y_train = generate_linear_regression_data(n=n_samples, d=2, coef=[5,5],
    intercept=intercept, sigma=5)
x_test,  y_test  = generate_linear_regression_data(n=50, d=2, coef=[5,5],
    intercept=intercept, sigma=5)
```

```
plt.figure(figsize=(10,5));
plt.subplot(1,2,1);
plt.scatter(x_train[:,0],  y_train);
plt.xlabel("x1");
plt.ylabel("y");
plt.subplot(1,2,2);
plt.scatter(x_train[:,1],  y_train);
plt.xlabel("x2");
plt.ylabel("y");
```



Fit a linear regression

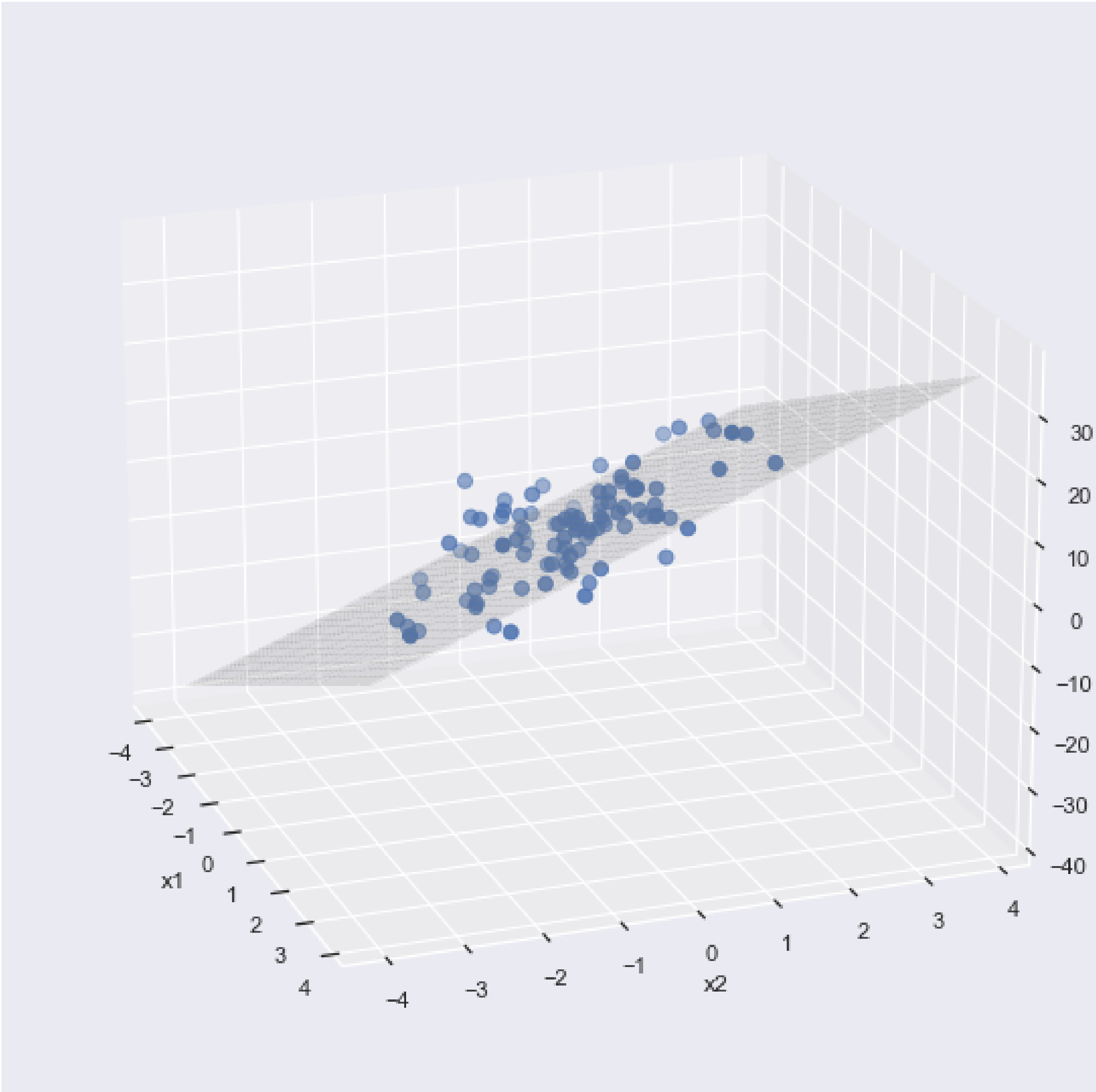
```
reg_multi_noisy = LinearRegression().fit(x_train, y_train)
print("Coefficient list: ", reg_multi_noisy.coef_)
print("Intercept: " , reg_multi_noisy.intercept_)
```

```
Coefficient list:  [4.56318915 4.70989482]
Intercept:  1.0570036948008308
```

Plot hyperplane

```
def plot_3D(elev=20, azim=-20, X=x_train, y=y_train):
    plt.figure(figsize=(10,10))
    ax = plt.subplot(projection='3d')


    X1 = np.arange(-4, 4, 0.2)
    X2 = np.arange(-4, 4, 0.2)
    X1, X2 = np.meshgrid(X1, X2)
    Z = X1*reg_multi_noisy.coef_[0] + X2*reg_multi_noisy.coef_[1]

    # Plot the surface.
    ax.plot_surface(X1, X2, Z, alpha=0.1, color='gray',
                    linewidth=0, antialiased=False)
    ax.scatter3D(X[:, 0], X[:, 1], y, s=50)

    ax.view_init(elev=elev, azim=azim)
    ax.set_xlabel('x1')
    ax.set_ylabel('x2')
    ax.set_zlabel('y')
```

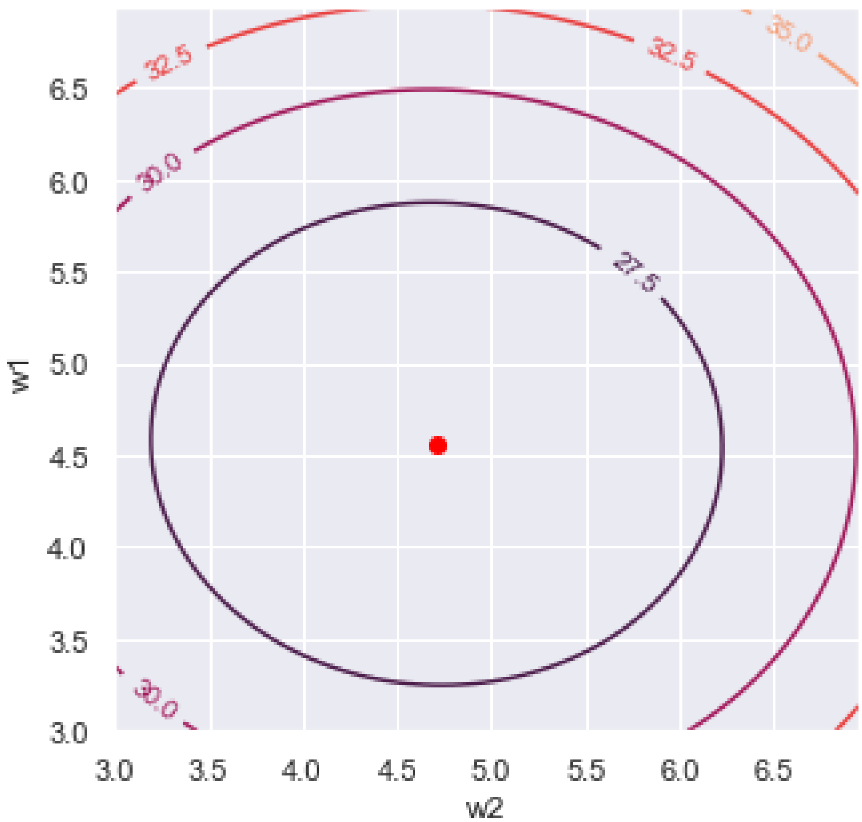
```
interact(plot_3D, elev=np.arange(-90,90,10), azim=np.arange(-90,90,10),
         X=fixed(x_train), y=fixed(y_train));
```



MSE contour

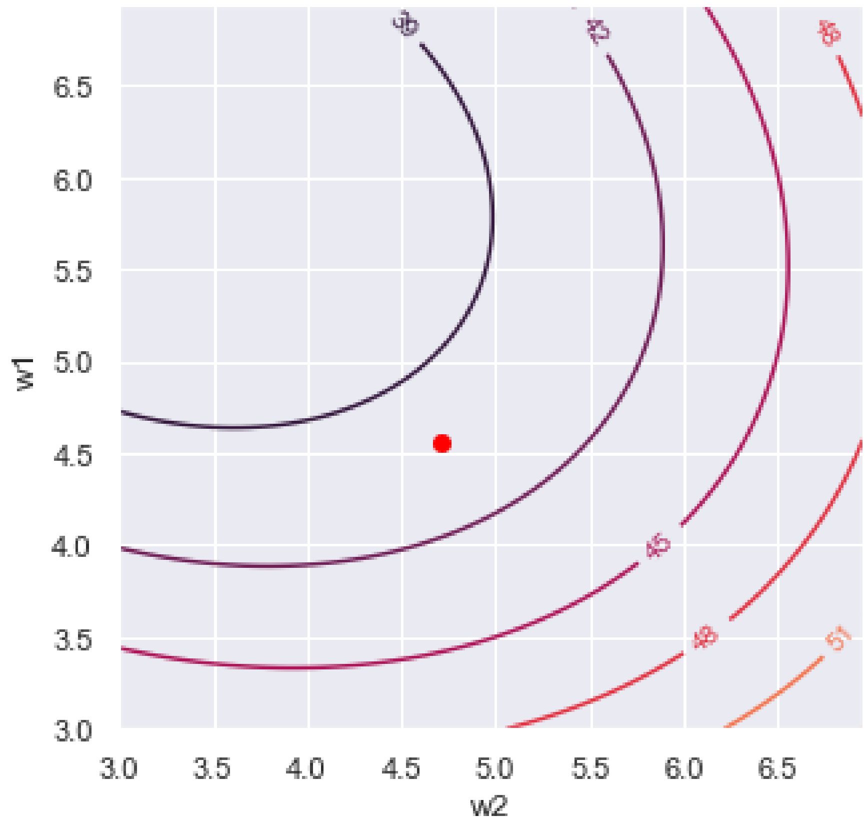
```
coefs = np.arange(3.0, 7.0, 0.05)
mses_train = np.zeros((len(coefs), len(coefs)))

for idx_1, c_1 in enumerate(coefs):
  for idx_2, c_2 in enumerate(coefs):
    y_train_hat_c = (reg_multi_noisy.intercept_ + np.dot(x_train,[c_1, c_2])).squeeze()
    mses_train[idx_1,idx_2] =  1.0/(len(y_train_hat_c)) * np.sum((y_train -
        y_train_hat_c)**2)
```

```
plt.figure(figsize=(5,5));
X1, X2 = np.meshgrid(coefs, coefs)
p = plt.scatter(x=reg_multi_noisy.coef_[1], y=reg_multi_noisy.coef_[0], c='red')
p = plt.contour(X1, X2, mses_train, levels=5);
plt.clabel(p, inline=1, fontsize=10);
plt.xlabel('w2');
plt.ylabel('w1');
```




```
coefs = np.arange(3.0, 7.0, 0.05)
mses_test = np.zeros((len(coefs), len(coefs)))

for idx_1, c_1 in enumerate(coefs):
  for idx_2, c_2 in enumerate(coefs):
    y_test_hat_c = (reg_multi_noisy.intercept_ + np.dot(x_test,[c_1, c_2])).squeeze()
    mses_test[idx_1,idx_2] =  1.0/(len(y_test_hat_c)) * np.sum((y_test - y_test_hat_c)**2)
```

```
plt.figure(figsize=(5,5));
X1, X2 = np.meshgrid(coefs, coefs)
p = plt.scatter(x=reg_multi_noisy.coef_[1], y=reg_multi_noisy.coef_[0], c='red')
p = plt.contour(X1, X2, mses_test, levels=5);
plt.clabel(p, inline=1, fontsize=10);
plt.xlabel('w2');
plt.ylabel('w1');
```



Linear basis function regression

The assumptions of the linear model (that the target variable can be predicted as a linear combination of the features) can be restrictive. We can capture more complicated relationships using linear basis function regression.

Generate some data

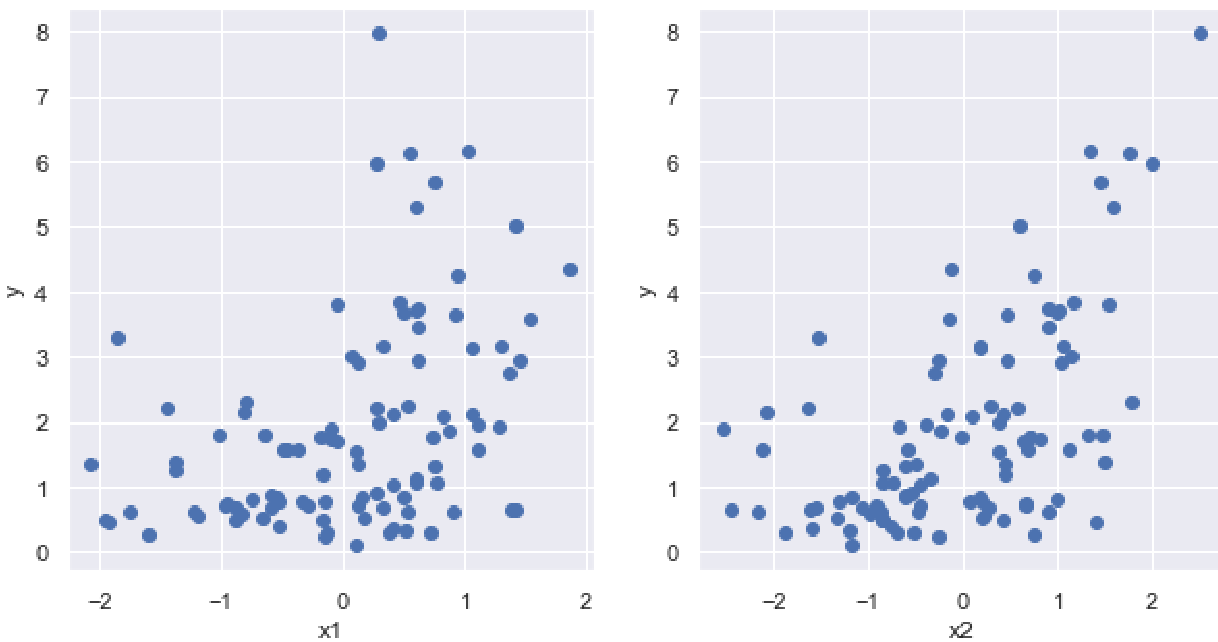
```
#@title Data generating function

import itertools

def generate_linear_basis_data(n=100, d=2, coef=[1,1,0.5,0.5,1], intercept=1, sigma=0):
  x = np.random.randn(n,d)
  x = np.column_stack((x, x**2 ))
  for pair in list(itertools.combinations(range(d), 2)):
    x = np.column_stack((x, x[:,pair[0]]*x[:,pair[1]]))
  y = (np.dot(x, coef) + intercept).squeeze() + sigma * np.random.randn(n)
  return x[:,:d], y
```

```
x_train, y_train = generate_linear_basis_data(sigma=0.2)
x_test,  y_test  = generate_linear_basis_data(n=50, sigma=0.2)
```

```
print(x_train.shape)
print(y_train.shape)
```

```
(100, 2)
(100,)
```

```
plt.figure(figsize=(10,5));
plt.subplot(1,2,1);
plt.scatter(x_train[:,0],  y_train);
plt.xlabel("x1");
plt.ylabel("y");
plt.subplot(1,2,2);
plt.scatter(x_train[:,1],  y_train);
plt.xlabel("x2");
plt.ylabel("y");
```



Fit a linear regression

```
reg_lbf = LinearRegression().fit(x_train, y_train)
print("Intercept: " , reg_lbf.intercept_)
print("Coefficient list: ", reg_lbf.coef_)
```

```
Intercept:  1.8599783475563312
Coefficient list:  [0.78381543 0.87641356]
```

Evaluate model

```
y_train_hat = reg_lbf.predict(x_train)
print("Training MSE: ", metrics.mean_squared_error(y_train, y_train_hat))
print("Training R2:  ", metrics.r2_score(y_train, y_train_hat))
```

```
Training MSE:  1.2385626463254227
Training R2:   0.503964789379802
```

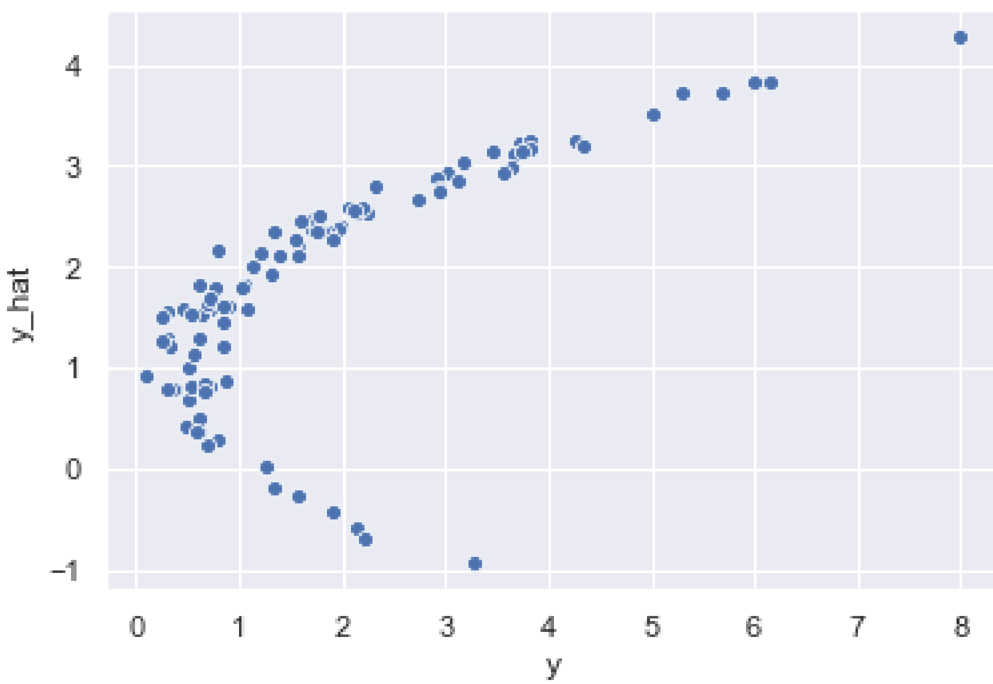
```
y_test_hat = reg_lbf.predict(x_test)
print("Test MSE: ", metrics.mean_squared_error(y_test, y_test_hat))
print("Test R2:  ", metrics.r2_score(y_test, y_test_hat))
```

```
Test MSE:  1.1355446695074995
Test R2:   0.6177904806012954
```

Residual analysis

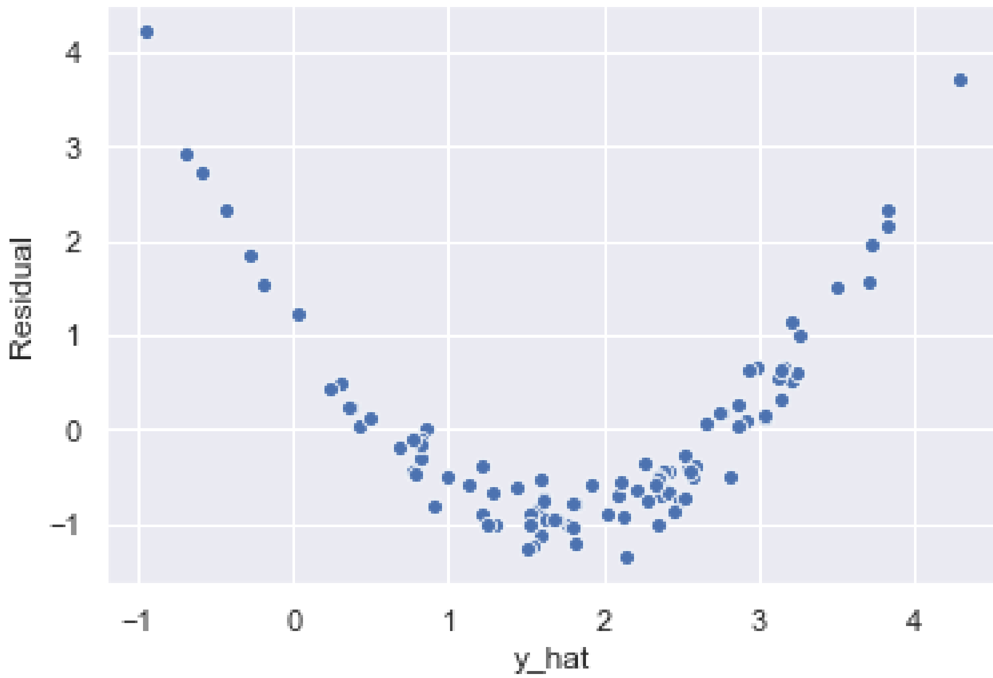
```
residual_train = y_train - y_train_hat
```

```
_ = sns.scatterplot(x=y_train, y=y_train_hat)
_ = plt.xlabel('y')
_ = plt.ylabel('y_hat')
```



Is the error random? Or does it look systematic?

```
_ = sns.scatterplot(x=y_train_hat, y=residual_train)
_ = plt.xlabel('y_hat')
_ = plt.ylabel('Residual')
```

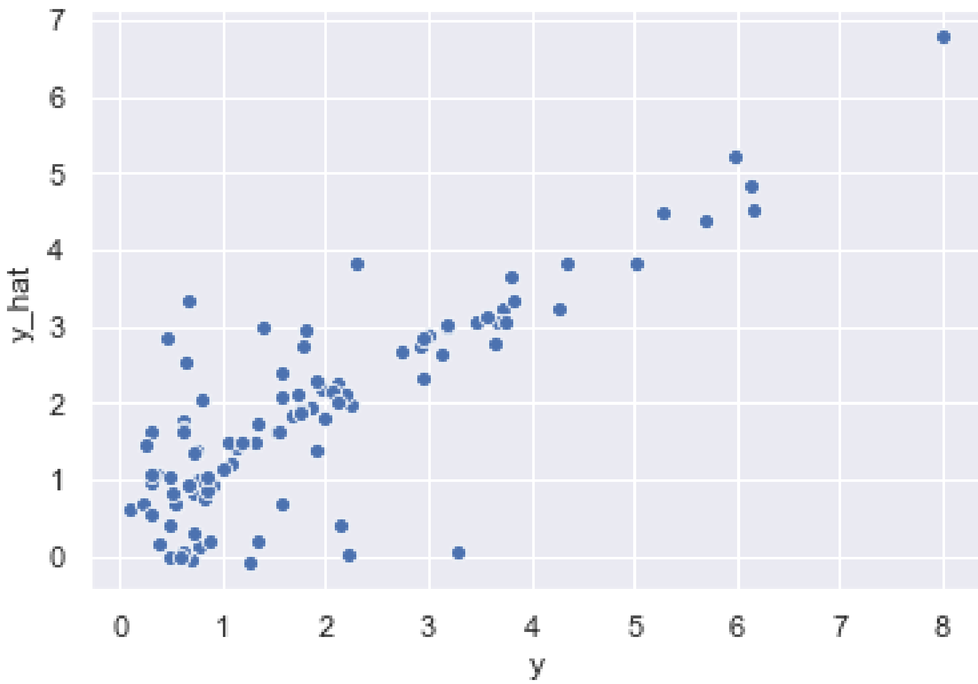


Since there is clearly some non-linearity, we can try to fit a model to a non-linear transformation of the features.

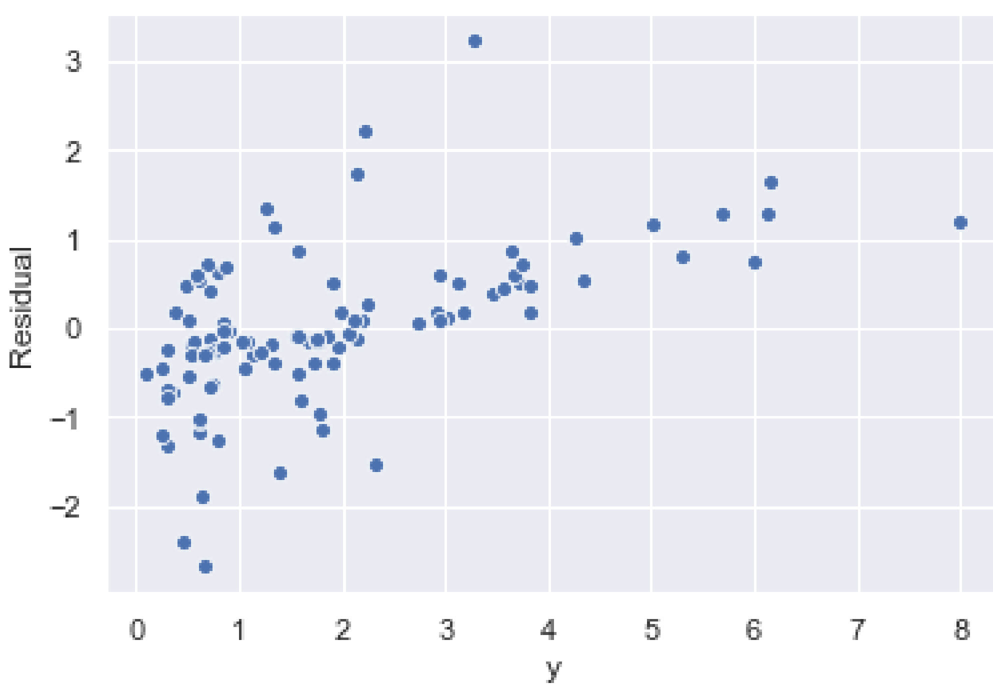
```
x_train_trans = np.column_stack((x_train, x_train**2))

reg_lbf_trans = LinearRegression().fit(x_train_trans, y_train)
print("Intercept: " , reg_lbf_trans.intercept_)
print("Coefficient list: ", reg_lbf_trans.coef_)

y_train_trans_hat = reg_lbf_trans.predict(x_train_trans)
print("Training MSE: ", metrics.mean_squared_error(y_train, y_train_trans_hat))
print("Training R2:  ", metrics.r2_score(y_train, y_train_trans_hat))

residual_train_trans = y_train - y_train_trans_hat
```

```
Intercept:  1.0707809989554227
Coefficient list:  [0.92040724 1.01062473 0.33382976 0.46107233]
Training MSE:  0.7722337515828896
Training R2:   0.690726074493773
```

```
_ = sns.scatterplot(x=y_train, y=y_train_trans_hat)
_ = plt.xlabel('y')
_ = plt.ylabel('y_hat')
```

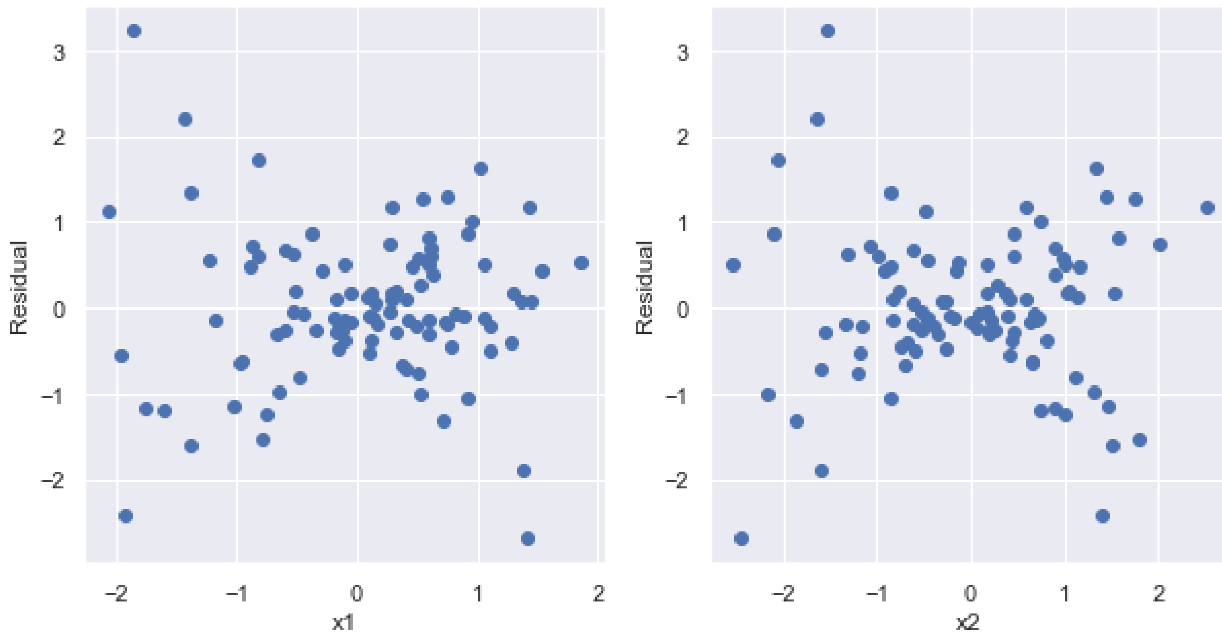



```
_ = sns.scatterplot(x=y_train, y=residual_train_trans)
_ = plt.xlabel('y')
_ = plt.ylabel('Residual')
```




```
plt.figure(figsize=(10,5));
plt.subplot(1,2,1);
plt.scatter(x_train[:,0],  residual_train_trans);
plt.xlabel("x1");
```

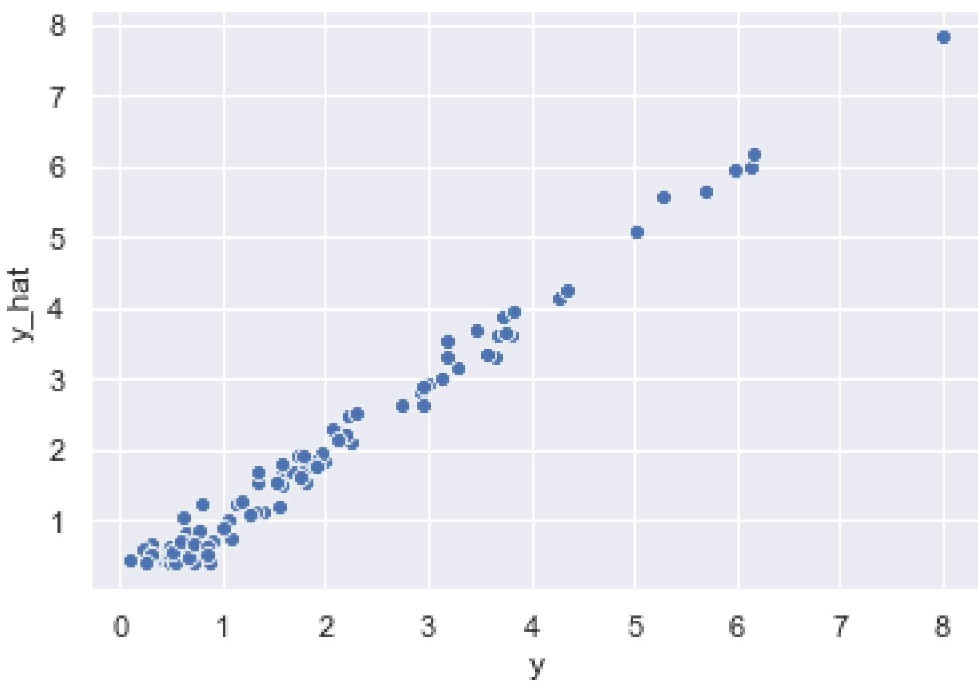
```
plt.ylabel("Residual");
plt.subplot(1,2,2);
plt.scatter(x_train[:,1],  residual_train_trans);
plt.xlabel("x2");
plt.ylabel("Residual");
```



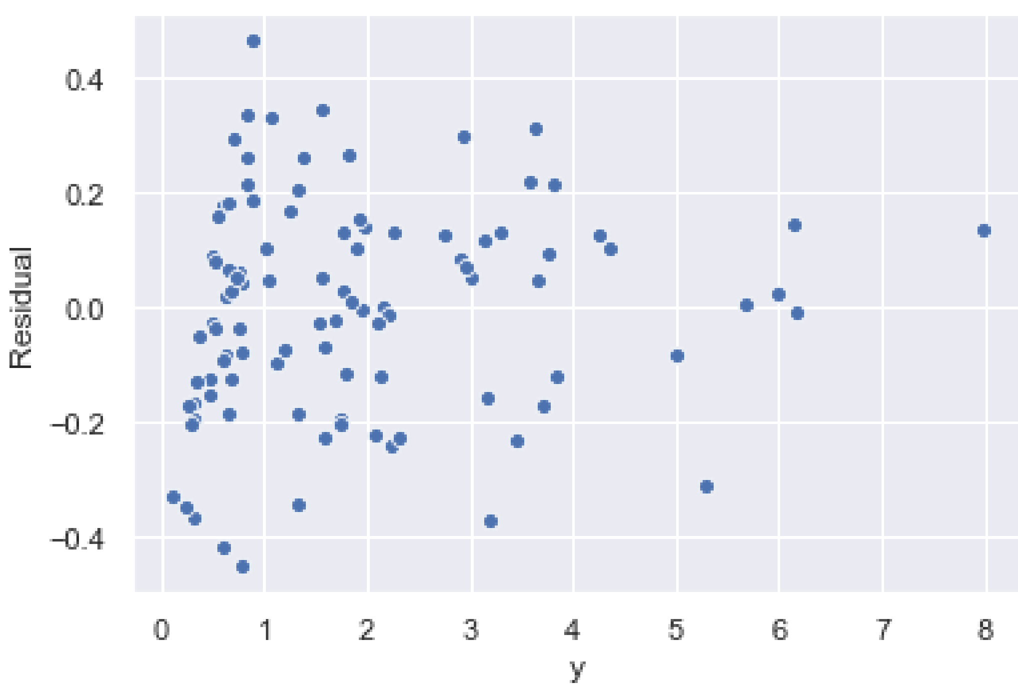

```
x_train_inter = np.column_stack((x_train_trans, x_train[:,0]*x_train[:,1]))

reg_lbf_inter = LinearRegression().fit(x_train_inter, y_train)
print("Intercept: " , reg_lbf_inter.intercept_)
print("Coefficient list: ", reg_lbf_inter.coef_)

y_train_inter_hat = reg_lbf_inter.predict(x_train_inter)
print("Training MSE: ", metrics.mean_squared_error(y_train, y_train_inter_hat))
print("Training R2:  ", metrics.r2_score(y_train, y_train_inter_hat))

residual_train_inter = y_train - y_train_inter_hat
```

```
Intercept:  0.9318430901150943
Coefficient list:  [1.04702793 1.03297183 0.50037422 0.5195507  0.98437995]
Training MSE:  0.03520822856000707
Training R2:   0.9858993639755397
```

```
_ = sns.scatterplot(x=y_train, y=y_train_inter_hat)
_ = plt.xlabel('y')
_ = plt.ylabel('y_hat')
```

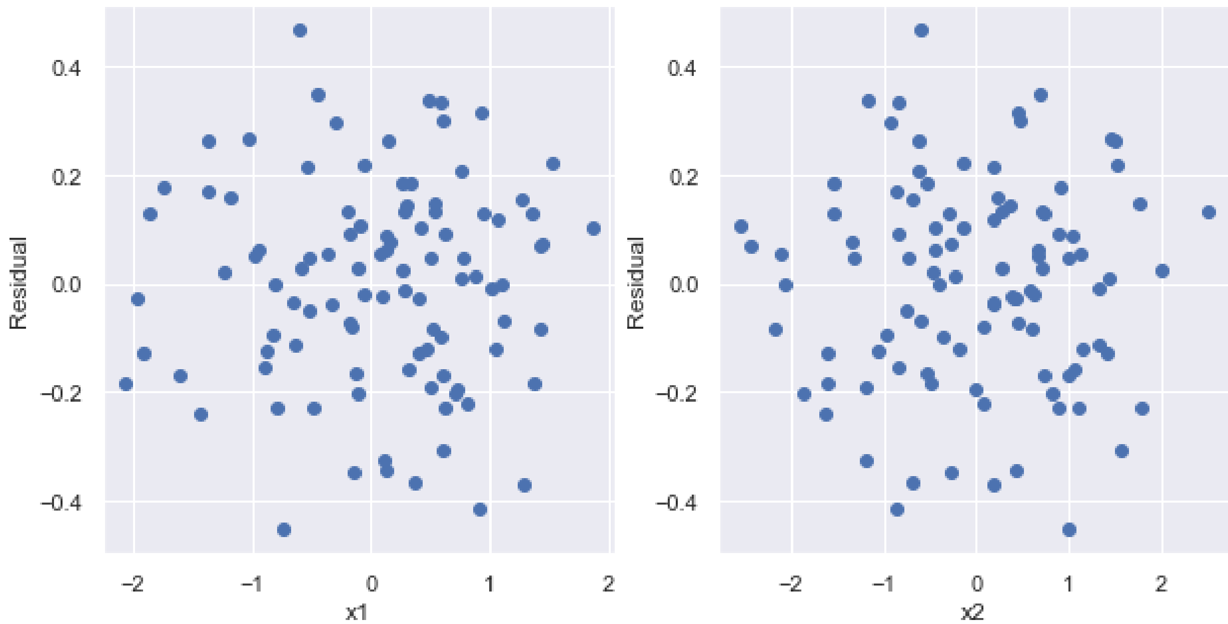



```
_ = sns.scatterplot(x=y_train, y=residual_train_inter)
_ = plt.xlabel('y')
_ = plt.ylabel('Residual')
```




```
plt.figure(figsize=(10,5));
plt.subplot(1,2,1);
plt.scatter(x_train[:,0],  residual_train_inter);
plt.xlabel("x1");
```

```
plt.ylabel("Residual");
plt.subplot(1,2,2);
plt.scatter(x_train[:,1],  residual_train_inter);
plt.xlabel("x2");
plt.ylabel("Residual");
```



Evaluate on test set again

```
x_test_inter = np.column_stack((x_test, x_test**2))
x_test_inter = np.column_stack((x_test_inter, x_test[:,0]*x_test[:,1]))

y_test_hat = reg_lbf_inter.predict(x_test_inter)
print("Test MSE: ", metrics.mean_squared_error(y_test, y_test_hat))
print("Test R2:  ", metrics.r2_score(y_test, y_test_hat))
```

```
Test MSE:  0.048320232670661156
Test R2:   0.9837360401556928
```