Regression 1

Industrial AI Lab.

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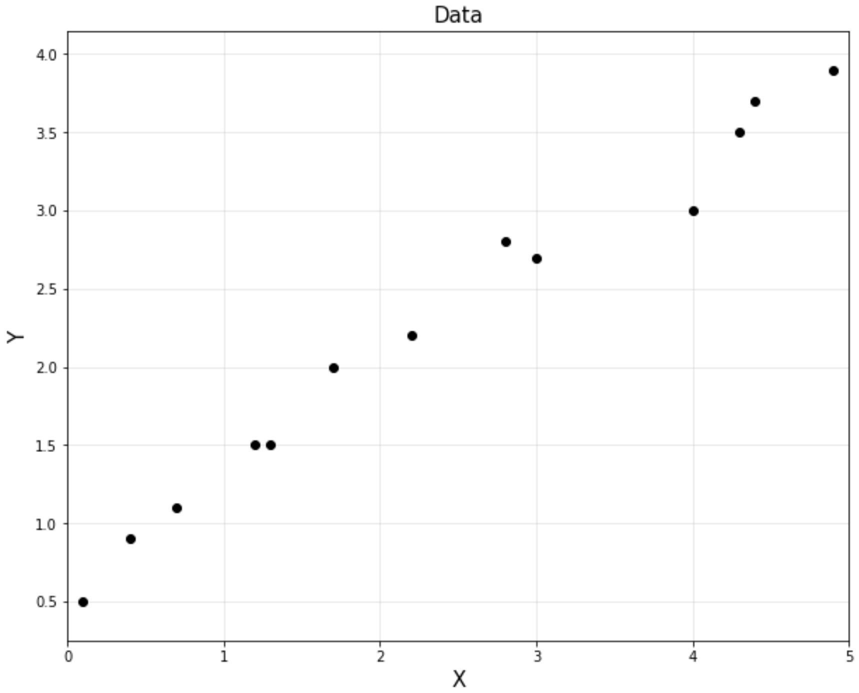
Assumption: Linear Model

$$\hat{y}_i = f(x_i\,; \theta) \ \text{ in general}$$

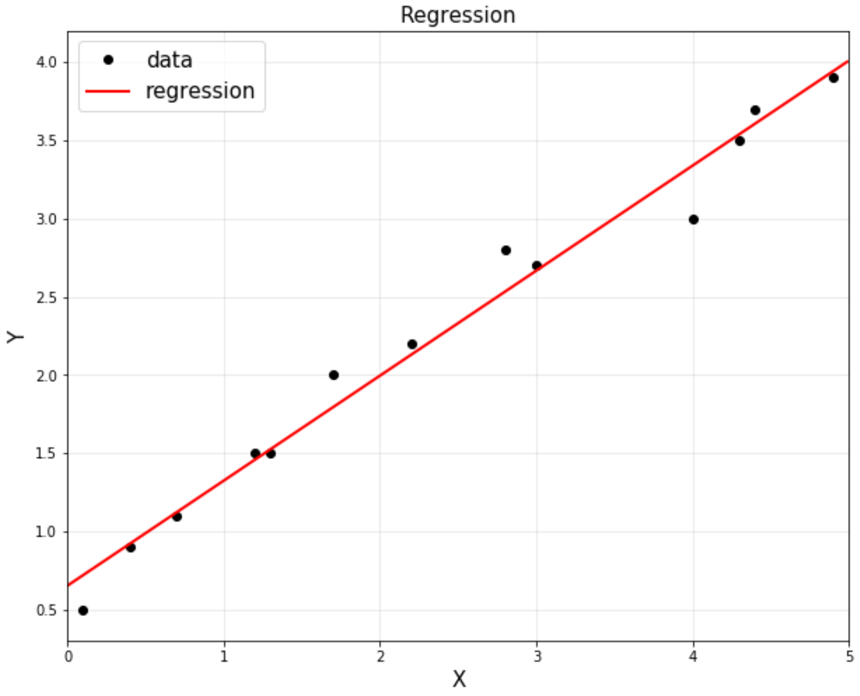


- In many cases, a linear model is used to predict y_i

$$\hat{y}_i = \theta_1 x_i + \theta_2$$

Assumption: Linear Model

$$\hat{y}_i = f(x_i\,;\theta) \quad \text{in general}$$



- In many cases, a linear model is used to predict y_i

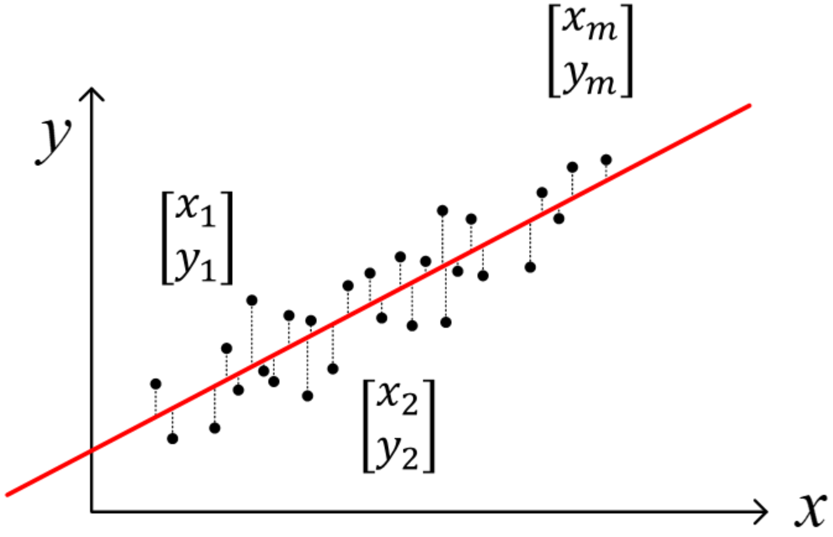
$$\hat{y}_i = \theta_1 x_i + \theta_2$$

Linear Regression

- $\hat{y}_i = f(x_i, \theta)$ in general
- In many cases, a linear model is assumed to predict y_i

Given $\begin{cases} x_i : \text{inputs} \\ y_i : \text{outputs} \end{cases}$, Find θ_0 and θ_1

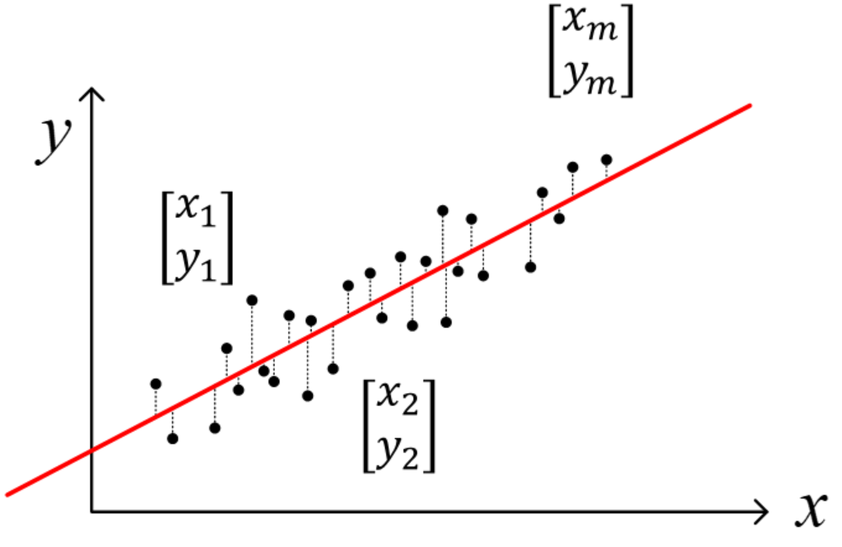
$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}, \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \approx \hat{y}_i = \theta_0 + \theta_1 x_i$$



- $\hat{y}_i$: predicted output
- $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$: model parameters

Linear Regression as Optimization

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}, \qquad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \approx \hat{y}_i = \theta_0 + \theta_1 x_i$$



- How to find model parameters $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$
- Optimization problem

$$\hat{y}_i = \theta_0 + \theta_1 x_i \qquad \text{such that} \qquad \min_{\theta_0, \theta_1} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2$$

$$\min_X \|E\|^2 = \min_X \|AX - B\|^2$$

$$X^* = \left(A^T A\right)^{-1} A^T B$$

$$B^* = AX^* = A\left(A^T A\right)^{-1} A^T B$$

Re-cast Problem as Least Squares

- For convenience, we define a function that maps inputs to feature vectors, ϕ

$$\begin{aligned}\hat{y}_i &= \theta_0 + x_i\theta_1 = 1 \cdot \theta_0 + x_i\theta_1 \\ &= \begin{bmatrix} 1 & x_i \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \\ &= \begin{bmatrix} 1 \\ x_i \end{bmatrix}^T \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} \\ &= \phi^T(x_i)\theta\end{aligned}$$

$$\text{feature vector } \phi(x_i) = \begin{bmatrix} 1 \\ x_i \end{bmatrix}$$

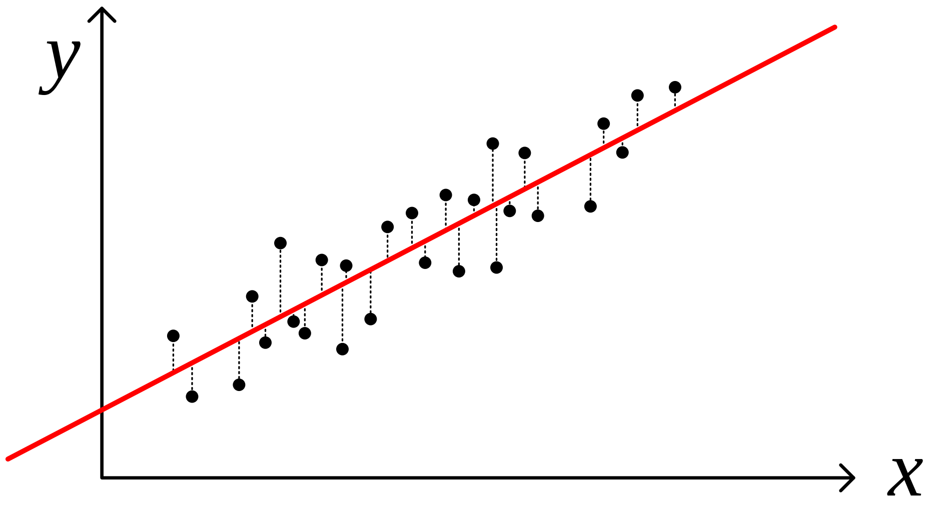
$$\begin{aligned}\min_X \|E\|^2 &= \min_X \|AX - B\|^2 \\ X^* &= \left(A^T A\right)^{-1} A^T B \\ B^* = AX^* &= A\left(A^T A\right)^{-1} A^T B\end{aligned}$$

$$\Phi = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_m \end{bmatrix} = \begin{bmatrix} \phi^T(x_1) \\ \phi^T(x_2) \\ \vdots \\ \phi^T(x_m) \end{bmatrix} \quad \Longrightarrow \quad \hat{y} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_m \end{bmatrix} = \Phi\theta$$

Optimization

$$\min_{\theta_0,\theta_1} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2 = \min_{\theta} ||\Phi\theta - y||_2^2 \qquad \left(\text{same as } \min_{x} ||Ax - b||_2^2\right)$$

$$\text{solution } \theta^* = (\Phi^T \Phi)^{-1} \Phi^T y$$



Optimization: Note

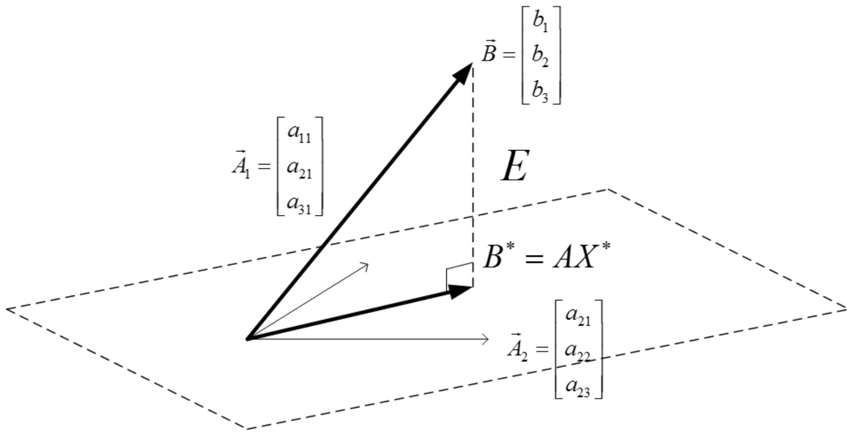
$$\begin{array}{ccccc} \text{input} & & \text{feature} & & \text{predicted output} \\ x_i & \rightarrow & \begin{bmatrix} 1 \\ x_i \end{bmatrix} & \rightarrow & \hat{y}_i \end{array}$$

$$\begin{array}{cc} \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_m \end{bmatrix} & \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} \end{array}$$

$$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ \vec{A}_1 & \vec{A}_2 & \vec{x} & \vec{B} \end{array}$$

over-determined or projection

$$A(=\Phi) = \left[\vec{A}_1 \; \vec{A}_2\right]$$



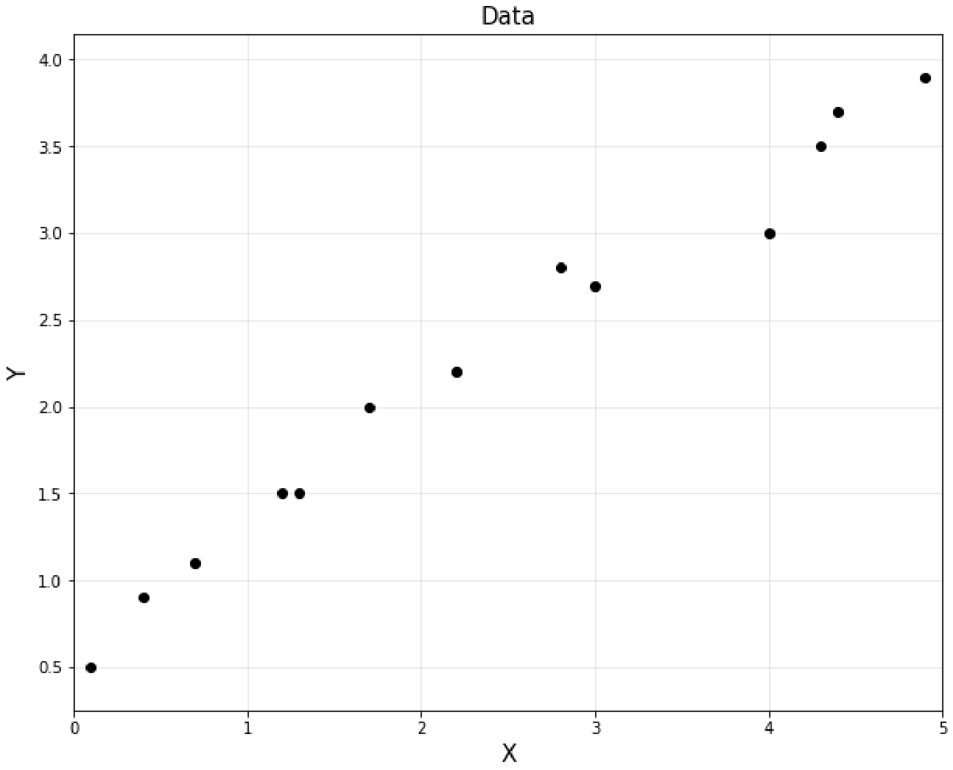
the same principle in a higher dimension

1. Solve using Linear Algebra

- known as *least square*

$$\theta = (A^T A)^{-1} A^T y$$

```
# data points in column vector [input, output]
x = np.array([0.1, 0.4, 0.7, 1.2, 1.3, 1.7, 2.2, 2.8, 3.0, 4.0, 4.3, 4.4, 4.9]).reshape(-1, 1)
y = np.array([0.5, 0.9, 1.1, 1.5, 1.5, 2.0, 2.2, 2.8, 2.7, 3.0, 3.5, 3.7, 3.9]).reshape(-1, 1)
```



1. Solve using Linear Algebra

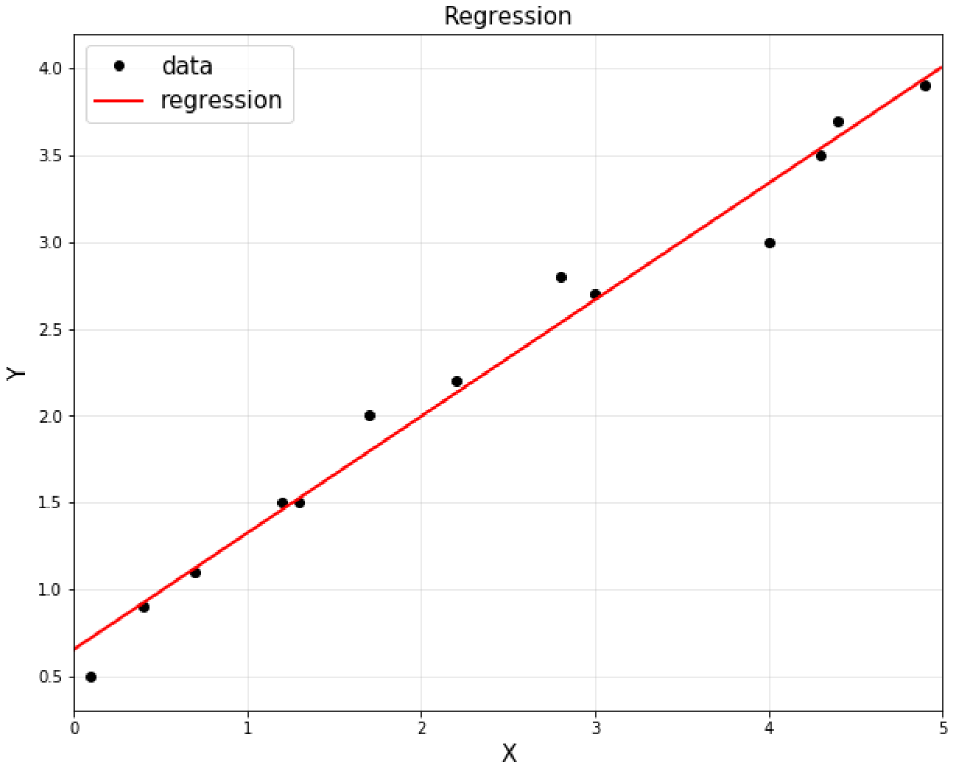
- known as *least square*

$$\theta = (A^T A)^{-1} A^T y$$

```
m = y.shape[0]
#A = np.hstack([np.ones([m, 1]), x])
A = np.hstack([x**0, x])
A = np.asmatrix(A)

theta = (A.T*A).I*A.T*y

print('theta:\n', theta)
```

```
theta:
 [[0.65306531]
 [0.67129519]]
```

```
# to plot
plt.figure(figsize=(10, 8))
plt.title('Regression', fontsize=15)
plt.xlabel('X', fontsize=15)
plt.ylabel('Y', fontsize=15)
plt.plot(x, y, 'ko', label="data")

# to plot a straight line (fitted line)
xp = np.arange(0, 5, 0.01).reshape(-1, 1)
yp = theta[0,0] + theta[1,0]*xp
```



2. Solve using Gradient Descent

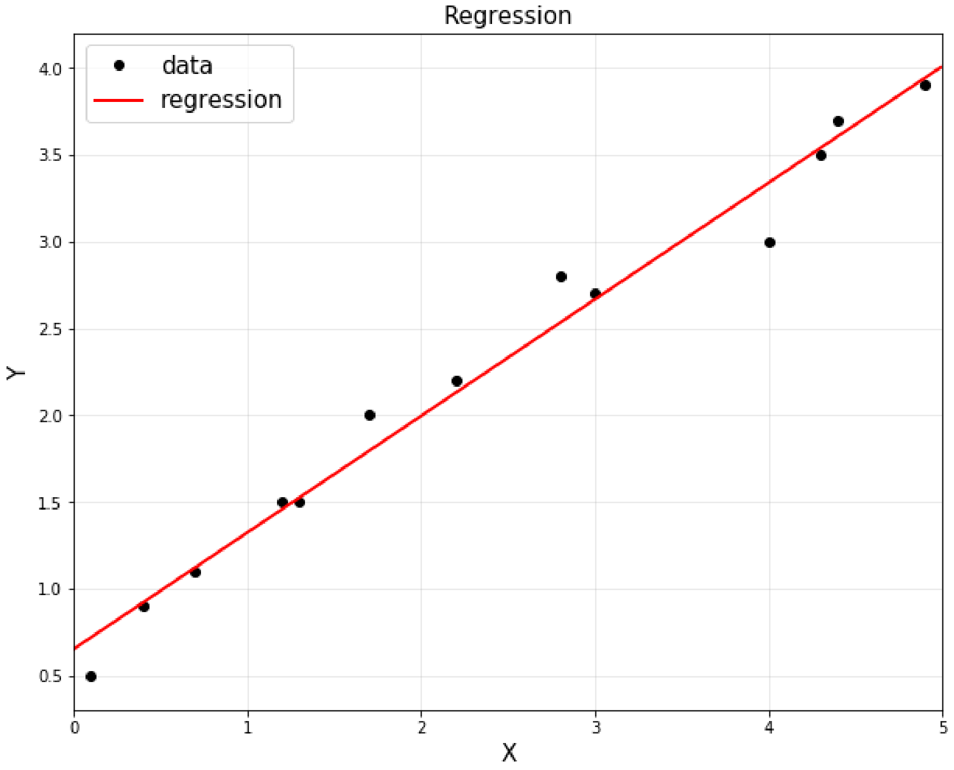
$$f = (A\theta - y)^T(A\theta - y) = (\theta^T A^T - y^T)(A\theta - y)$$
$$= \theta^T A^T A\theta - \theta^T A^T y - y^T A\theta + y^T y$$

$$\min_\theta \ \|\hat{y} - y\|_2^2 = \min_\theta \ \|A\theta - y\|_2^2$$

$$\nabla f = A^T A\theta + A^T A\theta - A^T y - A^T y = 2(A^T A\theta - A^T y)$$

$$\theta \leftarrow \theta - \alpha \nabla f$$

```
theta = np.random.randn(2,1)
theta = np.asmatrix(theta)

alpha = 0.001

for _ in range(1000):
    df = 2*(A.T*A*theta - A.T*y)
    theta = theta - alpha*df

print (theta)
```



3. Solve using CVXPY Optimization

```
theta2 = cvx.Variable([2, 1])
obj = cvx.Minimize(cvx.norm(A*theta2-y, 2))
cvx.Problem(obj,[]).solve()

print('theta:\n', theta2.value)
```

$$\boxed{\min_{\theta} \ \|\hat{y} - y\|_2 = \min_{\theta} \ \|A\theta - y\|_2}$$

```
theta:
 [[0.65306531]
 [0.67129519]]
```

POSTECH

3. Solve using CVXPY Optimization

```
theta2 = cvx.Variable([2, 1])
obj = cvx.Minimize(cvx.norm(A*theta2-y, 2))
cvx.Problem(obj,[]).solve()

print('theta:\n', theta2.value)
```

```
theta:
 [[0.65306531]
 [0.67129519]]
```

$$\boxed{\min_{\theta} \ \lVert \hat{y} - y \rVert_2 = \min_{\theta} \ \lVert A\theta - y \rVert_2}$$

- By the way, do we have to use only L_2 norm? No.
  - Let's use L_1 norm

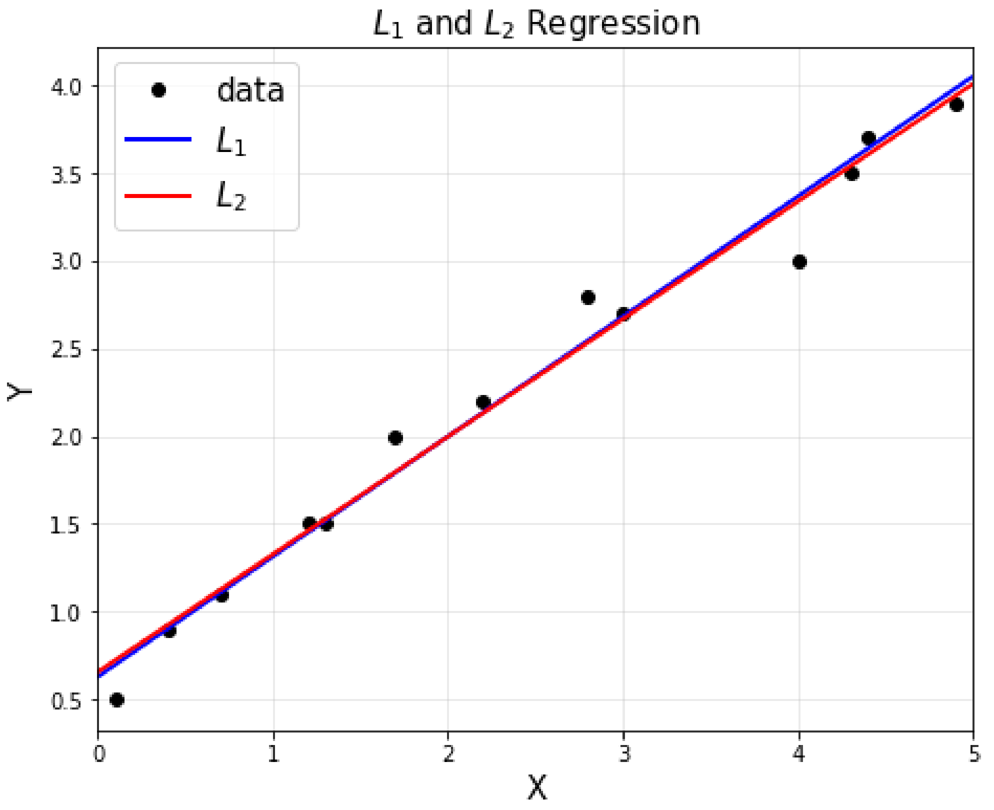
```
theta1 = cvx.Variable([2, 1])
obj = cvx.Minimize(cvx.norm(A*theta1-y, 1))
cvx.Problem(obj).solve()

print('theta:\n', theta1.value)
```

```
theta:
 [[0.628129  ]
 [0.68520147]]
```

$$\boxed{\min_{\theta} \ \lVert \hat{y} - y \rVert_1 = \min_{\theta} \ \lVert A\theta - y \rVert_1}$$

L_2 Norm vs. L_1 Norm

- L_1 norm also provides a decent linear approximation.



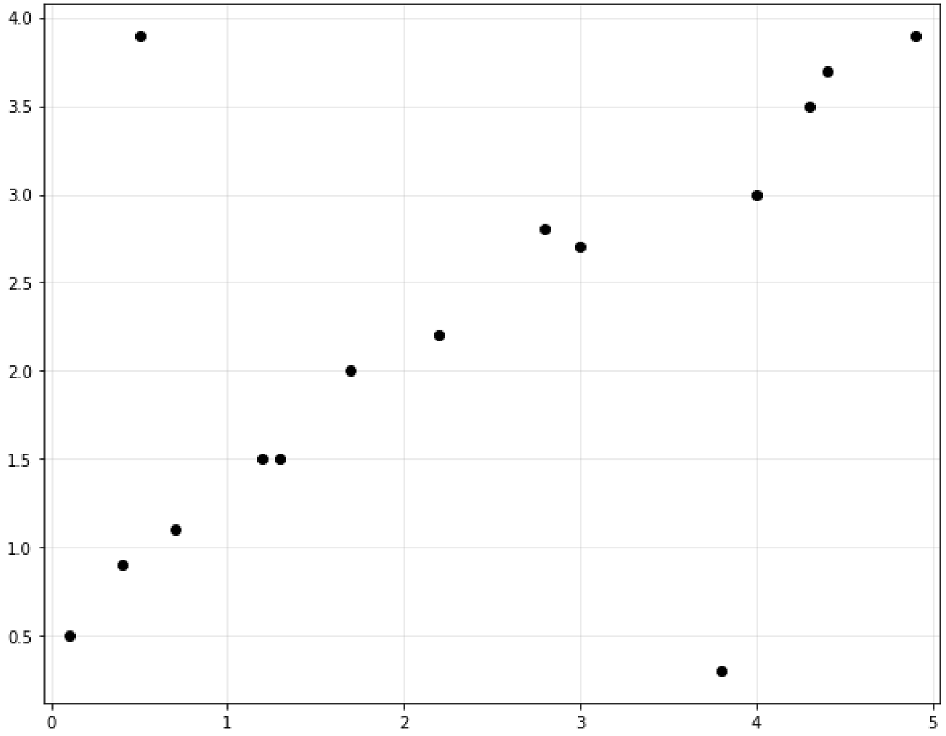
Regression with Outliers

- L_1 norm also provides a decent linear approximation.

- **What if outliers exist?**
  - Fitting with the different norms
  - source:
    - Week 9 of Computational Methods for Data Analysis by Coursera of Univ. of Washington
    - Chapter 17, online book available

Regression with Outliers

```
# add outliers
x = np.vstack([x, np.array([0.5, 3.8]).reshape(-1, 1)])
y = np.vstack([y, np.array([3.9, 0.3]).reshape(-1, 1)])

A = np.hstack([x**0, x])
A = np.asmatrix(A)
```



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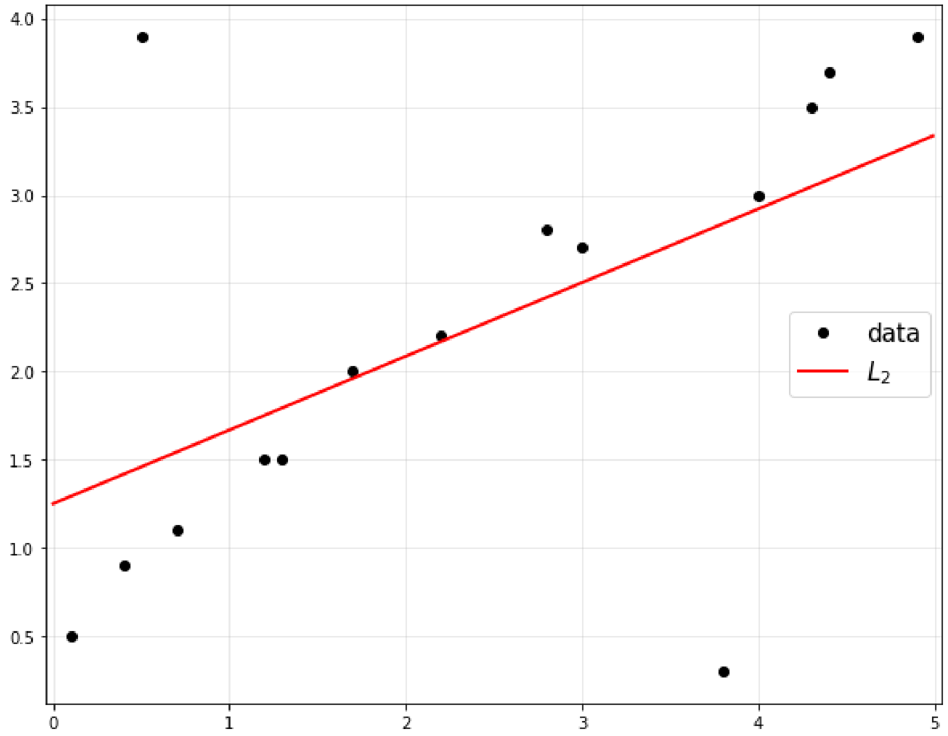
L_2 Norm vs. L_1 Norm

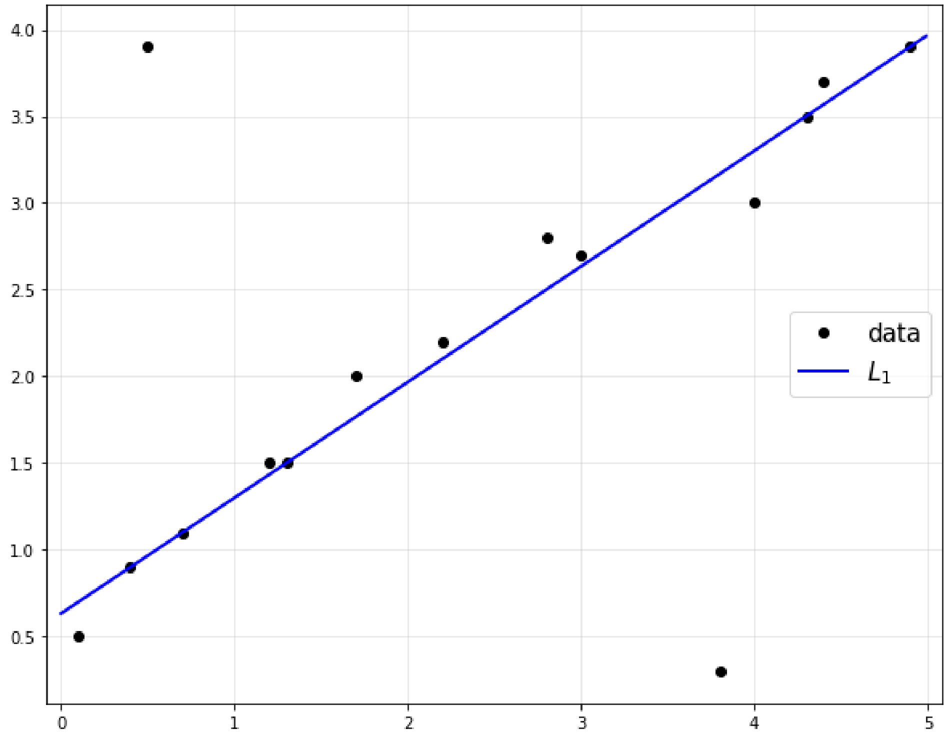
$$\min_{\theta} \; \|A\theta - y\|_2$$

```
theta2 = cvx.Variable([2, 1])
obj2 = cvx.Minimize(cvx.norm(A*theta2-y, 2))
prob2 = cvx.Problem(obj2).solve()
```



$$\min_{\theta} \; \|A\theta - y\|_1$$

```
theta1 = cvx.Variable([2, 1])
obj1 = cvx.Minimize(cvx.norm(A*theta1-y, 1))
prob1 = cvx.Problem(obj1).solve()
```

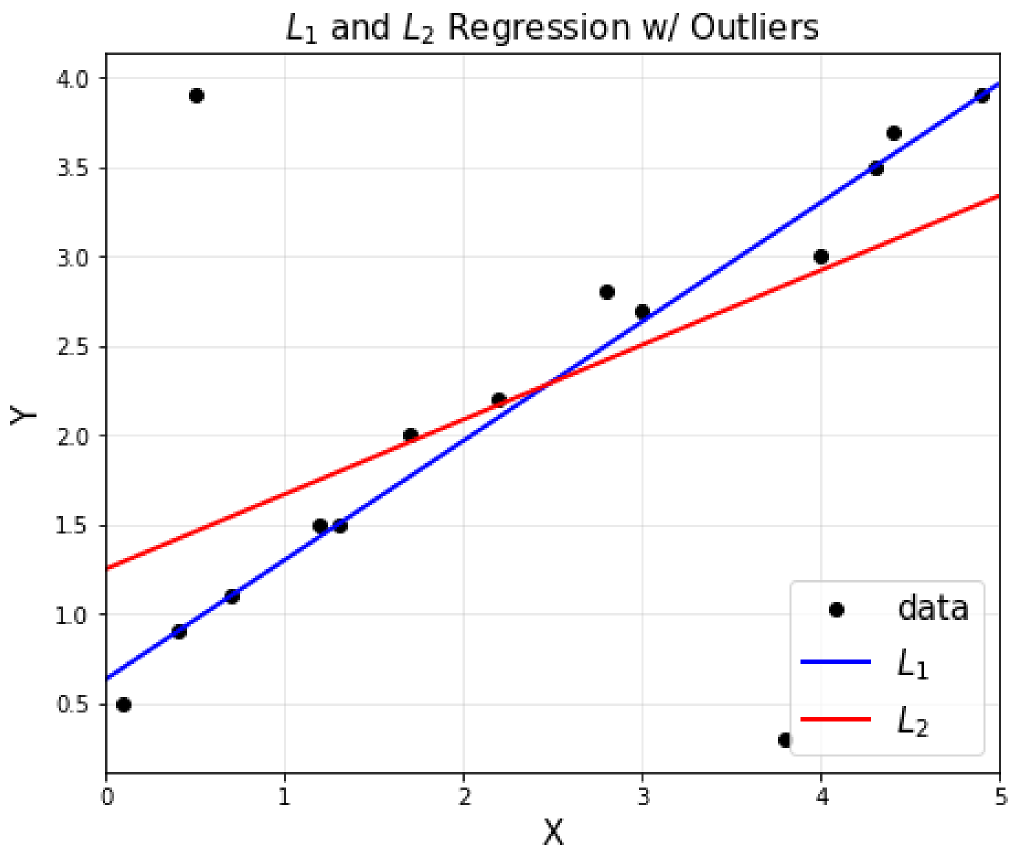


Think About What Makes Different

- It is important to understand what makes them different

$$\min_{\theta} \ \|A\theta - y\|_1$$

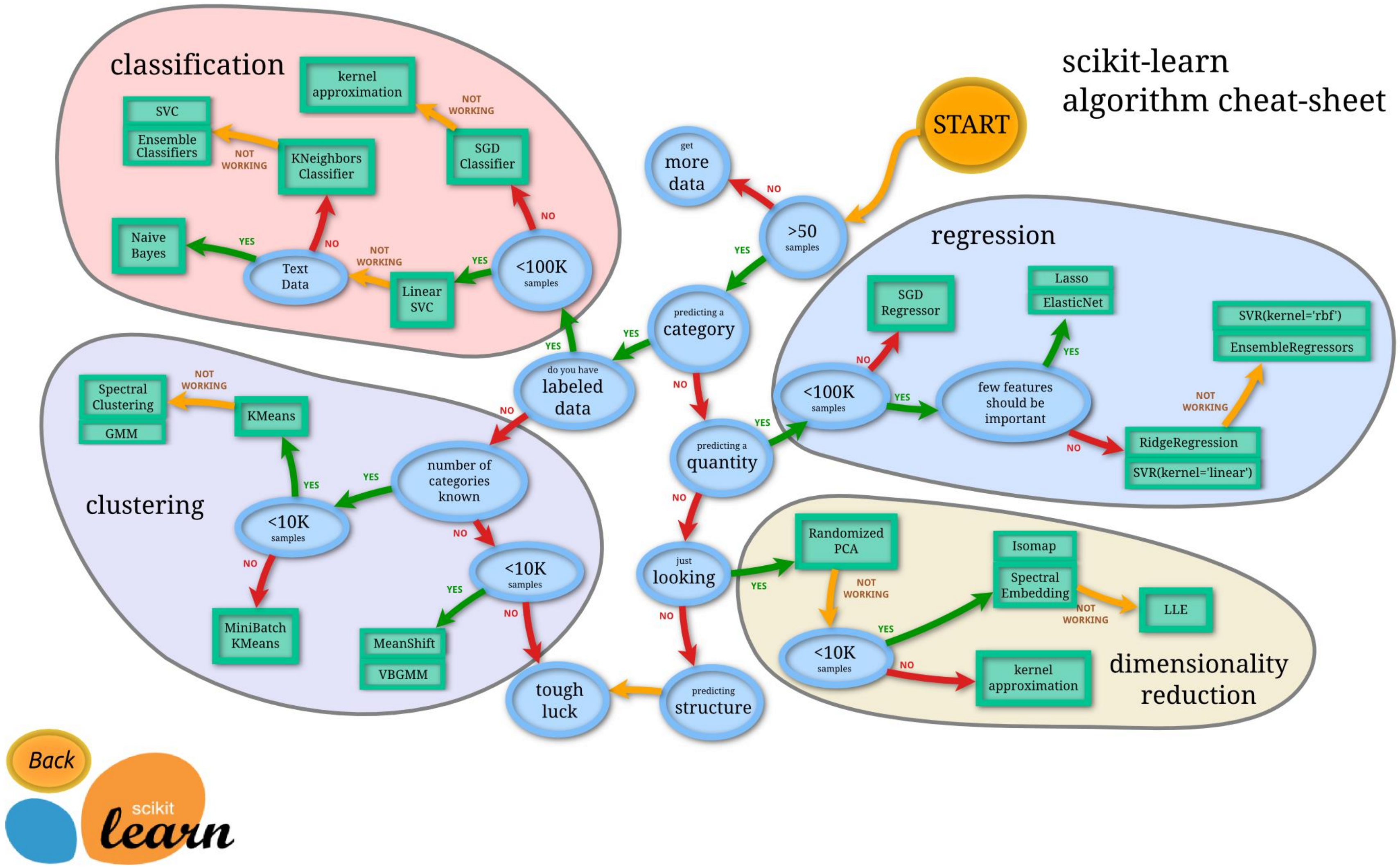
$$\min_{\theta} \ \|A\theta - y\|_2$$



Scikit-Learn

- Machine Learning in Python
- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license
- https://scikit-learn.org/stable/index.html#

Scikit-Learn



Scikit-Learn: Regression

```
from sklearn import linear_model
```

```
reg = linear_model.LinearRegression()
reg.fit(x, y)
```

```
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,
         normalize=False)
```

```
reg.coef_
```

```
array([[0.67129519]])
```

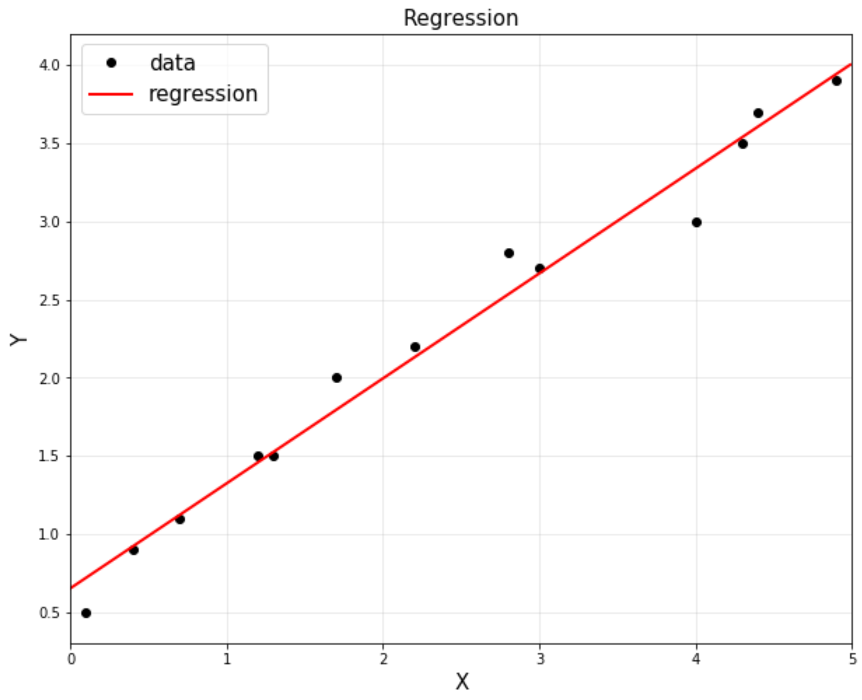
```
reg.intercept_
```

```
array([0.65306531])
```

Scikit-Learn: Regression

```python
# to plot
plt.figure(figsize=(10, 8))
plt.title('Regression', fontsize=15)
plt.xlabel('X', fontsize=15)
plt.ylabel('Y', fontsize=15)
plt.plot(x, y, 'ko', label="data")

# to plot a straight line (fitted line)
plt.plot(xp, reg.predict(xp), 'r', linewidth=2, label="regression")
plt.legend(fontsize=15)
plt.axis('equal')
plt.grid(alpha=0.3)
plt.xlim([0, 5])
plt.show()
```



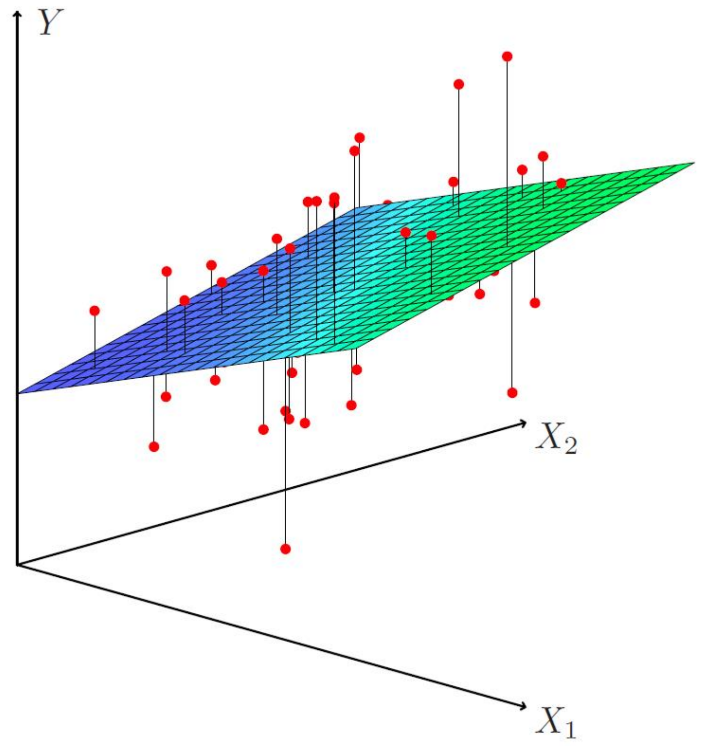
Multivariate Linear Regression

- Linear regression for multivariate data

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

$$\phi\left(x^{(i)}\right) = \begin{bmatrix} 1 \\ x_1^{(i)} \\ x_2^{(i)} \end{bmatrix} \quad\Longrightarrow\quad \theta^* = (\Phi^T\Phi)^{-1}\Phi^T y$$

$$\Phi = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} \\ \vdots & & \\ 1 & x_1^{(m)} & x_2^{(m)} \end{bmatrix} \quad\Longrightarrow\quad \hat{y} = \begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix} = \Phi\theta$$



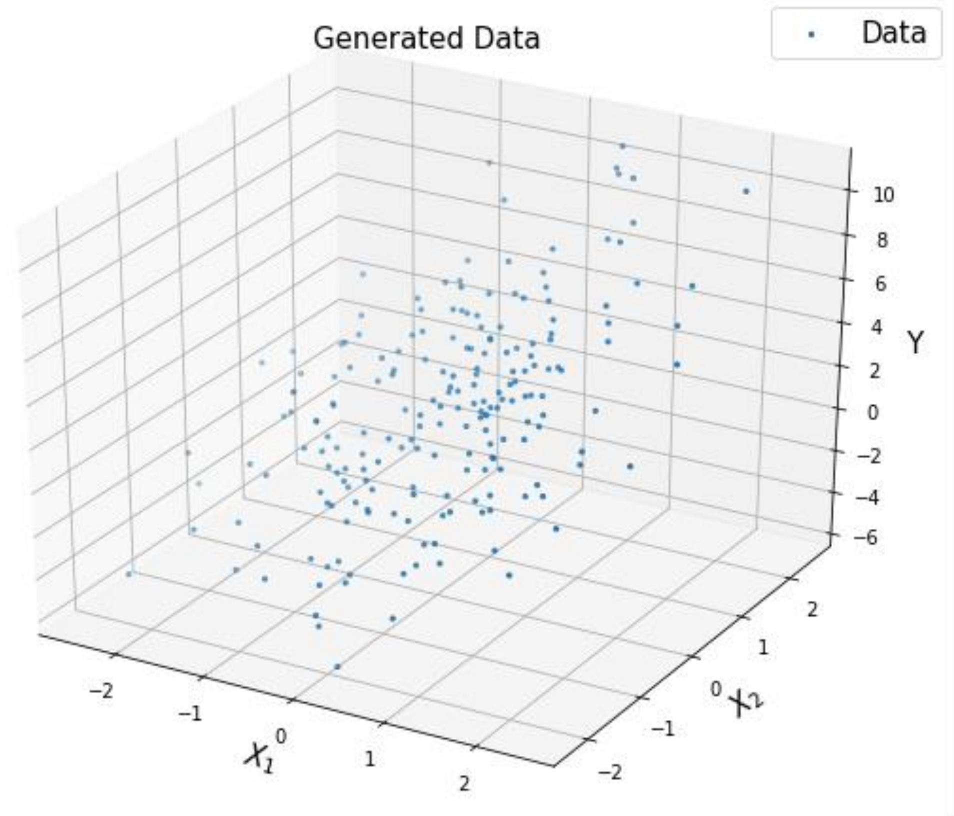
- Same in matrix representation

Multivariate Linear Regression

```
# y = theta0 + theta1*x1 + theta2*x2 + noise

n = 200
x1 = np.random.randn(n, 1)
x2 = np.random.randn(n, 1)
noise = 0.5*np.random.randn(n, 1);

y = 2 + 1*x1 + 3*x2 + noise
```



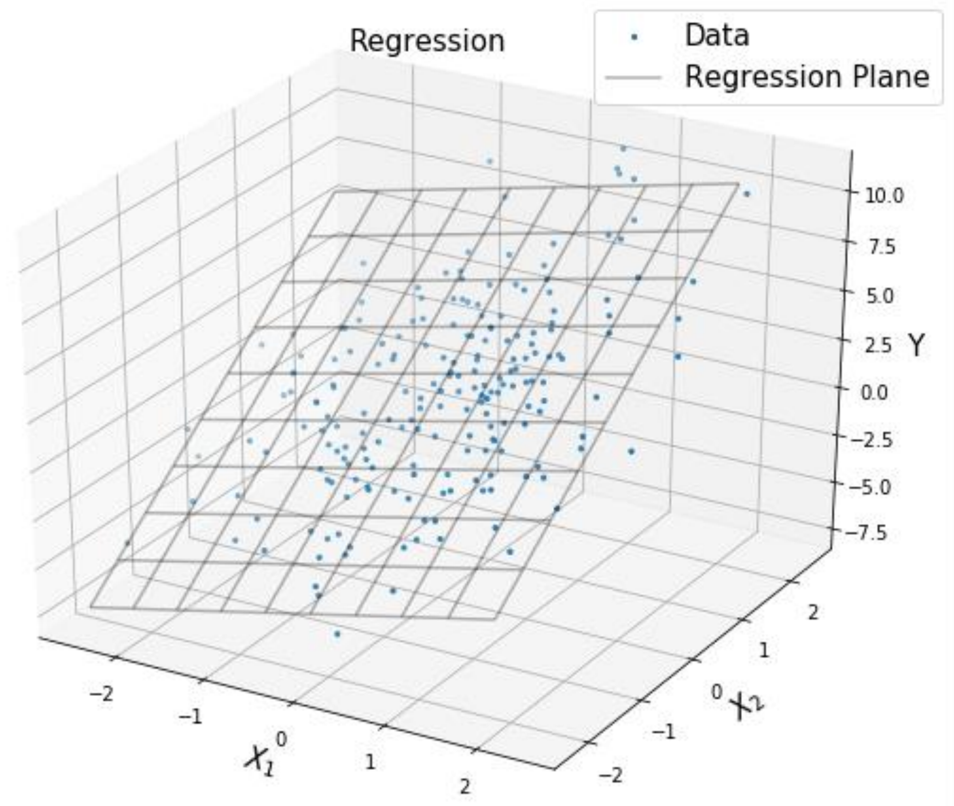
Multivariate Linear Regression

$$\Phi = \begin{bmatrix} 1 & x_1^{(1)} & x_2^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} \\ \vdots & & \\ 1 & x_1^{(m)} & x_2^{(m)} \end{bmatrix} \implies \hat{y} = \begin{bmatrix} \hat{y}^{(1)} \\ \hat{y}^{(2)} \\ \vdots \\ \hat{y}^{(m)} \end{bmatrix} = \Phi\theta$$

$$\implies \theta^* = (\Phi^T\Phi)^{-1}\Phi^T y$$

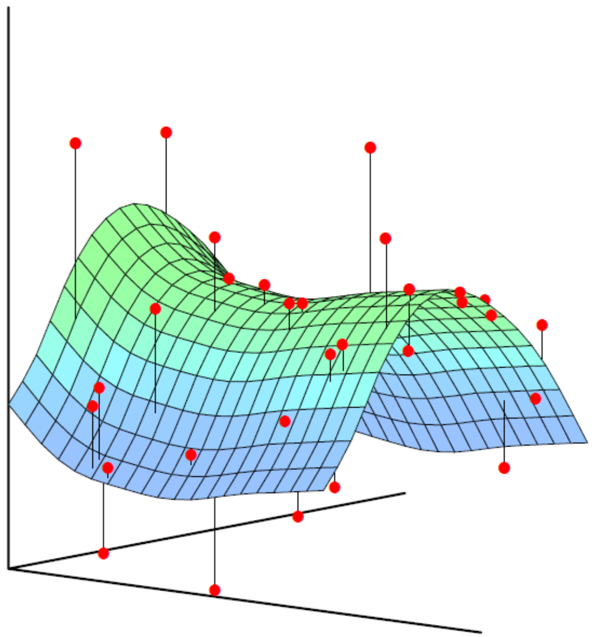
```
A = np.hstack([np.ones((n, 1)), x1, x2])
A = np.asmatrix(A)
theta = (A.T*A).I*A.T*y

X1, X2 = np.meshgrid(np.arange(np.min(x1), np.max(x1), 0.5),
                     np.arange(np.min(x2), np.max(x2), 0.5))
YP = theta[0,0] + theta[1,0]*X1 + theta[2,0]*X2
```



Nonlinear Regression

- Linear regression for non-linear data



- Same as linear regression, just with non-linear features

- Method 1: constructing explicit feature vectors
  - polynomial features
  - Radial basis function (RBF) features

- Method 2: implicit feature vectors, kernel trick

Nonlinear Regression

- Polynomial (here, quad is used as an example)

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \text{noise}$$

$$\phi(x_i) = \begin{bmatrix} 1 \\ x_i \\ x_i^2 \end{bmatrix}$$

$$\Phi = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & & \\ 1 & x_m & x_m^2 \end{bmatrix} \quad \Longrightarrow \quad \hat{y} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_m \end{bmatrix} = \Phi\theta$$

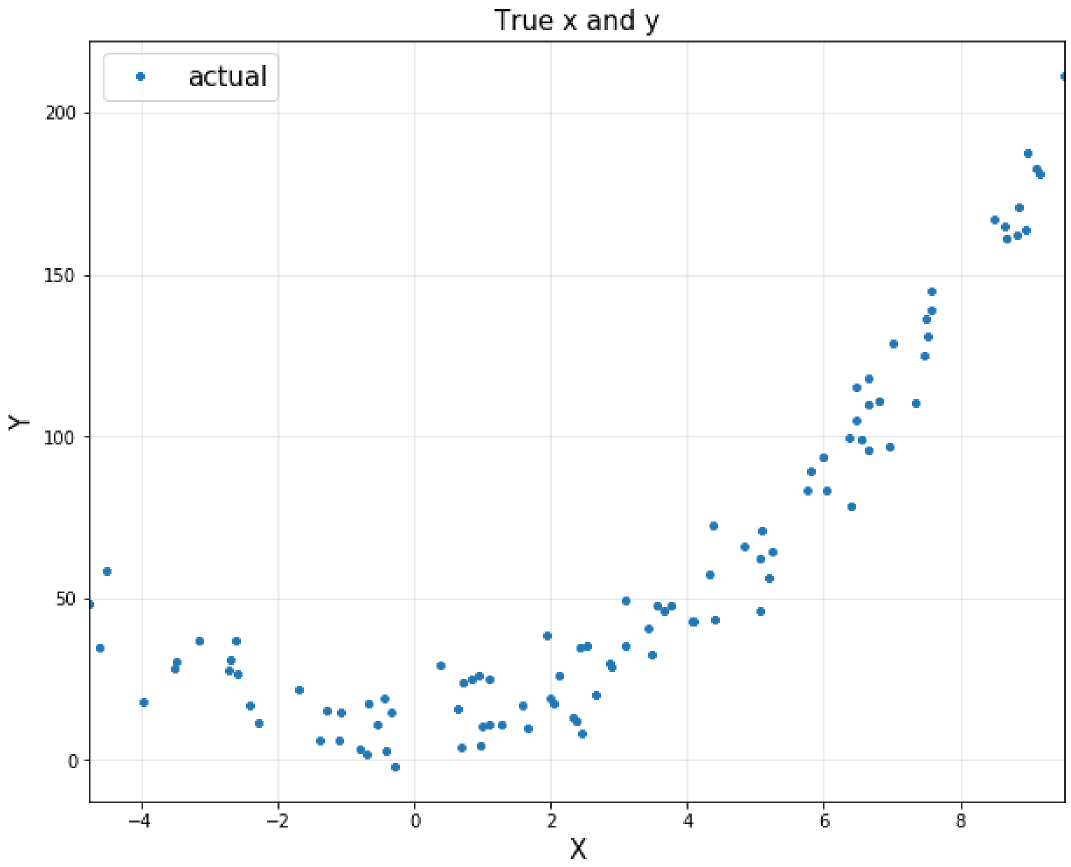
$$\Longrightarrow \quad \theta^* = (\Phi^T \Phi)^{-1} \Phi^T y$$

Polynomial Regression

```
# y = theta0 + theta1*x + theta2*x^2 + noise

n = 100
x = -5 + 15*np.random.rand(n, 1)
noise = 10*np.random.randn(n, 1)

y = 10 + 1*x + 2*x**2 + noise
```

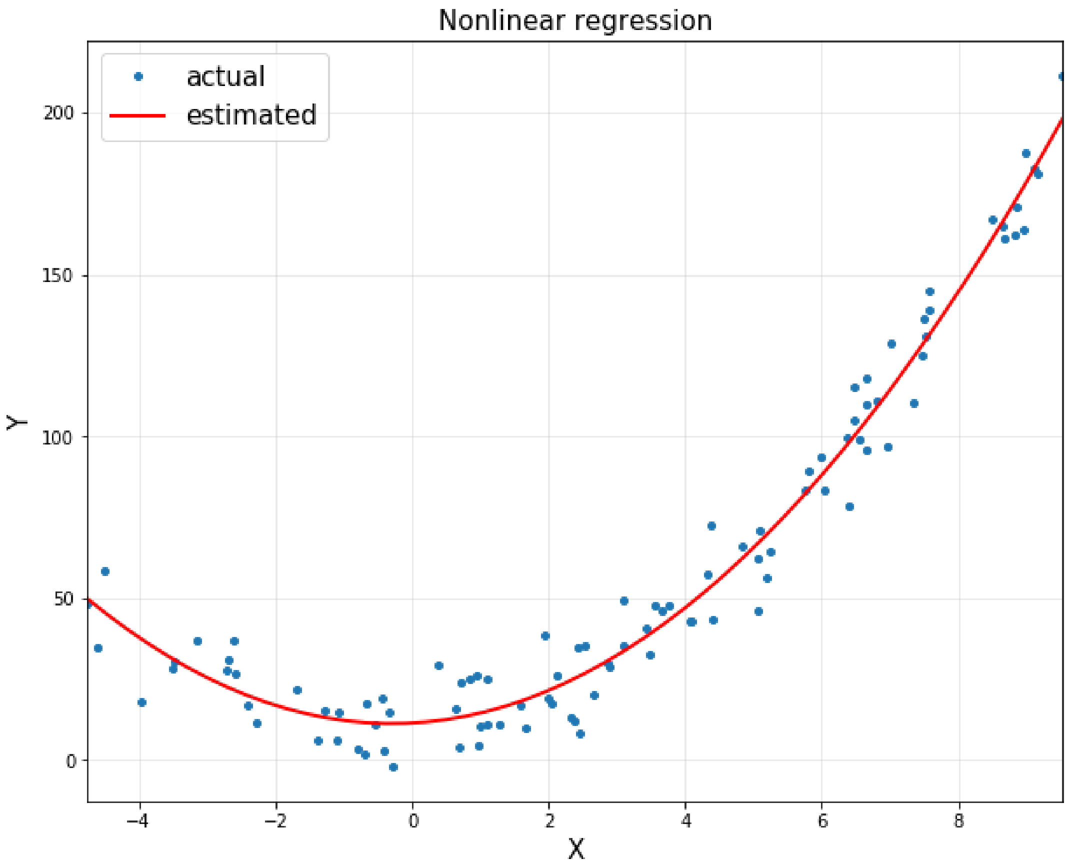


Polynomial Regression

$$\boxed{\theta = (A^T A)^{-1} A^T y}$$

```
A = np.hstack([x**0, x, x**2])
A = np.asmatrix(A)

theta = (A.T*A).I*A.T*y
print('theta:\n', theta)
```



Function Approximation

- Select coefficients among a well-defined function (basis) that closely matches a target function in a task-specific way

Recap: Nonlinear Regression

- Polynomial (here, quad is used as an example)

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \text{noise}$$

Different perspective:
- Approximate a target function as a linear combination of basis

$$\phi(x_i) = \begin{bmatrix} 1 \\ x_i \\ x_i^2 \end{bmatrix}$$

$$\hat{y} = \sum_{i=0}^{d} \theta_i b_i(x) = \Phi\theta$$

$$\Phi = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & & \\ 1 & x_m & x_m^2 \end{bmatrix} \implies \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \\ 1 & x_m & x_m^2 \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} \Rightarrow \begin{bmatrix} | & | & | \\ b_0(x) & b_1(x) & b_2(x) \\ | & | & | \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix}$$

$$\implies \theta^* = (\Phi^T \Phi)^{-1} \Phi^T y$$

Construct Explicit Feature Vectors

- Consider linear combinations of fixed nonlinear functions
  - Polynomial
  - Radial Basis Function (RBF)

$$\hat{y} = \sum_{i=0}^{d} \theta_i b_i(x) = \Phi\theta$$

$$\Phi = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & & \\ 1 & x_m & x_m^2 \end{bmatrix} \implies \hat{y} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_m \end{bmatrix} = \Phi\theta$$

Polynomial Basis

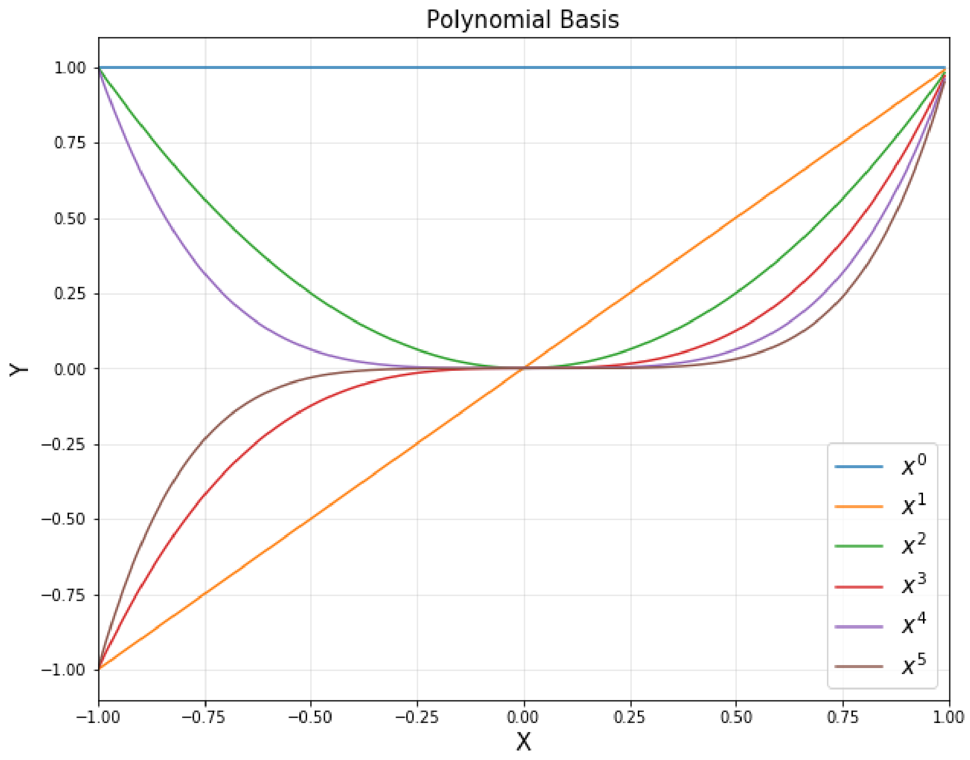
1) Polynomial functions

$$b_i(x) = x^i, \quad i = 0, \cdots, d$$

```
xp = np.arange(-1, 1, 0.01).reshape(-1, 1)
polybasis = np.hstack([xp**i for i in range(6)])

plt.figure(figsize=(10, 8))

for i in range(6):
    plt.plot(xp, polybasis[:,i], label = '$x^{}$'.format(i))
```



RBF Basis

2) Radial Basis Functions (RBF) with bandwidth σ and k RBF centers $\mu_i \in \mathbb{R}^n, \qquad i = 1, 2, \cdots, k$

$$b_i(x) = \exp\left(-\frac{\|x - \mu_i\|^2}{2\sigma^2}\right)$$

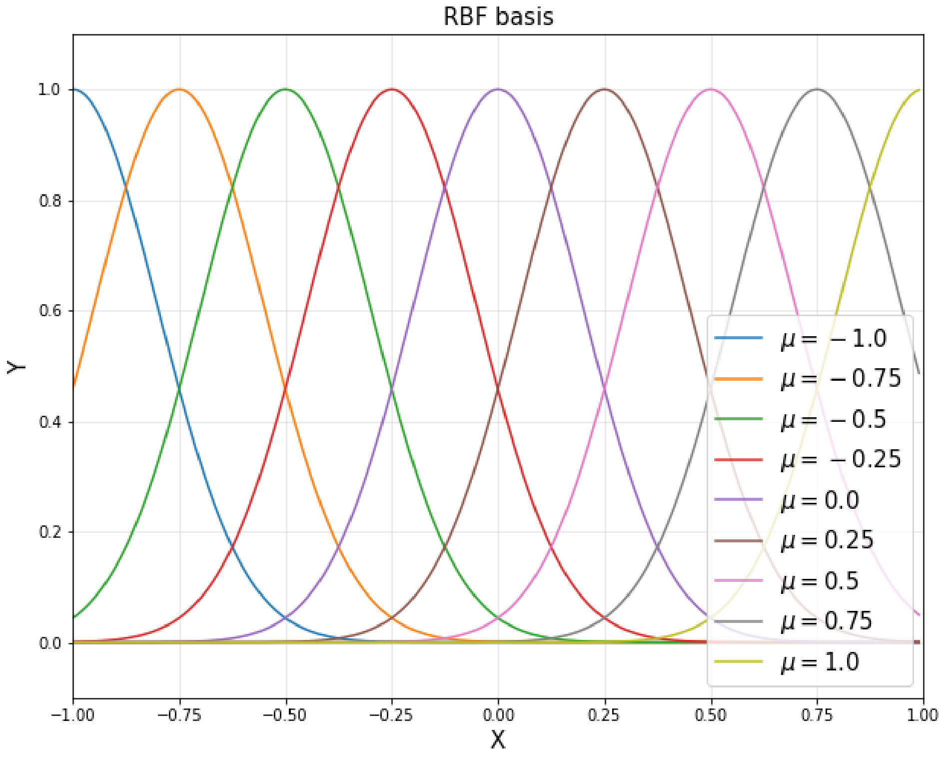
```
d = 9

u = np.linspace(-1, 1, d)
sigma = 0.2

rbfbasis = np.hstack([np.exp(-(xp-u[i])**2/(2*sigma**2)) for i in range(d)])

plt.figure(figsize=(10, 8))

for i in range(d):
    plt.plot(xp, rbfbasis[:,i], label='$\mu = {}$'.format(u[i]))
```



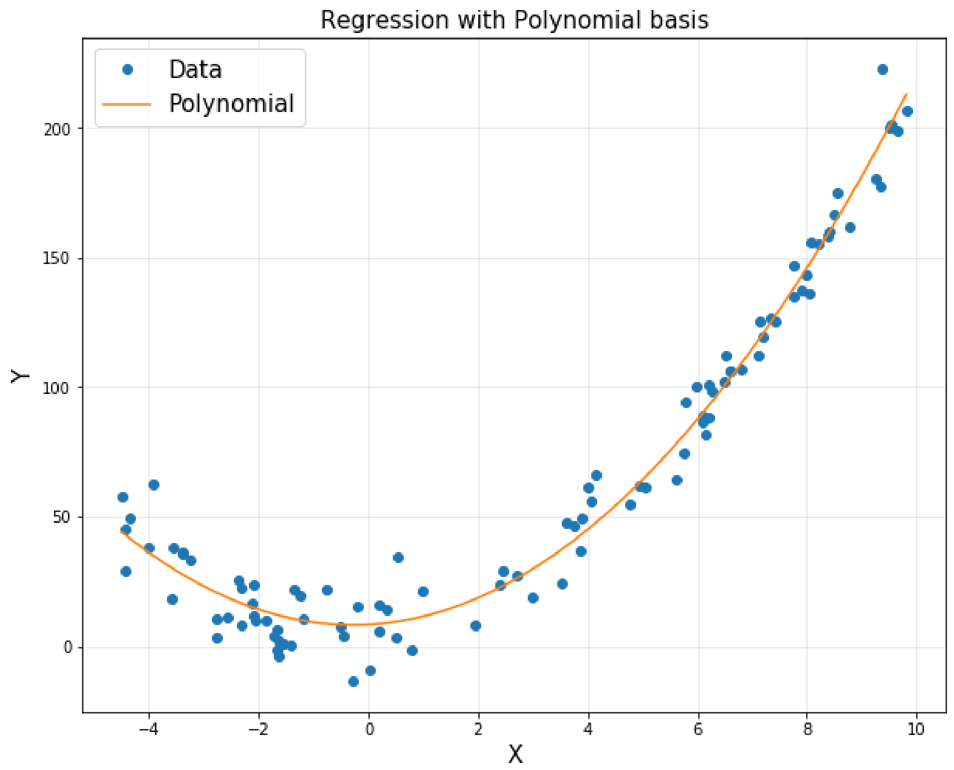
Nonlinear Regression with Polynomial Functions

```
xp = np.arange(np.min(x), np.max(x), 0.01).reshape(-1, 1)

d = 3
polybasis = np.hstack([xp**i for i in range(d)])
polybasis = np.asmatrix(polybasis)

A = np.hstack([x**i for i in range(d)])
A = np.asmatrix(A)

theta = (A.T*A).I*A.T*y
yp = polybasis*theta
```



Nonlinear Regression with RBF Functions

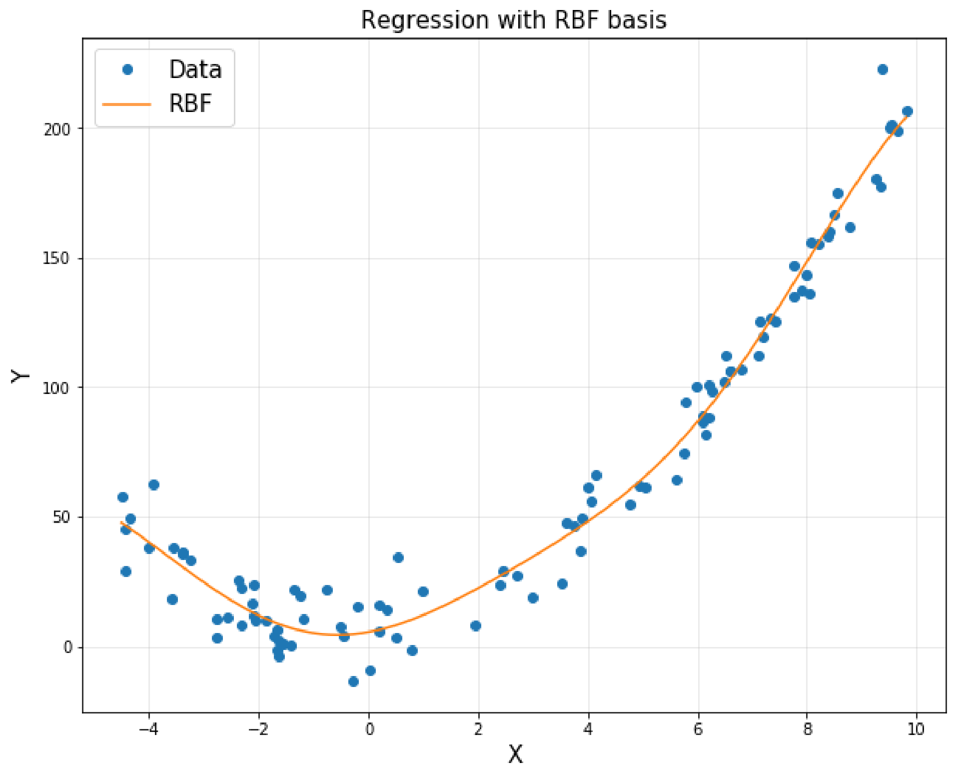
```
xp = np.arange(np.min(x), np.max(x), 0.01).reshape(-1, 1)

d = 6
u = np.linspace(np.min(x), np.max(x), d)
sigma = 4

rbfbasis = np.hstack([np.exp(-(xp-u[i])**2/(2*sigma**2)) for i in range(d)])
A = np.hstack([np.exp(-(x-u[i])**2/(2*sigma**2)) for i in range(d)])

rbfbasis = np.asmatrix(rbfbasis)
A = np.asmatrix(A)

theta = (A.T*A).I*A.T*y
yp = rbfbasis*theta
```



Summary: Linear Regression

- Though linear regression may seem limited, it is very powerful, since the input features can themselves include non-linear features of data

- Linear regression on non-linear features of data

- For least-squares loss, optimal parameters still are

$$\theta^* = (\Phi^T \Phi)^{-1} \Phi^T y$$