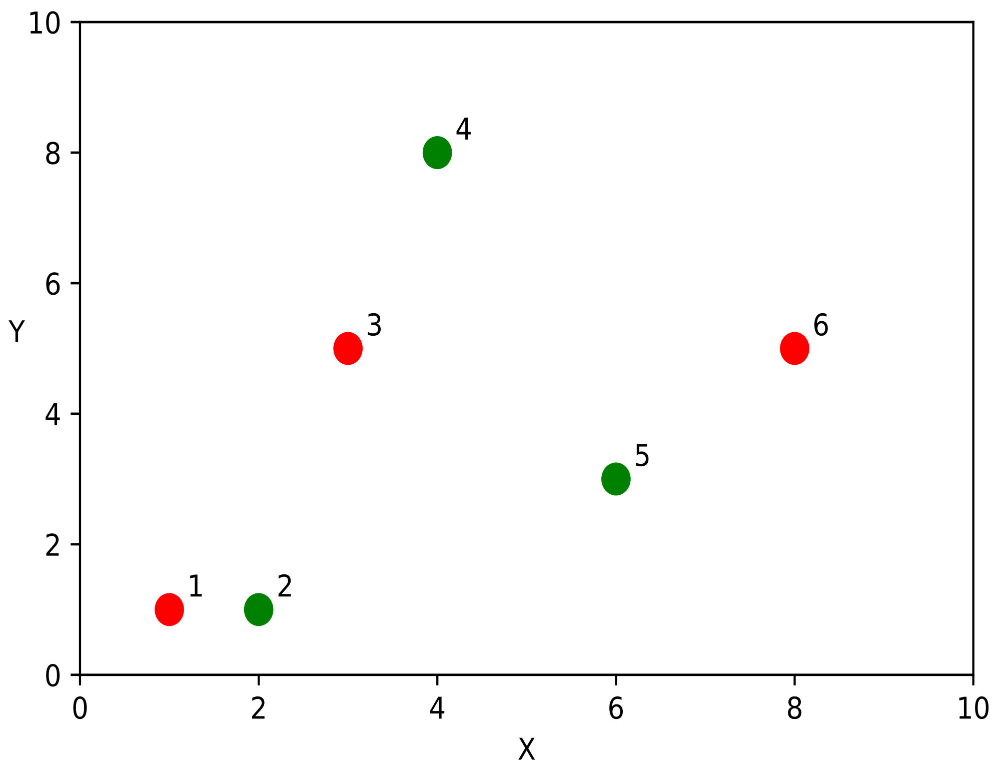
LINEAR REGRESSION

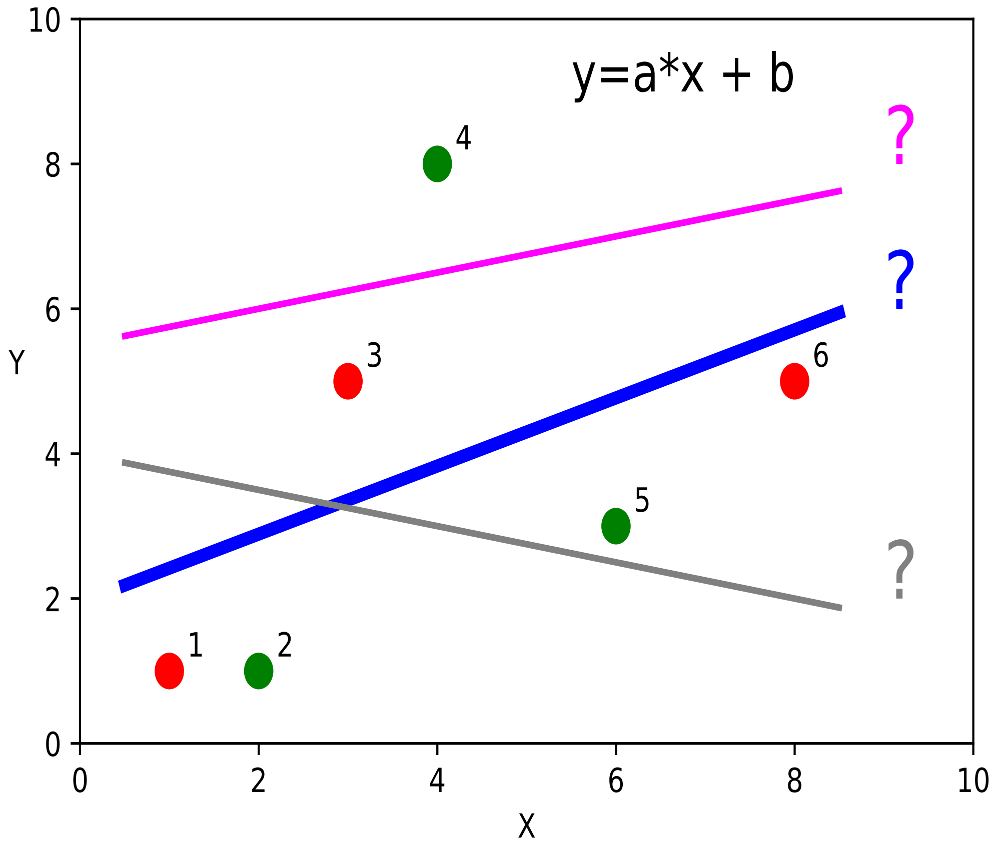
Linear Relationship



- want to establish a linear relationship:

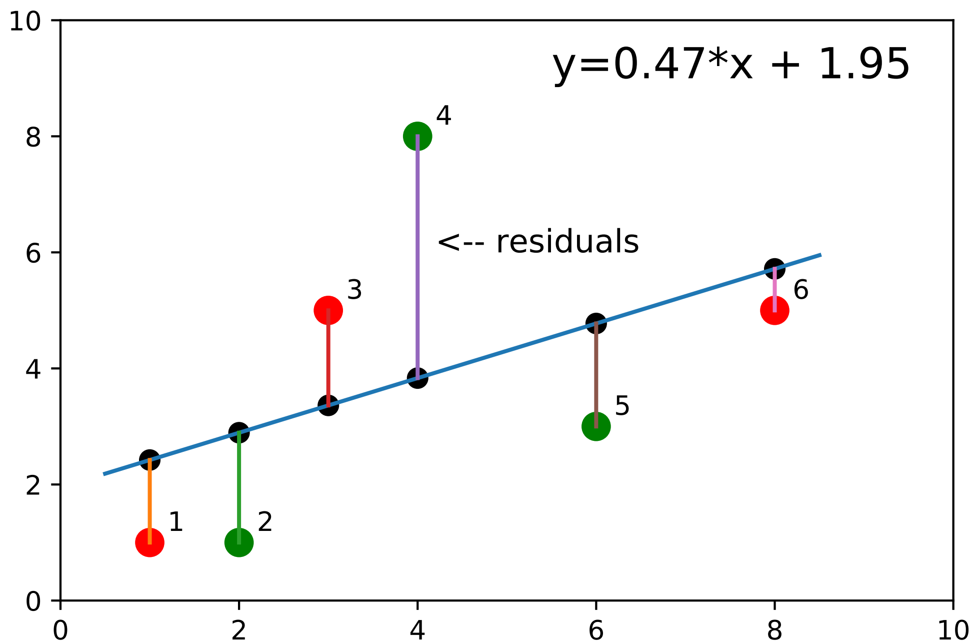
$$y = ax + b + e$$

Where is the difficulty?



- need a criteria to compute slope a and intercept b

How do we choose?



- choose line to minimize sum of squared residuals ("loss")

$$Q = \sum_{i=1}^{n} e_i^2$$

Python Code

```
import numpy as np
from sklearn.linear_model import LinearRegression

x = np.array([1,2,3,4,6,8])
y = np.array([1,1,5,8,3,5])
x_2 = x_2 = x[:,np.newaxis]
lin_reg = LinearRegression(fit_intercept=True)
lin_reg.fit(x_2, y)
```

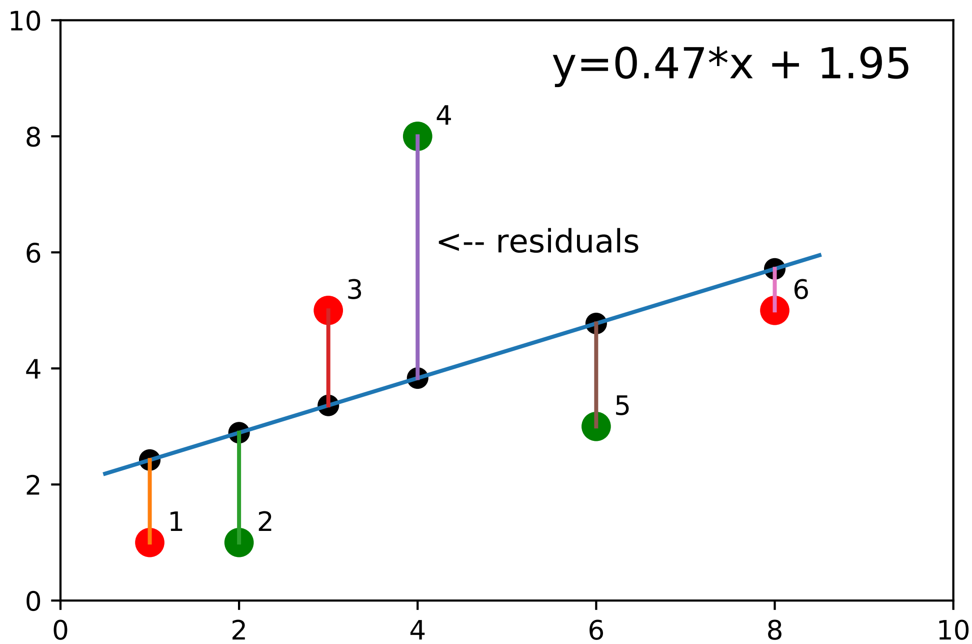
```
> x
array([1, 2, 3, 4, 6, 8])
> x_2
array([[1],
       [2],
       [3],
       [4],
       [6],
       [8]])
```

Python Code

```
import numpy as np
from sklearn.linear_model import LinearRegression

x = np.array([1,2,3,4,6,8])
y = np.array([1,1,5,8,3,5])

x_2 = x_2 = x[:,np.newaxis]
lin_reg = LinearRegression(fit_intercept=True)
lin_reg.fit(x_2, y)
```

```
> lin_reg.score(x_2,y)
 0.20441841895129076
> lin_reg.coef_
array([ 0.47058824])
> lin_reg.intercept_
1.9509803921568625
```

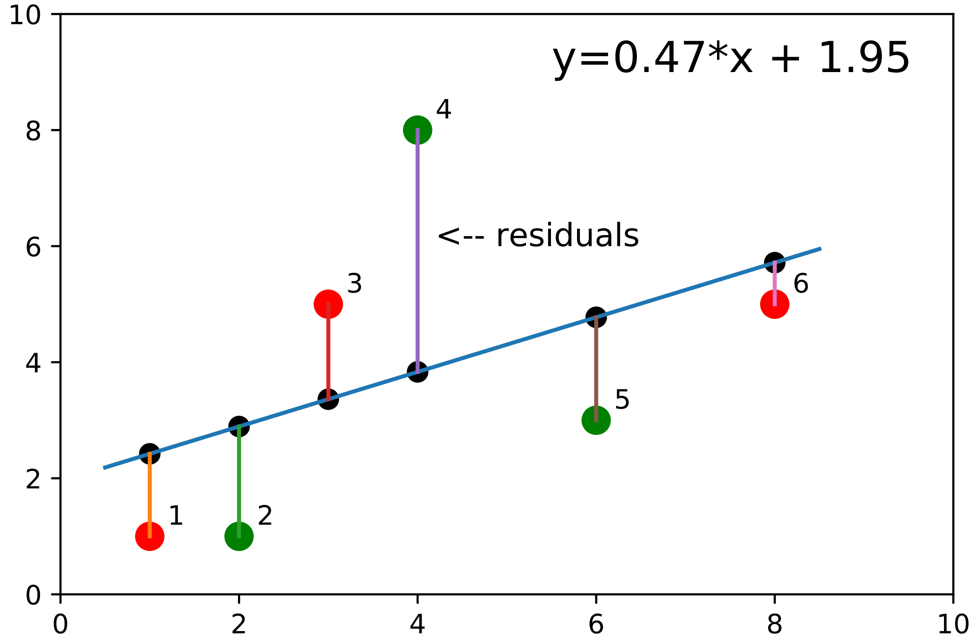
Derivation



- want to minimize loss function (sum of squares)

$$Q = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \big(y_i - (ax_i + b)\big)^2$$

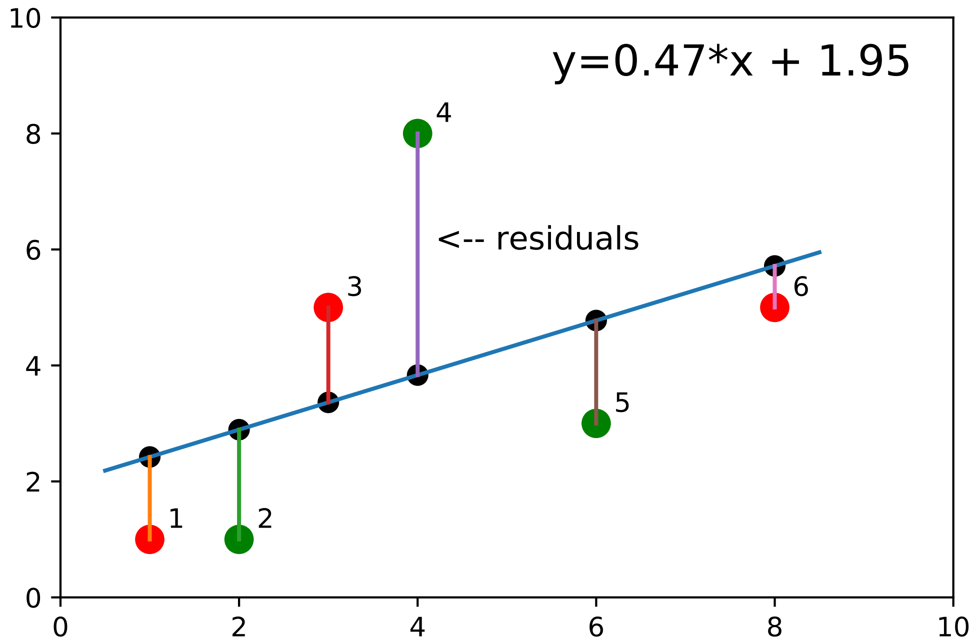
Derivation



- need to solve

$$\frac{\partial Q}{\partial a} = 0, \quad \frac{\partial Q}{\partial b} = 0$$

Derivation



- define means μ_x and μ_y
- define (co)variances σ_x^2 and σ_{xy}^2

Derivation

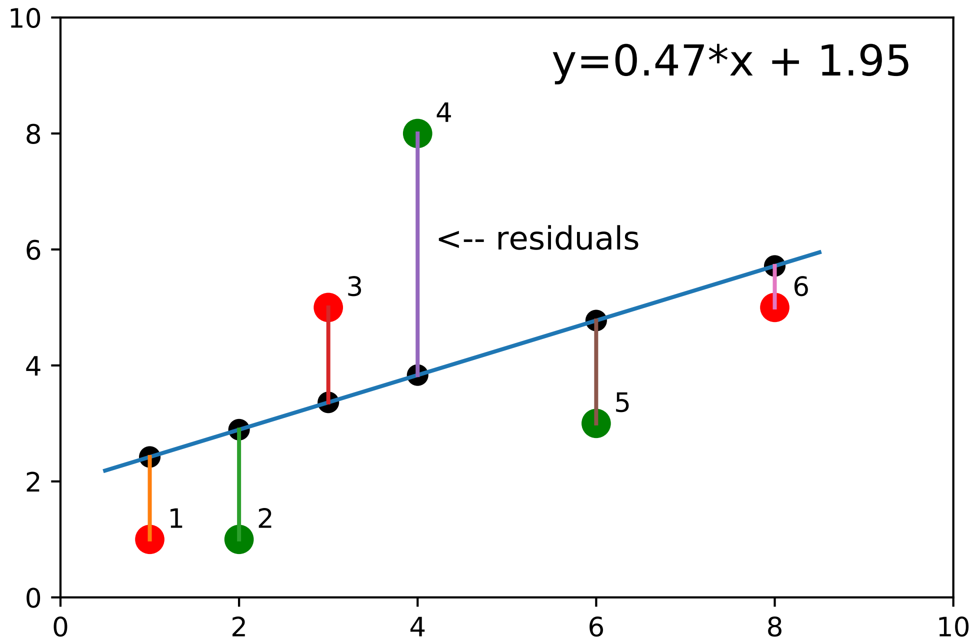
- define means:

$$\mu_x = \frac{x_1 + \cdots + x_n}{n}$$
$$\mu_y = \frac{y_1 + \cdots + y_n}{n}$$

and (co)variances

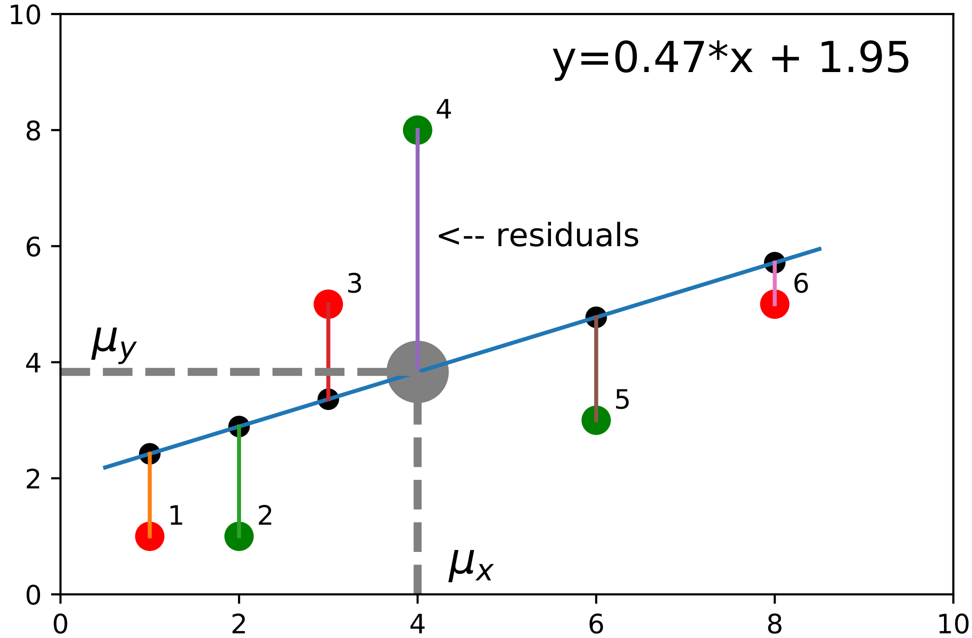
$$\sigma^2_{xy} = \frac{\left(x_1 y_1 + \cdots + x_n y_n\right)}{n} - \mu_x \mu_y$$
$$\sigma^2_x = \frac{\left(x_1^2 + \cdots + x_n^2\right)}{n} - \mu_x^2$$

Derivation for b



$$\frac{\partial Q}{\partial b} = -2\sum_{i=1}^{n}\left(y_i - \left(ax_i + b\right)\right)$$
$$= 2n\left(b + a\mu_x - \mu_y\right) = 0$$

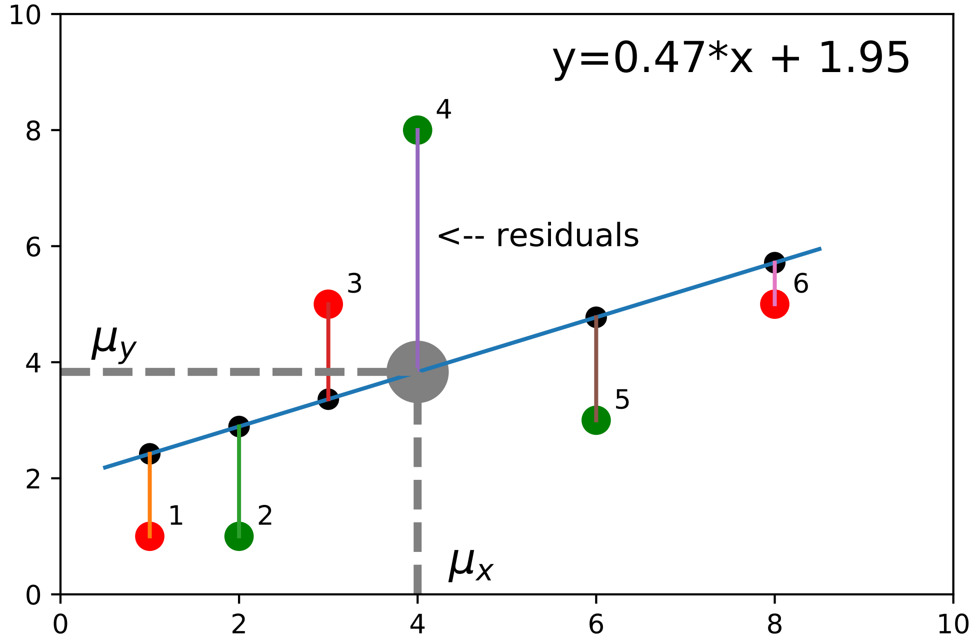
Derivation for b



- line must go through μ_x amd μ_y

$$b = \mu_y - a\mu_x$$

Derivation for a



- solve for b from

$$\frac{\partial Q}{\partial b} = 0$$

Derivation for a

$$\frac{\partial Q}{\partial b} = -2\sum_{i=1}^{n} x_i\Big(y_i - \big(ax_i + b\big)\Big)$$

$$= -2\sum_{i=1}^{n}\Big(x_i y_i - x_i\mu_y + ax_i\mu_x - ax_i^2\Big)$$

$$= -2\Big[\sum_{i=1}^{n}\Big(x_i y_i - x_i\mu_y\Big)$$

$$+ a\sum_{i=1}^{n}\Big(x_i^2 - \mu_x x_i\Big)\Big]$$

$$= -2\Big(\sigma_{xy}^2 - a\cdot\sigma_x^2\Big) = 0$$

- we obtain:

$$a = \sigma_{xy}^2 \cdot \left(\sigma_x^2\right)^{-1}$$

Summary of Derivation

- define:

$$\mu_x = \frac{x_1 + \cdots + x_n}{n}$$

$$\mu_y = \frac{y_1 + \cdots + y_n}{n}$$

$$\sigma_{xy}^2 = \frac{\left(x_1 y_1 + \cdots + x_n y_n\right)}{n} - \mu_x \mu_y$$

$$\sigma_x^2 = \frac{\left(x_1^2 + \cdots + x_n^2\right)}{n} - \mu_x^2$$

- compute slope and intercept:

$$a = \left[\sigma_{xy}^2 \cdot \left(\sigma_x^2\right)^{-1}\right]$$

$$b = \mu_y - \left[\sigma_{xy}^2 \cdot \left(\sigma_x^2\right)^{-1}\right] \mu_x$$

Correlation and Slope

- (Pearson) correlation

$$\rho_{xy} = \frac{\sigma^2_{xy}}{\sigma_x \sigma_y}$$

- correlation $-1 \leq \rho_{xy} \leq 1$
- X, Y independent $\rightarrow \rho_{xy} = 0$
- inverse is not true!
- slope of regression:

$$a = \left[\sigma^2_{xy} \cdot \left(\sigma^2_x\right)^{-1}\right] = \rho_{xy} \cdot \frac{\sigma_y}{\sigma_x}$$

- variance of residuals

$$\sigma^2_e = (1 - \rho^2_{xy})\sigma^2_y$$

Assumptions of Linear Regression

- existence of a linear relationship between x and y
- variance of residuals is the same ("*homoscedasticity*" - same scatter)
- residuals are normally distributed
- observations are independent
- contrast with "*heteroscedicity*" - varying variance

Python Code

```
import numpy as np
import matplotlib.pyplot as plt

def estimate_coef(x, y):
    n = np.size(x)
    mu_x, mu_y = np.mean(x), np.mean(y)
    SS_xy = np.sum(y*x) - n* mu_y * mu_x
    SS_xx = np.sum(x*x) - n *mu_x* mu_x
    slope = SS_xy / SS_xx
    intercept = mu_y - slope*mu_x
    return(slope, intercept)

def plot_regression(x, y, slope, intercept):
    plt.scatter(x, y, color = "blue",
                marker = "o", s = 100)
    y_pred = slope * x + intercept
    plt.plot(x, y_pred, color = "green", lw = 3)
    plt.xlabel("x")
    plt.ylabel("y")
    plt.show()
```

Python Code (cont'd)

```
x = np.array([1,2,3,4,6,8])
y = np.array([1,1,5,8,3,5])
slope, intercept = estimate_coef(x,y)
plot_regression(x,y,slope, intercept)
```

Equivalent Derivation

$$\frac{\partial Q}{\partial a} = -2\sum_{i=1}^{n} x_i\big(y_i - \big(ax_i + b\big)\big)$$

$$= -2\sum_{i=1}^{n} x_i e_i = 0$$

$$\frac{\partial Q}{\partial b} = -2\sum_{i=1}^{n} \big(y_i - \big(ax_i + b\big)\big)$$

$$= -2\sum_{i=1}^{n} e_i = 0$$

- these are equivalent to

$$E\big(Xe\big) = 0 \quad \text{and} \quad E\big(e\big) = 0$$

Numerical Computation

- use gradient descent algorithm
- have two equations

$$\frac{\partial Q}{\partial a} = -2\sum_{i=1}^{n} x_i(y_i - e_i) = 0$$

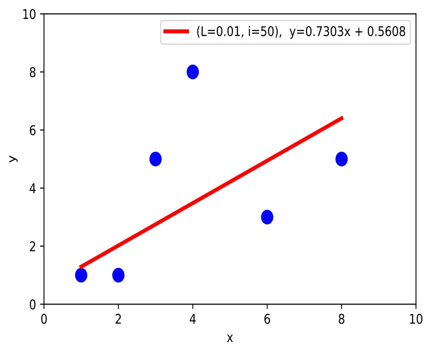
$$\frac{\partial Q}{\partial b} = -2\sum_{i=1}^{n} e_i = 0$$

- choose learning rate L

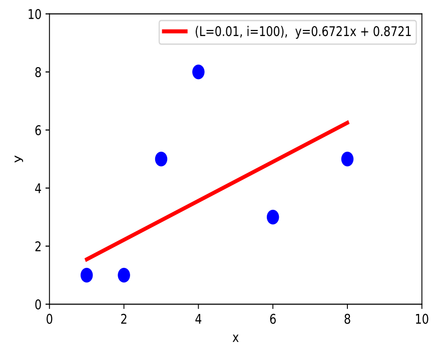
Numerical Computation

```
x = np.array([1,2,3,4,6,8])
y = np.array([1,1,5,8,3,5])

a = 0      # initial estimates
b = 0
L = 0.01   # learning rate
n = len(x);
epochs = 100
error  = []

for i in range(epochs):
    y_pred = slope * x + intercept
    error = sum((y-y_pred)*(y-y_pred))
    D_slope = (-2.0/n)* sum(x*(y-y_pred))
    D_intercept=(-2.0/n)*sum(y-y_pred)
    a = a - L * D_slope
    b = b - L * D_intercept
```

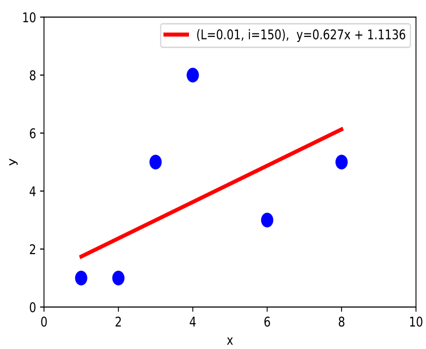
Gradient Descent



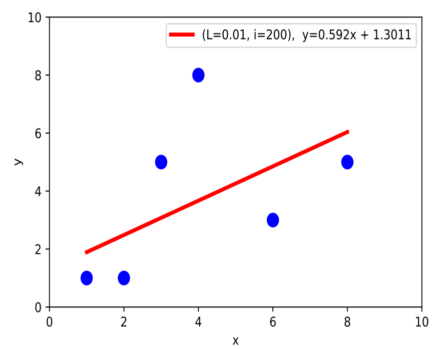
(a) iterations=50



(b) iterations=100



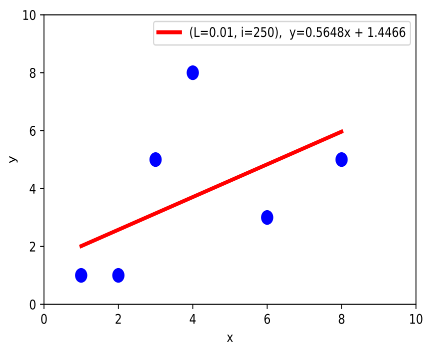
(a) iterations=150



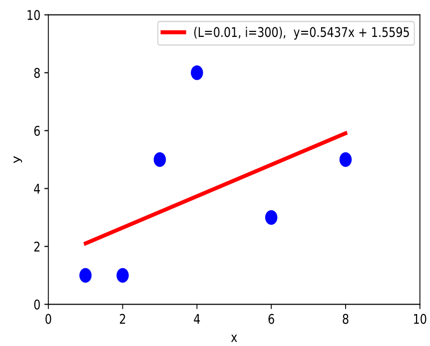
(b) iterations=200

- learning rate $L = 0.01$

Gradient Descent



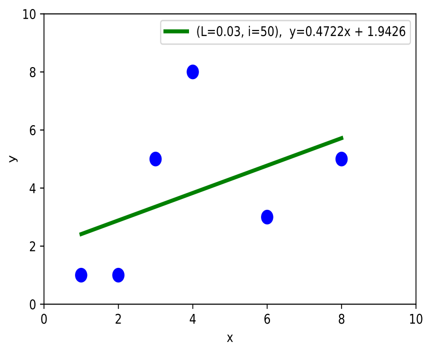
(a) iterations=50



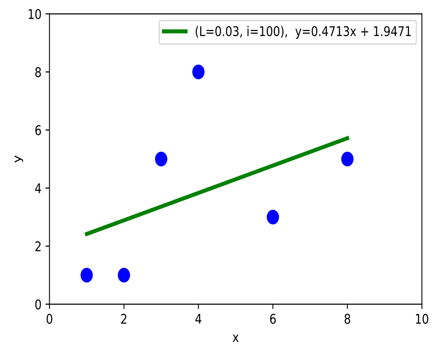
(b) iterations=100

- learning rate $L = 0.01$
- no significant changes to loss after 250 interations

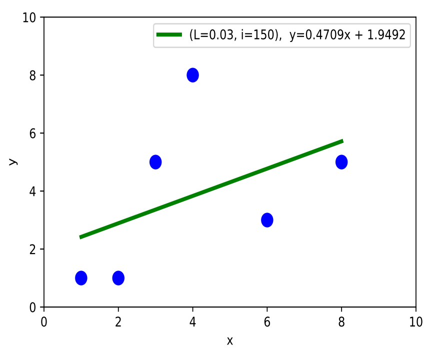
Gradient Descent



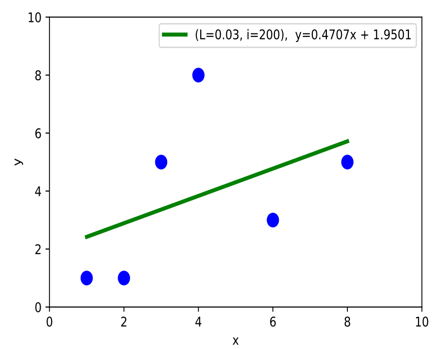
(a) iterations=50



(b) iterations=100



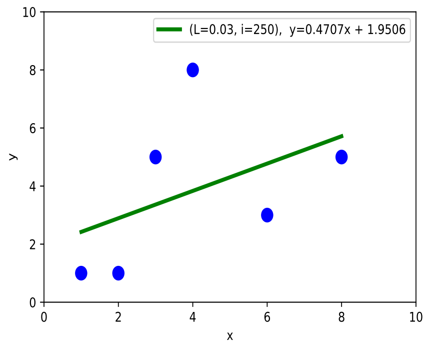
(a) iterations=150



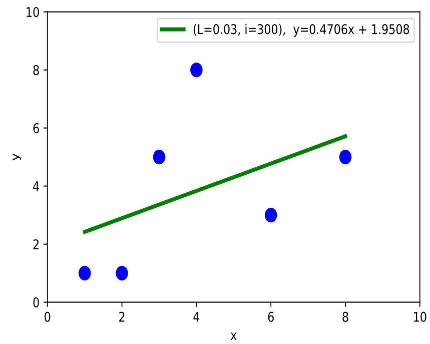
(b) iterations=200

- learning rate $L = 0.03$

Gradient Descent



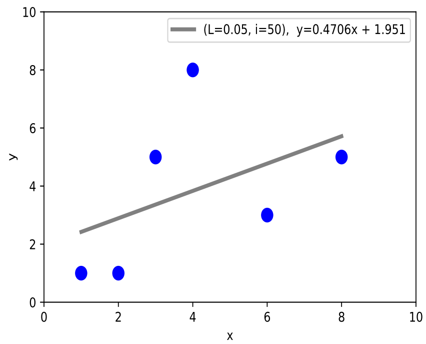
(a) iterations=50



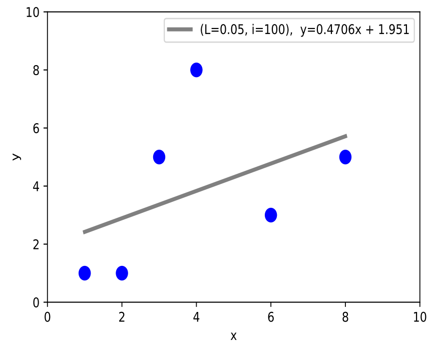
(b) iterations=100

- learning rate $L = 0.03$
- no significant changes to loss after 200 interations
- faster convergence for $L = 0.03$ than for $L = 0.01$

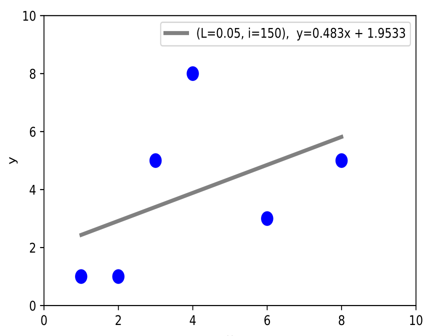
Gradient Descent



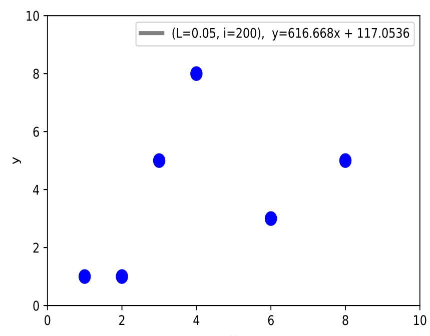
(a) iterations=50



(b) iterations=100



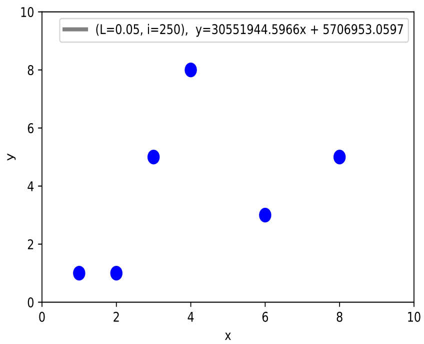
(a) iterations=150



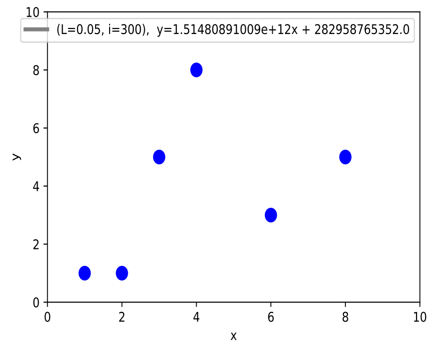
(b) iterations=200

- learning rate $L = 0.05$

Gradient Descent



(a) iterations=50



(b) iterations=100

- learning rate $L = 0.05$
- no convergence - rate is too high

Concepts Check:

(a) linear prediction
(b) residuals and loss function
(c) geometric meaning of slope and intercept
(d) correlation and covariance
(e) error variance
(f) computation of parameters