

Weighted least squares

Weighted least squares

Example: heteroscedastic errors

Iteratively reweighted least squares

Iteratively reweighted least squares

Example: ℓ_1 regression

Ordinary least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\|^2 = \sum_{i=1}^m (a_i^T x - y_i)^2$$

Ordinary least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\|^2 = \sum_{i=1}^m (a_i^T x - y_i)^2$$

- ▶ linear measurements of unknown vector $x \in \mathbb{R}^n$:

$$y_i = a_i^T x + \epsilon_i, \quad i = 1, \dots, m$$

Ordinary least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\|^2 = \sum_{i=1}^m (a_i^T x - y_i)^2$$

- ▶ linear measurements of unknown vector $x \in \mathbb{R}^n$:

$$y_i = a_i^T x + \epsilon_i, \quad i = 1, \dots, m$$

where

- ▶ y_i is i th measurement

Ordinary least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\|^2 = \sum_{i=1}^m (a_i^T x - y_i)^2$$

- ▶ linear measurements of unknown vector $x \in \mathbb{R}^n$:

$$y_i = a_i^T x + \epsilon_i, \quad i = 1, \dots, m$$

where

- ▶ y_i is i th measurement
- ▶ $a_i \in \mathbb{R}^n$ describes how i th measurement depends on x

Ordinary least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\|^2 = \sum_{i=1}^m (a_i^T x - y_i)^2$$

- ▶ linear measurements of unknown vector $x \in \mathbb{R}^n$:

$$y_i = a_i^T x + \epsilon_i, \quad i = 1, \dots, m$$

where

- ▶ y_i is i th measurement
- ▶ $a_i \in \mathbb{R}^n$ describes how i th measurement depends on x
- ▶ ϵ_i is noise or error in i th measurement

Ordinary least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\|^2 = \sum_{i=1}^m (a_i^T x - y_i)^2$$

- ▶ linear measurements of unknown vector $x \in \mathbb{R}^n$:

$$y_i = a_i^T x + \epsilon_i, \quad i = 1, \dots, m$$

where

- ▶ y_i is i th measurement
 - ▶ $a_i \in \mathbb{R}^n$ describes how i th measurement depends on x
 - ▶ ϵ_i is noise or error in i th measurement
- ▶ choose value of x that minimizes sum of squared errors:

$$\|\epsilon\|^2 = \sum_{i=1}^m \epsilon_i^2 = \sum_{i=1}^m (a_i^T x - y_i)^2$$

Weighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

Weighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

- ▶ ordinary least squares (OLS):

Weighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

- ▶ ordinary least squares (OLS):
equal weight for each measurement ($w_i = 1$)

Weighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

- ▶ ordinary least squares (OLS):
equal weight for each measurement ($w_i = 1$)
- ▶ weighted least squares (WLS):

Weighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

- ▶ ordinary least squares (OLS):
equal weight for each measurement ($w_i = 1$)
- ▶ weighted least squares (WLS):
different weight for each measurement

Weighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

- ▶ ordinary least squares (OLS):
equal weight for each measurement ($w_i = 1$)
- ▶ weighted least squares (WLS):
different weight for each measurement
- ▶ $w_i \in \mathbb{R}_+$ is weight of the i th measurement

Weighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

- ▶ ordinary least squares (OLS):
equal weight for each measurement ($w_i = 1$)
- ▶ weighted least squares (WLS):
different weight for each measurement
- ▶ $w_i \in \mathbb{R}_+$ is weight of the i th measurement
- ▶ more accurate or reliable measurements receive larger weight

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2$$

$$= \left\| \begin{bmatrix} \sqrt{w_1} (a_1^T x - y_1) \\ \vdots \\ \sqrt{w_m} (a_m^T x - y_m) \end{bmatrix} \right\|^2$$

Solving weighted least-squares problems

$$\begin{aligned}
 & \sum_{i=1}^m w_i (a_i^T x - y_i)^2 \\
 &= \left\| \begin{bmatrix} \sqrt{w_1} (a_1^T x - y_1) \\ \vdots \\ \sqrt{w_m} (a_m^T x - y_m) \end{bmatrix} \right\|^2 \\
 &= \left\| \begin{bmatrix} \sqrt{w_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{w_m} \end{bmatrix} \begin{bmatrix} a_1^T \\ \vdots \\ a_m^T \end{bmatrix} x - \begin{bmatrix} \sqrt{w_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{w_m} \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix} \right\|^2
 \end{aligned}$$

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}} Ax - W^{\frac{1}{2}} y\|^2$$

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}}Ax - W^{\frac{1}{2}}y\|^2$$

where

$$W = \text{diag}(w_1, \dots, w_m), \quad W^{\frac{1}{2}} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_m})$$

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}}Ax - W^{\frac{1}{2}}y\|^2$$

where

$$W = \text{diag}(w_1, \dots, w_m), \quad W^{\frac{1}{2}} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_m})$$

- ▶ ordinary least-squares problem!

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}}Ax - W^{\frac{1}{2}}y\|^2$$

where

$$W = \text{diag}(w_1, \dots, w_m), \quad W^{\frac{1}{2}} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_m})$$

- ▶ ordinary least-squares problem!
 - ▶ measurement matrix: $W^{\frac{1}{2}}A$

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}}Ax - W^{\frac{1}{2}}y\|^2$$

where

$$W = \text{diag}(w_1, \dots, w_m), \quad W^{\frac{1}{2}} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_m})$$

- ▶ ordinary least-squares problem!
 - ▶ measurement matrix: $W^{\frac{1}{2}}A$
 - ▶ observation vector: $W^{\frac{1}{2}}y$

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}}Ax - W^{\frac{1}{2}}y\|^2$$

where

$$W = \text{diag}(w_1, \dots, w_m), \quad W^{\frac{1}{2}} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_m})$$

- ▶ ordinary least-squares problem!
 - ▶ measurement matrix: $W^{\frac{1}{2}}A$
 - ▶ observation vector: $W^{\frac{1}{2}}y$
- ▶ solution:

x

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}}Ax - W^{\frac{1}{2}}y\|^2$$

where

$$W = \text{diag}(w_1, \dots, w_m), \quad W^{\frac{1}{2}} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_m})$$

- ▶ ordinary least-squares problem!
 - ▶ measurement matrix: $W^{\frac{1}{2}}A$
 - ▶ observation vector: $W^{\frac{1}{2}}y$
- ▶ solution:

$$x = ((W^{\frac{1}{2}}A)^T(W^{\frac{1}{2}}A))^{-1}(W^{\frac{1}{2}}A)^T(W^{\frac{1}{2}}y)$$

Solving weighted least-squares problems

$$\sum_{i=1}^m w_i (a_i^T x - y_i)^2 = \|W^{\frac{1}{2}}Ax - W^{\frac{1}{2}}y\|^2$$

where

$$W = \text{diag}(w_1, \dots, w_m), \quad W^{\frac{1}{2}} = \text{diag}(\sqrt{w_1}, \dots, \sqrt{w_m})$$

- ▶ ordinary least-squares problem!
 - ▶ measurement matrix: $W^{\frac{1}{2}}A$
 - ▶ observation vector: $W^{\frac{1}{2}}y$
- ▶ solution:

$$\begin{aligned} x &= ((W^{\frac{1}{2}}A)^T(W^{\frac{1}{2}}A))^{-1}(W^{\frac{1}{2}}A)^T(W^{\frac{1}{2}}y) \\ &= (A^TWA)^{-1}A^TWy \end{aligned}$$

Example: heteroscedastic errors

- ▶ measurement model:

$$y_i = mx_i + b + \epsilon_i, \quad i = 1, \dots, N$$

Example: heteroscedastic errors

- ▶ measurement model:

$$y_i = mx_i + b + \epsilon_i, \quad i = 1, \dots, N$$

- ▶ error model:

$$\epsilon_i \sim \mathcal{N}(0, i^2), \quad i = 1, \dots, N$$

Example: heteroscedastic errors

- ▶ measurement model:

$$y_i = mx_i + b + \epsilon_i, \quad i = 1, \dots, N$$

- ▶ error model:

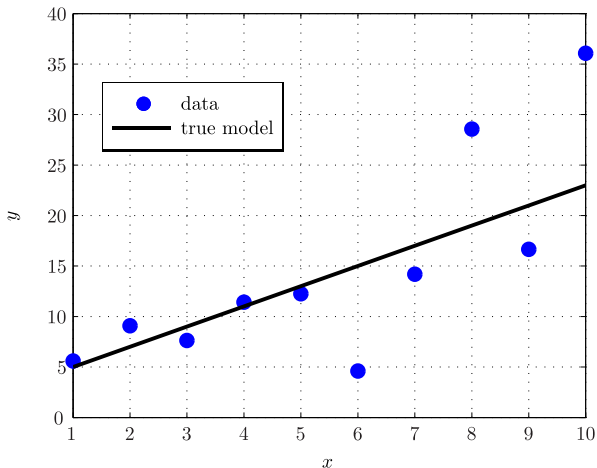
$$\epsilon_i \sim \mathcal{N}(0, i^2), \quad i = 1, \dots, N$$

- ▶ weights:

$$w_i = \frac{1}{i}, \quad i = 1, \dots, N$$

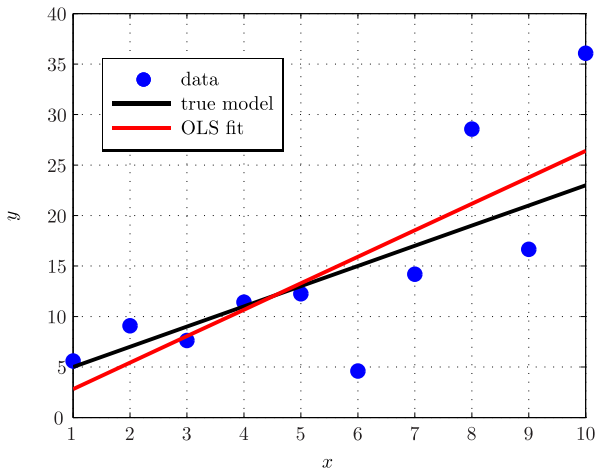
Example: heteroscedastic errors

example data: $m = 2$, $b = 3$



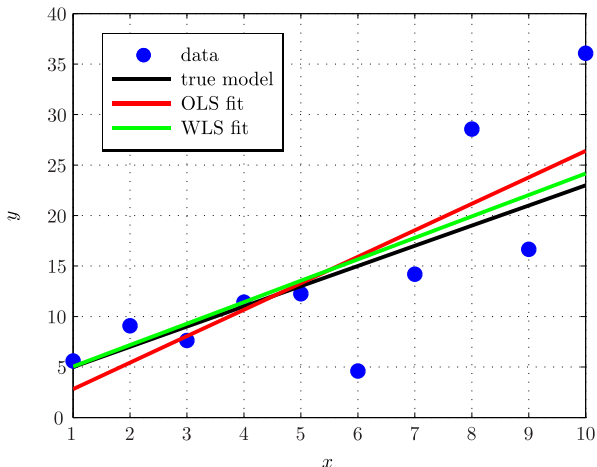
Example: heteroscedastic errors

ordinary least-squares fit: $m_{\text{ols}} = 2.6223$, $b_{\text{ols}} = 0.1845$



Example: heteroscedastic errors

weighted least-squares fit: $m_{\text{wls}} = 2.1234$, $b_{\text{wls}} = 2.9287$



Weighted least squares

Weighted least squares

Example: heteroscedastic errors

Iteratively reweighted least squares

Iteratively reweighted least squares

Example: ℓ_1 regression

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m \phi(a_i^T x - y_i)$$

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m \phi(a_i^T x - y_i)$$

- ▶ $\phi : \mathbb{R} \rightarrow \mathbb{R}_+$ is penalty function

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m \phi(a_i^T x - y_i)$$

- ▶ $\phi : \mathbb{R} \rightarrow \mathbb{R}_+$ is penalty function
- ▶ write as weighted least-squares problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m \phi(a_i^\top x - y_i)$$

- ▶ $\phi : \mathbb{R} \rightarrow \mathbb{R}_+$ is penalty function
- ▶ write as weighted least-squares problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^\top x - y_i)^2$$

- ▶ where weight function is

$$w_i(x) = \frac{\phi(a_i^\top x - y_i)}{(a_i^\top x - y_i)^2}$$

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

- ▶ the weights $w_i(x)$ depend on x

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

- ▶ the weights $w_i(x)$ depend on x
- ▶ choose initial guess $x^{(0)}$

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

- ▶ the weights $w_i(x)$ depend on x
- ▶ choose initial guess $x^{(0)}$
- ▶ solve a sequence of weighted least-squares problems:

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

- ▶ the weights $w_i(x)$ depend on x
- ▶ choose initial guess $x^{(0)}$
- ▶ solve a sequence of weighted least-squares problems:
 - ▶ for $k = 0, 1, 2, \dots$

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

- ▶ the weights $w_i(x)$ depend on x
- ▶ choose initial guess $x^{(0)}$
- ▶ solve a sequence of weighted least-squares problems:
 - ▶ for $k = 0, 1, 2, \dots$
 - ▶ compute weights using previous estimate for x :

$$W(x^{(k)}) = \text{diag}(w_1(x^{(k)}), \dots, w_m(x^{(k)}))$$

Iteratively reweighted least squares

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \sum_{i=1}^m w_i(x) (a_i^T x - y_i)^2$$

- ▶ the weights $w_i(x)$ depend on x
- ▶ choose initial guess $x^{(0)}$
- ▶ solve a sequence of weighted least-squares problems:
 - ▶ for $k = 0, 1, 2, \dots$
 - ▶ compute weights using previous estimate for x :

$$W(x^{(k)}) = \text{diag}(w_1(x^{(k)}), \dots, w_m(x^{(k)}))$$

- ▶ solve weighted-least squares problem for next estimate of x :

$$x^{(k+1)} = (A^T W(x^{(k)}) A)^{-1} A^T W(x^{(k)}) y$$

Example: ℓ_1 regression

ℓ_1 regression problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\| = \sum_{i=1}^m |a_i^\top x - y_i|$$

Example: ℓ_1 regression

ℓ_1 regression problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\| = \sum_{i=1}^m |a_i^T x - y_i|$$

iteratively reweighted least squares:

Example: ℓ_1 regression

ℓ_1 regression problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\| = \sum_{i=1}^m |a_i^\top x - y_i|$$

iteratively reweighted least squares:

- penalty function:

$$\phi(d) = |d|$$

Example: ℓ_1 regression

ℓ_1 regression problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\| = \sum_{i=1}^m |a_i^\top x - y_i|$$

iteratively reweighted least squares:

- ▶ penalty function:

$$\phi(d) = |d|$$

- ▶ weight function:

$$w_i(x) = \frac{\phi(a_i^\top x - y_i)}{(a_i^\top x - y_i)^2} = \frac{1}{|a_i^\top x - y_i|}$$

Example: ℓ_1 regression

ℓ_1 regression problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} : \|Ax - y\| = \sum_{i=1}^m |a_i^T x - y_i|$$

iteratively reweighted least squares:

- ▶ penalty function:

$$\phi(d) = |d|$$

- ▶ weight function:

$$w_i(x) = \frac{\phi(a_i^T x - y_i)}{(a_i^T x - y_i)^2} = \frac{1}{|a_i^T x - y_i|}$$

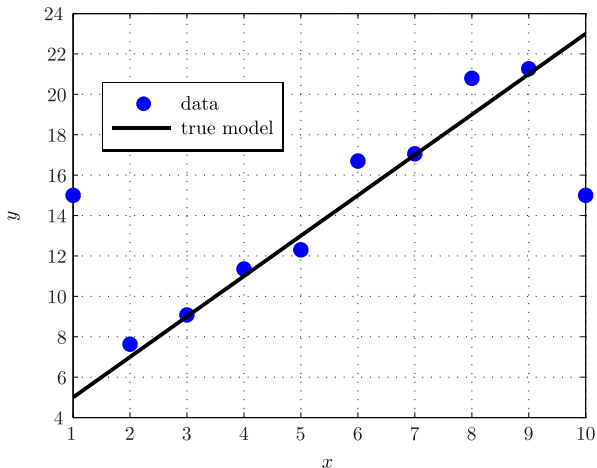
- ▶ practical weight function:

$$w_i(x) = \frac{1}{\max\{|a_i^T x - y_i|, \delta\}}$$

where δ is small, positive constant

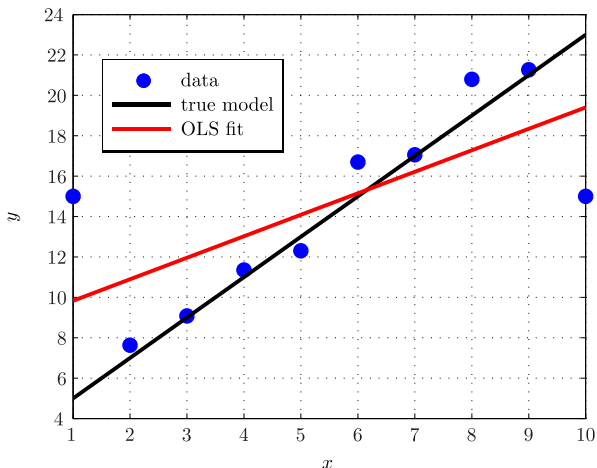
Example: ℓ_1 regression

example data: $m = 2$, $b = 3$



Example: ℓ_1 regression

ordinary least-squares fit: $m_{\text{ols}} = 1.0642$, $b_{\text{ols}} = 8.7645$



Example: ℓ_1 regression

weighted least-squares fit: $m_{\ell_1} = 1.8864$, $b_{\ell_1} = 3.8539$

