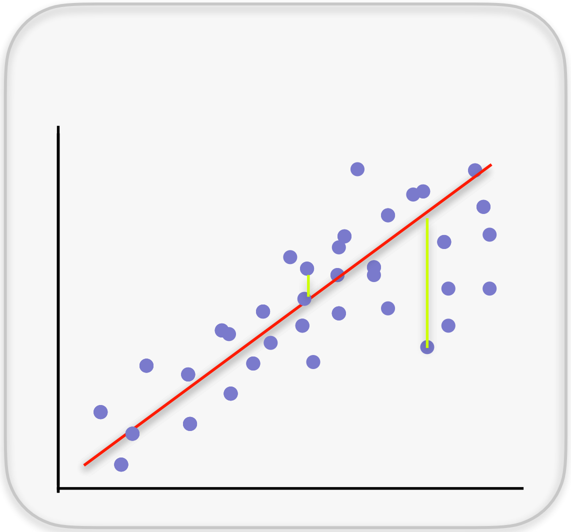
Lecture 3

The regression problem in matrix notation

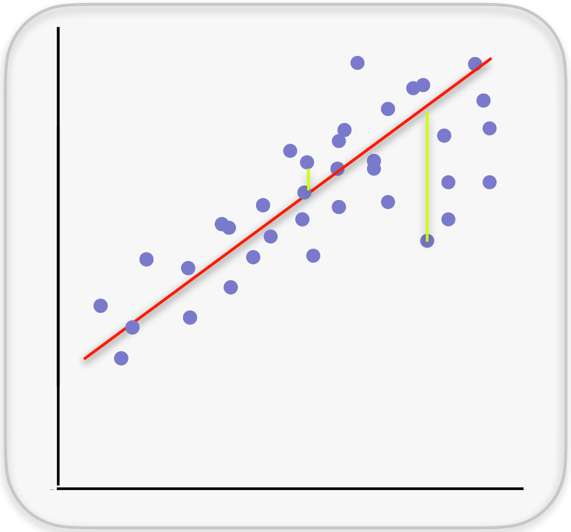
Linear model: $y_i = x_i^T w + \epsilon_i$

Least squares solution:

$$\widehat{w}_{LS} = \arg\min_w ||\mathbf{y} - \mathbf{X}w||_2^2$$
$$= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

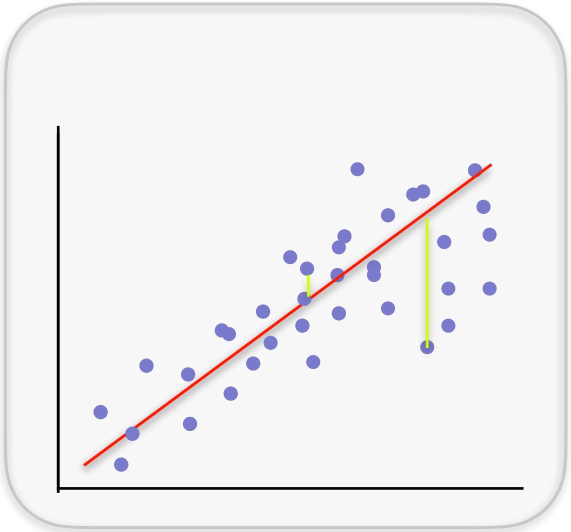


What about an offset (a.k.a intercept)?



The regression problem in matrix notation

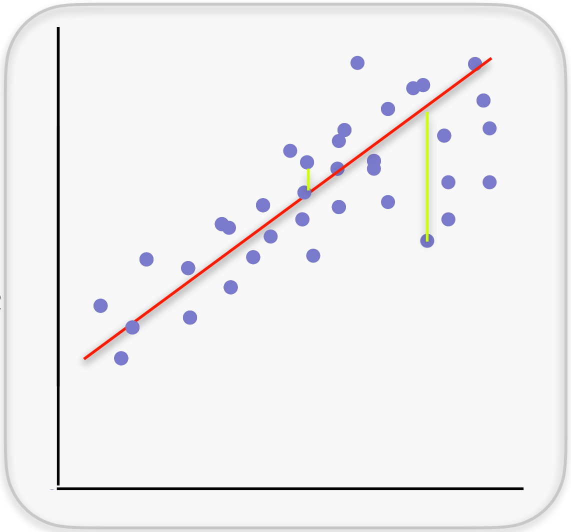
Linear model: $y_i = x_i^T w + \epsilon_i$



Least squares solution:

$$\begin{aligned}\widehat{w}_{LS} &= \arg\min_w ||\mathbf{y} - \mathbf{X}w||_2^2 \\ &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}\end{aligned}$$

Affine model: $y_i = x_i^T w + b + \epsilon_i$



Least squares solution:

$$\begin{aligned}\widehat{w}_{LS}, \widehat{b}_{LS} &= \arg\min_{w,b} \sum_{i=1}^n \left(y_i - (x_i^T w + b)\right)^2 \\ &= \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2\end{aligned}$$

Dealing with an offset

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

Set gradient w.r.t. w and b to zero to find the minima:

Dealing with an offset

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

$$\mathbf{X}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{X}^T\mathbf{1} = \mathbf{X}^T\mathbf{y}$$

$$\mathbf{1}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{1}^T\mathbf{1} = \mathbf{1}^T\mathbf{y}$$

If $\mathbf{X}^T\mathbf{1} = 0$, if the features have zero mean,

$$\widehat{w}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

$$\widehat{b}_{LS} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

Dealing with an offset

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

$$\mathbf{X}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{X}^T\mathbf{1} = \mathbf{X}^T\mathbf{y}$$
$$\mathbf{1}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{1}^T\mathbf{1} = \mathbf{1}^T\mathbf{y}$$

If $\mathbf{X}^\mathbf{T}\mathbf{1} = 0$,

$$\widehat{w}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

$$\widehat{b}_{LS} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

In general, when $\mathbf{X}^T\mathbf{1} \neq 0$,

Dealing with an offset

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

$$\mathbf{X}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{X}^T\mathbf{1} = \mathbf{X}^T\mathbf{y}$$
$$\mathbf{1}^T\mathbf{X}\widehat{w}_{LS} + \widehat{b}_{LS}\mathbf{1}^T\mathbf{1} = \mathbf{1}^T\mathbf{y}$$

If $\mathbf{X^T1} = 0$,

$$\widehat{w}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

$$\widehat{b}_{LS} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

In general, when $\mathbf{X}^T\mathbf{1} \neq 0$,

$$\mu = \frac{1}{n}\mathbf{X}^T\mathbf{1}$$
$$\widetilde{\mathbf{X}} = \mathbf{X} - \mathbf{1}\mu^T$$
$$\widehat{w}_{\text{LS}} = (\widetilde{\mathbf{X}}^T\widetilde{\mathbf{X}})^{-1}\widetilde{\mathbf{X}}^T\mathbf{y}$$
$$\widehat{b}_{\text{LS}} = \frac{1}{n}\sum_{i=1}^{n} y_i - \mu^T\widehat{w}_{\text{LS}}$$

Process

Decide on a **model:** $y_i = x_i^T w + b + \epsilon_i$

Choose a loss function - least squares

Pick the function which minimizes loss on data

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} \sum_{i=1}^{n} \left(y_i - (x_i^T w + b)\right)^2$$

Use function to make prediction on new examples

$$\hat{y}_{\text{new}} = x_{\text{new}}^T \hat{w}_{LS} + \hat{b}_{LS}$$

Another way of dealing with an offset

$$\widehat{w}_{LS}, \widehat{b}_{LS} = \arg\min_{w,b} ||\mathbf{y} - (\mathbf{X}w + \mathbf{1}b)||_2^2$$

reparametrize the problem as $\overline{\mathbf{X}} = [\mathbf{X}, \mathbf{1}]$ and $\overline{w} = \begin{bmatrix} w \\ b \end{bmatrix}$

$$\overline{\mathbf{X}}\,\overline{w} =$$

Why is least squares a good loss function?

$$\widehat{w}_{LS} = \arg\min_w ||\mathbf{y} - \mathbf{X}w||_2^2$$
$$= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Consider $\quad y_i = x_i^T w + \epsilon_i \quad$ where $\quad \epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$

$\implies y_i \sim$

$\implies P(y_i; x_i, w, \sigma) \; =$

Why is least squares a good loss function?

Maximum Likelihood Estimator:

$$\begin{aligned}\widehat{w}_{\text{MLE}} &= \arg\max_w \; \log P(\{y_i\}_{i=1}^n; \{x_i\}_{i=1}^n, w, \sigma) \\ &= \arg\max_w \; -n\log(\sigma\sqrt{2\pi}) + \sum_{i=1}^n -\frac{(y_i - x_i^T w)^2}{2\sigma^2}\end{aligned}$$

Why is least squares a good loss function?

Maximum Likelihood Estimator:

$$\widehat{w}_{\text{MLE}} = \arg\max_w \log P(\{y_i\}_{i=1}^n; \{x_i\}_{i=1}^n, w, \sigma)$$

$$= \arg\max_w -n\log(\sigma\sqrt{2\pi}) + \sum_{i=1}^n -\frac{(y_i - x_i^T w)^2}{2\sigma^2}$$

$$= \arg\min_w \sum_{i=1}^n (y_i - x_i^T w)^2$$

Recall: $$\widehat{w}_{LS} = \arg\min_w \sum_{i=1}^n \left(y_i - x_i^T w\right)^2$$

$$\widehat{w}_{LS} = \widehat{w}_{MLE} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

Recap of linear regression

$$\text{Data } \{(x_i, y_i)\}_{i=1}^n$$

Minimize the loss
(Empirical Risk Minimization)

Choose a loss
e.g., $(y_i - x_i^T w)^2$

Solve $\widehat{w}_{\text{LS}} = \arg\min_w \sum_{i=1}^n (y_i - x_i^T w)^2$

Maximize the likelihood
(MLE)

Choose a Hypothesis class
e.g., $y_i = x_i^T w + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^w)$

Maximize the likelihood,

$$\widehat{w}_{\text{MLE}} = \arg\max_w \left\{ -n \log(\sigma\sqrt{2\pi}) - \sum_{i=1}^n \frac{(y_i - x_i^T w)^2}{2\sigma^2} \right\}$$

Analysis of Error under additive Gaussian noise

$$\text{if} \quad y_i = x_i^T w + \epsilon_i \quad \text{and} \quad \epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2) \qquad \mathbf{Y} = \mathbf{X}w + \epsilon$$

$$\begin{aligned}
\widehat{w}_{MLE} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\
&= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}w + \epsilon) \\
&= w + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon
\end{aligned}$$

Maximum Likelihood Estimator is unbiased:

Analysis of Error under additive Gaussian noise

if $\quad y_i = x_i^T w + \epsilon_i \quad$ and $\quad \epsilon_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2) \qquad \mathbf{Y} = \mathbf{X}w + \epsilon$

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&= w + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon
\end{aligned}$$

Covariance is:

Analysis of Error under additive Gaussian noise

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$$\begin{aligned}\widehat{w}_{MLE} &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \\ &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}w + \epsilon) \\ &= w + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon\end{aligned}$$

$$\mathbb{E}[\widehat{w}_{MLE}] = w$$

$$\text{Cov}(\widehat{w}_{MLE}) = \mathbb{E}[(\widehat{w} - \mathbb{E}[\widehat{w}])(\widehat{w} - \mathbb{E}[\widehat{w}])^T] = (\mathbf{X}^T\mathbf{X})^{-1}$$

$$\widehat{w}_{MLE} \sim \mathcal{N}(w, (\mathbf{X}^T\mathbf{X})^{-1})$$

Questions?