About Regression

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Start with two **classification** type regression:

- ► Logistic Regression
- Softmax(Multinomial) regression

the BIG idea in here

Assume there is four classes that the classifier is capable to classify:

- if data x_1 has label $y_1 = 1$, then y_1 can be written as $[1, 0, 0, 0]^{\top}$.
- if data x_2 has label $y_2 = 2$, then y_2 can be written as $[0, 1, 0, 0]^{\top}$.
- if data x_3 has label $y_3 = 2$, then y_3 can be written as $[0, 1, 0, 0]^{\top}$.
- if data x_4 has label $y_4 = 3$, then y_4 can be written as $[0, 0, 1, 0]^{\top}$.
- if data x_5 has label $y_5 = 4$, then y_5 can be written as $[0, 0, 0, 1]^{\top}$.
- **>** ...

So basically, we want to build a classifer $f(x, \theta)$, such that:

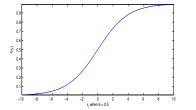
- $(y_1 = 1) \implies f(x_1, \theta)$ should be as close to $[1, 0, 0, 0]^{\top}$ as possible, e.g., $f(x_1, \theta) = [0.99, 0.005, 0.005, 0]^{\top}$
- $(y_2 = 2) \implies f(x_2, \theta)$ should be as close to $[0, 1, 0, 0]^{\top}$ as possible, e.g., $f(x_2, \theta) = [0.005, 0.99, 0.005, 0]^{\top}$
- $(y_3 = 2) \implies f(x_3, \theta)$ should be as close to $[0, 1, 0, 0]^{\top}$ as possible, e.g., $f(x_3, \theta) = [0.005, 0.99, 0.005, 0]^{\top}$
- $(y_4 = 3) \implies f(x_4, \theta)$ should be as close to $[0, 0, 1, 0]^{\top}$ as possible, e.g., $f(x_4, \theta) = [0.005, 0.005, 0.099, 0]^{\top}$
- $(y_5 = 4) \implies f(x_5, \theta)$ should be as close to $[0, 0, 0, 1]^{\top}$ as possible, e.g., $f(x_5, \theta) = [0.005, 0.005, 0, 0.99]^{\top}$
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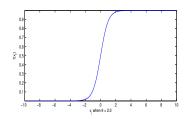
Let's see the mechanism to achieve this.



Standard Sigmoid function: logistic function

$$\sigma(t) = \frac{1}{1 + \exp(-t)} = \frac{\exp(t)}{\exp(t) + 1} \qquad \rightarrow \qquad \sigma(\mathbf{x}_i^\top \theta) = \frac{1}{1 - \exp(\mathbf{x}_i^\top \theta + \theta_0)}$$





It's a **squashing function** that maps any real number to a value between 0 . . . 1.

Properties of logistic function

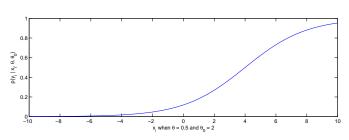
$$1 - \sigma(t) = 1 - \frac{1}{1 + \exp(-t)} = \frac{1 + \exp(-t) - 1}{1 + \exp(-t)} = \frac{\exp(-t)}{1 + \exp(-t)} = \sigma(-t)$$

$$\frac{\mathrm{d}\sigma(t)}{\mathrm{d}t} = \frac{\mathrm{d}\left(\frac{1}{1+\exp(-t)}\right)}{\mathrm{d}t} = \frac{\exp(-t)}{(1+\exp(-t))^2} = \left(\frac{1}{1+\exp(-t)}\right)\left(\frac{\exp(-t)}{1+\exp(-t)}\right)$$
$$= \sigma(t)(1-\sigma(t)) \qquad \qquad \text{it's always positive}$$

$$\frac{\mathrm{d}\sigma(-t)}{\mathrm{d}t} = \frac{\mathrm{d}\left(\frac{1}{1+\exp(t)}\right)}{\mathrm{d}t} = \frac{-\exp(t)}{(1+\exp(t))^2} = -\underbrace{\left(\frac{1}{1+\exp(t)}\right)}_{\sigma(-t) \text{ or } 1-\sigma(t)} \underbrace{\left(\frac{\exp(t)}{1+\exp(t)}\right)}_{\sigma(t)}$$
$$= -\sigma(t)(1-\sigma(t)) \qquad \text{it's always negative}$$

Logistic Regression

Finding a **single** Bernoulli probability: $\Pr(y_i = 1 | \underbrace{x_i^T \theta})$:



▶ Write $\{x_i, 1\} \rightarrow x_i$ and $\{\theta, \theta_0\} \rightarrow \theta$:

$$Pr(\mathbf{Y}|\mathbf{X}, \boldsymbol{\theta}) = \prod_{i=1}^{n} \left[\frac{1}{1 + \exp(-x_i^T \boldsymbol{\theta})} \right]^{y_i} \left[1 - \frac{1}{1 + \exp(-x_i^T \boldsymbol{\theta})} \right]^{1 - y_i}$$

Maximization is performed on the log space:

$$\mathcal{C}(\boldsymbol{\theta}) = -\log[p(\mathbf{Y}|\mathbf{X}, \boldsymbol{\theta})] = -\left(\sum_{i=1}^{n} y_{i} \log\left[\frac{1}{1 + \exp(-x_{i}^{T}\boldsymbol{\theta})}\right] + (1 - y_{i}) \log\left[1 - \frac{1}{1 + \exp(-x_{i}^{T}\boldsymbol{\theta})}\right]\right)$$

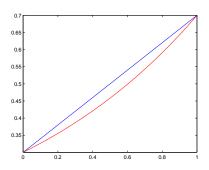


Think Bernoulli again

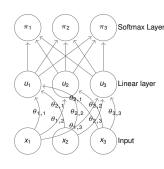
Both functions are the same at end-points $\{0, 1\}$:

$$f_p(x) = (1 - p)^{(1-x)} p^x$$

 $f_p(x) = (1 - p)(1 - x) + px$



Expand to multiple classes: Softmax



$$\pmb{\theta}_1 = \{\theta_{1,1}, \theta_{1,2}, \theta_{1,3}\} \quad \pmb{\theta}_2 = \{\theta_{2,1}, \theta_{2,2}, \theta_{2,3}\} \quad \pmb{\theta}_3 = \{\theta_{3,1}, \theta_{3,2}, \theta_{3,3}\}$$

Linear Layer

$$u_1 = \mathbf{x}^T \boldsymbol{\theta}_1 = \sum_{i=1}^3 x_{1,i} \theta_{1,i}$$

$$u_2 = \mathbf{x}^T \boldsymbol{\theta}_2 = \sum_{i=1}^3 x_{2,i} \theta_{2,i}$$

$$u_3 = \mathbf{x}^T \boldsymbol{\theta}_3 = \sum_{i=1}^3 x_{3,i} \theta_{3,i}$$

Softmax Layer

$$\pi_{1} \equiv \text{Pr}(y_{i} = 1 | \mathbf{x}_{i}, \boldsymbol{\theta}) = \frac{\exp(u_{1})}{\sum_{k=1}^{3} \exp(u_{k})} = \frac{\exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{1})}{\sum_{k=1}^{3} \exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{k})}$$

$$\pi_{2} \equiv \text{Pr}(y_{i} = 2 | \mathbf{x}_{i}, \boldsymbol{\theta}) = \frac{\exp(u_{2})}{\sum_{k=1}^{3} \exp(u_{k})} = \frac{\exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{2})}{\sum_{k=1}^{3} \exp(\mathbf{y}_{i}^{T}\boldsymbol{\theta}_{k})}$$

$$\pi_{3} \equiv \text{Pr}(y_{i} = 3 | \mathbf{x}_{i}, \boldsymbol{\theta}) = \frac{\exp(u_{3})}{\sum_{k=1}^{3} \exp(u_{k})} = \frac{\exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{3})}{\sum_{k=1}^{3} \exp(\mathbf{y}_{i}^{T}\boldsymbol{\theta}_{k})}$$

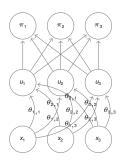
- easily extend them to multiple K arbitary classes



Relationship between 2-class Softmax and Logistic regression

$$\begin{split} \pi_1 &\equiv \pi(y_i = 1 | \mathbf{x}_i, \boldsymbol{\theta}) = \frac{\exp(\mathbf{x}^T \boldsymbol{\theta}_1)}{\exp(\mathbf{x}^T \boldsymbol{\theta}_1) + \exp(\mathbf{x}^T \boldsymbol{\theta}_2)} \\ &= \frac{1}{1 + \exp\left(\mathbf{x}^T (\boldsymbol{\theta}_2 - \boldsymbol{\theta}_1)\right)} \\ &= \frac{1}{1 + \exp\left(\mathbf{x}^T (\boldsymbol{\theta}_2)\right)} \\ &= \frac{\exp\left(\mathbf{x}^T \boldsymbol{\theta}\right)}{\exp\left(\mathbf{x}^T \boldsymbol{\theta}\right) + 1} \end{split}$$

Softmax in our three class example



$$\begin{split} \pi_{\text{1:Data Scientist}} &= \frac{\exp(u_1)}{\sum_{l=1}^3 u_l} = \frac{\exp(\mathbf{x}^T\boldsymbol{\theta}_1)}{\sum_{l=1}^3 \exp(\mathbf{x}^T\boldsymbol{\theta}_1)} \\ \pi_{\text{2:Scholar}} &= \frac{\exp(u_2)}{\sum_{l=1}^3 u_l} = \frac{\exp(\mathbf{x}^T\boldsymbol{\theta}_2)}{\sum_{l=1}^3 \exp(\mathbf{x}^T\boldsymbol{\theta}_2)} \\ \pi_{\text{3:CEO}} &= \frac{\exp(u_3)}{\sum_{l=1}^3 u_l} = \frac{\exp(\mathbf{x}^T\boldsymbol{\theta}_3)}{\sum_{l=1}^3 \exp(\mathbf{x}^T\boldsymbol{\theta}_1)} \end{split}$$

	attribute 1	attribute 2	attribute 3	Occupation
Attendee 1	50	64	1.2	Data scientist
Attendee 2	23	23	15	Scholar
Attendee 3	50	80	3.2	Data scientist
Attendee N	5	90	25	CEO
Attendee N+1	60	43	12	?

So, substitute into the neural network, you hope to get a set of $oldsymbol{ heta}$, such that:

$$\begin{aligned} \mathbf{x}^{(1)} &= (50, 64, 1.2) \implies (\pi_{1:\text{Data Scientist}} = \mathbf{1}, \, \pi_{2:\text{Scholar}} = 0, \, \pi_{3:\text{CEO}} = 0) \\ \mathbf{x}^{(2)} &= (23, 23, 15) \implies (\pi_{1:\text{Data Scientist}} = 0, \, \pi_{2:\text{Scholar}} = \mathbf{1}, \, \pi_{3:\text{CEO}} = 0) \\ \mathbf{x}^{(3)} &= (50, 80, 3.2) \implies (\pi_{1:\text{Data Scientist}} = \mathbf{1}, \, \pi_{2:\text{Scholar}} = 0, \, \pi_{3:\text{CEO}} = 0) \\ & \dots \\ \mathbf{x}^{(N)} &= (5, 90, 25) \implies (\pi_{1:\text{Data Scientist}} = 0, \, \pi_{2:\text{Scholar}} = 0, \, \pi_{3:\text{CEO}} = \mathbf{1}) \end{aligned}$$

An unique perfect $\boldsymbol{\theta}$ suitable for all the data obviously do NOT exist. We need to find a $\boldsymbol{\theta}$ which minimize the sum of cost.



Minimize cost function example: Softmax

Logistic regression:

$$\rho(\mathbf{Y}|\mathbf{X},\,\boldsymbol{\theta}) = \prod_{i=1}^{N} \left[\frac{1}{1 + \exp(-\mathbf{x}_i^T\boldsymbol{\theta})} \right]^{y_i} \left[1 - \frac{1}{1 + \exp(-\mathbf{x}_i^T\boldsymbol{\theta})} \right]^{1-y_i}$$

Softmax:

$$\begin{split} \rho(\mathbf{Y}|\mathbf{X},\boldsymbol{\theta}) &= \prod_{i=1}^{N} \prod_{k=1}^{K} \left[\frac{\exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{k})}{\sum_{l=1}^{K} \exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{l})} \right]^{Y_{i},k} & \text{we write } y_{i} \text{ as an indicator vector, e.g., [100], [101]} \\ \mathcal{C}(\boldsymbol{\theta}) &= -\sum_{i=1}^{N} \sum_{k=1}^{K} y_{i,k} \log \left[\frac{\exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{k})}{\sum_{l=1}^{K} \exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{l})} \right] & \text{note the cross entropy form: } H(p,q) = -\sum_{X} p(x) \log(q(x)) \\ &= -\sum_{i=1}^{N} \sum_{k=1}^{K} y_{i,k} \left[\log \exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{k}) - \log \sum_{l=1}^{K} \exp(\mathbf{x}_{i}^{T}\boldsymbol{\theta}_{l}) \right] \end{split}$$

What is cross entropy?



Cost function: Cross Entropy

Minimize the cost function: Cross Entropy can be thought of "how much" deviates between the "true" density p(x) and recovered density "q(x)".

$$\begin{aligned} H(p, q) &= \mathsf{E}_p[-\log q] \\ &= -\sum_{x} p(x) \, \log q(x) \\ &= \sum_{x} \left[\underbrace{-p(x) \, \log q(x) + p(x) \log(p(x)) - p(x) \log(p(x))}_{q} \right] \\ &= \sum_{x} \underbrace{-p(x) \, \log p(x) + \sum_{x} p(x) \, \log \frac{p(x)}{q(x)}}_{q} \\ &= H(p) + D_{\mathrm{KL}}(p||q), \end{aligned}$$

Question If minimising **cross entropy loss** is equivalent of maximising multinomial likelihood estimation, then minimising **square loss** is equivalent of maximising what likelihood estimation?

Softmax or multinomial regression objective function

$$C(\theta) = -\sum_{i=1}^{N} \sum_{k=1}^{K} y_{i,k} \left[\log \left(\frac{\exp(\mathbf{x}_{i}^{T} \theta_{k})}{\sum_{l=1}^{K} \exp(\mathbf{x}_{i}^{T} \theta_{l})} \right) \right]$$

How may we find:

$$\underset{\boldsymbol{\theta}}{\operatorname{arg\,min}}\,\mathcal{C}(\boldsymbol{\theta})$$

We solve it using Gradient descend.

Find the derivatives of Multinomial regression

$$\mathcal{C}(\boldsymbol{\theta}) = -\sum_{i=1}^{N} \sum_{k=1}^{K} y_{i,k} \left[\log \left(\frac{\exp(\mathbf{x}_{i}^{T} \boldsymbol{\theta}_{k})}{\sum_{i=1}^{K} \exp(\mathbf{x}_{i}^{T} \boldsymbol{\theta}_{i})} \right) \right]$$

Let $Z_k = \mathbf{x}_i^T \boldsymbol{\theta}_k$, we have,

$$\begin{split} \frac{\partial \mathcal{C}(\boldsymbol{\theta})}{\partial \mathcal{Z}_k} &= \sum_{i=1}^N \frac{\partial \left(-\sum_{k=1}^K y_{i,k} \left\lfloor \log \left(\frac{\exp(\mathcal{Z}_i)}{\sum_{i=1}^K \exp(\mathcal{Z}_i)} \right) \right\rfloor \right)}{\partial \mathcal{Z}_k} \\ &= \sum_{i=1}^N \left[\frac{\exp(\mathcal{Z}_i)}{\sum_{i=1}^K \exp(\mathcal{Z}_i)} - y_{i,k} \right] & \text{see next page} \\ \Rightarrow & \frac{\partial \mathcal{C}(\boldsymbol{\theta})}{\partial \mathcal{Z}} &= \sum_{i=1}^N \left[\frac{\exp(\mathcal{Z}_i)}{\sum_{i=1}^K \exp(\mathcal{Z}_i)} - y_{i,1} \right] \\ &= \sum_{i=1}^N \left(\frac{\exp(\mathcal{Z}_i)}{\sum_{i=1}^K \exp(\mathcal{Z}_i)} - y_{i,k} \right) \end{split}$$

If we were to differentiate with respect to θ :

$$\frac{\partial \mathcal{C}(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \frac{\partial \mathcal{C}(\boldsymbol{\theta})}{\partial Z} \frac{\partial Z}{\partial \boldsymbol{\theta}} = \sum_{i=1}^{N} \mathbf{x}_{i} \left[\frac{\exp(\mathbf{x}_{i}^{\mathsf{T}} \boldsymbol{\theta})}{\sum_{l=1}^{K} \exp(\mathbf{x}_{i}^{\mathsf{T}} \boldsymbol{\theta}_{l})} - y_{i} \right]^{\mathsf{T}}$$



Derivative for Softmax regression

$$\rho_k = \frac{\exp^{z_k}}{\sum_l \exp^{z_l}} \qquad \qquad \mathcal{C} = -\sum_k y_k \log \rho_k, \qquad \qquad \text{where } \sum_k y_k = 1$$

when k = i:

$$\frac{\partial \rho_k}{\partial z_k} = \frac{\partial \left(\frac{\exp^{r_k}}{\sum_l \exp^{r_l}}\right)}{\partial z_k} = \frac{\partial \left(\frac{\exp^{r_k}}{\exp^{r_k} + \sum_{l \neq k} \exp^{r_l}}\right)}{\partial \exp(z_k)} \times \frac{\partial \exp^{z_k}}{\partial z_k}$$

We know the identity:

$$\frac{\partial \frac{x}{x+c}}{\partial x} = \frac{\partial x(x+c)^{-1}}{\partial x} = (x+c)^{-1} - x(x+c)^{-2} = \frac{(x+c)-x}{(x+c)^2} = \frac{c}{(x+c)^2}$$

Therefore.

$$\begin{split} \frac{\partial p_k}{\partial z_k} &= \frac{\partial \left(\frac{\exp^{z_k}}{\exp^{z_k} + \sum_{i \neq k} \exp^{z_i}}\right)}{\partial \exp(z_k)} \times \frac{\partial \exp^{z_k}}{\partial z_k} &= \frac{\sum_{l \neq k} \exp^{z_l}}{\left(\sum_{l=1}^K \exp^{z_l}\right)^2} \times \exp^{z_k} \\ &= \frac{\sum_{l \neq k} \exp^{z_l}}{\left(\sum_{l=1}^K \exp^{z_l}\right)} \times \frac{\exp^{z_k}}{\left(\sum_{l=1}^K \exp^{z_l}\right)} &= p_k (1 - p_k) \end{split}$$



Derivative for Softmax regression

when $k \neq i$, We know the identity:

$$\frac{\partial \frac{y}{z+c}}{\partial z} = \frac{\partial y(z+c)^{-1}}{\partial z} = -\frac{y}{(z+c)^2}$$

$$\begin{split} \frac{\partial p_k}{\partial z_i} &= \frac{\left(\partial \frac{\exp^{z_k}}{\exp^{z_i} + \sum_{i \neq i} \exp^{z_i}}\right)}{\partial \exp(z_i)} \times \frac{\partial \exp^{z_i}}{\partial z_i} \\ &= -\frac{\exp^{z_k}}{\left(\sum_{l=1}^K \exp^{z_l}\right)^2} \times \exp^{z_l} \\ &= -\frac{\exp^{z_l}}{\left(\sum_{l=1}^K \exp^{z_l}\right)} \times \frac{\exp^{z_k}}{\left(\sum_{l=1}^K \exp^{z_l}\right)} = -\rho_l \rho_k \end{split}$$

Derivative for Softmax regression

$$\frac{\partial p_k}{\partial z_i} = \begin{cases} p_i(1-p_i), & i=k\\ -p_ip_k, & i\neq k \end{cases}$$

$$\frac{\partial C}{\partial z_i} = -\sum_k y_k \frac{\partial \log p_k}{\partial z_i}$$

$$= -\sum_k y_k \frac{1}{p_k} \frac{\partial p_k}{\partial z_i}$$

$$= -y_i(1-p_i) - \sum_{k\neq i} y_k \frac{1}{p_k} (-p_kp_i)$$

$$= -y_i(1-p_i) + \sum_{k\neq i} y_k(p_i)$$

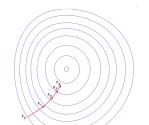
$$= -y_i + y_ip_i + \sum_{k\neq i} y_k(p_i)$$

$$= p_i \left(\sum_k y_k\right) - y_i$$

$$= p_i - y_i$$

Gradient Descend for multinomial regression

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \nabla f(\mathbf{x}_n), \ n \ge 0$$



$$\mathcal{C}(\boldsymbol{\theta}) = -\sum_{i=1}^{N} \sum_{k=1}^{K} y_{i,k} \log \left[\frac{\exp(\mathbf{x}_{i}^{T} \boldsymbol{\theta}_{k})}{\sum_{i=1}^{K} \exp(\mathbf{x}_{i}^{T} \boldsymbol{\theta}_{i})} \right] + \frac{\lambda}{2} \sum_{k=1}^{K} \sum_{j=1}^{m} \boldsymbol{\theta}_{k,j}^{2}$$

$$\boldsymbol{\theta}^{n+1} = \boldsymbol{\theta}^n - \alpha_n \left(\sum_{i=1}^N \mathbf{x}_i \left[\frac{\exp(\mathbf{x}_i^T \boldsymbol{\theta})}{\sum_{i=1}^K \exp(\mathbf{x}_i^T \boldsymbol{\theta}_i)} - y_i \right]^\top + \lambda \boldsymbol{\theta}^n \right), \ n \geq 0$$

What's this $\frac{\lambda}{2} \sum_{k=1}^K \sum_{j=1}^m \theta_{k,j}^2$ business? It's the **regulariser** we added.

Linear Regression

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

where

$$\mathbf{y} = \begin{pmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_n \end{pmatrix} \qquad \qquad \mathbf{X} = \begin{pmatrix} \mathbf{x}_1^{\mathsf{T}} \\ \mathbf{x}_2^{\mathsf{T}} \\ \vdots \\ \mathbf{x}_n^{\mathsf{T}} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_{11} & \cdots & \mathbf{x}_{1p} \\ \mathbf{x}_{21} & \cdots & \mathbf{x}_{2p} \\ \vdots & \ddots & \vdots \\ \mathbf{x}_{n1} & \cdots & \mathbf{x}_{np} \end{pmatrix} \qquad \qquad \boldsymbol{\beta} = \begin{pmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \\ \vdots \\ \boldsymbol{\beta}_p \end{pmatrix} \qquad \qquad \boldsymbol{\varepsilon} = \begin{pmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \\ \vdots \\ \boldsymbol{\varepsilon}_n \end{pmatrix}$$

You have seen it so many times! There is an analytical solution to it:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y} = \left(\sum \mathbf{x}_{i}\mathbf{x}_{i}^{\mathrm{T}}\right)^{-1}\left(\sum \mathbf{x}_{i}y_{i}\right).$$



Linear Regression

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$$\mathbf{y} = \begin{pmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_n \end{pmatrix} \qquad \qquad \mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{pmatrix} = \begin{pmatrix} \mathbf{x}_{11} & \cdots & \mathbf{x}_{1p} \\ \mathbf{x}_{21} & \cdots & \mathbf{x}_{2p} \\ \vdots & \ddots & \vdots \\ \mathbf{x}_{n1} & \cdots & \mathbf{x}_{np} \end{pmatrix} \qquad \qquad \boldsymbol{\beta} = \begin{pmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \\ \vdots \\ \boldsymbol{\beta}_p \end{pmatrix} \qquad \qquad \boldsymbol{\varepsilon} = \begin{pmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \\ \vdots \\ \boldsymbol{\varepsilon}_n \end{pmatrix}$$

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$$R^{2} = 1 - \frac{\sum_{i} \left(y_{i} - \hat{y}_{i} \right)^{2}}{\sum_{i} (y_{i} - \bar{y})^{2}}$$

- the better linear regression fits the data relative to a simple average, the closer the value of R² is to 1.
- ▶ If the chosen model fits worse than a horizontal line, then R^2 is negative

Polynomial Regression

For each of the data pairs (x_i, y_i) :

$$y_i = a_0 + a_1 x_i + a_2 x_i^2 + \cdots + a_m x_i^m + \varepsilon_i$$

The model can be written as a system of linear equations:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^m \\ 1 & x_2 & x_2^2 & \dots & x_2^m \\ 1 & x_3 & x_3^2 & \dots & x_3^m \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^m \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \vdots \\ \varepsilon_n \end{bmatrix},$$

or,

$$\vec{y} = \mathbf{X}\vec{a} + \vec{\varepsilon}.$$

Ordinary least squares estimation is:

$$\widehat{\vec{a}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \vec{y}.$$



Mixed effect model

Imagine we have the following setting:

A particular company "develops and markets products for the early detection of target organ damage and management of cardiovascular and renal disease.". In five years time, this company will have 10000 employees worldwide, HR needs a good model to reward its employees:

- ▶ has N = 10000 number of employees.
- ▶ has q = 45 working departments throughout the world.
- each department has N_q number of employees, i.e, $N = \sum_{i=1}^{q} n_i$
- ▶ The HR has collected p = 6 attributes from each employees, including:
 - utilisation hours
 - vrs of experience
 - salary
 - last year's rating
 - number of awards received
 - market value
- ightharpoonup each y_i is the amount of "shared" profit each employee should receive.



Mixed effect model

In the matrix form:

$$\mathbf{y} = X\beta + Z\gamma + \varepsilon$$

write down the dimensionality:

substitute numbers into:

z_i is a **one-hot** vector, indicating which Department the employee belong to.

