

Prob. 1

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- Assume that you are given the following sample . Estimate the weight of people whose heights are 150, 155, 165, and 190 cm, using KNN with $k = 3$:

$$\hat{y}_{KNN} = \frac{y_1 + y_2 + \cdots + y_k}{k}$$

where y_1, y_2, \dots, y_k are the labels of the k nearest neighbors to your test instance. (10 pts)

Person	Height (cm)	Weight (kg)
1	171	80
2	168	78
3	191	100
4	182	80
5	150	65
6	178	83

⊕ calc a person's weight w/ height 150

$$\text{Euclidean distance} = d = \sqrt{(h_t - h_{obr})^2}$$

$$d_1 = \sqrt{(150 - 171)^2} = \sqrt{(-21)^2} = 21$$

$$d_2 = \sqrt{(150 - 168)^2} = 18$$

$$d_3 = \sqrt{(150 - 191)^2} = 41$$

$$d_4 = \sqrt{(150 - 182)^2} = 32$$

$$d_5 = \sqrt{(150 - 150)^2} = 0$$

$$d_6 = \sqrt{(150 - 178)^2} = 28$$

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	21	80
2	168	18	78
3	191	41	100
4	182	32	80
5	150	0	65
6	178	28	83
7	150	N/A	74.33

⊕ find 3 near neighbors as $k=3$, so from the table,

people with heights 171, 168, 150

Therefore, to calc the est weight \hat{y}_{kNN} is

$$\hat{y}_{kNN} = \frac{y_1 + y_2 + y_3}{3} = \frac{80 + 78 + 65}{3} = 74.33 \checkmark \checkmark$$

④ repeat the same calculation

④ calc a person's weight w/ height 155

$$\text{Euclidean distance} = d = \sqrt{(h_t - h_{obs})^2}$$

$$d_1 = \sqrt{(155 - 171)^2} = 16$$

$$d_2 = \sqrt{(155 - 168)^2} = 13$$

$$d_3 = \sqrt{(155 - 191)^2} = 36$$

$$d_4 = \sqrt{(155 - 182)^2} = 27$$

$$d_5 = \sqrt{(155 - 150)^2} = 5$$

$$d_6 = \sqrt{(155 - 178)^2} = 23$$

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	16	80
2	168	13	78
3	191	36	100
4	182	27	80
5	150	5	65
6	178	23	83
7	155	N/A	74.33

④ find 3 near neighbors as $k=3$, so from the table, people with heights 171, 168, 150

Therefore, to calc the est weight \hat{y}_{kNN} is

$$\hat{y}_{kNN} = \frac{y_1 + y_2 + y_3}{3} = \frac{80 + 78 + 65}{3} = 74.33 \checkmark \checkmark$$

④ repeat the same calculation

④ calc a person's weight w/ height 165

$$\text{Euclidean distance} = d = \sqrt{(h_t - h_{\text{obs}})^2}$$

$$d_1 = \sqrt{(165 - 171)^2} = 6$$

$$d_2 = \sqrt{(165 - 168)^2} = 3$$

$$d_3 = \sqrt{(165 - 191)^2} = 26$$

$$d_4 = \sqrt{(165 - 182)^2} = 17$$

$$d_5 = \sqrt{(165 - 150)^2} = 15$$

$$d_6 = \sqrt{(165 - 178)^2} = 13$$

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	6	80
2	168	3	78
3	191	26	100
4	182	17	80
5	150	15	65
6	178	13	83
7	165	N/A	80.33

④ find 3 near neighbors as $k=3$, so from the table, people with heights 171, 168, 178

Therefore, to calc the est weight \hat{y}_{kNN} is

$$\hat{y}_{\text{kNN}} = \frac{y_1 + y_2 + y_3}{3} = \frac{80 + 78 + 83}{3} = 80.33 \quad \checkmark$$

④ repeat the same calculation

④ calc a person's weight w/ height 165

$$\text{Euclidean distance} = d = \sqrt{(h_t - h_{\text{obs}})^2}$$

$$d_1 = \sqrt{(190 - 171)^2} = 19$$

$$d_2 = \sqrt{(190 - 168)^2} = 22$$

$$d_3 = \sqrt{(190 - 191)^2} = 1$$

$$1 \quad \boxed{1, 19, 22, 1}$$

$$d_3 = \sqrt{(190 - 191)^2} = 1$$

$$d_4 = \sqrt{(190 - 182)^2} = 8$$

$$d_5 = \sqrt{(190 - 150)^2} = 40$$

$$d_6 = \sqrt{(190 - 178)^2} = 12$$

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	19	80
2	168	22	78
3	191	1	100
4	182	8	80
5	150	40	65
6	178	12	83
7	190	N/A	87.67

④ find 3 near neighbors as $k=3$, so from the table, people with heights 191, 182, 178

Therefore, to calc the est weight \hat{y}_{kNN} is

$$\hat{y}_{kNN} = \frac{y_1 + y_2 + y_3}{3} = \frac{100 + 80 + 83}{3} = 87.67 \checkmark$$

Prob. 2

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2. Repeat 1, but instead of using the simple average of the labels of k nearest neighbors, which is use the following weighted average:

$$\hat{y}_{KNN} = \frac{w_1 y_1 + w_2 y_2 + \cdots + w_k y_k}{w_1 + w_2 + \cdots + w_k}$$

where the weight w_i for the label y_i of instance i is determined as $1/d_i$, where d_i the distance between the instance i and the test instance. (10 pts)

(*) the distances for Person's weight 150

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	21	80
2	168	18	78
3	191	41	100
4	182	32	80
5	150	0	65
6	178	28	83
7	150	N/A	66.3

$$w_1 = \frac{1}{d_1} = \frac{1}{21}, \quad w_2 = \frac{1}{d_2} = \frac{1}{18}, \quad w_3 = \frac{1}{d_3} = \frac{1}{0} = \infty$$

Note: w_3 is a large number, and since $w_i \in (0, 1)$, we can assume that $w_3 = 1$

Now, calculate the estimated weight

$$\hat{y}_{KNN} = \frac{w_1 y_1 + w_2 y_2 + w_3 y_3}{w_1 + w_2 + w_3} = \frac{\frac{80}{21} + \frac{78}{18} + 65}{\frac{1}{21} + \frac{1}{18} + 1} = 66.3 \text{ vv}$$

(*) the distances for Person's weight 155

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	16	80
2	168	13	78
3	191	36	100
4	182	27	80
5	150	5	65
6	178	23	83
7	155	N/A	66.3

$$w_1 = \frac{1}{21}, \quad w_2 = \frac{1}{18}, \quad w_3 = 1 \rightarrow \text{by assumption}$$

Now, calculate the estimated weight

$$\hat{y}_{hNN} = \frac{w_1 y_1 + w_2 y_2 + w_3 y_3}{w_1 + w_2 + w_3} = \frac{\frac{80}{21} + \frac{78}{18} + 65}{\frac{1}{21} + \frac{1}{18} + 1} = 66.3 \text{ vv}$$

(*) the distances for Person's weight 165

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	6	80
2	168	3	78
3	191	26	100
4	182	17	80
5	150	15	65
6	178	13	83
7	165	N/A	79.24

$$w_1 = \frac{1}{6}, \quad w_2 = \frac{1}{3}, \quad w_3 = \frac{1}{13}$$

Now, calculate the estimated weight

$$\hat{y}_{hNN} = \frac{w_1 y_1 + w_2 y_2 + w_3 y_3}{w_1 + w_2 + w_3} = \frac{\frac{80}{6} + \frac{78}{3} + \frac{83}{13}}{\frac{1}{6} + \frac{1}{3} + \frac{1}{13}} = 79.24$$

(*) the distances for Person's weight 190

Person	Height (cm)	Distance (Euclidean)	Weight (kg)
1	171	19	80
2	168	22	78
3	191	1	100
4	182	8	80
5	150	40	65
6	178	12	83
7	190	N/A	96.76

$$w_1 = 1, \quad w_2 = 1/8, \quad w_3 = 1/12$$

Now, calculate the estimated weight

$$\hat{y}_{hNN} = \frac{w_1 y_1 + w_2 y_2 + w_3 y_3}{w_1 + w_2 + w_3} = \frac{100 + 10 + \frac{83}{12}}{1 + \frac{1}{8} + \frac{1}{12}} = 96.76$$

Prob. 3

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3. Assume that $J(\mathbf{x}) = \mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{d}^T \mathbf{x} + c$ where $\mathbf{Q} = \mathbf{Q}^T \in \mathbb{R}^{n \times n}$, $\mathbf{x}, \mathbf{d} \in \mathbb{R}^n$, and $c \in \mathbb{R}$. Show that $\nabla_{\mathbf{x}} J(\mathbf{x}) = 2\mathbf{Q}\mathbf{x} + \mathbf{d}$ and $\mathbf{H} = \frac{\partial^2 J}{\partial \mathbf{x} \partial \mathbf{x}^T} = 2\mathbf{Q}$. $\mathbf{H}_{ij} = \frac{\partial^2 J}{\partial x_i \partial x_j}$ and \mathbf{H} is called the Hessian matrix of J . (10 pts)

PROVE $\nabla_{\mathbf{x}} J(\mathbf{x}) = 2\mathbf{Q}\mathbf{x} + \mathbf{d}$

$$\nabla_{\mathbf{x}} J(\mathbf{x}) = \frac{\partial J}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{x}} (\mathbf{x}^T \mathbf{Q} \mathbf{x} + \mathbf{d}^T \mathbf{x} + c)$$

since \mathbf{Q} is symmetric and the function is linear, we can treat $\mathbf{x}^T \mathbf{Q} \mathbf{x}$ as $\frac{1}{2} \mathbf{x}^2$ and $\mathbf{d}^T \mathbf{x} = \mathbf{d} \cdot \mathbf{x}$

$$\therefore \nabla_{\mathbf{x}} J(\mathbf{x}) = \frac{\partial J}{\partial \mathbf{x}} = 2\mathbf{Q}\mathbf{x} + \mathbf{d} \quad \checkmark \checkmark$$

PROVE $\mathbf{H} = \frac{\partial^2 J}{\partial \mathbf{x} \partial \mathbf{x}^T} = 2\mathbf{Q}$

$$\frac{\partial^2 J}{\partial \mathbf{x} \partial \mathbf{x}^T} = \frac{\partial}{\partial \mathbf{x}^T} (2\mathbf{Q}\mathbf{x} + \mathbf{d}) = \frac{\partial}{\partial \mathbf{x}^T} [(2\mathbf{x}^T \mathbf{Q}^T + \mathbf{d}^T)]$$

$$= \frac{\partial}{\partial \mathbf{x}^T} [(2\mathbf{x}^T \mathbf{Q} + \mathbf{d}^T)] = 2\mathbf{Q} \quad \checkmark \checkmark$$

Prob. 4

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4. Write down the prediction \hat{y} for a test row vector $\mathbf{x}'_{1 \times p}$ made by a linear regression model in terms of \mathbf{y} the vector of labels of the training set and $\mathbf{X}_{n \times (p+1)}$, the (augmented) feature matrix, and explain why \hat{y} can be viewed as a special case of KNN regression. (10 pts)

$$\hat{y} = \mathbf{x}' \hat{\beta} = \underbrace{\mathbf{x}' (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' \mathbf{y}}_H = H\mathbf{y}$$

The linear regression model is a form of KNN. We can define KNN Regression model as $y_{KNN} = \frac{y}{k}$ where $y = [y_1, y_2, \dots, y_n]$. Comparing to the linear regression model \hat{y} , simply, $H = \frac{1}{k}$ if x_i 's are the nearest k point and zero elsewhere.

Let's take $y_0 = \hat{f}(x_0) = [x_0 \ 1]' \hat{\beta} = \underbrace{[x_0 \ 1] (\mathbf{X}' \mathbf{X})^{-1} \mathbf{X}' y}_H$

We can define H as

$$H = (x_0 \ 1)' (\mathbf{X}' \mathbf{X})^{-1} \begin{pmatrix} 1 \\ x_i \end{pmatrix}, \quad i \in \{1, 2, \dots, n\} \rightarrow *$$

Simplify $\mathbf{X}' \mathbf{X}$

$$\mathbf{X}' \mathbf{X} = \begin{pmatrix} \cdots & \cdots \\ \cdots & \cdots \\ \mathbf{x}'_i & \cdots \\ \cdots & \cdots \end{pmatrix}_{2 \times n} \begin{pmatrix} \vdots & \vdots \\ \vdots & \vdots \\ x'_i & \vdots \\ \vdots & \vdots \end{pmatrix}_{n \times 2} = \begin{pmatrix} \sum x_i & \sum x_i^2 \\ \sum x_i^2 & \sum x_i^4 \end{pmatrix}$$

$$= \begin{pmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{pmatrix}$$

To find the inverse, $(\mathbf{X}' \mathbf{X})^{-1}$

$$|X^T X| = n \sum x_i^2 - \sum x_i^2 = (n-1) \sum x_i^2$$

$$\therefore (X^T X)^{-1} = \frac{1}{(n-1) \sum x_i^2} \begin{pmatrix} \sum x_i^2 & -\sum x_i \\ -\sum x_i & n \end{pmatrix} \rightarrow D$$

Plug ① into *:

$$H = \frac{1}{(n-1) \sum x_i^2} (x_0 - 1) \begin{pmatrix} \sum x_i^2 & -\sum x_i \\ -\sum x_i & n \end{pmatrix} \begin{pmatrix} 1 \\ -x_0 \end{pmatrix}_{2 \times 2}$$


This should equal $\frac{1}{n}$ but it seems I missed some steps

$$= \frac{1}{(n-1) \sum x_i^2} (x_0 - 1) \begin{pmatrix} \sum x_i^2 - \sum x_i^2 \\ -\sum x_i + n \sum x_i \end{pmatrix}$$

$$= \frac{1}{(n-1) \sum x_i^2} (x_0 - 1) \begin{pmatrix} 0 \\ (n-1) \sum x_i \end{pmatrix} = \frac{1}{\sum x_i} (x_0 - 1) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= \frac{1}{\sum_{i=1}^n x_i}$$

Prob. 5

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5. Show that for $\mathbf{y} \in \mathbb{R}^n$, $\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ is a member of the column space of \mathbf{X} , i.e. is a linear combination of the columns of $\mathbf{X} \in \mathbb{R}^{n \times (p+1)}$. (10 pts)

$$\mathbf{X} \in \mathbb{R}^{n \times (p+1)}, \text{ where } (p+1) \leq n$$

$$\mathbf{H}_{n \times n} = \mathbf{X} \begin{pmatrix} \mathbf{X}^T \mathbf{X} \end{pmatrix}^{-1} \mathbf{X}^T_{(p+1) \times n}$$

note that $\mathbf{H}_{n \times n}$ has a rank of $p+1$

Suppose we have two vectors:

i) \mathbf{v} is the column space of \mathbf{X}

ii) \mathbf{w} is orthogonal to $\text{Col}(\mathbf{X})$

then we can prove from i) and ii) the following

i) Suppose $\mathbf{v} = \mathbf{X} \mathbf{u}_{(p+1) \times 1}$

$$\therefore \mathbf{H} \mathbf{v} = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{v} = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{X} \mathbf{u}$$

$$= \mathbf{X} (\mathbf{X}^{-1} (\mathbf{X}^T)^{-1}) \mathbf{X}^T \mathbf{X} \mathbf{u} = \underbrace{(\mathbf{X} \mathbf{X}^{-1})}_{\mathbf{I}} \underbrace{(\mathbf{X}^{-1} \mathbf{X})^T}_{\mathbf{I}^T} \mathbf{X} \mathbf{u} = \mathbf{X} \mathbf{u} = \mathbf{v}$$

ii)

$$\mathbf{H} \mathbf{w} = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \underbrace{\mathbf{X}^T \mathbf{w}}_0 = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{0} = \mathbf{0}$$

So we conclude that

$$\mathbf{H} \mathbf{v} = \lambda_1 \mathbf{v} \quad \text{where } \lambda_1 = 1 - \dots$$

$$Hv = \lambda_1 v \quad \text{where } \begin{cases} \lambda_1 = 1 \\ \lambda_2 = 0 \end{cases} \} \text{ e-values}$$
$$Hw = \lambda_2 w$$

and v, w are e-vectors, which span the whole space of $X \in \mathbb{R}^{n \times p+1}$

Prob. 6

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6. Show that in linear regression, if $\hat{\beta}$ minimizes $\text{RSS}(\beta)$, then $\mathbf{y} - \hat{\mathbf{y}}$ is orthogonal to the column space of \mathbf{X} . (10 pts)

$$\mathbf{y} = \mathbf{X}\beta + \varepsilon = \begin{bmatrix} 1 & x_{11} & \cdots & x_{n1} \\ 1 & x_{21} & \cdots & x_{n2} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{nn} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

In order to minimize $\text{RSS}(\beta)$

$$\text{RSS}(\beta) = \varepsilon^\top \varepsilon = (\mathbf{y} - \mathbf{X}\beta)^\top (\mathbf{y} - \mathbf{X}\beta)$$

$$= (\mathbf{y}^\top - \beta^\top \mathbf{X}^\top) (\mathbf{y} - \mathbf{X}\beta)$$

$$= \mathbf{y}^\top \mathbf{y} - \underbrace{\mathbf{y}^\top \mathbf{X}\beta}_{-2\mathbf{y}^\top \mathbf{X}\beta} - \underbrace{\beta^\top \mathbf{X}^\top \mathbf{y}}_{\beta^\top \mathbf{X}^\top \mathbf{X}\beta} + \beta^\top \mathbf{X}^\top \mathbf{X}\beta$$

$$= \mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{X}\beta + \beta^\top \mathbf{X}^\top \mathbf{X}\beta$$

$$\therefore \frac{\partial \text{RSS}(\beta)}{\partial \beta} = \frac{\partial}{\partial \beta} (\mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{X}\beta + \beta^\top \mathbf{X}^\top \mathbf{X}\beta)$$

$$= -2\mathbf{y}^\top \mathbf{X} + 2\beta^\top \mathbf{X}^\top \mathbf{X}$$

$$-2\mathbf{y}^\top \mathbf{X} + 2\beta^\top \mathbf{X}^\top \mathbf{X} = 0$$

$$2\beta^\top \mathbf{X}^\top \mathbf{X} = 2\mathbf{y}^\top \mathbf{X}$$

take \rightarrow
 transpose
 on both
 sides

$$\mathbf{X}^\top \mathbf{X}\beta = \mathbf{X}^\top \mathbf{y} \rightarrow \text{Normal equation}$$

assume $X^T X$ is linearly independent, then

$$(X^T X)^{-1} (X^T X) \hat{\beta} = (X^T X)^{-1} X^T y$$

$$\therefore \hat{\beta} = (X^T X)^{-1} X^T y$$

$$\therefore X \varepsilon = X(y - \hat{y}) = X(y - X\hat{\beta}) = 0 \rightarrow \text{orthogonality}$$