Artificial Intelligence: HW 2

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1 Linear Regression

1.a

Let f be the target function. I'll use the superscript with parenthesis to describe the n-th sample vector.

 $f(\boldsymbol{\omega}, \overline{\boldsymbol{x}^{(n)}}) = \sum_{n} \frac{1}{2} \left(t^{(n)} - \boldsymbol{\omega}^T \overline{\boldsymbol{x}^{(n)}} \right)^2$ (1)

To minimize f, differentiate it by ω and find the ω_0 which makes the derivative zero. To make expression simple, I used the Einstein notation.

$$\begin{split} \frac{\partial f}{\partial \omega_j} &= -(t^{(n)} - \boldsymbol{\omega}^T \overline{\boldsymbol{x}^{(n)}}) \cdot \frac{\partial}{\partial \omega_j} \boldsymbol{\omega}^T \bar{\boldsymbol{x}}^{(n)} \\ &= -(t^{(n)} - \boldsymbol{\omega}^T \overline{\boldsymbol{x}^{(n)}}) x_j^{(n)} \\ &= 0 \end{split}$$

By enumerating the $\frac{\partial f}{\partial \omega_i}$ horizontally, one can get $\frac{\partial f}{\partial \omega}$.

$$\sum_{n} t^{(n)} \begin{pmatrix} x_1^{(n)} \\ \vdots \\ x_M^{(n)} \end{pmatrix}^T = \sum_{n} \begin{pmatrix} \boldsymbol{\omega}^T \overline{\boldsymbol{x}^{(n)}} x_1^{(n)} \\ \vdots \\ \boldsymbol{\omega}^T \overline{\boldsymbol{x}^{(n)}} x_M^{(n)} \end{pmatrix}^T$$
(2)

The left hand side is simply $\sum_n t^{(n)} \overline{\boldsymbol{x}^{(n)}}^T$. From the linearity of vector summation rule, the right hand side is $\left(\left(\sum_n \overline{\boldsymbol{x}^{(n)}} \cdot \overline{\boldsymbol{x}^{(n)}}^T\right) \boldsymbol{\omega}\right)^T$. By taking transpose to both sides, one can get the following equation.

$$\left[\sum_{n} \overline{\boldsymbol{x}^{(n)}} \cdot \overline{\boldsymbol{x}^{(n)}}^{T}\right] \boldsymbol{\omega} = \sum_{n} t^{(n)} \overline{\boldsymbol{x}^{(n)}}$$
(3)

Therefore, $\mathbf{A} = \sum_n \overline{\mathbf{x}^{(n)}} \cdot \overline{\mathbf{x}^{(n)}}^T$ and $\mathbf{b} = \sum_n t^{(n)} \overline{\mathbf{x}^{(n)}}$

1.b

$$\overline{\boldsymbol{x}^{(1)}} = (1,0)^T, t^{(1)} = 1. \ \overline{\boldsymbol{x}^{(2)}} = (1,\epsilon)^T, t^{(2)} = 1. \ \boldsymbol{A} = \overline{\boldsymbol{x}^{(1)}} \cdot \overline{\boldsymbol{x}^{(1)}}^T + \overline{\boldsymbol{x}^{(1)}} \cdot \overline{\boldsymbol{x}^{(2)}}^T = \begin{pmatrix} 2 & \epsilon \\ \epsilon & \epsilon^2 \end{pmatrix}$$
$$\boldsymbol{b} = \overline{\boldsymbol{x}^{(1)}} + \overline{\boldsymbol{x}^{(2)}} = (2,\epsilon)^T. \text{ Since } \boldsymbol{A} \text{ is invertible(determinant is nonzero.)},$$

$$\boldsymbol{\omega} = \boldsymbol{A}^{-1}\boldsymbol{b} \tag{4}$$

$$= \frac{1}{\epsilon^2} \begin{pmatrix} \epsilon^2 & -\epsilon \\ -\epsilon & 2 \end{pmatrix} \begin{pmatrix} 2 \\ \epsilon \end{pmatrix} \tag{5}$$

$$= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{6}$$

1.c

 \boldsymbol{A} is same to the above one. $\boldsymbol{b} = (1+\epsilon) \cdot \overline{\boldsymbol{x}^{(1)}} + \overline{\boldsymbol{x}^{(2)}} = (2+\epsilon,\epsilon)^T$

$$\boldsymbol{\omega} = \boldsymbol{A}^{-1}\boldsymbol{b} \tag{7}$$

$$= \frac{1}{\epsilon^2} \begin{pmatrix} \epsilon^2 & -\epsilon \\ -\epsilon & 2 \end{pmatrix} \begin{pmatrix} 2+\epsilon \\ \epsilon \end{pmatrix} \tag{8}$$

$$= \begin{pmatrix} 1+\epsilon\\-1 \end{pmatrix} \tag{9}$$

1.d

 $\boldsymbol{\omega}_b = (1,0)^T, \boldsymbol{\omega}_c = (1.1,-1)^T$. The difference of $\Delta \boldsymbol{\omega} = \boldsymbol{\omega}_c - \boldsymbol{\omega}_b = (\epsilon,-1)^T = (0.1,-1)^T$

2 Linear Regression with Regularization

2.a

Claim 1: A is positive semi-definite. proof

 $m{A}$ is trivially symmetry matrix. $\forall m{v} \in \mathbb{R}^n, m{v}^T m{A} m{v} = \sum_n m{v}^T \overline{m{x}^{(n)}} \cdot \overline{m{x}^{(n)}}^T m{v} = \sum_n \|m{v}^T \overline{m{x}^{(n)}}\|^2 \ge 0.$

Claim 2: $Ax = \lambda x \iff A^{-1}x = \lambda^{-1}x$ where $\lambda \neq 0$ and A is invertible. proof

 $Ax = \lambda x \iff A^{-1}Ax = \lambda A^{-1}x \iff \lambda^{-1}x = A^{-1}x.$

Let S(A) be the set of all eigenvalues of A.

$$S(\mathbf{A}) \equiv \{\lambda_i | \text{for some } \mathbf{x} \in \mathbb{R}, \ \mathbf{A}\mathbf{x} = \lambda_i \mathbf{x} \}$$
 (10)

 $\forall \tilde{\lambda} \in S(\boldsymbol{A} + \lambda \boldsymbol{I}) \text{ s.t. } (\boldsymbol{A} + \lambda I)\boldsymbol{x} = \tilde{\lambda}\boldsymbol{x}.$

By multiplying \mathbf{x}^T , \mathbf{x}^T $(\mathbf{A} + \lambda \mathbf{I})\mathbf{x} = \mathbf{x}^T \mathbf{A} \mathbf{x} + \lambda = \tilde{\lambda} \ge \lambda$. (: \mathbf{A} is positive semi-definite.)

This implies that $\min(S(\boldsymbol{A} + \lambda \boldsymbol{I})) \geq \lambda$. Equivalently, due to the **Claim 2**, this also means that $\max(S((\boldsymbol{A} + \lambda I)^{-1})) \leq \lambda^{-1}$. By noticing that $\max(S((\boldsymbol{A} + \lambda I)^{-1})) = \rho((\boldsymbol{A} + \lambda I)^{-1})$, the proof is done. Note that for the equality, $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{0}$ must have nontrivial solution.

2.b

For both problems, the $\mathbf{A} + \lambda \mathbf{I}$ is following.

$$\mathbf{A} + \lambda \mathbf{I} = \begin{pmatrix} 2 + \lambda & \epsilon \\ \epsilon & \epsilon^2 + \lambda \end{pmatrix} \tag{11}$$

Since (11) is invertible, one can get ω_b, ω_c .

$$\omega_{b} = \frac{1}{(1+\lambda)\epsilon^{2} + \lambda(\lambda+2)} \cdot \begin{pmatrix} \epsilon^{2} + \lambda & -\epsilon \\ -\epsilon & 2 + \lambda \end{pmatrix} \cdot \begin{pmatrix} 2 \\ \epsilon \end{pmatrix}$$
$$= \frac{1}{(1+\lambda)\epsilon^{2} + \lambda(\lambda+2)} \cdot \begin{pmatrix} \epsilon^{2} + 2\lambda \\ \epsilon \lambda \end{pmatrix}$$
$$= \begin{pmatrix} 0.973 \\ 0.044 \end{pmatrix}$$

$$\omega_{c} = \frac{1}{(1+\lambda)\epsilon^{2} + \lambda(\lambda+2)} \cdot \begin{pmatrix} \epsilon^{2} + \lambda & -\epsilon \\ -\epsilon & 2 + \lambda \end{pmatrix} \cdot \begin{pmatrix} 2 + \epsilon \\ \epsilon \end{pmatrix}$$

$$= \frac{1}{(1+\lambda)\epsilon^{2} + \lambda(\lambda+2)} \cdot \begin{pmatrix} \epsilon^{3} + \epsilon^{2} + \lambda\epsilon + 2\lambda \\ -\epsilon^{2} + \lambda\epsilon \end{pmatrix}$$

$$= \begin{pmatrix} 1.026 \\ -0.044 \end{pmatrix}$$

Furthemore, $\Delta \boldsymbol{\omega} = \boldsymbol{\omega_c} - \boldsymbol{\omega_b}$ can be obtained.

$$\Delta \omega = \frac{1}{(1+\lambda)\epsilon^2 + \lambda(\lambda+2)} \begin{pmatrix} \epsilon^3 + \lambda \epsilon \\ -\epsilon^2 \end{pmatrix} = \begin{pmatrix} 0.0531 \\ -0.088 \end{pmatrix}$$
 (12)

2.c

One can notice that $\Delta \omega$ with regularization is much smaller than $\Delta \omega$ without regularization. This implies that regularization makes the parameters less variable with respect to small noise in input data. This can be verified by the following figure.

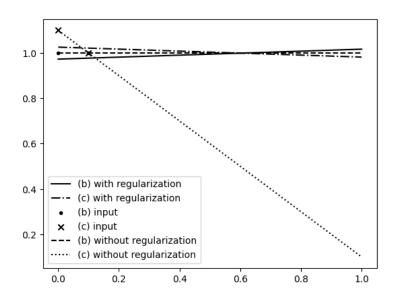


Figure 1: The linear regression result of (b) and (c)

3 LR with Regularization: A Probabilistic Perspective

$$\Pr(\boldsymbol{\omega}) = \mathcal{N}(\boldsymbol{0}, \frac{1}{\lambda} \boldsymbol{I})$$

$$= \frac{\lambda^{N/2}}{2\pi^{N/2}} \exp\left(-\frac{1}{2} \boldsymbol{\omega}^T \lambda \boldsymbol{\omega}\right)$$

$$t^{(i)} = \boldsymbol{\omega}^T \boldsymbol{x}^{(i)} + \epsilon^{(i)} \quad \& \quad \Pr(\epsilon^{(i)}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\epsilon^{(i)^2}/2\sigma^2\right)$$

$$\Rightarrow \Pr\left(t^{(i)} \mid \boldsymbol{\omega}, \boldsymbol{x}^{(i)}\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-(t^{(i)} - \boldsymbol{\omega}^T \boldsymbol{x}^{(i)})^2/2\sigma^2\right)$$

$$\begin{aligned} \Pr(\boldsymbol{t} \mid \boldsymbol{\omega}^T \boldsymbol{x}^{(i)}) &= \prod_{i=1}^N \Pr(t^{(i)} \mid \boldsymbol{\omega}^T, \boldsymbol{x}) \\ &= \frac{1}{2\pi^{N/2} \sigma^N} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^N (t^{(i)} - \boldsymbol{\omega}^T \boldsymbol{x}^{(i)})^2\right) \end{aligned}$$

From the discussion above, the posterior probability is following.

$$\Pr(\boldsymbol{\omega} \mid \boldsymbol{x}, \boldsymbol{t}) \propto \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^{N} (t^{(i)} - \boldsymbol{\omega}^T \boldsymbol{x}^{(i)})^2 - \frac{\lambda}{2} \boldsymbol{\omega}^T \boldsymbol{\omega}\right)$$
(13)

Minimizing (13) is equivalent to minimizing its logarithm.

$$\log \left(\Pr(\boldsymbol{\omega} \mid \boldsymbol{x}, \boldsymbol{t}) \right) \propto -\frac{1}{2\sigma^2} \sum_{i=1}^{N} \left(t^{(i)} - \boldsymbol{\omega}^T \boldsymbol{x}^{(i)} \right)^2 - \frac{\lambda}{2} \boldsymbol{\omega}^T \boldsymbol{\omega}$$
 (14)

One can see from (14) that maximizing logarithm of posterior is equivalent to minimizing the target function of linear regression with L2 regularization.

4 Logistic Regression

$$\log L(\boldsymbol{\omega}) = -\sum_{i} \left[t^{(i)} \log \left(\frac{1}{1 + e^{-\boldsymbol{\omega}^{T} \boldsymbol{x}^{(i)}}} \right) + (1 - t^{(i)}) \log \left(\frac{e^{-\boldsymbol{\omega}^{T} \boldsymbol{x}^{(i)}}}{1 + e^{\boldsymbol{\omega}^{T} \boldsymbol{x}^{(i)}}} \right) \right]$$
(15)

To minimize (15), one can differentiate it about ω to find the ω_0 that makes the derivative zero. By denoting $P^{(n)} = (1 + e^{\omega^T \boldsymbol{x}^{(n)}})^{-1} = \sigma(\boldsymbol{\omega}^T \boldsymbol{x}^{(n)})$

$$\begin{split} \frac{\partial}{\partial \omega_{i}} \log L(\boldsymbol{\omega}) &= -\sum_{n} \frac{\partial}{\partial \omega_{i}} \left[t^{(n)} \log P^{(n)} + (1 - t^{(n)}) \log (1 - P^{(n)}) \right] \\ &= -\sum_{n} \left[\frac{t^{(n)}}{P^{(n)}} - \frac{1 - t^{(n)}}{1 - P^{(n)}} \right] \cdot \frac{\partial P^{(n)}}{\partial \omega_{i}} \\ &= -\sum_{n} \left[t^{(n)} / P^{(n)} - (1 - t^{(n)}) / P^{(n)} \right] \cdot P^{(n)} (1 - P^{(n)}) \cdot \frac{\partial}{\partial \omega_{i}} \boldsymbol{\omega}^{T} \boldsymbol{x}^{(n)} \\ &= -\sum_{n} \left[t^{(n)} (1 - P^{(n)}) - (1 - t^{(n)}) P^{(n)} \right] x_{i}^{(n)} \\ &= -\sum_{n} (t^{(n)} - P^{(n)}) x_{i}^{(n)} = 0 \end{split}$$

Note that $d\sigma(x)/dx = \sigma(x)(1-\sigma(x))$. The result of the last equation above can be written in vector form.

$$\sum_{n} (t^{(n)} - \sigma(\boldsymbol{\omega}^{T} \boldsymbol{x})) \boldsymbol{x}^{(n)} = 0$$
(16)

The equation (16) can be written as following equation.

$$\sum_{n} t^{(n)} \boldsymbol{x}^{(n)} = \sum_{n} \sigma(\boldsymbol{\omega}^{T} \boldsymbol{x}) \boldsymbol{x}^{(n)}$$
(17)

Unfortunately, since sigmoid function σ is non-linear function, the equation (17) is non-linear equation that doesn't have the closed form of solution in general.