

# [EECS 545] HW1

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## 1. Derivation and Proof

(a) We are given the loss function

$$L = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - h(x^{(i)}))^2,$$

where  $h(x) = w_1x + w_0$ . To find optimal parameters, we want to constrain  $\nabla L = 0$ .

First, we want to find optimal  $w_0$ .

$$\begin{aligned} \frac{\partial L}{\partial w_0} &= \frac{\partial}{\partial w_0} \left[ \frac{1}{2} \sum_{i=1}^N (y^{(i)} - w_1x^{(i)} - w_0)^2 \right] \\ &= - \sum_{i=1}^N (y^{(i)} - w_1x^{(i)} - w_0) = 0 \\ \implies \sum_{i=1}^N y^{(i)} - w_1 \sum_{i=1}^N x^{(i)} - Nw_0 &= 0 \\ \implies Nw_0 &= \sum_{i=1}^N y^{(i)} - w_1 \sum_{i=1}^N x^{(i)} \\ \implies w_0 &= \frac{1}{N} \sum_{i=1}^N y^{(i)} - w_1 \cdot \frac{1}{N} \sum_{i=1}^N x^{(i)} \end{aligned}$$

Therefore,  $w_0 = \bar{Y} - w_1\bar{X}$ .

Then, we find optimal  $w_1$ . We have

$$\begin{aligned} \frac{\partial L}{\partial w_1} &= \frac{\partial}{\partial w_1} \left[ \frac{1}{2} \sum_{i=1}^N (y^{(i)} - w_1x^{(i)} - w_0)^2 \right] \\ &= - \sum_{i=1}^N x^{(i)} (y^{(i)} - w_1x^{(i)} - w_0) = 0. \\ \implies \sum_{i=1}^N x^{(i)} y^{(i)} - w_1 \sum_{i=1}^N (x^{(i)})^2 - w_0 \sum_{i=1}^N x^{(i)} &= 0 \end{aligned}$$

Substituting  $w_0 = \bar{Y} - w_1 \bar{X}$ , we have

$$\begin{aligned}
& \sum_{i=1}^N x^{(i)} y^{(i)} - w_1 \sum_{i=1}^N (x^{(i)})^2 - (\bar{Y} - w_1 \bar{X}) \sum_{i=1}^N x^{(i)} = 0 \\
\Rightarrow & \sum_{i=1}^N x^{(i)} y^{(i)} - w_1 \sum_{i=1}^N (x^{(i)})^2 - \bar{Y} \cdot N \bar{X} + w_1 \bar{X} \cdot N \bar{X} = 0 \\
& \Rightarrow \sum_{i=1}^N x^{(i)} y^{(i)} - N \bar{Y} \bar{X} = w_1 \left[ \sum_{i=1}^N (x^{(i)})^2 - N \bar{X}^2 \right] \\
& \Rightarrow w_1 = \frac{\sum_{i=1}^N x^{(i)} y^{(i)} - N \bar{Y} \bar{X}}{\sum_{i=1}^N (x^{(i)})^2 - N \bar{X}^2} \\
& \Rightarrow w_1 = \frac{\frac{1}{N} \sum_{i=1}^N x^{(i)} y^{(i)} - \bar{Y} \bar{X}}{\frac{1}{N} \sum_{i=1}^N (x^{(i)})^2 - \bar{X}^2}.
\end{aligned}$$

(b)

i. Proof that a real symmetric  $d \times d$  matrix  $\mathbf{A}$  is positive definite if and only if all eigenvalues  $\lambda_i > 0$ .

( $\Rightarrow$ ) Suppose  $\mathbf{A}$  is positive definite. For each eigenvector  $\mathbf{u}_i$  with eigenvalue  $\lambda_i$ , we have  $\mathbf{A}\mathbf{u}_i = \lambda_i \mathbf{u}_i$ . Since eigenvectors are nonzero, we have that

$$\mathbf{u}_i^\top \mathbf{A} \mathbf{u}_i = \mathbf{u}_i^\top (\lambda_i \mathbf{u}_i) = \lambda_i \|\mathbf{u}_i\|^2 > 0.$$

As  $\|\mathbf{u}_i\|^2 > 0$ ,  $\lambda_i > 0$  for all  $i$ .

( $\Leftarrow$ ) Assume all  $\lambda_i > 0$ . For any nonzero  $\mathbf{z} \in \mathbb{R}^d$ , we have

$$\mathbf{z}^\top \mathbf{A} \mathbf{z} = \mathbf{z}^\top \mathbf{U} \mathbf{\Lambda} \mathbf{U}^\top \mathbf{z} = (\mathbf{U}^\top \mathbf{z})^\top \mathbf{\Lambda} (\mathbf{U}^\top \mathbf{z}).$$

Let  $\mathbf{c} = \mathbf{U}^\top \mathbf{z} = [c_1, c_2, \dots, c_d]^\top$ . Since  $\mathbf{U}$  is orthogonal,  $\mathbf{c} \neq \mathbf{0}$  iff  $\mathbf{z} \neq \mathbf{0}$ . Thus

$$\mathbf{z}^\top \mathbf{A} \mathbf{z} = \sum_{i=1}^d \lambda_i c_i^2 > 0$$

since  $\lambda_i > 0$  for all  $i$  and at least one  $c_i \neq 0$ .

ii. Let  $\mathbf{u}_i$  be an eigenvector of  $\mathbf{\Phi}^\top \mathbf{\Phi}$  with eigenvalue  $\lambda_i$ ,

$$(\mathbf{\Phi}^\top \mathbf{\Phi} + \beta \mathbf{I}) \mathbf{u}_i = \mathbf{\Phi}^\top \mathbf{\Phi} \mathbf{u}_i + \beta \mathbf{u}_i = \lambda_i \mathbf{u}_i + \beta \mathbf{u}_i = (\lambda_i + \beta) \mathbf{u}_i.$$

Therefore,  $\mathbf{u}_i$  remains an eigenvector of  $\mathbf{\Phi}^\top \mathbf{\Phi} + \beta \mathbf{I}$  with eigenvalue  $\lambda_i + \beta$ .

Since  $\mathbf{\Phi}^\top \mathbf{\Phi}$  is positive semi-definite, all  $\lambda_i \geq 0$ . Therefore, the eigenvalues of  $\mathbf{\Phi}^\top \mathbf{\Phi} + \beta \mathbf{I}$  are  $\lambda_i + \beta > 0$  for any  $\beta > 0$ .

From property proved in part i, this implies  $\mathbf{\Phi}^\top \mathbf{\Phi} + \beta \mathbf{I}$  is positive definite.

(c) We show that maximizing the log-likelihood is equivalent to minimizing the given loss function.

$$\begin{aligned}
\log P(y^{(n)} | \mathbf{x}^{(n)}) &= \mathbb{I}(y^{(n)} = 1) \log P(y^{(n)} = 1 | \mathbf{x}^{(n)}) \\
&\quad + \mathbb{I}(y^{(n)} = -1) \log P(y^{(n)} = -1 | \mathbf{x}^{(n)}).
\end{aligned}$$

Since probabilities must sum to 1, we have

$$P(y = -1 | \mathbf{x}) = 1 - P(y = 1 | \mathbf{x}) = 1 - \frac{1}{1 + \exp(-\mathbf{w}^\top \phi(\mathbf{x}))} = \frac{1}{1 + \exp(\mathbf{w}^\top \phi(\mathbf{x}))}$$

We can express  $P(y | \mathbf{x}) = \frac{1}{1 + \exp(-y \mathbf{w}^\top \phi(\mathbf{x}))}$  for  $y \in \{-1, +1\}$

We have

$$\begin{aligned} \log P(y^{(n)}|\mathbf{x}^{(n)}) &= -\log(1 + \exp(-y^{(n)}\mathbf{w}^\top \phi(\mathbf{x}^{(n)}))) \\ \implies \sum_{n=1}^N \log P(y^{(n)}|\mathbf{x}^{(n)}) &= -\sum_{n=1}^N \log(1 + \exp(-y^{(n)}\mathbf{w}^\top \phi(\mathbf{x}^{(n)}))) \end{aligned}$$

So maximizing the log-likelihood of the logistic regression is equivalent to minimizing the loss function

$$\sum_{n=1}^N \log(1 + \exp(-y^{(n)}\mathbf{w}^\top \phi(\mathbf{x}^{(n)})))$$

## 2.1 GD and SGD

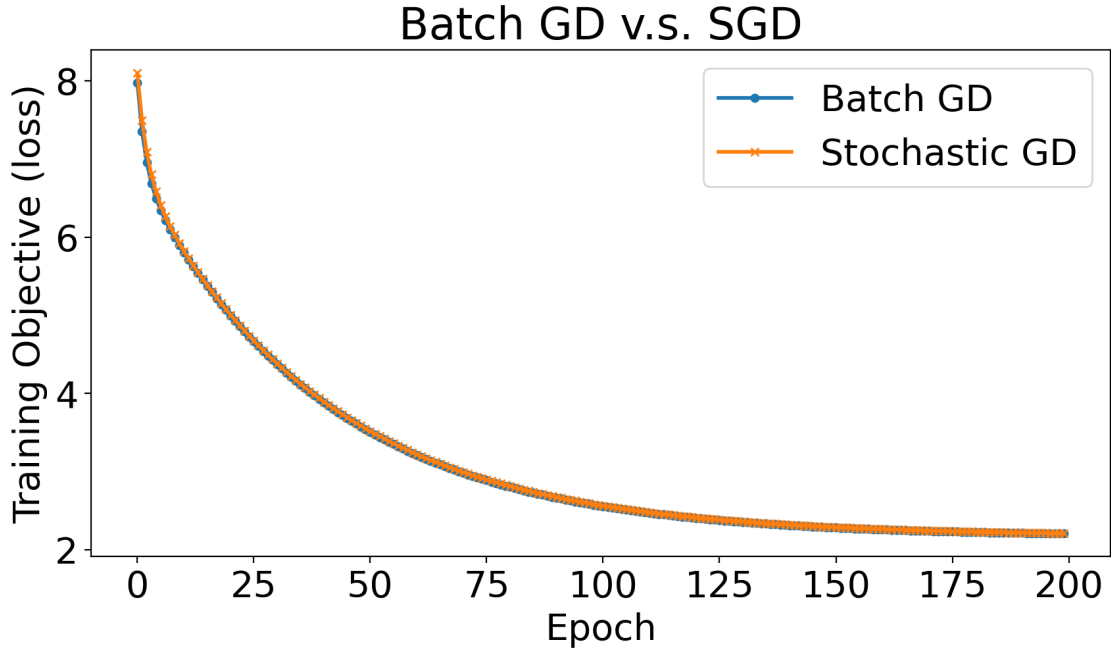


Figure 1: Training objective (loss) versus epoch for Batch GD and SGD.

From the printed runtimes, Batch GD is faster (about 0.00 s vs. 0.02 s for SGD). Meanwhile, SGD achieves the lower test objective  $E(\mathbf{w}_{\text{test}})$  (about 0.1340 vs. 0.1351 for Batch GD).

## 2.2 Over-fitting study

(b) The RMS error curves (training and test) for polynomial feature dimension  $M \in \{1, \dots, 10\}$  are shown below.

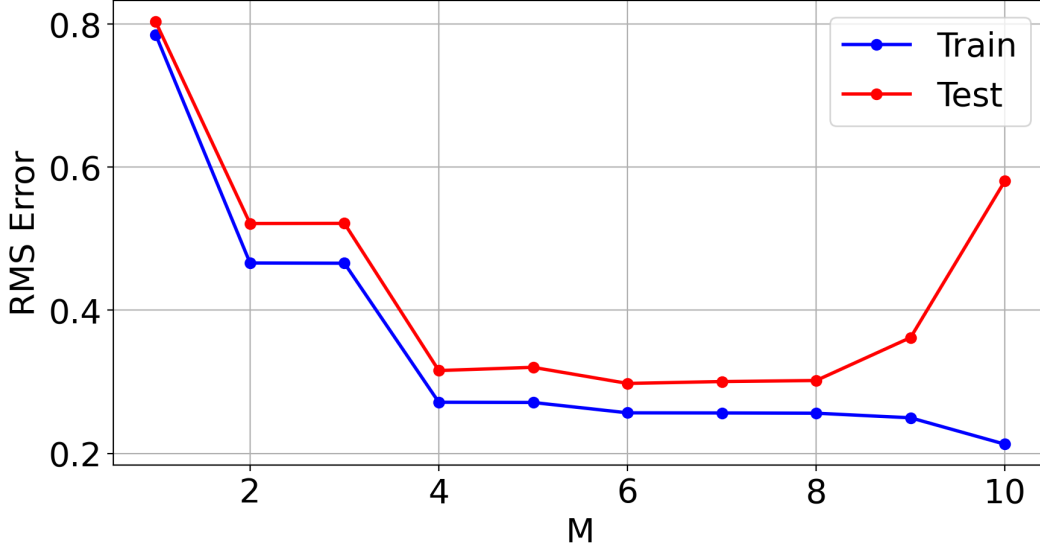


Figure 2: RMS error versus number of features  $M$  on training and test sets

(c) From the plot, the training RMS generally decreases as  $M$  increases, while the test RMS decreases at first and then increases for larger  $M$ . The smallest test RMS is achieved around  $M = 6$  while the training RMS is also relatively small, so a polynomial with degree of 6 would best fit the data. For small  $M$  ( $M = 1, 2$ ), both training and test RMS are relatively high which shows underfitting, whereas for large  $M$  (10) the training RMS becomes very small but the test RMS increases, which is evident to overfitting.

## 2.3 Regularization (Ridge Regression)

(b) The training and test RMS errors as a function of the regularization factor  $\lambda$  are shown below.

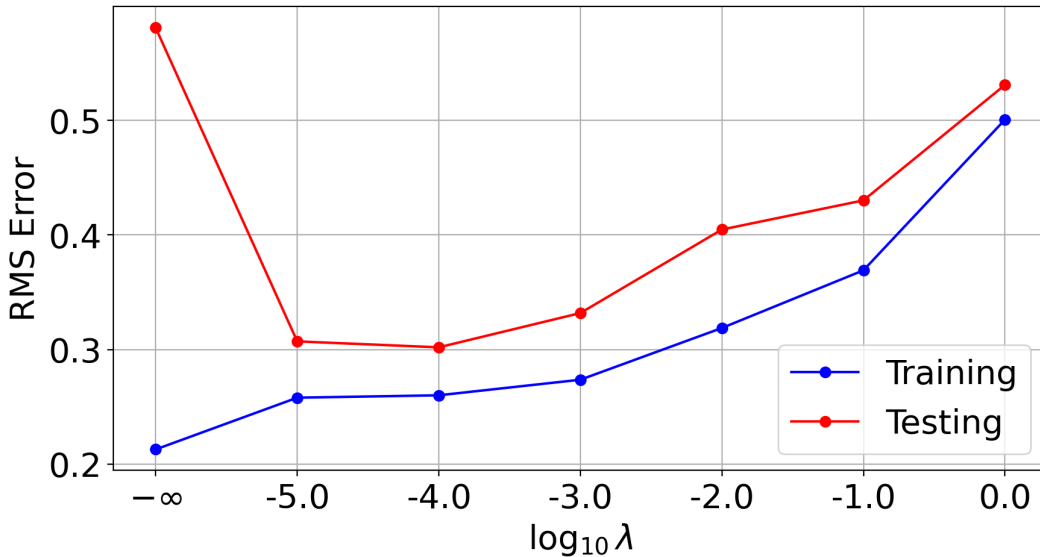


Figure 3: RMS error versus regularization factor  $\lambda$  (ridge regression) on training and test sets

(c) From the plot, the training RMS is slightly lower at  $\log_{10}(\lambda) = -5$  than that of  $\log_{10}(\lambda) = -4$ , but the test RMS achieves its minimum at  $\log_{10}(\lambda) = -4$ . Hence,  $\lambda = 10^{-4}$  stands out as the best choice for the

degree-9 polynomial.

### 3. Locally weighted linear regression

Consider the objective

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N r^{(i)} (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)})^2$$

(a) Let  $\mathbf{X} \in \mathbb{R}^{D \times N}$  be the data matrix whose  $i$ -th column is  $\mathbf{x}^{(i)}$ , and let  $\mathbf{y} \in \mathbb{R}^{N \times 1}$  be the vector whose  $i$ -th entry is  $y^{(i)}$ . We define the diagonal matrix

$$\mathbf{R} \triangleq \frac{1}{2} \text{diag}(r^{(1)}, \dots, r^{(N)}) \in \mathbb{R}^{N \times N}$$

Then  $\mathbf{w}^\top \mathbf{X} - \mathbf{y}^\top$  is a  $1 \times N$  row vector whose  $i$ -th entry equals  $\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}$ , and hence

$$E_D(\mathbf{w}) = (\mathbf{w}^\top \mathbf{X} - \mathbf{y}^\top) \mathbf{R} (\mathbf{w}^\top \mathbf{X} - \mathbf{y}^\top)^\top$$

(b) Given

$$E_D(\mathbf{w}) = (\mathbf{X}^\top \mathbf{w} - \mathbf{y})^\top \mathbf{R} (\mathbf{X}^\top \mathbf{w} - \mathbf{y}),$$

and the fact that  $\mathbf{R}$  is symmetric, we have

$$\nabla_{\mathbf{w}} E_D(\mathbf{w}) = 2\mathbf{X}\mathbf{R}(\mathbf{X}^\top \mathbf{w} - \mathbf{y})$$

Setting the gradient to zero gives the weighted normal equation

$$\mathbf{X}\mathbf{R}\mathbf{X}^\top \mathbf{w} = \mathbf{X}\mathbf{R}\mathbf{y}$$

Assuming  $\mathbf{X}\mathbf{R}\mathbf{X}^\top$  is invertible, then the closed form solution is

$$\mathbf{w}^* = (\mathbf{X}\mathbf{R}\mathbf{X}^\top)^{-1} \mathbf{X}\mathbf{R}\mathbf{y}.$$

(c) The conditional likelihood for each example is

$$p(y^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}) = \frac{1}{\sqrt{2\pi} \sigma^{(i)}} \exp\left(-\frac{(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)})^2}{2(\sigma^{(i)})^2}\right)$$

Assuming the  $N$  examples are independent, the likelihood of the full dataset is given by

$$\mathcal{L}(\mathbf{w}) = \prod_{i=1}^N p(y^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}).$$

Hence,

$$\begin{aligned} -\log \mathcal{L}(\mathbf{w}) &= -\sum_{i=1}^N \log p(y^{(i)} \mid \mathbf{x}^{(i)}; \mathbf{w}) \\ &= \sum_{i=1}^N \left[ \log(\sqrt{2\pi} \sigma^{(i)}) + \frac{(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)})^2}{2(\sigma^{(i)})^2} \right] \\ &= \underbrace{\sum_{i=1}^N \log(\sqrt{2\pi} \sigma^{(i)})}_{\text{constant w.r.t. } \mathbf{w}} + \sum_{i=1}^N \frac{(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)})^2}{2(\sigma^{(i)})^2} \end{aligned}$$

Therefore, dropping the constant term (independent of  $\mathbf{w}$ ), maximizing the likelihood is equivalent to minimizing

$$\sum_{i=1}^N \frac{(y^{(i)} - \mathbf{w}^\top \mathbf{x}^{(i)})^2}{2(\sigma^{(i)})^2} = \frac{1}{2} \sum_{i=1}^N r^{(i)} (\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)})^2,$$

where

$$r^{(i)} = \frac{1}{(\sigma^{(i)})^2}$$

(d)  
ii.

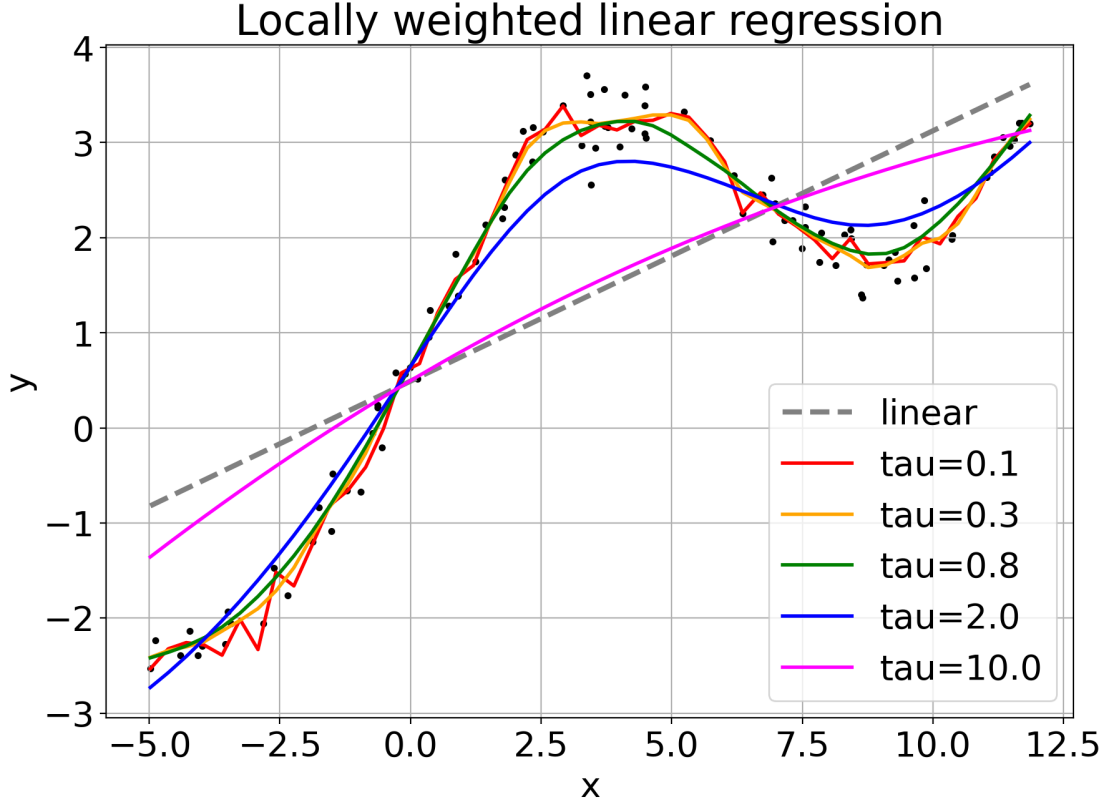


Figure 4: Locally weighted linear regression fits for different bandwidths  $\tau$

**iii.** When  $\tau$  is very small, the weights concentrate on points extremely close to the query  $x$ , so the fit has high variance and can overfit. When  $\tau$  is very large, however, the weights become nearly uniform, so the fit approaches ordinary least squares and becomes overly smooth, which corresponds to high bias and can underfit.