

Popular Machine Learning Methods: Idea, Practice and Math

Part 2, Chapter 2, Section 2:
Training Shallow Models

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Reference

- This set of slides was largely built on the following 7 wonderful books and a wide range of fabulous papers:
 - HML Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow (2nd Edition)
 - PML Python Machine Learning (3rd Edition)
 - ESL The Elements of Statistical Learning (2nd Edition)
 - PRML Pattern Recognition and Machine Learning
 - NND Neural Network Design (2nd Edition)
 - LFD Learning From Data
 - RL Reinforcement Learning: An Introduction (2nd Edition)
- For most materials covered in the slides, we will specify their corresponding books and papers for further reference.

Code Example & Case Study

- See related code example in github repository:
[/p2_c2_s2_training_shallow_models/code_example](#)
- See related case study of Kaggle Competition in github repository:
[/p2_c2_s2_training_shallow_models/case_study](#)

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Learning Objectives: Expectation

- It is expected to understand
 - the idea of Bias and Variance
 - the idea of Expected Test Error and its decomposition
 - the idea of Bias-Variance Tradeoff
 - the idea of Underfitting and Overfitting
 - the idea of Learning Curve
 - the takeaway of signs of underfitting and overfitting
 - the good practice for handling underfitting and overfitting
 - the idea of Regularization
 - the idea and implementation of popular regularization methods, including:
 - Lasso (a.k.a., L1 regularization)
 - Ridge (a.k.a., L2 regularization)
 - Elastic net
 - the good practice for using lasso / ridge / elastic net
 - the idea of Hyperparameter Tuning
 - the idea and usage of sklearn hyperparameter tuning tools, including:
 - GridSearchCV
 - RandomizedSearchCV
 - the good practice for using GridSearchCV and RandomizedSearchCV
 - the idea and implementation of model selection

Learning Objectives: Recommendation

- It is recommended to understand
 - the math of the decomposition of expected test error
 - the math of popular regularization methods, including:
 - lasso
 - ridge
 - elastic net

Kaggle Competition: Predicting House Price



Figure 1: Kaggle competition: predicting house price. Picture courtesy of Kaggle.

- House Prices (Advanced Regression Techniques) dataset:

- features: 79 explanatory variables describing (almost) every aspect of residential homes in Ames, Iowa
- target: the sale price of homes

Motivation

- In [/p2_c2_s1_linear_regression](#) we discussed two methods for training linear regression:
 - the normal equation, which solves the optimal solution analytically
 - gradient descent, which estimates the optimal solution iteratively
- While the two methods are different in many ways, there is one thing in common: they both train linear regression by minimizing the training error (e.g., mean squared error).
- Unfortunately, if we only cared about minimizing the training error, we might learn a model that:
 - on the one hand, has low training error (i.e., performs well on training data)
 - but on the other hand, has high test error (i.e., generalizes poorly on test data)
- The *Learning Theory* tells us:
 - why this is the case
 - and more importantly, what we can do to address this problem

Bias

- In learning theory, *Bias* measures the average difference between the predicted target value and real target value:

$$\text{Bias}(\hat{\mathbf{y}}, \mathbf{y}) = E[\hat{\mathbf{y}} - \mathbf{y}] = \frac{\sum_{i=1}^m (\hat{y}^i - y^i)}{m}. \quad (1)$$

Here:

- $\hat{\mathbf{y}}$ is the predicted target vector
- \mathbf{y} is the real target vector
- $E[\hat{\mathbf{y}} - \mathbf{y}]$ is the average of $\hat{\mathbf{y}} - \mathbf{y}$
- m is the number of samples in the data
- \hat{y}^i is the predicted target value of sample i
- y^i is the real target value of sample i

Variance

- Unlike bias that captures the difference between the predicted target value and real target value, *Variance* measures the difference between the predicted value themselves.
- More formally, variance is the average squared difference between the predicted target value and their mean:

$$\text{Var}(\hat{\mathbf{y}}) = E [(\hat{\mathbf{y}} - E[\hat{\mathbf{y}}])^2] = \frac{\sum_{i=1}^m (\hat{y}^i - \frac{\sum_{i=1}^m \hat{y}^i}{m})^2}{m}. \quad (2)$$

Here:

- $\hat{\mathbf{y}}$ is the predicted target vector
- $E[\hat{\mathbf{y}}]$ is the mean of the predicted target vector
- $E[(\hat{\mathbf{y}} - E[\hat{\mathbf{y}}])^2]$ is the average of $(\hat{\mathbf{y}} - E[\hat{\mathbf{y}}])^2$
- m is the number of samples in the data
- \hat{y}^i is the predicted target value of sample i

Expected Test Error

- Given a test sample, $[\mathbf{x} \ y]$, we:
 - draw m training sets, $[\mathbf{X}_1 \ y_1], \dots, [\mathbf{X}_m \ y_m]$, where the test sample and each training set come from the same distribution
 - train the same model H on each training set and obtain m models, H_1, \dots, H_m
- **Q:** What is the expected test error (across the m models)?

Decomposition of Expected Test Error

- **A:** It turns out that we can decompose the expected test error (across the m models) into the sum of squared bias and variance:

$$\underbrace{E[(\hat{\mathbf{y}} - \mathbf{y})^2]}_{\text{Expected test error}} = \underbrace{(E[\hat{\mathbf{y}} - \mathbf{y}])^2}_{\text{Bias}^2} + \underbrace{E[(\hat{\mathbf{y}} - E[\hat{\mathbf{y}}])^2]}_{\text{Variance}}. \quad (3)$$

Here:

- $\hat{\mathbf{y}} / \mathbf{y}$ is a $m \times 1$ predicted / real target vector across the m models:

$$\hat{\mathbf{y}} = [\hat{y}^1 \quad \dots \quad \hat{y}^m]^\top \quad \text{and} \quad \mathbf{y} = [y^1 \quad \dots \quad y^m]^\top, \quad (4)$$

where \hat{y}^i is predicted by model H_i and $y^i = y$ (with y being the target value in the test sample)

- bias is given in eq. (1)

$$\text{Bias}(\hat{\mathbf{y}}, \mathbf{y}) = E[\hat{\mathbf{y}} - \mathbf{y}] = \frac{\sum_{i=1}^m (\hat{y}^i - y^i)}{m} \quad (1)$$

- variance is given in eq. (2)

$$\text{Var}(\hat{\mathbf{y}}) = E[(\hat{\mathbf{y}} - E[\hat{\mathbf{y}}])^2] = \frac{\sum_{i=1}^m (y^i - \frac{\sum_{i=1}^m y^i}{m})^2}{m} \quad (2)$$

- See the proof of eq. (3) in Appendix (pages 53 to 55).

Bias-Variance Tradeoff

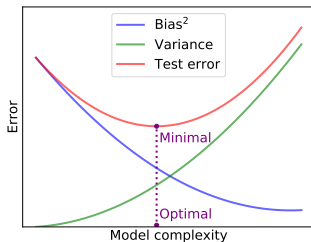


Figure 2: The bias-variance tradeoff.

- Fig. 2 shows the squared bias, variance and test error as a function of model complexity.
- Concretely, when the model complexity goes up
 - the squared bias goes down
 - the variance goes up
 - the test error, which can be decomposed into the sum of squared bias and variance (as shown in eq. (3)), first goes down then goes up
- The above relationship (between the squared bias / variance / test error and model complexity) is called the *Bias-Variance Tradeoff*.

Underfitting VS Overfitting

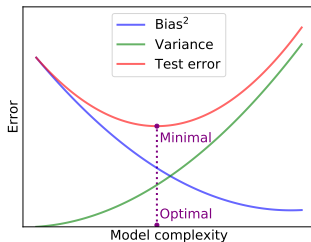


Figure 2: The bias-variance tradeoff.

- Fig. 2 also shows the minimal test error and the corresponding optimal model complexity.
- When model complexity < the optimal complexity, we call this *Underfitting*.
- When model complexity > the optimal complexity, we call this *Overfitting*.
- **Q:** Since the optimal complexity is usually unknown, how can we tell when we are underfitting and when we are overfitting?

Underfitting VS Overfitting

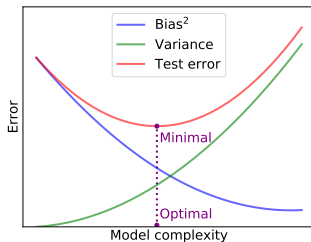


Figure 2: The bias-variance tradeoff.

- Fig. 2 also shows the minimal test error and the corresponding optimal model complexity.
- When model complexity $<$ the optimal complexity, we call this *Underfitting*.
- When model complexity $>$ the optimal complexity, we call this *Overfitting*.
- Q:** Since the optimal complexity is usually unknown, how can we tell when we are underfitting and when we are overfitting?
- A:** We can use the *Learning Curve* to do so.

Learning Curve



Figure 3: Learning Curve showing underfitting (left) and overfitting (right).

- The *Learning Curve* shows the training and validation error as a function of the number of training samples (or iterations).



Takeaway

- The left panel of fig. 3 shows the signs of underfitting:
 - training error is high
 - validation error is close to training error
- The right panel of fig. 3 shows the signs of overfitting:
 - training error is low
 - validation error is much higher than training error

Handling Underfitting and Overfitting: The Idea

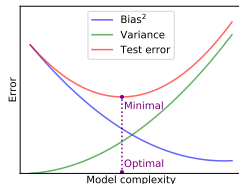


Figure 2: The bias-variance tradeoff.

- Underfitting indicates:
 - model complexity < the optimal complexity
 - we are on the left-hand side of the vertical dashed line in fig. 2
- Overfitting indicates:
 - model complexity > the optimal complexity
 - we are on the right-hand side of the vertical dashed line in fig. 2
- Both underfitting and overfitting result in higher test error (than the minimal).
- To handle underfitting, we should increase model complexity, so that we can significantly lower the squared bias and, in turn, the test error.
- To handle overfitting, we should decrease model complexity, so that we can significantly lower the variance and, in turn, the test error.

Handling Underfitting and Overfitting: The Methods



Good practice

- Methods for handling underfitting:
 - use more complex model + regularization (a.k.a., the *Stretch Pants* approach)
 - boosting (see [/p2_c2_s5_tree_based_models](#))
- Methods for handling overfitting:
 - regularization
 - bagging (see [/p2_c2_s5_tree_based_models](#))
 - (allocate or collect) more data for training

Further Reading

- See a very nice and detailed discussion of *Error Analysis* in this wonderful book by Andrew Ng: [Machine Learning Yearning](#).

Motivation

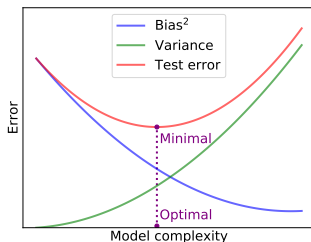


Figure 2: The bias-variance tradeoff.

- The idea of *Regularization* is handling overfitting by lowering model complexity.
- As shown in fig. 2, this allows us to significantly lower the variance and, in turn, lower the test error (i.e., the model will generalize better in reality).

Popular Regularization Methods

- For both shallow and deep learning:
 - Lasso (a.k.a., L1 regularization)
 - Ridge (a.k.a., L2 regularization)
 - Elastic net
 - Early stopping (see [/p2_c2_s5_tree_based_models](#))
- For deep learning only:
 - Batch normalization (see [/p3_c2_s2_training_deep_neural_networks](#))
 - Dropout (see [/p3_c2_s2_training_deep_neural_networks](#))
 - Data augmentation (see [/p3_c2_s2_training_deep_neural_networks](#))
- For most regularization methods, we will use Mini-Batch Gradient Descent (MBGD) as the default for gradient descent, since as discussed in [/p2_c2_s1_linear_regression](#):
 - in theory, MBGD reduces to Batch Gradient Descent (BGD) / Stochastic Gradient Descent (SGD) when the mini-batch contains all the samples / only one sample, so that we can slightly tweak the equations for MBGD (with respect to the mini-batch size) to get the equations for BGD and SGD
 - in practice, MBGD is more popular in deep learning

Lasso, Ridge and Elastic Net: Similarity

- The idea of lasso, ridge and elastic net are very similar: all of them aim to push parameter values toward zero, by adding the parameter values to the loss function.
- We will use linear regression in eq. (5) to show why this will decrease model complexity and variance (and finally the test error):

- Model complexity:
$$\hat{y}^i = b + w_1 x_1^i + \dots + w_n x_n^i. \quad (5)$$

- we can measure the complexity of linear equation as the number of features (i.e., x) in eq. (5)
- based on eq. (5), the more weights (i.e., w) are zero, the fewer features remain in the equation, hence the lower the model complexity

- Variance:

- the variance was given in eq. (2)

$$\text{Var}(\hat{\mathbf{y}}) = E[(\hat{\mathbf{y}} - E[\hat{\mathbf{y}}])^2] = \frac{\sum_{i=1}^m (\hat{y}^i - \frac{\sum_{i=1}^m \hat{y}^i}{m})^2}{m} \quad (2)$$

- by substituting eq. (5) into eq. (2), we have

$$\text{Var}(\hat{\mathbf{y}}) = \frac{\sum_{i=1}^m \left(\sum_{j=1}^n w_j (x_j^i - E[\mathbf{x}_j]) \right)^2}{m} \quad (6)$$

- based on eq. (6), generally the lower the (absolute value of the) weights, the lower the variance

Lasso, Ridge and Elastic Net: Difference

- While lasso, ridge and elastic net all add parameter values to the loss function, they do so in different ways.

- Lasso adds a weighted sum of the absolute value of the weights:

$$\alpha \sum_{j=1}^n |w_j|. \quad (7)$$

- Ridge adds a weighted sum of the squared value of the weights:

$$\frac{\alpha}{2} \sum_{j=1}^n w_j^2. \quad (8)$$

- Elastic net adds a weighted sum of the absolute value of the weights (first item in eq. (9)), and a weighted sum of the squared value of the weights (second item):

$$\alpha\gamma \sum_{j=1}^n |w_j| + \frac{\alpha(1-\gamma)}{2} \sum_{j=1}^n w_j^2. \quad (9)$$

- Here α (where $\alpha \geq 0$) and γ (where $0 \leq \gamma \leq 1$) are the regularization parameters.
- The larger the α , the stronger the regularization, in turn, the smaller the weights.
- The larger the γ , the similar the elastic net to lasso, whereas the smaller the γ , the similar the elastic net to ridge.
- Elastic net reduces to lasso / ridge when γ is 1 / 0.

MBGD + Lasso: Loss

- With the MBGD loss (second item in eq. (10)) and the regularization term of lasso (third item), the loss of MBGD + lasso is the sum of the two:

$$\underbrace{\mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)}_{\text{MBGD + lasso loss}} = \underbrace{\frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2}_{\text{MBGD loss}} + \underbrace{\alpha \sum_{j=1}^n |w_j|}_{\text{lasso term}}. \quad (10)$$

Here:

- $\boldsymbol{\theta}$ (where $\boldsymbol{\theta} = [b \ w_1 \cdots w_n]^\top$) is the parameter vector
- $|\mathbf{mb}^j|$ is the number of samples in mini-batch \mathbf{mb}^j
- y^i / \hat{y}^i is the real / predicted target value of sample i , where

$$\hat{y}^i = b + w_1 x_1^i + \dots + w_n x_n^i = [1 \ \mathbf{x}^i] [b \ w_1 \cdots w_n]^\top = [1 \ \mathbf{x}^i] \boldsymbol{\theta} \quad (11)$$

- α is the regularization parameter

MBGD + Lasso: Updating Rule

- The updating rule of MBGD was given in eq. (12)

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k - \eta_k \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top \big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}, \quad (12)$$

where the MBGD loss, $\mathcal{L}(\boldsymbol{\theta}^j)$, was given in eq. (13)

$$\mathcal{L}(\boldsymbol{\theta}^j) = \frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2. \quad (13)$$

- By replacing the MBGD loss in eq. (12), $\mathcal{L}(\boldsymbol{\theta}^j)$ (also the second item in eq. (10)), with MBGD + lasso loss, $\mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)$ (first item in eq. (10)), we can write the updating rule of MBGD + lasso as

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)^\top \big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}. \quad (14)$$

MBGD + Lasso: Updating Rule

- By deriving the gradient in eq. (14), $\nabla \mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)^\top|_{\boldsymbol{\theta}^j=\boldsymbol{\theta}_k^j}$, we can write eq. (14) as

$$\begin{aligned}\boldsymbol{\theta}_k^{j+1} &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} [1 \quad \mathbf{x}^i] (y^i - \widehat{y}^i) - \alpha [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top \right), \\ &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) - \alpha [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top \right).\end{aligned}\quad (15)$$

Here

- η_k is the learning rate in epoch k
- $|\mathbf{mb}^j|$ is the number of samples in mini-batch \mathbf{mb}^j
- y^i / \widehat{y}^i is the real / predicted target value of sample i , given in eq. (11)

$$\widehat{y}^i = b + w_1 x_1^i + \dots + w_n x_n^i = [1 \quad \mathbf{x}^i] [b \quad w_1 \cdots w_n]^\top = [1 \quad \mathbf{x}^i] \boldsymbol{\theta}_k^j \quad (11)$$

and $\mathbf{y}^j / \widehat{\mathbf{y}}^j$ is the $|\mathbf{mb}^j| \times 1$ real / predicted target vector, where

$$\widehat{\mathbf{y}}^j = b + w_1 \mathbf{x}_1 + \dots + w_n \mathbf{x}_n = [1 \quad \mathbf{X}^j] [b \quad w_1 \cdots w_n]^\top = [1 \quad \mathbf{X}^j] \boldsymbol{\theta}_k^j \quad (16)$$

- \mathbf{x}^i is the $1 \times n$ feature vector of sample i , and \mathbf{X}^j the $|\mathbf{mb}^j| \times n$ feature matrix of \mathbf{mb}^j
- sgn is the *Sign* function:

$$\text{sgn}(x) = \begin{cases} -1, & x < 0 \\ 0, & x = 0 \\ 1, & x > 0 \end{cases} \quad (17)$$

- See the proof of eq. (15) in Appendix (pages 56 to 60).

MBGD + Lasso: The Implementation

- See /models/p2_shallow_learning:
 - 1 cell 4

MBGD + Ridge: Loss

- With the MBGD loss (second item in eq. (18)) and the regularization term of ridge (third item), the loss of MBGD + ridge is the sum of the two:

$$\underbrace{\mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)}_{\text{MBGD + ridge loss}} = \underbrace{\frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2}_{\text{MBGD loss}} + \underbrace{\frac{\alpha}{2} \sum_{j=1}^n w_j^2}_{\text{ridge term}}. \quad (18)$$

Here:

- $\boldsymbol{\theta}$ (where $\boldsymbol{\theta} = [b \ w_1 \cdots w_n]^\top$) is the parameter vector
- $|\mathbf{mb}^j|$ is the number of samples in mini-batch \mathbf{mb}^j
- y^i / \hat{y}^i is the real / predicted target value of sample i , given in eq. (11)

$$\hat{y}^i = b + w_1 x_1^i + \cdots + w_n x_n^i = [1 \ \mathbf{x}^i] [b \ w_1 \cdots w_n]^\top = [1 \ \mathbf{x}^i] \boldsymbol{\theta} \quad (11)$$

- α is the regularization parameter

MBGD + Ridge: Updating Rule

- The updating rule of MBGD was given in eq. (12)

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top \big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}, \quad (12)$$

where the MBGD loss, $\mathcal{L}(\boldsymbol{\theta}^j)$, was given in eq. (13)

$$\mathcal{L}(\boldsymbol{\theta}^j) = \frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2. \quad (13)$$

- By replacing the MBGD loss in eq. (12), $\mathcal{L}(\boldsymbol{\theta}^j)$ (also the second item in eq. (18)), with MBGD + ridge loss, $\mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)$ (first item in eq. (18)), we can write the updating rule of MBGD + lasso as

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top \big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}. \quad (19)$$

MBGD + Ridge: Updating Rule

- By deriving the gradient in eq. (19), $\nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top|_{\boldsymbol{\theta}^j=\boldsymbol{\theta}_k^j}$, we can write eq. (19) as

$$\begin{aligned}\boldsymbol{\theta}_k^{j+1} &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} [1 \quad \mathbf{x}^i] (y^i - \widehat{y}^i) - \alpha [0 \quad w_1 \cdots w_n]^\top \right), \\ &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) - \alpha [0 \quad w_1 \cdots w_n]^\top \right).\end{aligned}\quad (20)$$

Here:

- η_k is the learning rate in epoch k
- $|\mathbf{mb}^j|$ is the number of samples in mini-batch \mathbf{mb}^j
- y^i / \widehat{y}^i is the real / predicted target value of sample i , given in eq. (11)

$$\widehat{y}^i = b + w_1 x_1^i + \dots + w_n x_n^i = [1 \quad \mathbf{x}^i] [b \quad w_1 \cdots w_n]^\top = [1 \quad \mathbf{x}^i] \boldsymbol{\theta}_k^j \quad (11)$$

and $\mathbf{y}^j / \widehat{\mathbf{y}}^j$ is the $|\mathbf{mb}^j| \times 1$ real / predicted target vector, given in eq. (16)

$$\widehat{\mathbf{y}}^j = b + w_1 \mathbf{x}_1 + \dots + w_n \mathbf{x}_n = [1 \quad \mathbf{X}^j] [b \quad w_1 \cdots w_n]^\top = [1 \quad \mathbf{X}^j] \boldsymbol{\theta}_k^j \quad (16)$$

- \mathbf{x}^i is the $1 \times n$ feature vector of sample i , and \mathbf{X}^j the $|\mathbf{mb}^j| \times n$ feature matrix of \mathbf{mb}^j

- See the proof of eq. (20) in Appendix (pages 61 to 63).

MBGD + Ridge: The Implementation

- See [/models/p2_shallow_learning:](#)
 - 1 cell 4

MBGD + Elastic Net: Loss

- With the MBGD loss (second item in eq. (21)) and the regularization term of elastic net (third item), the loss of MBGD + elastic net is the sum of the two:

$$\underbrace{\mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)}_{\text{MBGD + elastic net loss}} = \underbrace{\frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2}_{\text{MBGD loss}} + \underbrace{\alpha\gamma \sum_{j=1}^n |w_j| + \frac{\alpha(1-\gamma)}{2} \sum_{j=1}^n w_j^2}_{\text{elastic net term}}. \quad (21)$$

Here:

- $\boldsymbol{\theta}$ (where $\boldsymbol{\theta} = [b \ w_1 \cdots w_n]^\top$) is the parameter vector
- $|\mathbf{mb}^j|$ is the number of samples in mini-batch \mathbf{mb}^j
- y^i / \hat{y}^i is the real / predicted target value of sample i , where

$$\hat{y}^i = b + w_1 x_1^i + \dots + w_n x_n^i = [1 \ \mathbf{x}^i] [b \ w_1 \cdots w_n]^\top = [1 \ \mathbf{x}^i] \boldsymbol{\theta} \quad (11)$$

- α and γ are the regularization parameters

MBGD + Elastic Net: Updating Rule

- The updating rule of MBGD was given in eq. (12)

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top \big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}, \quad (12)$$

where the MBGD loss, $\mathcal{L}(\boldsymbol{\theta}^j)$, was given in eq. (13):

$$\mathcal{L}(\boldsymbol{\theta}^j) = \frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i)^2. \quad (13)$$

- By replacing the MBGD loss in eq. (12), $\mathcal{L}(\boldsymbol{\theta}^j)$ (also the second item in eq. (21)), with MBGD + elastic net loss, $\mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)$ (first item in eq. (21)), we can write the updating rule of MBGD + elastic net as

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)^\top \big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}. \quad (22)$$

MBGD + Elastic Net: Updating Rule

- By deriving the gradient in eq. (22), $\nabla \mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)^\top \big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}$, we can write eq. (22) as

$$\begin{aligned}\boldsymbol{\theta}_k^{j+1} &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2\eta_k}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} [1 \quad \mathbf{x}^i] (y^i - \widehat{y}^i) - \alpha\gamma [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top - \alpha(1-\gamma) [0 \quad w_1 \cdots w_n]^\top \right) \\ &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2\eta_k}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) - \alpha\gamma [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top - \alpha(1-\gamma) [0 \quad w_1 \cdots w_n]^\top \right).\end{aligned}\quad (23)$$

Here

- η_k is the learning rate in epoch k
- $|\mathbf{mb}^j|$ is the number of samples in mini-batch \mathbf{mb}^j
- y^i / \widehat{y}^i is the real / predicted target value of sample i , given in eq. (11)

$$\widehat{y}^i = b + w_1 x_1^i + \dots + w_n x_n^i = [1 \quad \mathbf{x}^i] [b \quad w_1 \cdots w_n]^\top = [1 \quad \mathbf{x}^i] \boldsymbol{\theta}_k^j \quad (11)$$

and $\mathbf{y}^j / \widehat{\mathbf{y}}^j$ is the $|\mathbf{mb}^j| \times 1$ real / predicted target vector, given in eq. (16)

$$\widehat{\mathbf{y}}^j = b + w_1 \mathbf{x}_1 + \dots + w_n \mathbf{x}_n = [1 \quad \mathbf{X}^j] [b \quad w_1 \cdots w_n]^\top = [1 \quad \mathbf{X}^j] \boldsymbol{\theta}_k^j \quad (16)$$

- \mathbf{x}^i is the $1 \times n$ feature vector of sample i , and \mathbf{X}^j the $|\mathbf{mb}^j| \times n$ feature matrix of \mathbf{mb}^j
- sgn is the sign function:

$$\text{sgn}(x) = \begin{cases} -1, & x < 0 \\ 0, & x = 0 \\ 1, & x > 0 \end{cases} \quad (17)$$

- See the proof of eq. (15) in Appendix (pages 64 to 66).

MBGD + Elastic Net: The Implementation

- See [/models/p2_shallow_learning:](#)
 - 1 cell 4

Lasso VS Ridge VS Elastic Net



Good practice

- Ridge is a good default.
- However, if across all the features only a few of them are relevant:
 - use elastic net or lasso, because they tend to push parameter values of irrelevant features to exact zero
 - elastic net is preferred, because lasso may perform badly when
 - the number of features is higher than the number of samples (i.e., $n > m$)
 - some features are strongly correlated

Lasso VS Ridge

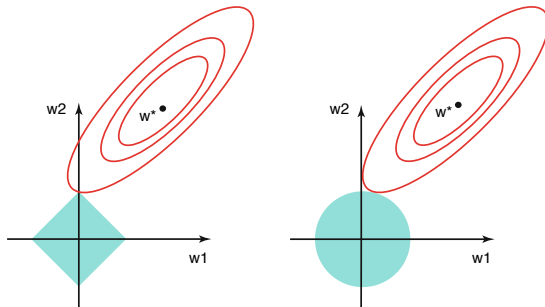


Figure 4: Contour plot of MSE and constraint of Lasso and Ridge. Picture courtesy of *An Introduction to Statistical Learning*.

- The ellipses are the contour plot of MSE (where w^* represents the optimal solution).
- The highlighted diamond and circle are the constraint region of the weights (w_1 and w_2) imposed by Lasso and Ridge (e.g., $|w_1| + |w_2| \leq s$ and $w_1^2 + w_2^2 \leq s$).
- The weights estimated by lasso and ridge regression are the first points where an ellipse contacts the constraint region.
- As lasso has corners on each axis, this intersection will usually occur on an axis, and so one of the estimates will be exactly zero.
- Conversely, as ridge has a circular constraint, this intersection will not generally occur on an axis, and so none of the estimates will be exactly zero.

Parameters

- Parameters of a model or training method are the unknowns that are:
 - not fixed
 - but updated during training
- For example, $\boldsymbol{\theta} = [b \quad w_1 \cdots w_n]^\top$ (bias and weights) are the parameters of linear regression in eq. (24)

$$\widehat{\mathbf{y}} = b + w_1 \mathbf{x}_1 + \dots + w_n \mathbf{x}_n = [\mathbf{1} \quad \mathbf{X}] [b \quad w_1 \cdots w_n]^\top = [\mathbf{1} \quad \mathbf{X}] \boldsymbol{\theta}. \quad (24)$$

- These parameters are:
 - not fixed
 - but updated using, say, the updating rule of MBGD + ridge in eq. (20)

$$\begin{aligned} \boldsymbol{\theta}_k^{j+1} &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} [\mathbf{1} \quad \mathbf{x}^i] (y^i - \widehat{y}^i) - \alpha [0 \quad w_1 \cdots w_n]^\top \right), \\ &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} [\mathbf{1} \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) - \alpha [0 \quad w_1 \cdots w_n]^\top \right). \end{aligned} \quad (20)$$

Hyperparameters

- Hyperparameters of a model or training method are the unknowns that are:
 - fixed
 - and not updated during training
- For example, η_k (learning rate) and α (regularization parameter) are the hyperparameters of the updating rule of MBGD + ridge in eq. (20)

$$\begin{aligned}\boldsymbol{\theta}_k^{j+1} &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} \begin{bmatrix} 1 & \mathbf{x}^i \end{bmatrix} (y^i - \widehat{y}^i) - \alpha \begin{bmatrix} 0 & w_1 \cdots w_n \end{bmatrix}^\top \right), \\ &= \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} \begin{bmatrix} 1 & \mathbf{X}^j \end{bmatrix}^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) - \alpha \begin{bmatrix} 0 & w_1 \cdots w_n \end{bmatrix}^\top \right).\end{aligned}\tag{20}$$

- These hyperparameters are:
 - fixed
 - and not updated during training
- It is worth noting that learning rate is not necessarily a hyperparameter:
 - we can use methods such as *Learning Rate Scheduling* to update it during training (see [/p3_c2_s2_training_deep_neural_networks](#))
 - in this case, learning rate is a parameter rather than a hyperparameter

Hyperparameter Tuning: Motivation

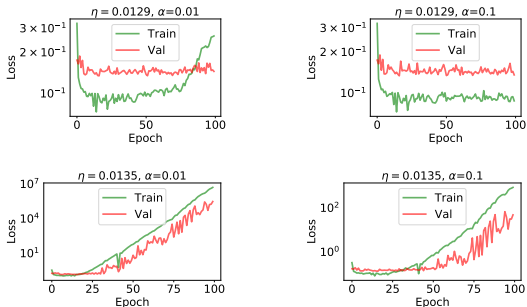


Figure 5: Training and validation loss of MBGD + ridge with different combinations of learning rate (η) and regularization parameter (α).

- By comparing the two rows in each column of fig. 5, we can see that the training and validation loss can be quite sensitive to η .
- By comparing the two columns in each row of fig. 5, we can see that the training and validation loss can be quite sensitive to α .
- The goal of hyperparameter tuning is finding hyperparameter values that lead to good validation performance (e.g., low validation loss).

Hyperparameter Tuning: Idea

Table 1: Combinations of learning rate (η) and regularization parameter (α) and their validation MSE. The best combination is highlighted in red.

η	α	Val MSE
0.001	0.01	0.138
0.001	0.1	0.139
0.02	0.1	2.35×10^{52}
0.02	0.01	5.94×10^{57}

- Let us use table 1 as an example to illustrate the idea of hyperparameter tuning:
 - ① we loop over each combination of η and α , and for each combination:
 - ① we train the model (on the training data) using the combination as the hyperparameter values
 - ② we get the validation MSE of the model (on the validation data)
 - ② we pick the first combination (highlighted in red) as the best hyperparameter values since it leads to the lowest validation MSE
 - ③ we retrain the model (on the combined training and validation data) with the best hyperparameter values picked earlier

Hyperparameter Tuning in Sklearn: Two Popular Methods

- There are two popular hyperparameter tuning methods in sklearn:
 - GridSearchCV
 - RandomizedSearchCV
- The key difference between the two methods lies in:
 - how they expect the user to propose values of a single hyperparameter
 - how they produce combinations of values of all the hyperparameters
- After producing the combinations of values, both methods:
 - ① loop over each combination, and for each combination:
 - ① train the model (on the training data) using the combination as the hyperparameter values
 - ② get the validation performance of the model (on the validation data)
 - ② pick the best hyperparameter values that lead to the best validation performance
 - ③ (when setting parameter `refit` as `True`) retrain the model (on the combined training and validation data) with the best hyperparameter values picked earlier

Hyperparameter Tuning in Sklearn: Good Practice



Good practice

- It is recommended to set `parameter refit` as `True` when using `GridSearchCV` and `RandomizedSearchCV`.
- This allows us to retrain the model (i.e., its parameters) on the combined training and validation data with the best hyperparameter values.
- While retraining model requires extra computational cost, doing so will usually improve model performance (which is often preferred).

GridSearchCV: Parameter Grid

Table 1: Combinations of learning rate (η) and regularization parameter (α) and their validation MSE. The best combination is highlighted in red.

η	α	Val MSE
0.001	0.01	0.138
0.001	0.1	0.139
0.02	0.1	2.35×10^{52}
0.02	0.01	5.94×10^{57}

- GridSearchCV expects a list of possible values for each hyperparameter.
- This list of values is also called *Parameter Grid* (hence the name of GridSearchCV).
- In table 1 we used the grid below for η and α (in MBGD + ridge):
 - η : [0.001, 0.02]
 - α : [0.01, 0.1]
- Based on the parameter grid of each hyperparameter, GridSearchCV produces all the possible combinations of hyperparameter values.
- With the grid of η and α above, we will have four combinations, shown in table 1.

GridSearchCV: Code Example

- See [/p2_c2_s2_training_shallow_models/code_example:](#)
 - ① cells 54 to 56
 - ② cells 57 to 61

GridSearchCV: Pros and Cons

- Pros:
 - we have full control:
 - we can use parameter grid to specify the exact hyperparameter values we want to fine-tune
- Cons:
 - it is not scalable:
 - assume there are n hyperparameters and for each hyperparameter we only fine-tune two values
 - the number of combination of hyperparameter values is 2^n

RandomizedSearchCV: Parameter Distribution

Table 2: Combinations of learning rate (η) and regularization parameter (α) and their validation MSE. The best combination is highlighted in red.

η	α	Val MSE
0.0124	0.0759	0.1350
0.0040	0.024	0.1355
0.0175	0.0152	5.31×10^{40}
0.0191	0.0437	1.11×10^{50}

- Unlike GridSearchCV that expects a list of possible values for each hyperparameter, RandomizedSearchCV expects a distribution for each hyperparameter.
- Possible values of a hyperparameter will then be randomly sampled from the distribution (hence the name of RandomizedSearchCV).
- In table 2 we used the distribution below for η and α (in MBGD + ridge):
 - η : uniform(loc=0.01, scale=0.003)
 - α : uniform(loc=0.01, scale=0.09)
- Based on the distribution of each hyperparameter, and parameter `n_iter`, RandomizedSearchCV produces `n_iter` combinations of hyperparameter values.
- With the distribution of η and α above, and `n_iter` = 4, we could have four combinations, shown in table 2.

RandomizedSearchCV: Code Example

- See [/p2_c2_s2_training_shallow_models/code_example:](#)
 - ① cells 54 to 56
 - ② cells 62 to 66

RandomizedSearchCV: Pros and Cons

- Pros:
 - it is scalable:
 - the number of combination of hyperparameter values is not determined by the number of hyperparameters
 - instead, it is determined by parameter `n_iter` of `RandomizedSearchCV`
- Cons:
 - we do not have full control:
 - hyperparameter values we want to fine-tune are randomly sampled from the parameter distributions

GridSearchCV VS RandomizedSearchCV: Good Practice



Good practice

- When there are many hyperparameters to fine-tune:
 - it is recommended to use `RandomizedSearchCV` (so that hyperparameter tuning can be scalable)
- When there are only a few hyperparameters to fine-tune:
 - it is recommended to use `GridSearchCV` (so that we can have full control of the hyperparameter values to fine-tune)

Model Selection: Motivation

- For a problem, (in theory) there are usually many models we can use.
- Take linear regression for example, we have sklearn models such as:
 - `LinearRegression`
 - `SGDRegressor`
 - `Lasso`
 - `Ridge`
 - `ElasticNet`
- While for certain problems some models are favored over others, we may not know for sure which model actually works the best.
- As a result, we may have to:
 - 1 try many models
 - 2 select the top-1 model or ensemble of top- k models for production
- The process of trying many models and selecting some of them is called *Model Selection*.

Model Selection: Idea

- The idea of model selection is as follows:
 - ① for each model:
 - ① we fine-tune its hyperparameters and select the best combination of hyperparameter values (ones with the best validation performance)
 - ② we retrain the model using the best combination selected earlier on the combined training and validation data
 - ② we select the top-1 retrained model or ensemble of top- k retrained models (based on the validation performance of the models)
 - ③ we test the selected retrained models on the test data to estimate how well they generalize in reality

Model Selection: Code Example

- See [/p2_c2_s2_training_shallow_models/code_example:](#)
 - 1 cell 67
 - 2 cell 69

Proof of Decomposition of Expected Test Error: Page 12

- The expected test error, $E[(\hat{y} - y)^2]$, can be written as

$$\underbrace{E[(\hat{y} - y)^2]}_{\text{Expected test error}} = E[\hat{y}^2 - 2\hat{y}y + y^2] = E[\hat{y}^2] - 2E[\hat{y}y] + E[y^2] \quad (25)$$

- Since \hat{y} and y are independent, we can write eq. (25) as

$$\underbrace{E[(\hat{y} - y)^2]}_{\text{Expected test error}} = E[\hat{y}^2] - 2E[\hat{y}]E[y] + E[y^2]. \quad (26)$$

- Let \mathbf{a} be a vector and $E[\mathbf{a}]$ the expectation of \mathbf{a} , then

$$\begin{aligned} E[(\mathbf{a} - E[\mathbf{a}])^2] &= E[\mathbf{a}^2 - 2\mathbf{a}E[\mathbf{a}] + E[\mathbf{a}]^2], \\ &= E[\mathbf{a}^2] - 2E[\mathbf{a}E[\mathbf{a}]] + E[E[\mathbf{a}]^2], \\ &= E[\mathbf{a}^2] - 2E[\mathbf{a}]^2 + E[\mathbf{a}]^2, \\ &= E[\mathbf{a}^2] - E[\mathbf{a}]^2. \end{aligned} \quad (27)$$

- Based on eq. (27), we have

$$E[\mathbf{a}^2] = E[(\mathbf{a} - E[\mathbf{a}])^2] + E[\mathbf{a}]^2. \quad (28)$$

Proof of Decomposition of Expected Test Error: Page 12

- Based on eq. (28), we can write $E [\hat{\mathbf{y}}^2]$ in eq. (25) as

$$E [\hat{\mathbf{y}}^2] = \underbrace{E [(\hat{\mathbf{y}} - E[\hat{\mathbf{y}}])^2]}_{\text{Variance}} + E[\hat{\mathbf{y}}]^2. \quad (29)$$

- Similarly, based on eq. (28), we can write $E [\mathbf{y}^2]$ in eq. (25) as:

$$E [\mathbf{y}^2] = E [(\mathbf{y} - E[\mathbf{y}])^2] + E[\mathbf{y}]^2. \quad (30)$$

- Based on eq. (4)

$$\mathbf{y} = [y^1 \quad \dots \quad y^m]^\top, \quad (4)$$

where $y^i = y$ and y is the target value in the test sample, we have

$$E [(\mathbf{y} - E[\mathbf{y}])^2] = 0. \quad (31)$$

- By substituting eq. (31) into eq. (30), we have

$$E [\mathbf{y}^2] = E[\mathbf{y}]^2. \quad (32)$$

Proof of Decomposition of Expected Test Error: Page 12

- By substituting eqs. (29) and (32) into eq. (26), we have

$$\begin{aligned}
 \underbrace{E[(\hat{y} - y)^2]}_{\text{Expected test error}} &= E[\hat{y}^2] - 2E[\hat{y}]E[y] + E[y^2], \\
 &= \underbrace{E[(\hat{y} - E[\hat{y}])^2]}_{\text{Variance}} + \left(E[\hat{y}]^2 - 2E[\hat{y}]E[y] + E[y]^2 \right), \\
 &= \underbrace{E[\hat{y} - E[\hat{y}]]^2}_{\text{Variance}} + (E[\hat{y}] - E[y])^2, \\
 &= \underbrace{E[\hat{y} - E[\hat{y}]]^2}_{\text{Variance}} + \underbrace{(E[\hat{y} - y])^2}_{\text{Bias}^2}.
 \end{aligned} \tag{33}$$

which proves the claim in eq. (3) on page 12. □

Proof of Updating Rule: Page 25

- The MBGD + lasso loss can be written as

$$\underbrace{\mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)}_{\text{MBGD + lasso loss}} = \underbrace{\mathcal{L}(\boldsymbol{\theta}^j)}_{\text{MBGD loss}} + \underbrace{\alpha \sum_{j=1}^n |w_j|}_{\text{lasso term}}, \quad (34)$$

where the MBGD loss, $\mathcal{L}(\boldsymbol{\theta}^j)$, was given in eq. (13)

$$\mathcal{L}(\boldsymbol{\theta}^j) = \frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2. \quad (13)$$

- The gradient of MBGD + lasso loss, $\nabla \mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)^\top$, can be written as the sum of the gradient of MBGD loss (second item in eq. (34)) and the gradient of lasso term (third item):

$$\nabla \mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)^\top = \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top + \left(\nabla \alpha \sum_{j=1}^n |w_j| \right)^\top. \quad (35)$$

Proof of Updating Rule: Page 25

- The gradient of MBGD loss (second item in eq. (35)), $\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top$, can be written as

$$\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top = \left[\frac{\partial}{\partial b} \mathcal{L}(\boldsymbol{\theta}^j) \quad \frac{\partial}{\partial w_1} \mathcal{L}(\boldsymbol{\theta}^j) \cdots \frac{\partial}{\partial w_n} \mathcal{L}(\boldsymbol{\theta}^j) \right]^\top. \quad (36)$$

- Based on eq. (13), we can write $\frac{\partial}{\partial b} \mathcal{L}(\boldsymbol{\theta}^j)$ as

$$\begin{aligned} \frac{\partial}{\partial b} \mathcal{L}(\boldsymbol{\theta}^j) &= \frac{\partial}{\partial b} \left(\frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i)^2 \right), \\ &= \frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i) \cdot \frac{\partial}{\partial b} (y^i - \widehat{y}^i), \\ &= \frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i) \cdot \frac{\partial}{\partial b} (y^i - (b + w_1 x_1^i + \dots + w_n x_n^i)), \\ &= \frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i) \cdot (-1). \end{aligned} \quad (37)$$

Proof of Updating Rule: Page 25

- Based on eq. (13), we can write $\frac{\partial}{\partial w_j} \mathcal{L}(\boldsymbol{\theta}^i)$ as

$$\begin{aligned}
 \frac{\partial}{\partial w_j} \mathcal{L}(\boldsymbol{\theta}^j) &= \frac{\partial}{\partial w_j} \left(\frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2 \right), \\
 &= \frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i) \cdot \frac{\partial}{\partial w_j} (y^i - \hat{y}^i), \\
 &= \frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i) \cdot \frac{\partial}{\partial w_j} (y^i - (b + w_1 x_1^i + \dots + w_n x_n^i)), \\
 &= \frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i) \cdot (-x_j^i).
 \end{aligned} \tag{38}$$

- By substituting eqs. (37) and (38) into eq. (36), we have

$$\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i) \begin{bmatrix} 1 & \mathbf{x}^i \end{bmatrix}^\top = -\frac{2}{|\mathbf{mb}^j|} \begin{bmatrix} \mathbf{1} & \mathbf{X}^j \end{bmatrix}^\top (\mathbf{y}^j - \hat{\mathbf{y}}^j). \tag{39}$$

Proof of Updating Rule: Page 25

- The gradient of the lasso term (third item in eq. (35)), $\nabla \alpha \sum_{j=1}^n |w_j|^\top$, can be written as

$$\left(\nabla \alpha \sum_{j=1}^n |w_j| \right)^\top = \alpha \left[\frac{\partial}{\partial b} \sum_{j=1}^n |w_j| \quad \frac{\partial}{\partial w_1} \sum_{j=1}^n |w_j| \cdots \frac{\partial}{\partial w_n} \sum_{j=1}^n |w_j| \right]^\top, \quad (40)$$

where

$$|w_j| = \begin{cases} -w_j, & w_j < 0 \\ 0, & w_j = 0 \\ w_j, & w_j > 0. \end{cases} \quad (41)$$

- Based on eq. (41), we have

$$\frac{\partial}{\partial b} \sum_{j=1}^n |w_j| = 0 \quad \text{and} \quad \frac{\partial}{\partial w_k} \sum_{j=1}^n |w_j| = \text{sgn}(w_k) = \begin{cases} -1, & w_k < 0 \\ 0, & w_k = 0 \\ 1, & w_k > 0 \end{cases} \quad (42)$$

where $1 \leq k \leq n$.

- By substituting eq. (42) into eq. (40), we have

$$\left(\nabla \alpha \sum_{j=1}^n |w_j| \right)^\top = \alpha \left[0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n) \right]^\top. \quad (43)$$

Proof of Updating Rule: Page 25

- By substituting eqs. (39) and (43) into eq. (35),

$$\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i) [1 \quad \mathbf{x}^i]^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j), \quad (39)$$

$$\left(\nabla \alpha \sum_{j=1}^n |w_j| \right)^\top = \alpha [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top, \quad (43)$$

$$\nabla \mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)^\top = \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top + \left(\nabla \alpha \sum_{j=1}^n |w_j| \right)^\top, \quad (35)$$

we have

$$\nabla \mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) + \alpha [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top. \quad (44)$$

- By substituting eq. (44) into eq. (14)

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}_{m+l_1}(\boldsymbol{\theta}^j)^\top \Big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}, \quad (14)$$

we have

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) - \alpha [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top \right), \quad (45)$$

which proves the claim in eq. (15) on page 25. \square

Proof of Updating Rule: Page 29

- The MBGD + ridge loss can be written as

$$\underbrace{\mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)}_{\text{MBGD + ridge loss}} = \underbrace{\mathcal{L}(\boldsymbol{\theta}^j)}_{\text{MBGD loss}} + \underbrace{\frac{\alpha}{2} \sum_{j=1}^n w_j^2}_{\text{ridge term}}, \quad (46)$$

where the MBGD loss, $\mathcal{L}(\boldsymbol{\theta}^j)$, was given in eq. (13)

$$\mathcal{L}(\boldsymbol{\theta}^j) = \frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2. \quad (13)$$

- The gradient of MBGD + ridge loss, $\nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top$, can be written as the sum of the gradient of MBGD loss (second item in eq. (46)) and the gradient of ridge term (third item):

$$\nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top = \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top + \left(\nabla \frac{\alpha}{2} \sum_{j=1}^n w_j^2 \right)^\top, \quad (47)$$

where the gradient of MBGD loss was given in eq. (39)

$$\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i) [1 \quad \mathbf{x}^i]^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \hat{\mathbf{y}}^j). \quad (39)$$

Proof of Updating Rule: Page 29

- The gradient of the ridge term (third item in eq. (47)), $\nabla \alpha \sum_{j=1}^n |w_j|^2$, can be written as

$$\left(\nabla \frac{\alpha}{2} \sum_{j=1}^n w_j^2 \right)^T = \frac{\alpha}{2} \left[\frac{\partial}{\partial b} \sum_{j=1}^n w_j^2 \quad \frac{\partial}{\partial w_1} \sum_{j=1}^n w_j^2 \cdots \frac{\partial}{\partial w_n} \sum_{j=1}^n w_j^2 \right]^T, \quad (48)$$

where

$$\frac{\partial}{\partial b} \sum_{j=1}^n w_j^2 = 0 \quad \text{and} \quad \frac{\partial}{\partial w_k} \sum_{j=1}^n w_j^2 = 2w_k \quad (49)$$

where $1 \leq k \leq n$.

- By substituting eq. (49) into eq. (48), we have

$$\left(\nabla \frac{\alpha}{2} \sum_{j=1}^n w_j^2 \right)^T = \alpha \begin{bmatrix} 0 & w_1 & \cdots & w_n \end{bmatrix}^T. \quad (50)$$

Proof of Updating Rule: Page 29

- By substituting eqs. (39) and (50) into eq. (47),

$$\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i) [1 \quad \mathbf{x}^i]^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j), \quad (39)$$

$$\left(\nabla \frac{\alpha}{2} \sum_{j=1}^n w_j^2 \right)^\top = \alpha [0 \quad w_1 \cdots w_n]^\top, \quad (50)$$

$$\nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top = \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top + \left(\nabla \frac{\alpha}{2} \sum_{j=1}^n w_j^2 \right)^\top, \quad (47)$$

we have

$$\nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) + \alpha [0 \quad w_1 \cdots w_n]^\top. \quad (51)$$

- By substituting eq. (51) into eq. (19)

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top \Big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}, \quad (19)$$

we have

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (\mathbf{y}^j - \widehat{\mathbf{y}}^j) - \alpha [0 \quad w_1 \cdots w_n]^\top \right), \quad (52)$$

which proves the claim in eq. (20) on page 29. □

Proof of Updating Rule: Page 33

- The MBGD + elastic net loss can be written as

$$\underbrace{\mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)}_{\text{MBGD + elastic net loss}} = \underbrace{\mathcal{L}(\boldsymbol{\theta}^j)}_{\text{MBGD loss}} + \underbrace{\alpha\gamma \sum_{j=1}^n |w_j| + \frac{\alpha(1-\gamma)}{2} \sum_{j=1}^n w_j^2}_{\text{elastic net term}}, \quad (53)$$

where the MBGD loss, $\mathcal{L}(\boldsymbol{\theta}^j)$, was given in eq. (13)

$$\mathcal{L}(\boldsymbol{\theta}^j) = \frac{1}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \hat{y}^i)^2. \quad (13)$$

- The gradient of MBGD + elastic net loss, $\nabla \mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)^\top$, can be written as the sum of the gradient of MBGD loss (second item in eq. (53)) and the gradient of elastic net term (third item):

$$\nabla \mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)^\top = \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top + \left(\nabla \alpha\gamma \sum_{j=1}^n |w_j| \right)^\top + \left(\nabla \frac{\alpha(1-\gamma)}{2} \sum_{j=1}^n w_j^2 \right)^\top. \quad (54)$$

Proof of Updating Rule: Page 33

- The gradient of MBGD loss was given in eq. (39)

$$\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i) [1 \quad \mathbf{x}^i]^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (y^j - \widehat{\mathbf{y}}^j). \quad (39)$$

- Based on the gradient of lasso term and ridge term given in eqs. (43) and (50)

$$\left(\nabla \alpha \sum_{j=1}^n |w_j| \right)^\top = \alpha [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top, \quad (43)$$

$$\left(\nabla \frac{\alpha}{2} \sum_{j=1}^n w_j^2 \right)^\top = \alpha [0 \quad w_1 \cdots w_n]^\top, \quad (50)$$

we can write the gradient of elastic net term as

$$\left(\nabla \alpha \gamma \sum_{j=1}^n |w_j| \right)^\top + \left(\nabla \frac{\alpha(1-\gamma)}{2} \sum_{j=1}^n w_j^2 \right)^\top = \alpha \gamma [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top + \alpha(1-\gamma) [0 \quad w_1 \cdots w_n]^\top. \quad (55)$$

Proof of Updating Rule: Page 33

- By substituting eqs. (39) and (55) into eq. (54),

$$\nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} \sum_{i \in \mathbf{mb}^j} (y^i - \widehat{y}^i) [1 \quad \mathbf{x}^i]^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (y^j - \widehat{y}^j), \quad (39)$$

$$\left(\nabla \alpha \gamma \sum_{j=1}^n |w_j| \right)^\top + \left(\nabla \frac{\alpha(1-\gamma)}{2} \sum_{j=1}^n w_j^2 \right)^\top = \alpha \gamma [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top + \alpha(1-\gamma) [0 \quad w_1 \cdots w_n]^\top, \quad (55)$$

$$\nabla \mathcal{L}_{m+l_{12}}(\boldsymbol{\theta}^j)^\top = \nabla \mathcal{L}(\boldsymbol{\theta}^j)^\top + \left(\nabla \alpha \gamma \sum_{j=1}^n |w_j| \right)^\top + \left(\nabla \frac{\alpha(1-\gamma)}{2} \sum_{j=1}^n w_j^2 \right)^\top, \quad (54)$$

we have

$$\nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top = -\frac{2}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (y^j - \widehat{y}^j) + \alpha \gamma [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top + \alpha(1-\gamma) [0 \quad w_1 \cdots w_n]^\top. \quad (56)$$

- By substituting eq. (56) into eq. (22)

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j - \eta_k \mathbf{g}_k^j = \boldsymbol{\theta}_k^j - \eta_k \nabla \mathcal{L}_{m+l_2}(\boldsymbol{\theta}^j)^\top \Big|_{\boldsymbol{\theta}^j = \boldsymbol{\theta}_k^j}, \quad (22)$$

we have

$$\boldsymbol{\theta}_k^{j+1} = \boldsymbol{\theta}_k^j + \eta_k \left(\frac{2\eta_k}{|\mathbf{mb}^j|} [1 \quad \mathbf{X}^j]^\top (y^j - \widehat{y}^j) - \alpha \gamma [0 \quad \text{sgn}(w_1) \cdots \text{sgn}(w_n)]^\top - \alpha(1-\gamma) [0 \quad w_1 \cdots w_n]^\top \right), \quad (57)$$

which proves the claim in eq. (23) on page 33. \square

Bibliography