Training Models

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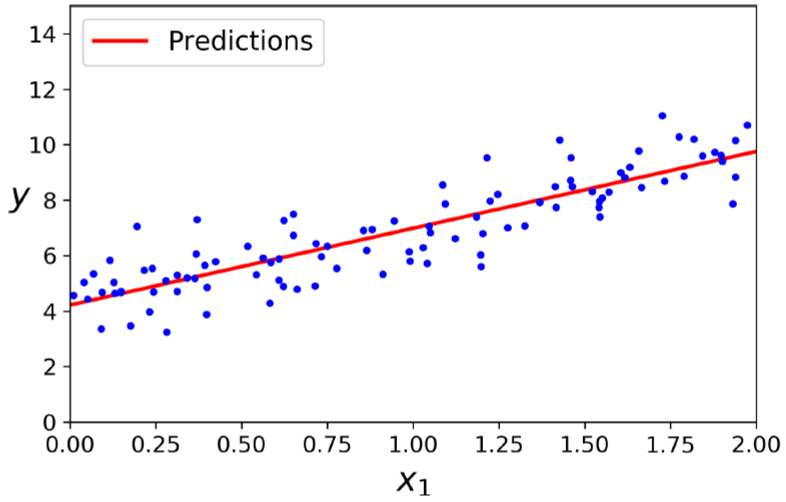
Reference: *Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow* by Aurélien Géron (O'Reilly). 2019, 978-1-492-03264-9.

Outline

1. Linear Regression
2. Gradient Descent
3. Gradient Descent Variants
    1. Batch Gradient Descent
    2. Stochastic Gradient Descent
    3. Mini-batch Gradient Descent
4. Learning Curves
5. Early Stopping
6. Exercises

Linear Regression

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$



- $\hat{y}$ is the predicted value.
- n is the number of features.
- x_i is the i^th feature value.
- θ_j is the j^th model parameter (including the bias term θ_0 and the feature weights $\theta_1, \theta_2, \cdots, \theta_n$).

$$\hat{y} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta} \cdot \mathbf{x}$$

Analytical Solution

- The Root Mean Square Error (RMSE) is used as cost function.

$$\text{MSE}(\mathbf{X}, h_{\boldsymbol{\theta}}) = \frac{1}{m}\sum_{i=1}^{m}\left(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)}\right)^2$$

- Minimizing this cost gives the following solution (normal function):

$$\hat{\boldsymbol{\theta}} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1} \ \mathbf{X}^T \ \mathbf{y}$$

Complexity $O(mn^2)$

- $\hat{\boldsymbol{\theta}}$ is the value of $\boldsymbol{\theta}$ that minimizes the cost function.
- $\mathbf{y}$ is the vector of target values containing $y^{(1)}$ to $y^{(m)}$.

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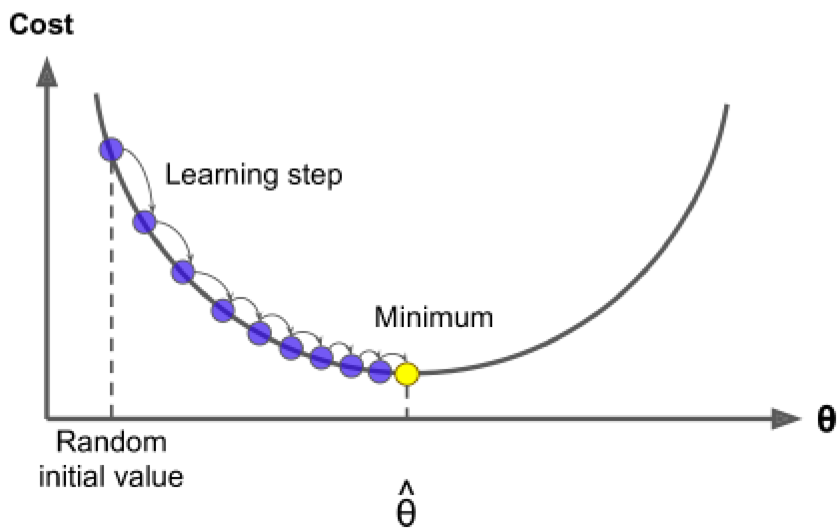
Gradient Descent

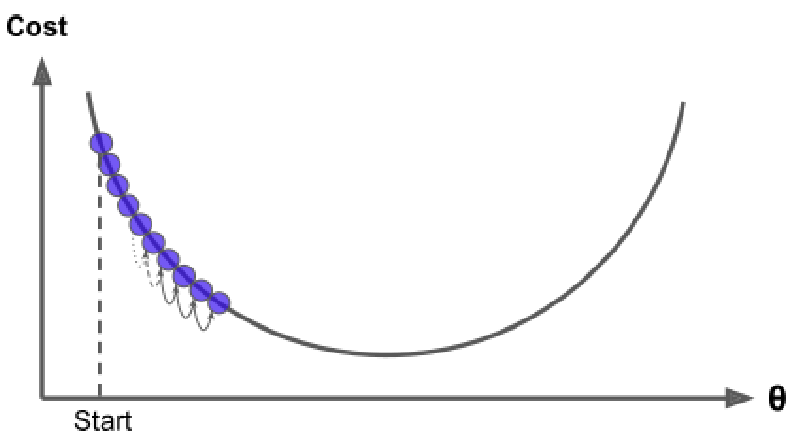
- Generic optimization algorithm capable of finding optimal solutions to a wide range of problems.
- Tweaks parameters iteratively in order to minimize a cost function.



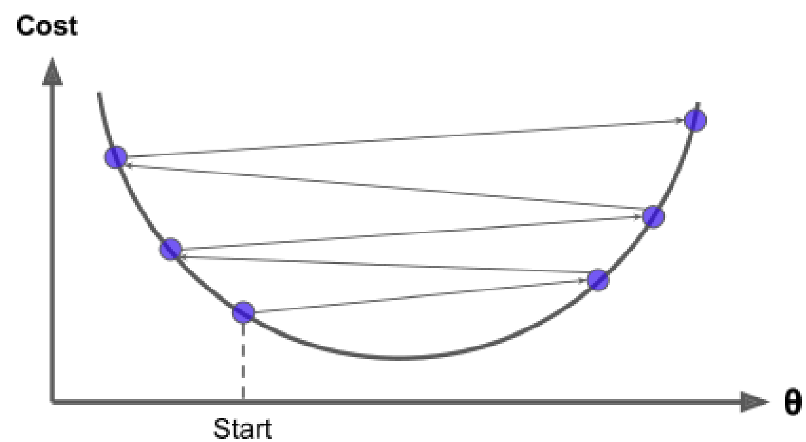
$$\theta^{(\text{next step})} = \theta - \eta \nabla_{\theta} \text{MSE}(\theta)$$

Learning Rate

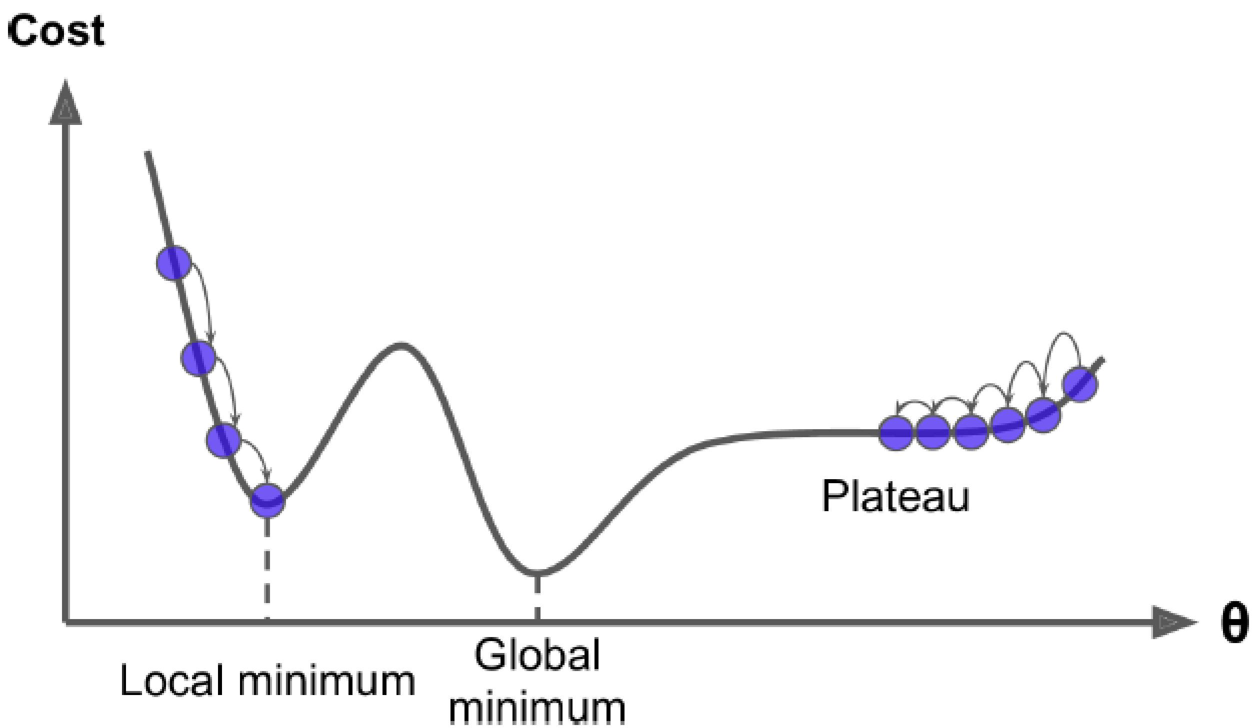
Too Small



Too Large

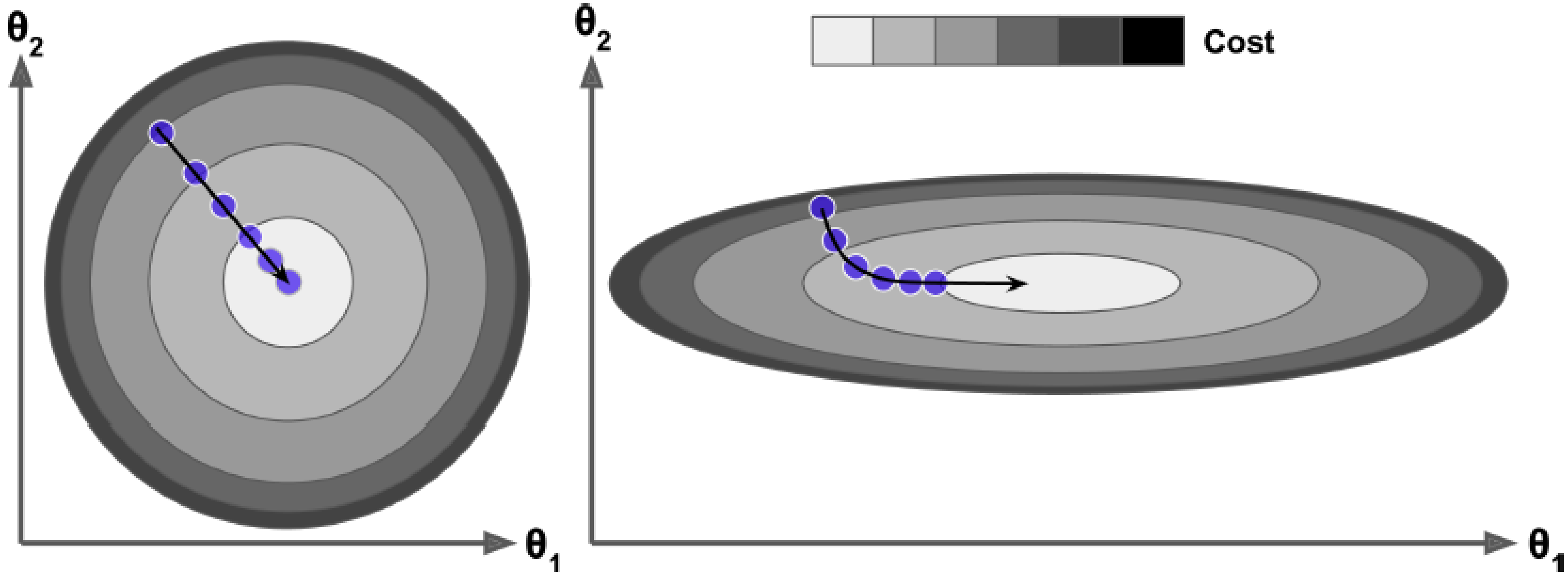


Gradient Descent Pitfalls



Feature Scaling

- Ensure that all features have a similar scale (e.g., using Scikit-Learn's `StandardScaler` class).
- Gradient Descent with and without feature scaling.



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Batch Gradient Descent

- Partial derivatives of the cost function in θ_j

$$\frac{\partial}{\partial \theta_j} \text{MSE}(\boldsymbol{\theta}) = \frac{2}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)} \right) x_j^{(i)}$$

- Gradient vector of the cost function

$$\nabla_{\boldsymbol{\theta}} \text{MSE}(\boldsymbol{\theta}) = \begin{pmatrix} \frac{\partial}{\partial \theta_0} \text{MSE}(\boldsymbol{\theta}) \\ \frac{\partial}{\partial \theta_1} \text{MSE}(\boldsymbol{\theta}) \\ \vdots \\ \frac{\partial}{\partial \theta_n} \text{MSE}(\boldsymbol{\theta}) \end{pmatrix} = \frac{2}{m} \mathbf{X}^T (\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$$

The entire training Batch

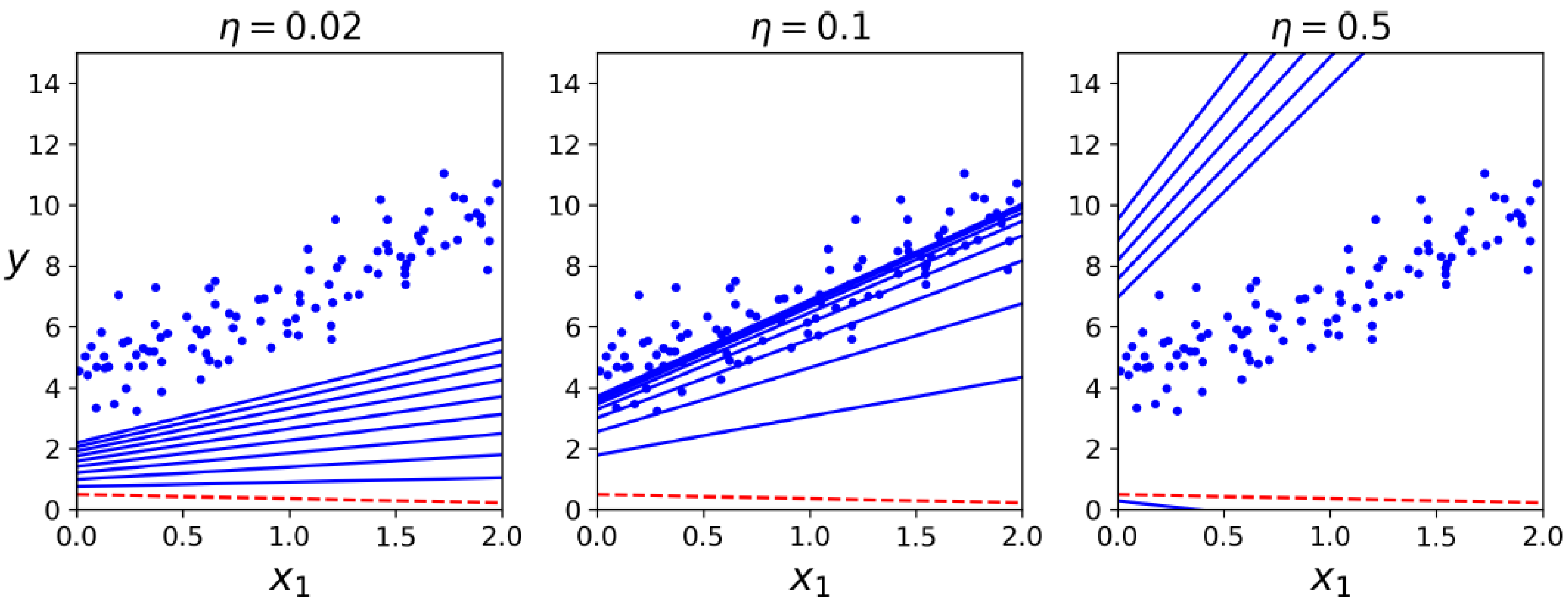
$$\boldsymbol{\theta}^{(\text{next step})} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \text{MSE}(\boldsymbol{\theta})$$

Batch Gradient Descent

- Gradient Descent step

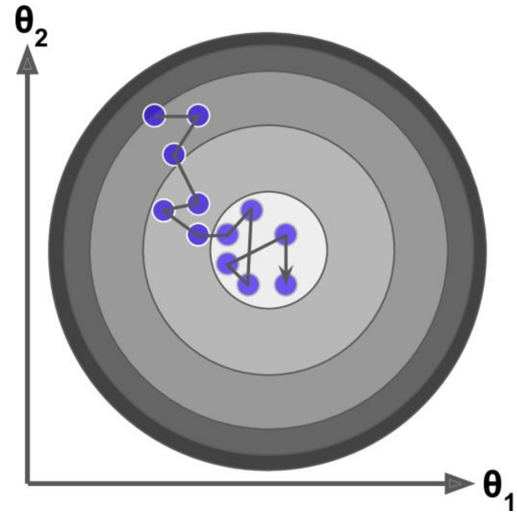
$$\theta^{(\text{next step})} = \theta - \eta \nabla_{\theta} \text{MSE}(\theta)$$

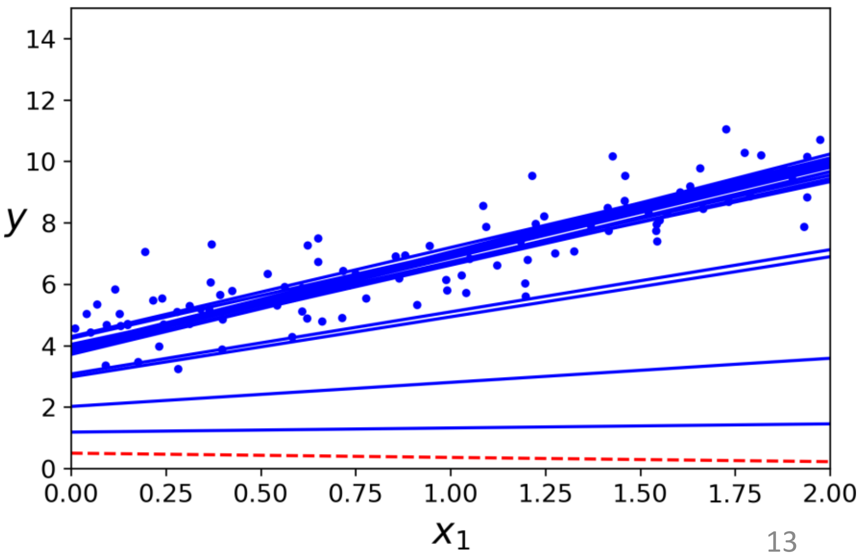
- Gradient Descent with various learning rates



Stochastic Gradient Descent

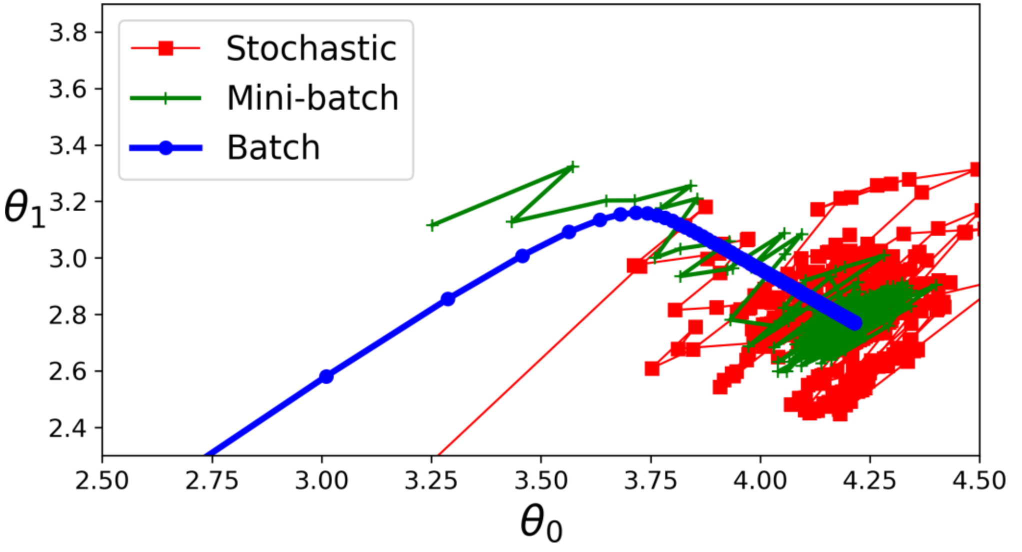
- SGD picks a random instance in the training set at every step and computes the gradients.
- SGD is faster when the training set is large.
- Is bouncy
- Eventually gives good solution
- Can escape local minima





Mini-batch Gradient Descent

- Computes the gradients on small random sets of instances called mini batches.
- Benefits from hardware accelerators (e.g., GPU).
- Less bouncy, better solution, escapes some local minima



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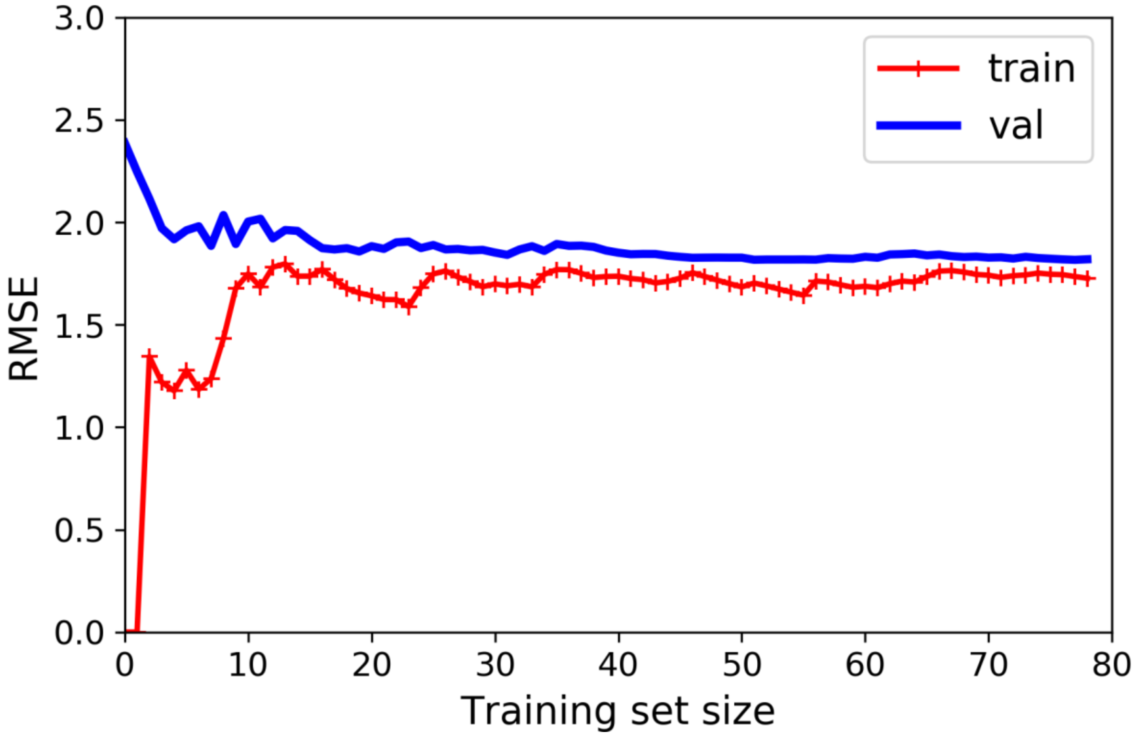
Learning Curves

- The accuracy on the validation set generally increases as the training set size increases.
- Overfitting decreases with larger training set.



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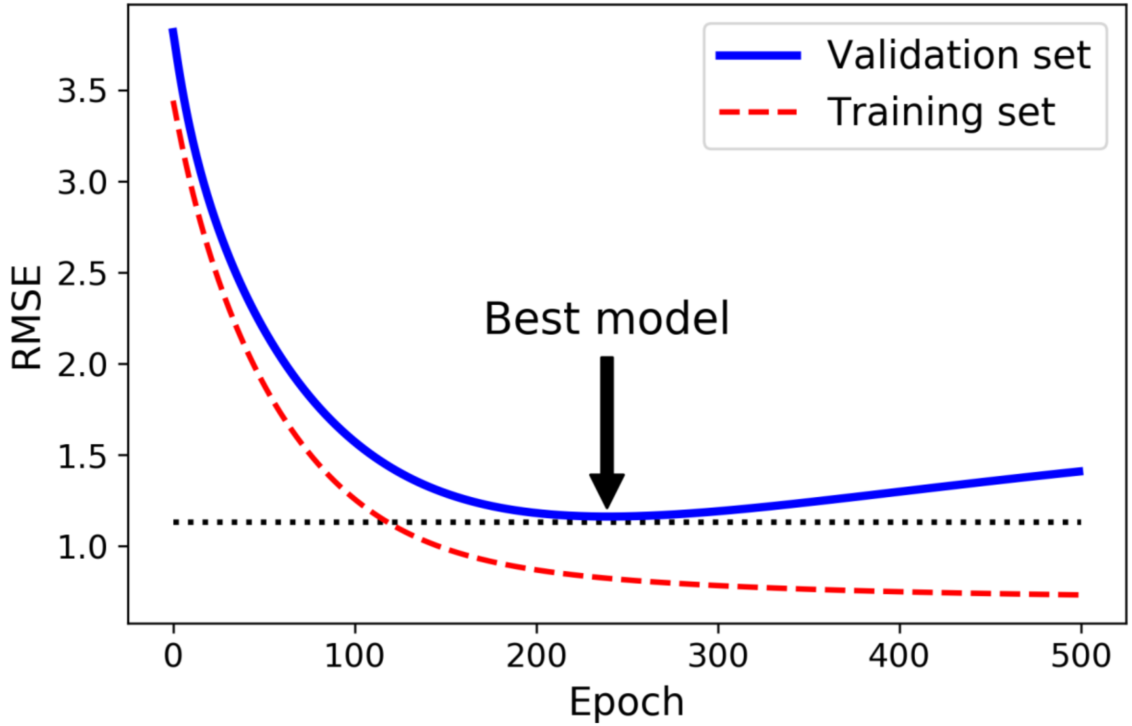
Early Stopping

- Stop training when the validation error reaches a minimum.
- Need to save the best model.



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Exercises

1. What Linear Regression training algorithm can you use if you have a training set with millions of features?
2. Suppose the features in your training set have very different scales. What algorithms might suffer from this, and how? What can you do about it?
3. Do all Gradient Descent algorithms lead to the same model provided you let them run long enough?

Summary

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