UNIVERSITY OF TORONTO
SCHOOL OF CONTINUING STUDIES

3253 Machine Learning

Module 5: Training Models and Feature Selection

Course Plan

Module Titles
Module 1 – Introduction to Machine Learning
Module 2 – End to End Machine Learning Project
Module 3 – Classification
Module 4 – Clustering and Unsupervised Learning
Module 5 – **Current Focus: Training Models and Feature Selection**
Module 6 – Support Vector Machines
Module 7 – Decision Trees and Ensemble Learning
Module 8 – Dimensionality Reduction
Module 9 – Introduction to TensorFlow
Module 10 – Introduction to Deep Learning and Deep Neural Networks
Module 11 – Distributing TensorFlow, CNNs and RNNs
Module 12 – Final Assignment and Presentations (no content)

Learning Outcomes for this Module

- Apply alternative learning strategies to regression
- Evaluate model learning using learning curves
- Employ regularized regression for automatic feature selection
- Learn a logistic regression model for categorical classification problems

Topics for this Module

- **5.1** Linear regression using the normal equations
- **5.2** Linear regression using gradient descent
- **5.3** Non-linear regression
- **5.4** Learning curves
- **5.5** Regularization and ridge regression
- **5.6** Logistic regression
- **5.7** Resources and Wrap-up

Module 5 – Section 1

Linear Regression Using the Normal Equations

Introduction

- So far we have treated Machine Learning models and their training algorithms mostly like black boxes.
  - you optimized a regression system,
  - you improved a digit image classifier,
  - All this without knowing how they actually work

- However, having a good understanding of how things work can help you quickly home in on the appropriate model, the right training algorithm to use, and a good set of hyperparameters for your task

Train a Linear Regression Model

- Using a direct “closed-form” equation that directly computes the model parameters that best fit the model to the training set
- Using an iterative optimization approach, called Gradient Descent (GD)
  - Variants:
    - Batch GD
    - Mini-batch GD
    - Stochastic GD

Linear Regression

- The target variable is continuous and expressed as a linear combination of predictors (features)

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

- The goal is to find the parameters -> θ_i which are those minimizing the function:

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

The Normal Equation

- To find the value of θ that minimizes the cost function, there is a closed-form solution

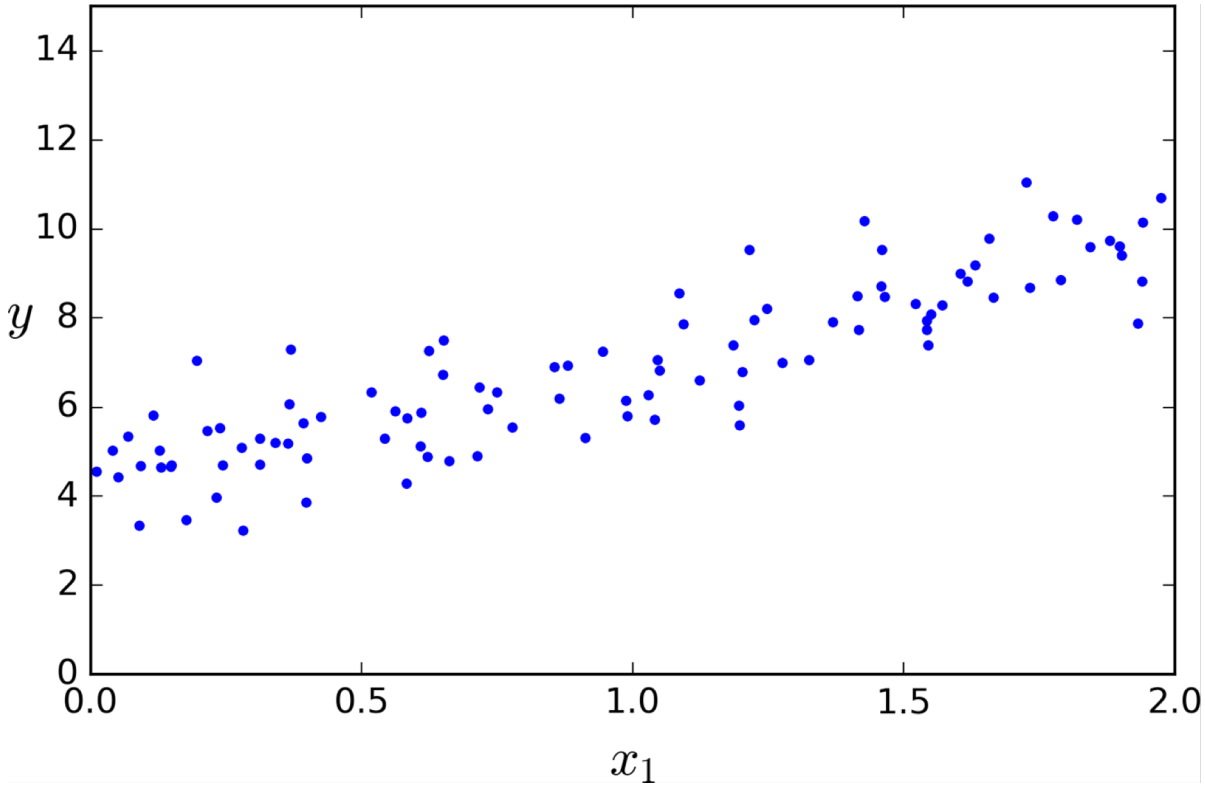
$$\hat{\theta} = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

- θhat is the value of theta that minimizes the cost function.

- y is the vector of target values containing y(1) to y(m).

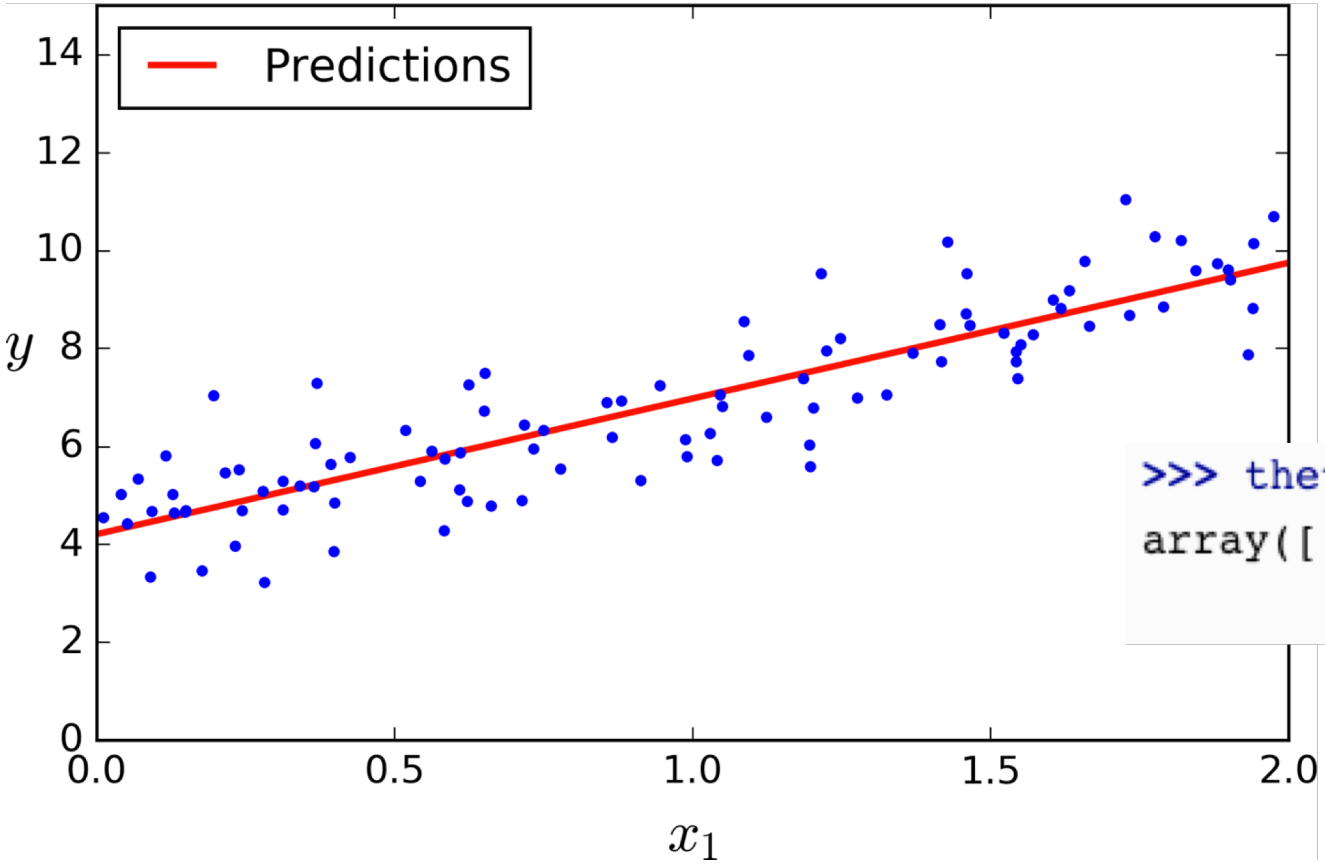
Generated Data

```
import numpy as np

X = 2 * np.random.rand(100, 1)
y = 4 + 3 * X + np.random.randn(100, 1)
```



Solve Using Normal Equation

```
X_b = np.c_[np.ones((100, 1)), X]  # add x0 = 1 to each instance
theta_best = np.linalg.inv(X_b.T.dot(X_b)).dot(X_b.T).dot(y)
```




```
>>> theta_best
array([[ 4.21509616],
       [ 2.77011339]])
```

Scikit-learn

```
>>> from sklearn.linear_model import LinearRegression
>>> lin_reg = LinearRegression()
>>> lin_reg.fit(X, y)
>>> lin_reg.intercept_, lin_reg.coef_
(array([ 4.21509616]), array([[ 2.77011339]]))
>>> lin_reg.predict(X_new)
array([[ 4.21509616],
       [ 9.75532293]])
```

Complexity

- The Normal Equation computes the inverse of $X^T \cdot X$, which is an n × n matrix
  - the computational complexity of inverting such a matrix is typically about $O(n^{2.4})$ to $O(n^3)$, depending on the implementation

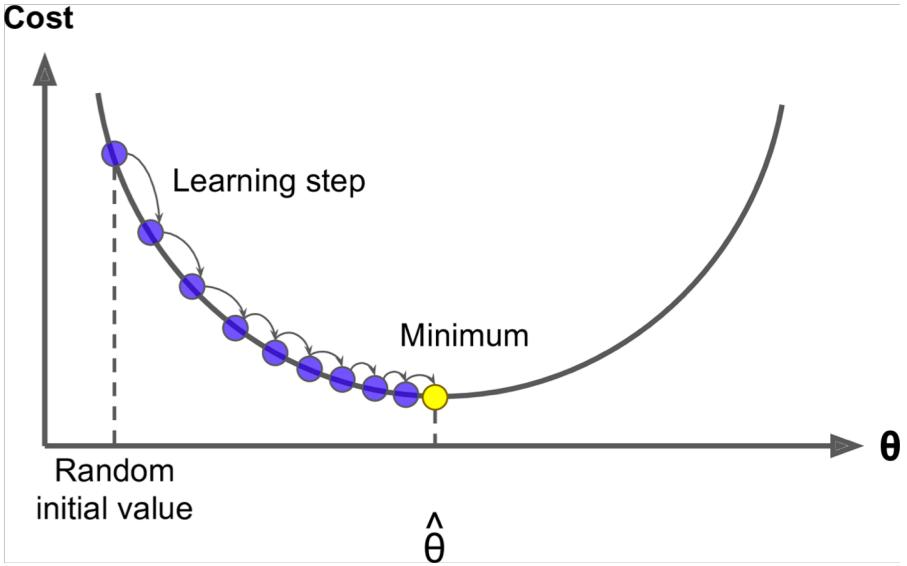
- What are some other ways of training a Linear Regression model?
  - better suited for cases where there are a large number of features
  - too many training instances to fit in memory.

Module 5 – Section 2

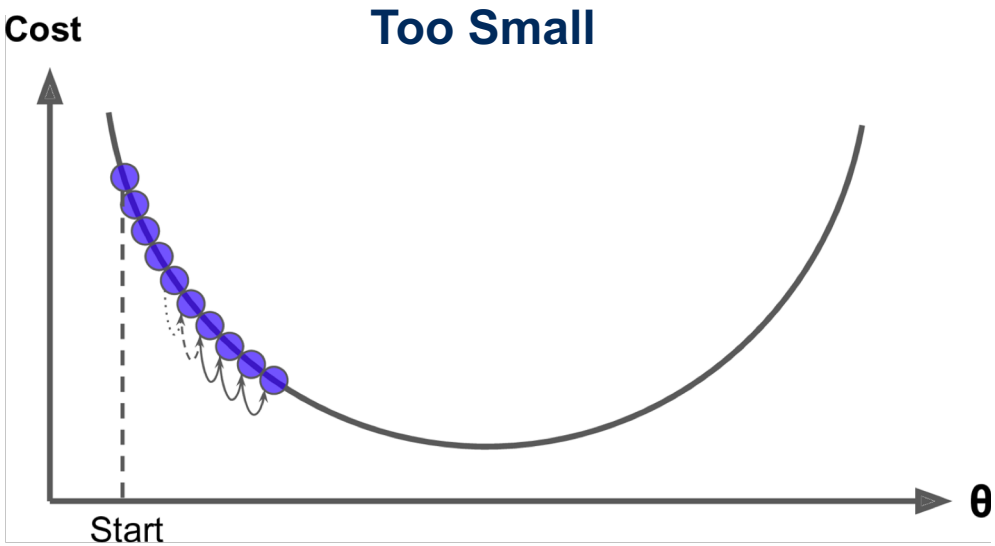
Linear Regression Using Gradient Descent

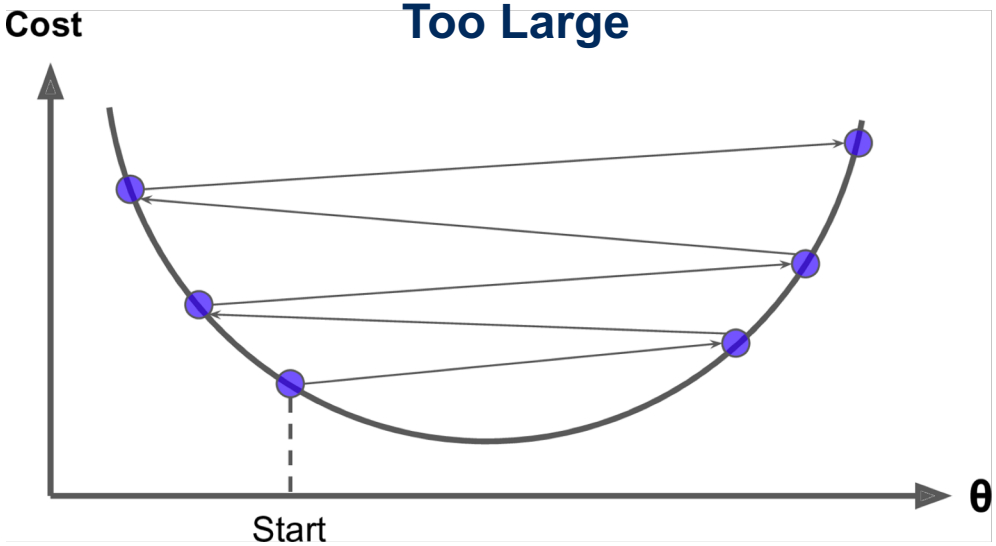
Gradient Descent

- Start by filling θ with random values
- Then you improve it gradually, by decreasing the cost function one step at a time (e.g. the MSE)
- Algorithm converges to a minimum

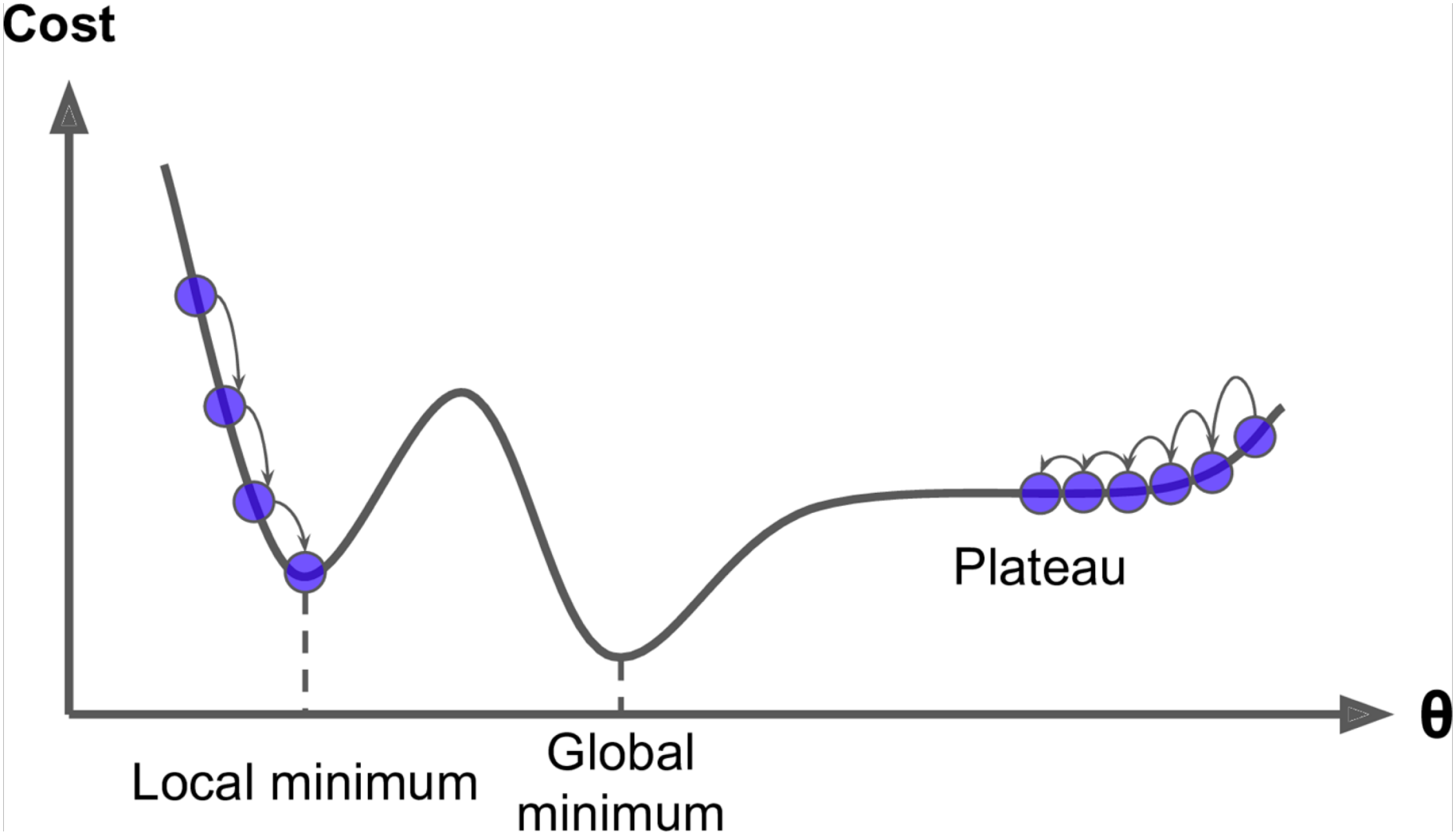


Step Size

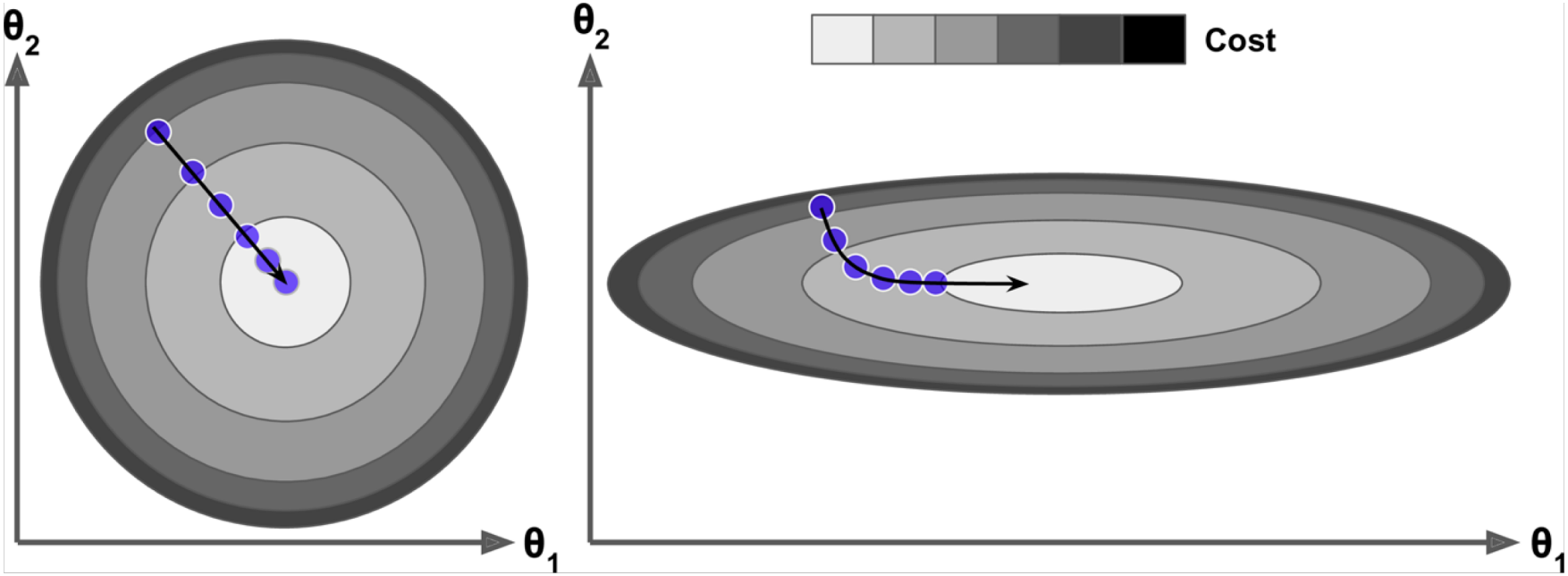




Local Minimum vs Global Minimum



MSE Cost Function is Convex



Ensure that all features have a similar scale or else it will take much longer to converge.

Batch Gradient Descent

- To implement Gradient Descent, you need to compute the gradient of the cost function with regards to each model parameter θ_j

$$\frac{\partial}{\partial \theta_j} \mathrm{MSE}(\theta) = \frac{2}{m} \sum_{i=1}^{m} (\theta^T \cdot \mathbf{x}^{(i)} - y^{(i)}) \, x_j^{(i)}$$

- Once you have the gradient vector, which points uphill, just go in the opposite direction to go downhill. This means subtracting $\nabla\theta_{MSE}(\theta)$ from θ

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

Batch Gradient Descent (cont'd)

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

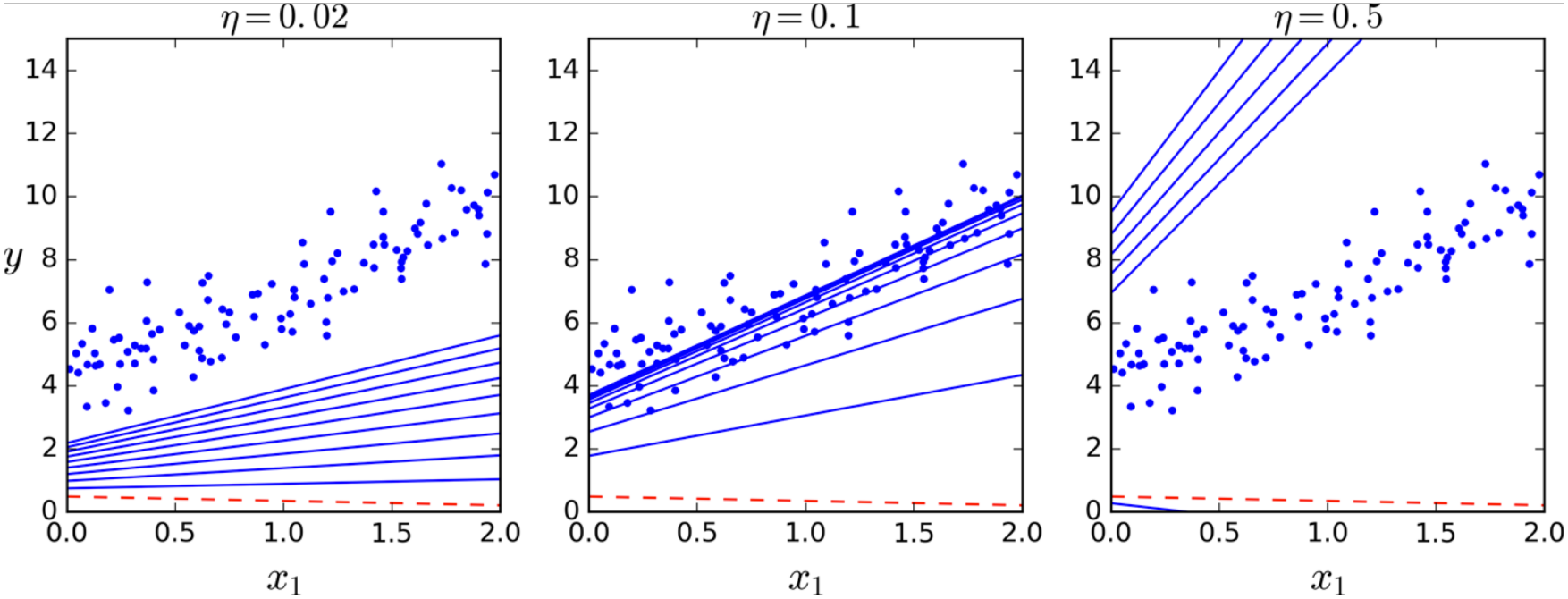
It uses the full dataset!

```
eta = 0.1  # learning rate
n_iterations = 1000
m = 100

theta = np.random.randn(2,1)  # random initialization

for iteration in range(n_iterations):
    gradients = 2/m * X_b.T.dot(X_b.dot(theta) - y)
    theta = theta - eta * gradients
```

```
>>> theta
array([[ 4.21509616],
       [ 2.77011339]])
```

Same result as Normal Eq.

Learning Rates

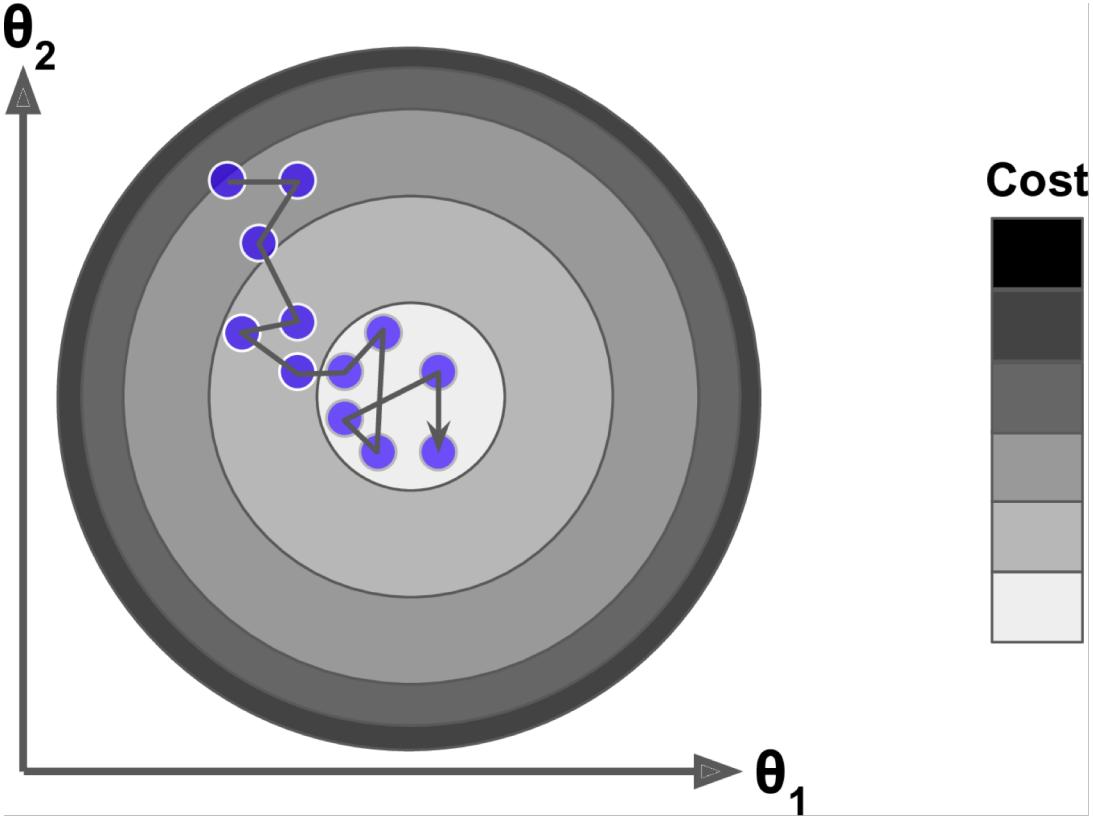


Too Small Just Right Too Big

Stochastic Gradient Descent

- Stochastic Gradient Descent picks a random instance in the training set at every step and computes the gradients based only on that single instance.
  - SGD is much faster since it has very little data to manipulate -> Makes it possible to train on huge training sets
  - SGD is much less regular than Batch Gradient Descent: instead of gently decreasing until it reaches the minimum, the cost function will bounce up and down. Over time it will end up very close to the minimum, but once it gets there it will continue to bounce around, never settling down
  - Once the algorithm stops, the final parameter values are good, but not optimal.

Stochastic Gradient Descent (cont'd)



When the cost function is very irregular, Stochastic Gradient Descent has a better chance of finding the global minimum than Batch Gradient Descent does.

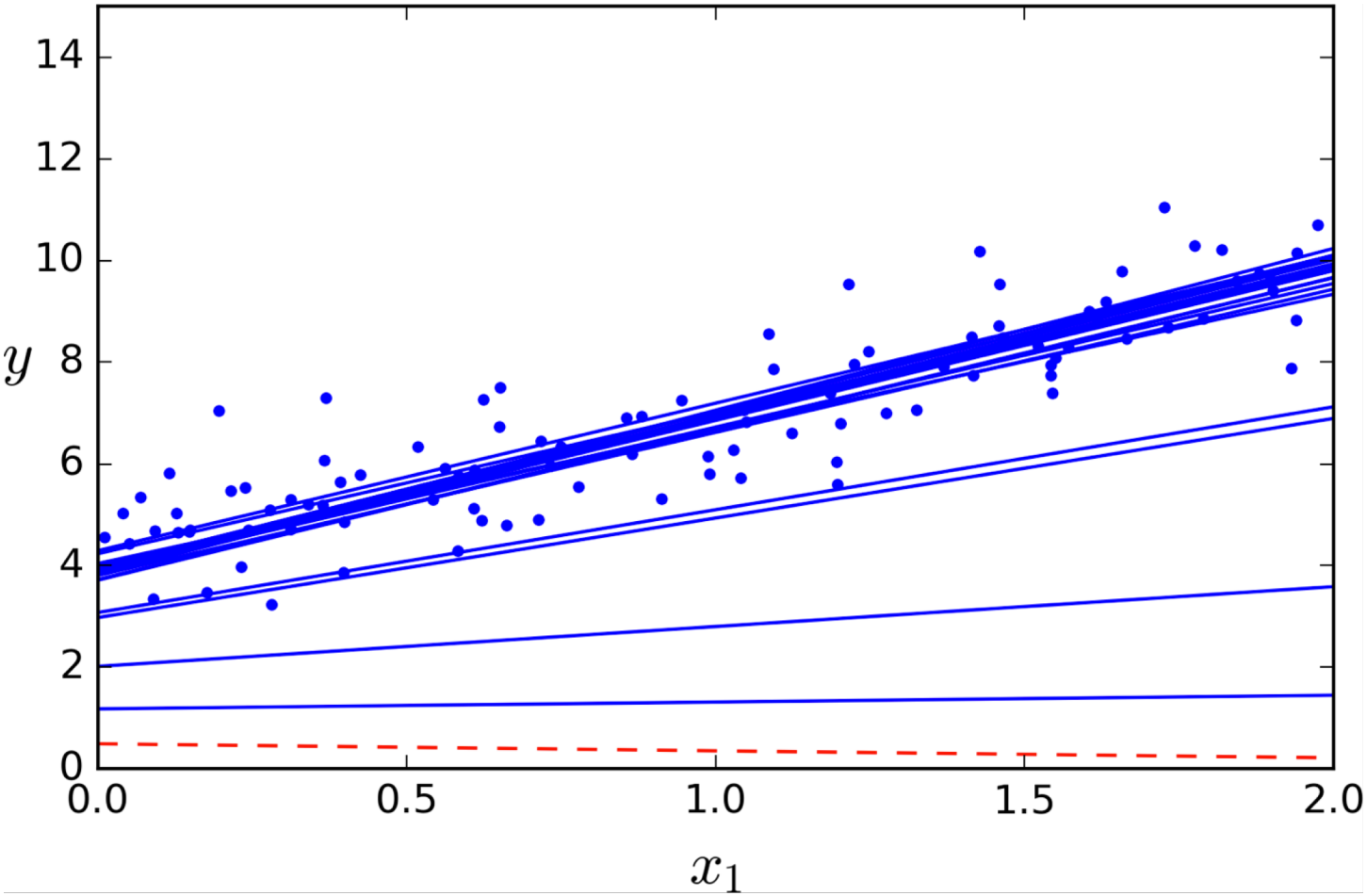
Simulated Annealing

- Randomness is good to escape from local optima, but bad because it means that the algorithm can never settle at the minimum.
- One solution to this dilemma is to gradually reduce the learning rate.
  - The steps start out large (which helps make quick progress and escape local minima)
  - Then get smaller and smaller, allowing the algorithm to settle at the global minimum.

Simulated Annealing (cont'd)

```
n_epochs = 50
t0, t1 = 5, 50  # learning schedule hyperparameters

def learning_schedule(t):
    return t0 / (t + t1)

theta = np.random.randn(2,1)  # random initialization

for epoch in range(n_epochs):
    for i in range(m):
        random_index = np.random.randint(m)
        xi = X_b[random_index:random_index+1]
        yi = y[random_index:random_index+1]
        gradients = 2 * xi.T.dot(xi.dot(theta) - yi)
        eta = learning_schedule(epoch * m + i)
        theta = theta - eta * gradients
```

Simulated Annealing (cont'd)



SGD with Scikit-Learn

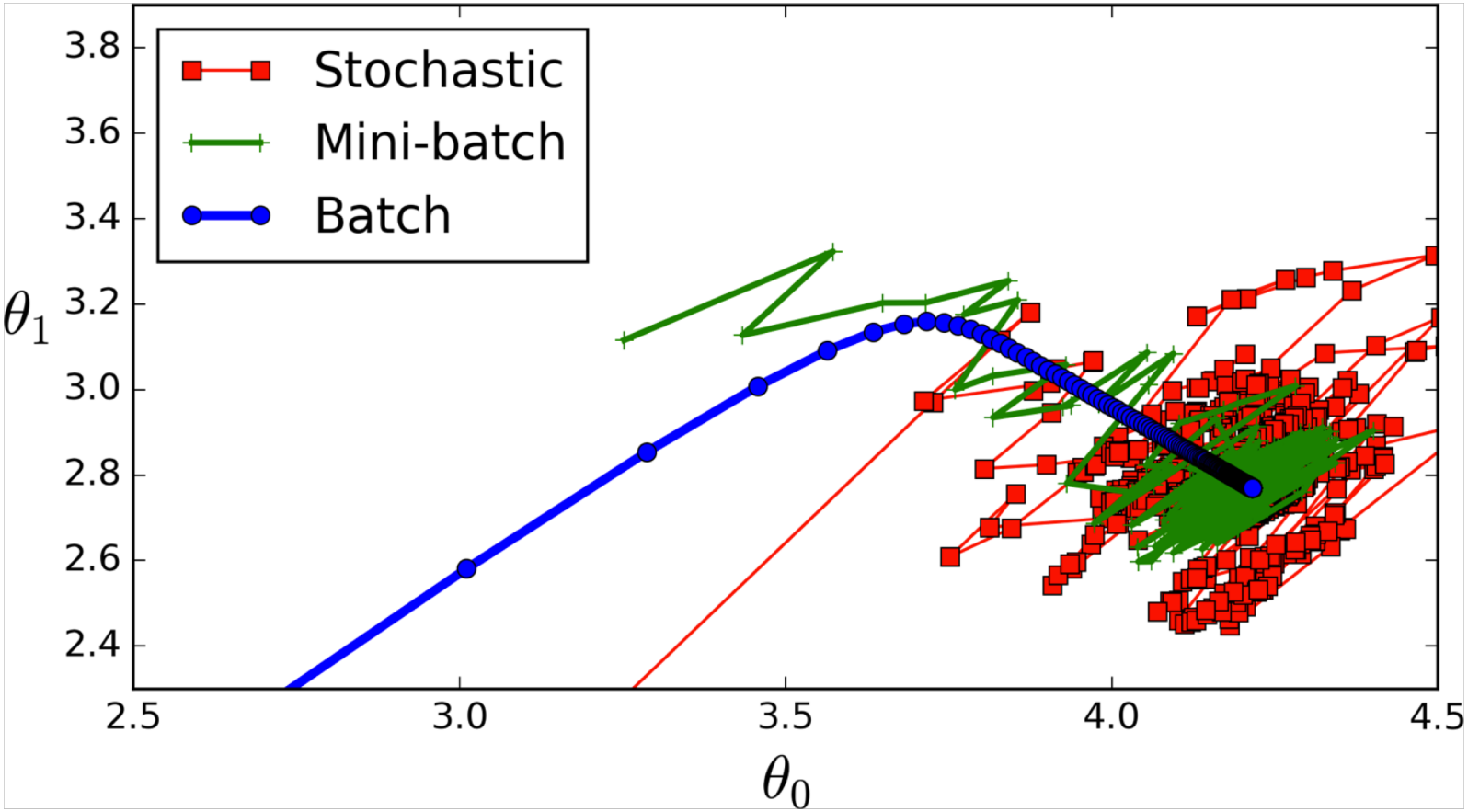
```
from sklearn.linear_model import SGDRegressor
sgd_reg = SGDRegressor(n_iter=50, penalty=None, eta0=0.1)
sgd_reg.fit(X, y.ravel())
```

```
>>> sgd_reg.intercept_, sgd_reg.coef_
(array([ 4.16782089]), array([ 2.72603052]))
```

Mini-Batch Gradient Descent

- Mini-batch GD computes the gradients on small random sets of instances called mini-batches.
- The main advantage of Mini-batch GD over Stochastic GD is that you can get a performance boost from hardware optimization of matrix operations.

Gradient Descent Comparison



Algorithm	Large *m*	Out-of-core support	Large *n*	Hyperparams	Scaling required	Scikit-Learn
Normal Equation	Fast	No	Slow	0	No	`LinearRegression`
Batch GD	Slow	No	Fast	2	Yes	n/a
Stochastic GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`
Mini-batch GD	Fast	Yes	Fast	≥2	Yes	n/a

Module 5 – Section 3

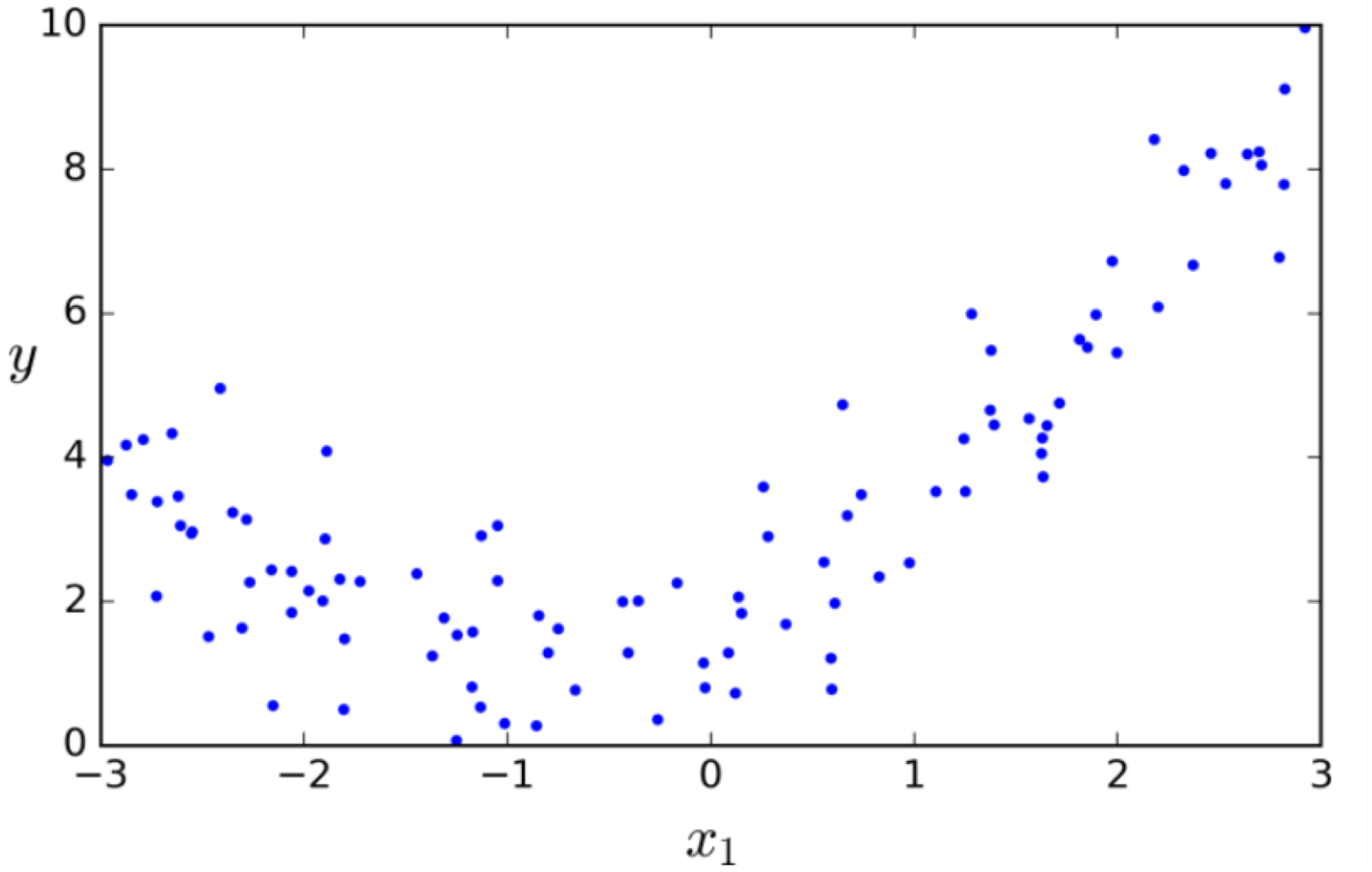
Non-Linear Regression

Polynomial Regression

- What if your data is actually more complex than a simple straight line?
  - You can actually use a linear model to fit nonlinear data by adding powers of each feature as new features, then train a linear model on this extended set of features.

Non-linear Data

```
X = 6 * np.random.rand(m, 1) - 3
y = 0.5 * X**2 + X + 2 + np.random.randn(m, 1)
```



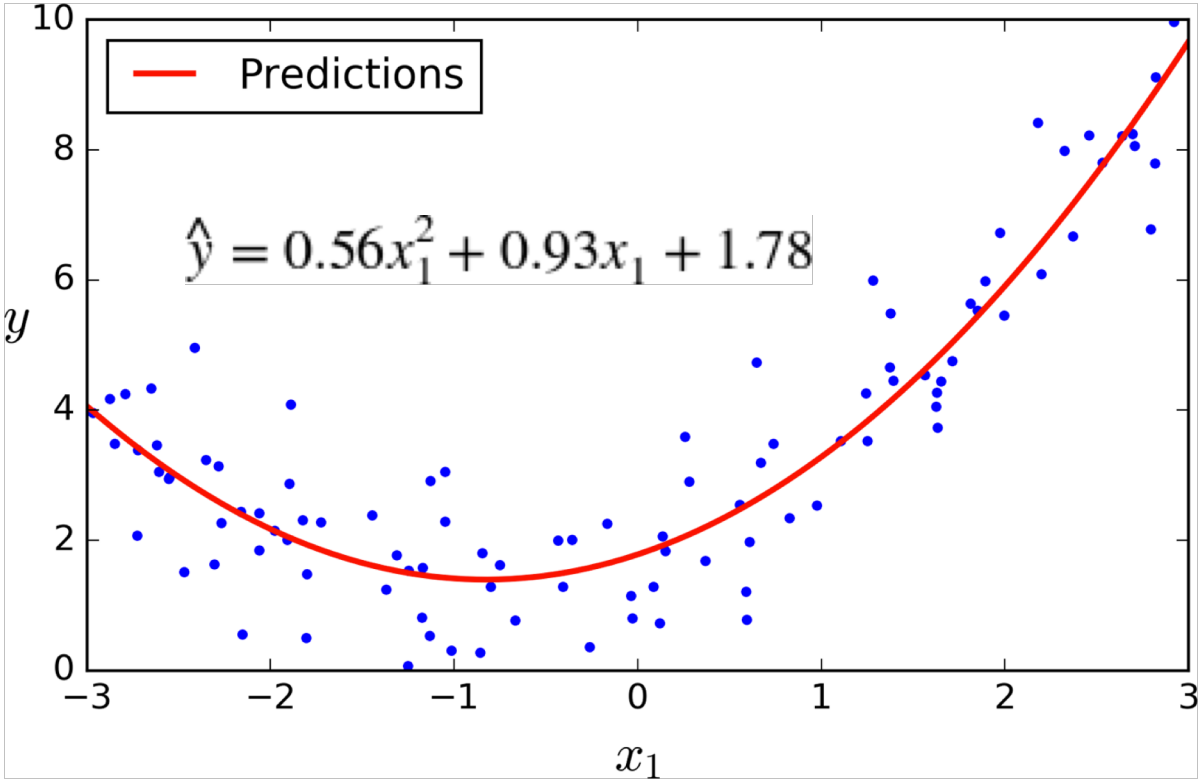
Regression

- $y = \theta_1 x^2 + \theta_2 x + c$

```
>>> from sklearn.preprocessing import PolynomialFeatures
>>> poly_features = PolynomialFeatures(degree=2, include_bias=False)
>>> X_poly = poly_features.fit_transform(X)
>>> X[0]
array([-0.75275929])
>>> X_poly[0]
array([-0.75275929,  0.56664654])
```

```
>>> lin_reg = LinearRegression()
>>> lin_reg.fit(X_poly, y)
>>> lin_reg.intercept_, lin_reg.coef_
(array([ 1.78134581]), array([[ 0.93366893,  0.56456263]]))
```

Non-linear Predictions



True data → $y = 0.5x_1^2 + 1.0x_1 + 2.0 +$ Gaussian noise

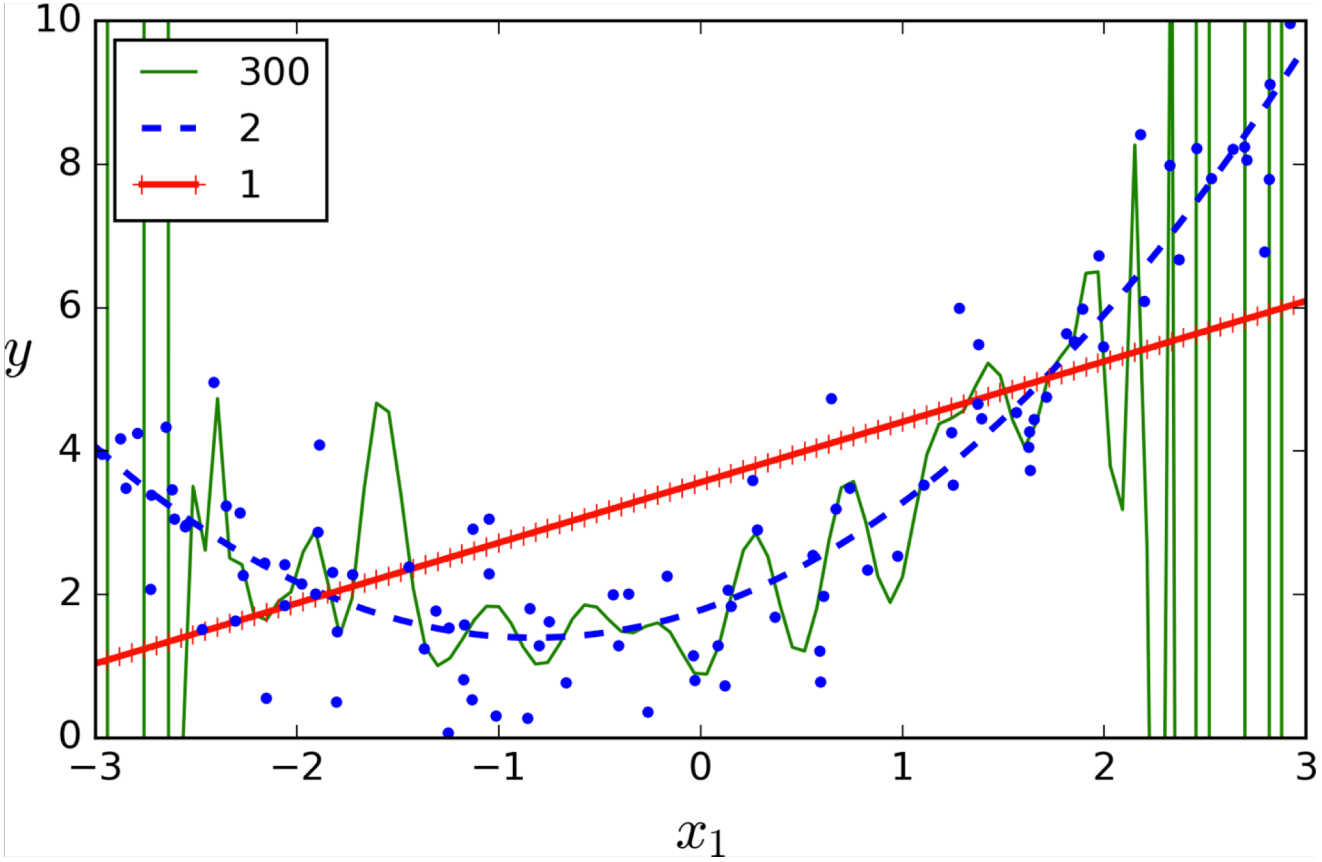
Module 5 – Section 4

Learning Curves

Learning Curves

- ML models can vary in complexity
- Linear regression is the simplest model
- Non-linear transformations of the features can increase the complexity
- The generalization error (on test data) of a model depends on the noise of the data (regardless of the model), and on the model itself

Learning Curves (cont'd)



Bias and Variance

- **Bias**: error due to wrong assumptions, such as assuming that the data is linear when it is actually quadratic. A high-bias model is most likely to underfit the training data.
- **Variance**: error due to the model's excessive sensitivity to small variations in the training data. A model with many degrees of freedom is likely to have high variance, and thus to overfit the training data.
- Irreducible error: due to the noisiness of the data itself. The only way to reduce this part of the error is to clean up the data.

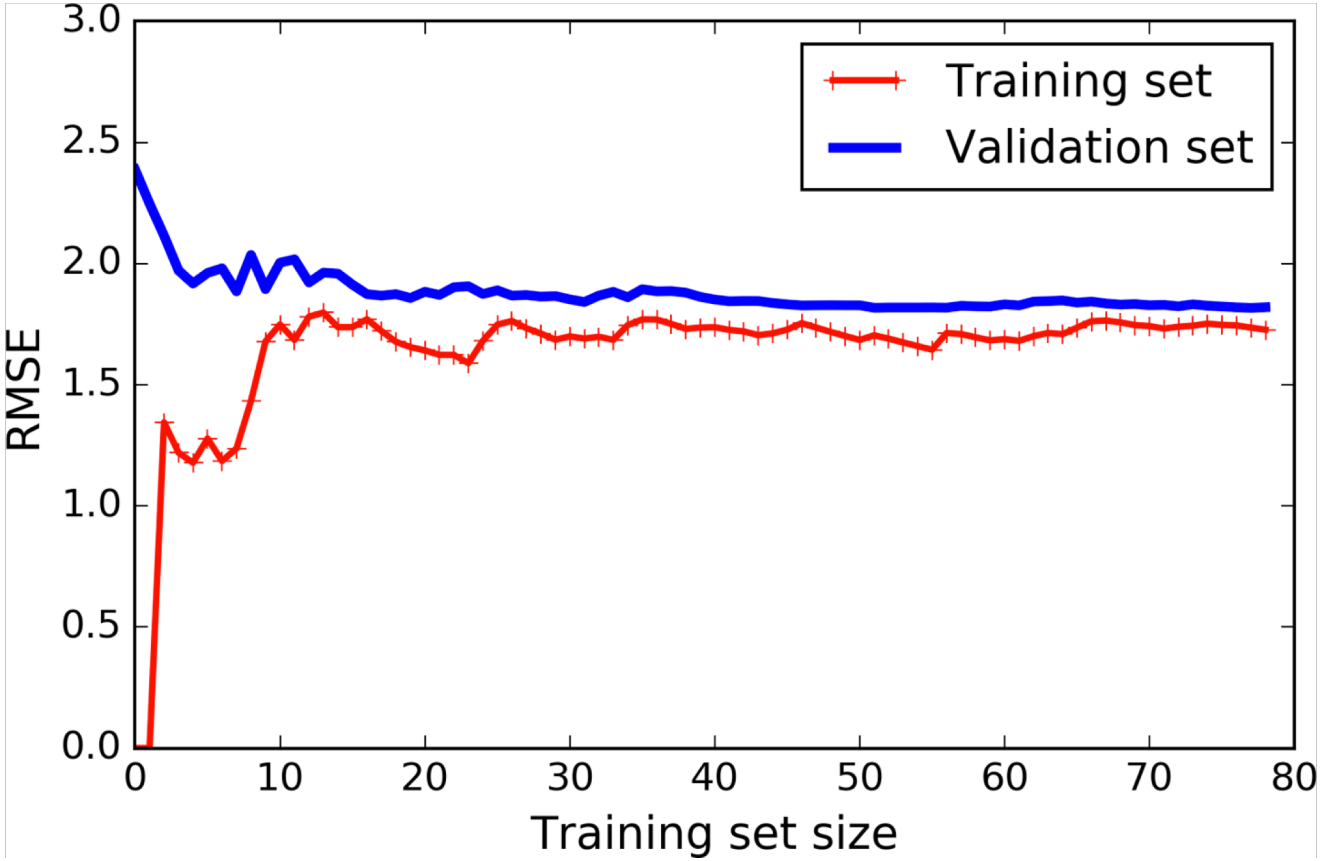
Learning Curves (cont'd)

- The model's contribution to the error is decomposed into: Bias + Variance
- Bias is the error due to a model simpler than the phenomena being predicted
- Variance is the error due to a model that learns the nuances/noise of the data
- Over-fitting relates to high variance models
- Underfitting relates to high bias models

Learning Curves (cont'd)

```
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import train_test_split

def plot_learning_curves(model, X, y):
    X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.2)
    train_errors, val_errors = [], []
    for m in range(1, len(X_train)):
        model.fit(X_train[:m], y_train[:m])
        y_train_predict = model.predict(X_train[:m])
        y_val_predict = model.predict(X_val)
        train_errors.append(mean_squared_error(y_train_predict, y_train[:m]))
        val_errors.append(mean_squared_error(y_val_predict, y_val))
    plt.plot(np.sqrt(train_errors), "r-+", linewidth=2, label="train")
    plt.plot(np.sqrt(val_errors), "b-", linewidth=3, label="val")
```

Learning Curves - Underfit



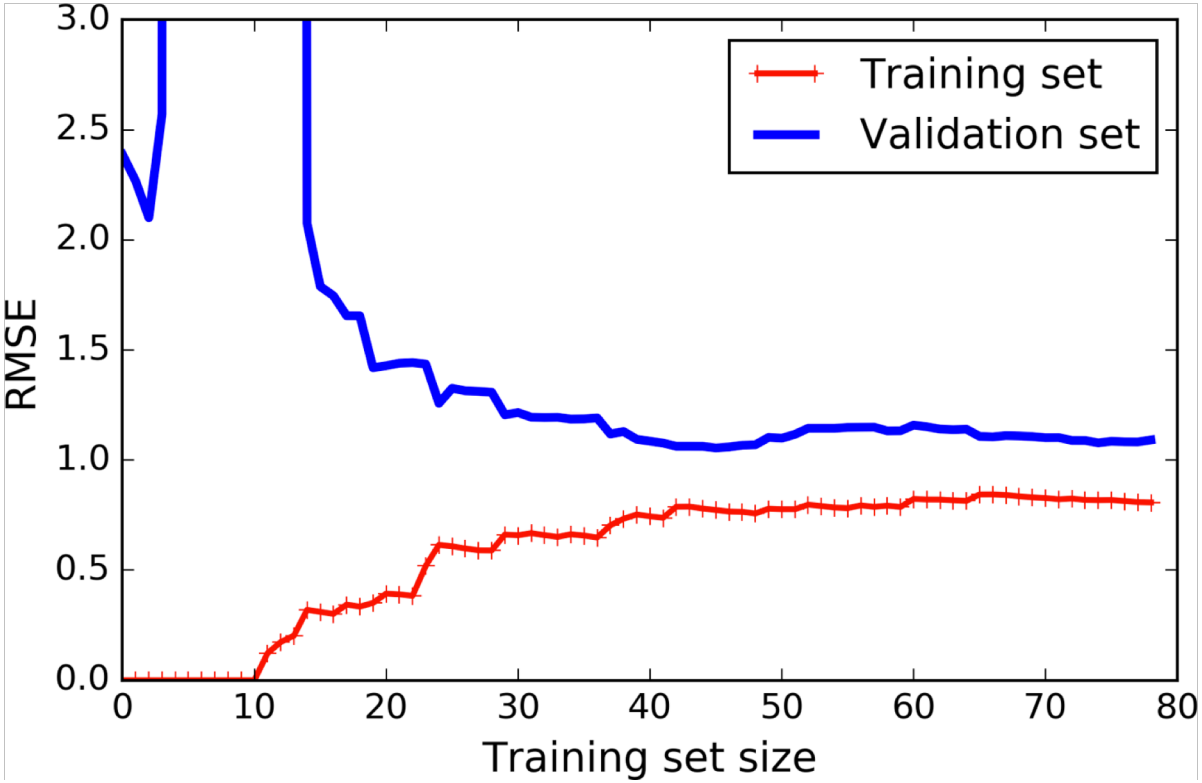
These learning curves are typical of an underfitting model. Both curves have reached a plateau; they are close and fairly high.

Learning Curves (cont'd)

- Now let's look at the learning curves of a 10th-degree polynomial model on the same data

```
from sklearn.pipeline import Pipeline

polynomial_regression = Pipeline([
        ("poly_features", PolynomialFeatures(degree=10, include_bias=False)),
        ("lin_reg", LinearRegression()),
    ])

plot_learning_curves(polynomial_regression, X, y)
```

Learning Curves - Overfit



One way to improve an overfitting model is to feed it more training data until the validation error reaches the training error.

Learning Curves (cont'd)

- Learning Curves helps figuring out if there is over-fit or under-fit
- The training and validation errors are plotted as a function of the training data size
- Under-fitting models have both high training and validation error
- Over-fitting models have low training error but high validation error

Module 5 – Section 5

Regularization and Ridge Regression

Regularization

- With too many features and their non-linear transformations, over-fitting is possible
- Learning Curves can detect over-fitting, but it is not a method to fix the problem
- Regularization is a method to fix it
- The idea is to penalize coefficients that do not contribute much reducing the generalization error (cross-validation)
- This helps not using the model to learn just nuances exclusive to the training set

Regularization

- Digression: Learning Curves on other hyperparameter values (instead of the training set size) can be used to fix over-fitting
- E.g.: Plot Learning Curves of train and valid error with respect to the number of hidden nodes in a 1-hidden layer NN

Ridge Regression

- The hyperparameter α controls how much you want to regularize the model.
  - If α = 0 then Ridge Regression is just Linear Regression.
  - If α is very large, then all weights end up very close to zero and the result is a flat line going through the data's mean.

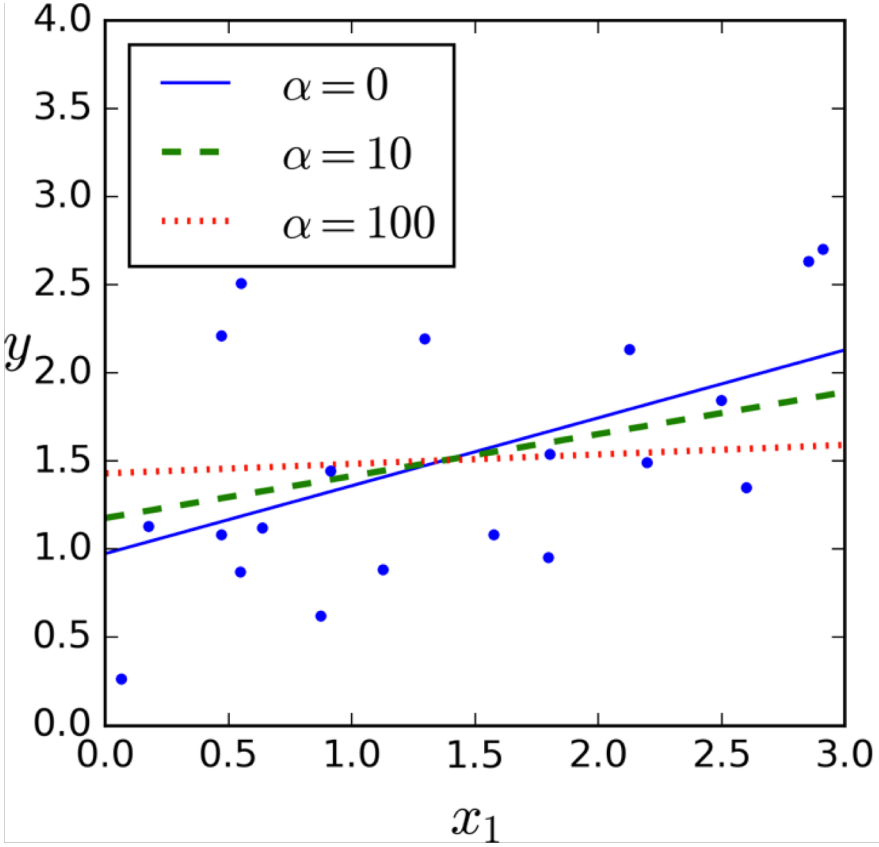
$$J(\theta) = \text{MSE}(\theta) + \alpha \frac{1}{2} \sum_{i=1}^{n} \theta_i^2$$

Ridge Regression (cont'd)

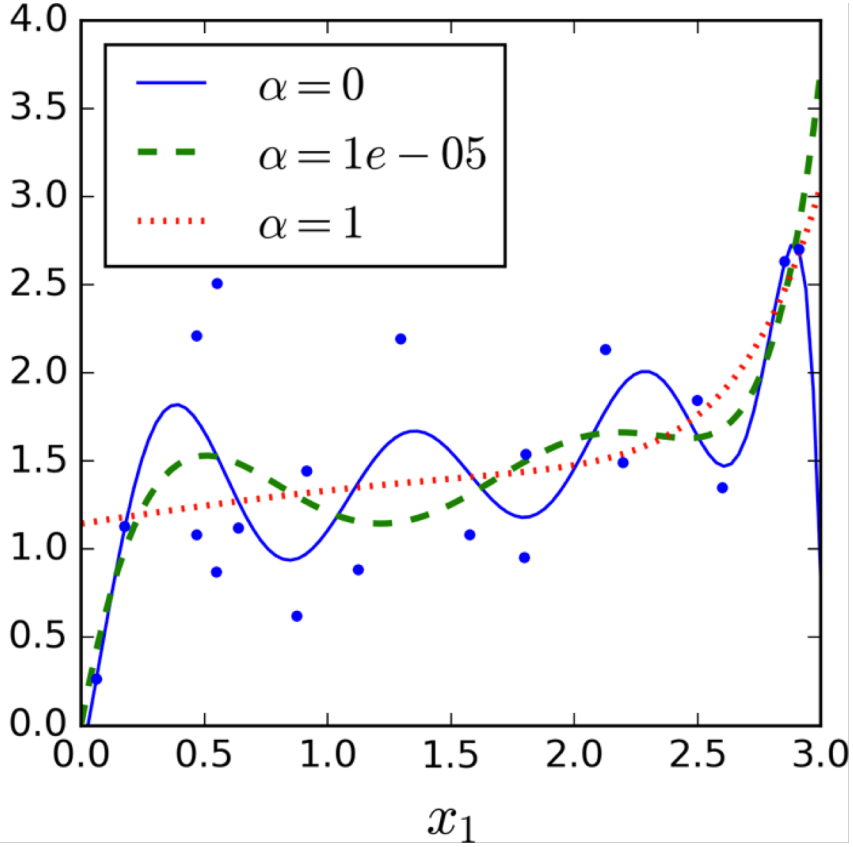
- The parameter alpha is calibrated via cross-validation (e.g. k-fold)
- Higher values of alpha increase bias
- Under all regularization methods, scaling features is recommended, since the solution is scale dependent
- Normal equation

$$\hat{\theta} = (\mathbf{X}^T \cdot \mathbf{X} + \alpha \mathbf{A})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

Ridge Regression (cont'd)



Various alpha values. Linear features



Data is first expanded using PolynomialFeatures(degree=10)

Lasso Regression

- Least Absolute Shrinkage and Selection Operator:
  - adds a regularization term to the cost function, but it uses the ℓ1 norm of the weight vector

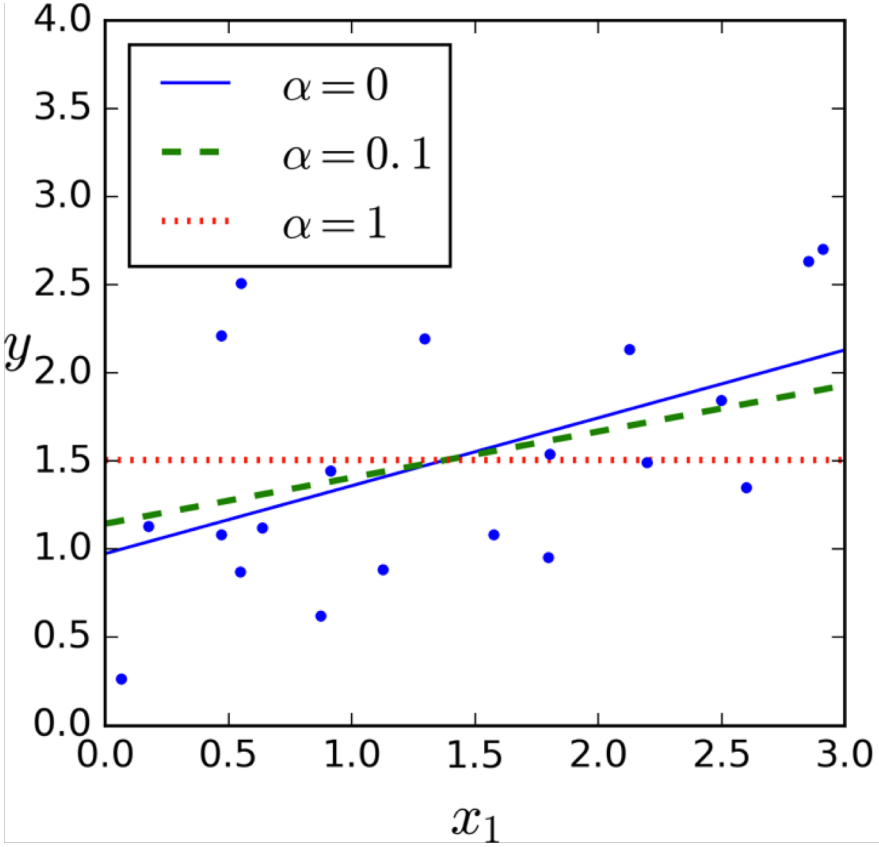
- Cost function

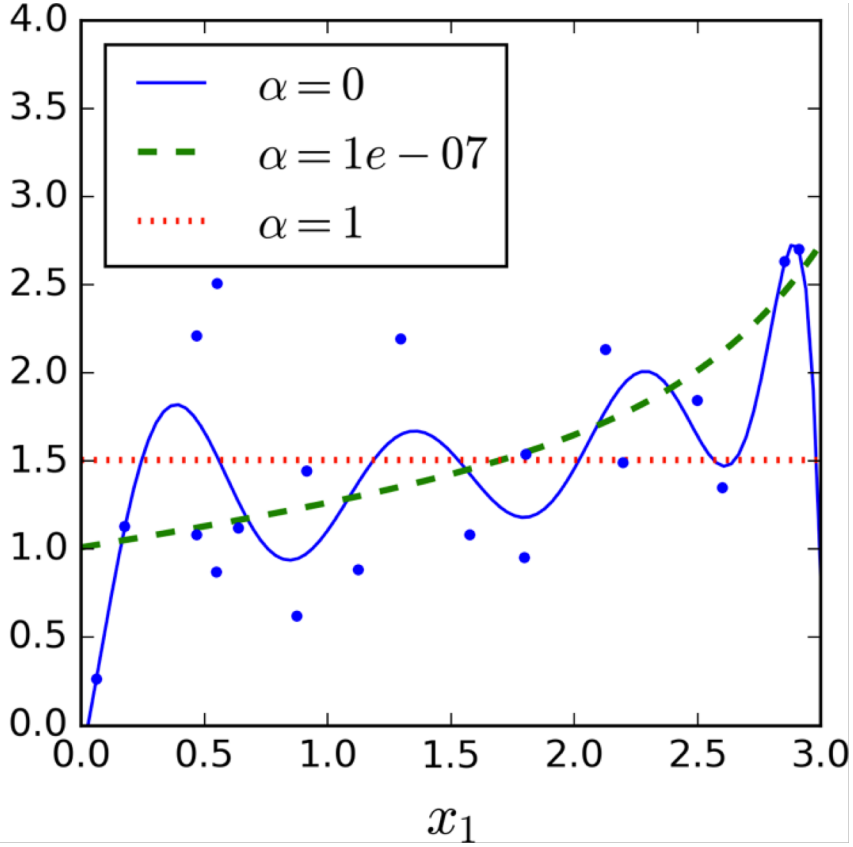
$$J(\theta) = \text{MSE}(\theta) + \alpha \sum_{i=1}^{n} | \theta_i |$$

Feature Selection with Lasso

- An important characteristic of Lasso Regression is that it tends to completely eliminate the weights of the least important features
  - Lasso Regression automatically performs feature selection and outputs a sparse model

Lasso Regression

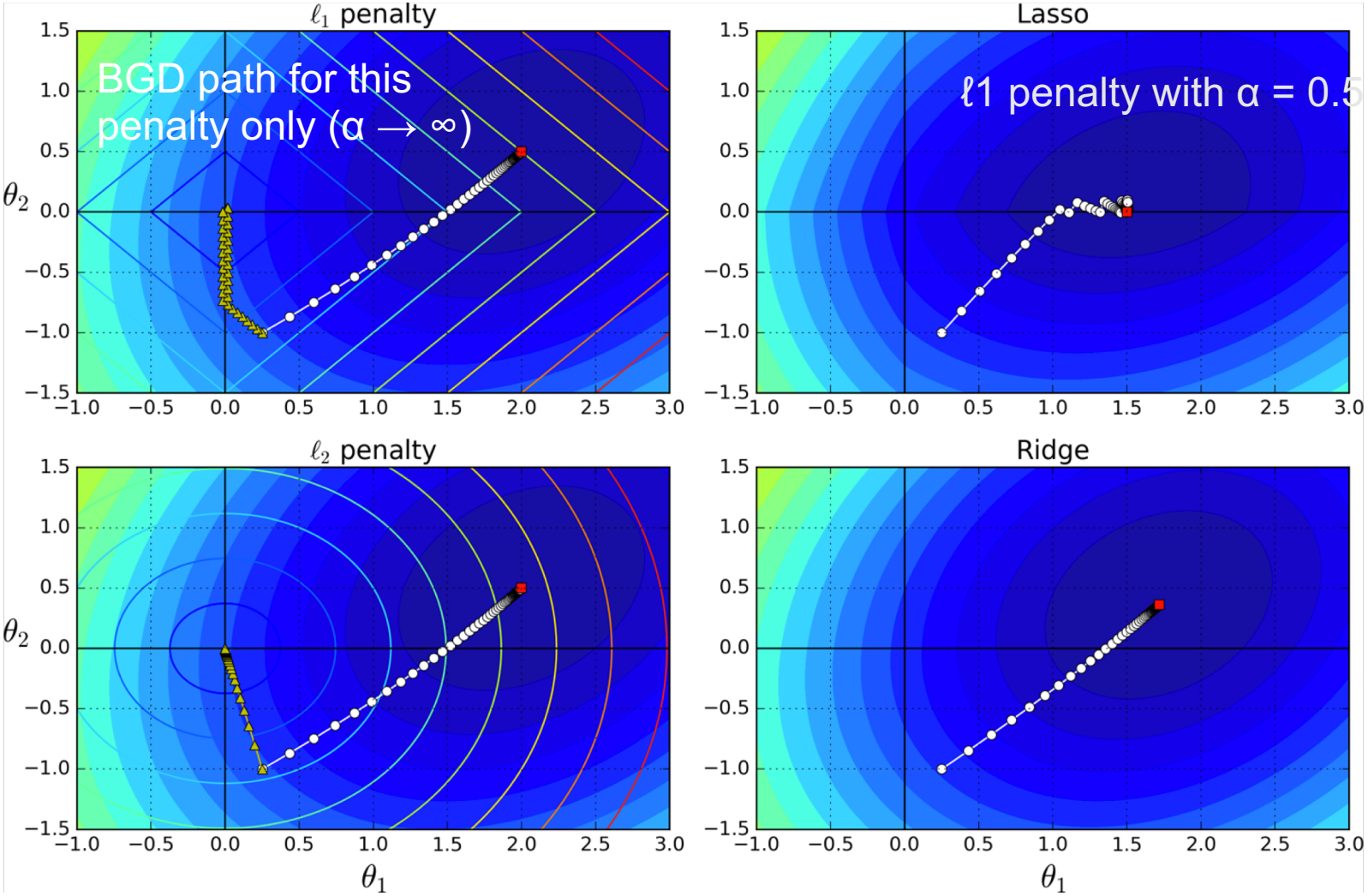




Various alpha values. Linear features

Data is first expanded using PolynomialFeatures(degree=10)

L1 vs. L2 Penalty



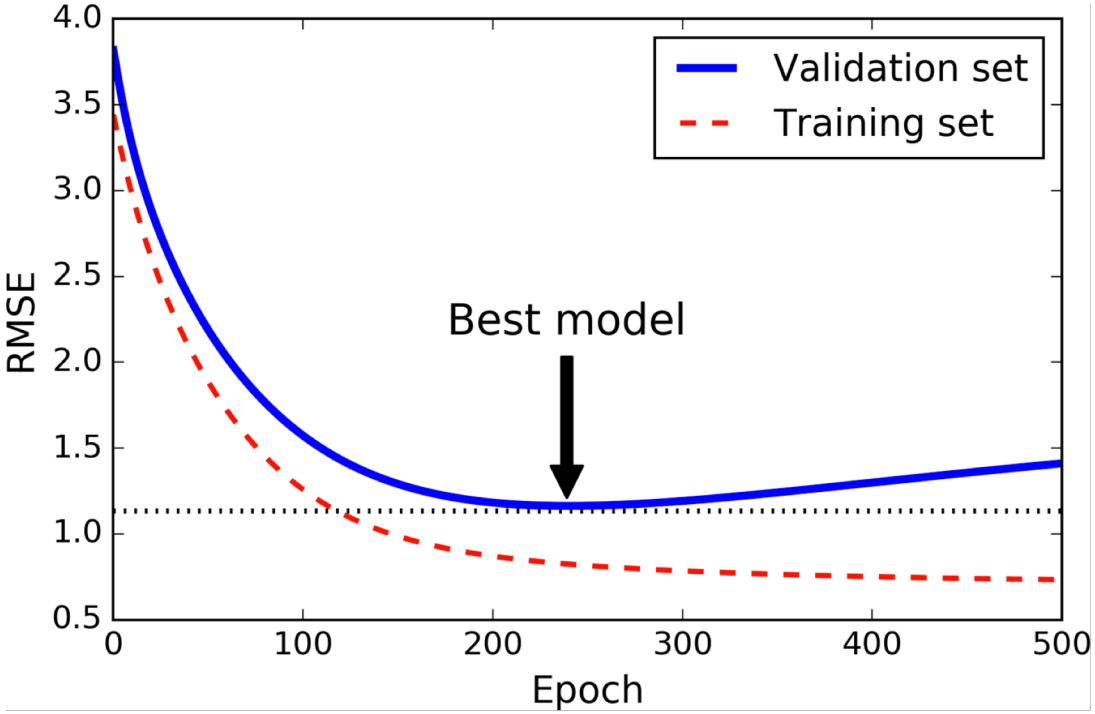
Elastic Net

- Middle ground between Ridge Regression and Lasso Regression.
  - The regularization term is a mix of both
  - You can control the mix ratio r.
    - When r = 0, Elastic Net is equivalent to Ridge Regression,
    - When r = 1, it is equivalent to Lasso Regression

$$J(\theta) = \text{MSE}(\theta) + r\alpha \sum_{i=1}^{n} |\theta_i| + \frac{1-r}{2}\alpha \sum_{i=1}^{n} \theta_i^2$$

Early Stopping

- Stop training as soon as the validation error reaches a minimum



Early Stopping

```
from sklearn.base import clone

sgd_reg = SGDRegressor(n_iter=1, warm_start=True, penalty=None,
                       learning_rate="constant", eta0=0.0005)

minimum_val_error = float("inf")
best_epoch = None
best_model = None
for epoch in range(1000):
    sgd_reg.fit(X_train_poly_scaled, y_train)  # continues where it left off
    y_val_predict = sgd_reg.predict(X_val_poly_scaled)
    val_error = mean_squared_error(y_val_predict, y_val)
    if val_error < minimum_val_error:
        minimum_val_error = val_error
        best_epoch = epoch
        best_model = clone(sgd_reg)
```

Module 5 – Section 6

Logistic Regression

Logistic Regression

- A linear model for binary classification
- It learns from examples with labels {0,1}
- Predicts probabilities of new examples having label 1
- A threshold on the probability yields a binary classification
- It is exactly the algorithm for a binary classification Neural Network with no hidden layers

Logistic Regression (cont'd)

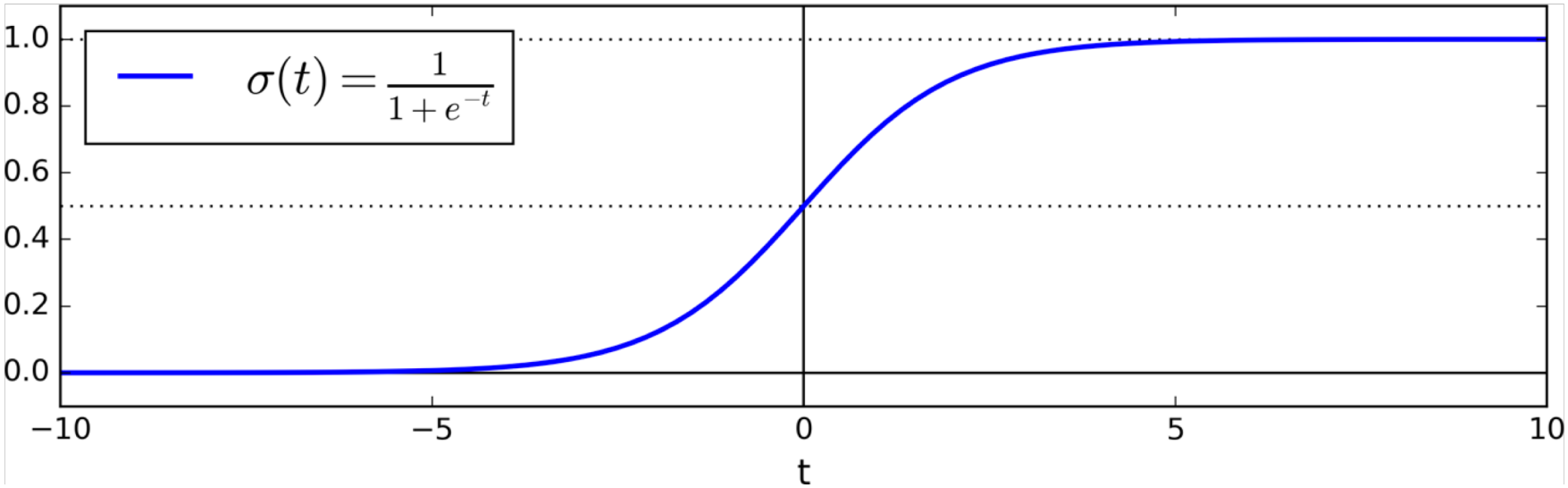
- The model computes a weighted sum of the input features (plus a bias term):
  - but instead of outputting the result directly, it outputs the logistic of this result

$$\hat{p} = h_\theta(\mathbf{x}) = \sigma(\theta^T \cdot \mathbf{x})$$

  - where

$$\sigma(t) = \frac{1}{1 + \exp(-t)}$$

Logistic Function



Cost Function

- The objective of training is to set the parameter vector θ so that the model estimates high probabilities for positive instances (y = 1) and low probabilities for negative instances (y = 0)

$$c(\theta) = \begin{cases} -\log(\hat{p}) & \text{if } y = 1, \\ -\log(1 - \hat{p}) & \text{if } y = 0. \end{cases}$$

- over the whole training set :

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}log(\hat{p}^{(i)}) + (1 - y^{(i)})log(1 - \hat{p}^{(i)})]$$

Logistic Regression (cont'd)

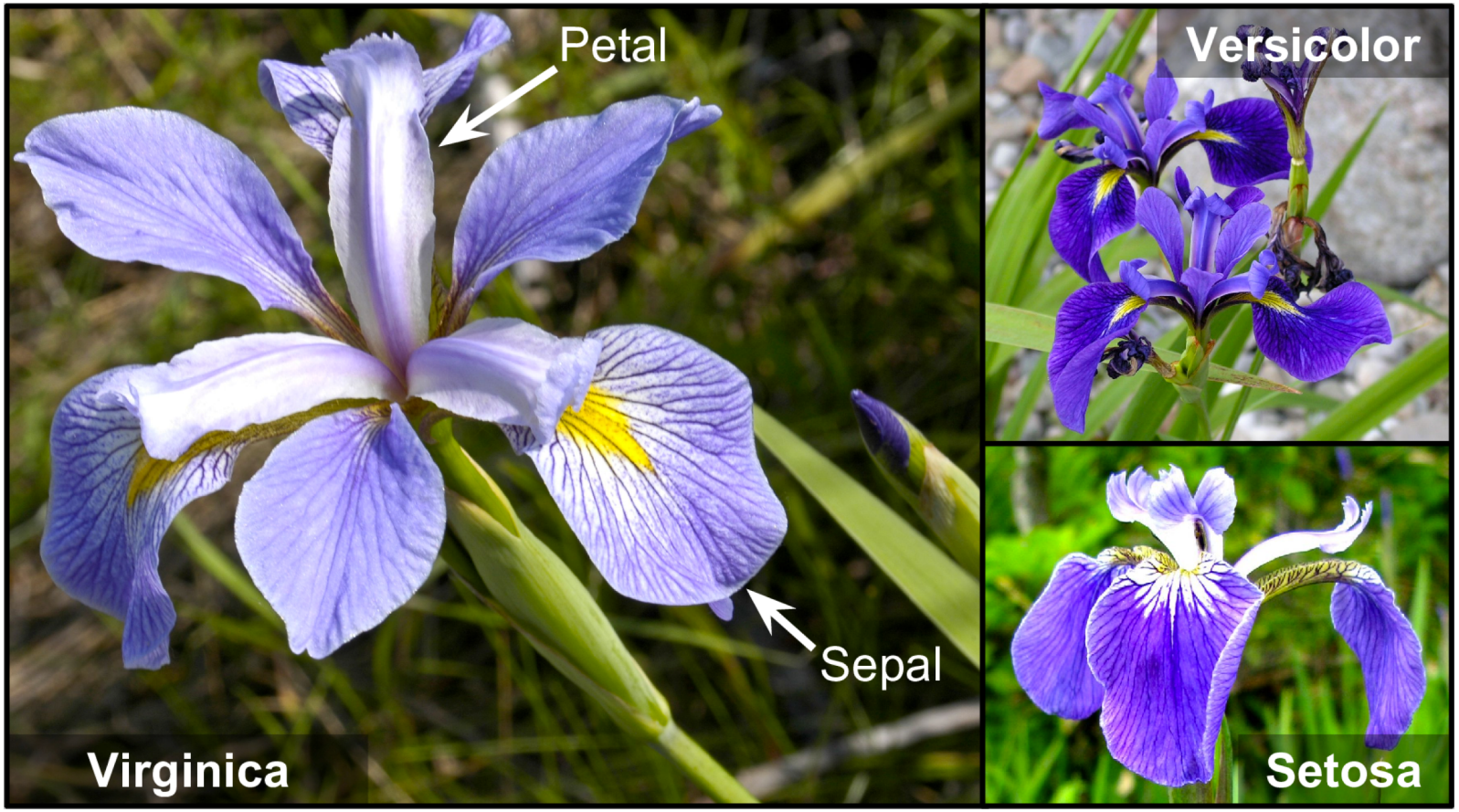
- The cost function is convex, so Gradient Descent is guaranteed to find the global minimum (if the learning rate is not too large and you wait long enough).

$$\frac{\partial}{\partial \theta_j} \mathrm{J}(\theta) = \frac{1}{m} \sum_{i=1}^{m} (\sigma(\theta^T \cdot \mathbf{x}^{(i)}) - y^{(i)})\, x_j^{(i)}$$

Logistic Regression (cont'd)

- The solution of logistic regression finds a hyperplane separating both classes
- The hyperplane is the decision boundary
- Points in the decision boundary:
  - If the product is negative, the class is 0, if it positive the class is 1
  - The sigmoid function maps the product to [0,1] (a probability)

1-d Logistic Example



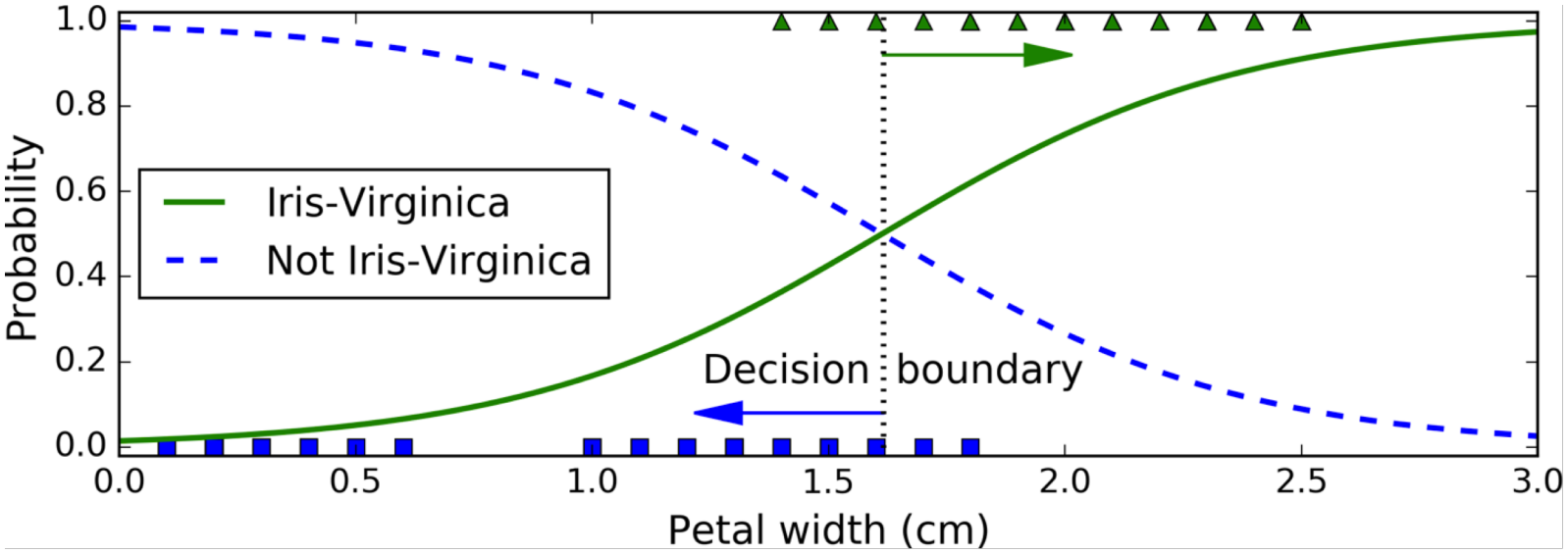
1-d Logistic Example

```
>>> from sklearn import datasets
>>> iris = datasets.load_iris()
>>> list(iris.keys())
['data', 'target_names', 'feature_names', 'target', 'DESCR']
>>> X = iris["data"][:, 3:]  # petal width
>>> y = (iris["target"] == 2).astype(np.int)  # 1 if Iris-Virginica, else 0
```

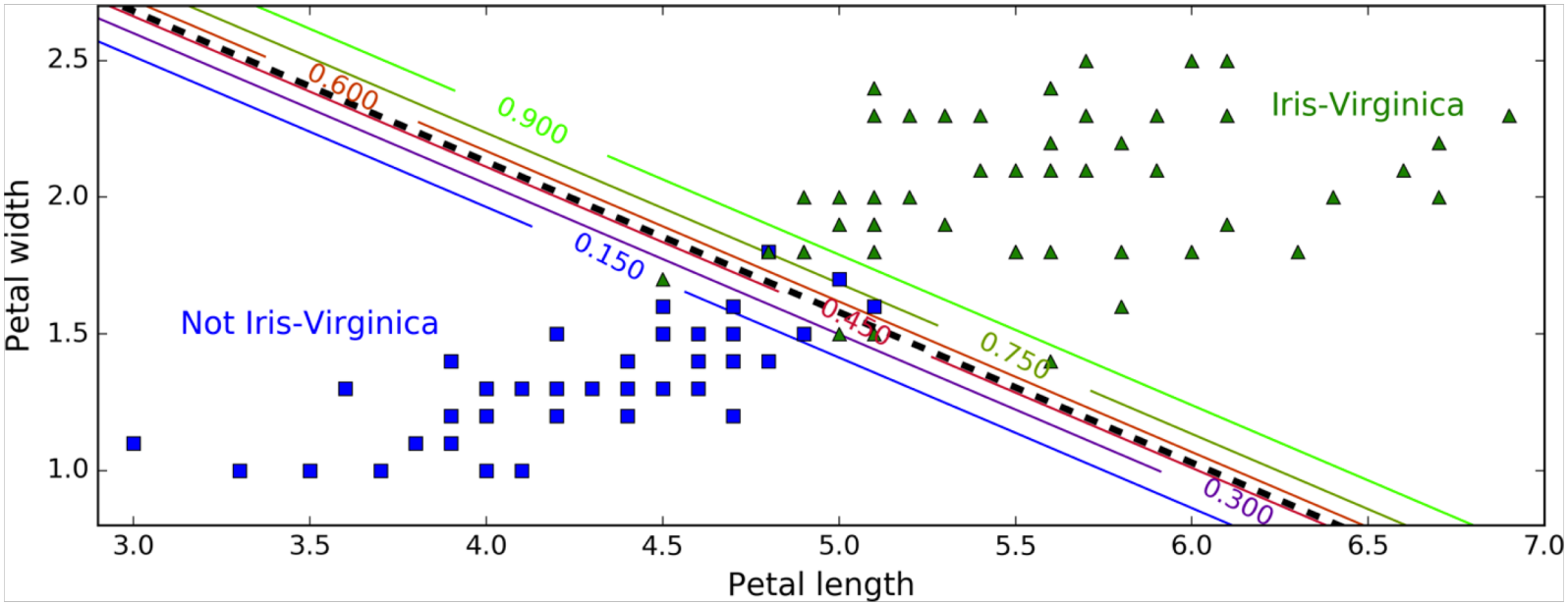
```
from sklearn.linear_model import LogisticRegression

log_reg = LogisticRegression()
log_reg.fit(X, y)
```

1-d Logistic Example

```
X_new = np.linspace(0, 3, 1000).reshape(-1, 1)
y_proba = log_reg.predict_proba(X_new)
plt.plot(X_new, y_proba[:, 1], "g-", label="Iris-Virginica")
plt.plot(X_new, y_proba[:, 0], "b--", label="Not Iris-Virginica")
```



2-d Logistic Example



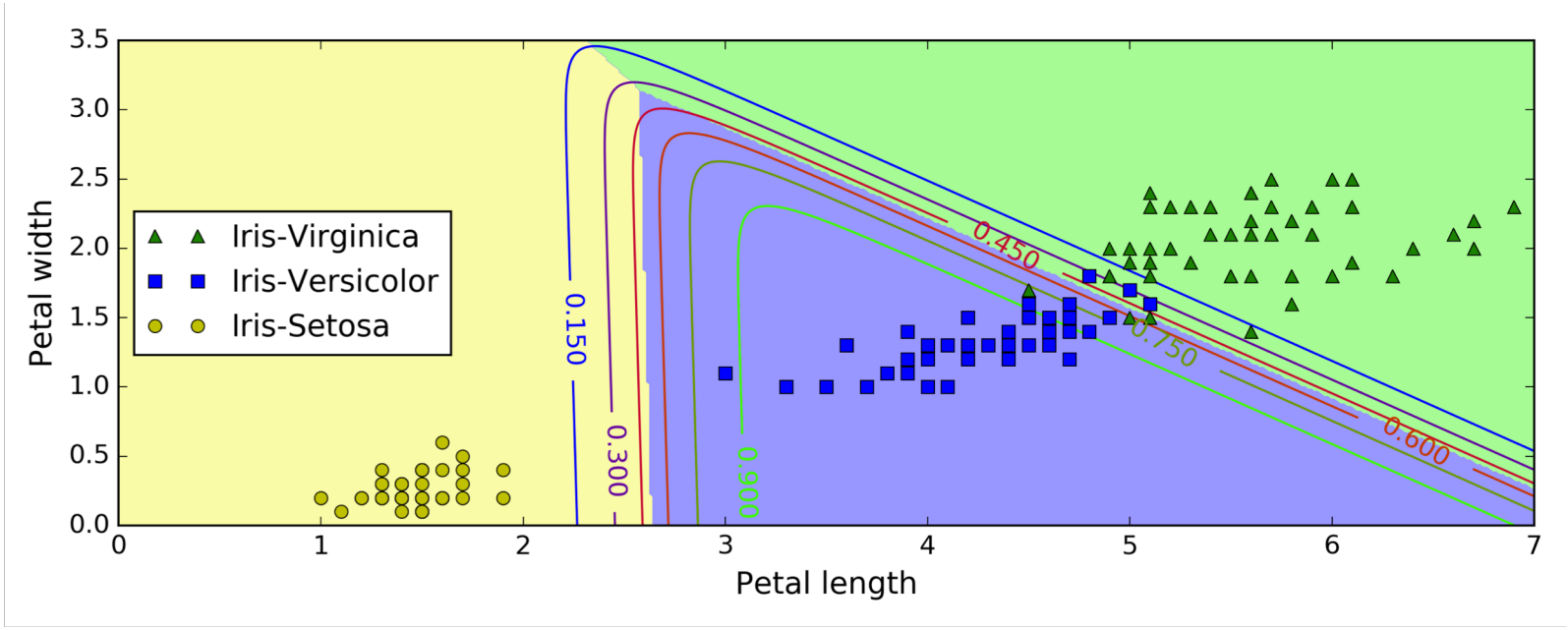
Softmax Regression

- LR model can be generalized to support multiple classes directly. This is called Softmax Regression, or Multinomial Logistic Regression.
- When given an instance x, the Softmax Regression model first computes a score $s_k(x)$ for each class k, then estimates the probability of each class by applying the softmax

$$s_k(\mathbf{x}) = (\theta^{(k)})^T \cdot \mathbf{x}$$

Softmax Regression (cont'd)

$$\hat{p}_k = \sigma(\mathbf{s}(\mathbf{x}))_k = \frac{\exp\left(s_k(\mathbf{x})\right)}{\sum_{j=1}^{K} \exp\left(s_j(\mathbf{x})\right)}$$



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Module 5 – Section 7

Resources and Wrap-up

Resources

- Hands-On Machine Learning with Scikit-Learn and TensorFlow

Homework

- Complete the notebook in the assignments section for this week

Next Class

- Support Vector Machines
  - Chapter 5 textbook

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