Advanced Data Analysis

DATA 71200

Class 6: k-Nearest Neighbors and Linear Models

Supervised Learning

- **Learning paradigm where we have example input/output pairs to learn from**
- **Classification predicts a class label**
  - Binary example: is this email spam? yes/no
  - Multiclass example: what is the species of this flower?
- **Regression predicts a *continuous* number**
  - Example: what is the value of a house given a set of features?

Generalization

- **Generalization - a model's ability to make accurate predictions on unseen data**
- **Typically we want to find the simplest effective model**
- **Model complexity**
  - **Underfitting - when a model is too simple to represent the training data**
  - **Overfitting - when a model is too specific to the training data to generalize to new data**

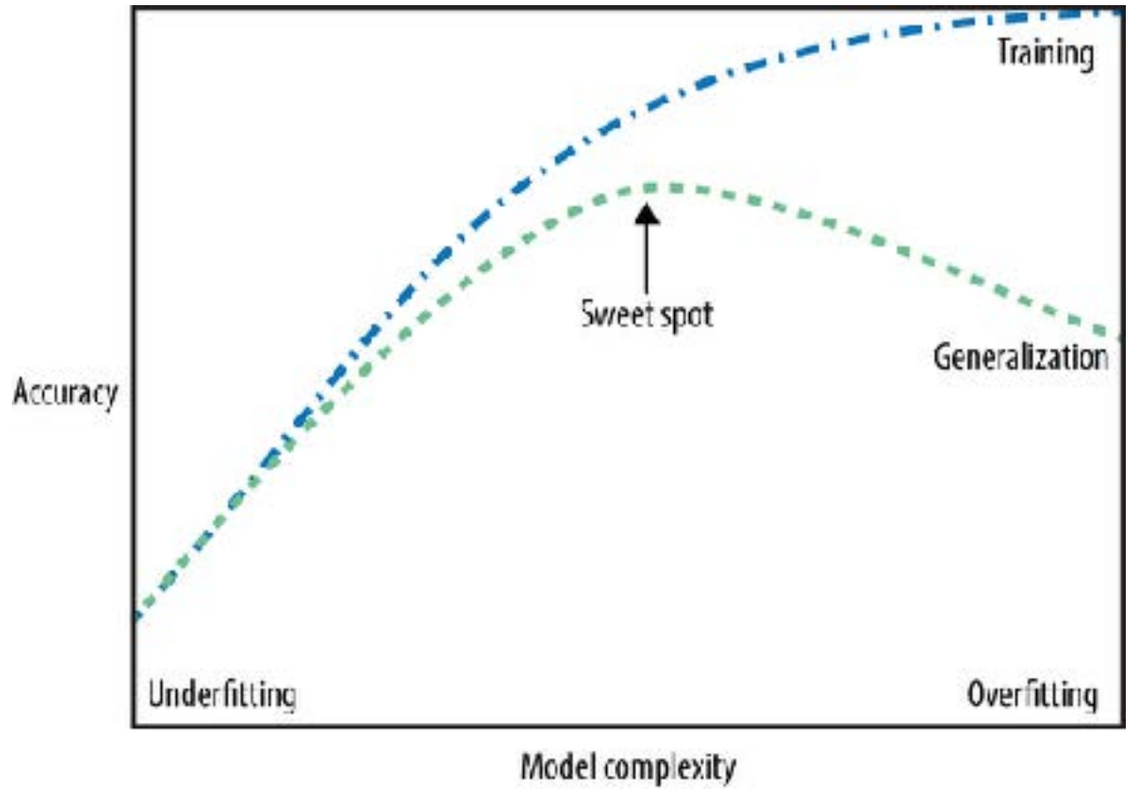


Figure 2-1. Trade-off of model complexity against training and test accuracy

Guido, Sarah and Andreas C. Muller. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

k-Nearest Neighbors Classification

- Classification of unlabeled points based on the closest labeled point(s)
- *k* is the number of points considered to determine the class of an unlabeled point
- When *k* = 1 the class of the nearest point

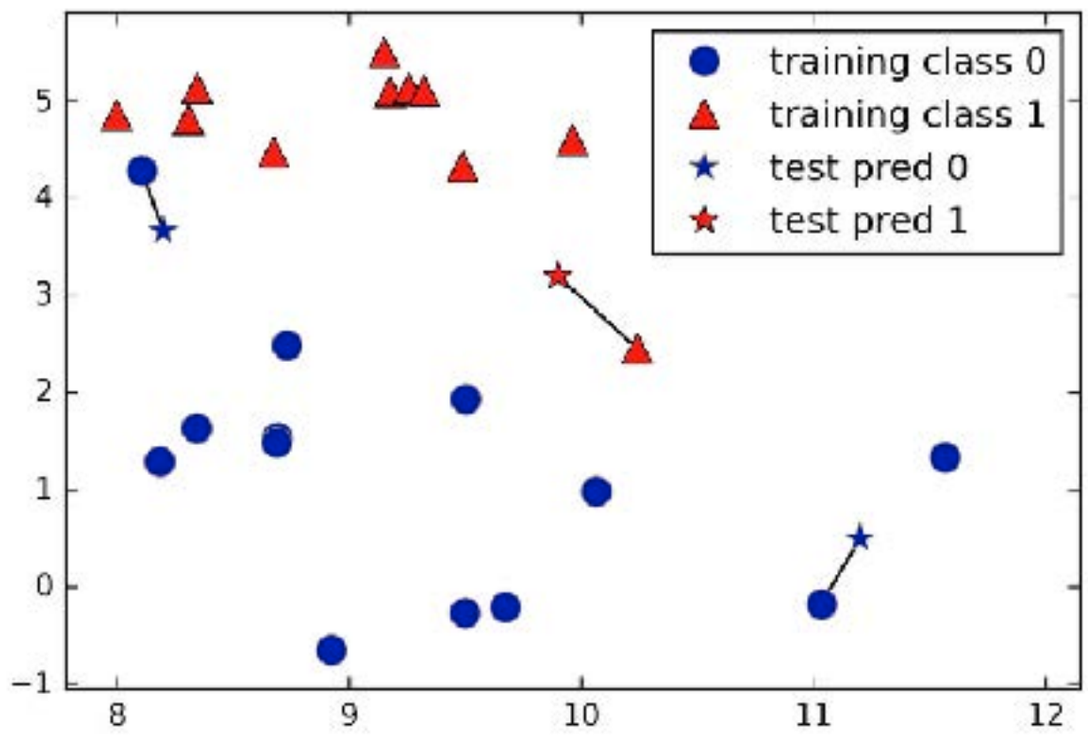


Figure 2-4. Predictions made by the one-nearest-neighbor model on the forge dataset

Jupyter Notebook 02-supervised-learning .ipynb [10]

Guido, Sarah and Andreas C. Muller. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

k-Nearest Neighbors Classification

- **When k > 1 the algorithm uses a simple voting paradigm**
  - Assigned class label is the most frequent label among the neighbors
  - *k* should be larger than the number of classes
  - *k* should not be a multiple of the number of classes

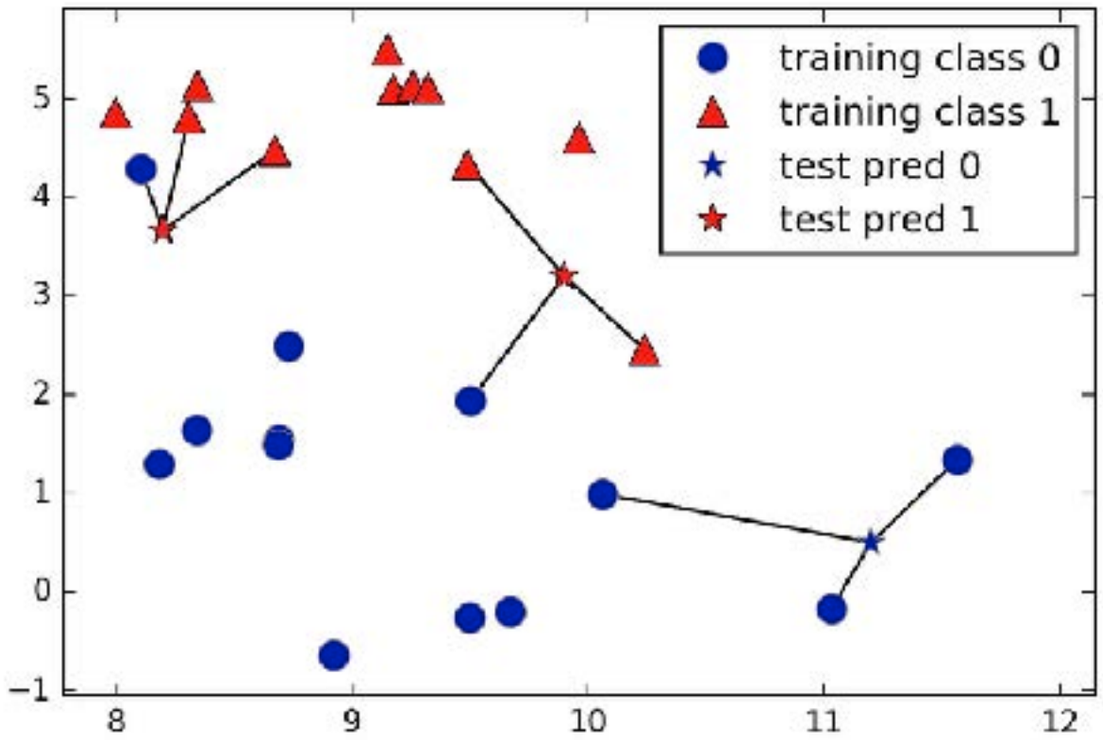


Figure 2-5. Predictions made by the three-nearest-neighbors model on the forge dataset

Jupyter Notebook 02-supervised-learning .ipynb [11–16]

Guido, Sarah and Andreas C. Muller. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

Size of *k*

- **When *k* is too small the model is too complex and tends to overfit**
- **When *k* is too large the model is too simple and tends to underfit**

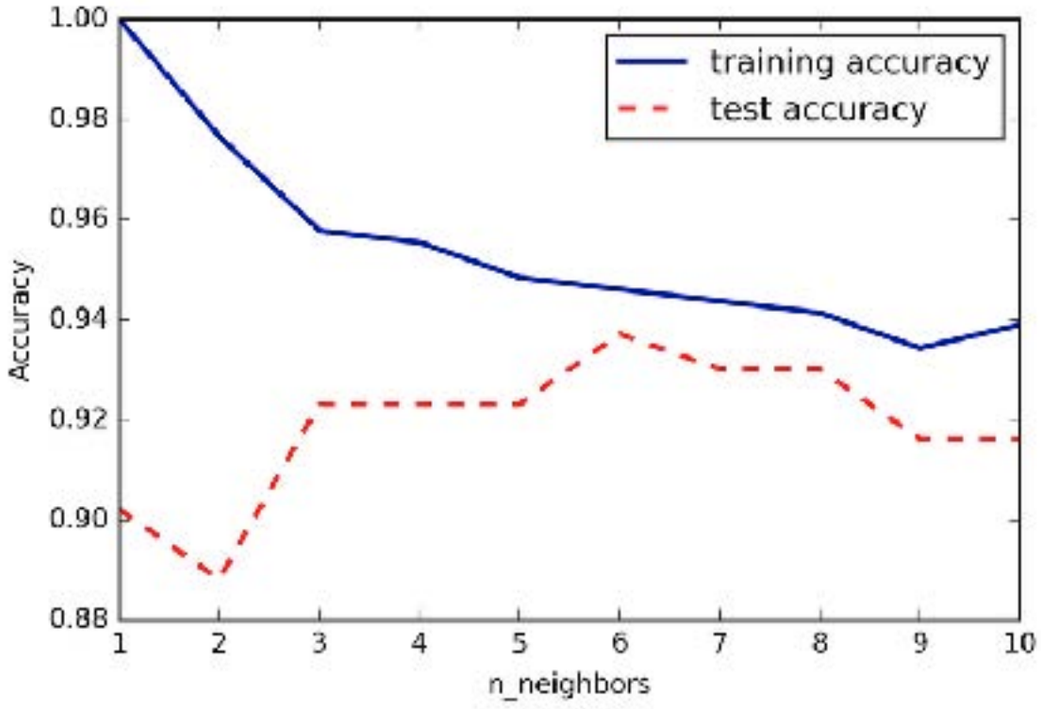


Figure 2-7. Comparison of training and test accuracy as a function of n_neighbors

Jupyter Notebook 02-supervised-learning .ipynb [18]

Guido, Sarah and Andreas C. Muller. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

k-Nearest Neighbors Overview

- **Assumptions**
  - *k*NNs do not make any assumptions about the distribution of the data
- **Parameters**
  - Number of neighbors
  - Distance measure (Euclidean, Manhattan, etc)
- **Strengths**
  - Easy to understand
  - Reasonable performance (at most twice as bad as the optimal classifier)
- **Weaknesses**
  - Prediction can be slow on large dataset
  - Often requires pre-processing
  - Performs poorly on datasets with a large number of features
  - Performs poorly on sparse datasets (where many values are 0)

Review from Class 5

- **(Linear) Regression**
  - Continuous predictive model created by estimating a linear relationship between features and response
- **Logistic Regression**
  - Predictive model of the probability of a certain class

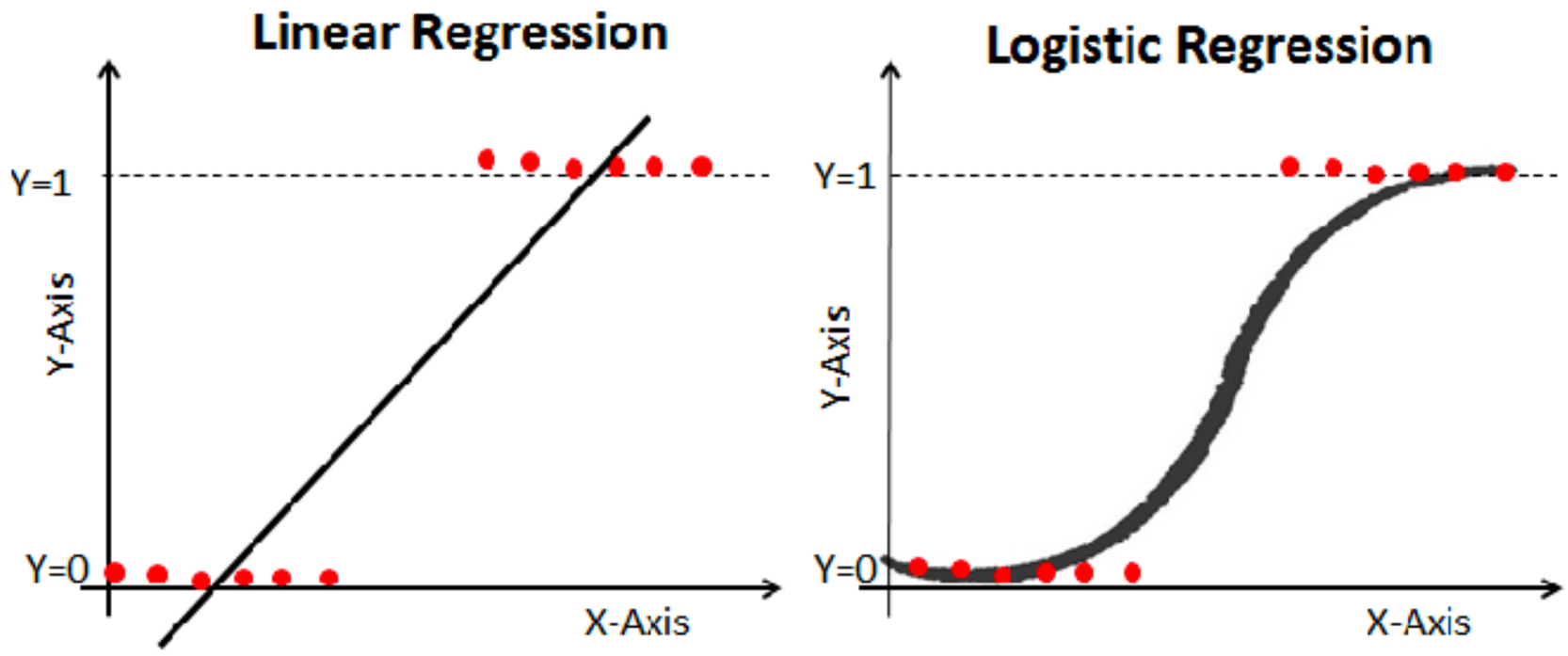
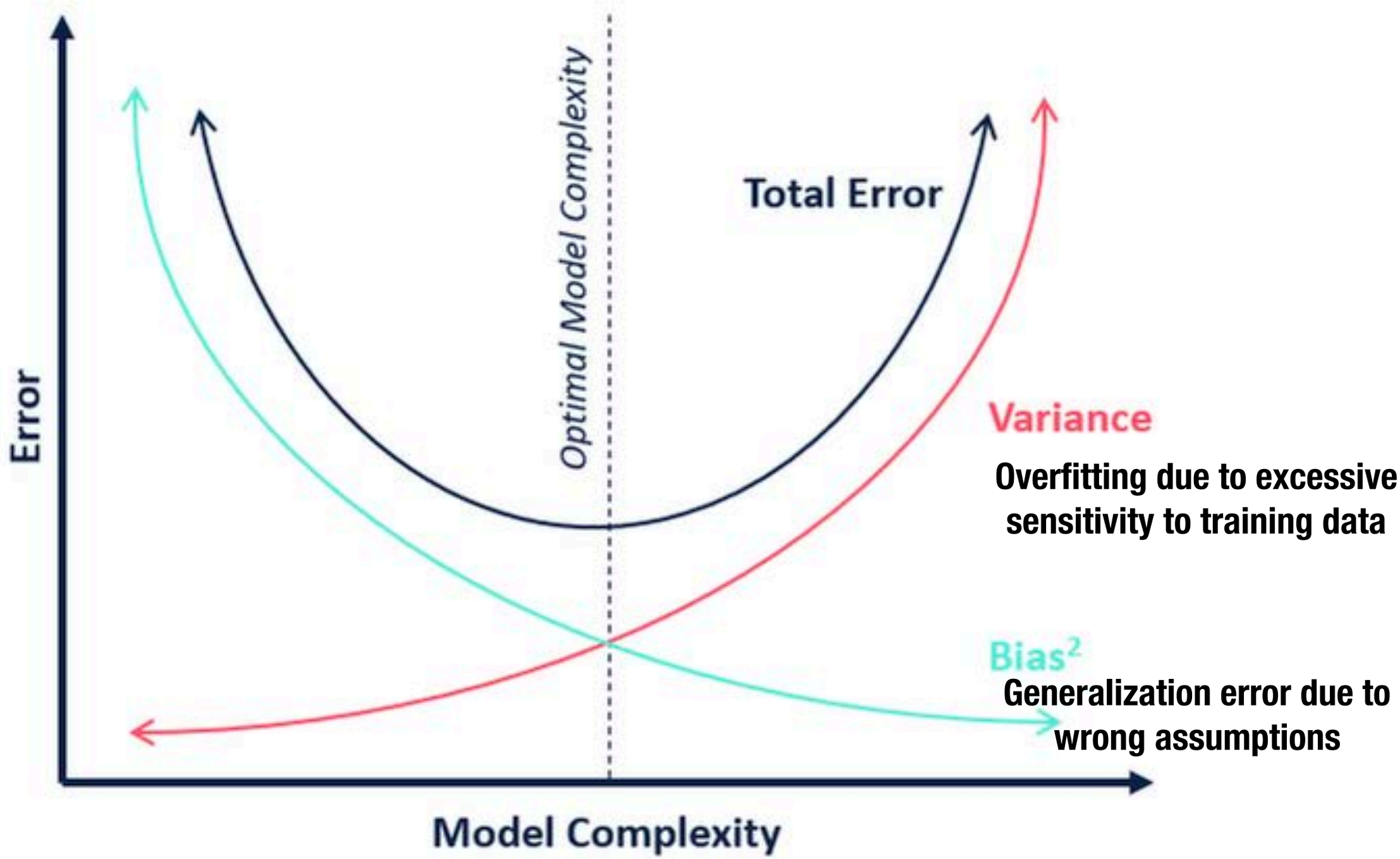


Image: https://medium.com/@hpsuresh12345/logistic-regression-60694a973bee

Bias/Variance Tradeoff



https://ai-pool.com/a/s/bias-variance-tradeoff-in-machine-learning

Ridge Regression

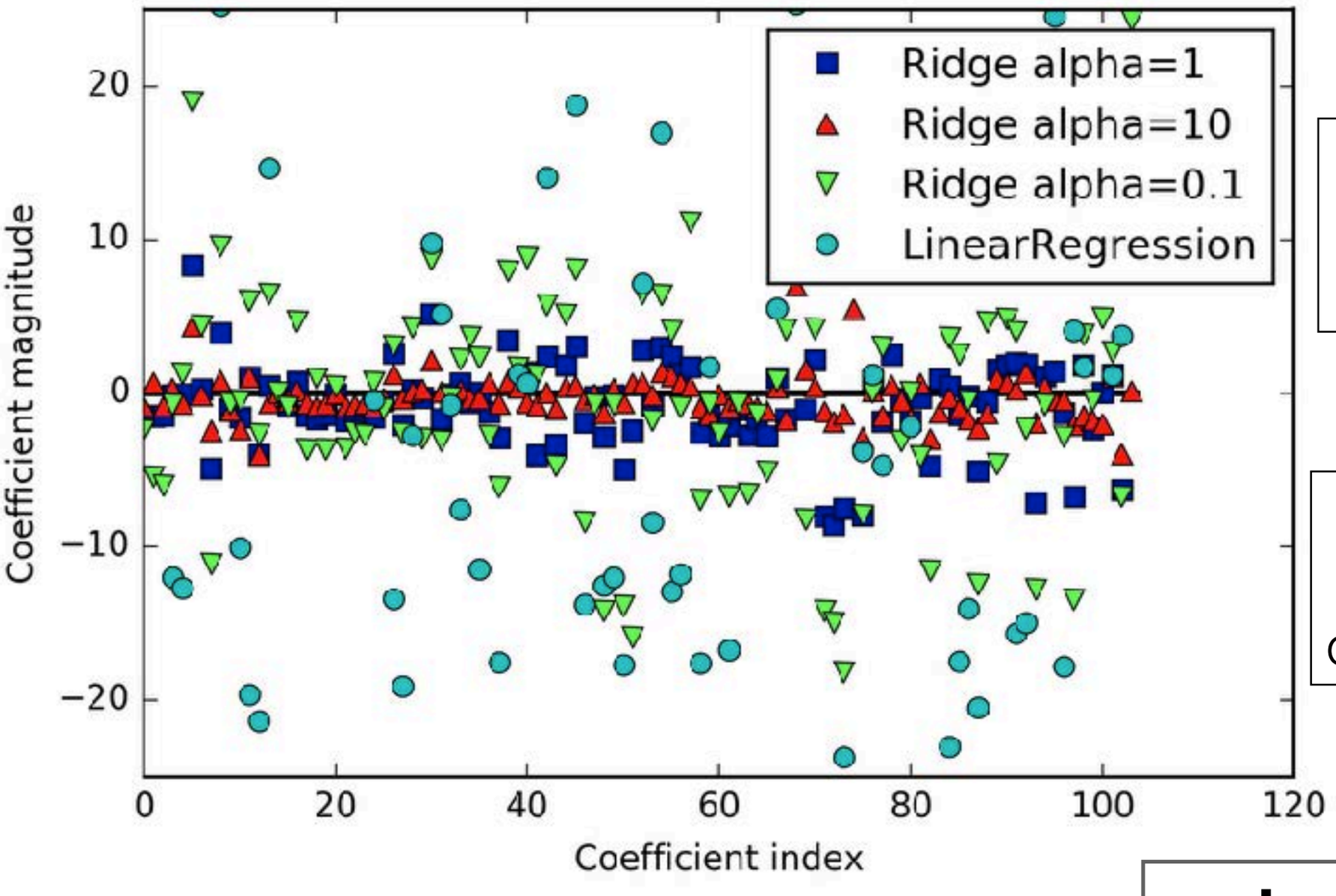


Figure 2-12. Comparing coefficient magnitudes for ridge regression with different values of alpha and linear regression

Trade off between model simplicity and model performance

Increasing alpha moves more coefficients towards 0

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Guido, Sarah and Andreas C. Muller. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

Ridge Regression

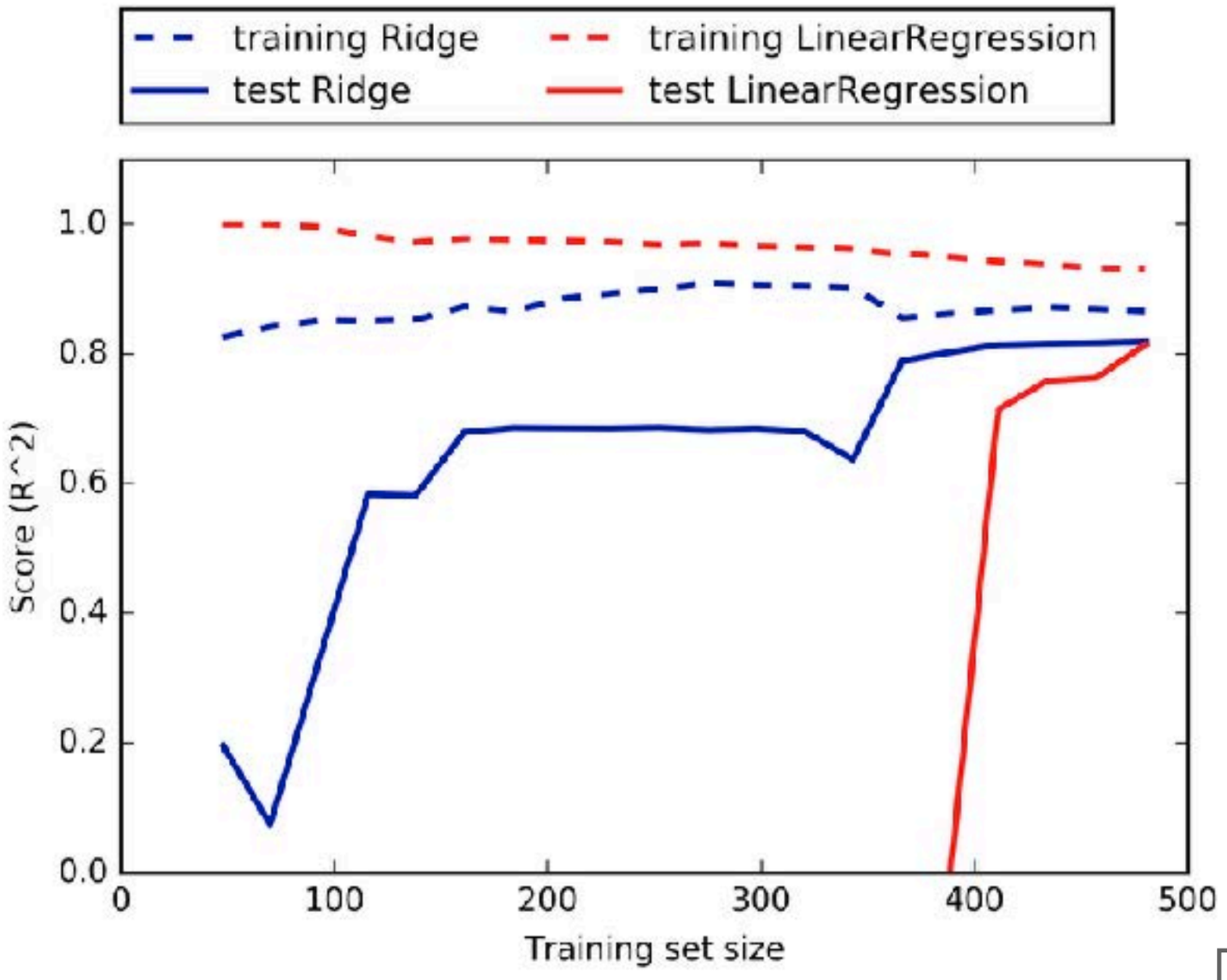

Figure 2-13. Learning curves for ridge regression and linear regression on the Boston Housing dataset

Ridge performs worse than OLS (MSE) on training set but better on testing set

OLS improves performance on testing set with more data (generalizes better so performance on training data declines)

Jupyter Notebook 02-supervised-learning .ipynb [34]

Lasso versus Ridge Regression

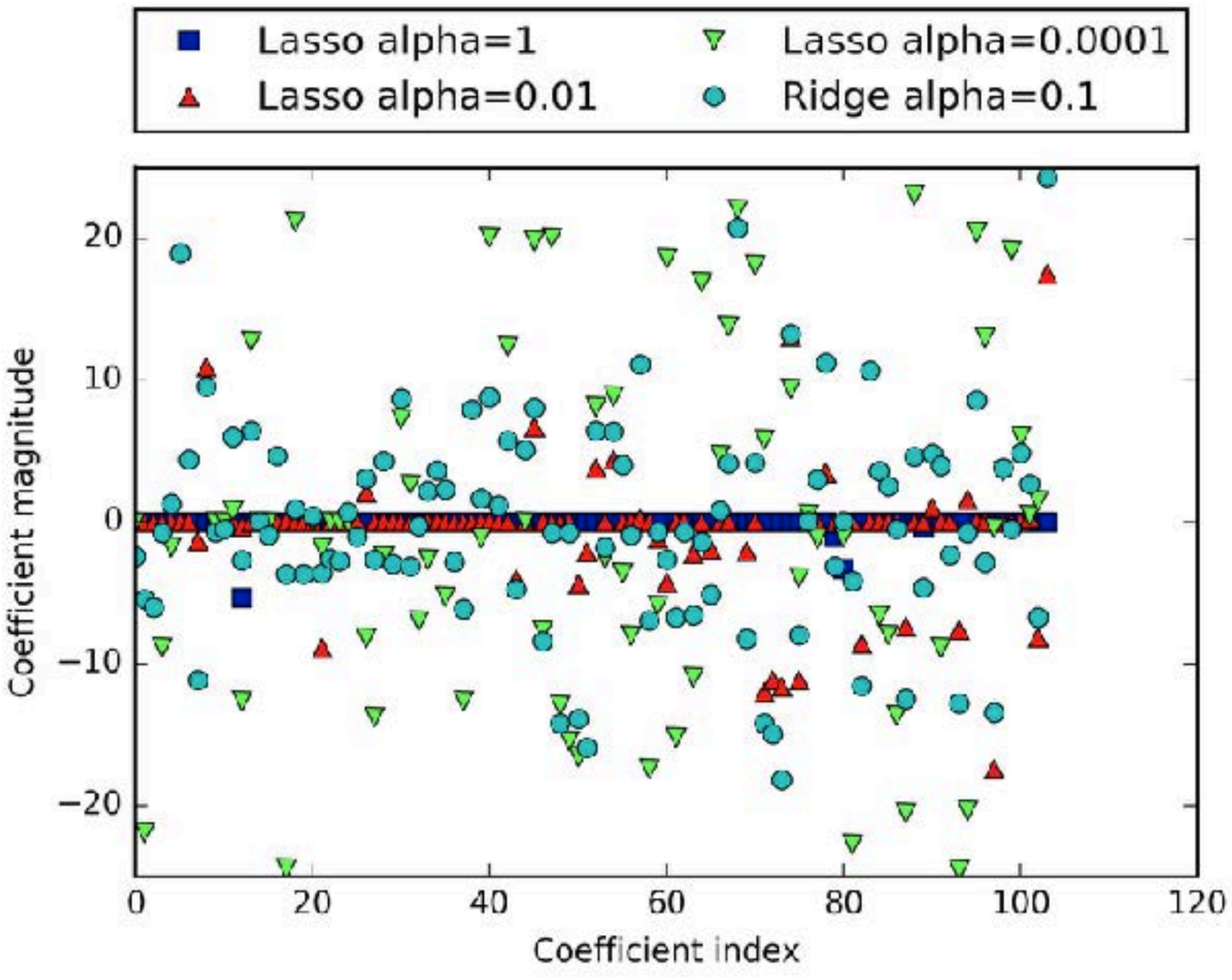

Figure 2-14. Comparing coefficient magnitudes for lasso regression with different values of alpha and ridge regression

When alpha is too high, too many features are zeroed out

When alpha is too low, the model is effectively unregularized

Lasso alpha=0.01 is similar to Ridge alpha=0.1 but some coefficients are zeroed out

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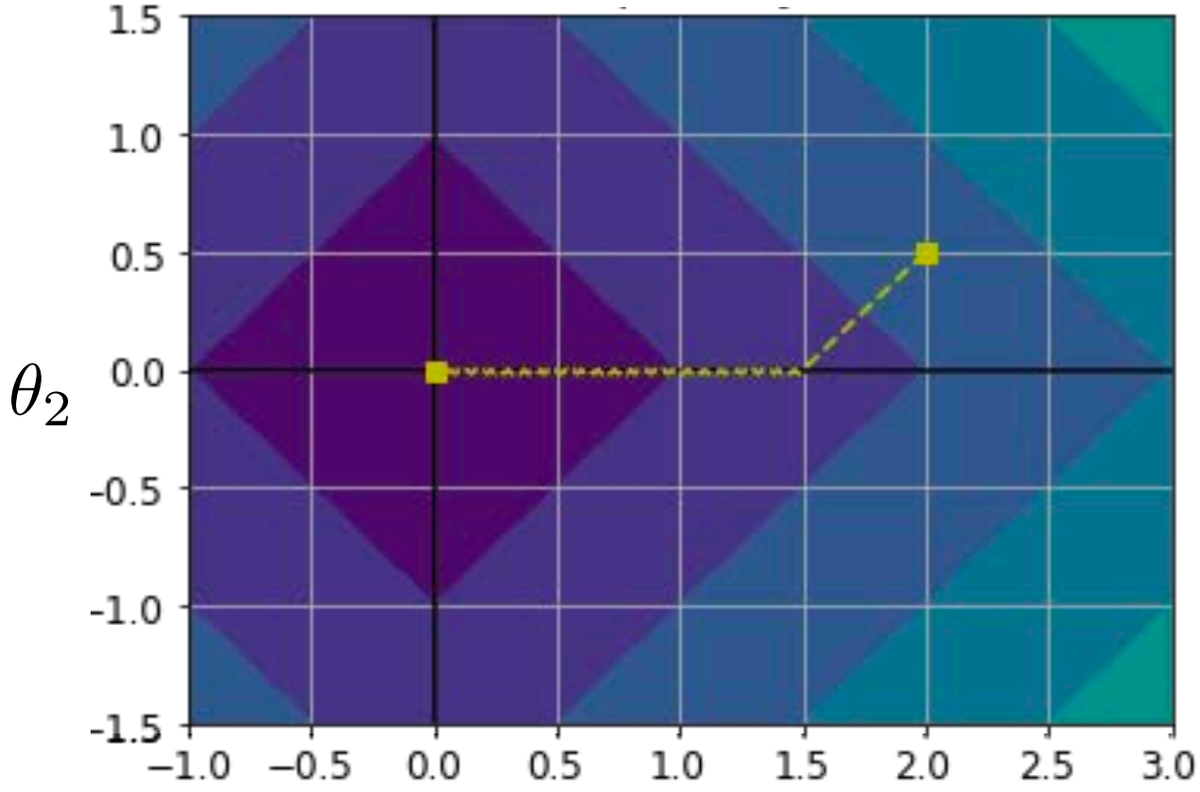
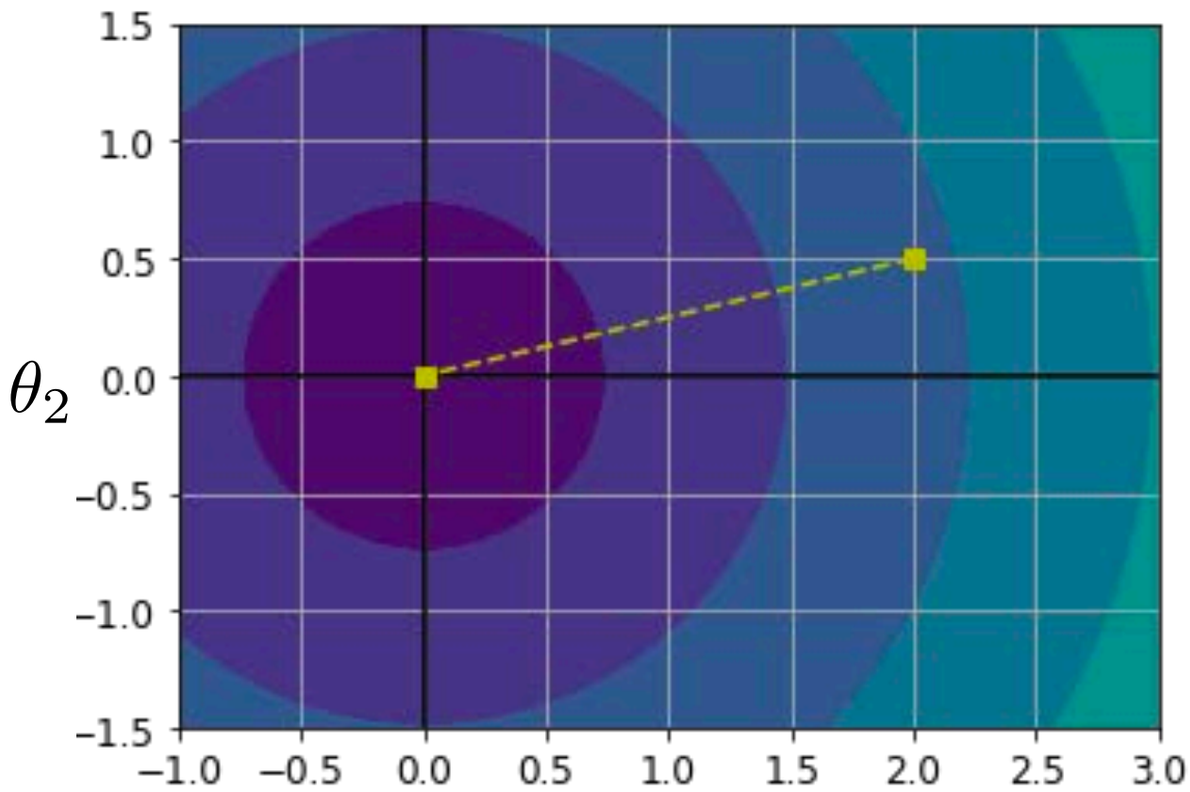
Guido, Sarah and Andreas C. Muller. (2016). Introduction to Machine Learning with Python, O'Reilly Media, Inc.

Lasso versus Ridge Regression

ℓ_1 penalty (Lasso)



ℓ_2 penalty (Ridge)

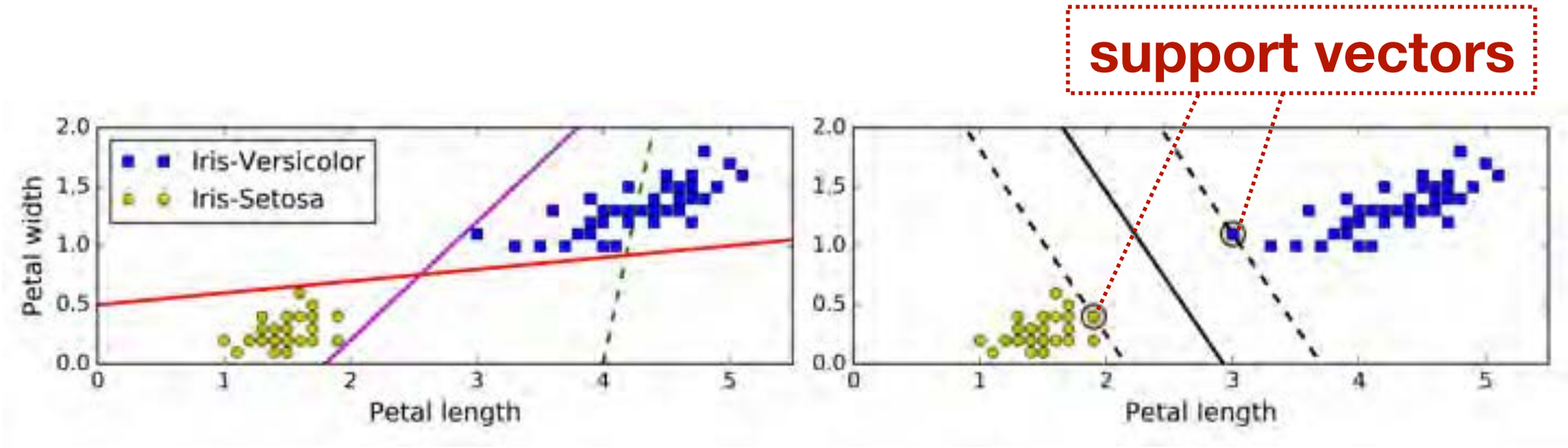


Observe that in Lasso θ_2 remains 0 until it reaches a minimum value (0.5) while in Ridge the value of θ_2 can be a value between 0 and 0.5

Géron, Aurélien. (2019). *Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow* O'Reilly Media, Inc.

Linear Support Vector Classifier

- **Find the linear classifier with the best separation (margin) between the two classes**
  - Operationally the data points used to make this calculation are the support vectors



Three possible linear classifiers

Linear classifier with the widest margin

Géron, Aurélien. (2019). *Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow* O'Reilly Media, Inc.

Logistic Reg versus Linear SVC

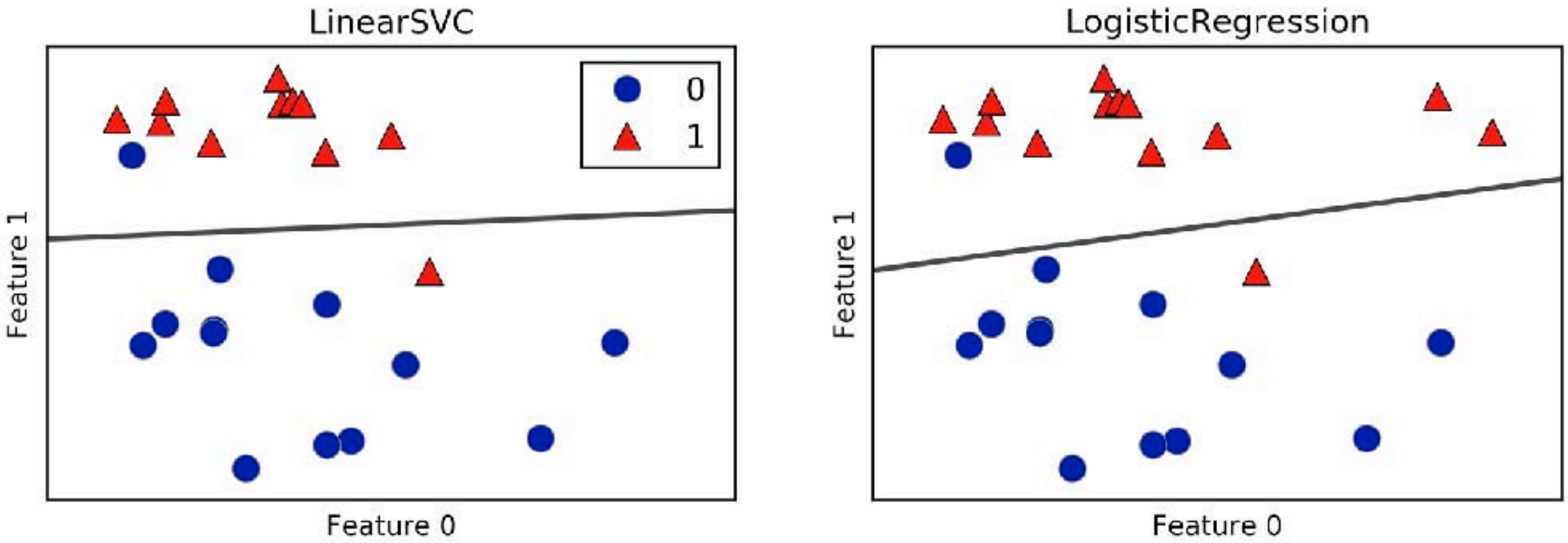


Figure 2-15. Decision boundaries of a linear SVM and logistic regression on the forge dataset with the default parameters

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Coefficient Magnitude

- C is the inverse of regularization strength

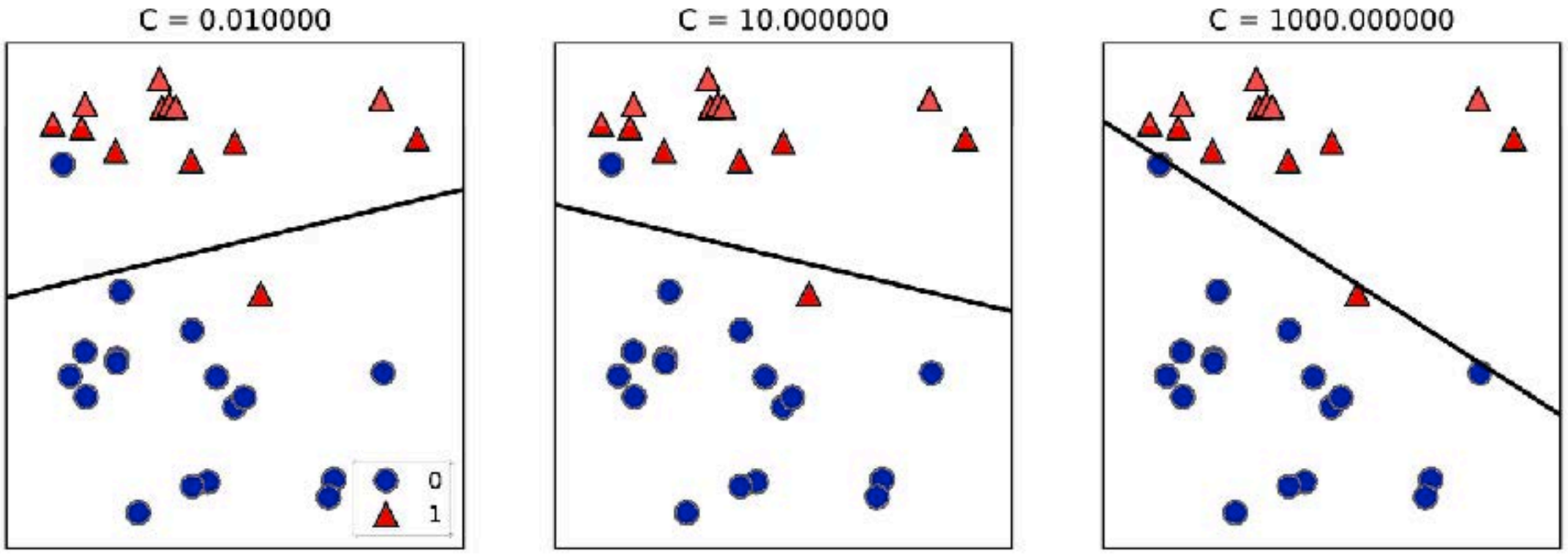

Figure 2-16. Decision boundaries of a linear SVM on the forge dataset for different values of C

Low values of C - algorithm adjusts to the majority of the data points

High values of C - algorithm attempts to correctly classify as many individual data points as possible

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One versus Rest Classification

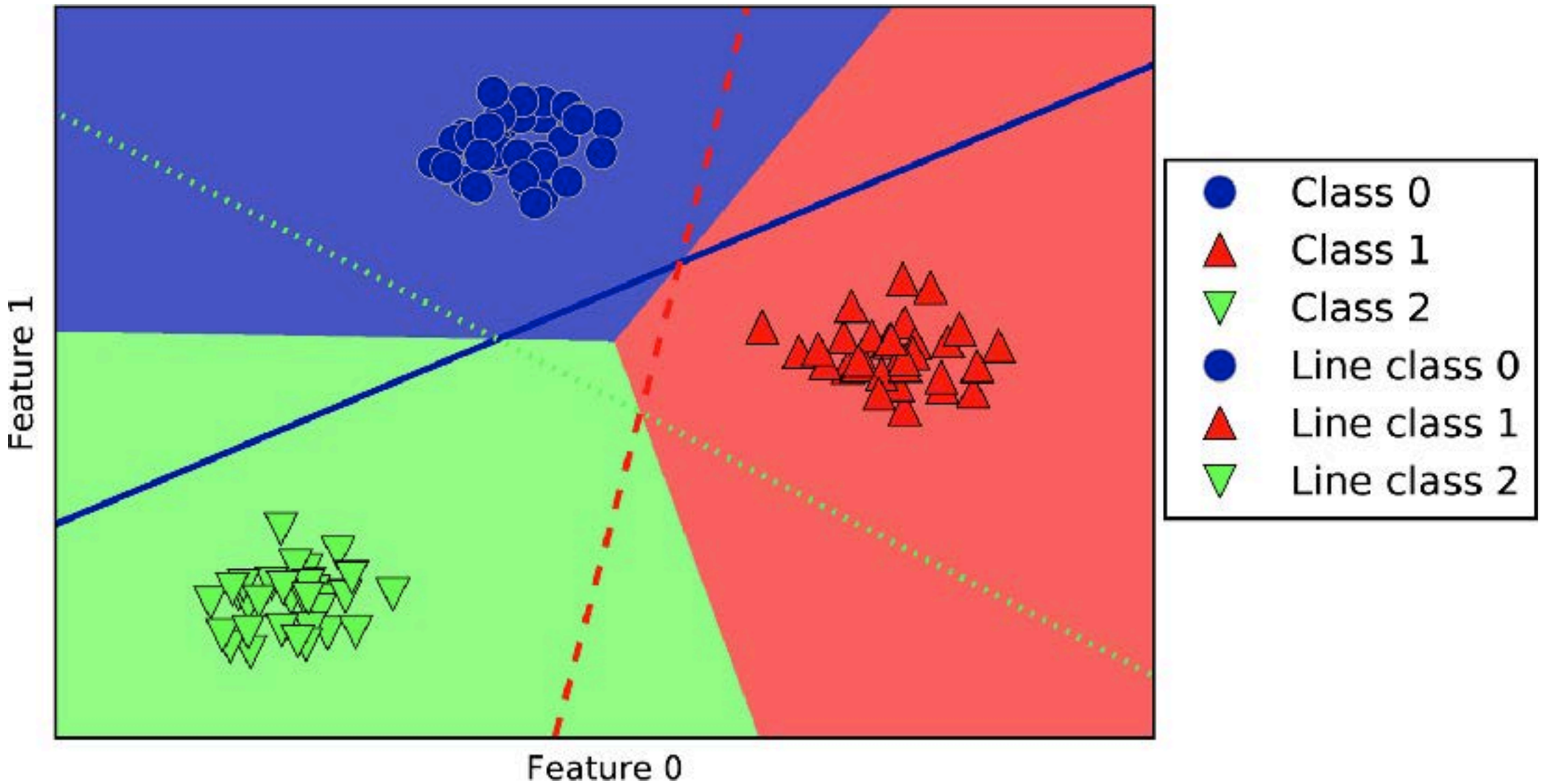

Figure 2-21. Multiclass decision boundaries derived from the three one-vs.-rest classifiers

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Linear Models Overview

- **Assumptions**
  - Linear relationship between input and output
  - No noise in input or output
  - Independence (lack of correlation in input)
  - Gaussian (normally) distributed data

- **Best Practices**
  - Scale inputs

Linear Models Overview

- **Parameters**
  - Regularization parameter: alpha (regression) or C (classification)
  - Type of regularization (L1 or L2)
- **Strengths**
  - Fast to train (good for large datasets)
  - Fast at prediction
  - Easy to understand the algorithm
  - Work well even when there are a large number of features compared to the number of samples
- **Weaknesses**
  - Not so easy to interpret a model's coefficients
  - Generalization may be poor with small number of features