Advanced Data Analysis

DATA 71200

Class 6

Weekly Schedule

7-Jun	Inspecting Data
8-Jun	Representing Data
9-Jun	**Evaluation Methods**
10-Jun	Async

Splitting the Data

- **Cross-validation**
  - Splitting the data into folds and iteratively switching up which fold is used for testing (while the remainder are used for training)
  - The data can be split up in a variety of ways

Splitting the Data

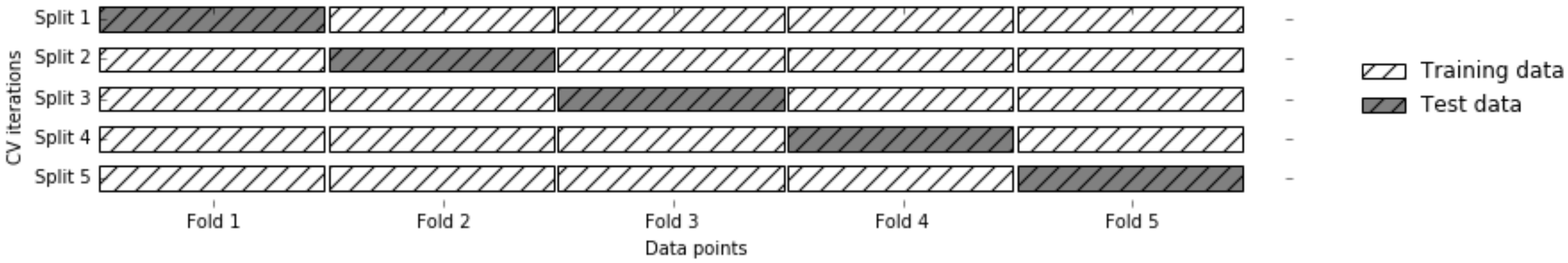

Figure 5-1. Data splitting in five-fold cross-validation

This will create issues if the data is ordered by class since some classes will appear disproportionately (or not at all) in either the testing or training sets

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Splitting the Data

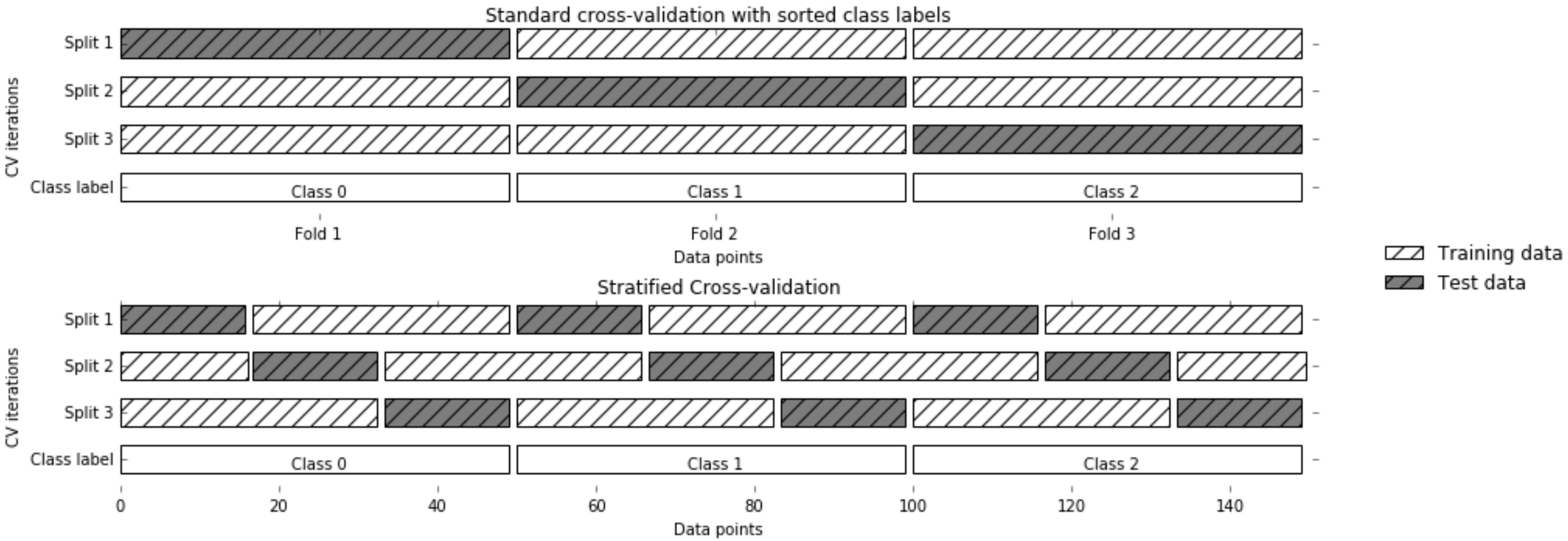

Figure 5-2. Comparison of standard cross-validation and stratified cross-validation when the data is ordered by class label

Stratified Cross-validation explicitly takes data from each class in order to count the issue of over-/under-sampling that can arise in standard cross-validation

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Splitting the Data

Small Data Sets

Leave-one out cross validation can be used where each fold is a single sample

Large Data Sets

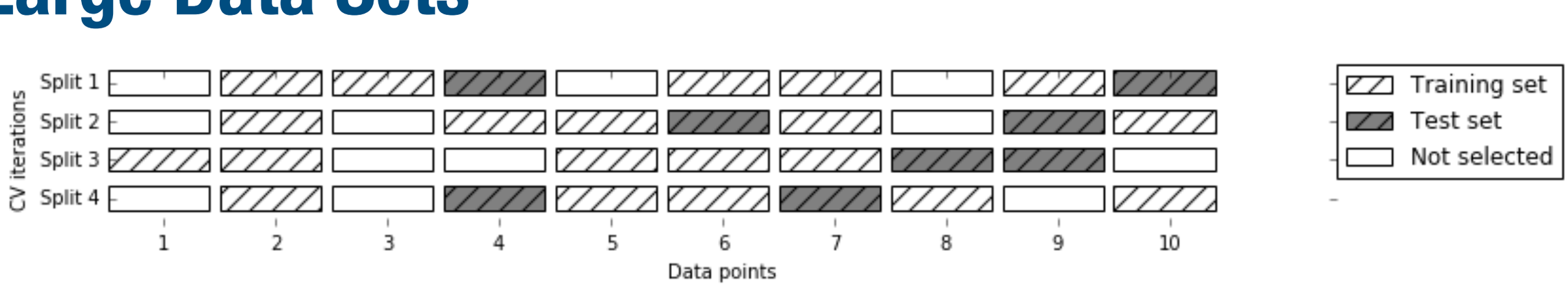

Figure 5-3. ShuffleSplit with 10 points, train_size=5, test_size=2, and n_splits=4

Shuffle-Split provides a system way to sample from your dataset without using all of the data

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Splitting the Data

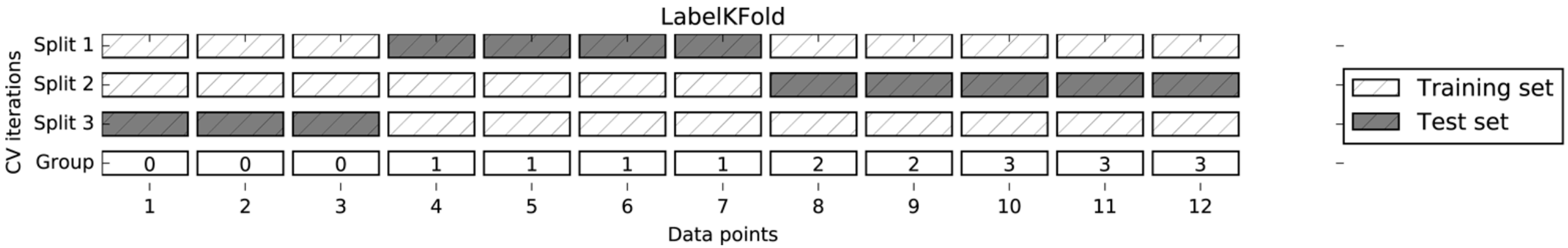

Figure 5-4. Label-dependent splitting with GroupKFold

When groups are highly related (e.g., individual speakers in speech recognition) you may not want to train and test on a single group

GroupKFold allows you select training and testing sets that either include or exclude an entire group

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Splitting the Data

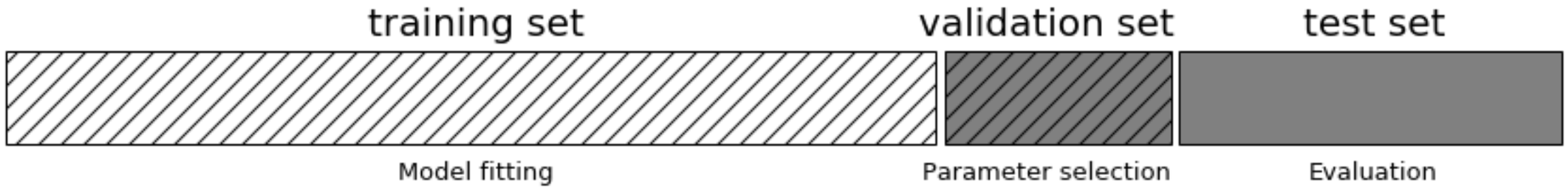

Figure 5-5. A threefold split of data into training set, validation set, and test set

If you are evaluating different models or tuning parameters (e.g., using Grid Search), you will want to have a reserved test set and then split the remaining data into training and validation sets

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Grid Search

Grid search can be performed simply (one split) or iteratively (cross-validation) - in the latter the optimal parameter values need to be summarized

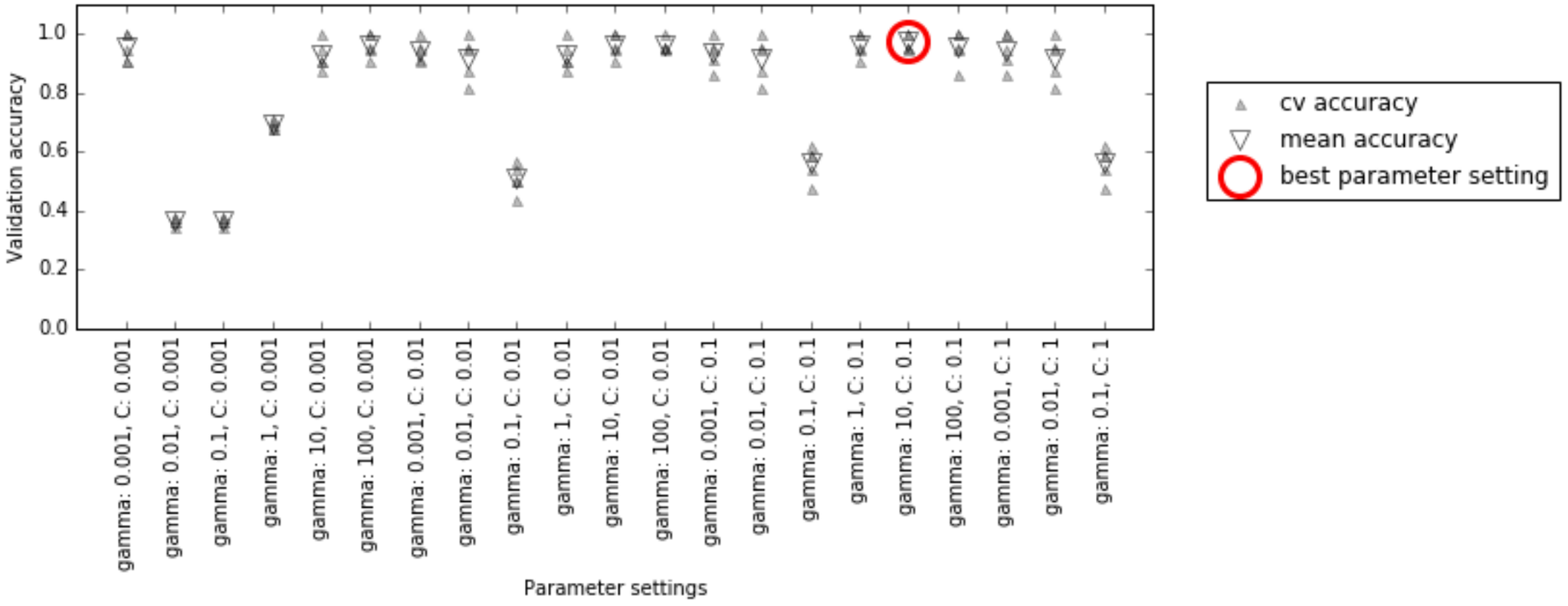

Figure 5-6. Results of grid search with cross-validation

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Grid Search

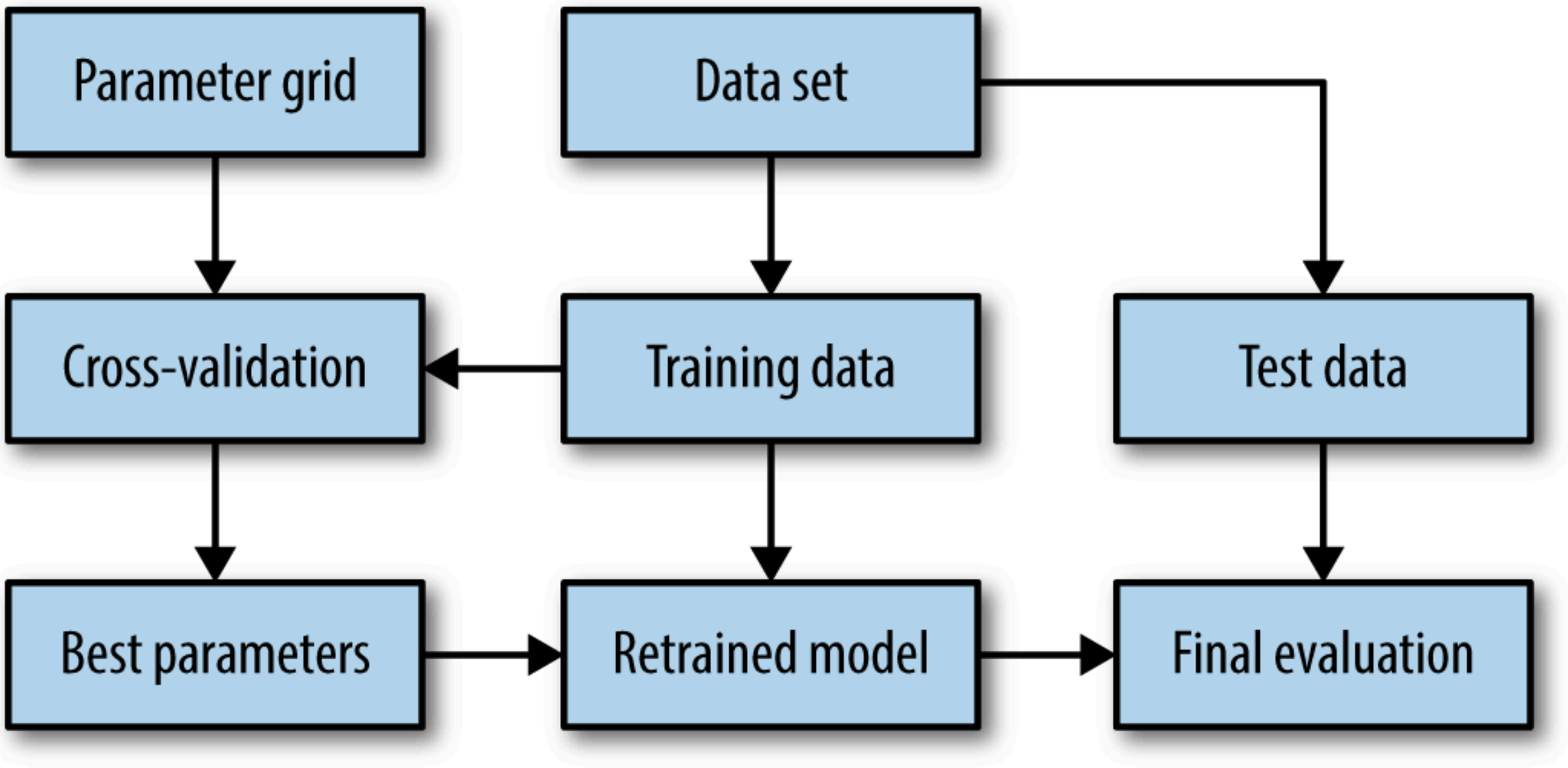

Figure 5-7. Overview of the process of parameter selection and model evaluation with GridSearchCV

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Grid Search

It is important than the parameter range reached is appropriate

Heat maps can help understand whether the range is appropriate

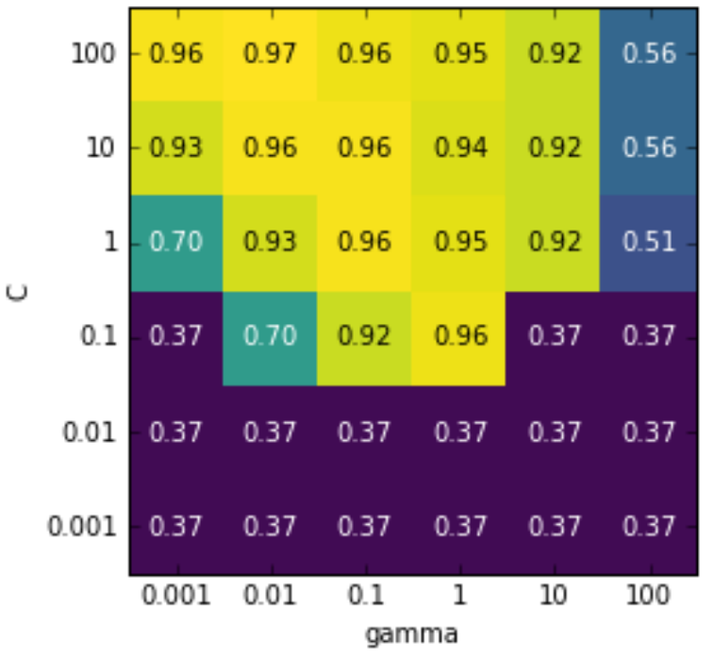

Figure 5-8. Heat map of mean cross-validation score as a function of C and gamma

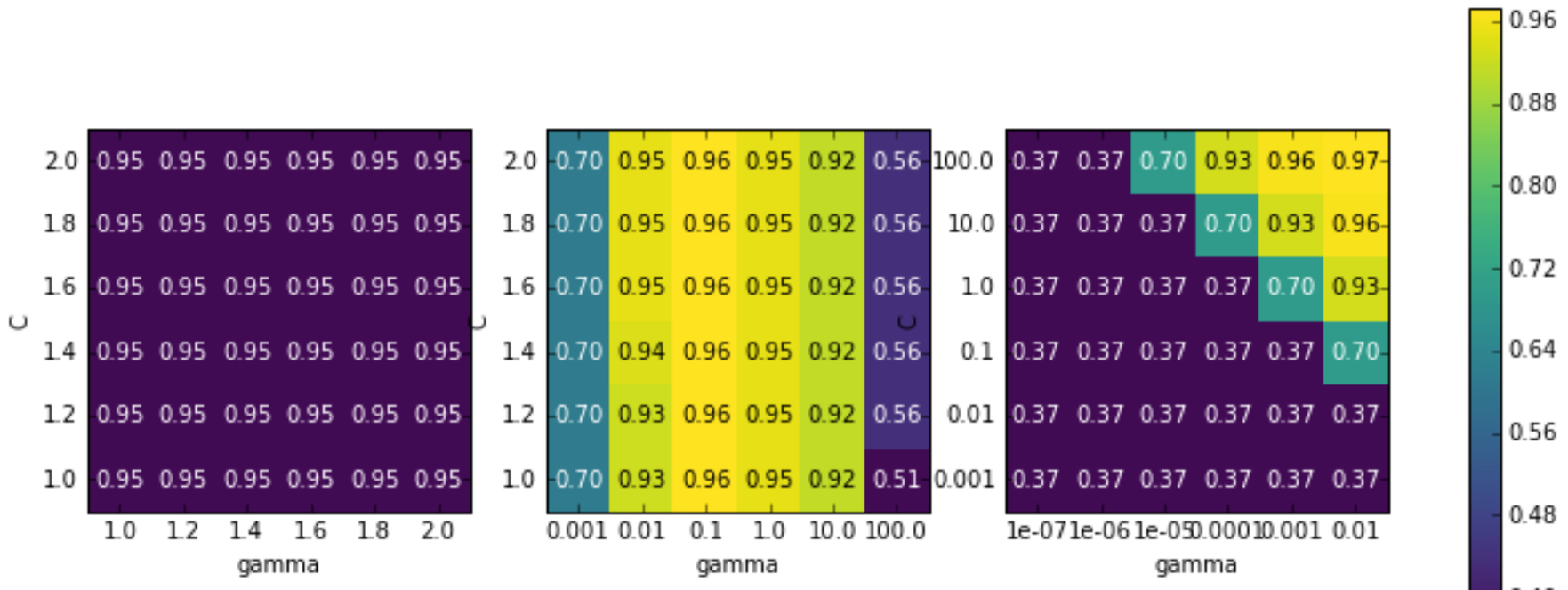

Figure 5-9. Heat map visualizations of misspecified search grids

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Accuracy

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

TP - true positive

TN - true negative

FP - false positive

FN - false negative

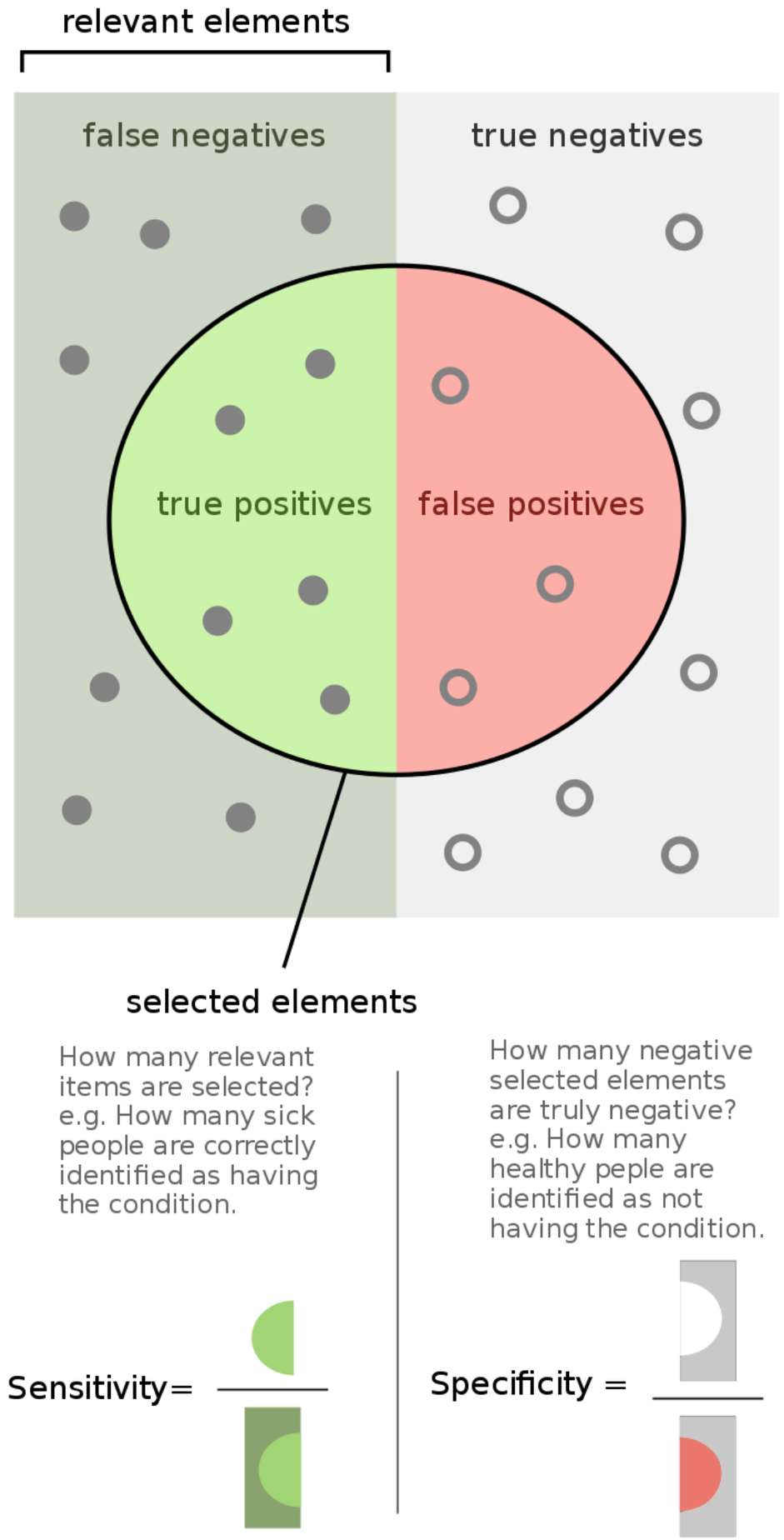
How many predictions were correct out of all the predictions made

Kinds of Errors

Type I: false positive

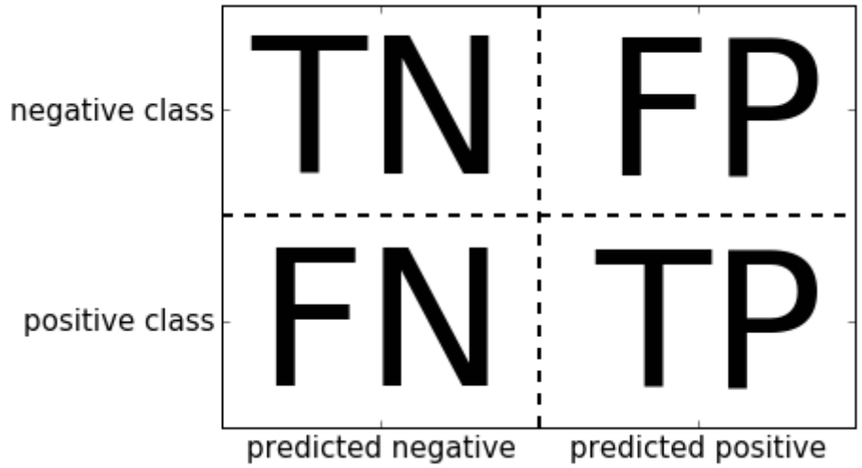
Type II: false negative

Balance of the classes in the dataset will influence how you interpret performance errors



https://commons.wikimedia.org/wiki/File:Precisionrecall.svg

Confusion Matrices



		True condition	
	Total population	Condition positive	Condition negative
Predicted condition	Predicted condition positive	**True positive**	**False positive**, Type I error
	Predicted condition negative	**False negative**, Type II error	**True negative**

Confusion matrices visualize not only how many correct estimates a model made but also what and how it mis-classified

https://en.wikipedia.org/wiki/Precision_and_recall

Precision

$$\text{Precision} = \frac{tp}{tp + fp}$$

tp - true positive

fp - false positive

Positive predictive value

Number of the positive predicted values that are actually positive

Recall

$$\text{Recall} = \frac{tp}{tp + fn}$$

tp - true positive

fn - false negative

Sensitivity

Proportion of the actually positives identified

F-1 Score (F-score, F-measure)

$$F_1 = 2 \cdot \frac{\mathrm{precision} \cdot \mathrm{recall}}{\mathrm{precision} + \mathrm{recall}}.$$

Harmonic mean of precision and recall

Summary measurement of the classifier's accuracy

Putting it All Together

		True condition			
	Total population	Condition positive	Condition negative	Prevalence = $\frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) = $\frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$
Predicted condition	Predicted condition positive	**True positive**	**False positive**, Type I error	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Predicted condition positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$
	Predicted condition negative	**False negative**, Type II error	**True negative**	False omission rate (FOR) = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Predicted condition negative}}$	Negative predictive value (NPV) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Predicted condition negative}}$
		True positive rate (TPR), Recall, Sensitivity, probability of detection, Power = $\frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm = $\frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) = $\frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) = $\frac{\text{LR+}}{\text{LR−}}$
		False negative rate (FNR), Miss rate = $\frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	Specificity (SPC), Selectivity, True negative rate (TNR) = $\frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) = $\frac{\text{FNR}}{\text{TNR}}$	F_1 score = $2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

https://en.wikipedia.org/wiki/Precision_and_recall

In-Class Activity

Calculate each of these metrics for the confusion matrix on the right

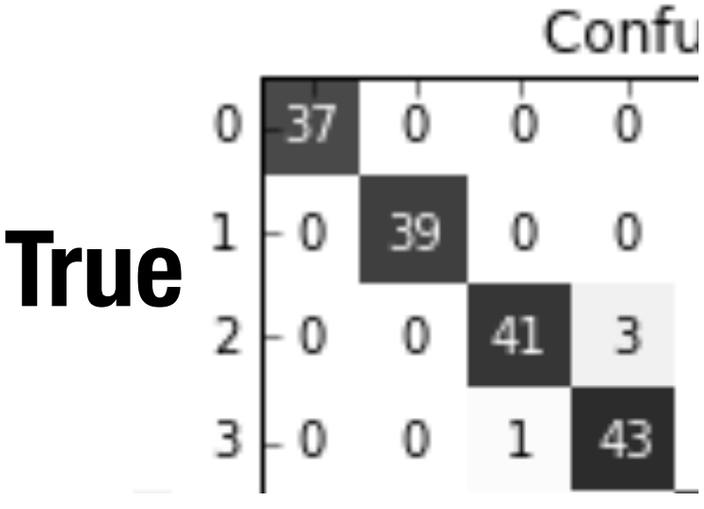


Figure 5-18. Confusion matrix for the 10-digit classification task

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

$$\text{Precision} = \frac{tp}{tp + fp}$$

$$\text{Recall} = \frac{tp}{tp + fn}$$

$$F_1 = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}.$$

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Precision Recall Curves

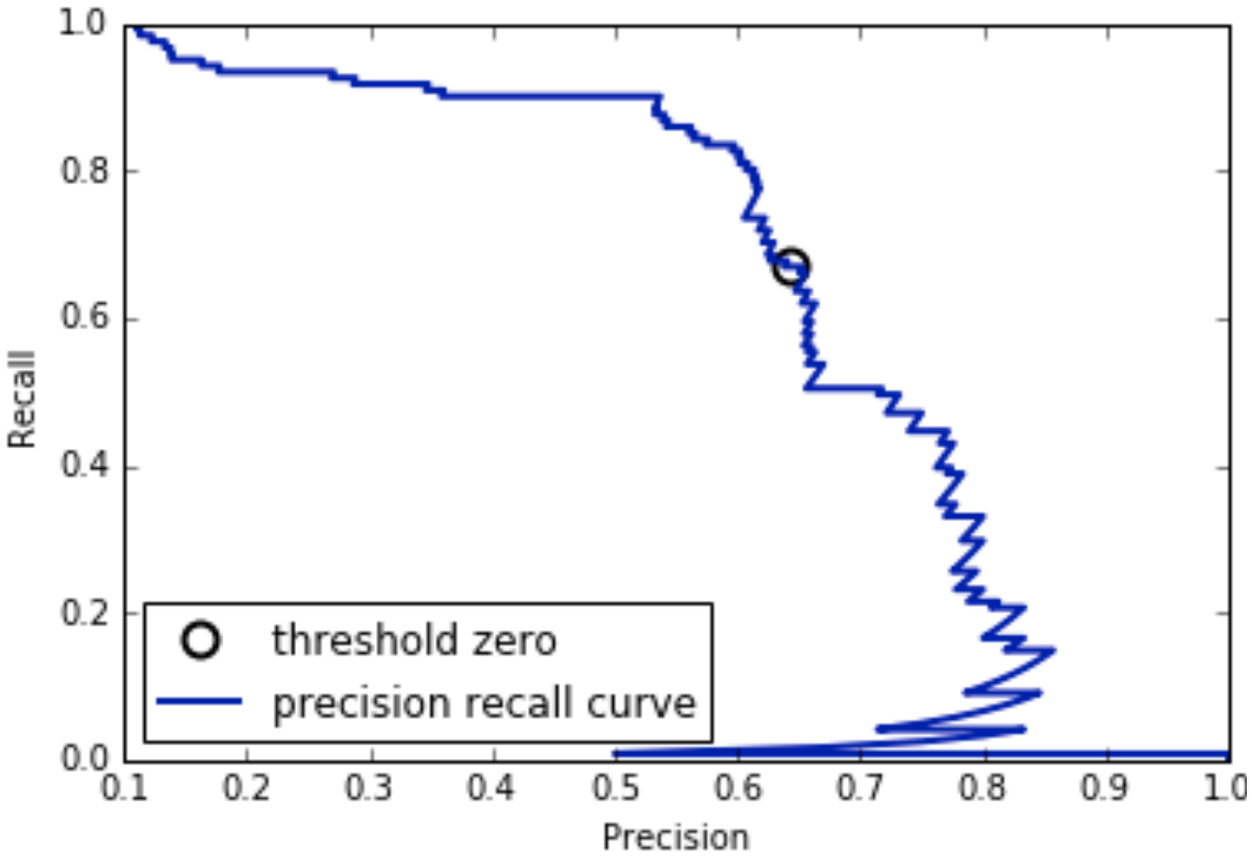

Figure 5-13. Precision recall curve for SVC(gamma=0.05)

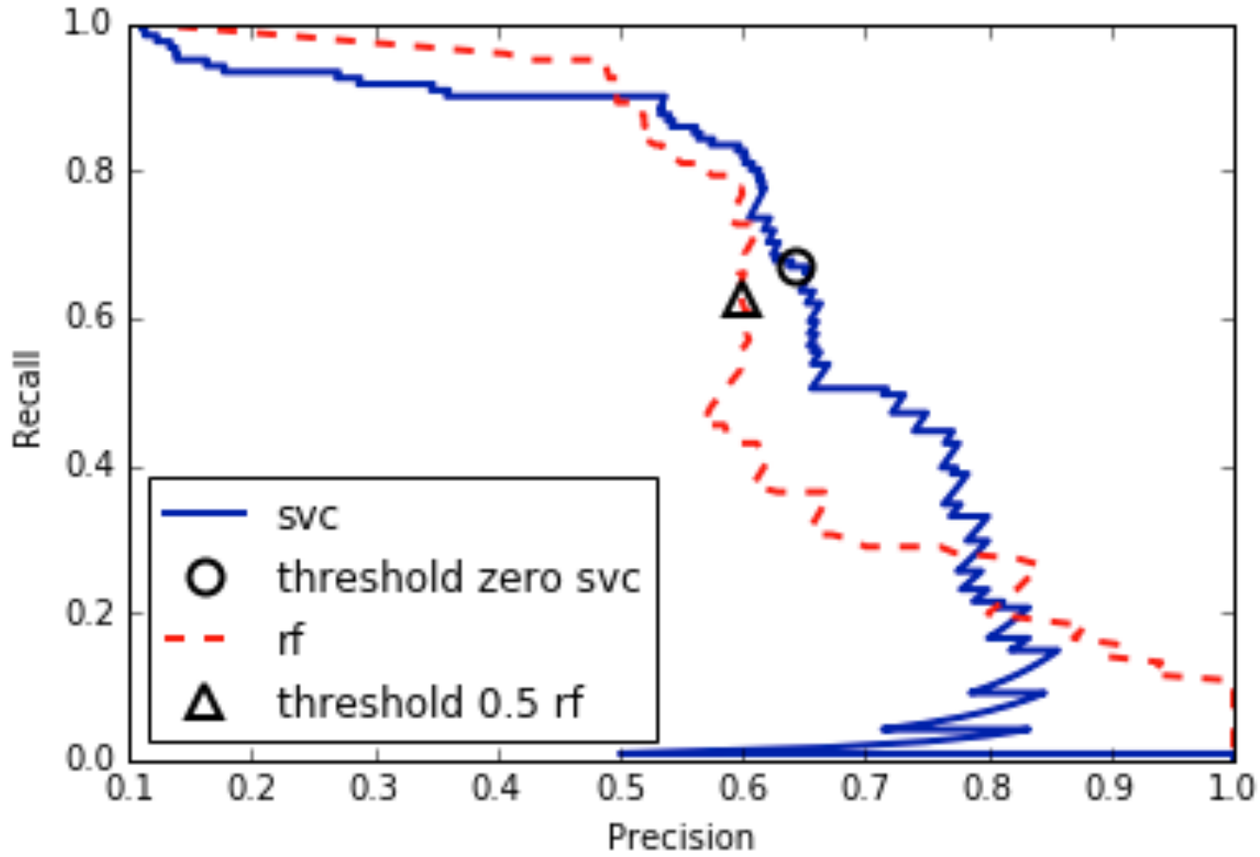

Figure 5-14. Comparing precision recall curves of SVM and random forest

Visualizes trade-off between positive predictive rate and true positive rate (sensitivity)

Area under curve summarizes this information

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ROC Curves

$$FPR = \frac{FP}{FP + TN}$$

TP - true positive
TN - true negative
FP - false positive

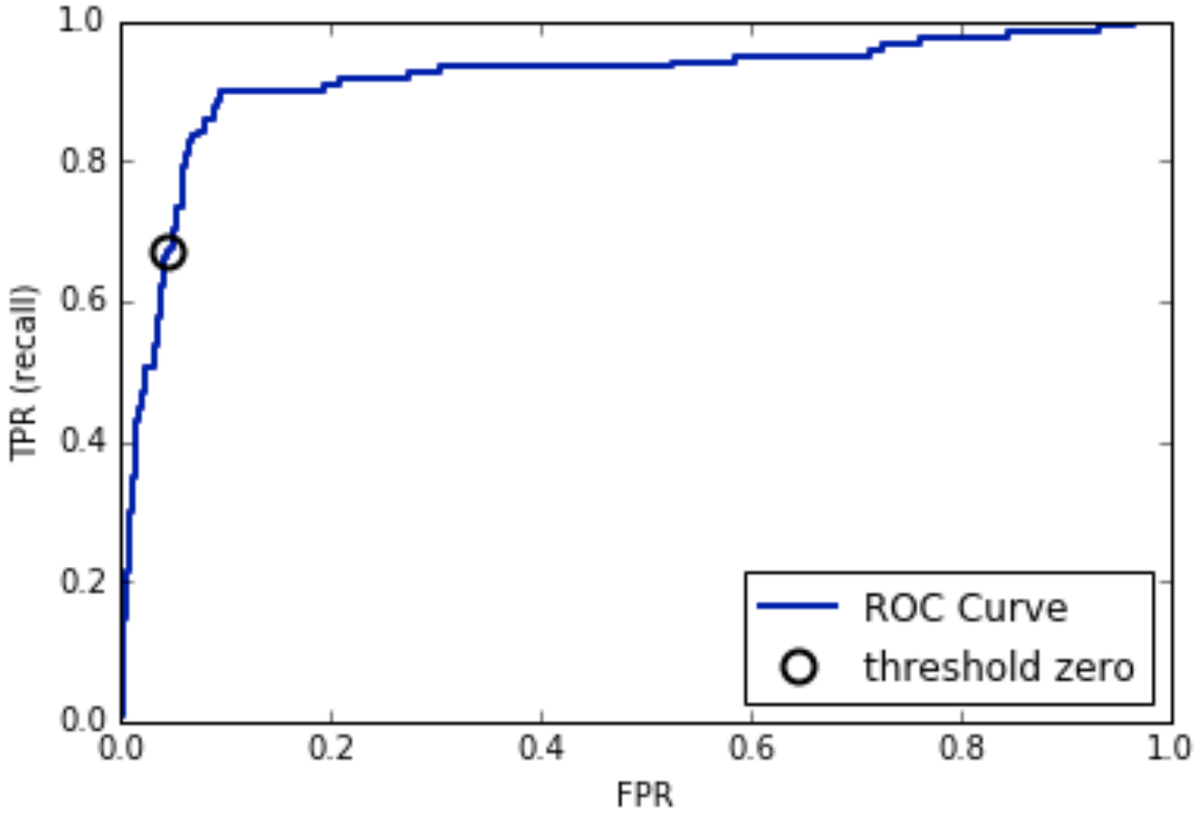

Figure 5-15. ROC curve for SVM

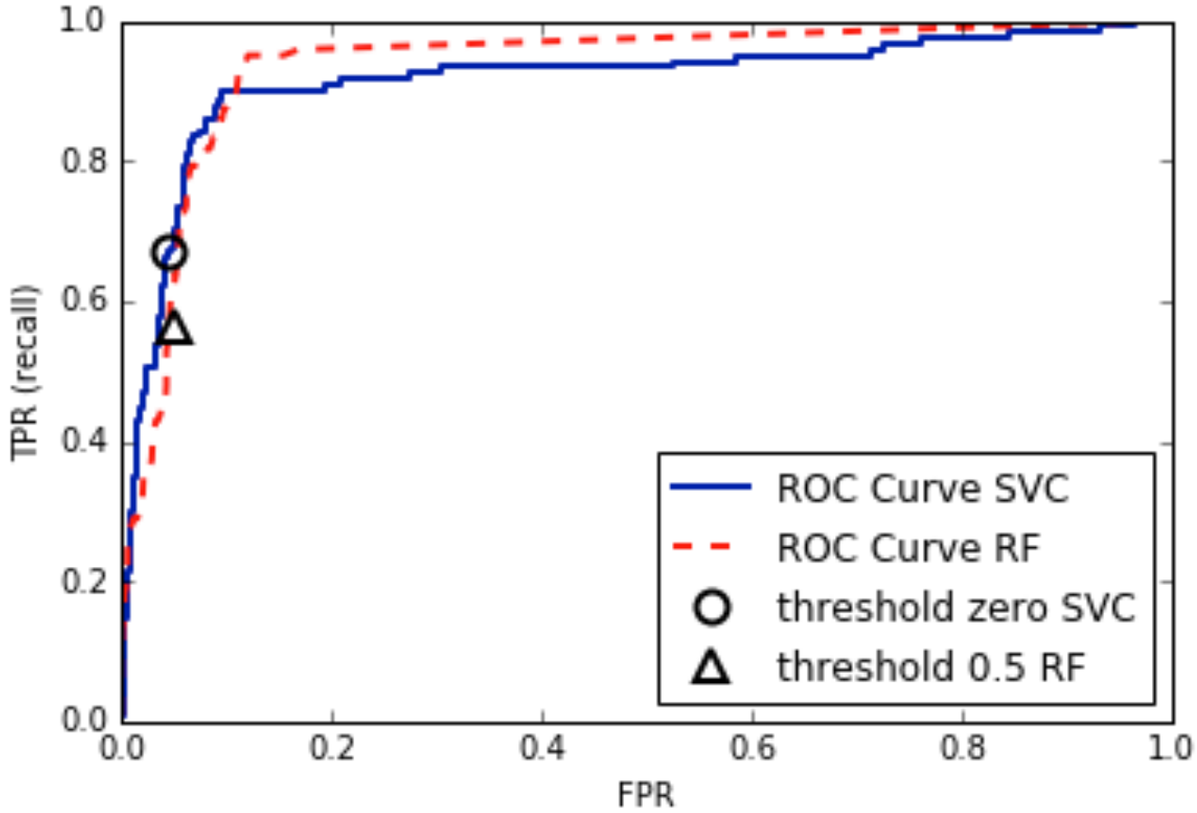

Figure 5-16. Comparing ROC curves for SVM and random forest

Receiver operating characteristics

Visualizes relationship between true positive rate (sensitivity) and false positive rate - the closer to the top right the better

Area under curve also useful to calculate here

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Decision Thresholds

How much uncertainty the classifier will permit to make a classification

Can be adjusted to change the prioritization between precision and recall

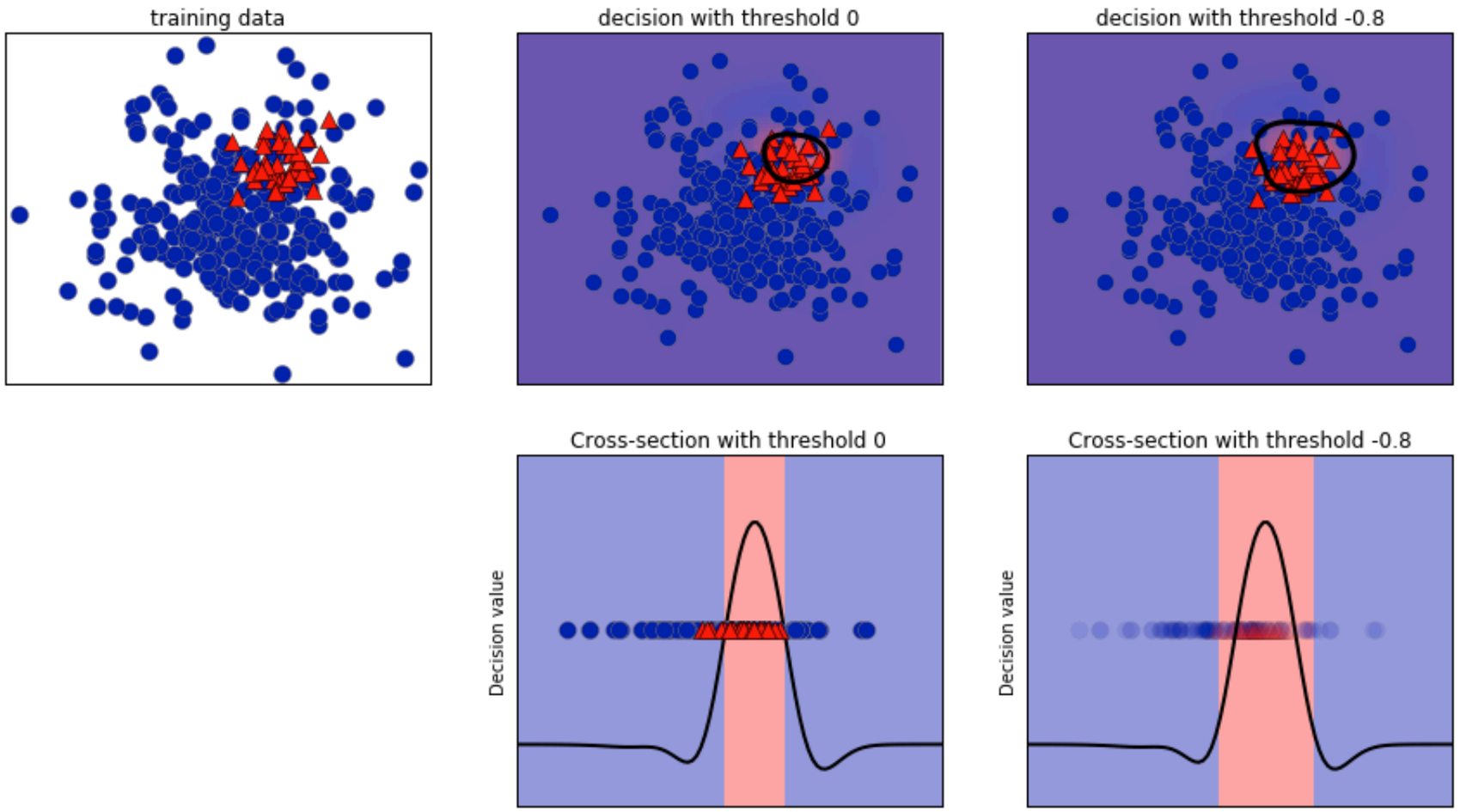

Figure 5-12. Heatmap of the decision function and the impact of changing the decision threshold

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Regression Performance Measures

Equation 2-1. Root Mean Square Error (RMSE)

$$\text{RMSE}(\mathbf{X}, h) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right)^2}$$

m

- m is the number of instances in the dataset you are measuring the RMSE on.
  - For example, if you are evaluating the RMSE on a validation set of 2,000 districts, then m = 2,000.

$\mathbf{x}^{(i)}$ $y^{(i)}$

- $\mathbf{x}^{(i)}$ is a vector of all the feature values (excluding the label) of the i^{th} instance in the dataset, and $y^{(i)}$ is its label (the desired output value for that instance).

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Regression Performance Measures

$\mathbf{X}^{(i)}$ $y^{(i)}$ — For example, if the first district in the dataset is located at longitude –118.29°, latitude 33.91°, and it has 1,416 inhabitants with a median income of $38,372, and the median house value is $156,400 (ignoring the other features for now), then:

$$\mathbf{x}^{(1)} = \begin{pmatrix} -118.29 \\ 33.91 \\ 1,416 \\ 38,372 \end{pmatrix}$$

and:

$$y^{(1)} = 156,400$$

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Regression Performance Measures

X

- **X** is a matrix containing all the feature values (excluding labels) of all instances in the dataset. There is one row per instance and the i^{th} row is equal to the transpose of $\mathbf{x}^{(i)}$, noted $(\mathbf{x}^{(i)})^T$.[6]
  - For example, if the first district is as just described, then the matrix **X** looks like this:

$$\mathbf{X} = \begin{pmatrix} \left(\mathbf{x}^{(1)}\right)^T \\ \left(\mathbf{x}^{(2)}\right)^T \\ \vdots \\ \left(\mathbf{x}^{(1999)}\right)^T \\ \left(\mathbf{x}^{(2000)}\right)^T \end{pmatrix} = \begin{pmatrix} -118.29 & 33.91 & 1,416 & 38,372 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

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Regression Performance Measures

h

- h is your system's prediction function, also called a *hypothesis*. When your system is given an instance's feature vector $\mathbf{x}^{(i)}$, it outputs a predicted value $\hat{y}^{(i)} = h(\mathbf{x}^{(i)})$ for that instance ($\hat{y}$ is pronounced "y-hat").
  - For example, if your system predicts that the median housing price in the first district is \$158,400, then $\hat{y}^{(1)} = h(\mathbf{x}^{(1)}) = 158{,}400$. The prediction error for this district is $\hat{y}^{(1)} - y^{(1)} = 2{,}000$.

$\text{RMSE}(\mathbf{X},h)$

- RMSE($\mathbf{X}$,h) is the cost function measured on the set of examples using your hypothesis h.

- Computing the root of a sum of squares (RMSE) corresponds to the *Euclidian norm*: it is the notion of distance you are familiar with. It is also called the ℓ_2 *norm*, noted $\| \cdot \|_2$ (or just $\| \cdot \|$).

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Regression Performance Measures

Equation 2-2. Mean Absolute Error

$$\mathrm{MAE}(\mathbf{X}, h) = \frac{1}{m}\sum_{i=1}^{m}\left|h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right|$$

m

- m is the number of instances in the dataset you are measuring the RMSE on.

$\mathbf{x}^{(i)}$ $y^{(i)}$

- $\mathbf{x}^{(i)}$ is a vector of all the feature values (excluding the label) of the i^{th} instance in the dataset, and $y^{(i)}$ is its label (the desired output value for that instance).

- Computing the sum of absolutes (MAE) corresponds to the ℓ_1 *norm*, noted $\| \cdot \|_1$. It is sometimes called the *Manhattan norm* because it measures the distance between two points in a city if you can only travel along orthogonal city blocks.

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Regression Performance Measures

RMSE is more sensitive to outliers than the MAE

- when outliers are exponentially rare (like in a bell-shaped curve), the RMSE performs very well and is generally preferred

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Assignments for next week

- **DataCamp**
  - Pre-processing for Machine Learning in Python course
  - Model Validation in Python course

- **Project 1**

- **Videos to watch (password: 71200)**
  - K-nearest Neighbors: https://vimeo.com/400660692
  - Linear Models: https://vimeo.com/403004687