

# Introduction to Machine Learning with Python

Andreas Müller  
Columbia University, scikit-learn

<https://github.com/amueller/quick-ml-intro>



What is machine learning?

loan_amnt	term	int_rate	grade	home_ownership	annual_inc
5000.0	36 months	10.65%	B	RENT	24000.0
2500.0	60 months	15.27%	C	RENT	30000.0
2400.0	36 months	15.96%	C	RENT	12252.0
10000.0	36 months	13.49%	C	RENT	49200.0
3000.0	60 months	12.69%	B	RENT	80000.0
5000.0	36 months	7.90%	A	RENT	36000.0
7000.0	60 months	15.96%	C	RENT	47004.0
3000.0	36 months	18.64%	E	RENT	48000.0
5600.0	60 months	21.28%	F	OWN	40000.0
5375.0	60 months	12.69%	B	RENT	15000.0



loan_status
Fully Paid
Charged Off
Fully Paid
Fully Paid
Fully Paid
Fully Paid
Fully Paid
Charged Off
Charged Off

# Supervised Learning

$$(x_i, y_i) \propto p(x, y) \quad \text{i.i.d.}$$

$$x_i \in \mathbb{R}^n$$

$$y_i \in \mathbb{R}$$

$$f(x_i) \approx y_i$$

# Classification and Regression

Classification:

- $y$  discrete

Will they subscribe?

Regression:

- $y$  continuous

How much will the  
returns be?

# Generalization

Not only

$$f(x_i) \approx y_i$$

Also for new data:

$$f(x) \approx y$$

## Documentation of scikit-learn 0.17

### Quick Start

A very short introduction into machine learning problems and how to solve them using scikit-learn. Introduced basic concepts and conventions.

### User Guide

The main documentation. This contains an in-depth description of all algorithms and how to apply them.

### Other Versions

- [scikit-learn 0.18 \(development\)](#)
- [scikit-learn 0.17 \(stable\)](#)
- [scikit-learn 0.16](#)
- [scikit-learn 0.15](#)

### Tutorials

Useful tutorials for developing a feel for some of scikit-learn's applications in the machine learning field.

### API

The exact API of all functions and classes, as given by the docstrings. The API documents expected types and allowed features for all functions, and all parameters available for the algorithms.

### Additional Resources

Talks given, slide-sets and other information relevant to scikit-learn.

### Contributing

Information on how to contribute. This also contains useful information for advanced users, for example how to build their own estimators.

### Flow Chart

A graphical overview of basic areas of machine learning, and guidance which kind of algorithms to use in a given situation.

### FAQ

Frequently asked questions about the project and contributing.

<http://scikit-learn.org/>

# Representing Data

one sample

$$X = \begin{pmatrix} 1.1 & 2.2 & 3.4 & 5.6 & 1.0 \\ 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \end{pmatrix}$$

one feature

$$y = \begin{pmatrix} 1.6 \\ 2.7 \\ 4.4 \\ 0.5 \\ 0.2 \\ 5.6 \\ 6.7 \end{pmatrix}$$

outputs / labels



# Training and Testing Data

training set

$$X = \begin{pmatrix} 1.1 & 2.2 & 3.4 & 5.6 & 1.0 \\ 6.7 & 0.5 & 0.4 & 2.6 & 1.6 \\ 2.4 & 9.3 & 7.3 & 6.4 & 2.8 \\ 1.5 & 0.0 & 4.3 & 8.3 & 3.4 \\ 0.5 & 3.5 & 8.1 & 3.6 & 4.6 \\ 5.1 & 9.7 & 3.5 & 7.9 & 5.1 \\ 3.7 & 7.8 & 2.6 & 3.2 & 6.3 \end{pmatrix}$$

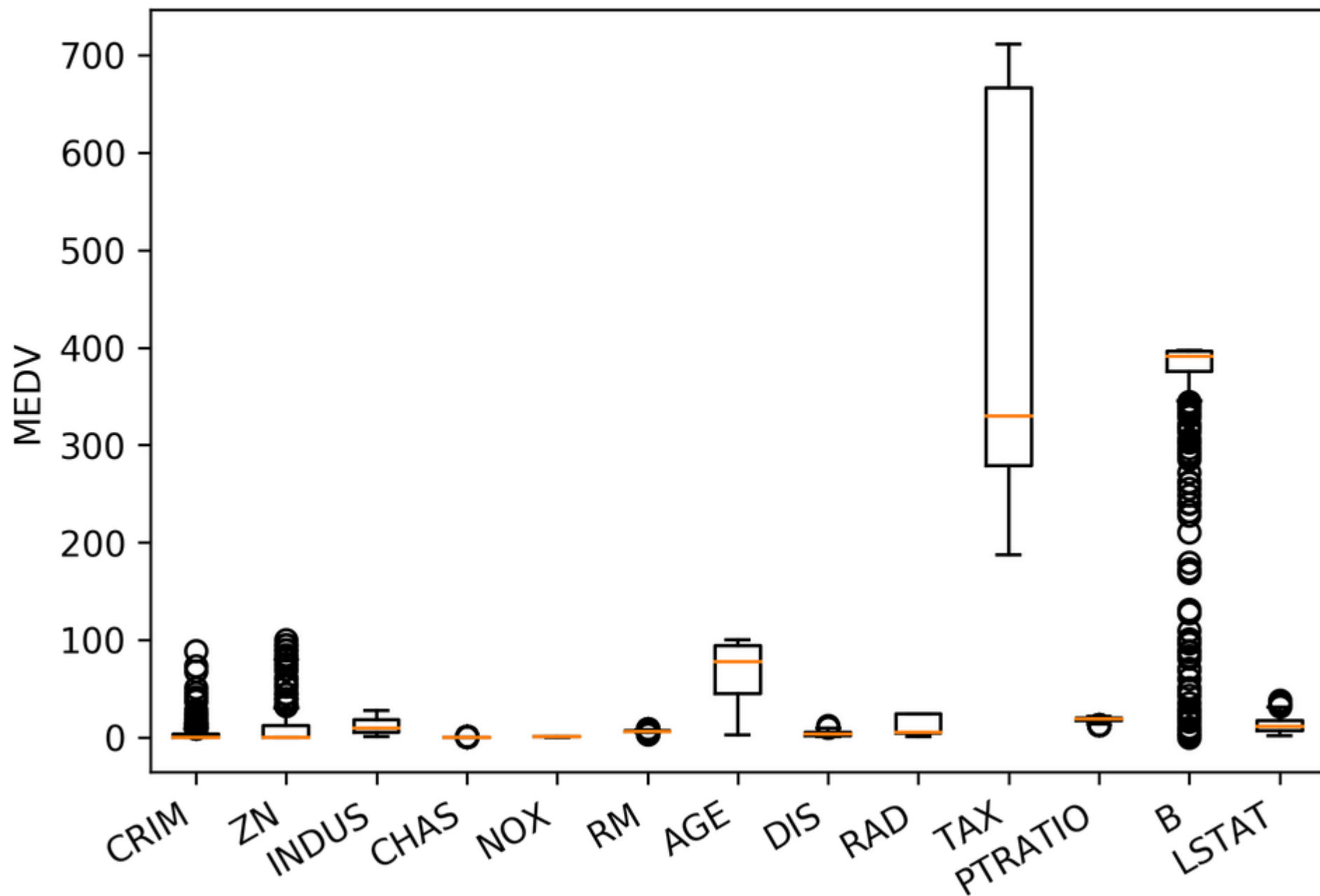
test set

$$y = \begin{pmatrix} 1.6 \\ 2.7 \\ 4.4 \\ 0.5 \\ 0.2 \\ 5.6 \\ 6.7 \end{pmatrix}$$

# IPython Notebook: Part 1 – Data Loading

# Preprocessing

```
: plt.boxplot(X)
plt.xticks(np.arange(1, X.shape[1] + 1), boston.feature_names, rotation=30, ha="right")
plt.ylabel("MEDV")
: <matplotlib.text.Text at 0x7f580303eac8>
```



# Categorical Features

# Categorical Features

$\{\text{"red"}, \text{"green"}, \text{"blue"}\} \subset \mathbb{R}^p$  ?

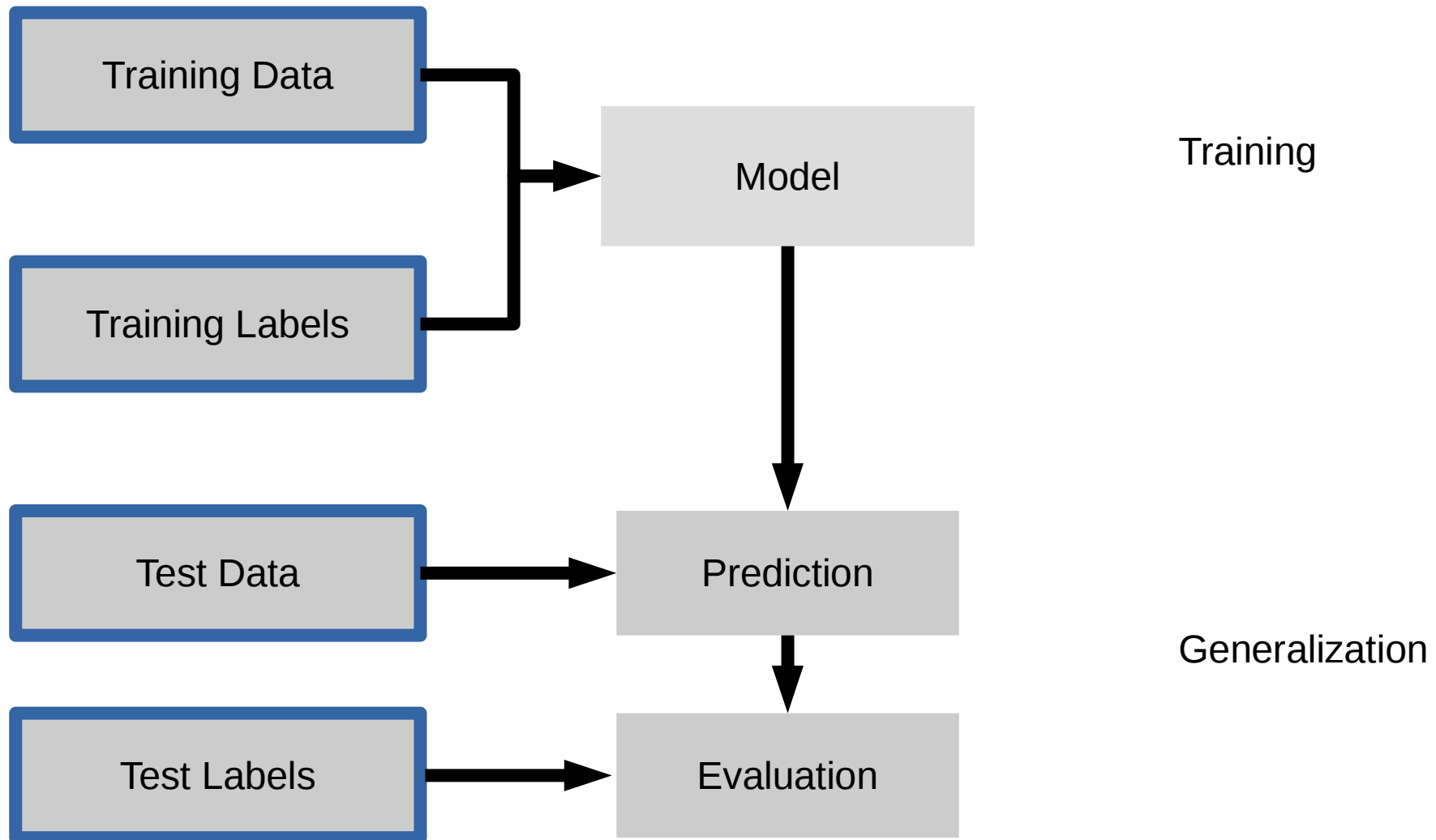
# Categorical Variables

	“red”	“green”	“blue”
	1	0	0
	0	1	0
	0	0	1

# IPython Notebook: Part 2 – Preprocessing



# Supervised Machine Learning

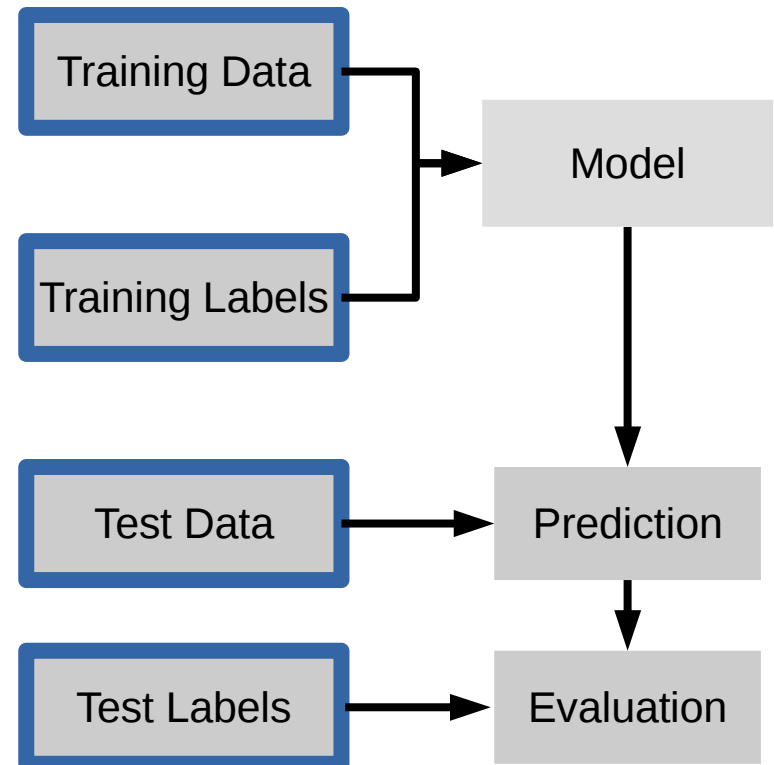


```
clf = RandomForestClassifier()
```

```
clf.fit(X_train, y_train)
```

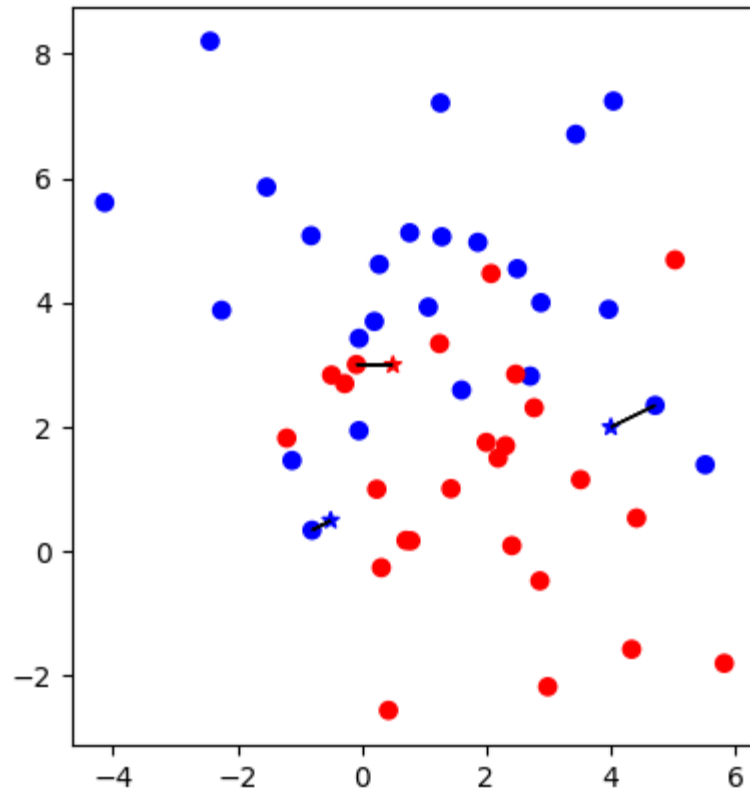
```
y_pred = clf.predict(X_test)
```

```
clf.score(X_test, y_test)
```



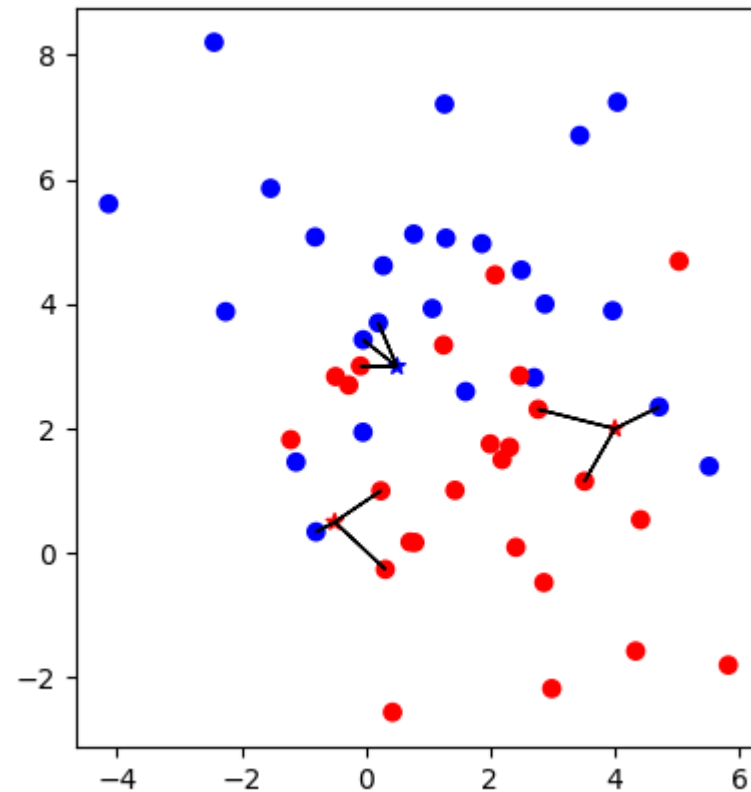
# IPython Notebook: Part 3 – Supervised Learning

# Nearest neighbors

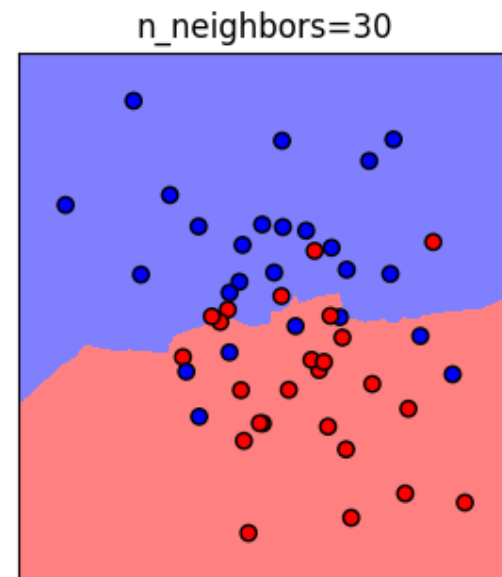
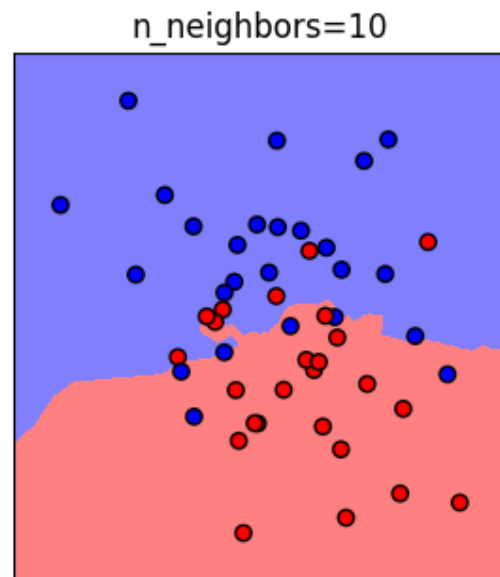
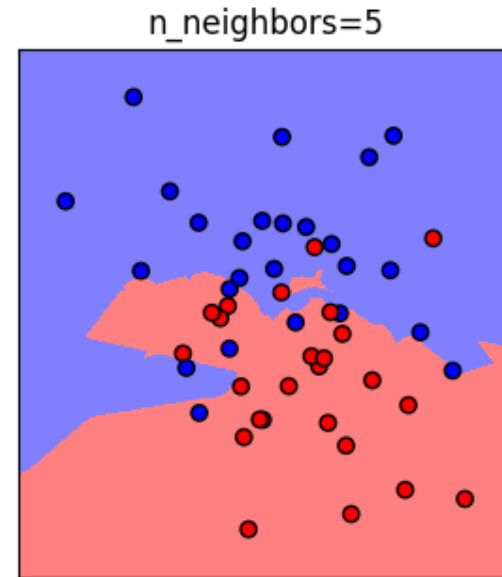
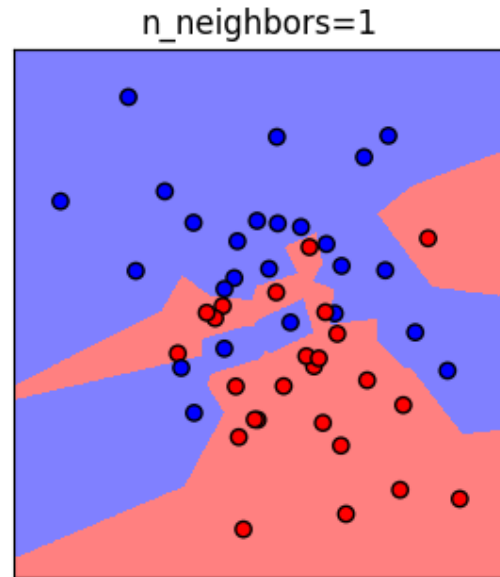


$$f(x) = y_i, i = \operatorname{argmin}_j ||x_j - x||$$

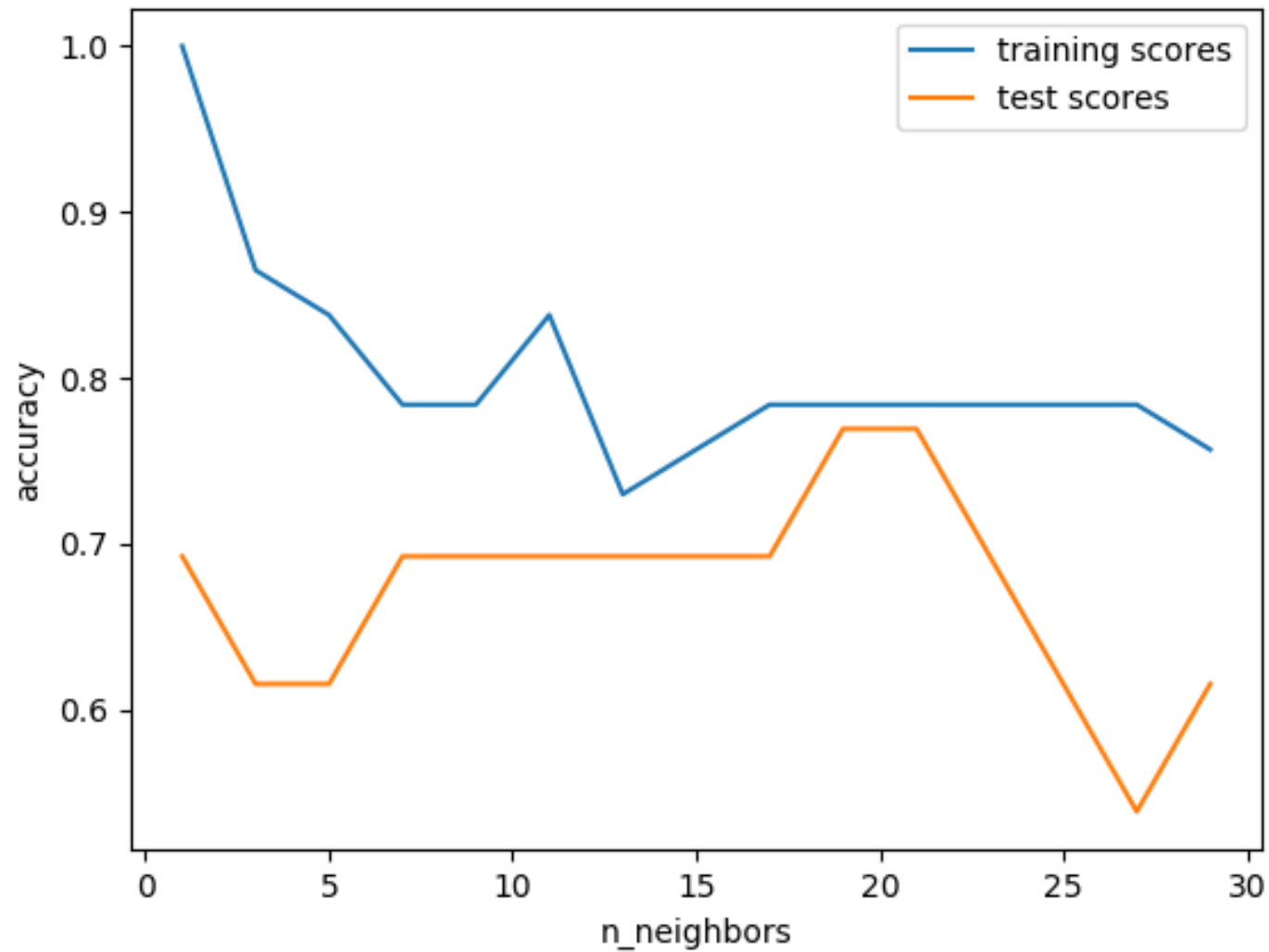
# Nearest neighbors



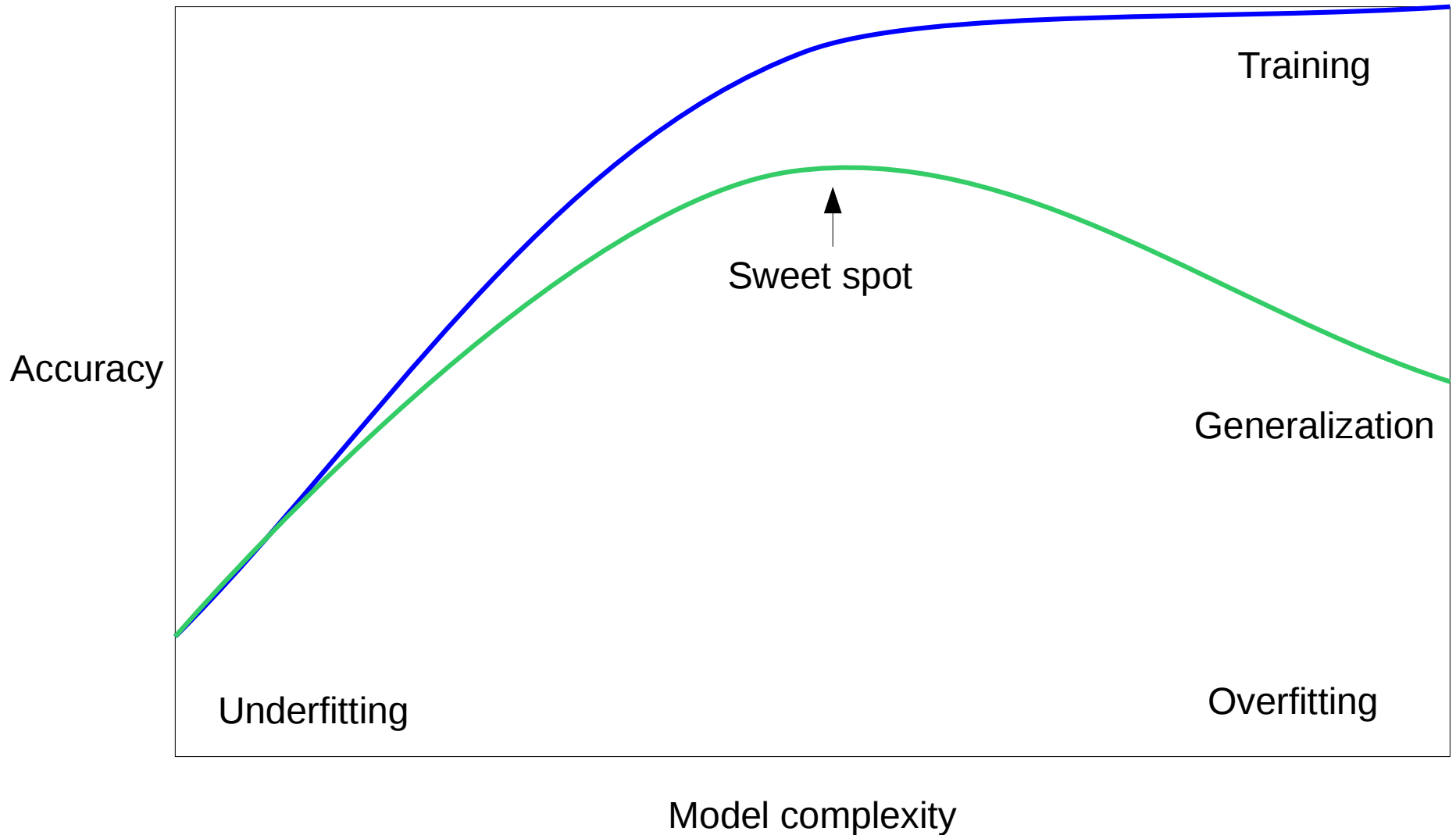
# Influence of $n\_neighbors$



# Model Complexity

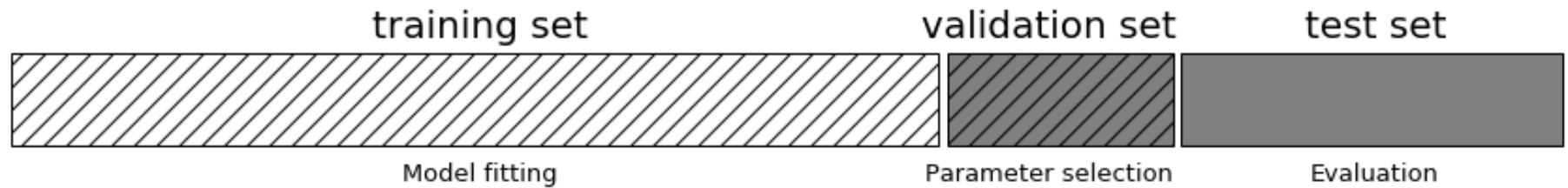


# Overfitting and Underfitting





# Three-fold split



pro: fast, simple

con: high variance, bad use of data.

```

val_scores = []
neighbors = np.arange(1, 15, 2)
for i in neighbors:
    knn = KNeighborsClassifier(n_neighbors=i)
    knn.fit(X_train, y_train)
    val_scores.append(knn.score(X_val, y_val))
print("best validation score: {:.3f}".format(np.max(val_scores)))
best_n_neighbors = neighbors[np.argmax(val_scores)]
print("best n_neighbors: {}".format(best_n_neighbors))

knn = KNeighborsClassifier(n_neighbors=best_n_neighbors)
knn.fit(X_trainval, y_trainval)
print("test-set score: {:.3f}".format(knn.score(X_test, y_test)))

```

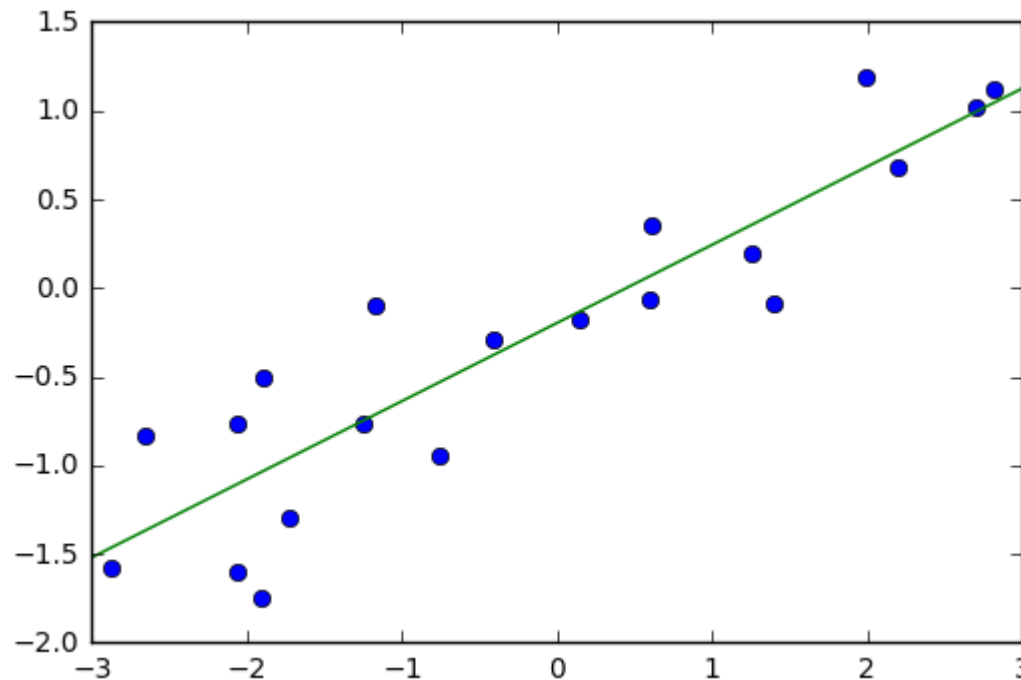
best validation score: 0.972

best n\_neighbors: 3

test-set score: 0.965

# Linear Models for Regression

# Linear Models for Regression



$$\hat{y} = w^T \mathbf{x} + b = \sum_{i=1}^p w_i x_i + b$$

# Linear Regression & Ridge Regression

$$\hat{y} = w^T \mathbf{x} + b = \sum_{i=1}^p w_i x_i + b$$

$$\min_{w \in \mathbb{R}^p} \sum_{i=1}^p ||w^T \mathbf{x}_i - y_i||^2$$

Unique solution if  $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_n)^T$  has full column rank.

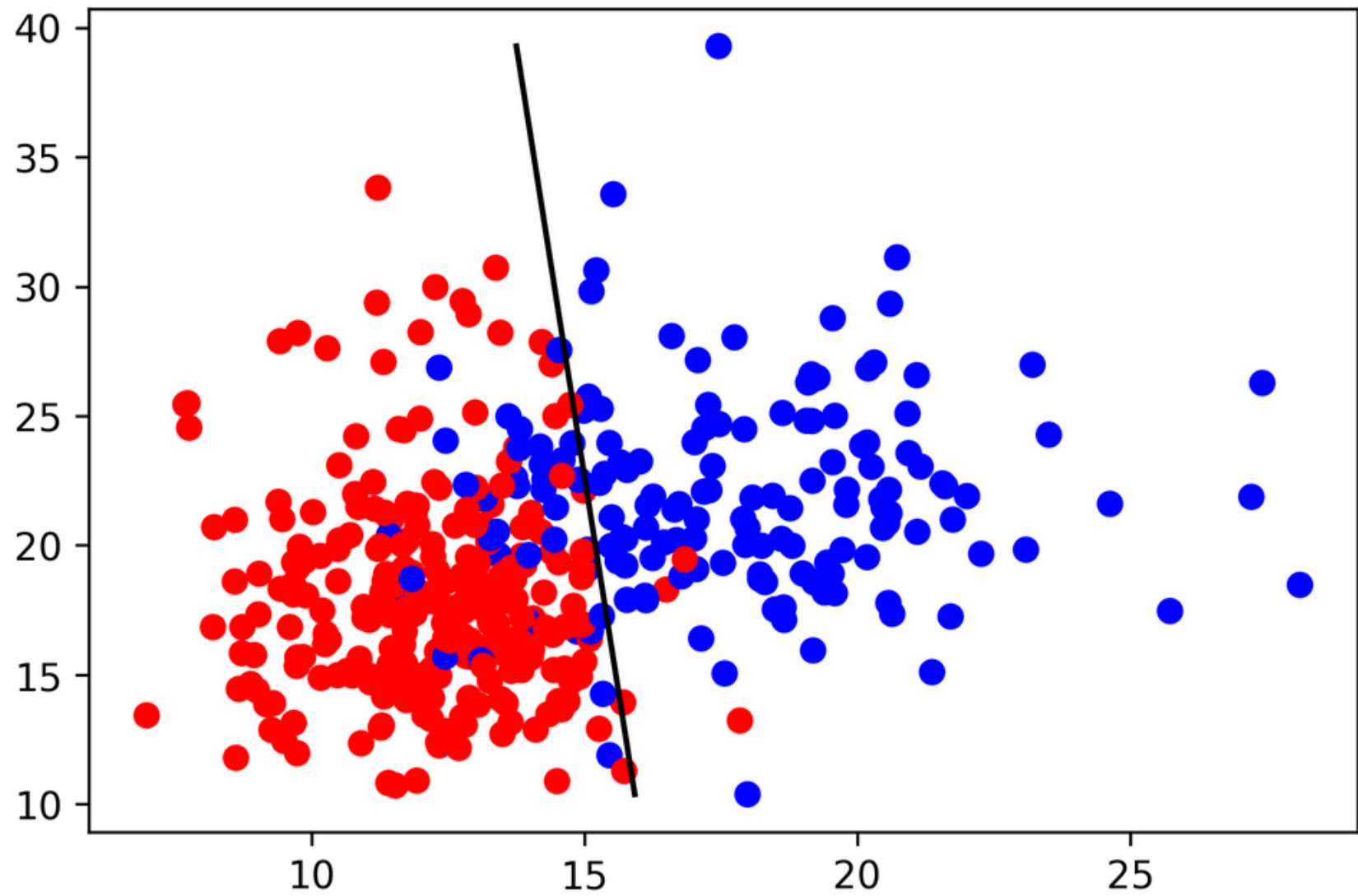
$$\min_{w \in \mathbb{R}^p} \sum_{i=1}^n ||w^T x_i - y_i||^2 + \alpha ||w||^2$$

Always has a unique solution.  
Tuning parameter alpha.

# IPython Notebook:

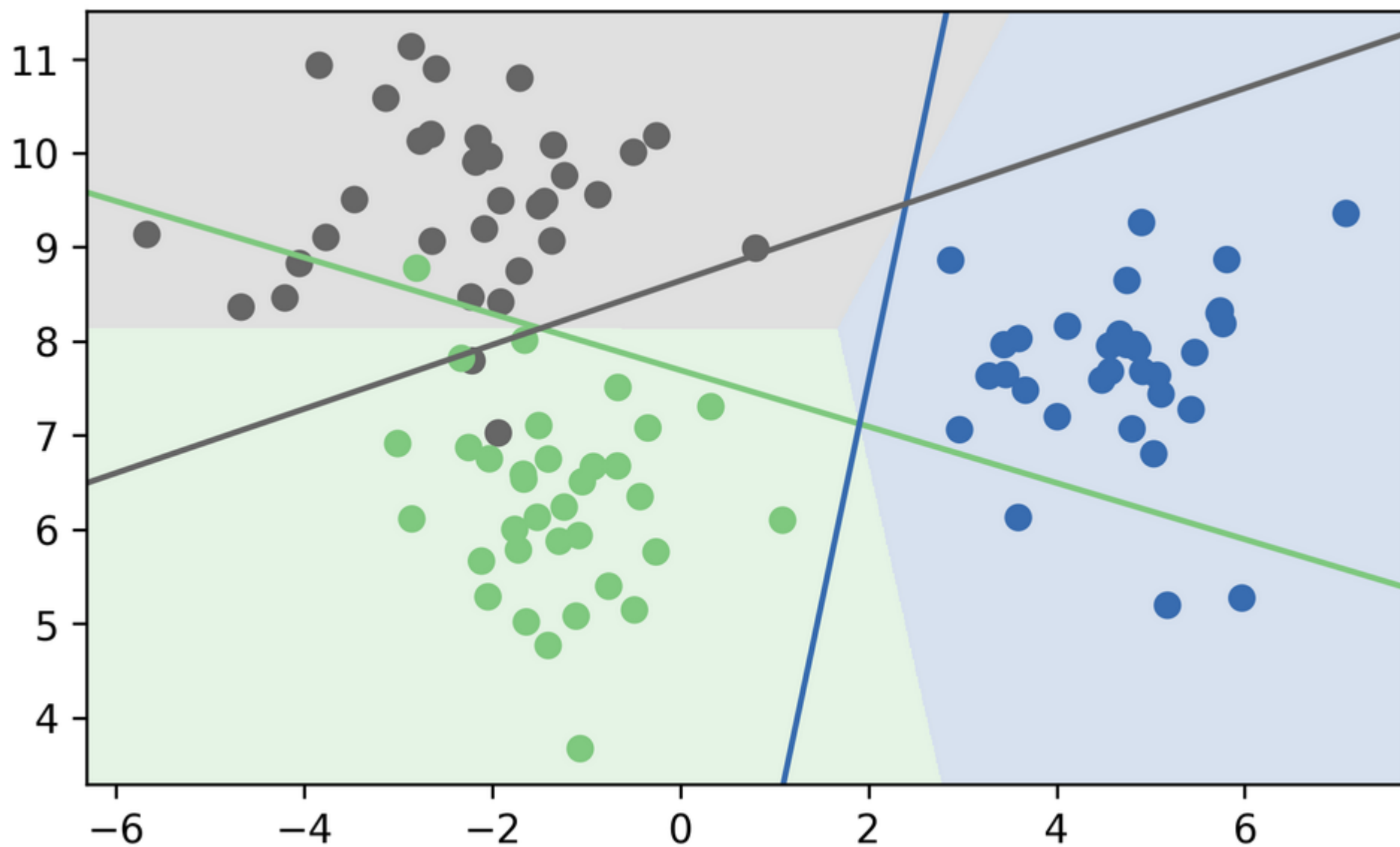
## Part 4 – Linear Models for Regression

# Linear Models for Classification



$$\hat{y} = \text{sign}(w^T \mathbf{x} + b) = \text{sign}\left(\sum_i w_i x_i + b\right)$$





$$\hat{y} = \arg \max_{i \in Y} \mathbf{w}_i \mathbf{x} + b_i$$

# IPython Notebook:

## Part 5 – Linear Models for Classification

# Basic API

**`estimator.fit(X, [y])`**

**`estimator.predict`**

**`estimator.transform`**

---

Classification

Preprocessing

Regression

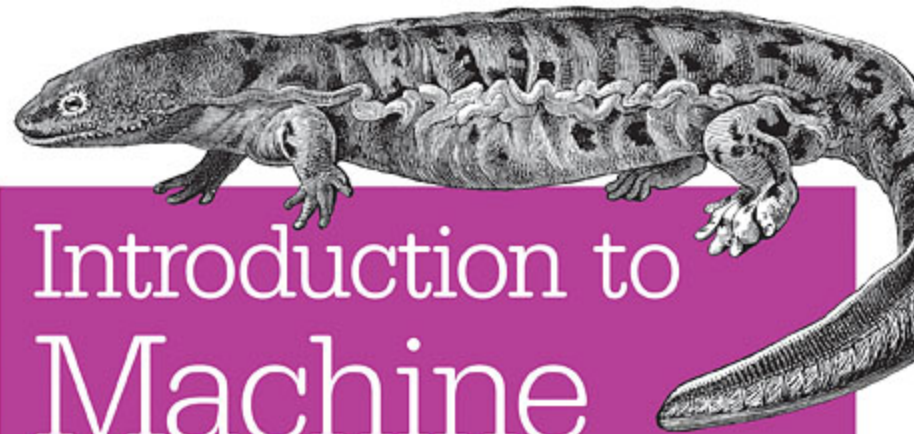
Dimensionality reduction

Clustering

Feature selection

Feature extraction

O'REILLY®



# Introduction to Machine Learning with Python

A GUIDE FOR DATA SCIENTISTS

Andreas C. Müller & Sarah Guido

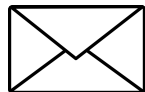
Thank you for your attention.



@amuellerm1



@amueller



importamueller@gmail.com



<http://amueller.github.io>