Introduction to regression

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George Boorman
Core Curriculum Manager, DataCamp

Predicting blood glucose levels

```python
import pandas as pd
diabetes_df = pd.read_csv("diabetes.csv")
print(diabetes_df.head())
```

	pregnancies	glucose	triceps	insulin	bmi	age	diabetes
0	6	148	35	0	33.6	50	1
1	1	85	29	0	26.6	31	0
2	8	183	0	0	23.3	32	1
3	1	89	23	94	28.1	21	0
4	0	137	35	168	43.1	33	1

Creating feature and target arrays

```
X = diabetes_df.drop("glucose", axis=1).values
y = diabetes_df["glucose"].values
print(type(X), type(y))
```

```
<class 'numpy.ndarray'> <class 'numpy.ndarray'>
```

Making predictions from a single feature

```
X_bmi = X[:, 3]
print(y.shape, X_bmi.shape)
```

```
(752,) (752,)
```

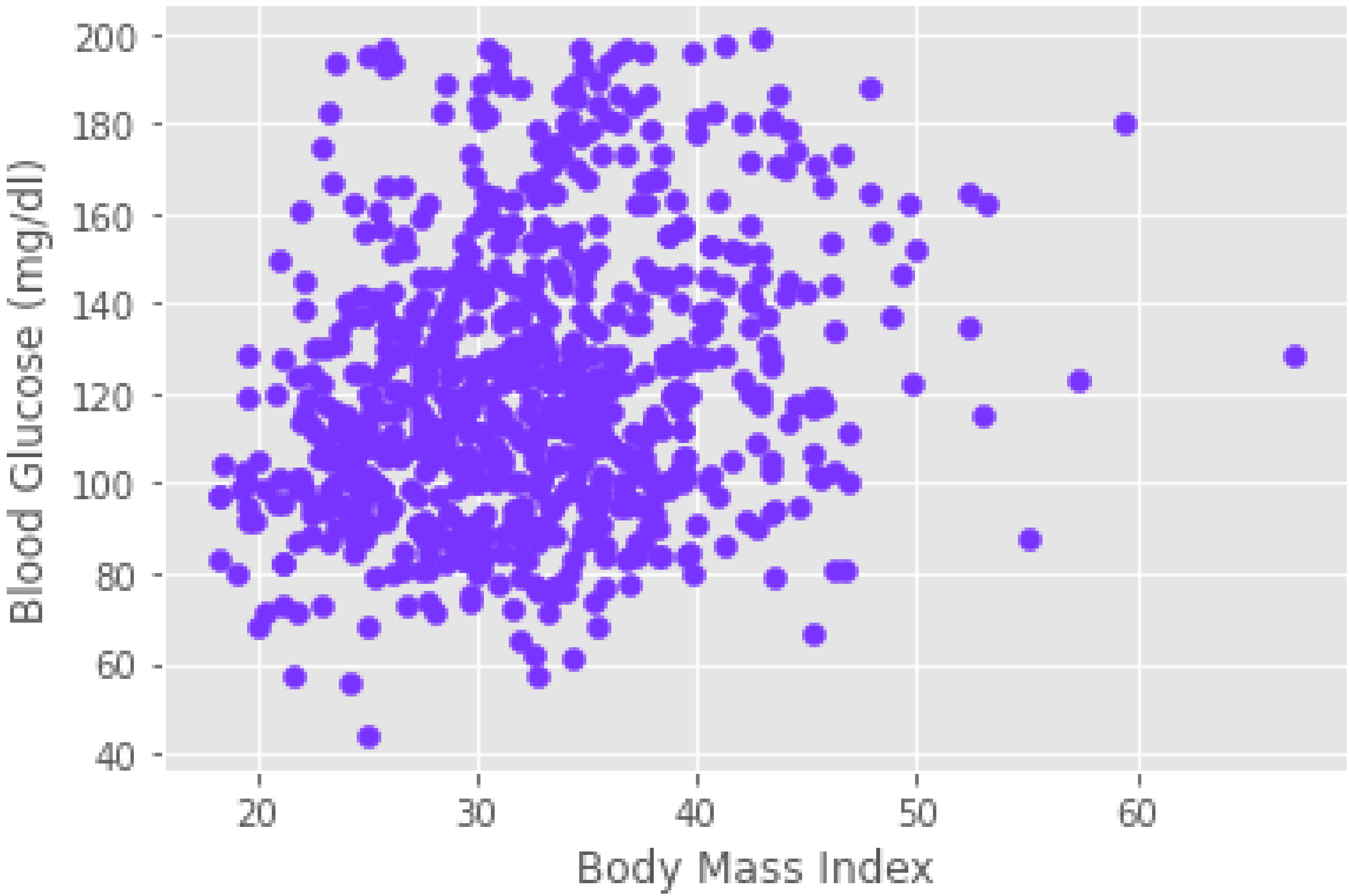
```
X_bmi = X_bmi.reshape(-1, 1)
print(X_bmi.shape)
```

```
(752, 1)
```

Plotting glucose vs. body mass index

```
import matplotlib.pyplot as plt
plt.scatter(X_bmi, y)
plt.ylabel("Blood Glucose (mg/dl)")
plt.xlabel("Body Mass Index")
plt.show()
```

Plotting glucose vs. body mass index



Fitting a regression model

```
from sklearn.linear_model import LinearRegression
reg = LinearRegression()
reg.fit(X_bmi, y)
predictions = reg.predict(X_bmi)
plt.scatter(X_bmi, y)
plt.plot(X_bmi, predictions)
plt.ylabel("Blood Glucose (mg/dl)")
plt.xlabel("Body Mass Index")
plt.show()
```

Fitting a regression model

Let's practice!

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The basics of linear regression

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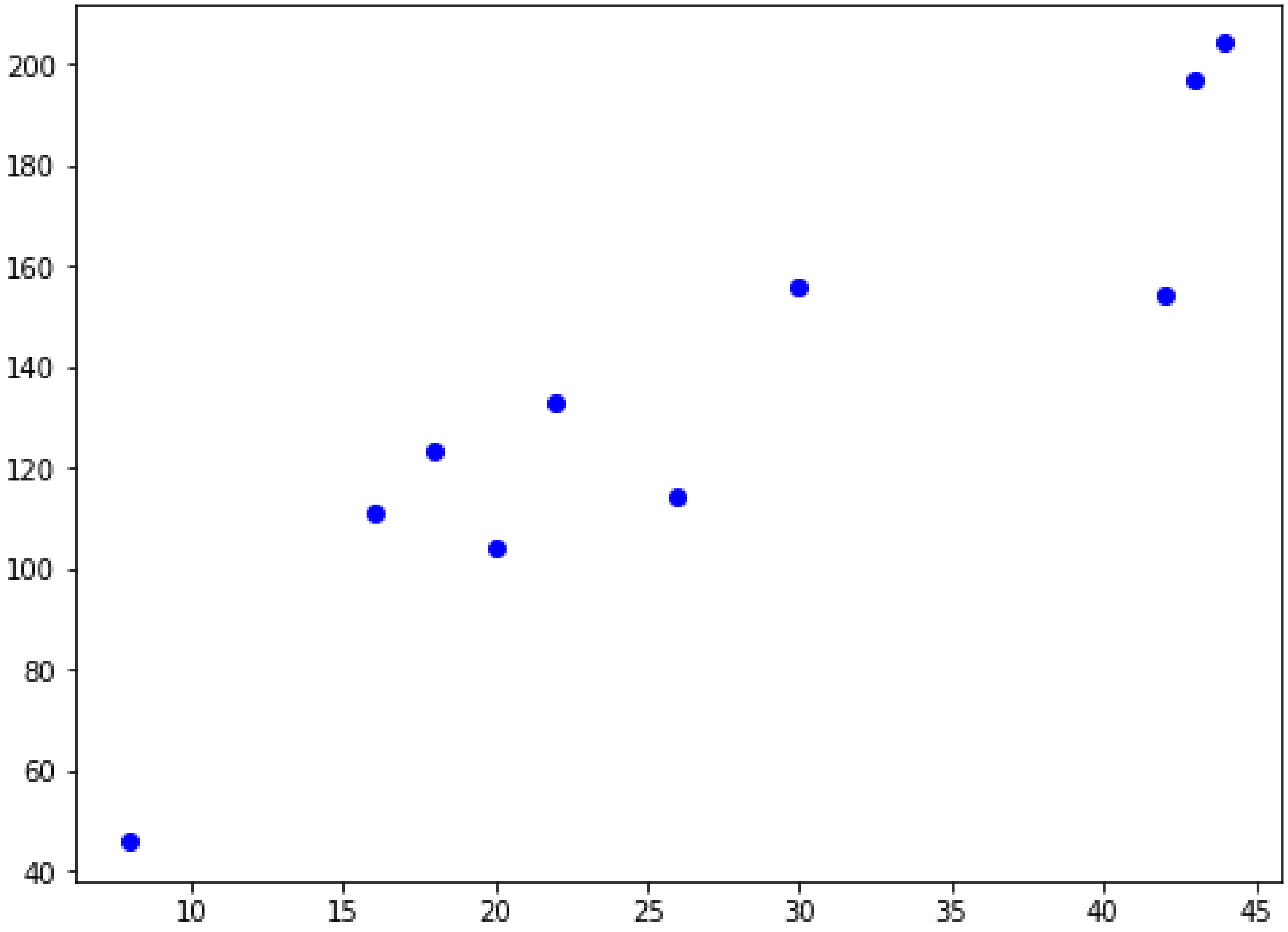
George Boorman
Core Curriculum Manager, DataCamp

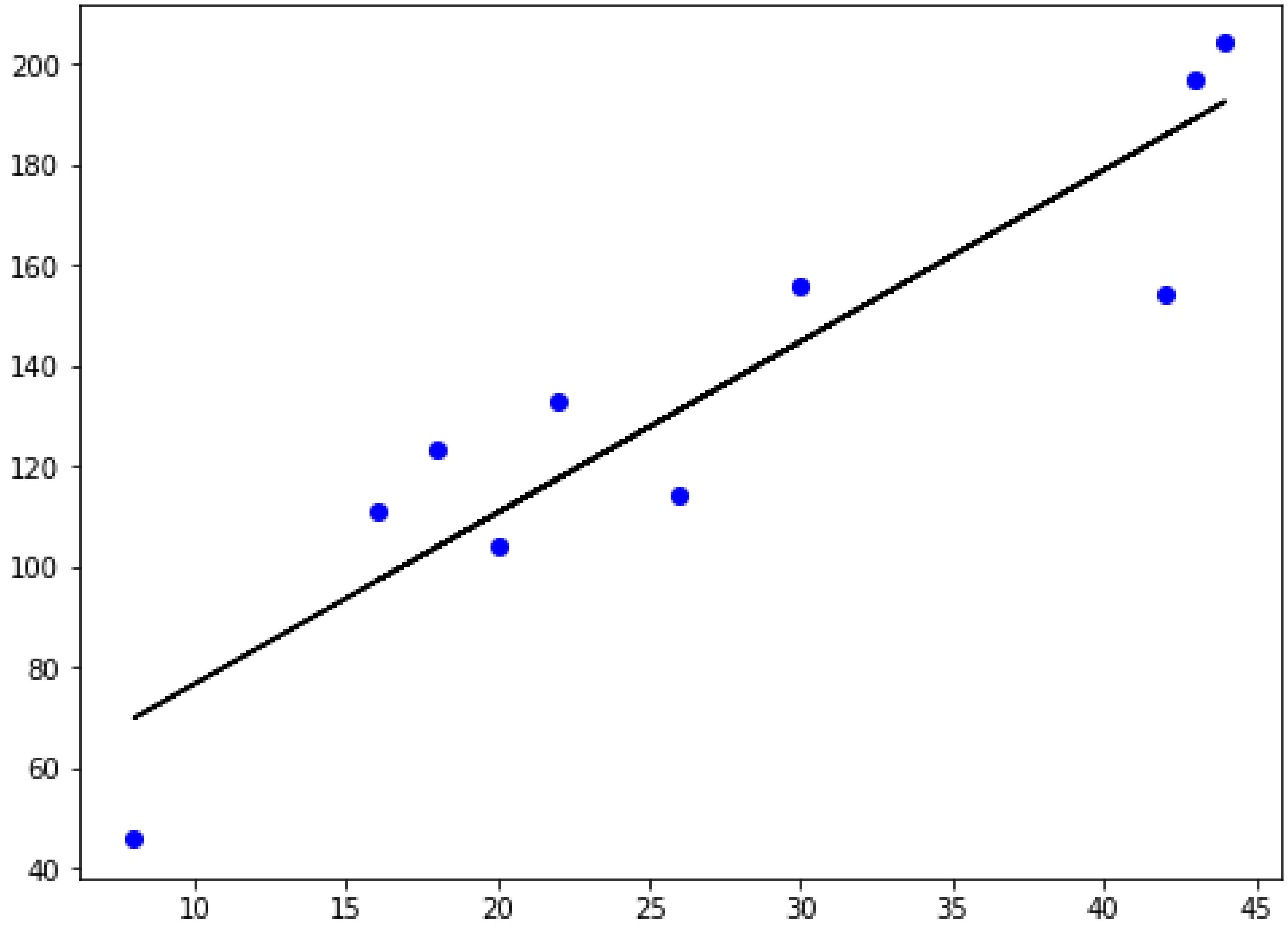
Regression mechanics

- $y = ax + b$
  - Simple linear regression uses one feature
    - y = target
    - x = single feature
    - a, b = parameters/coefficients of the model - slope, intercept
- How do we choose a and b?
  - Define an error function for any given line
  - Choose the line that minimizes the error function
- Error function = loss function = cost function

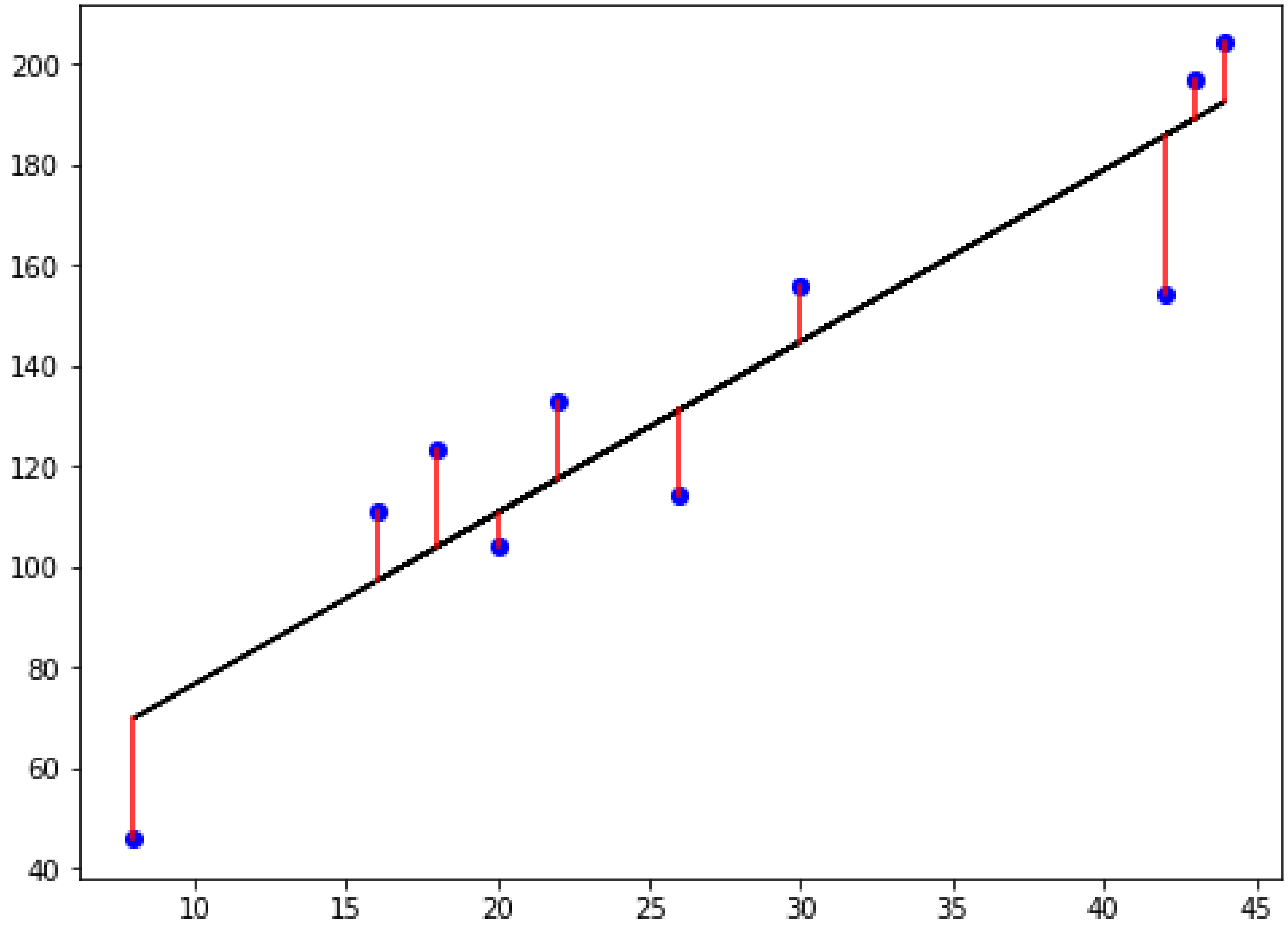
The loss function



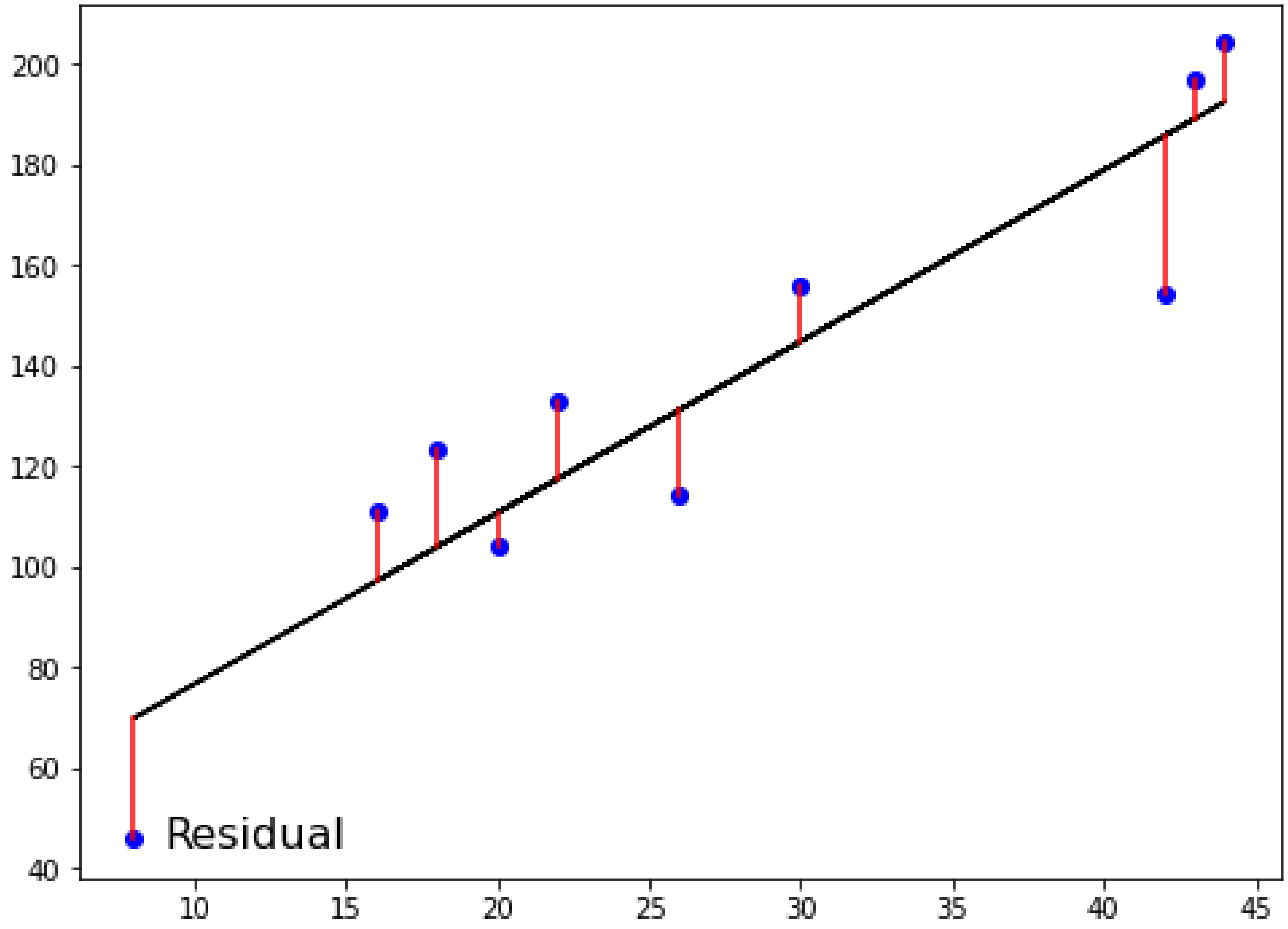
The loss function



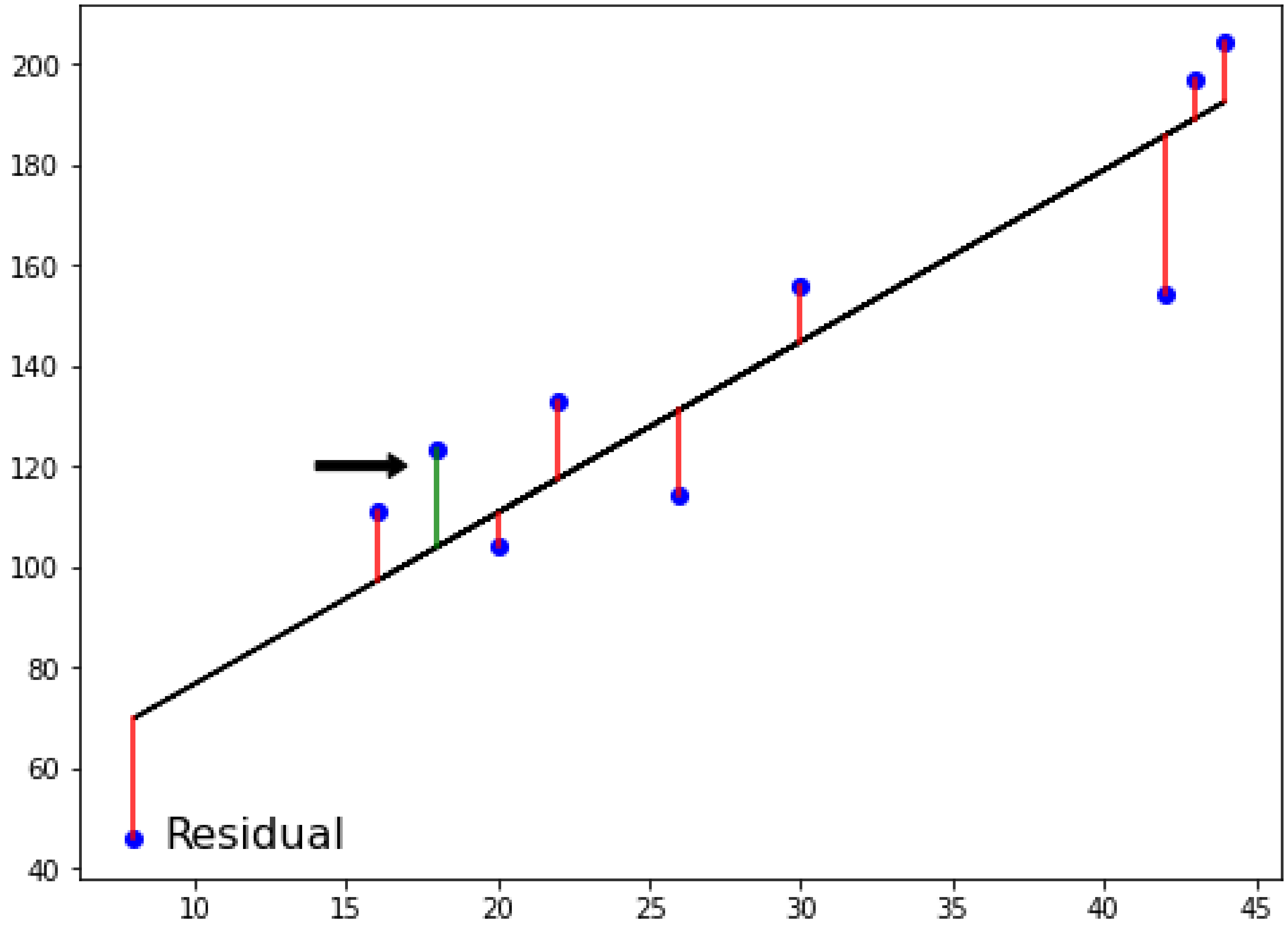
The loss function



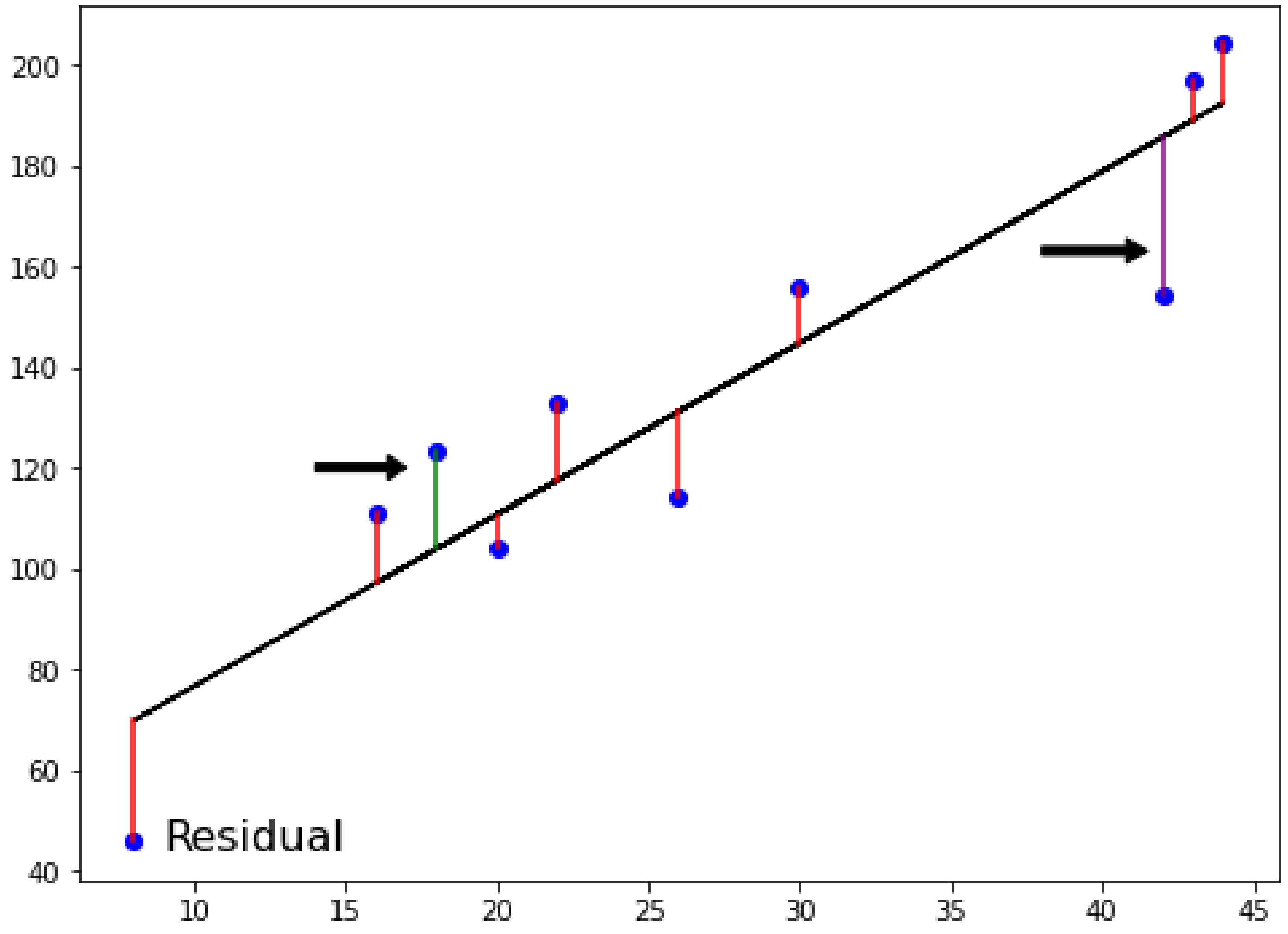
The loss function



The loss function



Ordinary Least Squares



$$RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Ordinary Least Squares (OLS): minimize RSS

Linear regression in higher dimensions

$$y = a_1x_1 + a_2x_2 + b$$

- To fit a linear regression model here:
  - Need to specify 3 variables: $a_1,\ a_2,\ b$
- In higher dimensions:
  - Known as multiple regression
  - Must specify coefficients for each feature and the variable b

$$y = a_1x_1 + a_2x_2 + a_3x_3 + \ldots + a_nx_n + b$$

- scikit-learn works exactly the same way:
  - Pass two arrays: features and target

Linear regression using all features

```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
                                                    random_state=42)
reg_all = LinearRegression()
reg_all.fit(X_train, y_train)
y_pred = reg_all.predict(X_test)
```

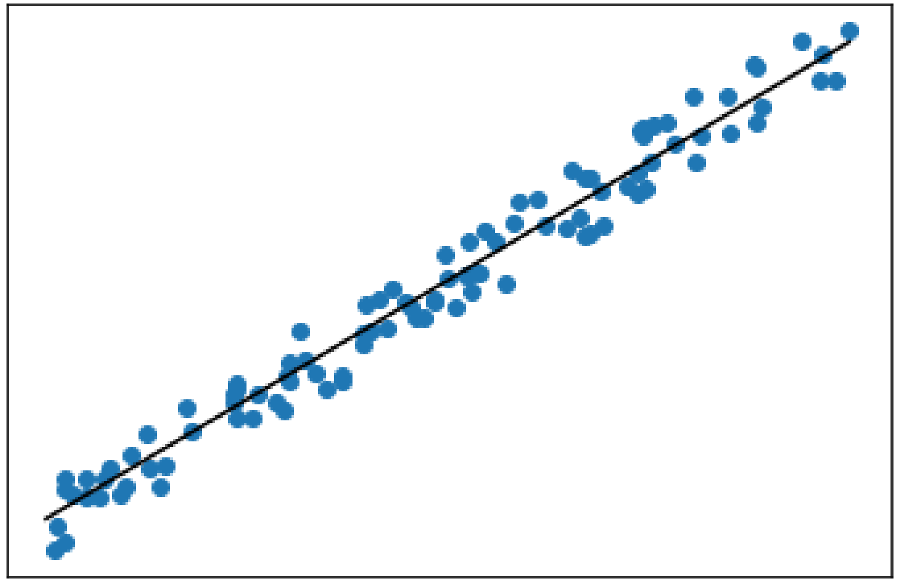
R-squared

- R^2: quantifies the variance in target values explained by the features
  - Values range from 0 to 1

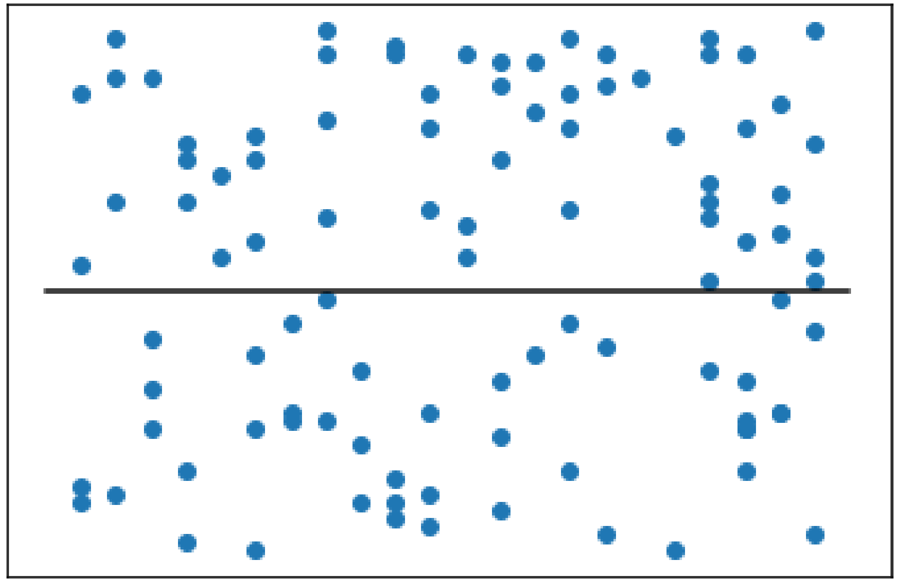
$$R^2 = 1 - \frac{SS_{residual}}{SS_{total}}$$

$$SS_{res} = \sum_{i=1}^{n} (y - \hat{y})^2$$

- High R^2:



- Low R^2:



$$SS_{tot} = \sum_{i=1}^{n} (y - \bar{y})^2$$

R-squared in scikit-learn

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

```
0.356302876407827
```

Mean squared error and root mean squared error

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

- MSE is measured in target units, squared

$$RMSE = \sqrt{MSE}$$

- Measure $RMSE$ in the same units at the target variable

RMSE in scikit-learn

```
from sklearn.metrics import mean_squared_error
mean_squared_error(y_test, y_pred, squared=False)
```

```
24.028109426907236
```

Let's practice!

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Cross-validation

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Core Curriculum Manager, DataCamp

Cross-validation motivation

- Model performance is dependent on the way we split up the data
- Not representative of the model's ability to generalize to unseen data
- Solution: Cross-validation!

Cross-validation basics

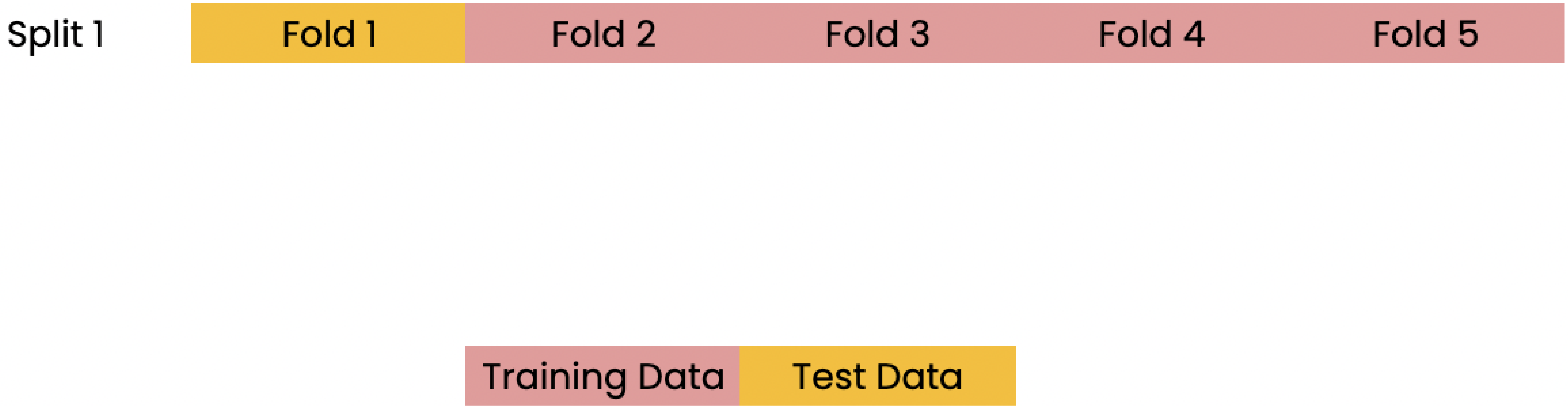
Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

Test Data

Cross-validation basics



Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1

Training Data	Test Data

Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	

Training Data | Test Data

Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	

Training Data	Test Data

Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 2

Training Data	Test Data

Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 2
Split 3	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 3

Training Data	Test Data

Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 2
Split 3	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 3
Split 4	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 4

Training Data	Test Data

Cross-validation basics

Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 1
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 2
Split 3	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 3
Split 4	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 4
Split 5	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Metric 5

Training Data	Test Data

Cross-validation and model performance

- 5 folds = 5-fold CV
- 10 folds = 10-fold CV
- k folds = k-fold CV
- More folds = More computationally expensive

Cross-validation in scikit-learn

```
from sklearn.model_selection import cross_val_score, KFold
kf = KFold(n_splits=6, shuffle=True, random_state=42)
reg = LinearRegression()
cv_results = cross_val_score(reg, X, y, cv=kf)
```

Evaluating cross-validation peformance

```python
print(cv_results)
```

```
[0.70262578, 0.7659624, 0.75188205, 0.76914482, 0.72551151, 0.73608277]
```

```python
print(np.mean(cv_results), np.std(cv_results))
```

```
0.7418682216666667 0.023330243960652888
```

```python
print(np.quantile(cv_results, [0.025, 0.975]))
```

```
array([0.7054865, 0.76874702])
```

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Regularized regression

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Core Curriculum Manager, DataCamp

Why regularize?

- Recall: Linear regression minimizes a loss function
- It chooses a coefficient, a, for each feature variable, plus b
- Large coefficients can lead to overfitting
- Regularization: Penalize large coefficients

Ridge regression

- Loss function = OLS loss function +

$$\alpha * \sum_{i=1}^{n} {a_i}^2$$

- Ridge penalizes large positive or negative coefficients
- α: parameter we need to choose
- Picking α is similar to picking `k` in KNN
- Hyperparameter: variable used to optimize model parameters
- α controls model complexity
  - α = 0 = OLS (Can lead to overfitting)
  - Very high α: Can lead to underfitting

Ridge regression in scikit-learn

```
from sklearn.linear_model import Ridge
scores = []
for alpha in [0.1, 1.0, 10.0, 100.0, 1000.0]:
    ridge = Ridge(alpha=alpha)
    ridge.fit(X_train, y_train)
    y_pred = ridge.predict(X_test)
    scores.append(ridge.score(X_test, y_test))
print(scores)
```

```
[0.2828466623222221, 0.28320633574804777, 0.2853000732200006,
 0.2642398481266813, 0.19292424694100963]
```

Lasso regression

- Loss function = OLS loss function +

$$\alpha * \sum_{i=1}^{n} |a_i|$$

Lasso regression in scikit-learn

```
from sklearn.linear_model import Lasso
scores = []
for alpha in [0.01, 1.0, 10.0, 20.0, 50.0]:
  lasso = Lasso(alpha=alpha)
  lasso.fit(X_train, y_train)
  lasso_pred = lasso.predict(X_test)
  scores.append(lasso.score(X_test, y_test))
print(scores)
```

```
[0.99991649071123, 0.99961700284223, 0.93882227671069, 0.74855318676232, -0.05741034640016]
```

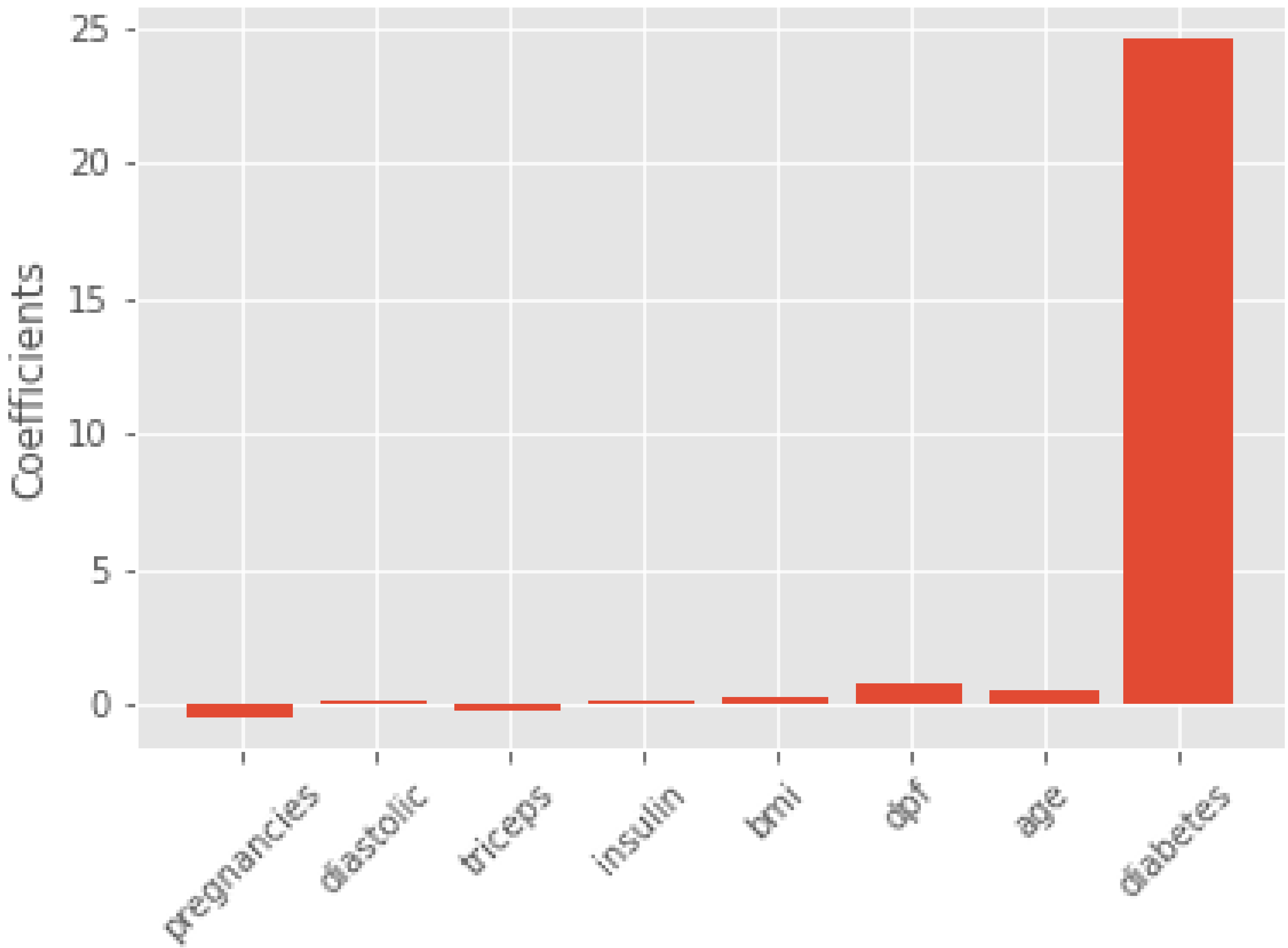
Lasso regression for feature selection

- Lasso can select important features of a dataset
- Shrinks the coefficients of less important features to zero
- Features not shrunk to zero are selected by lasso

Lasso for feature selection in scikit-learn

```
from sklearn.linear_model import Lasso
X = diabetes_df.drop("glucose", axis=1).values
y = diabetes_df["glucose"].values
names = diabetes_df.drop("glucose", axis=1).columns
lasso = Lasso(alpha=0.1)
lasso_coef = lasso.fit(X, y).coef_
plt.bar(names, lasso_coef)
plt.xticks(rotation=45)
plt.show()
```

Lasso for feature selection in scikit-learn



Let's practice!

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