# Getting Started with Machine Learning in Python

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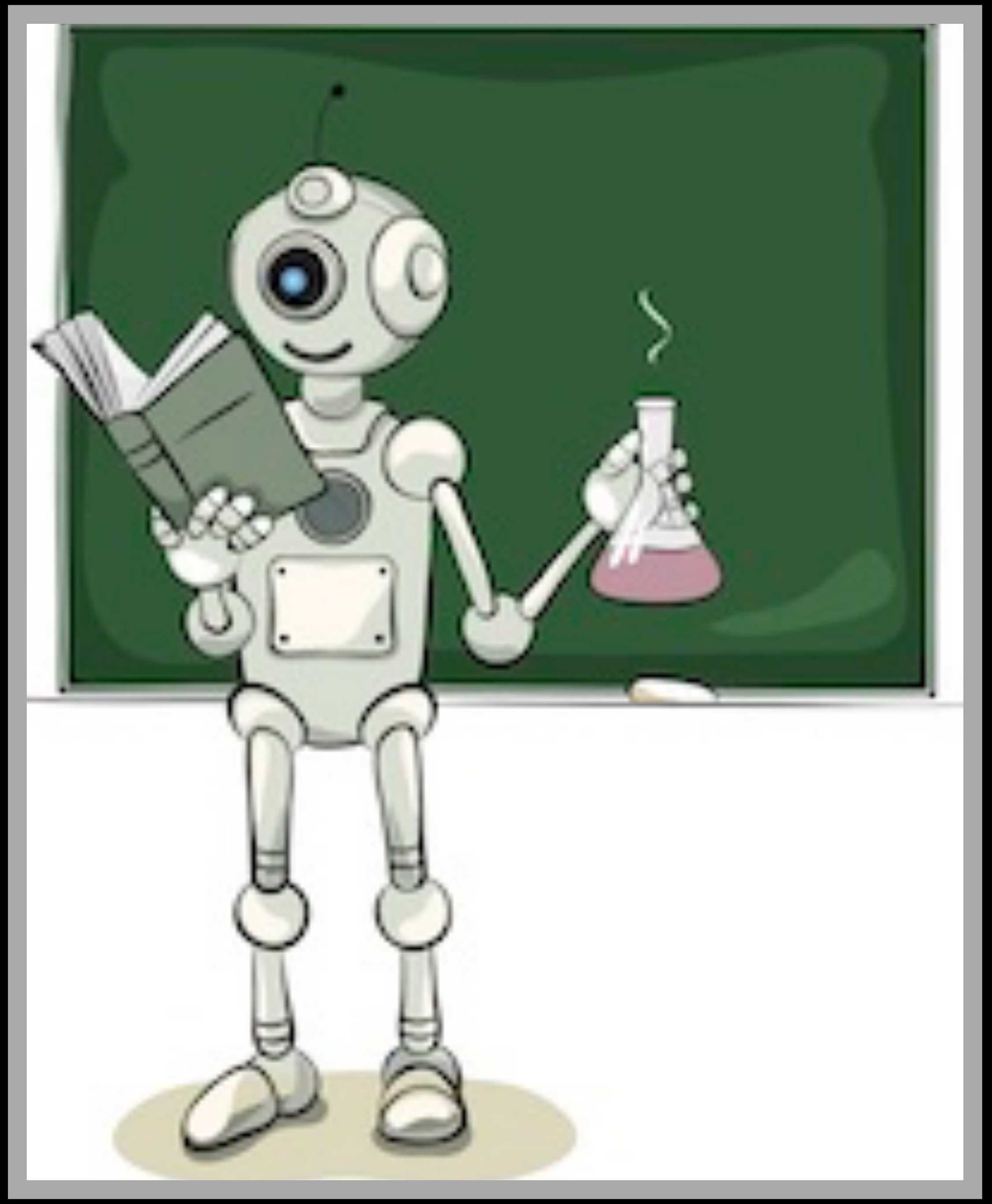
Wednesday, February 28, 2024 at 4:30-6:00 PM

**https://github.com/PrincetonUniversity/python_machine_learning**

Workshop materials created by Prof. Christina Peters

# What is machine learning?



A computer observes some data,
builds a model based on the data,
and uses the model as both a hypothesis about the world
and a piece of software that can solve problems.

*Artificial Intelligence: A Modern Approach*. Russell and Norvig, 2021. Pearson.

# Why use machine learning?

*Why not just program the model?*

- you may not know the model
- you want the model to be flexible and adapt as you have new data

# Why use <u>classical</u> machine learning?

- You want a physically interpretable model
- Your data isn’t images
- You have a simple-ish problem

# Supervised Machine Learning

Computer observes input-output pairs
and learns a function that maps input to output.

- *Labeled* data

# Supervised Machine Learning

Training set of N input-output pairs:

$(X_1,y_1), (X_2,y_2), \ldots (X_N,y_N)$

where each pair was generated by an unknown function $y = f(X)$.

Goal: learn a function $h$ that approximates the true function $f$.

# Unsupervised Machine Learning

Computer learns patterns/structure in input data.

- Without labels.

# Unsupervised Machine Learning

Training set of N inputs:

$X_1, X_2, \dots X_N$

Goal: learn structure/patterns in the data

# Supervised Machine Learning

- You have simulated data where you know the truth
- You have data labeled by a human

# Unsupervised Machine Learning

- You have experimental data
- You want to explore / visualize the data

# Common algorithms

| **Supervised** | **Unsupervised** |
|---|---|
| Regression | Clustering |
| Classification | Dimensionality Reduction |

# Common algorithms

| Supervised | Unsupervised |
| --- | --- |
| Regression | Clustering |
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# Regression

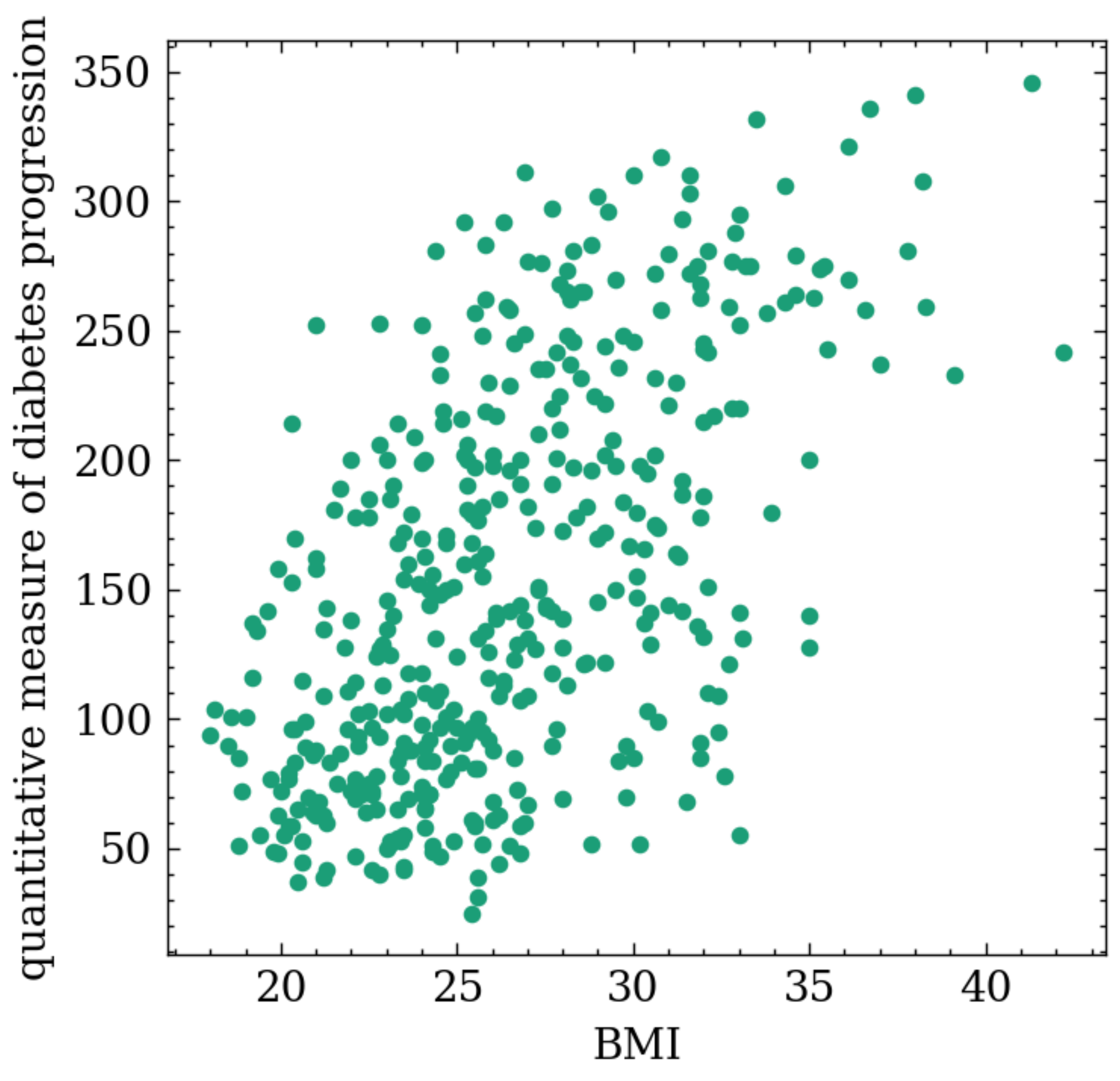
Training set of N input-output pairs:

$(X_1,y_1), (X_2,y_2), \ldots (X_N,y_N)$

where <u>desired output value is a continuous value</u>.

Goal: learn a function that approximates the true function *f*.

# Linear Regression




input-output pairs:

- $X_i$ , BMI
- $y_i$ , diabetes progression

Diabetes dataset:

*sklearn.datasets.load_diabetes*

Goal: learn a function $h$ that approximates the true function $f$:

*Predicted diabetes progression:* $\hat{y} = h(x)$

# Linear Regression

independent variables

dependent variable

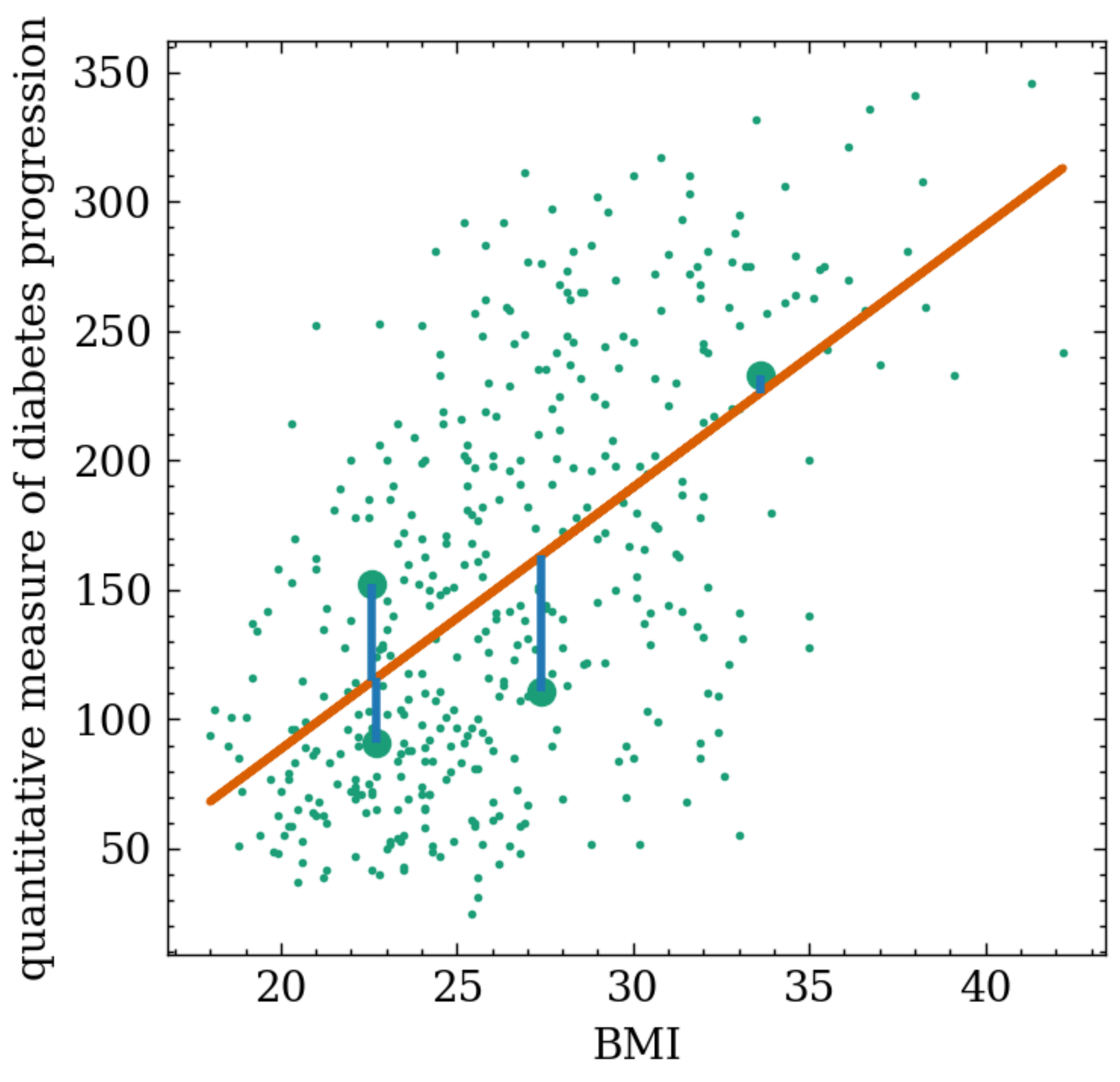
$$y = b + mx$$

$$y = X\beta$$

parameter vector

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \qquad X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix} \qquad \beta = \begin{bmatrix} b \\ m \end{bmatrix}$$

# Linear Regression



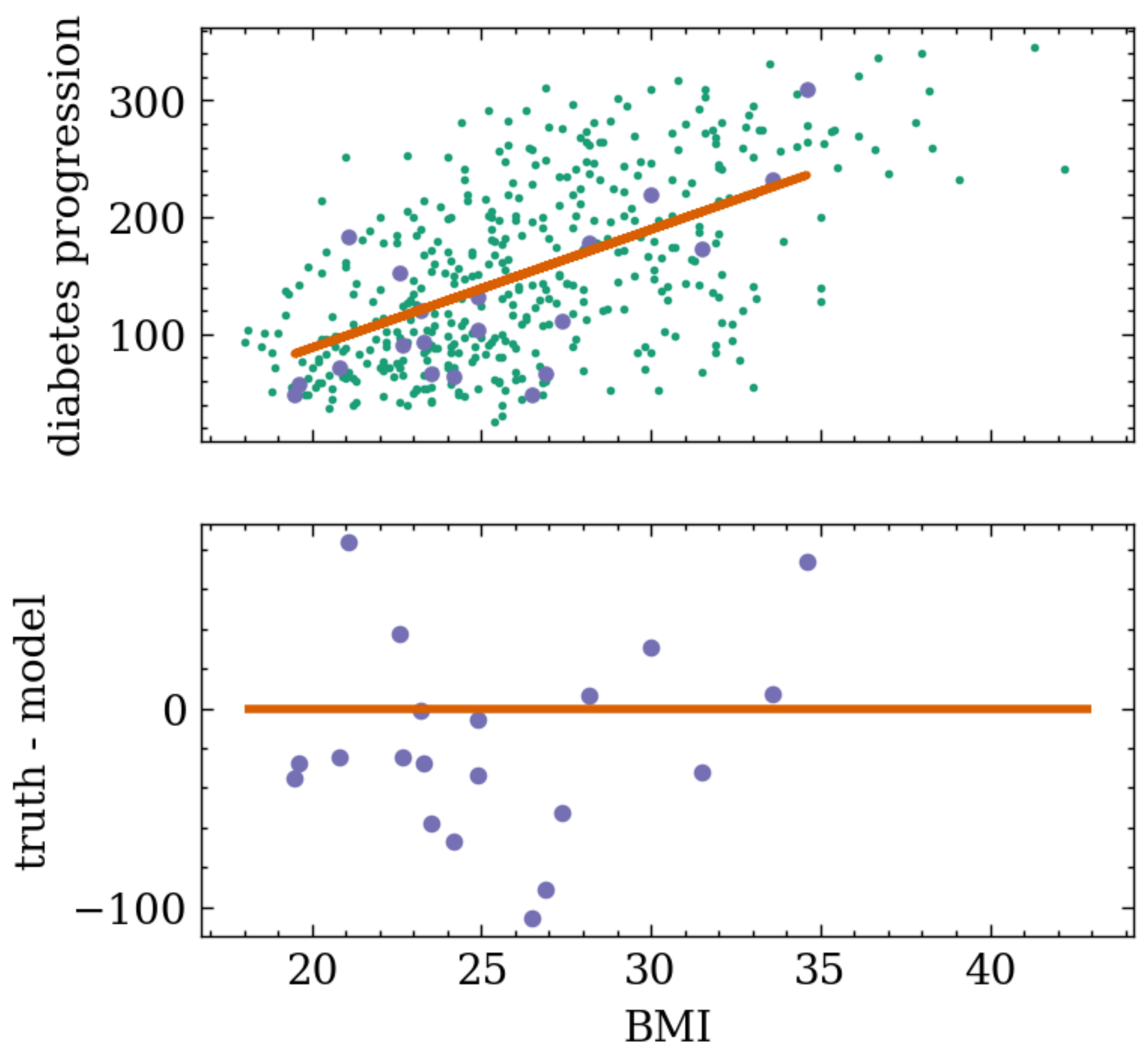

$$y = X\beta$$

**Ordinary Least Squares**

Compute the vector $\beta$ that minimizes:

$$\sum_{i}^{N} (y_i - X_i\ \beta)^2$$

# Linear Regression

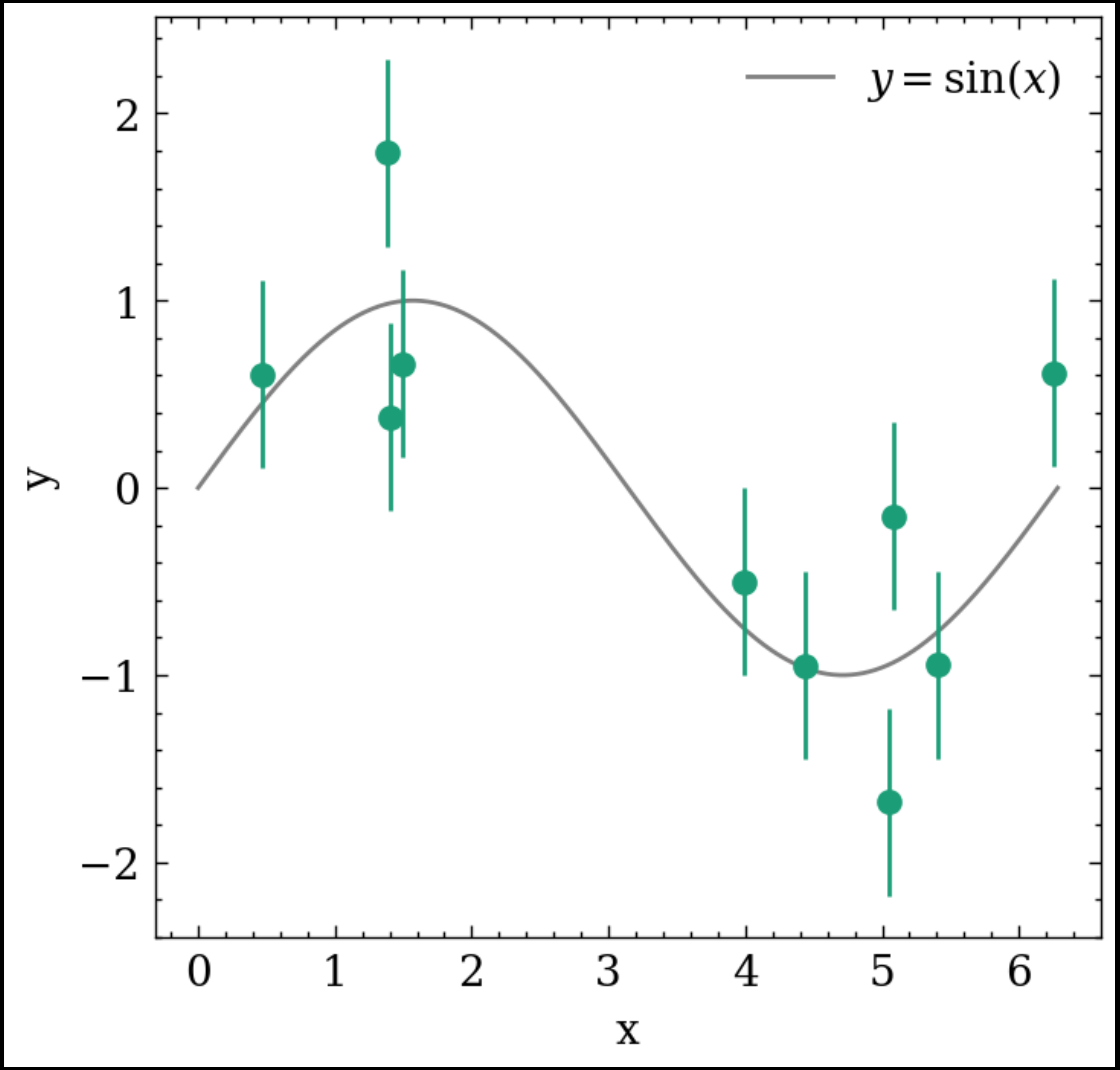



Evaluate the generalizability of the model with a test set of M input-output pairs:

$$(X_1,y_1),\ (X_2,y_2),\ \dots\ (X_M,y_M)$$

Test set data is not included in the training set.

# Gaussian Process Regression



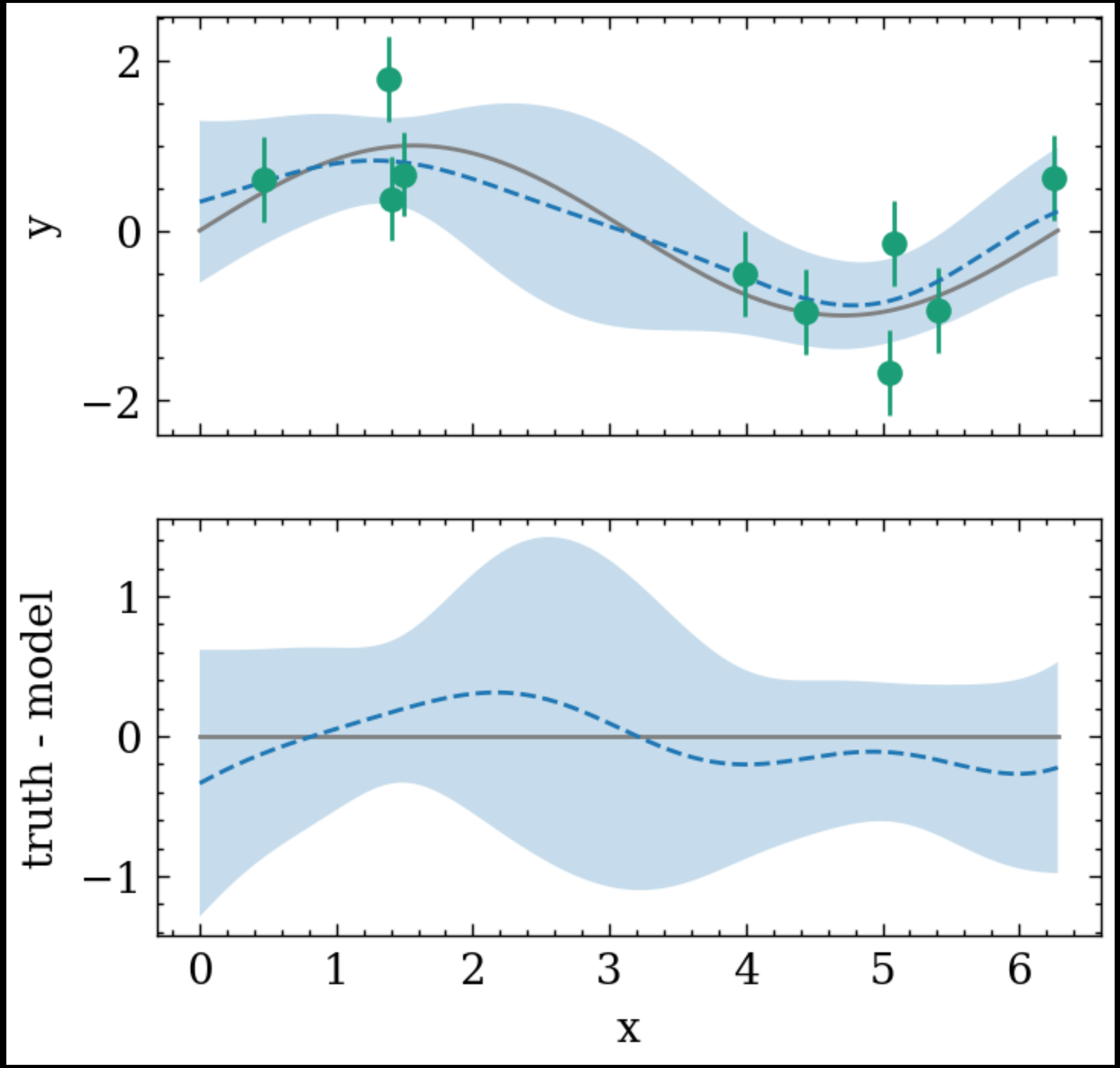

input-output pairs:

- $x_i$
- $y_i = \sin(x_i)$ + Gaussian noise

Goal: learn a function $h$ that approximates the true function $f$:

$$\hat{y} = h(x)$$

# Gaussian Process Regression




A regression method where the prediction is probabilistic

- Gaussian
- compute empirical confidence intervals

sklearn.gaussian_process.GaussianProcessRegressor

Carl Eduard Rasmussen and Christopher K.I. Williams, “Gaussian Processes for Machine Learning”, MIT Press 2006.

Examples of problems in your area of research where *regression* could be used?

# Common algorithms

| Supervised | Unsupervised |
| --- | --- |
| Regression | Clustering |
| Classification | Dimensionality Reduction |

# Classification

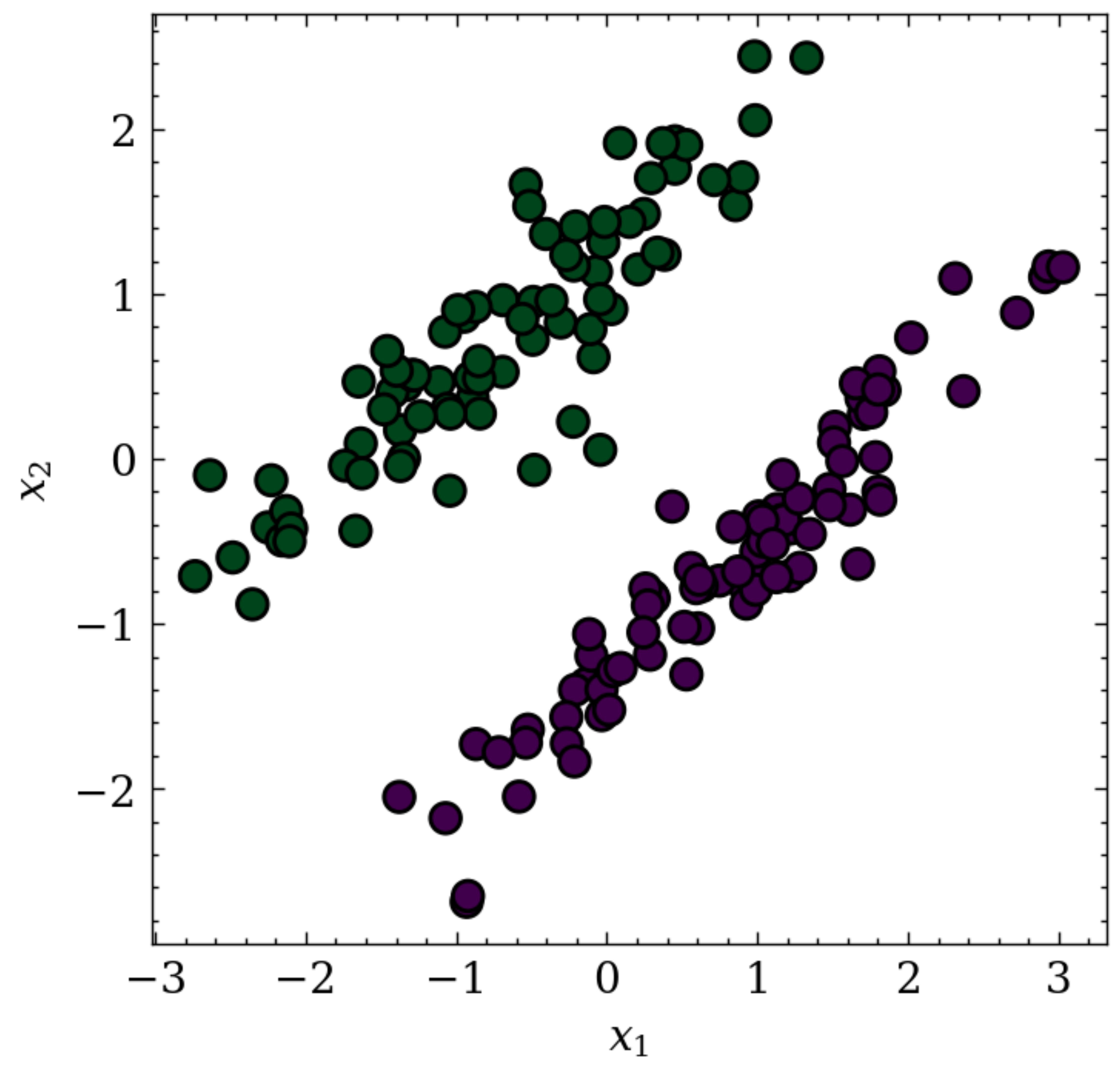
Training set of N input-output pairs:

$(X_1,y_1), (X_2,y_2), \ldots (X_N,y_N)$

where desired output value is a discrete value.

Goal: learn a function $h$ that approximates the true function $f$.

# Classification



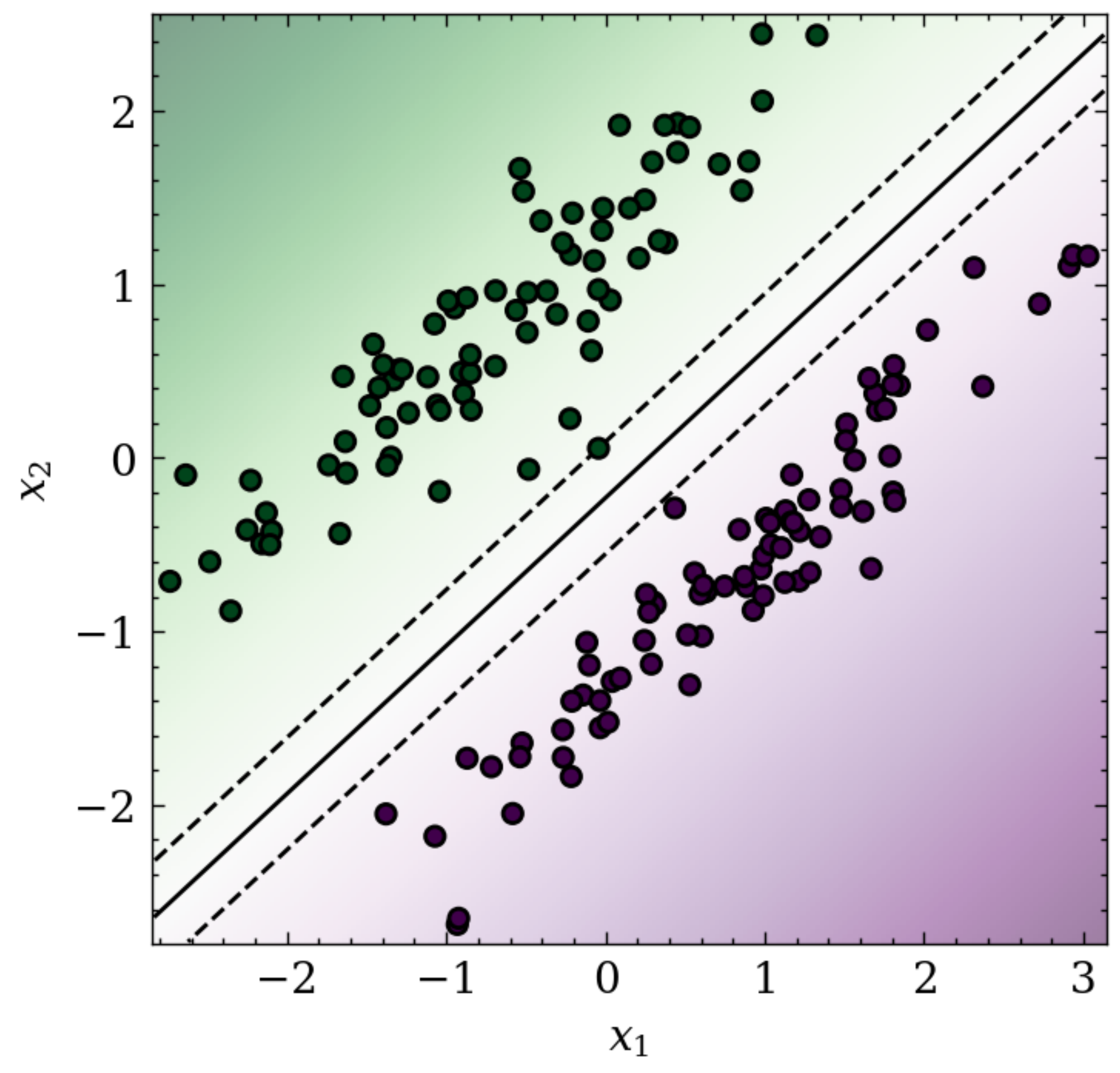

**input-output pairs:**

- $X_i = \{x_{i,1}, x_{i,2}\}$
- $y_i$ **, class label, either 1 or –1**

Goal: learn a function $h$ that approximates the true function *f:*

*predicted class label,* $\hat{y} = h(x_1, x_2)$

# Support Vector Classification



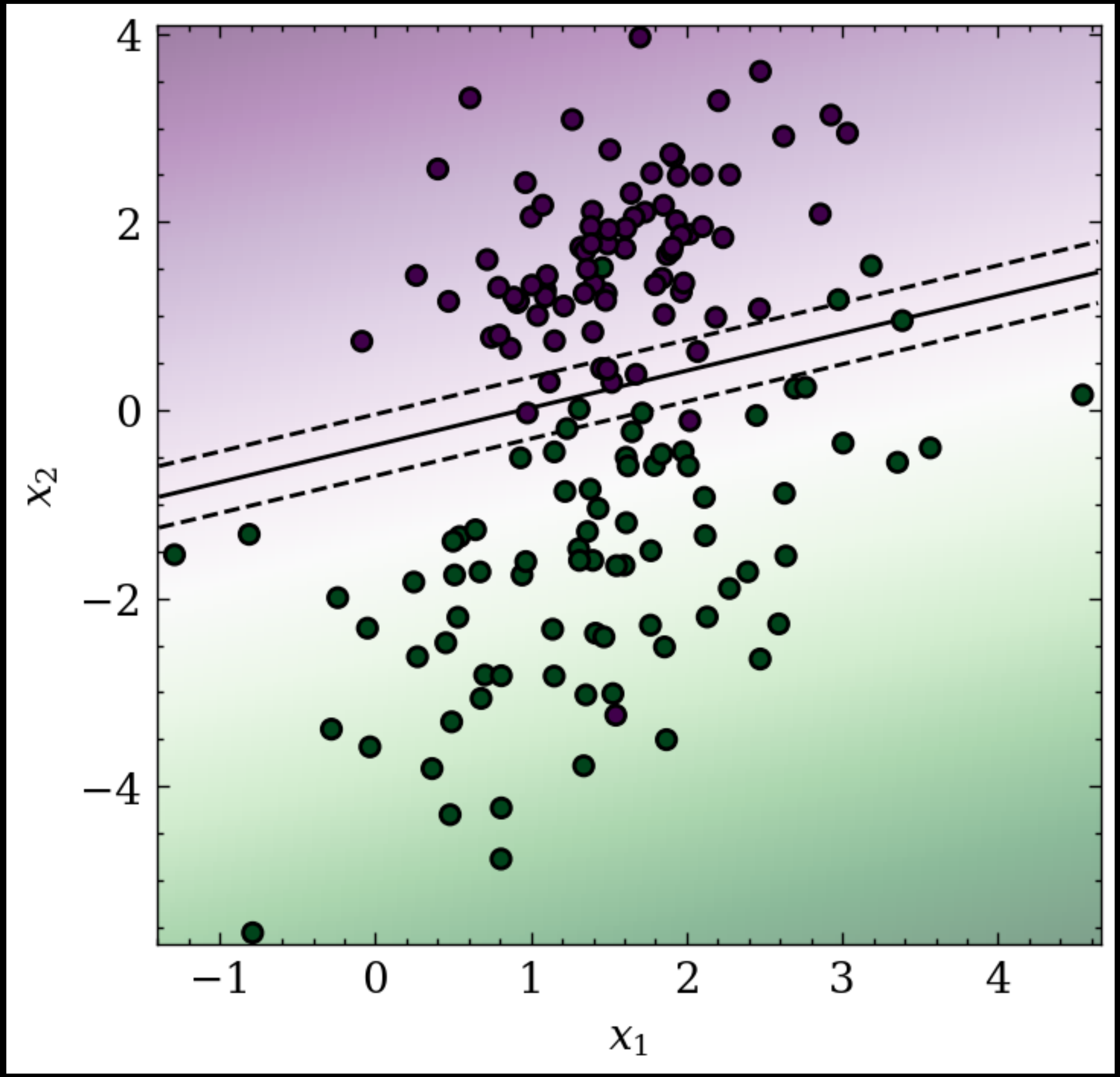

Calculate the line that separates the classes with the maximal margin.

Margin: area between two parallel lines that separate the two classes of data.

- 3-D :  plane
- > 3-D : hyperplane

*sklearn.svm.SVC*

# Support Vector Classification



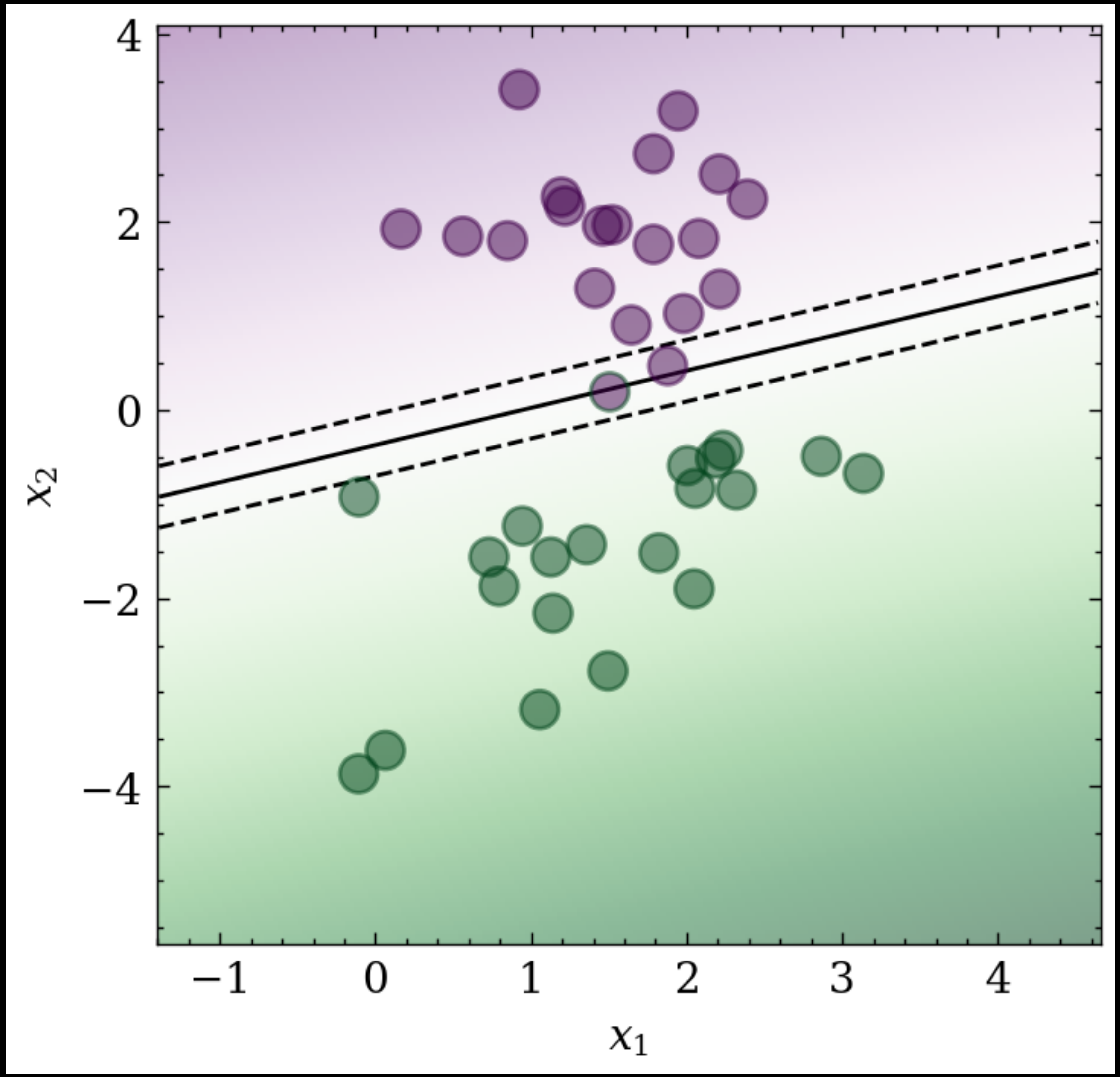

What if the data are not linearly separable?

Minimize a function that is a sum over values for all training data:

- 0 - if on correct side of margin
- value proportional to the distance from the margin

*sklearn.svm.SVC*

# Support Vector Classification




Evaluate the generalizability of the model with a <u>test set</u> of M input-output pairs:

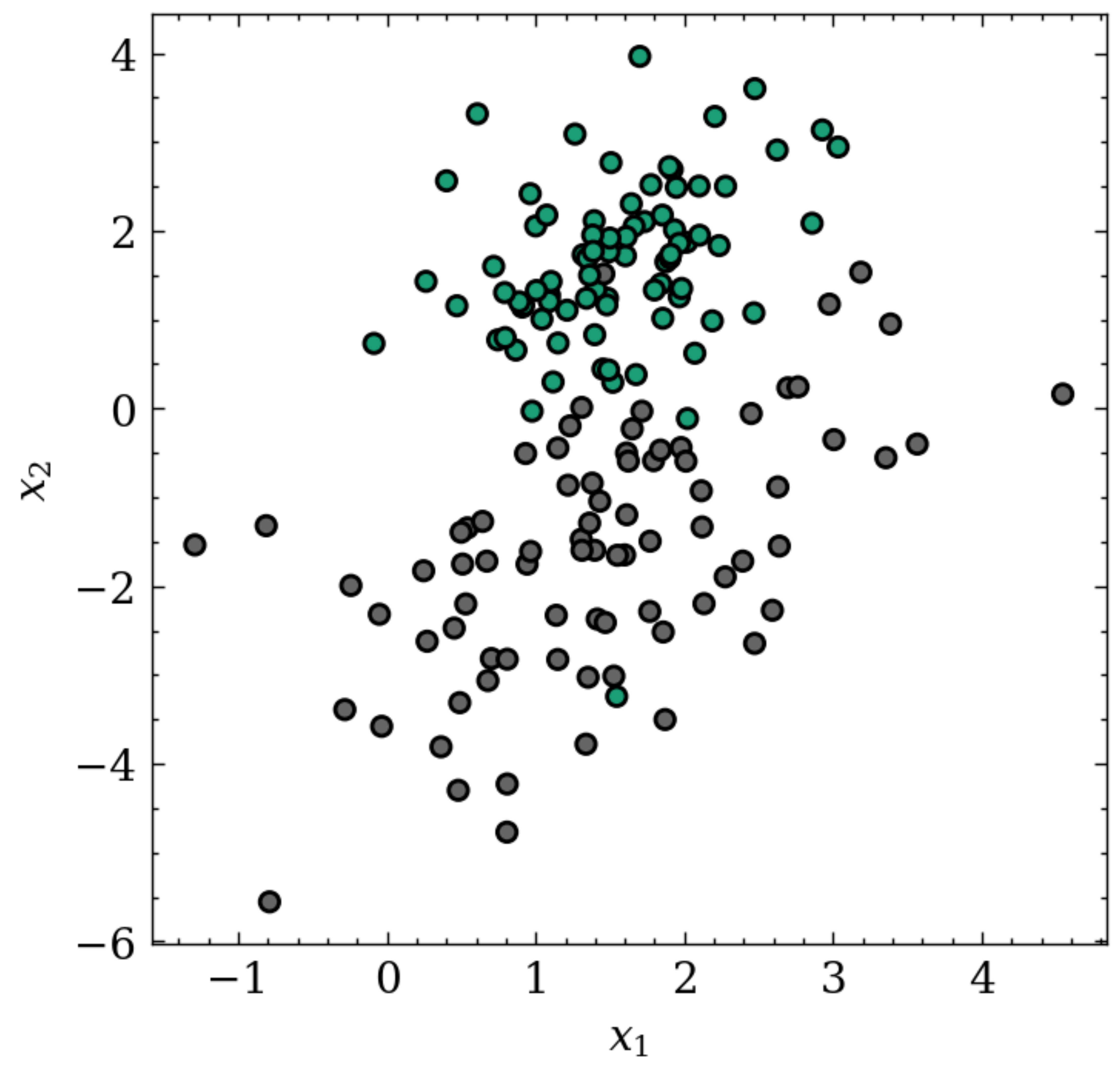
$$(X_1,y_1),\ (X_2,y_2),\ \ldots\ (X_M,y_M)$$

Test set data is not included in the training set.

$$\text{Accuracy} = \frac{1}{M}\sum_{i}^{M}(\hat{y}_i = y_i)$$

*sklearn.svm.SVC*

# K-Nearest Neighbors

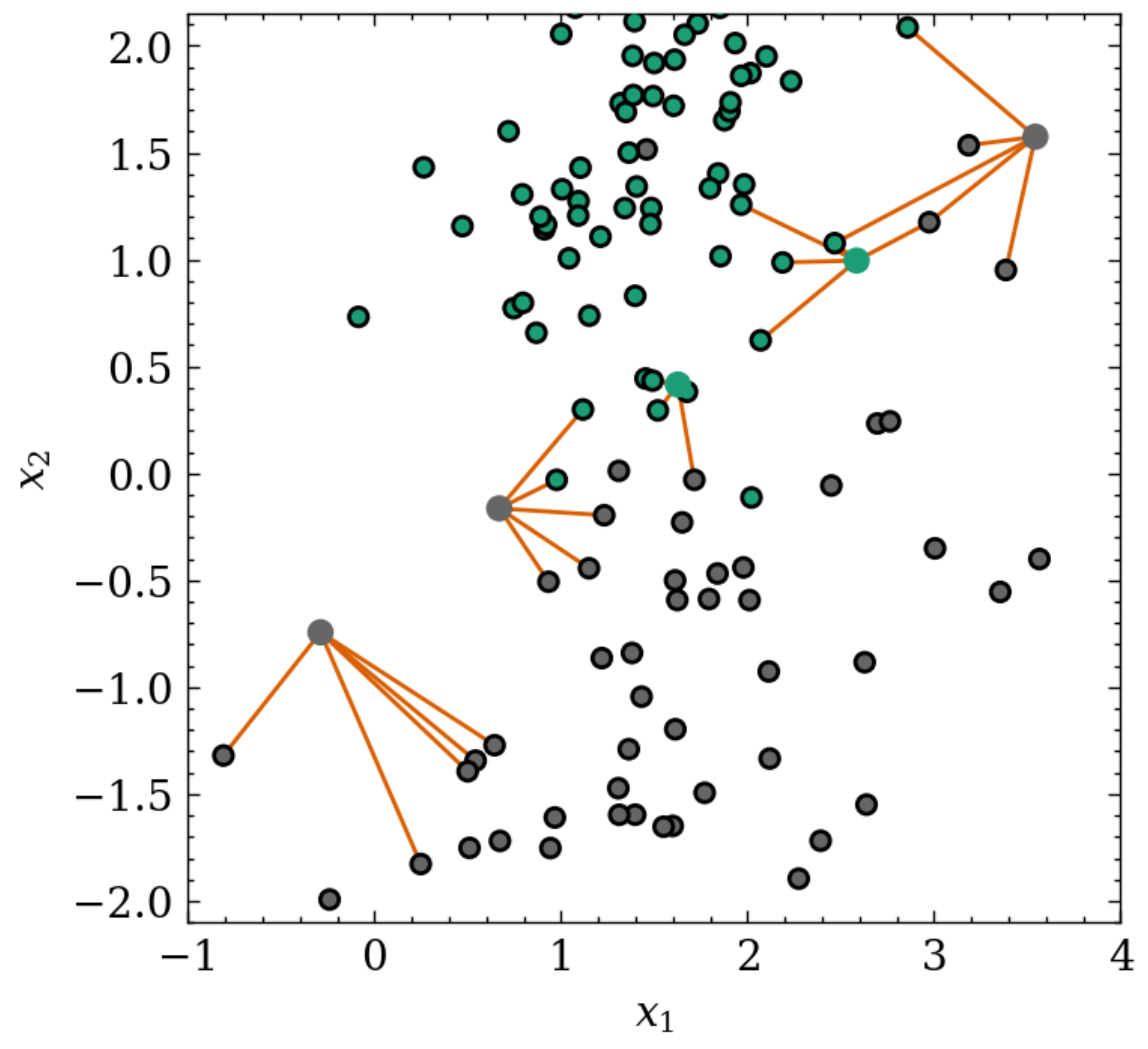



Classification is computed from a simple majority vote of the nearest neighbors of each point.

Does not construct a general model; instead stores the training data.

*sklearn.neighbors.KNeighborsClassifier*

# K-Nearest Neighbors




Classification is computed from a simple majority vote of the nearest neighbors of each point.

Does not construct a general model; instead stores the training data.

At left, the case where k = 5.

*sklearn.neighbors.KNeighborsClassifier*

Examples of problems in your area of research where *classification* could be used?

# Common algorithms

| Supervised | Unsupervised |
|---|---|
| Regression | Clustering |
| Classification | Dimensionality Reduction |

# Clustering

Training set of N inputs:

$x_1, x_2, \ldots x_N$ .

Goal: identify M clusters in the data.

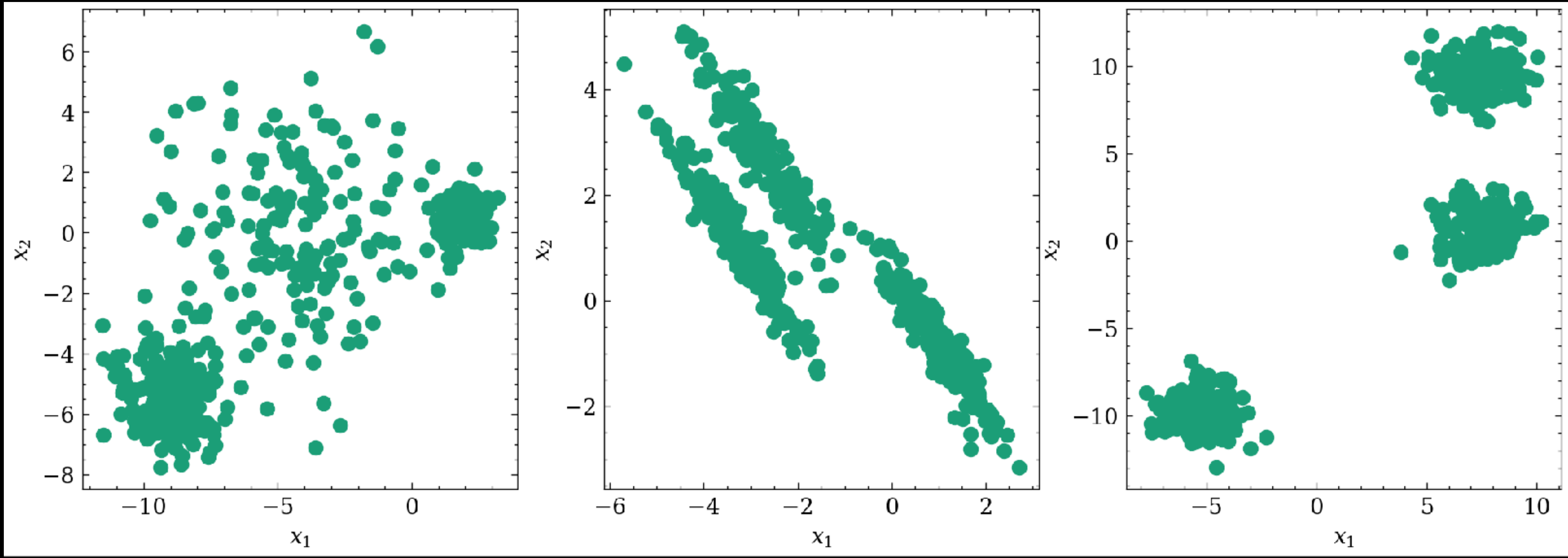
# Clustering

input:

- $x_1, x_2$

Goal: identify M clusters in the data:

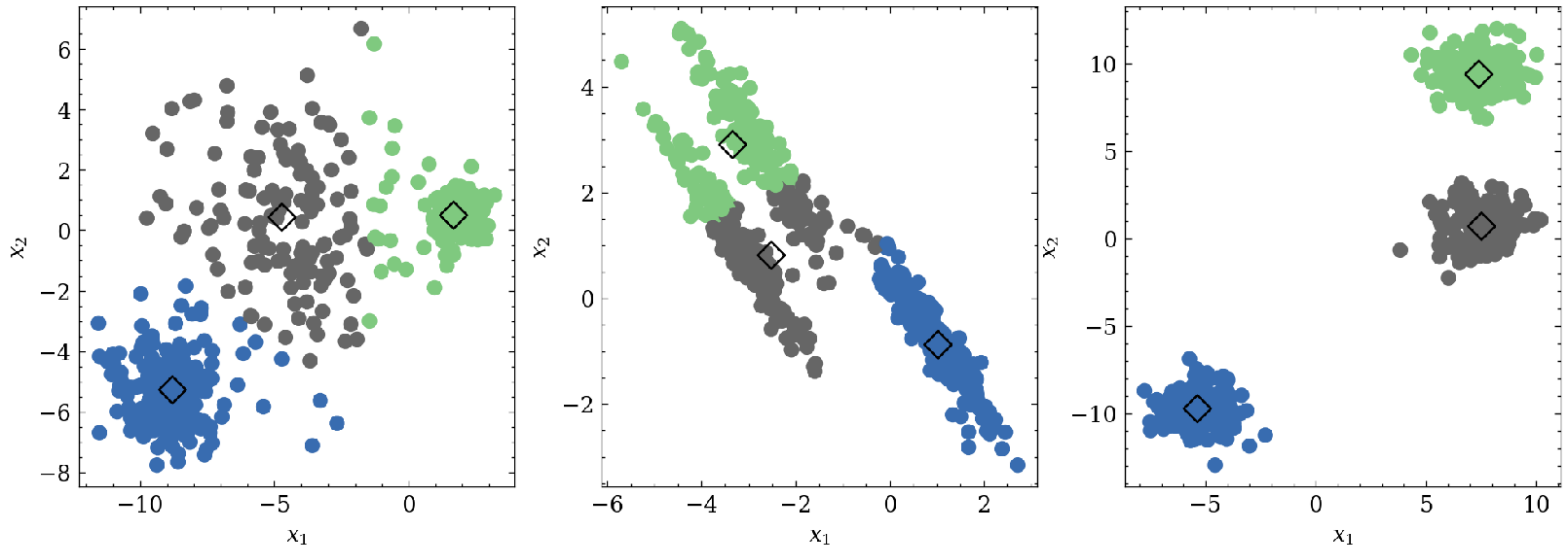
*predicted class label* $= h(x_1, x_2)$



# K-means Clustering

- requires the number of clusters to be specified
- separate samples in M clusters of equal variance
- choose centroids that minimize the inertia or within-cluster sum-of-squares

$$\sum_{i=0}^{N} \min_{\mu_j \in C} (x_i - \mu_j)^2$$






*sklearn.cluster.KMeans*

# K-means Clustering

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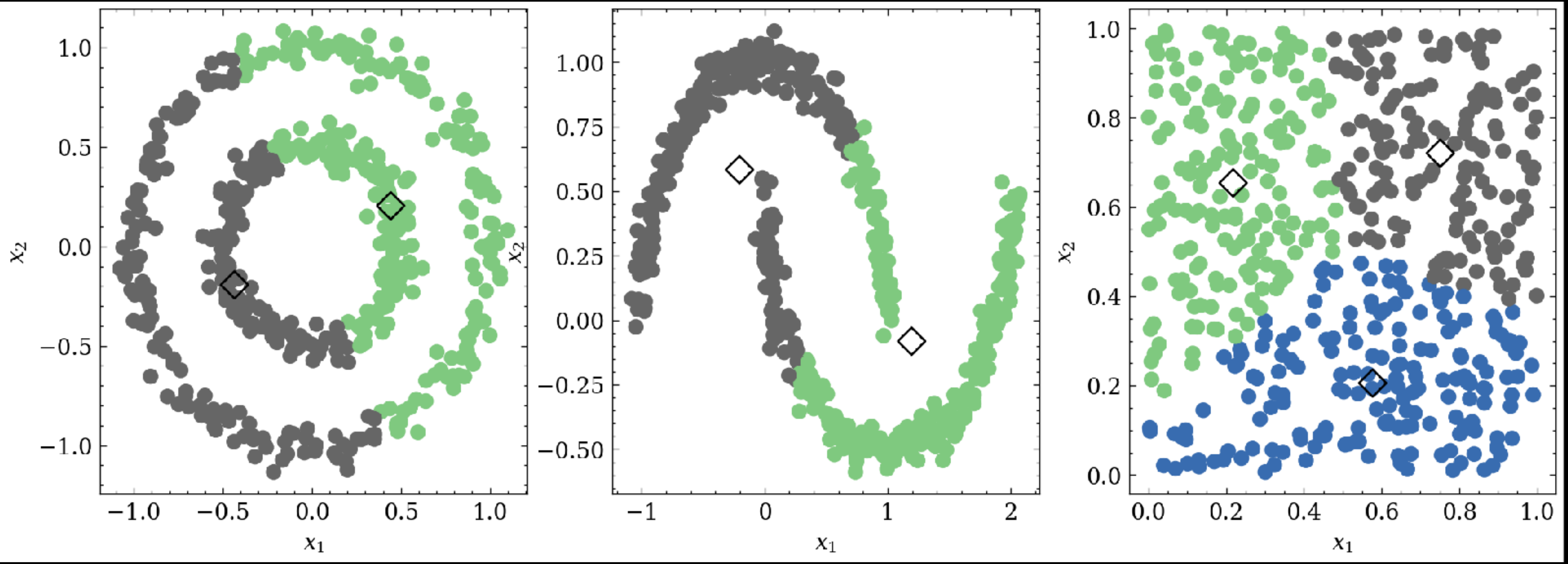




*sklearn.cluster.KMeans*

Examples of problems in your area of research where *clustering* could be used?

# Common algorithms

| Supervised | Unsupervised |
|---|---|
| Regression | Clustering |
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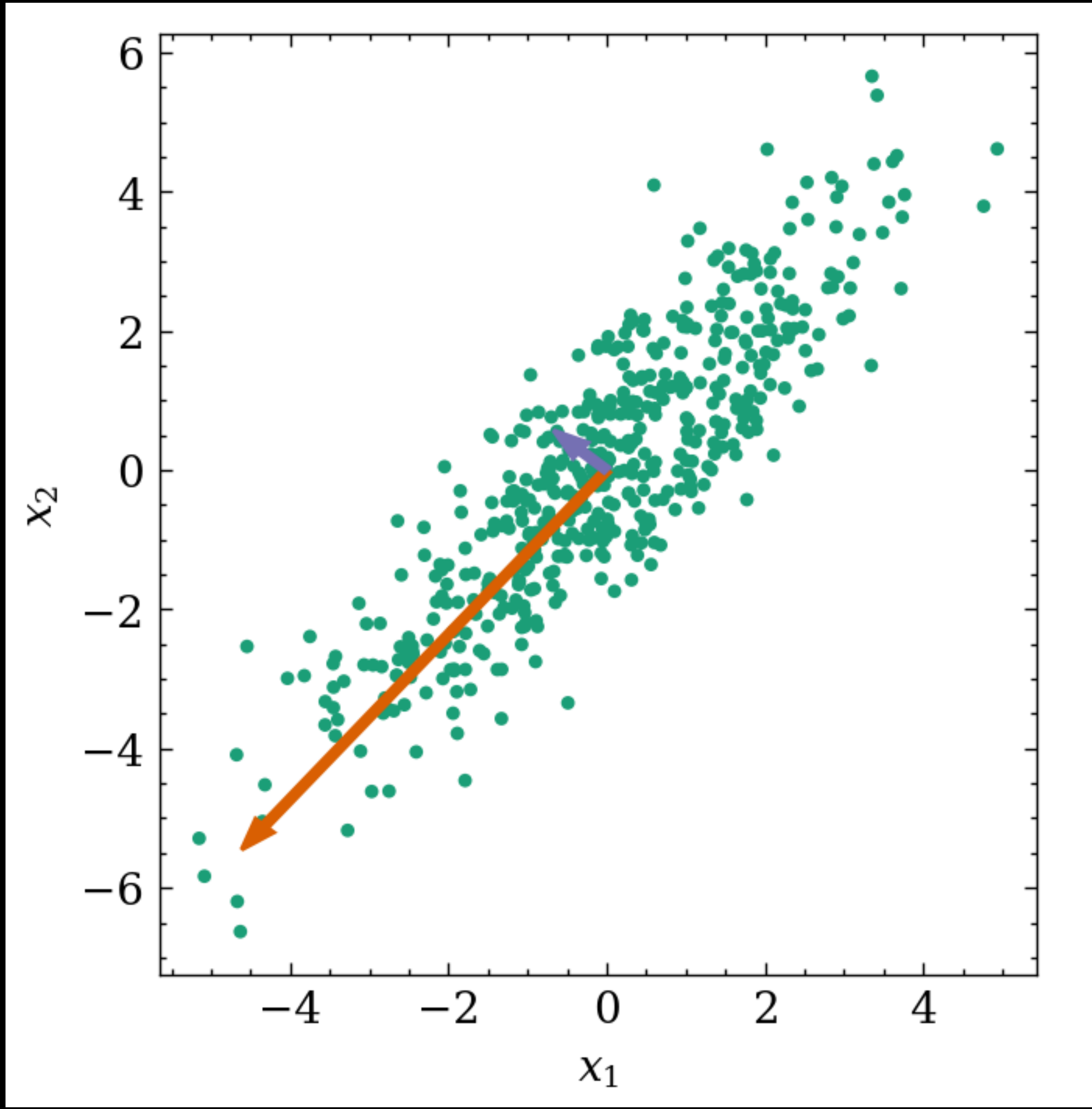
# Dimensionality Reduction

Training set of N inputs pairs:

$X_1, X_2, \ldots X_N$ .

Goal: data exploration / visualization

# Principal Component Analysis



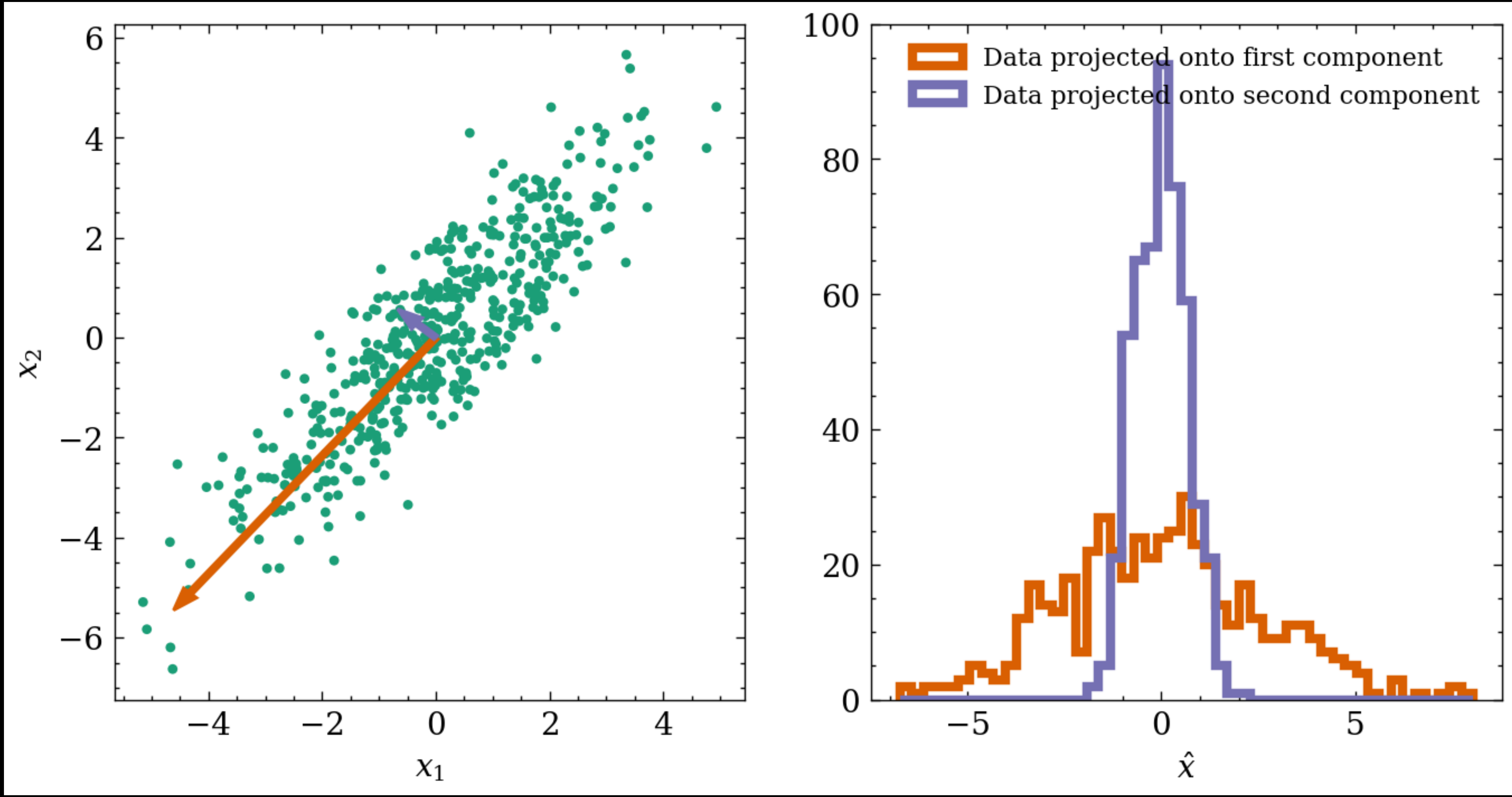

- First principal component: line that minimizes the average squared perpendicular distance from the points to the line.
- Second principal component: line orthogonal to first principal component, that does the same.

- Use the principal components to perform a change of coordinate system.

*sklearn.decomposition.PCA*

*Pearson, K. (1901). "On Lines and Planes of Closest Fit to Systems of Points in Space". Philosophical Magazine. 2 (11): 559–572.*

# Principal Component Analysis




*sklearn.decomposition.PCA*

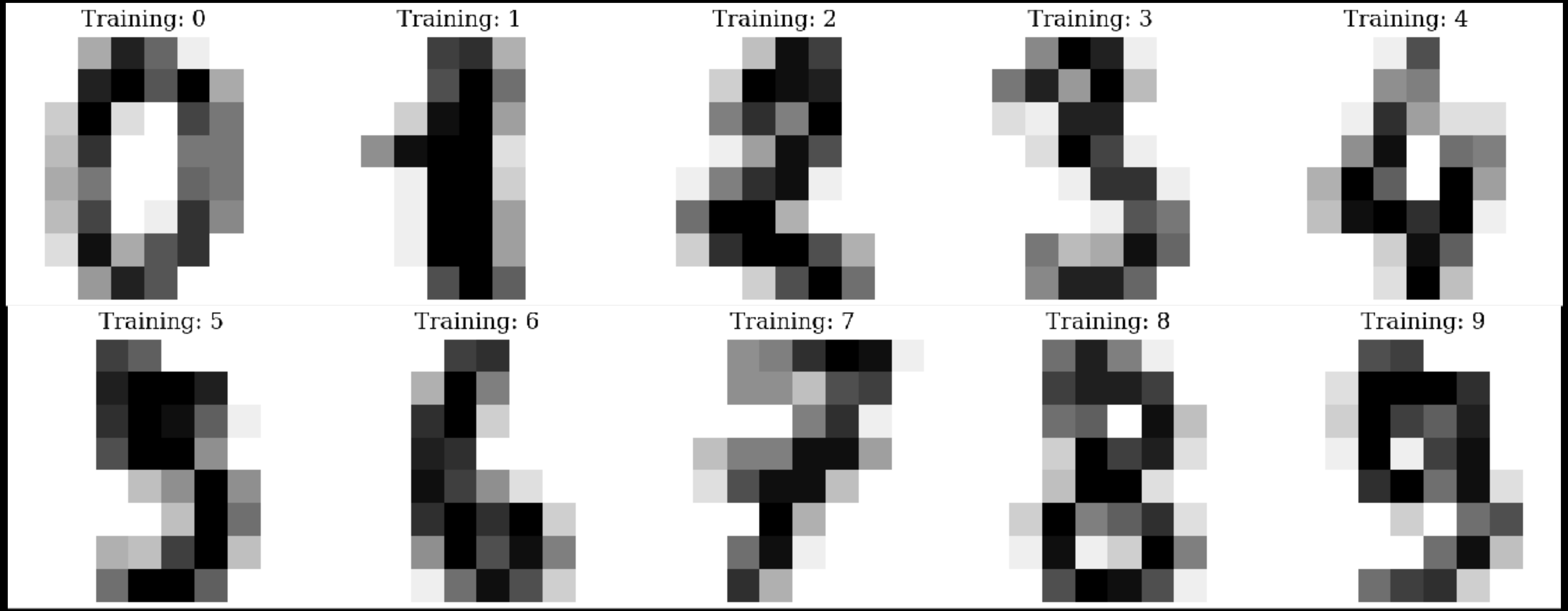
# Dimensionality Reduction

input:

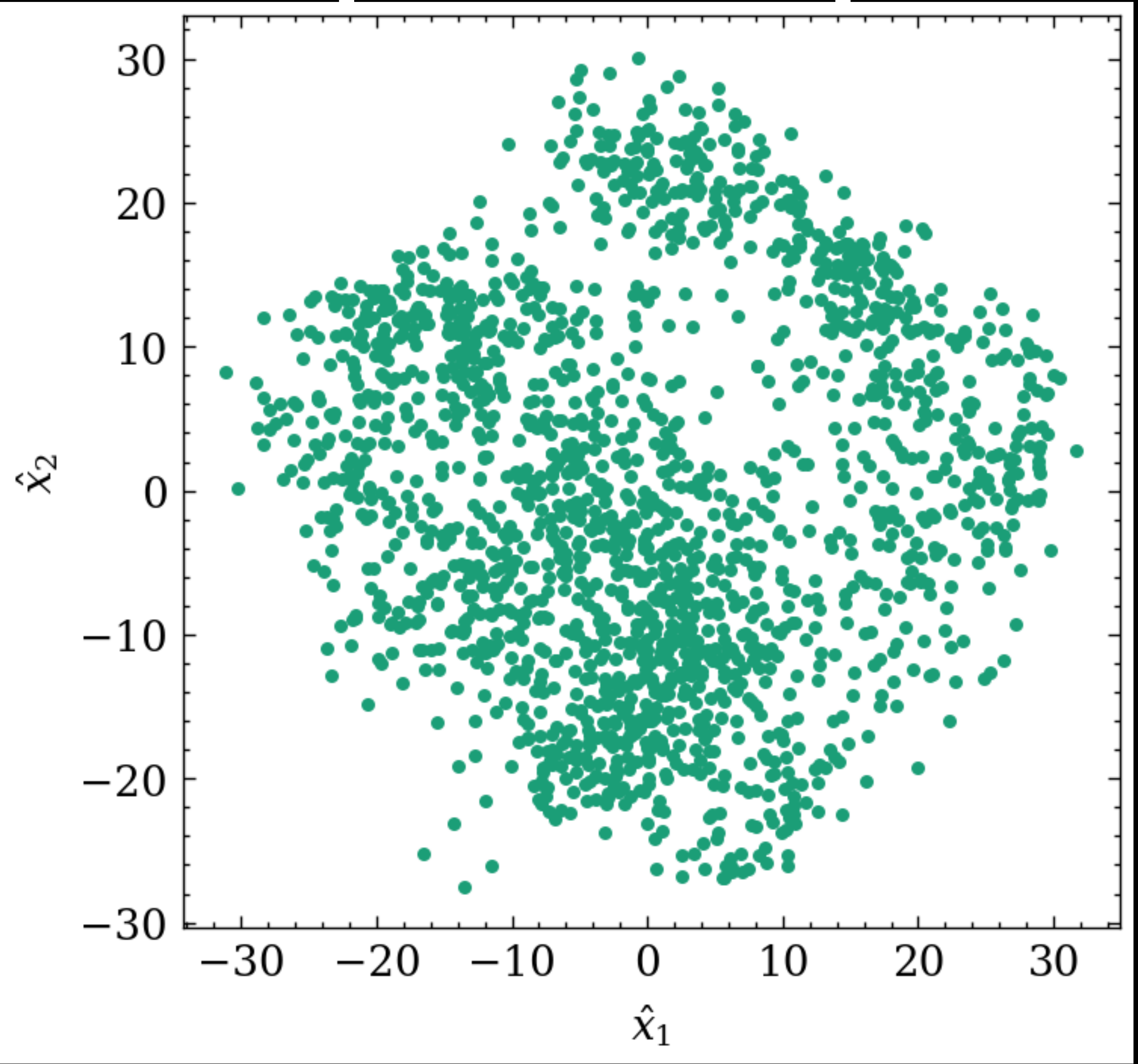
- $x_1, x_2, \ldots \; x_{64}$

Goal: visualize the data in two dimensions

$\hat{x}_1, \hat{x}_2 = h(x_1, x_2, \ldots x_{64})$



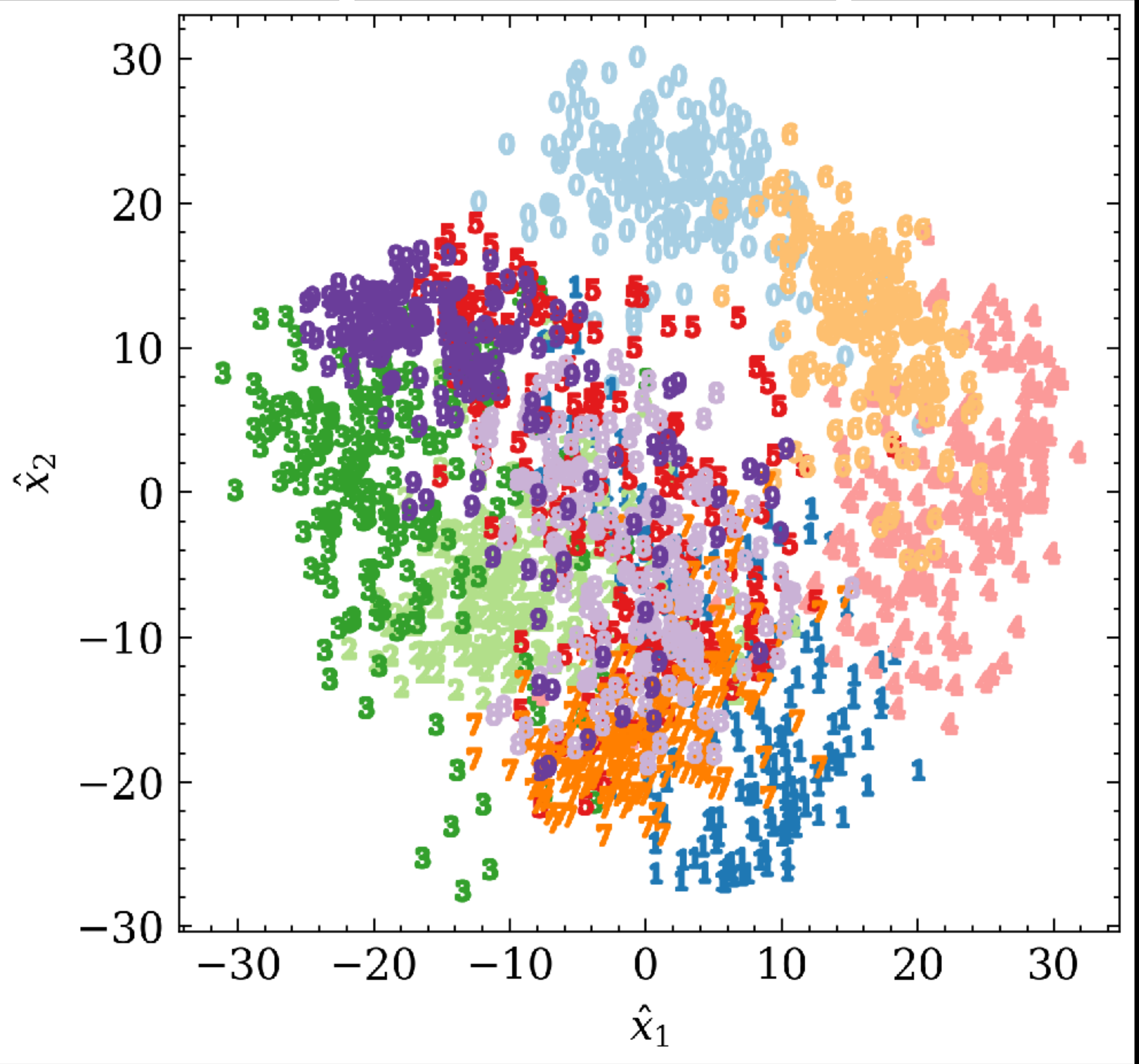
# Principal Component Analysis




The data set projected down onto the first two principal components

*sklearn.decomposition.PCA*

# Principal Component Analysis




The data set projected down onto the first two principal components, with labels.

*sklearn.decomposition.PCA*

Examples of problems in your area of research where *dimensionality reduction* could be used?