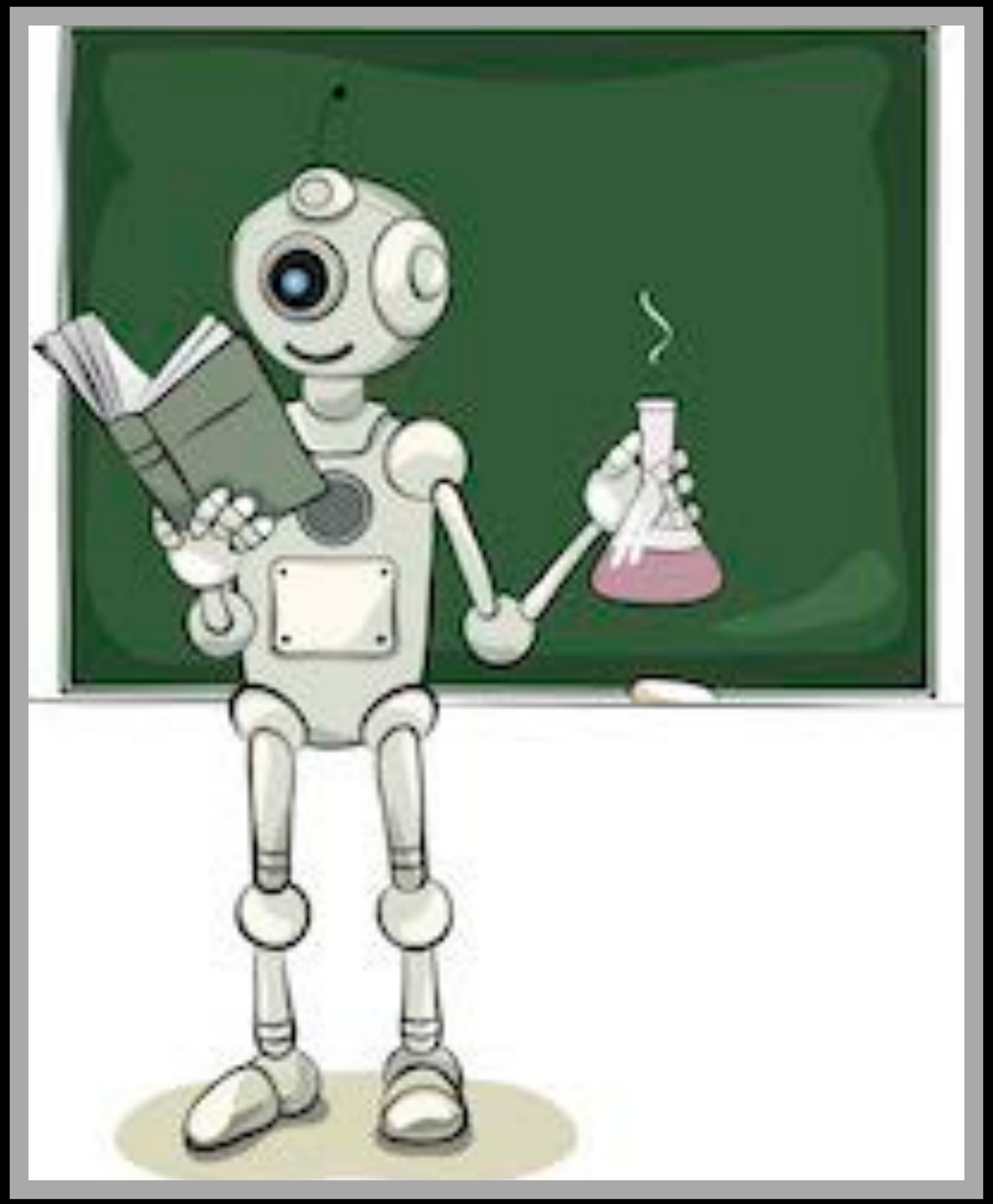
Getting Started with Machine Learning in Python

Julian Gold, DataX Data Scientist, CSML
Wednesday, September 25, 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 classical 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:

$X_1, X_2, \ldots X_N$

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

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Regression

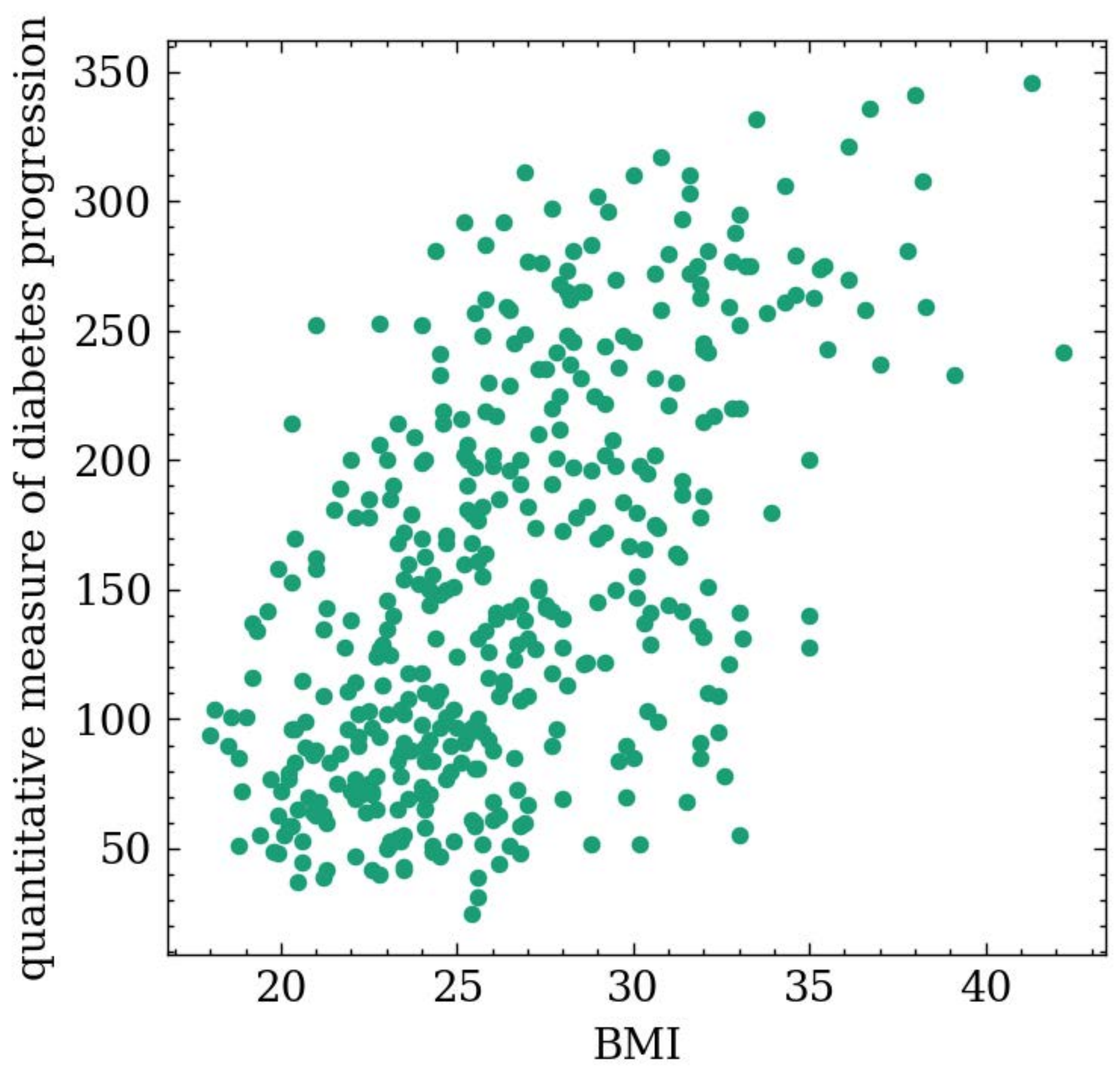
Training set of N input-output pairs:

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

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

$$y = b + mx$$

independent variables

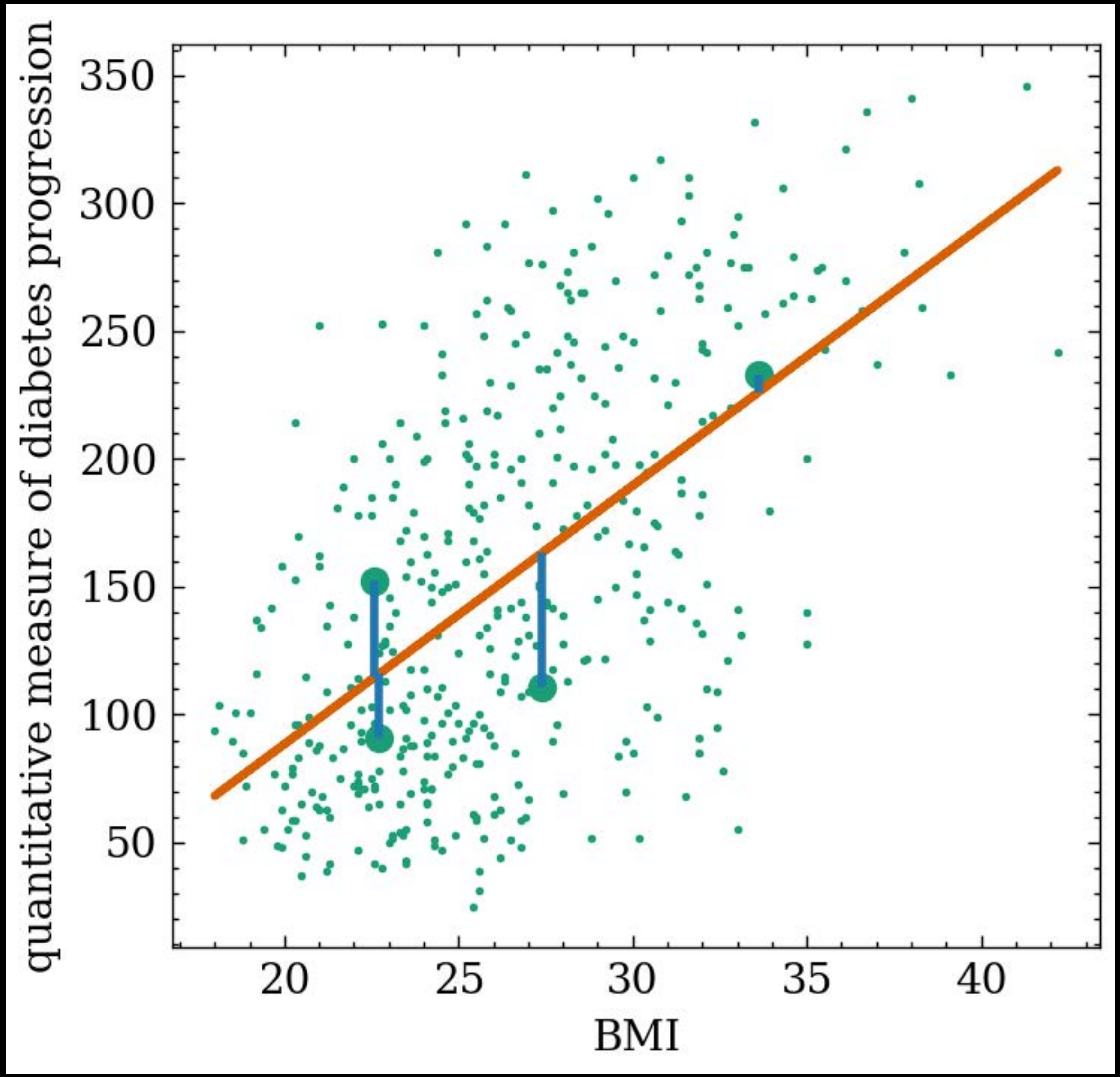
dependent variable

$$y = X\beta$$

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



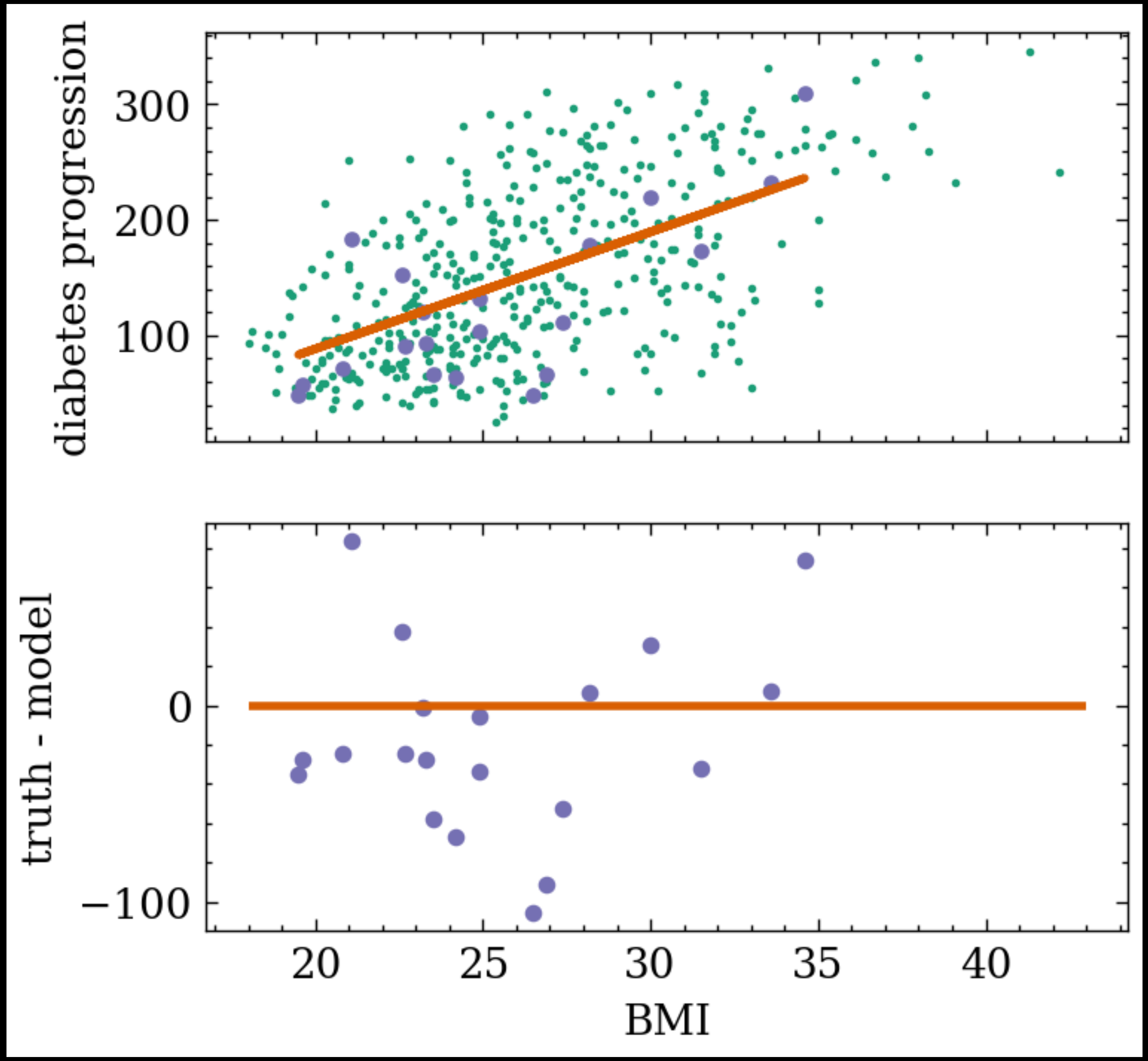
$$y = X\beta$$

Ordinary Least Squares

Compute the vector β that minimizes:

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

Linear Regression

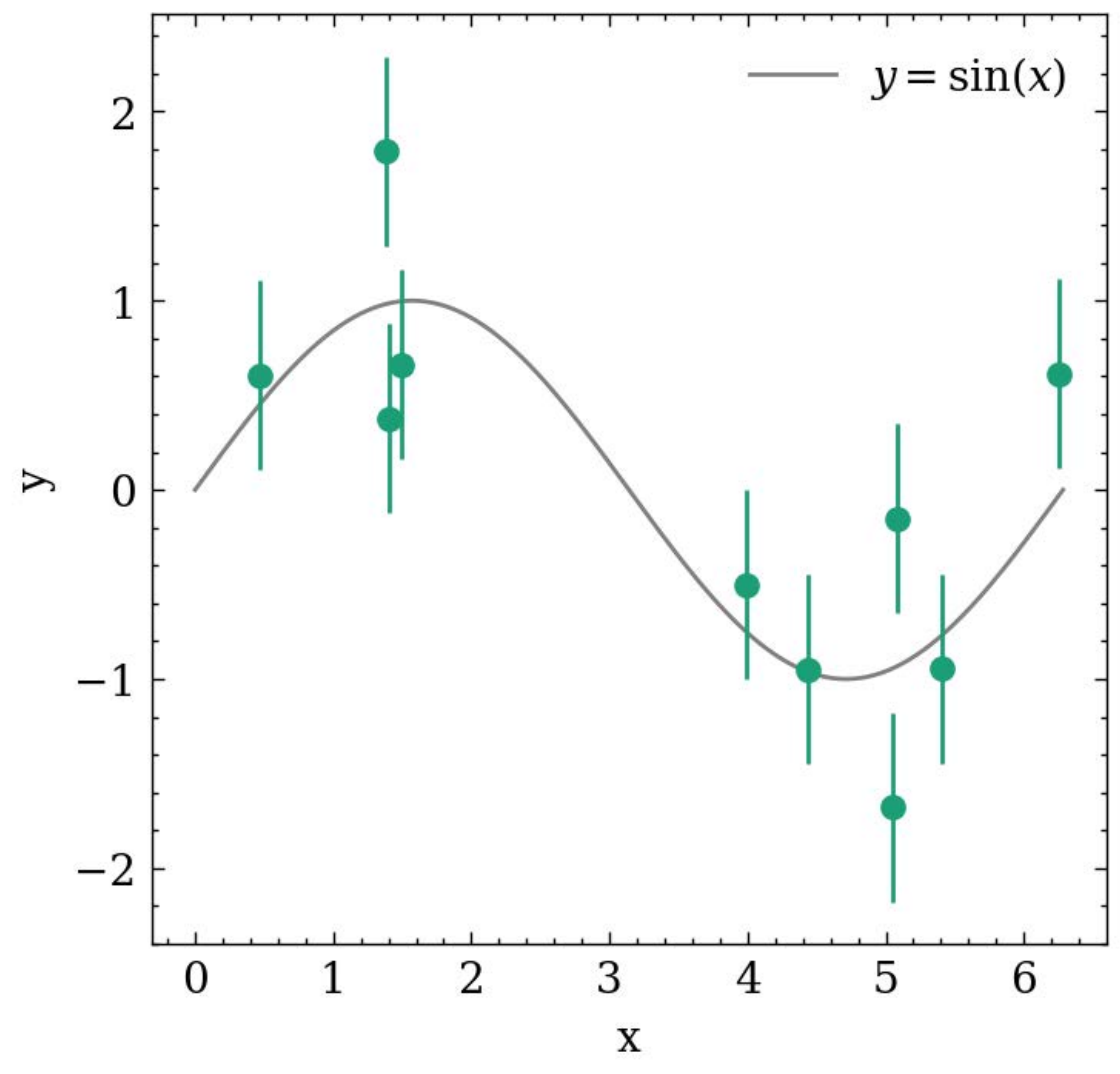


Evaluate the generalizability of the model with a <u>test set</u> of M input-output pairs:

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

Test set data is not included in the training set.

Gaussian Process Regression



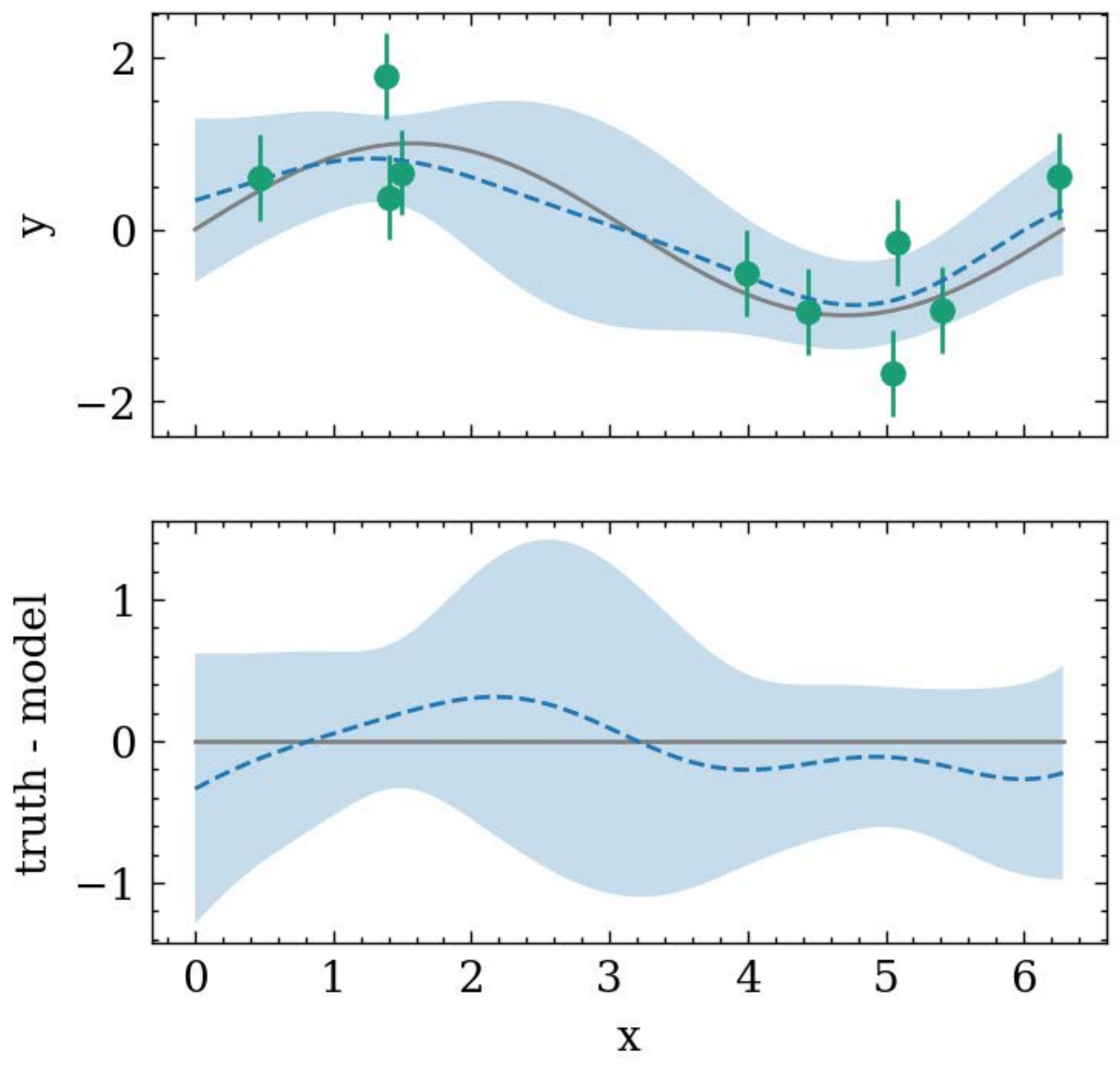
input-output pairs:

- 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

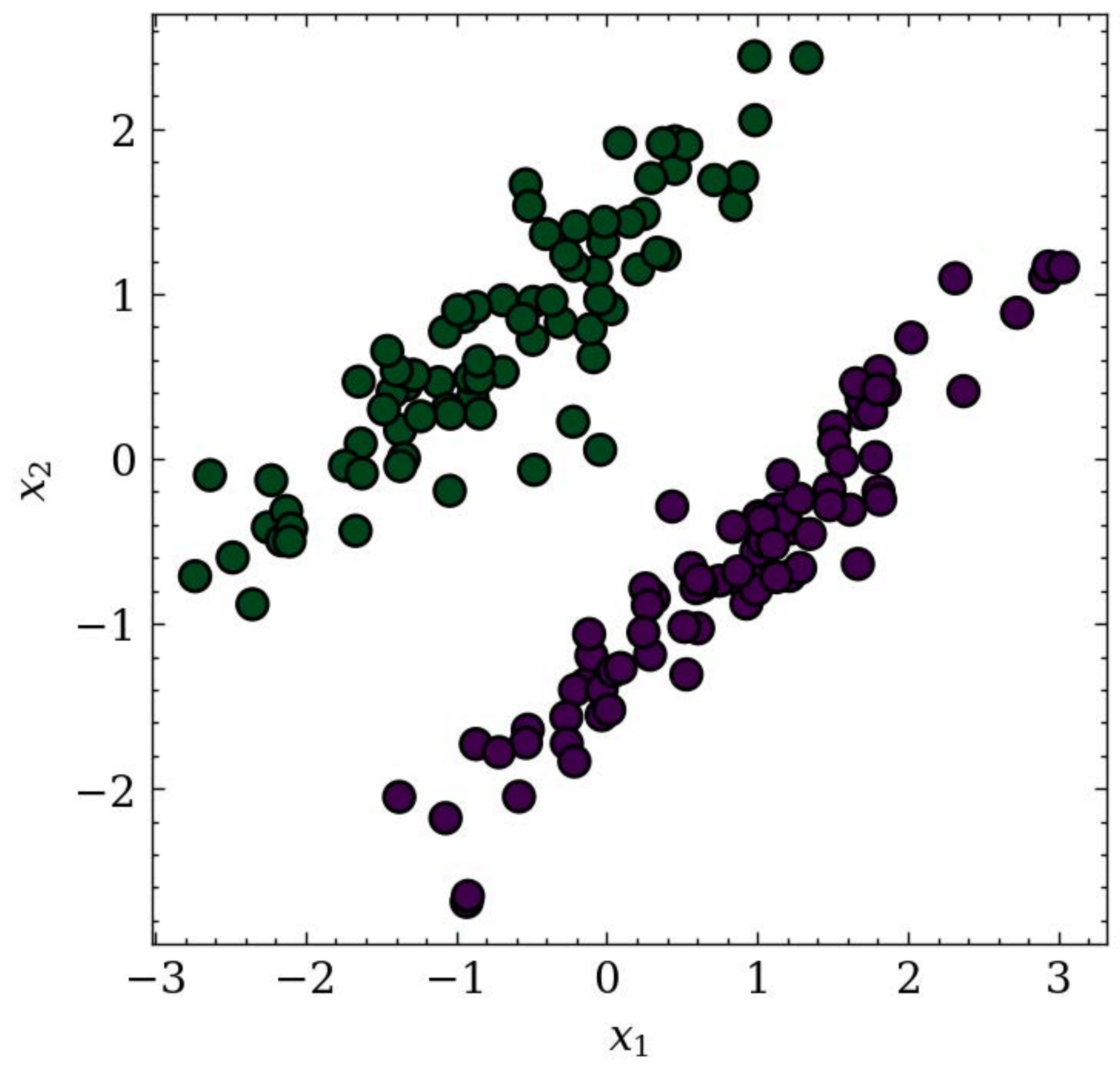
Training set of N input-output pairs:

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

where desired output value is a discrete value.

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

Classification



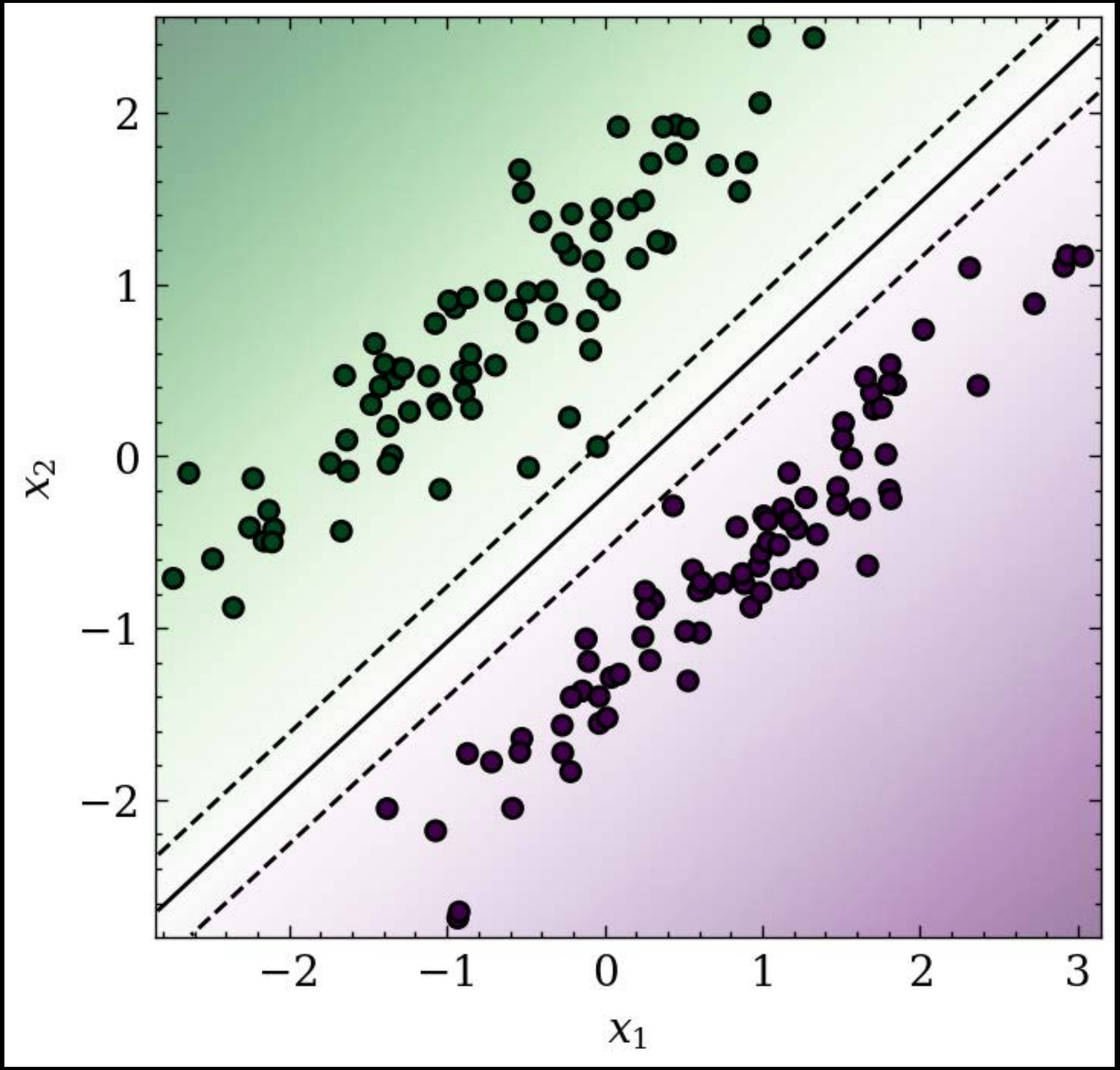
input-output pairs:

- $X_i = \{x_{i,1}, x_{i,2}\}$
- 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



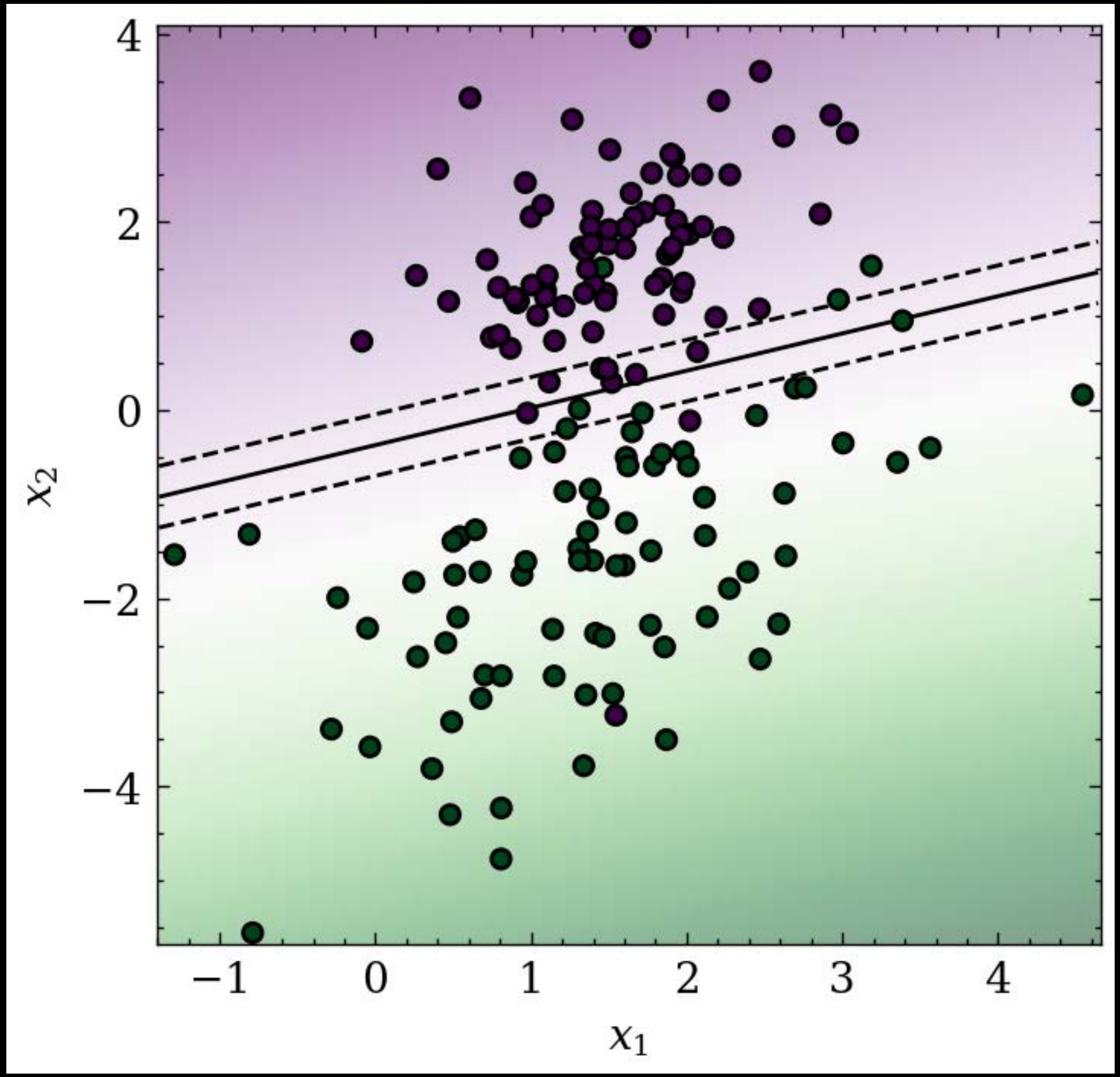
Calculate the line that separates the classes with the maximal margin.

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



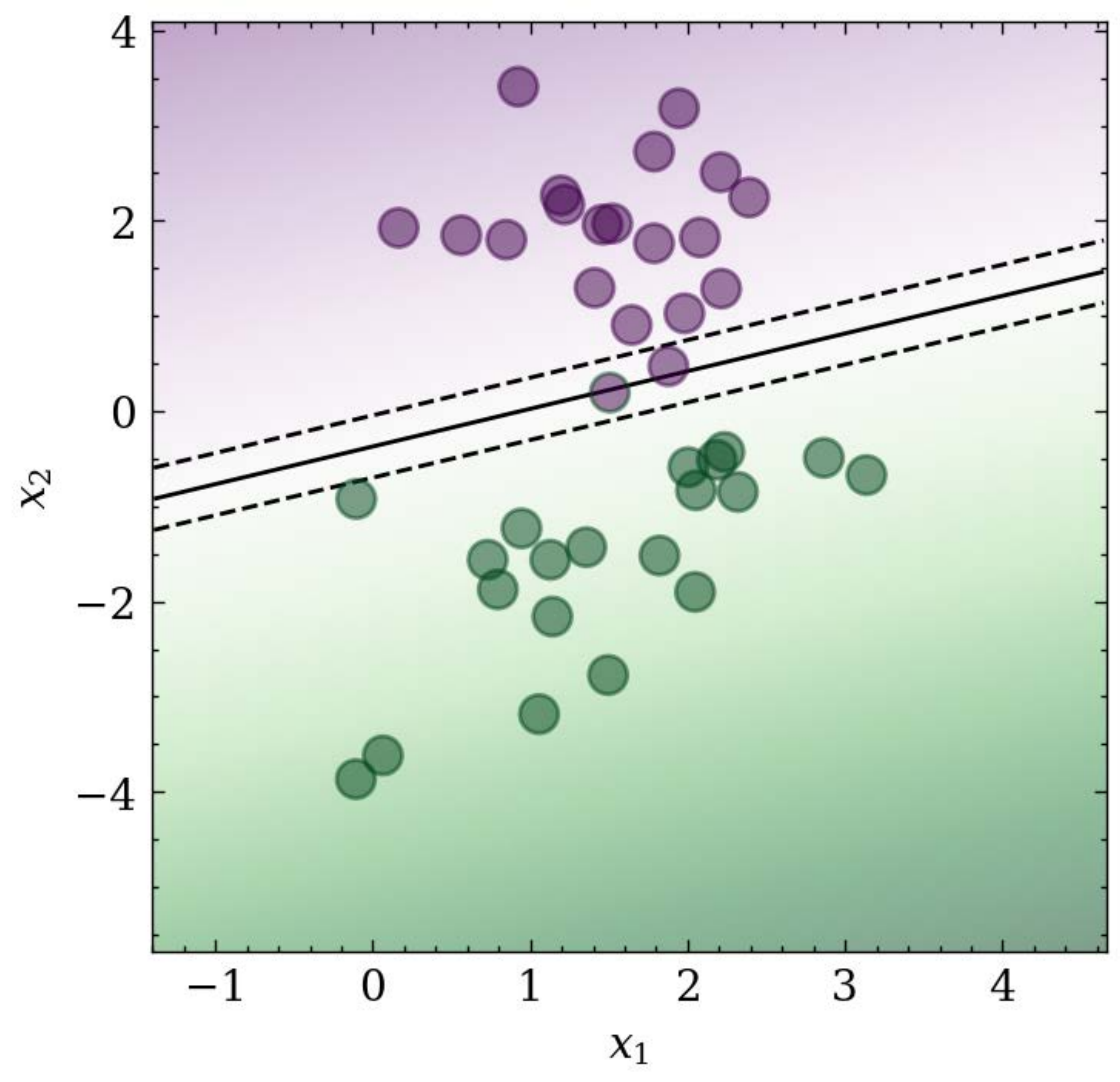
What if the data are not linearly separable?

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:

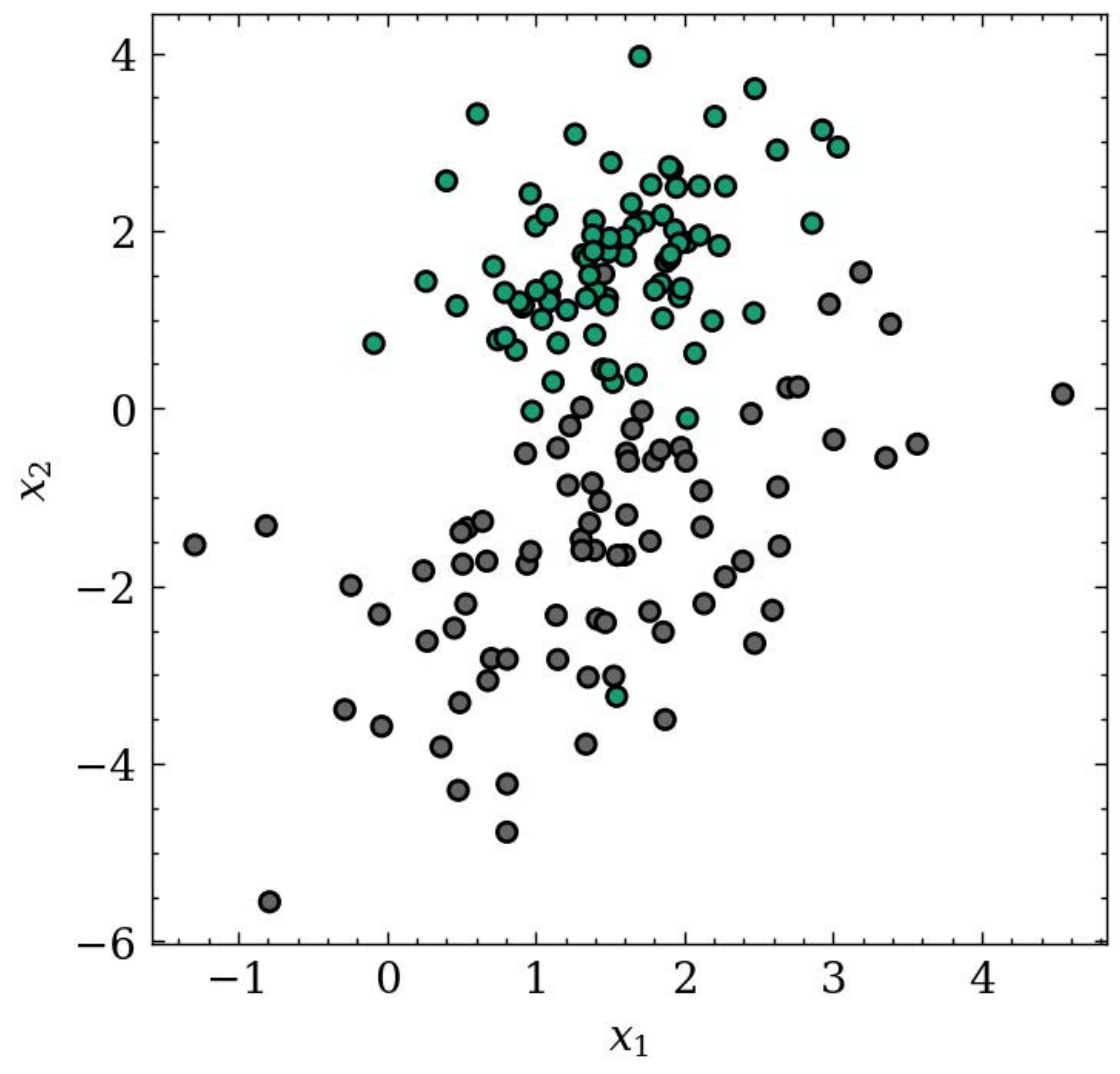
$$(X_1, y_1), (X_2, y_2), \ldots (X_M, y_M)$$

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

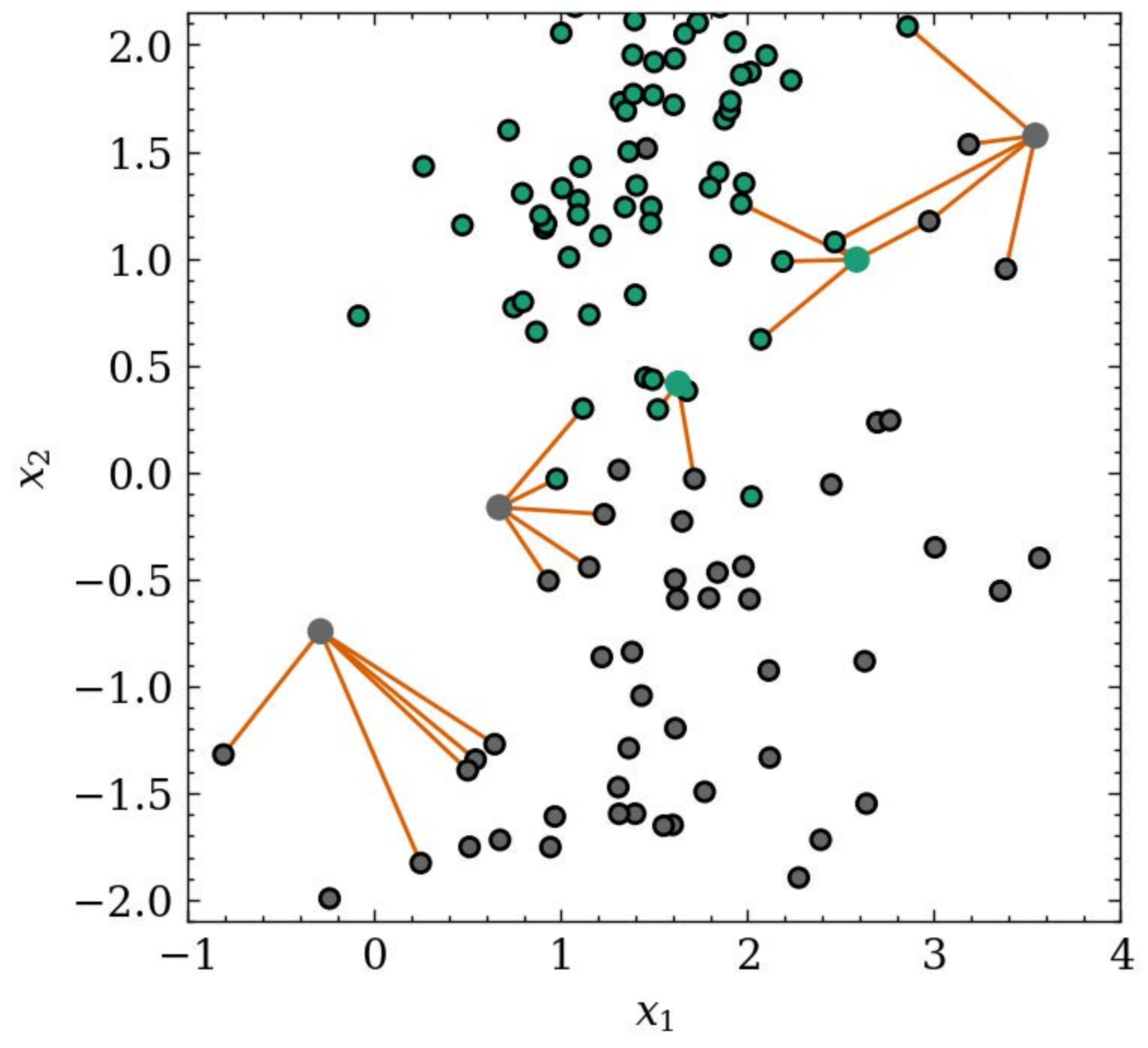


Classification is computed from a simple majority vote of the nearest neighbors of each point.

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
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Clustering

Training set of N inputs:

$X_1, X_2, \dots X_N$.

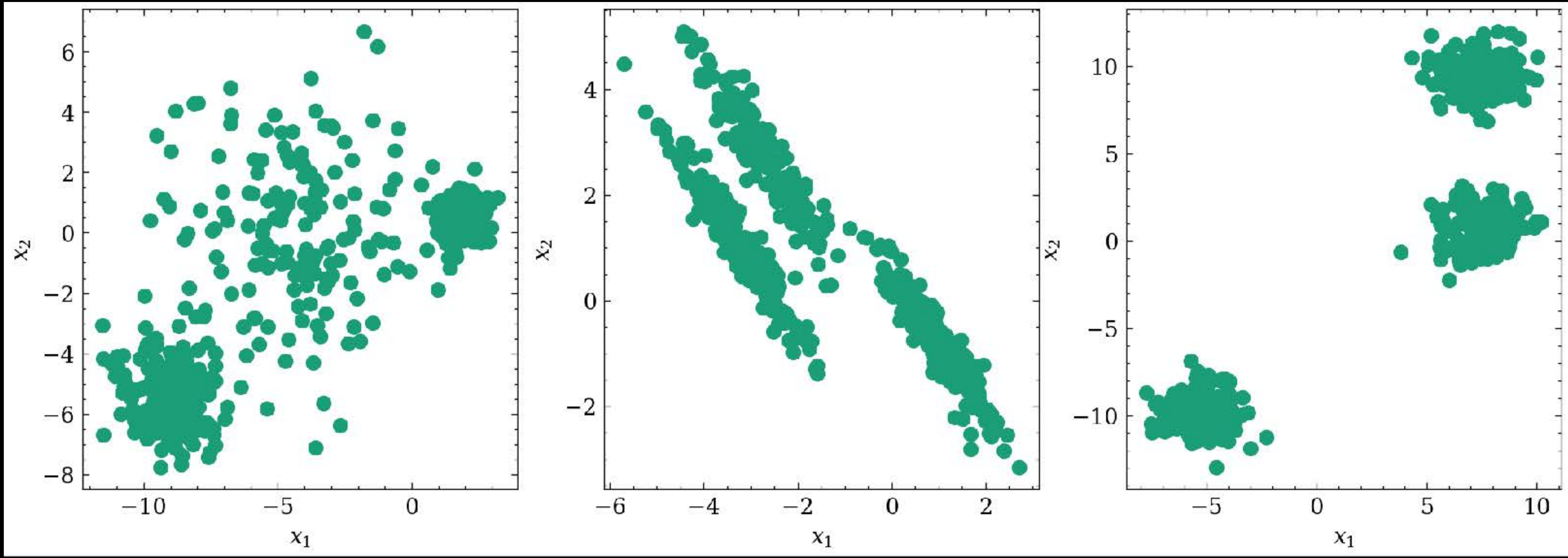
Goal: identify M clusters in the data.

Clustering

input:
- x_1, x_2

Goal: identify M clusters in the data*:*

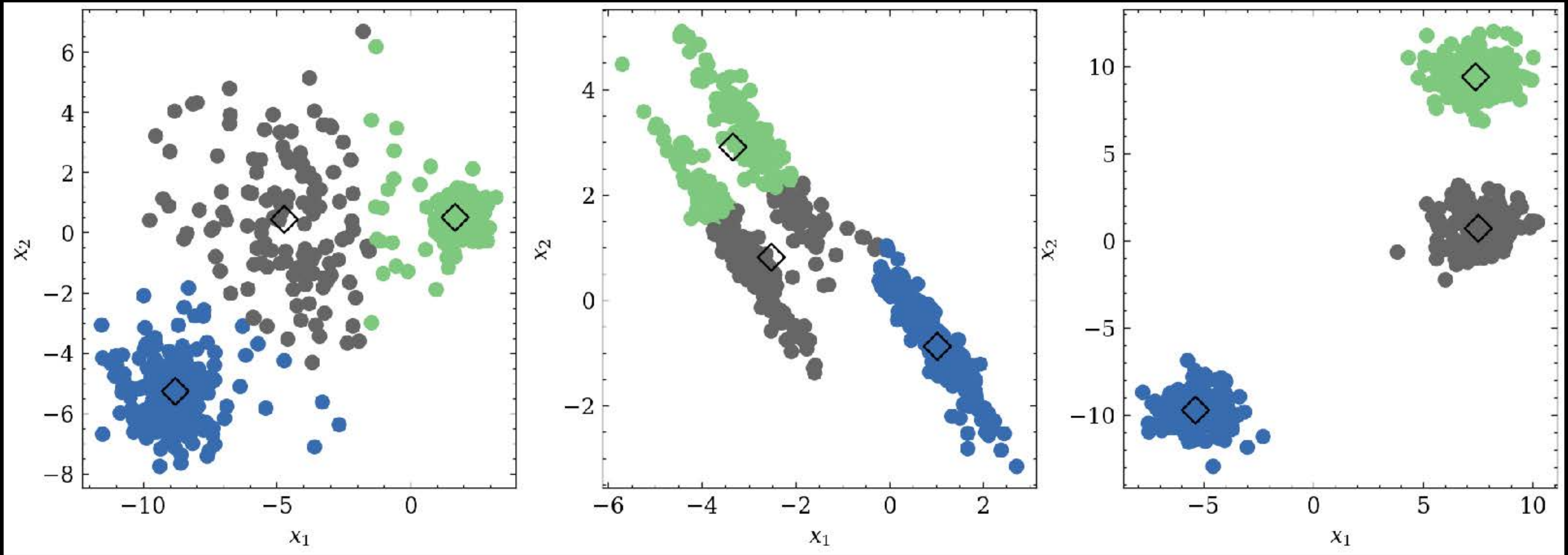
predicted class label $= h(x_1, x_2)$



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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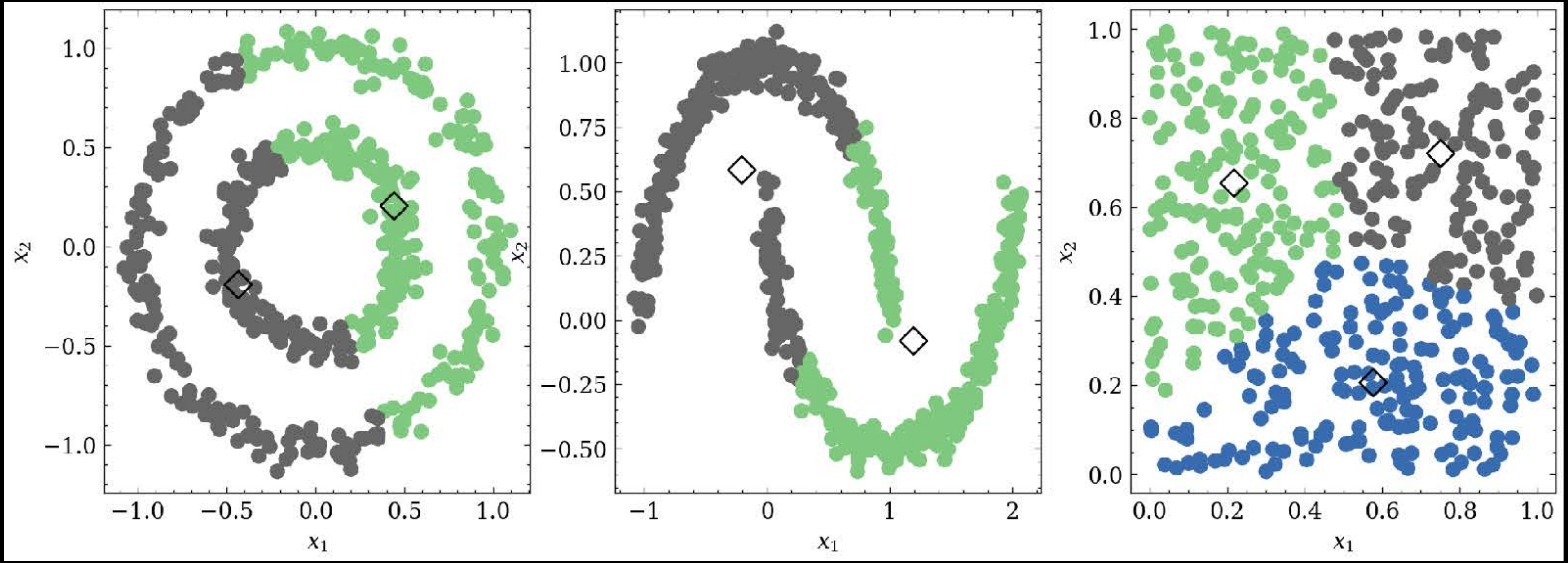

sklearn.cluster.KMeans

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

Common algorithms

Supervised	Unsupervised
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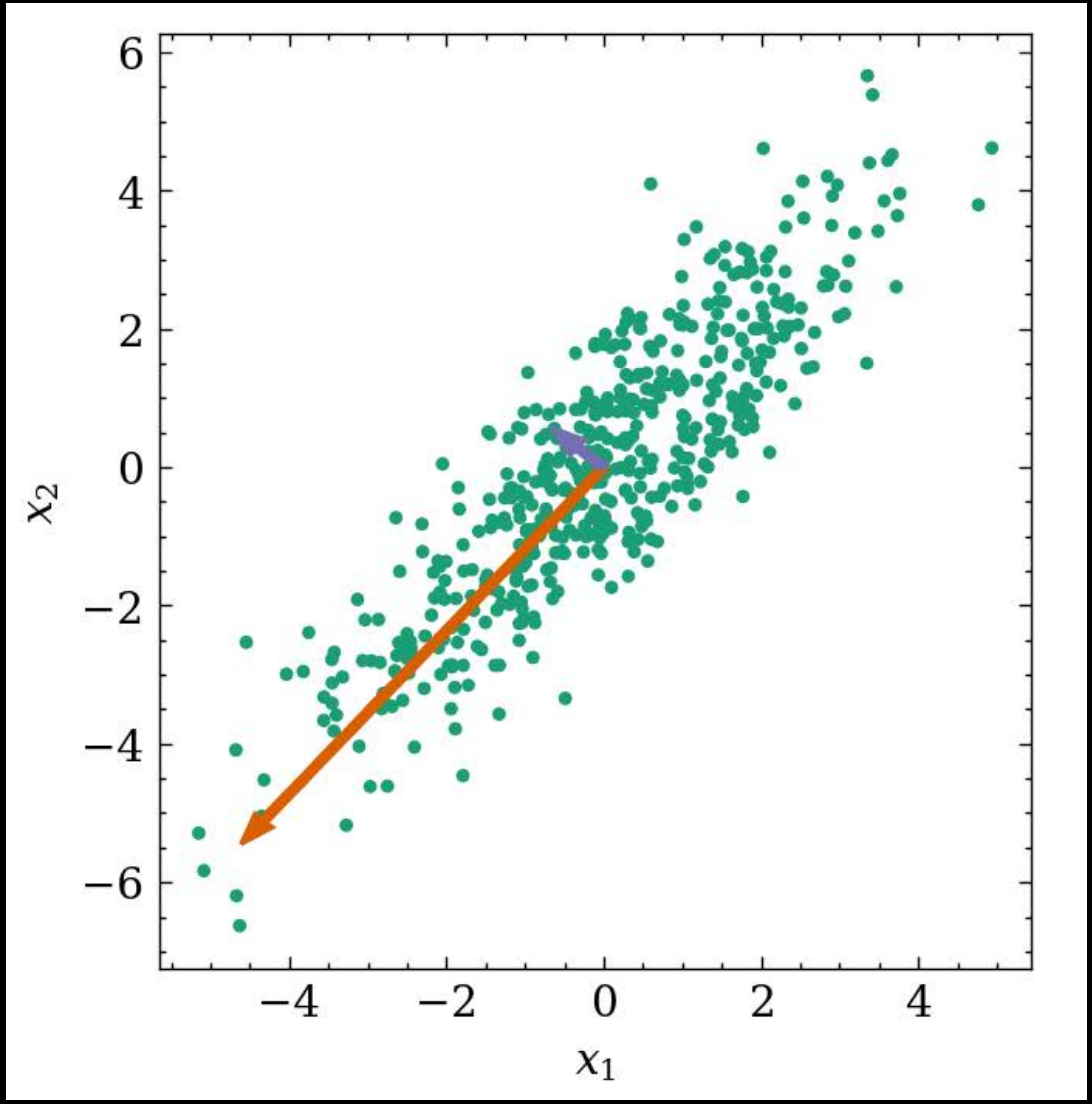
Dimensionality Reduction

Training set of N inputs pairs:

$X_1, X_2, \ldots X_N$.

Goal: data exploration / visualization

Principal Component Analysis

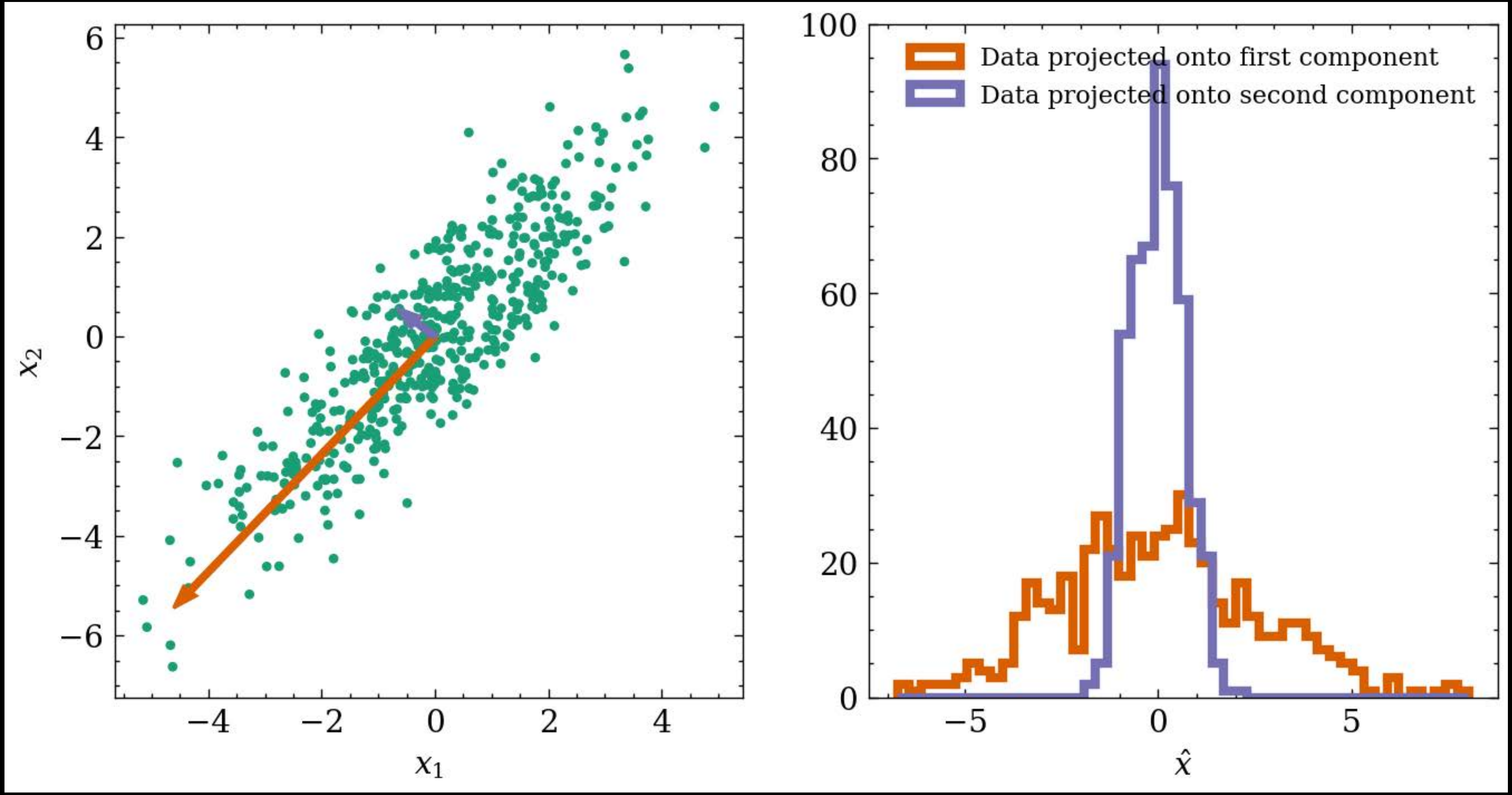


- First principal component: line that minimizes the average squared perpendicular distance from the points to the line.
- Second principal component: line orthogonal to first principal component, that does the same.
- Use the principal components to perform a change of coordinate system.

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

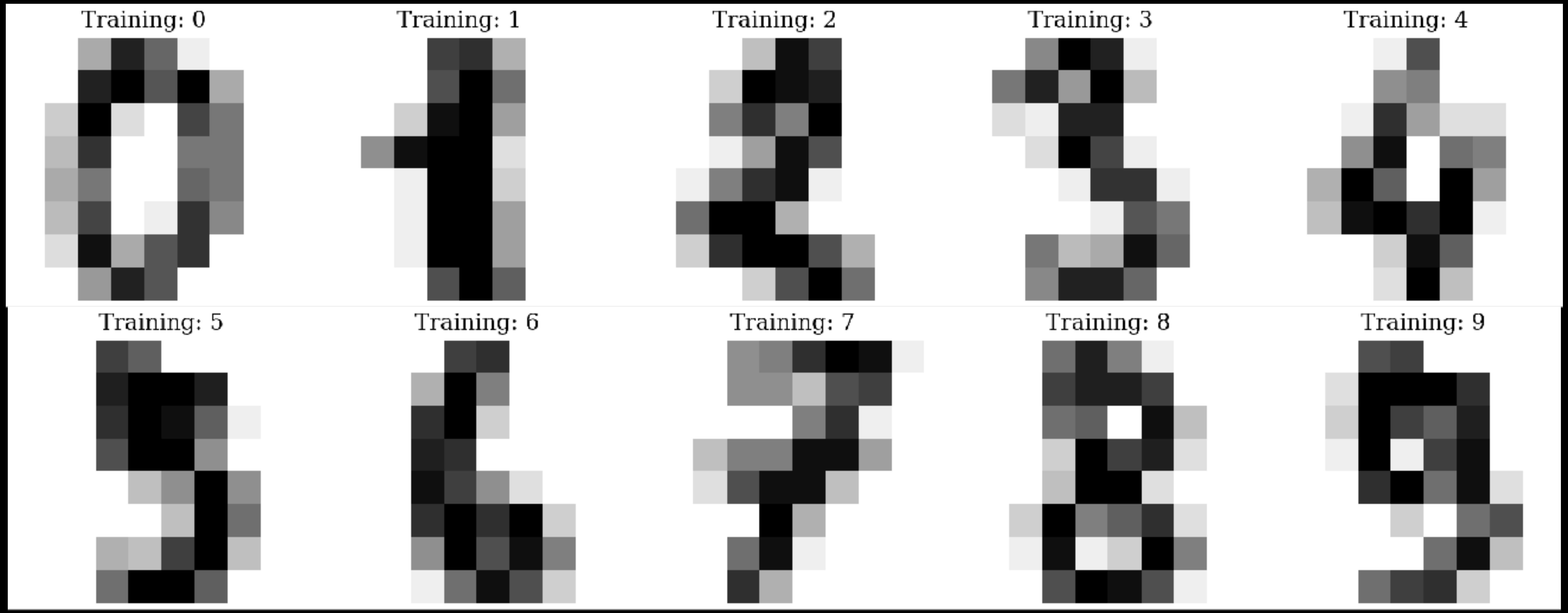
Dimensionality Reduction

input:

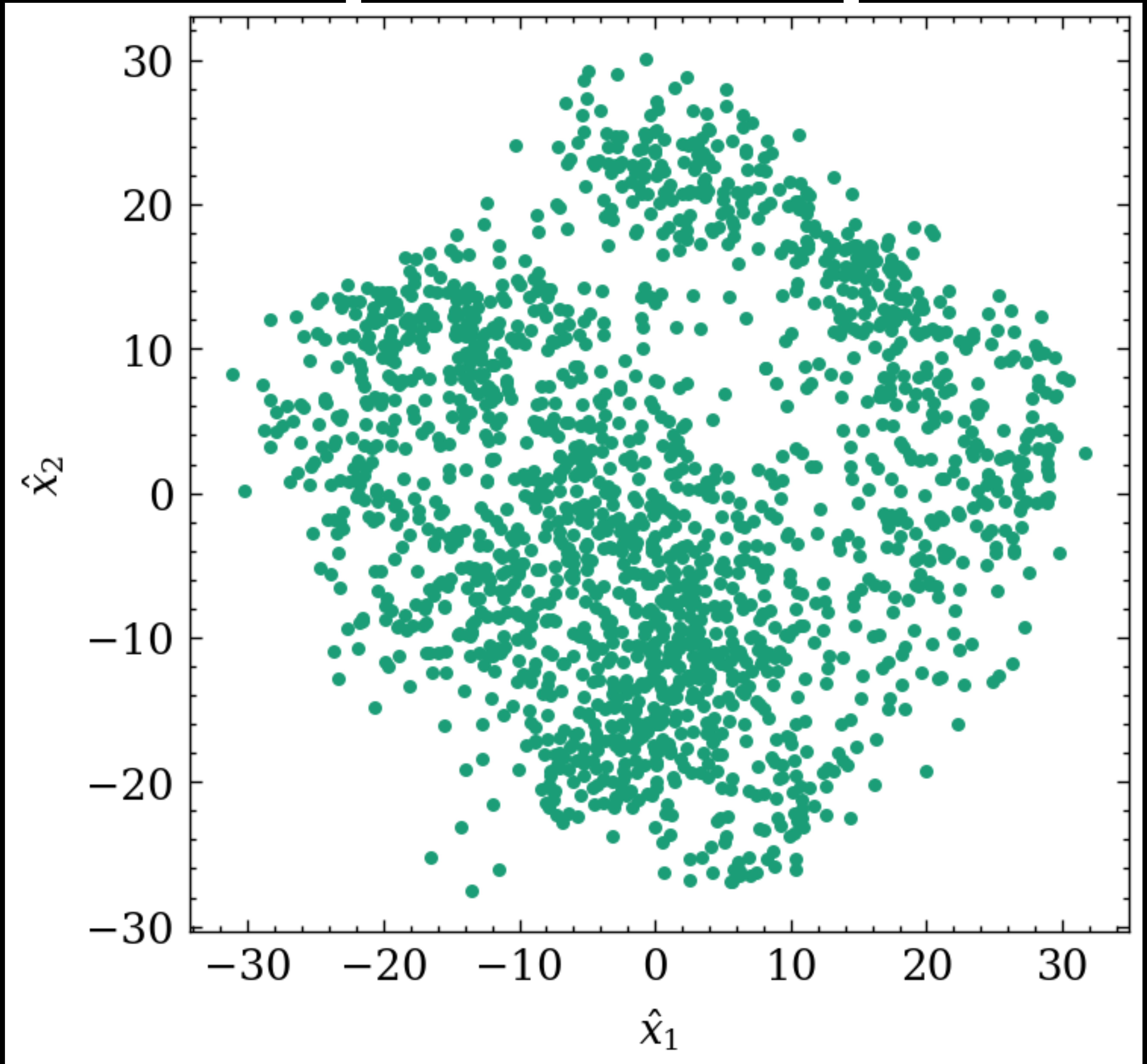
- $x_1, x_2, \ \dots \ x_{64}$

Goal: visualize the data in two dimensions

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



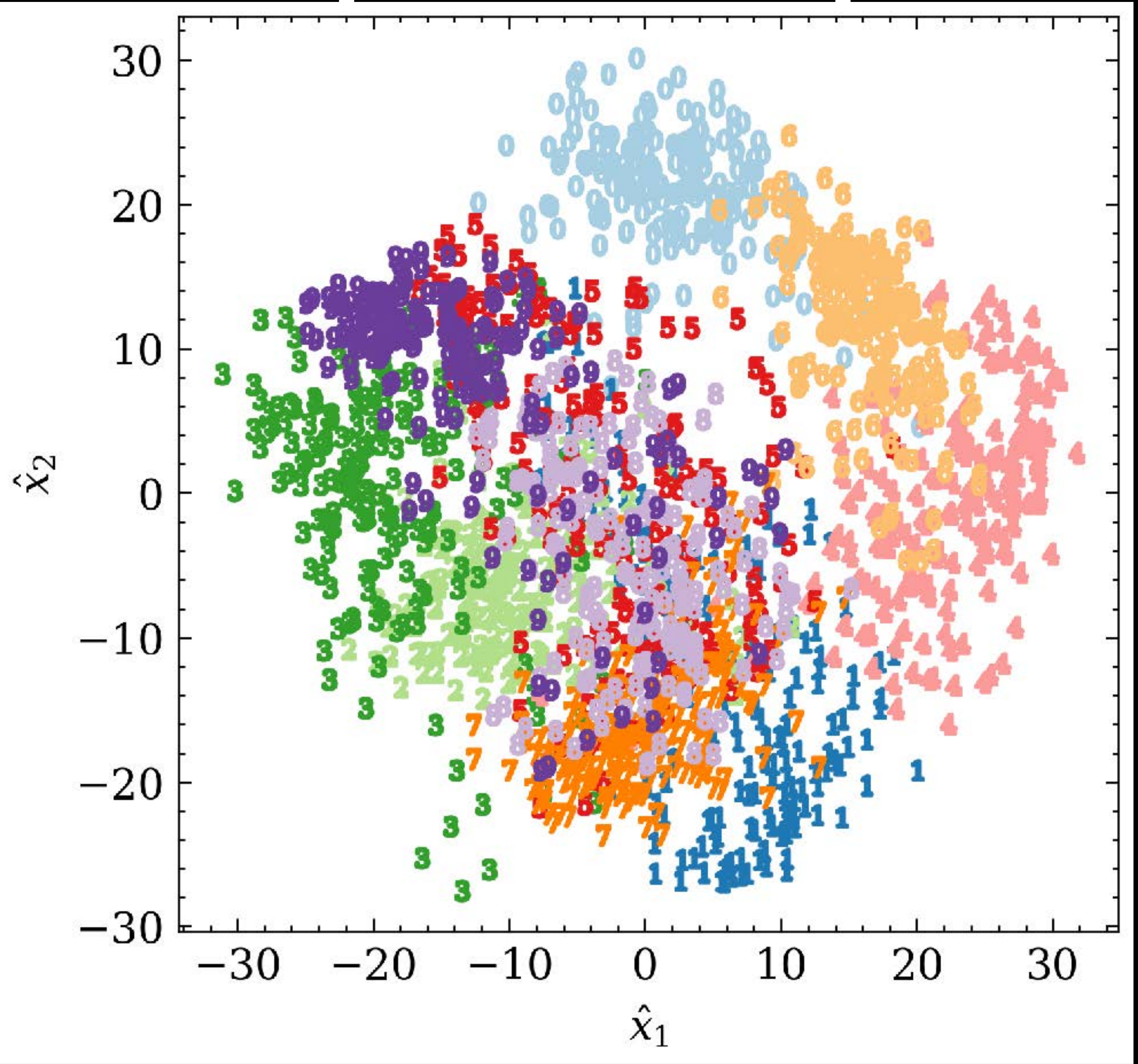
Principal Component Analysis



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?