Linear models I

Lecture 04

What makes a model linear?

How does least squares actually work?

How can we adapt linear models for classification?

Which of the following models are linear?

A $y = w_0$

B $y = w_0 + w_1 x_1$

C $y = w_0 + w_1 x_1 + w_2 x_2$

D $y = w_0 + w_1 x_1^2 + w_2 x_2^{0.4}$

E $y = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2$

F $y = w_0 + w_1 \int \sqrt[3]{x_1}\, dx_1 + w_2 g(x_2) + w_3 median(x_1, x_2, x_3)$

Which of the following models are linear?

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These are **ALL** linear in the **parameters, *w***

Linear models are linear in the **parameters**

They often model nonlinear relationships between features and targets

$$y_j = \sum_{i=0}^{p} w_i x_{i,j} + \epsilon$$

Linear regression assumptions

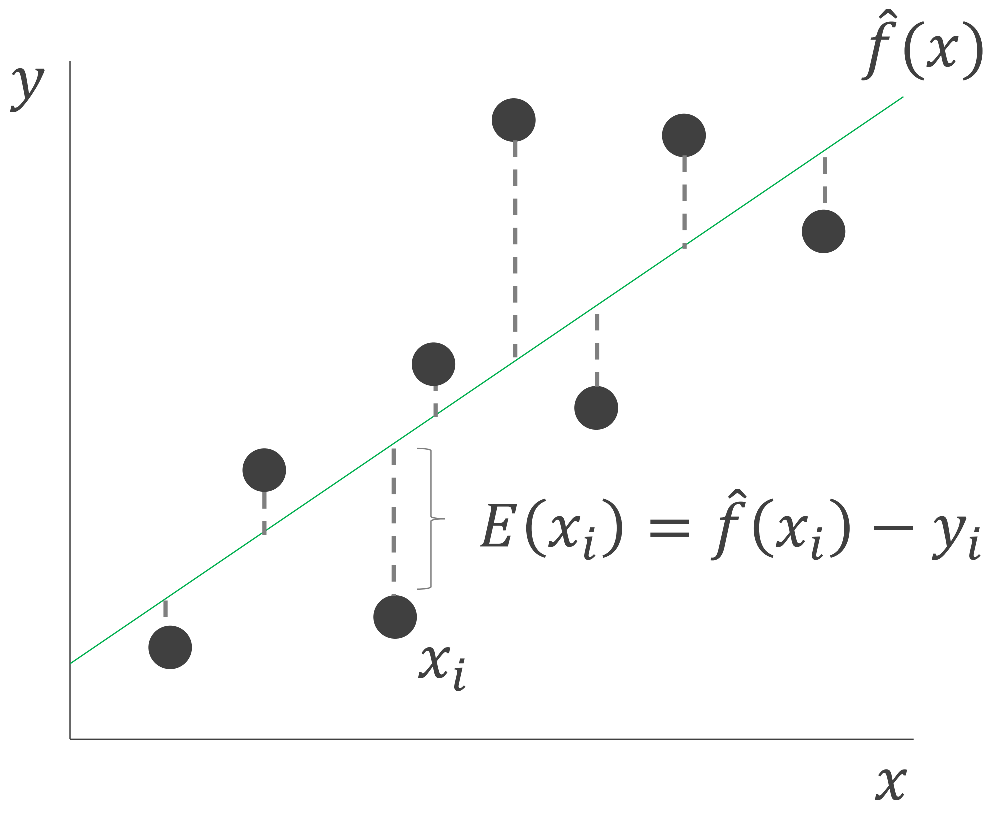
1. Linear relationship between feature and target variables
2. Error is normally distributed
3. Features are not correlated with one another (no multicollinearity)
4. Assumes observations are independent from one another (no autocorrelation)
5. Variance of the error is constant (homoscedastic)

Types of Linear Regression

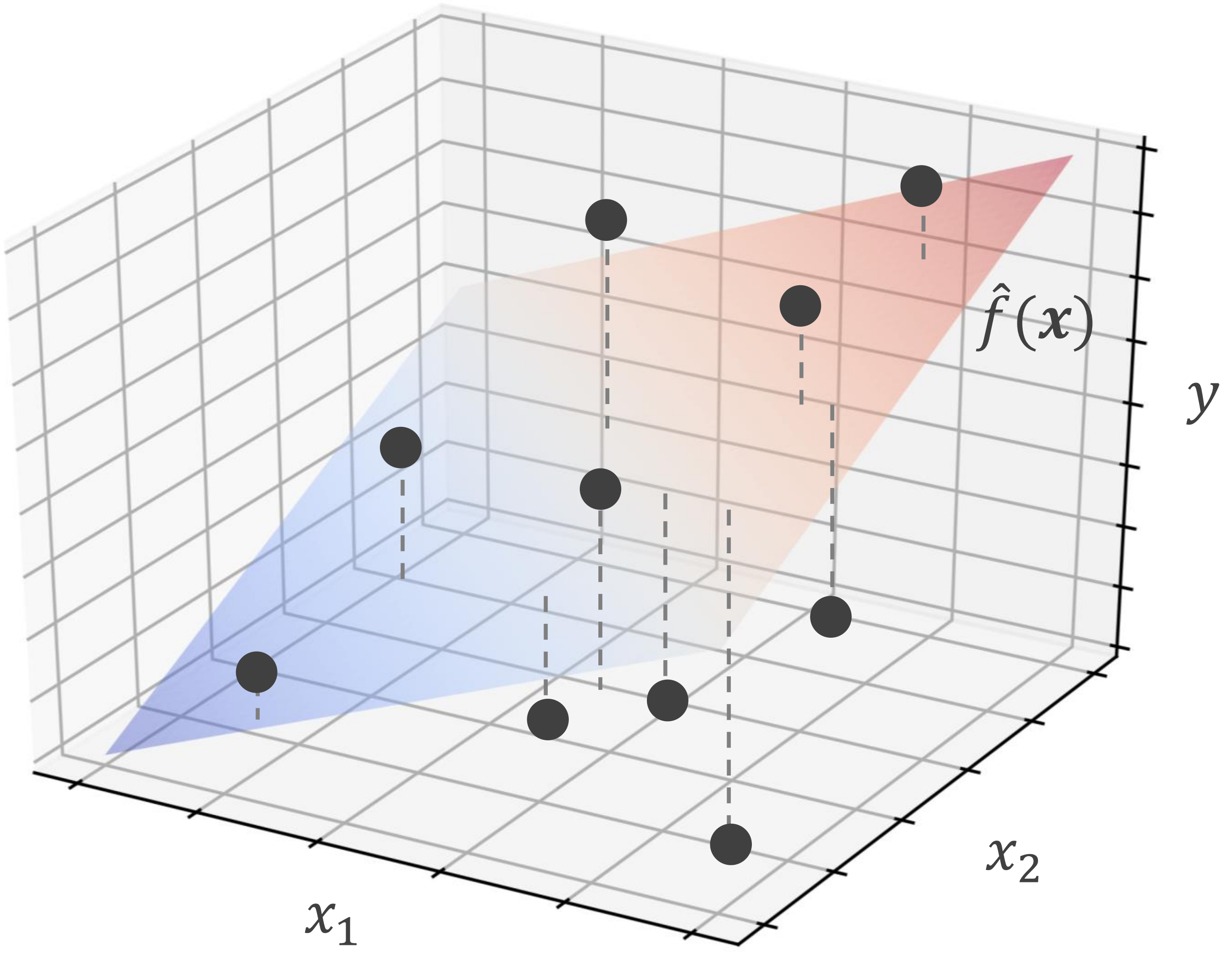
Here, $x_0 \triangleq 1$

	One feature variable	**One or more** feature variables
One target variable	**Simple Linear Regression** $y = w_0 + w_1 x_1$	**Multiple Linear Regression** $y = \sum_{i=0}^{p} w_i x_i$ or $y = \boldsymbol{w}^T \boldsymbol{x}$
One or more target variables	**Multivariate (Multiple) Linear Regression** $\boldsymbol{y} = \sum_{i=0}^{p} w_i \boldsymbol{x}_i$ or $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{w}$	

Linear models and error



simple linear regression



multiple linear regression

How do we fit a linear model to data?

We want the error between our estimates and predictions to be small

How do we measure error?

How well does $\hat{y} = \hat{f}(\boldsymbol{x}) = \sum_{i=0}^{p} w_i x_i$ approximate y ?

Error: difference between our estimate $\hat{y}$ and our training data y

$$\text{error} = \hat{y} - y$$

We use mean squared error to quantify training (in-sample) error:

Training (in-sample) error: $$E_{in}(\hat{f}) = \frac{1}{N} \sum_{n=1}^{N} \left(\hat{f}(\boldsymbol{x}_n) - y_n\right)^2$$

We call this our **Cost Function** (a.k.a. loss, error, or objective)

Cost Function: $$E_{in}(\hat{f}) = \frac{1}{N}\sum_{n=1}^{N}\left(\hat{f}(\boldsymbol{x}_n) - y_n\right)^2$$

Training error is a function of our **model** and the **training data**

We can’t change the data, we must adjust our model to minimize cost

We choose model **parameters** that minimize cost

This is an **optimization** problem

How to fit our model to the training data?

Equivalently: how do we choose $\boldsymbol{w}$ to minimize cost (error)

$$E_{in}(\hat{f}) = \frac{1}{N}\sum_{n=1}^{N}\left(\hat{f}(\boldsymbol{x}_n) - y_n\right)^2$$

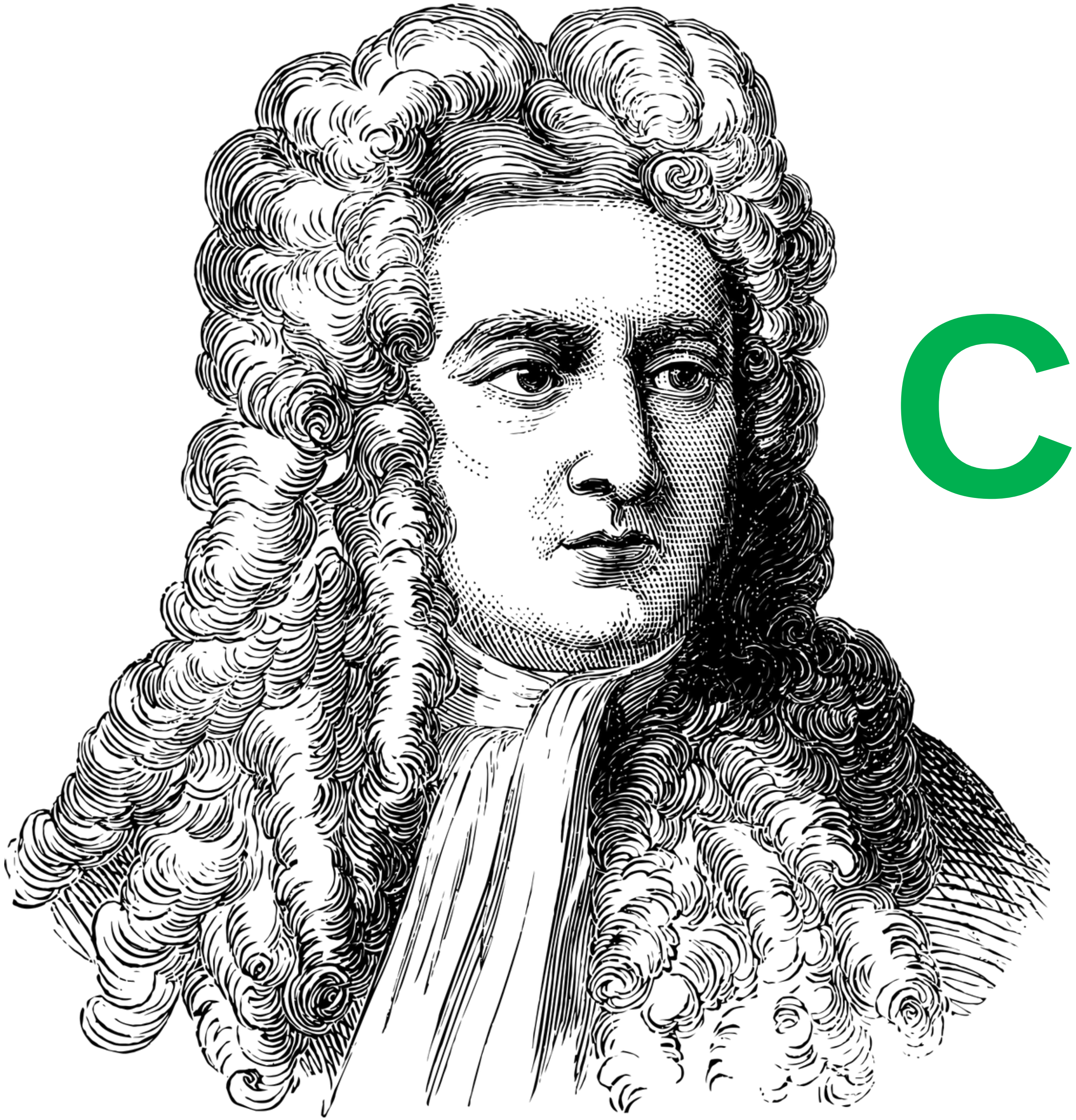
where $\hat{f}(\boldsymbol{x}_n) = \boldsymbol{w}^T\boldsymbol{x}_n$

We want to minimize

$$E_{in}(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{w}^T\boldsymbol{x}_n - y_n)^2$$

…by varying $\boldsymbol{w}$

How do we do that?



Calculus

A moment of calculus

Function of one variable

$$f(x) = ax + bx^2$$

Function of multiple variables

$$f(x_1, x_2) = ax_1 + bx_2$$

Derivative

$$\frac{df}{dx} = a + 2bx$$

Partial Derivative

$$\frac{\partial f}{\partial x_1} = a$$

$$\frac{\partial f}{\partial x_2} = b$$

Gradient

$$\nabla_{\boldsymbol{x}} f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{bmatrix}$$

$$= \begin{bmatrix} a \\ b \end{bmatrix}$$

May also treat parameters as variables and take their partial derivative $\frac{\partial f}{\partial b} = x_2$

How to fit our model to the training data?

Take the derivative with respect to $\boldsymbol{w}$, set it to zero, and solve for $\boldsymbol{w}$

$$\nabla_{\boldsymbol{w}} E_{in}(\boldsymbol{w}) = \nabla_{\boldsymbol{w}} \left(\frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{w}^T \boldsymbol{x}_n - y_n)^2 \right)$$

p = number of predictors
N = number of data points

$$\nabla_{\boldsymbol{w}} E_{in}(\boldsymbol{w}) = \begin{bmatrix} \frac{\partial E_{in}}{\partial w_0} \\ \frac{\partial E_{in}}{\partial w_1} \\ \vdots \\ \frac{\partial E_{in}}{\partial w_p} \end{bmatrix} = \boldsymbol{0}$$

Size: $[p+1 \times 1]$ or $\mathbb{R}^{p+1\times1}$

Here we walk through the **ordinary least squares** (OLS) closed-form solution.

Could have used an iterative approach like **gradient descent**

How to fit our model to the training data?

We can rewrite our objective function:

$$E_{in}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{w}^T\mathbf{x}_n - y_n)^2$$

Scalar

$$\mathbf{w}^T \in \mathbb{R}^{1\times p+1}$$

$$\mathbf{x}_n \in \mathbb{R}^{p+1\times 1}$$

We can rewrite our objective function:

$$E_{in}(\mathbf{w}) = \frac{1}{N}(\mathbf{X}\mathbf{w} - \mathbf{y})^T(\mathbf{X}\mathbf{w} - \mathbf{y})$$

Convenient definitions:

$$\mathbf{y} \in \mathbb{R}^{N\times 1}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix} \in \mathbb{R}^{N\times p+1}$$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_p \end{bmatrix} \in \mathbb{R}^{p+1\times 1}$$

p = number of predictors
N = number of data points

p = number of predictors
N = number of data points

1 Assume $p = 2$, $N = 4$

$$\boldsymbol{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} \qquad \boldsymbol{x}_i = \begin{bmatrix} x_{i,0} \\ x_{i,1} \\ x_{i,2} \end{bmatrix}$$

2

$$\boldsymbol{w}^T \boldsymbol{x}_i = \begin{bmatrix} w_0 & w_1 & w_2 \end{bmatrix} \begin{bmatrix} x_{i,0} \\ x_{i,1} \\ x_{i,2} \end{bmatrix}$$

$$= w_0 x_{i,0} + w_1 x_{i,1} + w_2 x_{i,2}$$

3

$$\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_1^T \\ \boldsymbol{x}_2^T \\ \boldsymbol{x}_3^T \\ \boldsymbol{x}_4^T \end{bmatrix} = \begin{bmatrix} x_{1,0} & x_{1,1} & x_{1,2} \\ x_{2,0} & x_{2,1} & x_{2,2} \\ x_{3,0} & x_{3,1} & x_{3,2} \\ x_{4,0} & x_{4,1} & x_{4,2} \end{bmatrix}$$

4

$$\boldsymbol{X}\boldsymbol{w} = \begin{bmatrix} x_{1,0} & x_{1,1} & x_{1,2} \\ x_{2,0} & x_{2,1} & x_{2,2} \\ x_{3,0} & x_{3,1} & x_{3,2} \\ x_{4,0} & x_{4,1} & x_{4,2} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} \boldsymbol{w}^T \boldsymbol{x}_1 \\ \boldsymbol{w}^T \boldsymbol{x}_2 \\ \boldsymbol{w}^T \boldsymbol{x}_3 \\ \boldsymbol{w}^T \boldsymbol{x}_4 \end{bmatrix}$$

Algebraic manipulations

4

$$\boldsymbol{X}\boldsymbol{w} = \begin{bmatrix} x_{1,0} & x_{1,1} & x_{1,2} \\ x_{2,0} & x_{2,1} & x_{2,2} \\ x_{3,0} & x_{3,1} & x_{3,2} \\ x_{4,0} & x_{4,1} & x_{4,2} \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} \boldsymbol{w}^T \boldsymbol{x}_1 \\ \boldsymbol{w}^T \boldsymbol{x}_2 \\ \boldsymbol{w}^T \boldsymbol{x}_3 \\ \boldsymbol{w}^T \boldsymbol{x}_4 \end{bmatrix}$$

5

$$(\boldsymbol{X}\boldsymbol{w})^T(\boldsymbol{X}\boldsymbol{w}) = \begin{bmatrix} \boldsymbol{w}^T \boldsymbol{x}_1 & \boldsymbol{w}^T \boldsymbol{x}_2 & \boldsymbol{w}^T \boldsymbol{x}_3 & \boldsymbol{w}^T \boldsymbol{x}_4 \end{bmatrix} \begin{bmatrix} \boldsymbol{w}^T \boldsymbol{x}_1 \\ \boldsymbol{w}^T \boldsymbol{x}_2 \\ \boldsymbol{w}^T \boldsymbol{x}_3 \\ \boldsymbol{w}^T \boldsymbol{x}_4 \end{bmatrix}$$

$$= \sum_{n=1}^{N} (\boldsymbol{w}^T \boldsymbol{x}_n)^2$$

Algebraic manipulations

How to fit our model to the training data?

We can rewrite our objective function:

$$E_{in}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N}(\underbrace{\mathbf{w}^T\mathbf{x}_n}_{\text{Scalar}} - y_n)^2$$

$$\mathbf{w}^T \in \mathbb{R}^{1\times p+1}$$

$$\mathbf{x}_n \in \mathbb{R}^{p+1\times 1}$$

We can rewrite our objective function:

$$E_{in}(\mathbf{w}) = \frac{1}{N}(\mathbf{X}\mathbf{w} - \mathbf{y})^T(\mathbf{X}\mathbf{w} - \mathbf{y})$$

Convenient definitions:

$$\mathbf{y} \in \mathbb{R}^{N\times 1}$$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_N^T \end{bmatrix} \in \mathbb{R}^{N\times p+1}$$

$$\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_p \end{bmatrix} \in \mathbb{R}^{p+1\times 1}$$

p = number of predictors
N = number of data points

How to fit our model to the training data?

$$E_{in}(\mathbf{w}) = \frac{1}{N}(\mathbf{X}\mathbf{w} - \mathbf{y})^T(\mathbf{X}\mathbf{w} - \mathbf{y})$$

$$\nabla_{\mathbf{w}} E_{in}(\mathbf{w}) = \frac{2}{N}(\mathbf{X}^T\mathbf{X}\mathbf{w} - \mathbf{X}^T\mathbf{y}) = \mathbf{0}$$

Univariate analogy:

$$f(w) = \frac{1}{N}(xw - y)^2$$

$$= \frac{1}{N}(x^2w^2 - 2xyw + y^2)$$

$$\frac{df(w)}{dw} = \frac{2}{N}(x^2w - xy)$$

$$\mathbf{X}^T\mathbf{X}\mathbf{w} - \mathbf{X}^T\mathbf{y} = \mathbf{0}$$

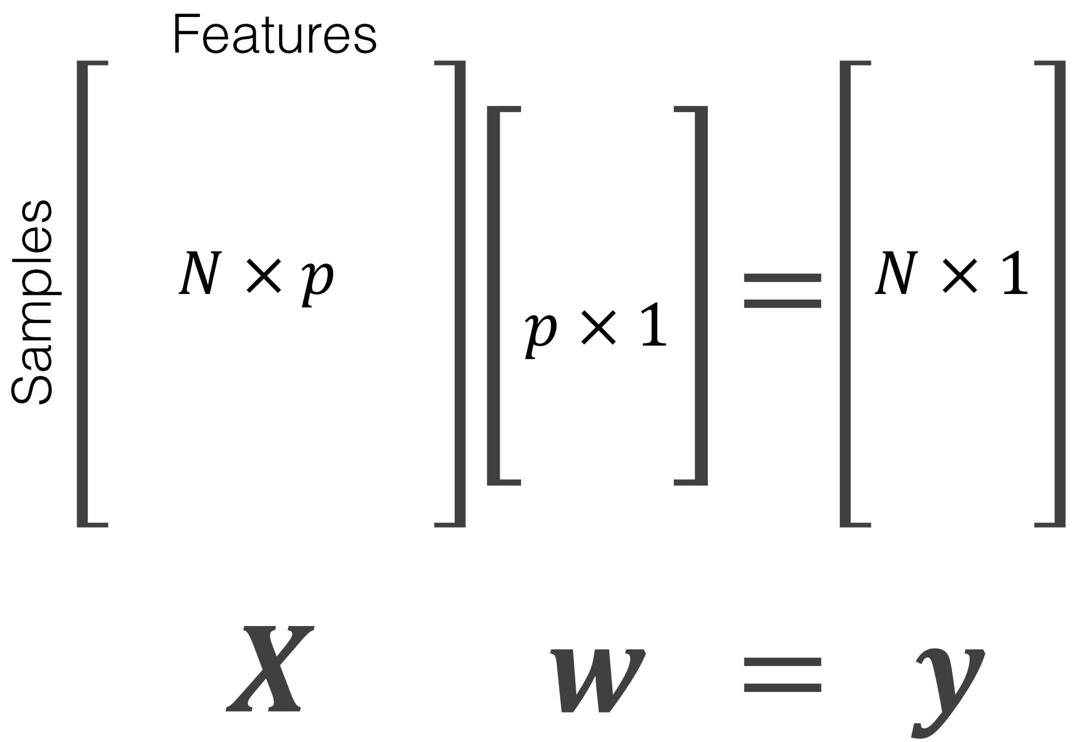
$$\mathbf{X}^T\mathbf{X}\mathbf{w} = \mathbf{X}^T\mathbf{y}$$ (normal equation)

$$\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Pseudoinverse $\mathbf{X}^\dagger = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$

$$\boxed{\mathbf{w}^* = \mathbf{X}^\dagger\mathbf{y}}$$

What is the pseudoinverse?



If $N = p$, then there are the same number of features as samples
(# equations = # unknowns)

If $N > p$, then the system of equations is overdetermined: more samples than features
(# equations > # unknowns)

Overdetermined systems

Example 1

Fully determined system

equations = # unknowns

$$w_1 = 2$$
$$w_2 = 1$$

Overdetermined system

equations > # unknowns

$$w_1 = 2$$
$$w_2 = 1$$
$$w_2 = 5$$

Example 2

Fully determined system

equations = # unknowns

$$2w_1 + 3w_2 = 2$$
$$6w_1 + 1w_2 = 0.63$$

Overdetermined system

equations > # unknowns

$$2w_1 + 3w_2 = 2$$
$$6w_1 + 1w_2 = 0.63$$
$$3w_1 + 2w_2 = 14$$
$$16w_1 - w_2 = 0.1$$

What is the pseudoinverse?

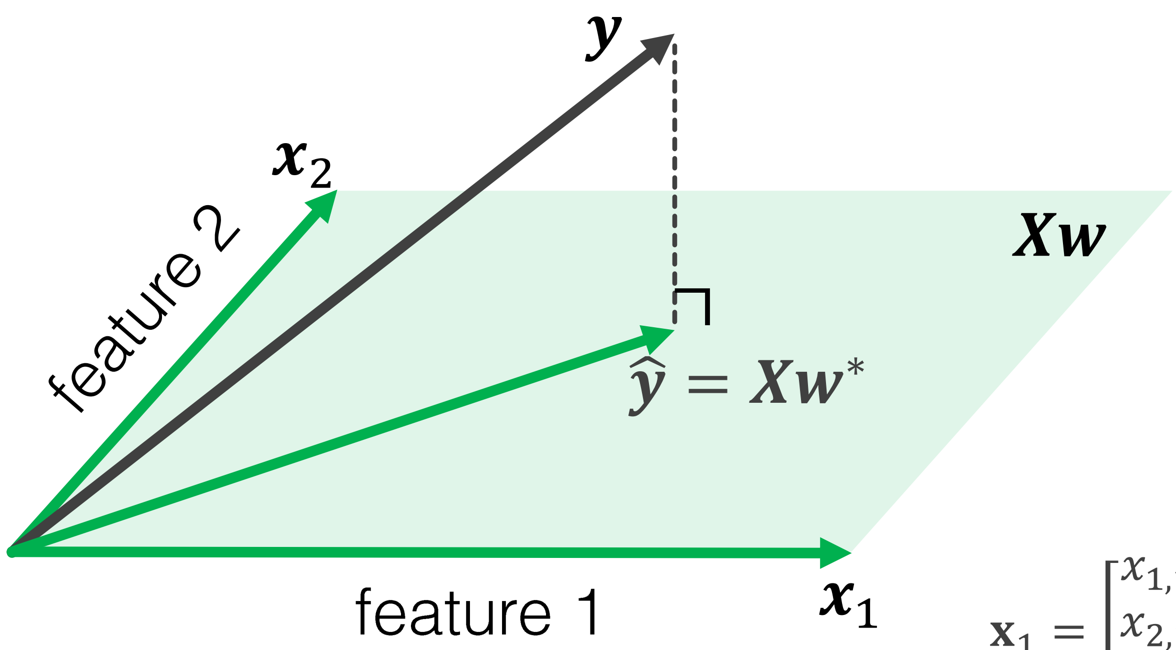
Consider the case when $N = 3$, $p = 2$

$$\begin{array}{cc} & \text{Features} \\ \text{Samples} & \begin{bmatrix} x_{1,1} & x_{1,2} \\ x_{2,1} & x_{2,2} \\ x_{3,1} & x_{3,2} \end{bmatrix} \end{array} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

$$\boldsymbol{X} \quad \boldsymbol{w} \neq \boldsymbol{y}$$

We CAN solve for the least squares solution: $\boldsymbol{X}^{\dagger}\boldsymbol{w}^* = \boldsymbol{y}$

The least squares solution is the best we can do given $N > p$



$$\mathbf{x}_1 = \begin{bmatrix} x_{1,1} \\ x_{2,1} \\ x_{3,1} \end{bmatrix}$$

Common paradigm for model fitting

1. Choose a **hypothesis set of models** to train
   (e.g. linear regression with 4 predictor variables)

2. Identify a **cost function** to measure the model fit to the training data
   (e.g. mean square error)

3. **Optimize** model **parameters** to minimize cost
   (e.g. closed form solution using the normal equations for OLS)

Much of machine learning is **optimizing** a **cost function**

What about classification?

Moving from regression to classification

Regression

$$y = \sum_{i=0}^{p} w_i x_i$$

Classification
(perceptron model)

$$y = sign\left(\sum_{i=0}^{p} w_i x_i\right)$$

$$y = \begin{cases} 1 & \sum_{i=0}^{p} w_i x_i > 0 \\ -1 & else \end{cases}$$

where

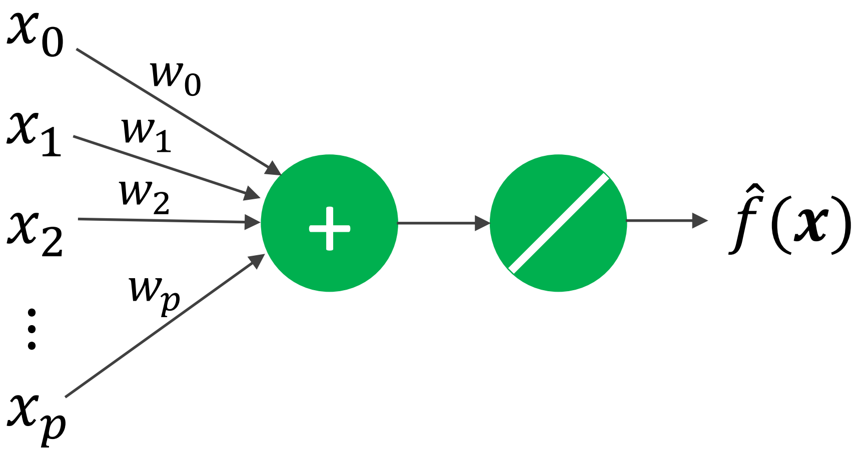
$$sign(x) = \begin{cases} 1 & x > 0 \\ -1 & else \end{cases}$$

Source: Abu-Mostafa, Learning from Data, Caltech

Moving from regression to classification

Linear Regression

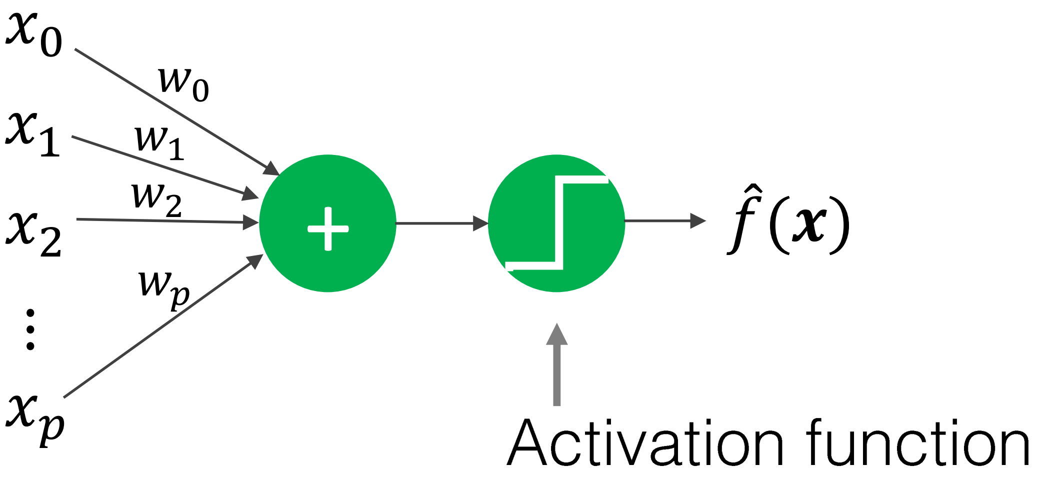
$$\hat{f}(\boldsymbol{x}) = \sum_{i=0}^{p} w_i x_i$$



Linear Classification

(perceptron)

$$\hat{f}(\boldsymbol{x}) = sign\left(\sum_{i=0}^{p} w_i x_i\right)$$



Source: Abu-Mostafa, Learning from Data, Caltech

Takeaways

Linear models are **linear in the weights**

Linear models can be used for **both regression and classification**

Model fitting/training (valid beyond linear models):

- Choose a hypothesis set of models to train
- Identify a cost function
- **Optimize the cost function** by adjusting model parameters