Feb 13

Important announcements

- midterm marks will be released on the weekend or early next week
- release solutions tonight
- Thank you for filling out the midterm evaluation survey

=> Our goal (from supervised learning lecture)

Defining $\mathcal{A}(D)$: Empirical Risk Minimization (ERM)

Estimation:

Use D to estimate $L(f)$ for all $f \in \mathcal{F} \subset \{f \mid f : \mathcal{X} \to \mathcal{Y}\}$

call the estimate $\hat{L}(f)$

Optimization:

pick $\hat{f}$ to be the $f \in \underbrace{\mathcal{F}}_{\text{Function class}}$ that minimizes $\hat{L}(f)$

Optimization

finding the best solution from a set of possible solutions

Usually this means finding the minimum or maximum value of some function

we will care about:

$$\min_{w \in \mathcal{W}} g(w)$$

minimum value of $g(w)$ over all $w \in \mathcal{W}$

or $$w^* = \underset{w \in \mathcal{W}}{\operatorname{argmin}}\ g(w)$$

the $w \in \mathcal{W}$ that achieves the minimum value of $g(w)$

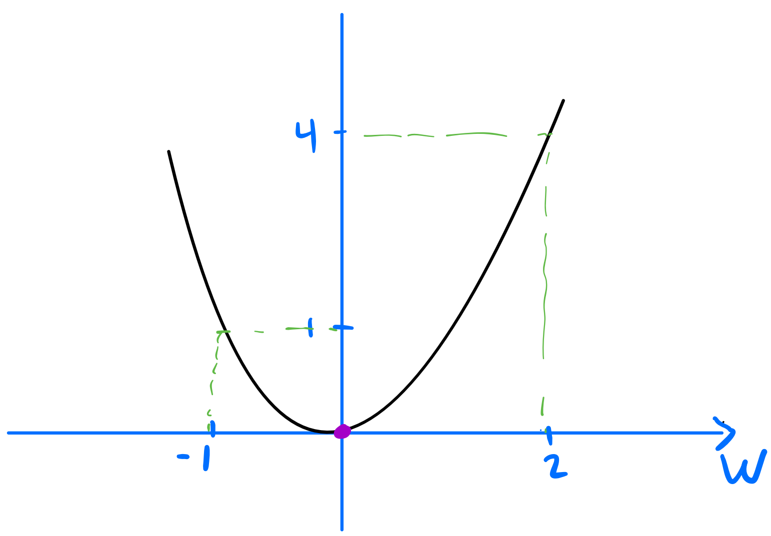
w^* is a "minimizer"

$$\min_{w \in \mathcal{W}} g(w) = g(w^*)$$

Ex: $g(w) = w^2$ $\quad \mathcal{W} = \mathbb{R}$

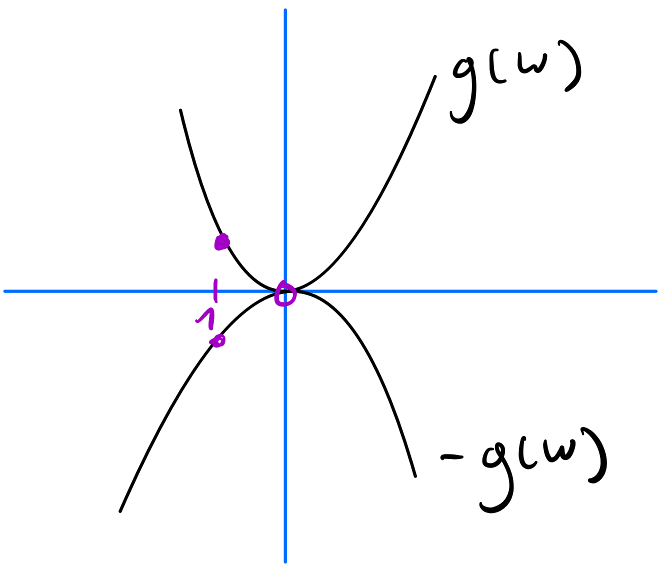
$w^* = \operatorname{argmin}\ g(w) = 0$

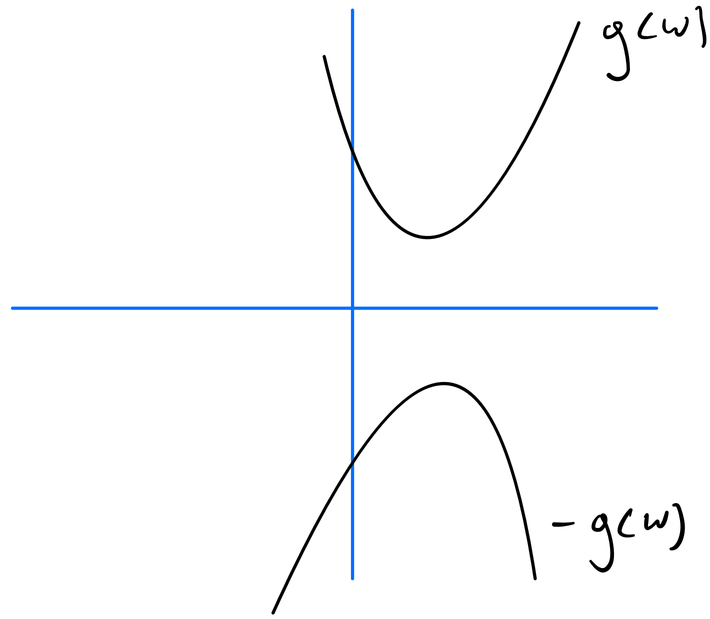
$\min_{w \in \mathcal{W}} g(w) = 0 = g(w^*)$



$W = \{-1, 2\}$ $\quad \min_{w \in W} g(w) = 1 = g(w^*)$ $\quad \arg\min_{w \in W} g(w) = -1 = w^*$

Note: There is a relationship between minimizing and maximizing





$$w^* = \arg\min_{w \in W} g(w) = \arg\max_{w \in W} -g(w)$$

$$g(w^*) = \min_{w \in W} g(w) = -\left(\max_{w \in W} -g(w)\right) = -\left(-g(w^*)\right) = g(w^*)$$

=> We can choose if we want to maximize a function or minimize its negative (of that function)

How do we solve minimization problems?

<u>Cases:</u>

1. If $\mathcal{W}$ is discrete
   we compare $g(w)$ for all $w \in \mathcal{W}$

2. If $\mathcal{W}$ is continuous we can sometimes
   use derivatives

$\Rightarrow$ <u>We will focus on $\mathcal{W}$ continuous</u>

Additional assumptions:

If $g(w)$ is convex and twice differentiable
then:

<u>Cases:</u> 1. If $\mathcal{W} = \mathbb{R}$ then w^* is the solution
to $g'(w) = 0$

2. If $\mathcal{W} = [a,b]$ then w^* is the solution
to $g'(w) = 0$ if this solution is in $[a,b]$
Otherwise, w^* is a or b.

Twice differentiable: The second derivative of $g(w)$ written $g''(w)$ exists for all $w \in \mathcal{W}$

Convex: $g(w)$ is convex if $g''(w) \geq 0$ for all $w \in \mathcal{W}$

"Usually $g(w)$ is bowl-shaped"

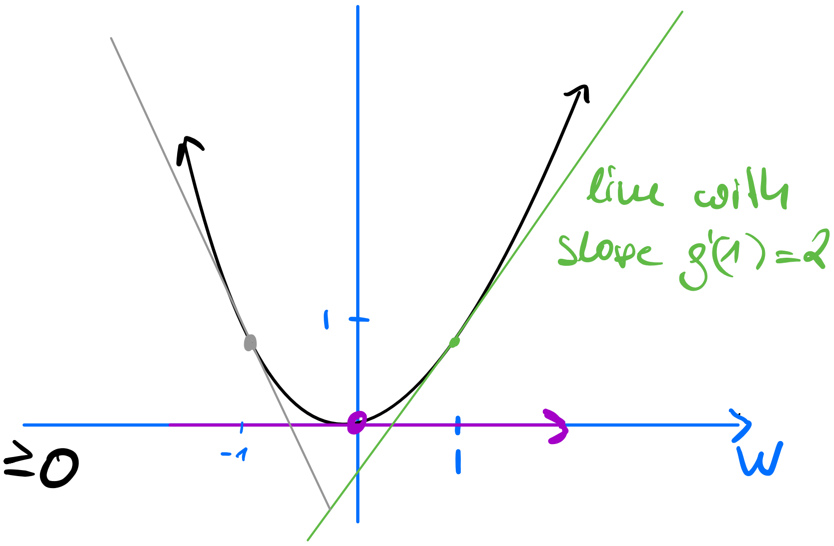
Ex: $g(w) = w^2$, $\mathcal{W} = \mathbb{R}$

$w^* = \underset{w}{\operatorname{argmin}}\, g(w)$

$g'(w) = 2w$, $g''(w) = 2$

$\Rightarrow g(w)$ is convex: $g''(w) = 2 \geq 0$

$g'(w) = 2w = 0 \rightarrow w^* = 0$



$g'(1) = 2 \cdot 1$

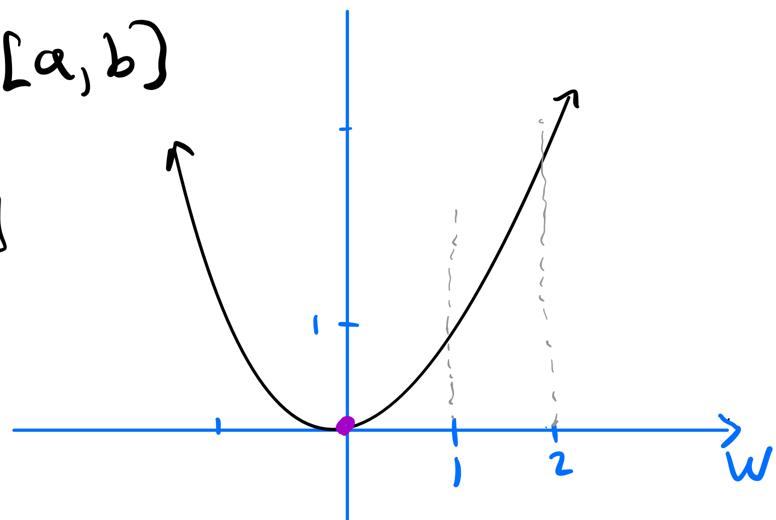
$g'(-1) = 2 \cdot (-1) = -2$

$g'(0) = 0$

Ex: $g(w) = w^2$, $\mathcal{W} = [1, 2] = [a, b]$

$g'(w) = 2w = 0 \rightarrow w = 0 \notin [1, 2]$

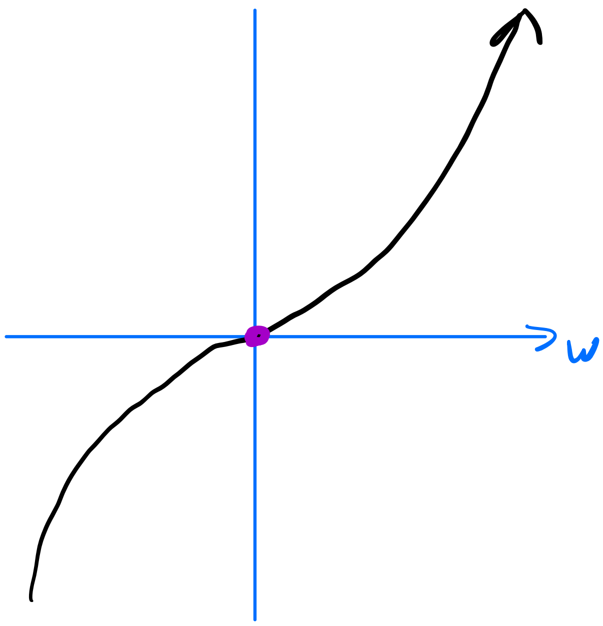
$g(1) = 1$, $g(2) = 4$



$w^* = 1 \rightarrow g(w^*) = \min_w g(w) =$

Ex: $g(w) = w^3$, $\mathcal{W} = \mathbb{R}$

$g'(w) = 3w^2$, $g''(w) = 6w$

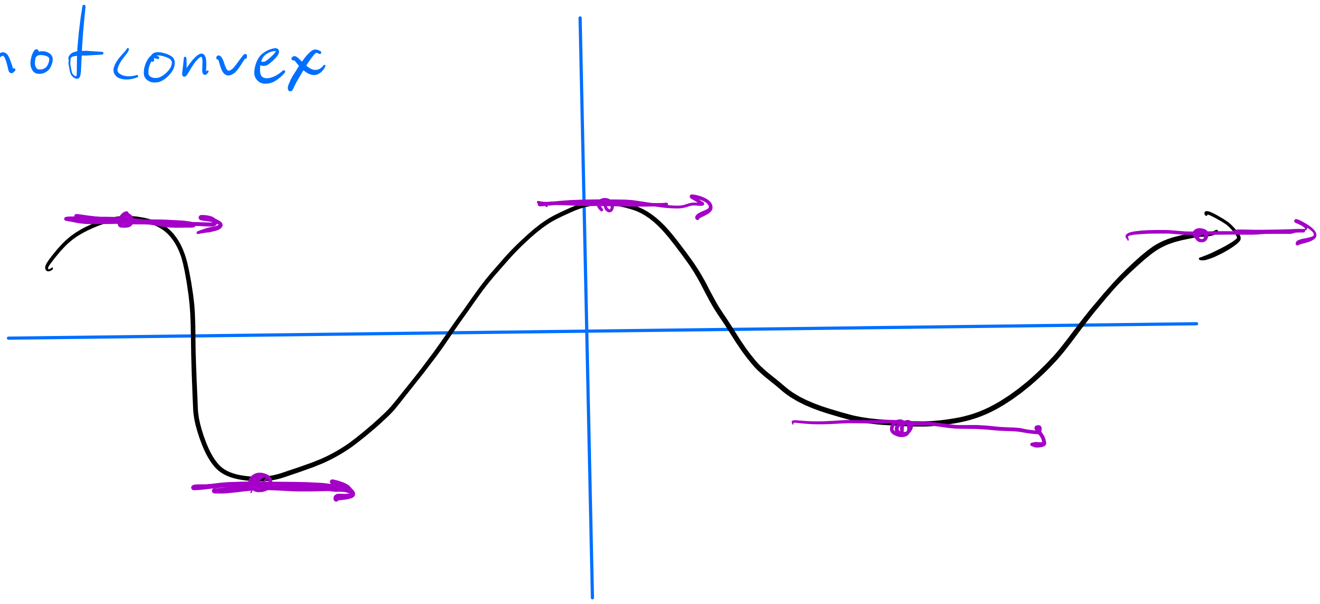


$g''(w) < 0$
when $w < 0$

$g'(w) = 3w^2 = 0$

w of the minimum

Ex: not convex



Multidimensional Minimization

If $\mathcal{W} = \mathbb{R}^d$ for $d > 1$, and $g(\vec{\omega})$ is convex

Note: it is more complex to check if $g(\vec{\omega})$ is convex if $d > 1$. So, I will tell you.

then we calculate

$$\vec{\omega}^* = (w_1^*, \dots, w_d^*)^T = \underset{\vec{\omega} \in \mathcal{W}}{\operatorname{argmin}} \; g(\vec{\omega})$$

by setting w_j^* as the solution to

$$\frac{\partial g(\vec{\omega})}{\partial w_j} = 0 \quad \text{for all } j \in \{1, \dots, d\}$$

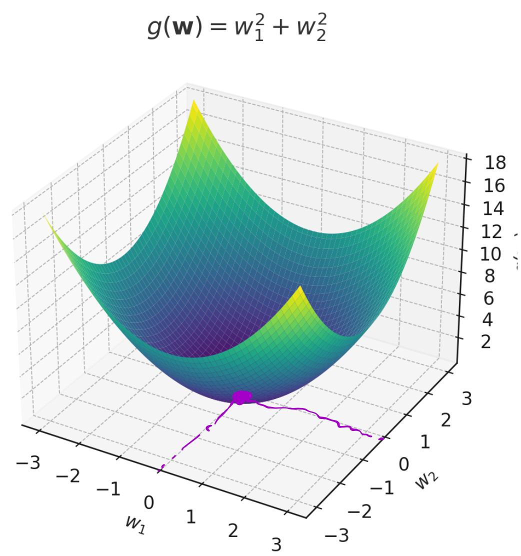
Ex: $g(\vec{w}) = g(w_1, w_2) = w_1^2 + w_2^2$, $\quad \mathcal{W} = \mathbb{R}^2$

$$\frac{\partial g(\vec{\omega})}{\partial w_1} = 2\omega_1 = 0 \Rightarrow \omega_1^* = 0$$

$$\frac{\partial g(\vec{\omega})}{\partial \omega_2} = 2\omega_2 = 0 \Rightarrow \omega_2^* = 0$$

$$\vec{\omega}^* = (w_1^*, w_2^*)^T = (0, 0)^T$$

$$g(\vec{\omega}^*) = \min_{\vec{\omega}} g(\vec{\omega})$$



Finding a good predictor (Linear Regression)

Optimization step of ERM

$\mathcal{X} = \mathbb{R}^{d+1}$, $\mathcal{Y} = \mathbb{R}$ (regression)

$\mathcal{F} \subset \{ f \mid f : \mathbb{R}^{d+1} \to \mathbb{R} \}$ function class

$D = ((\vec{x}_1, y_1), \dots, (\vec{x}_n, y_n))$ fixed dataset

$\hat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(\vec{x}_i), y_i)$ estimate of $L(f)$ for all $f \in \mathcal{F}$

(sample mean)

what we want

$$\boxed{\hat{f} = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \hat{L}(f)}$$

pick $\mathcal{F} = \{ f \mid f : \mathcal{X} \to \mathcal{Y} \text{ and } f(\vec{x}) = \vec{x}^T \vec{w} \text{ where } \vec{w} \in \mathbb{R}^{d+1} \}$

$\to$ "linear functions"

$$f(\vec{x}) = \vec{x}^T \vec{w} + b = (x_1, \dots, x_d)^T (w_1, \dots, w_d) + b$$

$$= \underset{\Rightarrow w_0}{b} + x_1 w_1 + \dots + x_d w_d$$

$b = w_0$

$x_0 = 1$

$$= x_0 w_0 + x_1 w_1 + \dots + x_d w_d$$

$$= (x_0, x_1, \dots, x_d)^T (w_0, w_1, \dots, w_d)$$

$$= \vec{x}_0^T \vec{w}_0$$

Assume $\vec{x} = (x_0 = 1, x_1, \dots, x_d) \in \mathbb{R}^{d+1}$

$\vec{x}_i = (x_{i,0} = 1, x_{i,1}, \dots, x_{i,d}) \in \mathbb{R}^{d+1}$ (dataset)

Notice $\hat{f} \in F$ so $\hat{f}(\vec{x}) = \vec{x}^T \hat{\vec{w}}$ for some $\hat{\vec{w}} \in \mathbb{R}^{d+1}$

$$\hat{\vec{w}} = \underset{\substack{\vec{w} \in \mathbb{R}^{d+1} \\ \downarrow \\ W}}{\arg\min} \; \underset{\substack{\downarrow \\ g}}{\hat{L}(\vec{w})} \quad \text{where } \hat{L}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(\vec{x}_i^T \vec{w}, y_i)$$

- searching over functions is equivalent to searching over parameters $\vec{w} \in \mathbb{R}^{d+1}$

=> multivariate optimization problem

Pick loss function ℓ to be the squared loss

→ $\hat{L}(\vec{w})$ is convex

$$\hat{L}(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} (\vec{x}_i^T \vec{w} - y_i)^2$$

$$= \frac{1}{n} \left[(\vec{x}_1^T \vec{w} - y_1)^2 + \dots + (\vec{x}_n^T \vec{w} - y_n)^2 \right]$$

$\vec{x}_i = (x_{i,0} = 1, x_{i,1}, \dots, x_{i,d})^T$, $\vec{w} = (w_0, w_1, \dots, w_d)^T$

$$= \frac{1}{n} \Big[(x_{1,0} w_0 + x_{1,1} w_1 + \dots + x_{1,d} w_d - y_1)^2 + \dots$$

$$+ (x_{n,0} w_0 + x_{n,1} w_1 + \dots + x_{n,d} w_d - y_n)^2 \Big]$$

$$= \frac{1}{n}\left[\hat{L}_1(\vec{w}) + \dots + \hat{L}_n(\vec{w}) \right]$$

$$\hat{L}_i(\vec{w}) = (x_i^T \vec{w} - y_i)^2 = (x_{i,0} w_0 + x_{i,1} w_1 + \dots - x_{i,d} w_d - y_i)^2$$

Take the derivative of the estimated loss w.r.t each w_j for all $j \in \{0, \dots, d\}$

$$\frac{\partial \hat{L}(\vec{w})}{\partial w_j} = \frac{1}{n}\left[\frac{\partial}{\partial w_j} L_1(\vec{w}) + \dots + \frac{\partial}{\partial w_j} \hat{L}_n(\vec{w}) \right]$$

applying the chain rule

$$\hat{L}_i(\vec{w}) = g(u_i) = u_i^2 \quad , \quad u_i = \vec{x}_i^T \vec{w} - y_i$$

$$\frac{\partial}{\partial w_j} \hat{L}_i(\vec{w}) = \frac{\partial g}{\partial u_i} \frac{\partial u_i(\vec{w})}{\partial w_j} = 2 u_i x_{i,j} = 2 x_{i,j} (\vec{x}_i^T \vec{w} - y_i)$$

$$= \frac{2}{n}\left[x_{1,j} (\vec{x}_1^T \vec{w} - y_1) + \dots + x_{n,j} (\vec{x}_n^T \vec{w} - y_n) \right]$$

$$= \frac{2}{n} \sum_{i=1}^{n} x_{i,j} (\vec{x}_i^T \vec{w} - y_i)$$

$$\frac{\partial \hat{L}(\vec{w})}{\partial w_j} = \frac{2}{n} \sum_{i=1}^{n} x_{i,j} (\vec{x}_i^T \vec{w} - y_i) = 0$$

-> solve for w_j

$$\Rightarrow \frac{2}{n} \sum_{i=1}^{n} x_{i,j} \vec{x}_i^T \vec{w} - \frac{2}{n} \sum_{i=1}^{n} x_{i,j} y_i = 0$$

$$\sum_{i=1}^{n} x_{i,j} \vec{x}_i^T \vec{w} = \sum_{i=1}^{n} x_{i,j} y_i \quad \text{for all } j \in \{0, \dots, d\}$$

→ system of d+1 equations

$$\sum_{i=1}^{n} x_{i,0}\, \vec{x}_i^{T} \vec{w} = \sum_{i=1}^{n} x_{i,0}\, y_i \qquad j=0$$

$$\vdots$$

$$\sum_{i=1}^{n} x_{i,d}\, \vec{x}_i^{T} \vec{w} = \sum_{i=1}^{n} x_{i,d}\, y_i \qquad j=d$$

→ compact formulation

$$\sum_{i=1}^{n} \vec{x}_i\, x_i^{T} \vec{w} = \sum_{i=1} \vec{x}_i\, y_i$$

$$A = \sum_{i=1}^{n} \overbrace{\vec{x}_i\, \vec{x}_i^{T}}^{\text{outer product}}$$

$$\vec{b} = \sum_{i=1}^{n} \vec{x}_i\, y_i$$

inverse of A

$$\underbrace{A^{-1} A}_{\substack{I \\ \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}}} \vec{w} = A^{-1} \vec{b}$$

$$\hat{\vec{w}} \overset{\text{def}}{=} \vec{w} = A^{-1} \vec{b} \qquad \text{if } A^{-1} \text{ exists}$$

What is the learner $\mathcal{A}(D)$?

$$D = \left((\vec{x}_1, y_1), \dots, (\vec{x}_n, y_n) \right) \in (\mathcal{X} \times \mathcal{Y})^n$$

$$\mathcal{A}(D) = \hat{f} \in \mathcal{F} \quad \text{where } \hat{f}(\vec{x}) = \vec{x}^{T} \vec{w} \qquad \vec{x} \in \mathcal{X}$$

$$\text{and } \hat{\vec{w}} = A^{-1} \vec{b}$$

Algorithm: Closed form linear regression learner

input: $D = ((\vec{x}_1, y_1), \dots, (\vec{x}_n, y_n))$

$$A \leftarrow \sum_{i=1}^{n} \vec{x}_i \vec{x}_i^T$$ (sum of the outer product of the features)

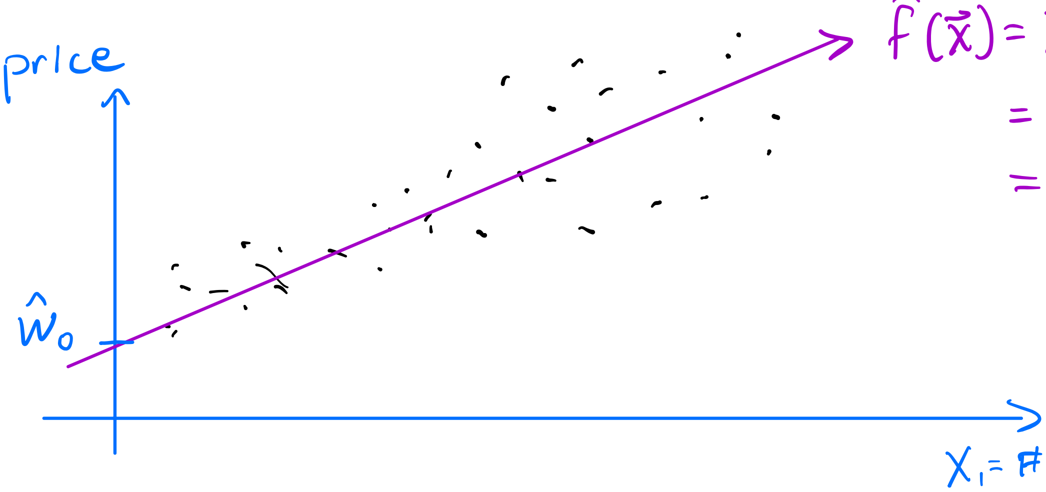
$$\vec{b} \leftarrow \sum_{i=1}^{n} \vec{x}_i y_i$$

$$\hat{\vec{w}} \leftarrow A^{-1} \vec{b}$$

returned $\hat{f}(\vec{x}) = \vec{x}^T \hat{\vec{w}}$

Ex: $d=1$, $\mathcal{X} = \mathbb{R}^{1+1} = \mathbb{R}^2$, $\mathcal{Y} = \mathbb{R}$, $\hat{\vec{w}} = (\hat{w}_0, \hat{w}_1)^T$

$$\mathcal{D} = ((\vec{x}_1, y_1), \dots, (\vec{x}_n, y_1))$$



$$\hat{f}(\vec{x}) = \vec{x}^T \hat{\vec{w}}$$
$$= x_0 \hat{w}_0 + x_1 \hat{w}_1$$
$$= \hat{w}_0 + x_1 \hat{w}_1$$