Math 390.4 Lec 6 2/20/18

Null model Alg.
$\mathcal{H} = \{0,1\}$
$g = \mathcal{A}(\mathbb{D}, \mathcal{H}) = \text{Mode}[\vec{y}]$

most likely category $\in \{0,1\}$
$\vec{x}$'s don't matter in null model

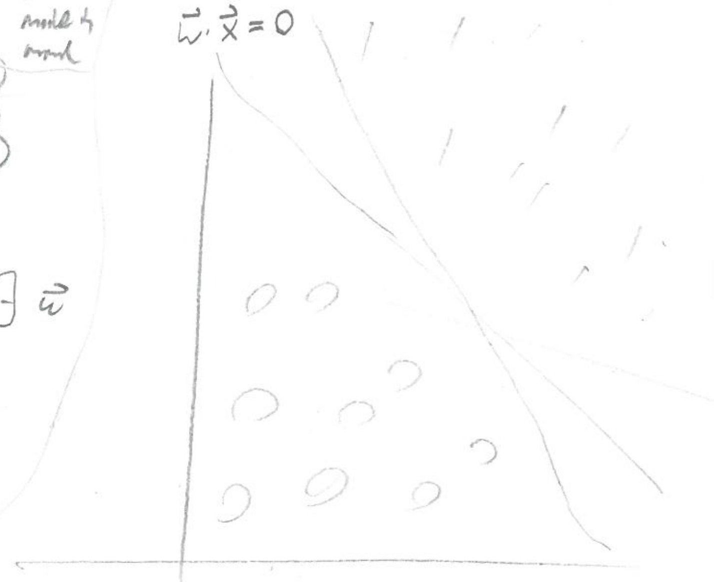
Always keep Null model in mind

Let's return to

$$\mathcal{H} = \{ \mathbb{1}_{\vec{w} \cdot \vec{x} > 0} : \vec{w} \in \mathbb{R}^{p+1} \}$$

$\vec{x}$ includes a 1

Assume "linearly separable" i.e. $\exists \vec{w}$ s.t. there would be no errors if g were used on obs's in $\mathbb{D}$.

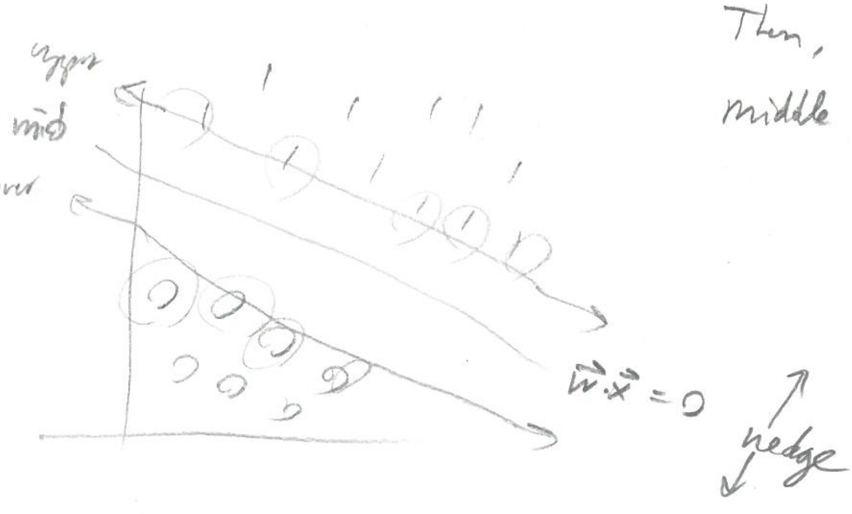


Consider a
New $\mathcal{A}$, different from perceptron learning algorithm.

Which hyperplane (i.e. $\vec{w}$) is best?

Why not create a wedge, large as possible using parallel hyperplanes.

Then, g is built from the $\vec{w}$ in the middle of this wedge.



The "max-margin hyperplane" (proven to be optimal linear classifier in 1990)

Which data pts most matter? Since data pts $\vec{x}_i$ are "vectors", these are called the "support vectors". The middleline model is then called the "support vector machine"

weird name ... if I were naming this now...

"support vector" $\Rightarrow$ "essential observation"
"machine" $\Rightarrow$ "model" + "separation"

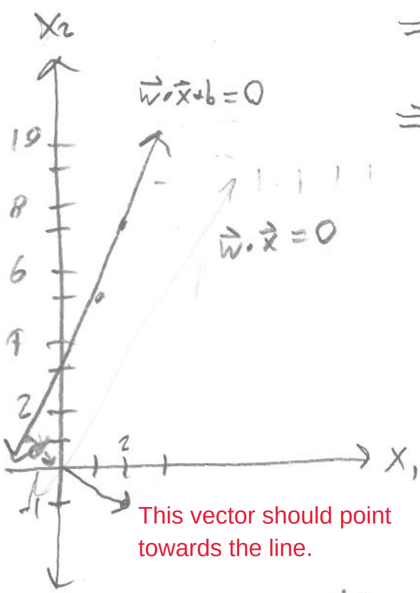
How to fit this?

Unfortunately, it is convenient to revert back to the ugly slope-intercept form,

$$\mathcal{H} = \left\{ \mathbb{1}_{\vec{w}\cdot\vec{x}+b>0} : \vec{w}\in\mathbb{R}^p, b\in\mathbb{R} \right\}$$

this is equivalent to before, it's just a slight reparameterization...

Let's first review 8th grade math.. Imagine the line $x_2 = 2x_1 + 3$



$$\Rightarrow 2x_1 - x_2 + 3 = 0$$

$$\Rightarrow \underbrace{\begin{bmatrix}2\\-1\end{bmatrix}}_{\vec{w}} \cdot \underbrace{\begin{bmatrix}x_1\\x_2\end{bmatrix}}_{\vec{x}} + \underbrace{3}_{b} = 0$$

Hesse Normal Form is wx - b = 0. Then the w vector will point towards the line. So the "b" here should be "-b".

where is $\vec{w}$ on this graph? It's the "normal vector" i.e. perpendicular to the line

If $p > 2$, $\vec{w}\cdot\vec{x}=0$ is a plane/hyperplane and $\vec{w}$ is $\perp$ to it.

Note: $\|\vec{w}\|$ indicates length of the vector $:= \sqrt{\sum_{j=1}^{p} w_j^2}$

And the normalized $\vec{w}$ vector is defined as the vector in same direction with length 1.

$$\vec{w}_0 := \frac{\vec{w}}{\|\vec{w}\|} \qquad \text{Proof: } \|\vec{w}_0\| = \sqrt{\sum_{j=1}^{p}\left(\frac{w_j}{\|\vec{w}\|}\right)^2} = \sqrt{\frac{1}{\|\vec{w}\|^2}\sum_{j=1}^{p} w_j^2} = \sqrt{\frac{1}{\|\vec{w}\|^2}\|\vec{w}\|^2} = 1$$

What is the length of the line $\vec{l} = \alpha \vec{w}_0$ where $\alpha \in \mathbb{R}$, constant?

$$\|\vec{x}\| = \sqrt{\sum_{j=1}^{p}(\alpha w_{0,j})^2} = \sqrt{\alpha^2 \sum_{j=1}^{p} w_{0_j}^2} = \sqrt{\alpha^2 \|\vec{w}_0\|^2} = |\alpha|$$ Makes sense... $\alpha \cdot 1 = 1$!

let $\vec{l}$ be the vector from the origin to the line $\vec{w}\cdot\vec{x}+b=0$, perpendicular to it

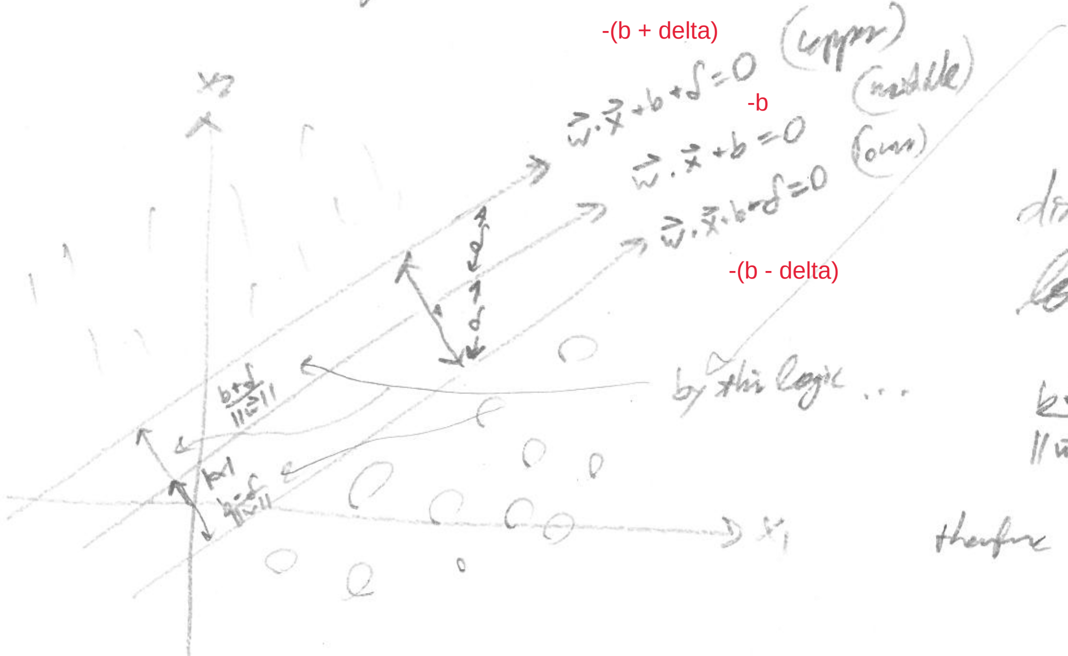
Let's solve for α.. $\vec{l}$ is on the line $\vec{w}\cdot\vec{x}+b=0$ "-b"

$\Rightarrow \vec{w}\cdot\vec{l} + b = 0 \Rightarrow \vec{w}\cdot\alpha\vec{w_0} + b = 0$ "-b"

$\Rightarrow \vec{w}\cdot\alpha\frac{\vec{w}}{\|\vec{w}\|} + b = 0 \Rightarrow \alpha\frac{\|\vec{w}\|^2}{\cancel{\|\vec{w}\|}} + b = 0 \Rightarrow \alpha = +\frac{b}{\|\vec{w}\|}$ No negative sign here.

$\Rightarrow |\alpha| = \frac{b}{\|\vec{w}\|}$

Now back to finding that "best" line:



distance between upper & lower lines is

$$\frac{b+\delta}{\|\vec{w}\|} - \frac{b-\delta}{\|\vec{w}\|} = \frac{2\delta}{\|\vec{w}\|}$$

this is still true now since alpha has correct sign

therefore

Since $c(\vec{w}\cdot\vec{x}+b)=0$, there are infinite solutions since $c\in\mathbb{R}$ (-b)

Coerce $\delta = 1$ ... now there's a unique solution to the equation

$\vec{w}\cdot\vec{x}+b+\delta=0 \Rightarrow \vec{w}\cdot\vec{x}+b+1=0$

-(b + delta) -b

$\Rightarrow$ margin $= \frac{2}{\|\vec{w}\|}$

Constrain all $y=1$'s to be $\geq$ upper; constrain all $y=0$'s to be $\leq$ lower

$\vec{w}\cdot\vec{x} - (b+1) \geq 0 \Rightarrow \vec{w}\cdot\vec{x} - b \geq +1 \Rightarrow \forall i$ s.t. $y_i = 1$ $\vec{w}\cdot\vec{x}_i - b \geq +1$

multiply both sides by $(y_i - \frac{1}{2})$

$(y_i - \frac{1}{2})(\vec{w}\cdot\vec{x}_i + b) \geq (y_i - \frac{1}{2}) \Rightarrow (y_i - \frac{1}{2})(\vec{w}\cdot\vec{x}_i - b) \geq +(1-\frac{1}{2})$ now positive

Now $y_i = 1$

$\Rightarrow (y_i - \frac{1}{2})(\vec{w}\cdot\vec{x}_i - b) \geq +\frac{1}{2}$ now positive

Now $\forall i$ s.t $y_i = 0$ $\quad \vec{w}\cdot\vec{x}_i - (b-1) \geq 0 \Rightarrow \vec{w}\cdot\vec{x}_i - b \geq -1$ now negative

multiply both sides by $(y_i - \frac{1}{2})$

now positive

$(y_i - \frac{1}{2})(\vec{w}\cdot\vec{x}_i + b) \geq -(y_i - \frac{1}{2})$ $\quad$ Now $y_i = 0 \Rightarrow \underbrace{(y_i - \frac{1}{2})(\vec{w}\cdot\vec{x}_i + b) \geq +\frac{1}{2}}$

Same condition for $y \in \{0,1\} \Rightarrow \forall i$ $\quad$ Condition of perfect separability. If the pt on the line, $= +\frac{1}{2}$. If not, $> +\frac{1}{2}$.

Then we solve the following optimization problem:

Maximize $\frac{2}{\|\vec{w}\|} \Rightarrow$ $\boxed{\text{Minimize } \|\vec{w}\| \text{ subj. to. } \forall i \ (y_i - \frac{1}{2})(\vec{w}\cdot\vec{x}_i + b) \geq +\frac{1}{2} \quad \text{over } \vec{w} \in \mathbb{R}^p, b \in \mathbb{R}}$

the $\{\vec{w}, b\}$ solution is the support vector machine

This approach assumes perfect linear separability. In the real world... who has this luxury? We need to "upgrade" $\mathcal{A}$.

We need a loss function. Previously we employed $SAE = \sum_{i=1}^{n} \mathbb{1}_{\hat{y}_i \neq y_i}$ and then allowed the computer to find $\vec{w}$. This is okay but we can do better. We can make the loss dependent on how bad the error is. Consider the following for the i^{th} obs:

$$H_i := \max\left\{0, +\frac{1}{2} - (y_i - \frac{1}{2})(\vec{w}\cdot\vec{x}_i - b)\right\}$$ termed "hinge loss"

Let's see why this makes sense...

Imagine the pt is correctly classified and thus it respects the inequality. Consider it is above the inequality by $d \geq 0$.

$$\Rightarrow \left(y_i - \tfrac{1}{2}\right)\left(\vec{w} \cdot \vec{x}_i + b\right) = +\tfrac{1}{2} + d \geq +\tfrac{1}{2}$$ correct!

$$\Rightarrow H_i = \max\left\{0, +\tfrac{1}{2} - \left(+\tfrac{1}{2} + d\right)\right\} = \max\{0, -d\} = 0$$

makes sense .. if it is correctly classified then there should be zero error

Imagine the pt. is incorrectly classified and hence does not respect the inequality. Let's say its below by $d > 0$.

$$\Rightarrow \left(y_i - \tfrac{1}{2}\right)\left(\vec{w} \cdot \vec{x}_i - b\right) = +\tfrac{1}{2} - d < +\tfrac{1}{2}$$ incorrect!

$$\Rightarrow H_i = \max\left\{0, +\tfrac{1}{2} - \left(+\tfrac{1}{2} - d\right)\right\} = \max\{0, d\} = d > 0$$

makes sense .. you make a mistake, the worse it is, the more you pay.

minimize;

$$SHE = \sum_{i=1}^{n} \max\left\{0, +\tfrac{1}{2} - \left(y_i - \tfrac{1}{2}\right)\left(\vec{w} \cdot \vec{x}_i - b\right)\right\}$$

One more wrinkle... Recall we were trying to maximize the margin $|\alpha| = \frac{1}{\|\vec{w}\|}$ i.e. minimize $\|w\|$. You can't minimize two things! You need one objective function / loss function. Here is Vapnik's (1963) idea: Minimize:

$$\underbrace{\frac{1}{n} \sum \max\left\{0, +\tfrac{1}{2} - \left(y_i - \tfrac{1}{2}\right)\left(\vec{w} \cdot \vec{x}_i - b\right)\right\}}_{\text{min. avg. hinge loss}} + \underbrace{\lambda \|\vec{w}\|^2}_{\text{max. margin}}$$

tradeoff between these two goals.

What are the params? $\vec{w} \in \mathbb{R}^p$, $b \in \mathbb{R}$. Still $p+1$ parameters.

What is λ? A predefined constant called a "hyperparameter."

$g = \mathcal{A}(\mathbb{D}, \mathcal{H}, \lambda, \ldots)$

It is considered a tuning knob on the $\mathcal{A}$ itself. It is a new idea. Recall $g(\vec{x}) = \mathbb{1}\, \vec{w} \cdot \vec{x} + b$ there is no λ here!

Perceptron's max iter could be a λ.

λ only affects which $g \in \mathcal{H}$ will be selected.

We will discuss how the value of hyperparameters are selected later in the course. For now, what does λ do?

- If $\lambda \approx 0$, we only care about errors and not a max. margin. One error far away can ruin our nice separation line.
- If $\lambda \approx \infty$, we only care about the best line of separation and not about errors... this makes no sense! I can just make $\|\vec{w}\| \to 0$

Considering λ is picked "reasonably". How do we solve for $\{\vec{w}, b\}$ our params? Use modern numerical optimization methods:

- quadratic programming
- sub-gradient descent
- coordinate descent

which we will likely not study. Lucky for us, R packages already implement this for us.