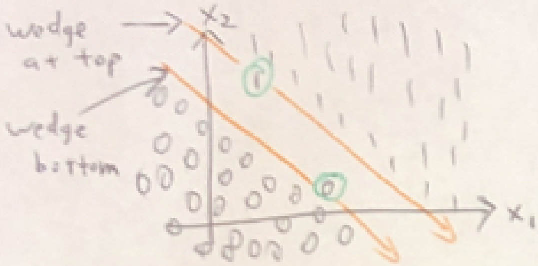
Lecture 5   2/10/21

$$\mathcal{Y} = \{0,1\},\quad p+1=3,\quad \mathcal{H} = \{ \mathbb{1}_{\vec{w}\cdot\vec{x} \geq 0} : \vec{w} \in \mathbb{R}^3 \}$$

Assume the data is linearly separable so it looks like:



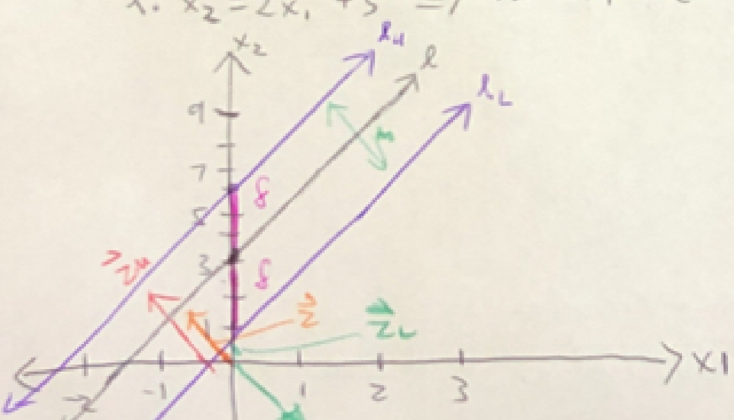
We need an algorithm that locates the middle of that wedge. Let the top of the wedge be the linearly separable model "closest" to the $y=1$'s and the bottom of the wedge be the linearly separable model "closest" to the $y=0$'s. The "max margin hyperplane" is the parallel line in the center of the top and bottom.

Note: there are two critical observations (the ~~critical~~ circled points). Since observations are x-vectors, these critical observations are called "support vectors" and hence the final model is called a "support vector machine" (SVM). "Machine" is a fancy word meaning "complex model." So "machine learning" just means "learning complex models." To find the SVM...

First rewrite $\mathcal{H} = \{ \mathbb{1}_{\vec{w}\cdot\vec{x} - b \geq 0} : \vec{w} \in \mathbb{R}^p, b \in \mathbb{R} \}$

Note $\underbrace{\vec{w}\cdot\vec{w} - b = 0}_{\text{Hesse Normal Form}}$ defines a line / hyperplane

$$\ell: x_2 = 2x_1 + 3 \implies \ell: 2x_1 - x_2 + 3 = 0 \to \ell: \overbrace{\begin{bmatrix} 2 \\ -1 \end{bmatrix}}^{\vec{w}} \cdot \vec{x} - \overbrace{(-3)}^{b} = 0$$



The w vector is perpendicular to line ℓ and called the "normal vector."

Let $\vec{w}_0 := \dfrac{\vec{w}}{\|\vec{w}\|}$

The direction of the w vector with unit length.

Let $m>0$ be the perpendicular distance between ℓ_u and ℓ_L and Let $\delta>0$ be the distance between ℓ_u and ℓ (and ℓ_L and ℓ) on the x_2 axis.

$\vec{z}=\alpha\vec{w}_0$, $\vec{z}\in\ell$

$\vec{w}\cdot\vec{z}-b=0$

$\vec{w}\cdot(\alpha\vec{w}_0)-b=0 \Rightarrow \frac{\alpha}{\|\vec{w}\|}\|\vec{w}\|^2-b=0$

$\Rightarrow \alpha=\frac{b}{\|\vec{w}\|} \Rightarrow \vec{z}=\frac{b}{\|\vec{w}\|}\vec{w}_0$

$\ell_u: \vec{w}\cdot\vec{x}-(b+\delta)=0$, $\vec{z}_u=\frac{b+\delta}{\|\vec{w}\|}\vec{w}_0$

$\ell_L: \vec{w}\cdot\vec{x}-(b-\delta)=0$, $\vec{z}_L=\frac{b-\delta}{\|\vec{w}\|}\vec{w}_0$

$$m=\|\vec{z}_u-z_L\|=\left\|\frac{b+\delta}{\|\vec{w}\|}\vec{w}_0-\frac{b-\delta}{\|\vec{w}\|}\vec{w}_0\right\|=\frac{1}{\|\vec{w}\|}2\delta\|\vec{w}_0\|=\frac{2\delta}{\|\vec{w}\|}$$

Goal is to make m as large as possible (maximum margin) $\Leftrightarrow$ making the w vector as small as possible.

The Hesse Normal form is not unique. There are infinite equivalent specification of a line:

$$\forall c\neq 0 \quad c(\vec{w}\cdot\vec{x}-b)=0. \quad \text{Let } c=\frac{1}{\delta}$$

$$\Downarrow$$

$$m=\frac{2}{\|\vec{w}\|}$$

Now we need 2 conditions

(I) All $y=1$'s are above or equal to ℓ_u:

$\forall_i$ such that $y_i=1$ $\quad \vec{w}\cdot\vec{x}_i-(b+1)\geq 0 \Rightarrow \vec{w}\cdot\vec{x}_i-b\geq 1$

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

$$\Downarrow$$

$$(y_i-\tfrac{1}{2})(\vec{w}\cdot\vec{x}_i-b)\geq\tfrac{1}{2}$$

(II) All $y=0$'s are below or equal to ℓ_L:

$\forall_i$ such that $y_i=0$ $\quad \vec{w}\cdot\vec{x}_i-(b-1)\leq 0 \Rightarrow \vec{w}\cdot\vec{x}_i-b\leq -1$

$\Rightarrow \frac{1}{2}(\vec{w}\cdot\vec{x}_i-b)\leq-\frac{1}{2}$

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

$$\Downarrow$$

$$(y_i-\tfrac{1}{2})(\vec{w}\cdot\vec{x}_i-b)\geq\tfrac{1}{2}$$

Note how both inequalities are the same for both I and II. Thus this inequality satisfies both constraints. So all observations will be in their right places.

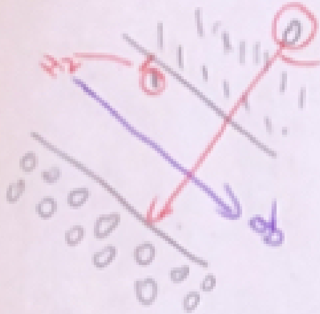
$\forall_i \; (y_i - \frac{1}{2})(\vec{w} \cdot \vec{x}_i - b) \geq \frac{1}{2} \Rightarrow$ line is linearly separable

You compute the SVM by optimizing the following problem:

$\min \|\vec{w}\|$ such that $\forall$ is true, and return resulting w vector and b. There is no analytical solution. You need optimization algorithms. It can be solved with quadratic programming and other procedures as well.

Note: everything we did above generalizes to $p > 2$. Note: most textbooks have 1's in the place of our $\frac{1}{2}$'s that's because they assumed $y = \{-1, 1\}$ but we assumed binary.

What if the data is not linearly separable? You can never satisfy that constraint... So this whole thing doesn't work.



We will use a new objective function / loss function / error-tallying function called "hinge loss," H:

$$H_i := \max\{0, \tfrac{1}{2} - \underbrace{(y_i - \tfrac{1}{2})(\vec{w} \cdot \vec{x}_i - b)}_{\text{should be } \geq \frac{1}{2}}\}$$

Let's say a point is d away from where it should be.

$$(y_i - \tfrac{1}{2})(\vec{w} \cdot \vec{x}_i - b) = \tfrac{1}{2} - d$$

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

With this loss function, it is clear we wish to minimize the sum of the hinge errors:

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

But we also want to maximize the margin. So we combine both considerations together into the objective function of Vapnik (1963):

$$\underset{\vec{w}, b}{\operatorname{argmin}} \{ \underbrace{\tfrac{1}{n} SHE}_{\text{minimizing distance errors}} + \lambda \underbrace{\|\vec{w}\|^2}_{\text{maximizing the width of the wedge}} \}$$

Once λ is set, the computer can do the optimization to find the resulting SVM even using out of the box R packages.

What is λ? It is a positive "hyperparameter," "tuning parameter." It is set by you! It controls the tradeoff between these two considerations.

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

What if you have the modeling setting where $\mathcal{Y} = \{1, 2, \ldots, L\}$, a normal categorical response with $L > 2$ levels. The model will still be a "classification model" but not a "binary classification model" and it's sometimes called a "multinomial classification model." What is the null model g_0? Again, $g_0 = \text{Sample Mode}[y]$.

Consider a model that predicts on a new x_* by looking through the training data and finding the "closest" x_i vector and returning its y_i as the predicted response value. This is called a "nearest neighbor" model. Further, you may also want to find the K closest observations and return the mode of these K observations as the predicted response value (randomize ties). That's called "K nearest neighbors" (KNN) model where K is a natural number hyperparameter. There is another hyperparameter that must be specified, the "distance function" $d : \mathcal{X}^2 \to \mathbb{R}_{\geq 0}$. The typical distance function is Euclidean distance squared:

$$d(\vec{x}_*, \vec{x}_i) := \sum_{j=1}^{p} (x_{i,j} - x_{*,j})^2$$

What is $\mathcal{H}$? $\mathcal{A}$?