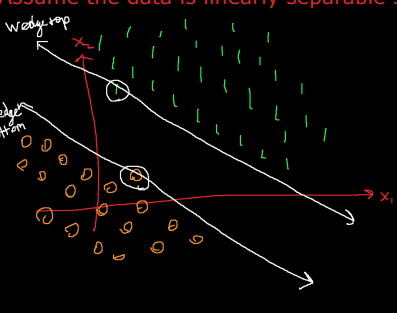
$y = \{0,1\}$, $p+1 = 3$, $\mathcal{H} = \{\mathbb{1}_{\vec{w}\cdot\vec{x}\geq 0} : \vec{w}\in\mathbb{R}^3\}$

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.

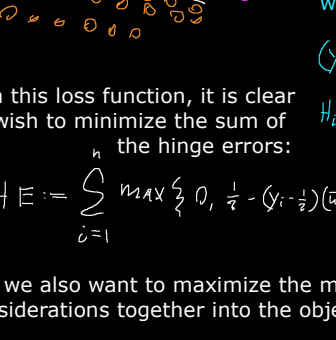
Note: there are two critical observations (the circled points). Since observations are x-vectors, these critical observations are called "support vectors" and hence the final model is called a "support vector machine" (SVM). "Machine" is a fancy word meaning "complex model". So "machine learning" just 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 $\vec{w}\cdot\vec{x}-b=0$ defines a line / hyperplane.

Hesse Normal Form

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



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

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

The direction of the w vector with unit length.

Let m > 0 be the perpendicular distance between l_U and l_L and let δ > 0 be the distance between l_U and l (and l_L and l) on the x_2 axis.

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

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

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

$l_U: \vec{w}\cdot\vec{x}-(b+\delta)=0,\ \vec{z}_U = \frac{b+\delta}{\|\vec{w}\|}\vec{w}_0 \Rightarrow \alpha = \frac{b}{\|\vec{w}\|} \Rightarrow \vec{z} = \frac{b}{\|\vec{w}\|}\vec{w}_0$

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

$\Downarrow$

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

Goal is to make m as large as possible (maximum margin) <=> making the w vector as small as possible.

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

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

$\Downarrow$

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

Now we need two conditions
(I) All y=1's are above or equal to l_U:

$\forall i \text{ s.t. } y_i=1 \quad \vec{w}\cdot\vec{x}_i-(b+1)\geq 0 \Rightarrow \vec{w}\cdot\vec{x}_i-b\geq 1 \Rightarrow \frac{1}{2}(\vec{w}\cdot\vec{x}_i-b)\geq\frac{1}{2}$

$\Downarrow$

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

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

$\forall i \text{ s.t. } y_i=0 \quad \vec{w}\cdot\vec{x}_i-(b-1)\leq 0 \Rightarrow \vec{w}\cdot\vec{x}_i-b\leq -1 \Rightarrow \frac{1}{2}(\vec{w}\cdot\vec{x}_i-b)\leq -\frac{1}{2}$

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

$\Downarrow$

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

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

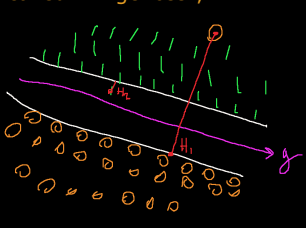
You compute the SVM by optimizing the following problem:

$\min \|\vec{w}\| \text{ s.t. } \leftarrow$ is true

and return the 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 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:



Should be $\geq\frac{1}{2}$

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

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

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

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

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

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

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

$\underset{\vec{w},b}{\text{argmin}} \left\{\frac{1}{n}SHE + \lambda\|\vec{w}\|^2\right\}$

minimizing distance errors

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 positve "hyperparameter", "tuning parameter". It is set by you! It controls the tradeoff between these two considerations.

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

What if you have the modeling setting where $y = \{1,2,...,L\}$, a nominal 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 = SampleMode[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 $\mathcal{H}$? A?