CPSC 340: Machine Learning and Data Mining

Linear Classifiers

Last Time: L1-Regularization

- We discussed L1-regularization:

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_1$$

  - Also known as "LASSO" and "basis pursuit denoising".
  - Regularizes 'w' so we decrease our test error (like L2-regularization).
  - Yields sparse 'w' so it selects features (like L0-regularization).
- Properties:
  - It's convex and fast to minimize (with "proximal-gradient" methods).
  - Solution is not unique (sometimes people do L2- and L1-regularization).
  - Usually includes "correct" variables but tends to yield false positives.

L1-loss vs. L1-regularization

- Don't confuse the L1 loss with L1-regularization!
  - L1-loss is robust to outlier data points.
    - You can use this instead of removing outliers.
  - L1-regularization is robust to irrelevant features.
    - You can use this instead of removing features.
- And note that you can be robust to outliers and irrelevant features:

$$f(w) = \underbrace{\|Xw - y\|_1}_{L_1\text{-loss}} + \underbrace{\lambda\|w\|_1}_{L_1\text{-regularizer}}$$

- Can we smooth and use "Huber regularization"?
  - Huber regularizer is still robust to irrelevant features.
  - But it's the non-smoothness that sets weights to exactly 0.

L*-Regularization

- L0-regularization (AIC, BIC, Mallow's Cp, Adjusted R^2, ANOVA):
  - Adds penalty on the number of non-zeros to select features.

$$f(w) = \|Xw - y\|^2 + \lambda \|w\|_0$$

- L2-regularization (ridge regression):
  - Adding penalty on the L2-norm of 'w' to decrease overfitting:

$$f(w) = \|Xw - y\|^2 + \frac{\lambda}{2} \|w\|^2$$

- L1-regularization (LASSO):
  - Adding penalty on the L1-norm decreases overfitting and selects features:

$$f(w) = \|Xw - y\|^2 + \lambda \|w\|_1$$

L0- vs. L1- vs. L2-Regularization

	Sparse 'w' (Selects Features)	Speed	Unique 'w'	Coding Effort	Irrelevant Features
L0-Regularization	Yes	Slow	No	Few lines	Not Sensitive
L1-Regularization	Yes*	Fast*	No	1 line*	Not Sensitive
L2-Regularization	No	Fast	Yes	1 line	A bit sensitive

- L1-Regularization isn't as sparse as L0-regularization.
  - L1-regularization tends to give more false positives (selects too many).
  - And it's only "fast" and "1 line" with specialized solvers.
- Cost of L2-regularized least squares is $O(nd^2 + d^3)$.
  - Changes to $O(ndt)$ for 't' iterations of gradient descent (same for L1).
- "Elastic net" (L1- and L2-regularization) is sparse, fast, and unique.
- Using L0+L2 does not give a unique solution.

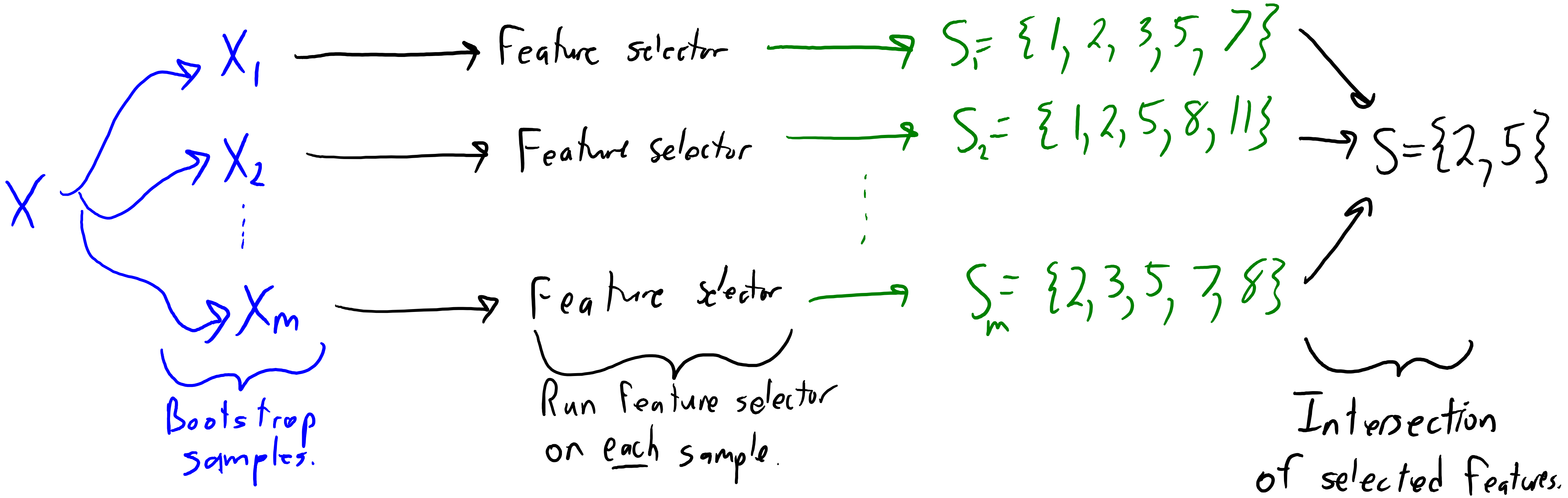
Ensemble Feature Selection

- We can also use ensemble methods for feature selection.
  - Usually designed to reduce false positives or reduce false negatives.

- In this case of L1-regularization, we want to reduce false positives.
  - Unlike L0-regularization, the non-zero w_j are still "shrunk".
    - "Irrelevant" variables can be included before "relevant" w_j reach best value.

- A bootstrap approach to reducing false positives:
  - Apply the method to bootstrap samples of the training data.
  - Only take the features selected in all bootstrap samples.

Ensemble Feature Selection

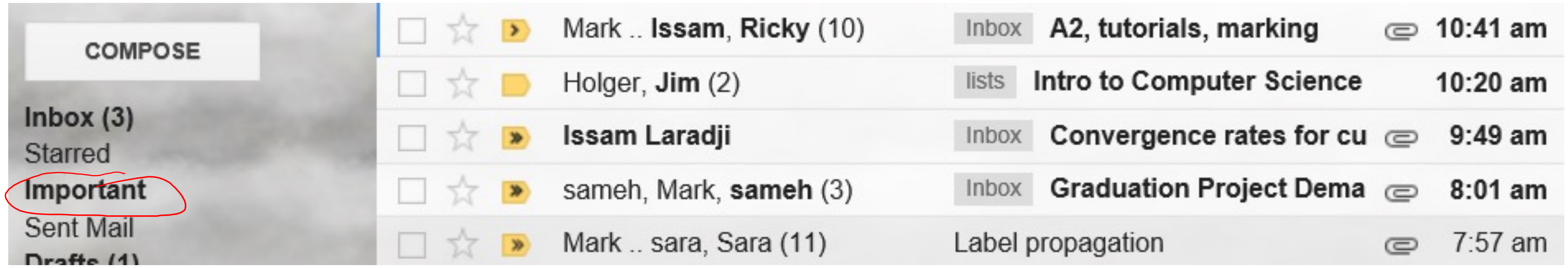

X
X_1
X_2
X_m
Bootstrap samples.
Feature selector
Feature selector
Feature selector
Run feature selector on each sample.
$S_1 = \{1, 2, 3, 5, 7\}$
$S_2 = \{1, 2, 5, 8, 11\}$
$S_m = \{2, 3, 5, 7, 8\}$
$S = \{2, 5\}$
Intersection of selected features.

- Example: bootstrapping plus L1-regularization (“BoLASSO”).
  - Reduces false positives.
  - It’s possible to show it recovers “correct” variables with weaker conditions.
    - Can replace “intersection” with “selected frequency” if has false negatives too.

Next Topic: Linear Classifiers

Motivation: Identifying Important E-mails

- How can we automatically identify 'important' e-mails?



Mark .. Issam, Ricky (10)	Inbox	A2, tutorials, marking	10:41 am
Holger, Jim (2)	lists	Intro to Computer Science	10:20 am
Issam Laradji	Inbox	Convergence rates for cu	9:49 am
sameh, Mark, sameh (3)	Inbox	Graduation Project Dema	8:01 am
Mark .. sara, Sara (11)		Label propagation	7:57 am

- A binary classification problem ("important" vs. "not important").
  - Labels are approximated by whether you took an "action" based on mail.
  - High-dimensional feature set (that we'll discuss later).

- Gmail uses regression for this binary classification problem.

Binary Classification Using Regression?

- Can we apply linear models for binary classification?
  - Set $y_i = +1$ for one class ("important").
  - Set $y_i = -1$ for the other class ("not important").
- At training time, fit a linear regression model:

Define the "output" $o_i = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id}$

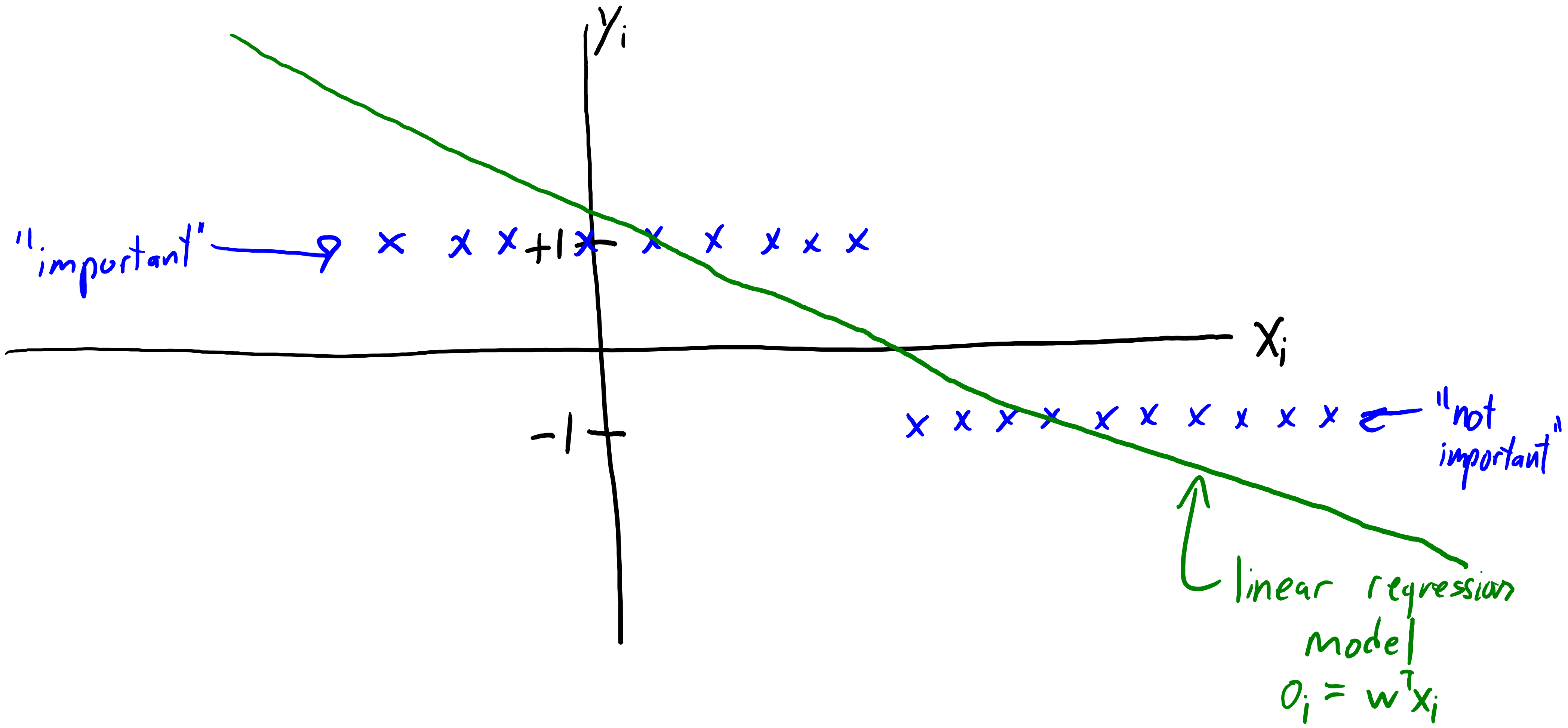
$$= w^T x_i$$

  - And try to minimize squared error between output o_i and labels y_i.
- The model will try to make:
  - Output $o_i = w^T x_i = +1$ for "important" e-mails,
  - Output $o_i = w^T x_i = -1$ for "not important" e-mails.

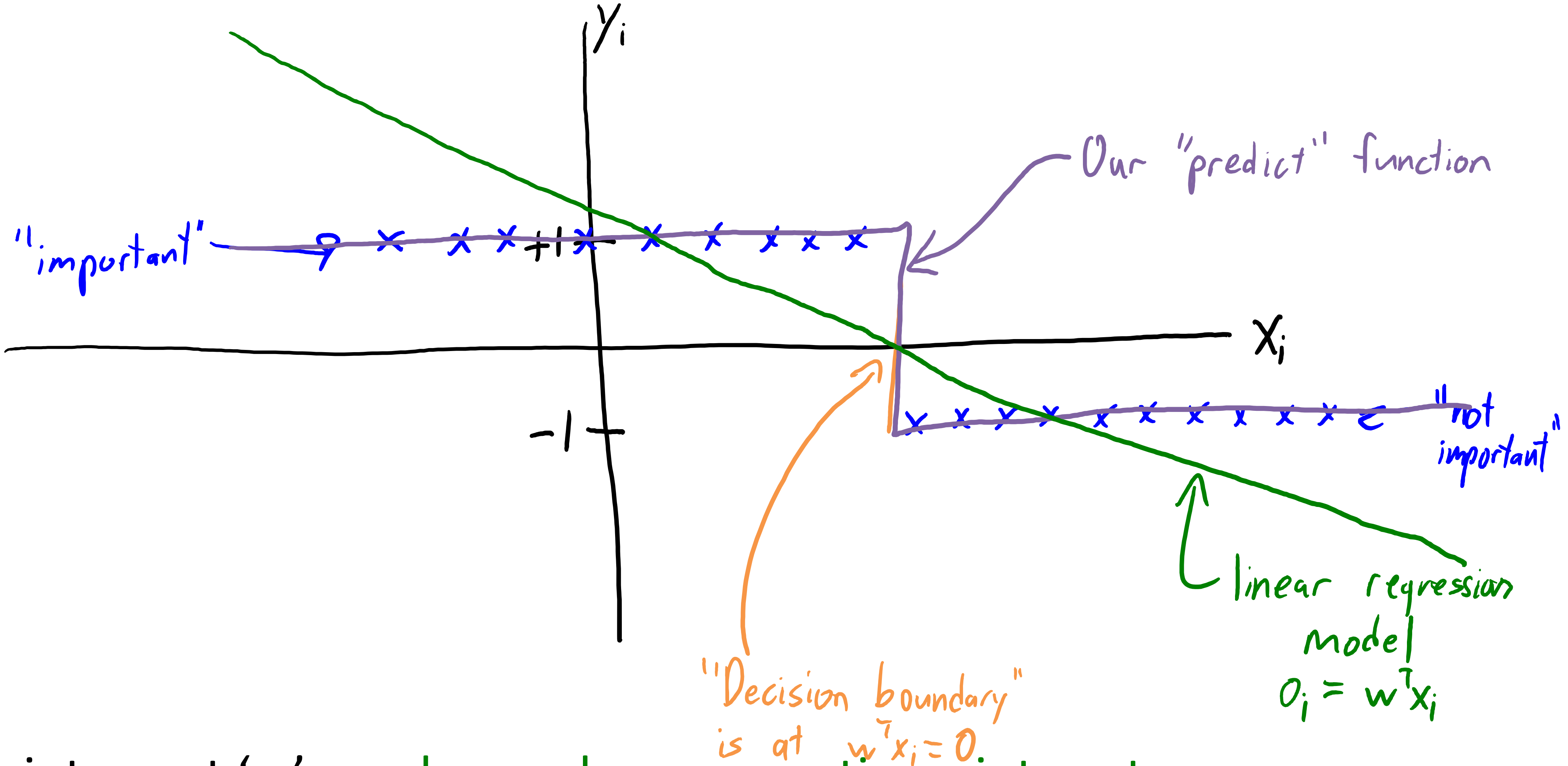
Binary Classification Using Regression?

- Can we apply linear models for binary classification?
  - Set $y_i = +1$ for one class ("important").
  - Set $y_i = -1$ for the other class ("not important").
- Linear model gives real numbers like 0.9, -1.1, and so on.
- So to predict, we look at whether $o_i = w^T x_i$ is closer to +1 or -1.
  - If $o_i = 0.9$, predict $\hat{y}_i = +1$.
  - If $o_i = -1.1$, predict $\hat{y}_i = -1$.
  - If $o_i = 0.1$, predict $\hat{y}_i = +1$.
  - If $o_i = -100$, predict $\hat{y}_i = -1$.
  - We write this operation (rounding to +1 or -1) as $\hat{y}_i = \text{sign}(o_i)$.

Decision Boundary in 1D



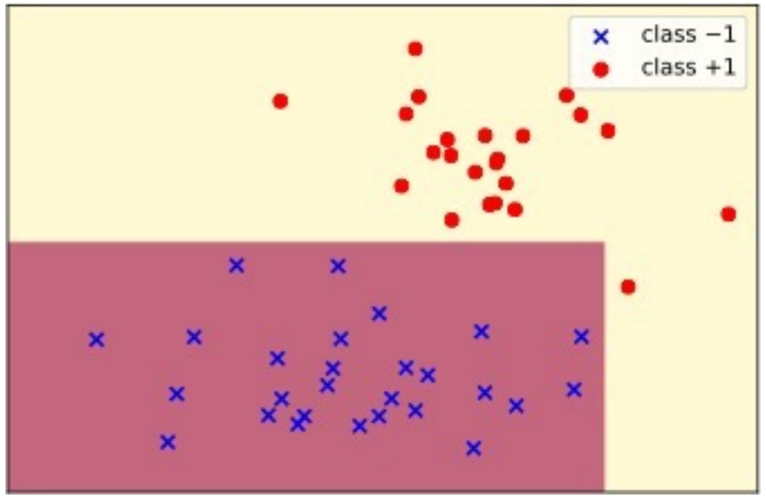
Decision Boundary in 1D


y_i
x_i
+1
-1
"important"
"not important"
Our "predict" function
"Decision boundary" is at $w^Tx_i = 0$
linear regression model $o_i = w^Tx_i$

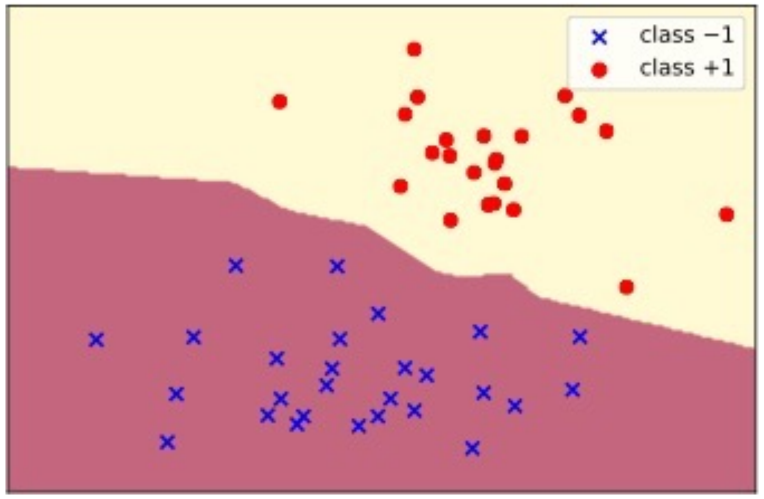
- We can interpret ‘w’ as a hyperplane separating x into sets:
  - Set where $w^Tx_i > 0$ and set where $w^Tx_i < 0$.

Decision Boundary in 2D

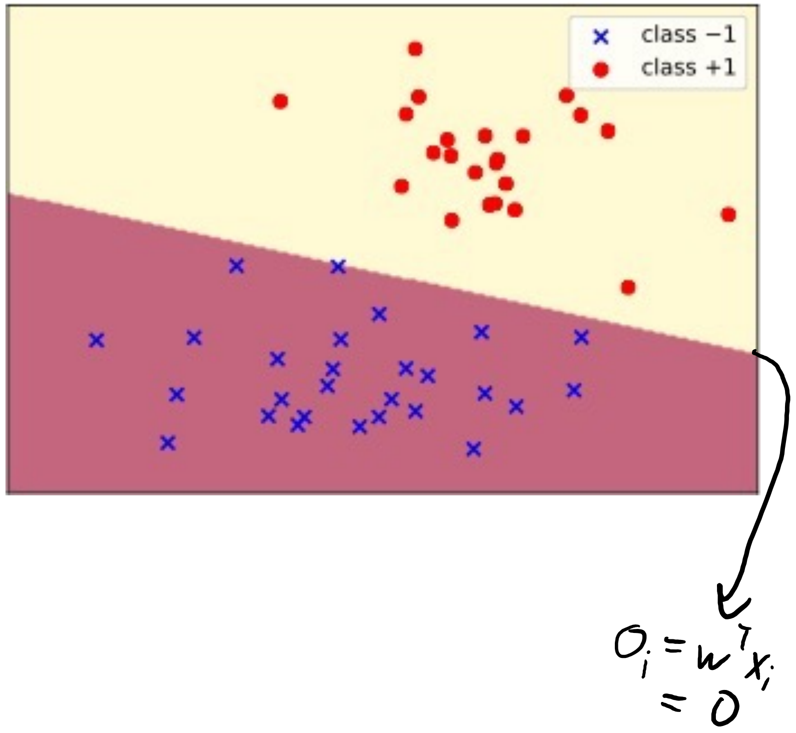
decision tree



KNN



linear classifier



- Linear classifier would be a $o_i = w^T x_i$ function
  - And the boundary is at $o_i = w^T x_i = 0$.

Should we use least squares for classification?

- Consider training by minimizing squared error with y_i that are +1 or -1:

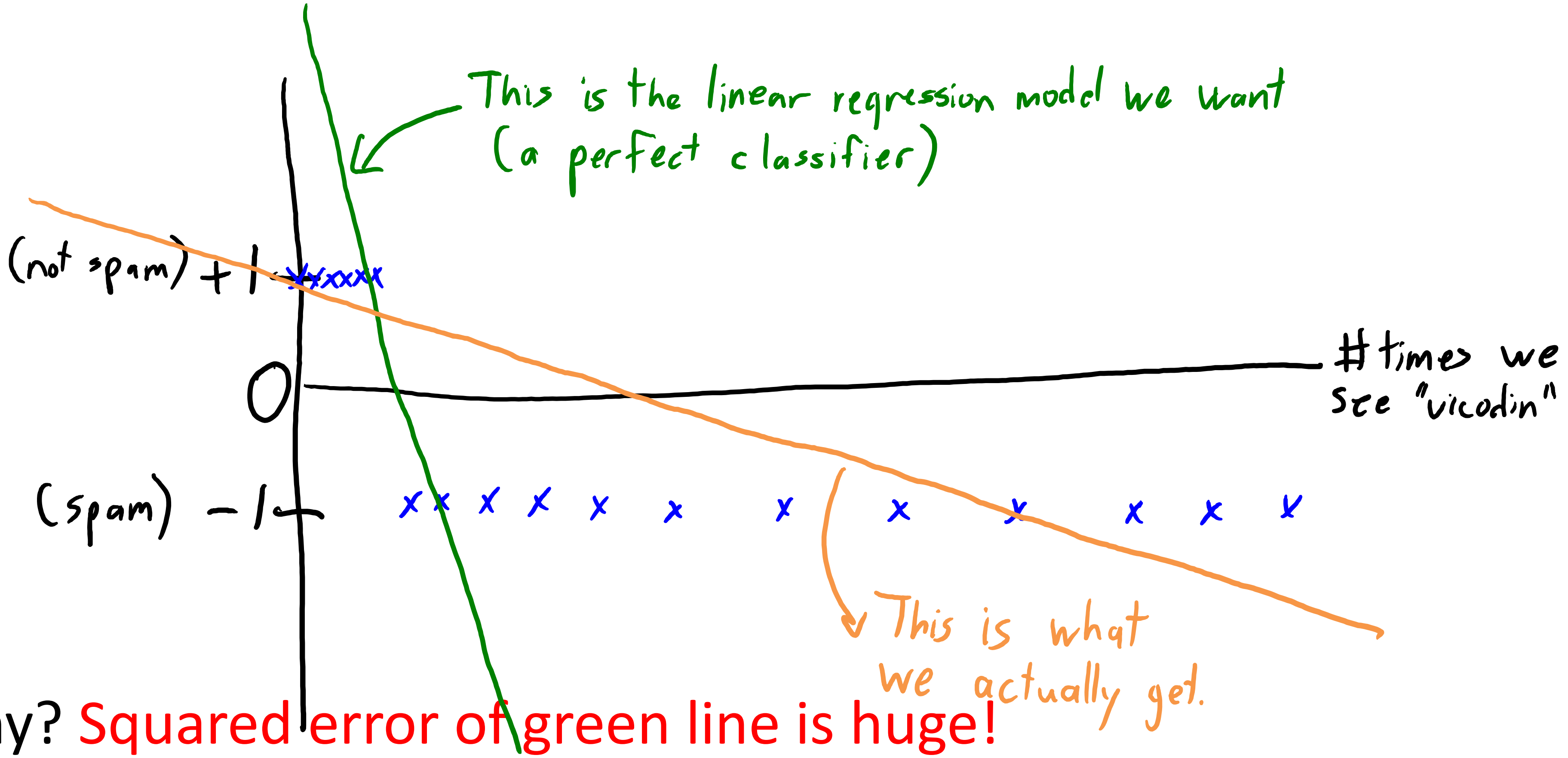
$$f(w) = \frac{1}{2}\|Xw - \underbrace{y}_{}\|^2 \qquad y = \begin{bmatrix}+1\\+1\\-1\\+1\\-1\end{bmatrix}$$

- If we predict $o_i = +0.9$ and $y_i = +1$, error is small: $(0.9 - 1)^2 = 0.01$.
- If we predict $o_i = -0.8$ and $y_i = +1$, error is bigger: $(-0.8 - 1)^2 = 3.24$.
- If we predict $o_i = +100$ and $y_i = +1$, error is huge: $(100 - 1)^2 = 9801$.
  - But it shouldn't be, the prediction is correct.

- Least squares penalized for being "too right".
  - +100 has the right sign, so the error should not be large.

Should we use least squares for classification?

- Least squares can behave weirdly when applied to classification:

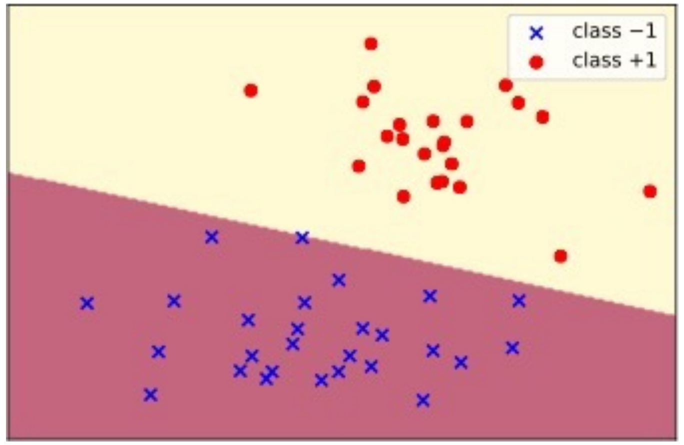


- Why? Squared error of green line is huge!
  - Make sure you understand why the green line achieves 0 training error.

“0-1 Loss” Function: Minimizing Classification Errors

- Could we instead minimize number of classification errors?
  - This is called the 0-1 loss function:
    - You either get the classification wrong (error of 1) or right (error of 0).
  - We can write using the L0-norm as $||\text{sign}(o_i) - y||_0$.
    - Unlike regression, in classification it’s reasonable we exactly match y_i (it’s +1 or -1).

- Important special case: “linearly separable” data.
  - Classes can be “separated” by a hyper-plane.
  - So a perfect linear classifier exists.



Perceptron Algorithm for Linearly-Separable Data

- One of the first "learning" algorithms was the "perceptron" (1957).
  - Searches for a 'w' such that sign(w^Tx_i) = y_i for all i.

- Perceptron algorithm:
  - Start with $w^0 = 0$.
  - Go through examples in any order until you make a mistake predicting y_i.
    - Set $w^{t+1} = w^t + y_ix_i$.
  - Keep going through examples until you make no errors on training data.

- If a perfect classifier exists, this algorithm finds one in finite number of steps.

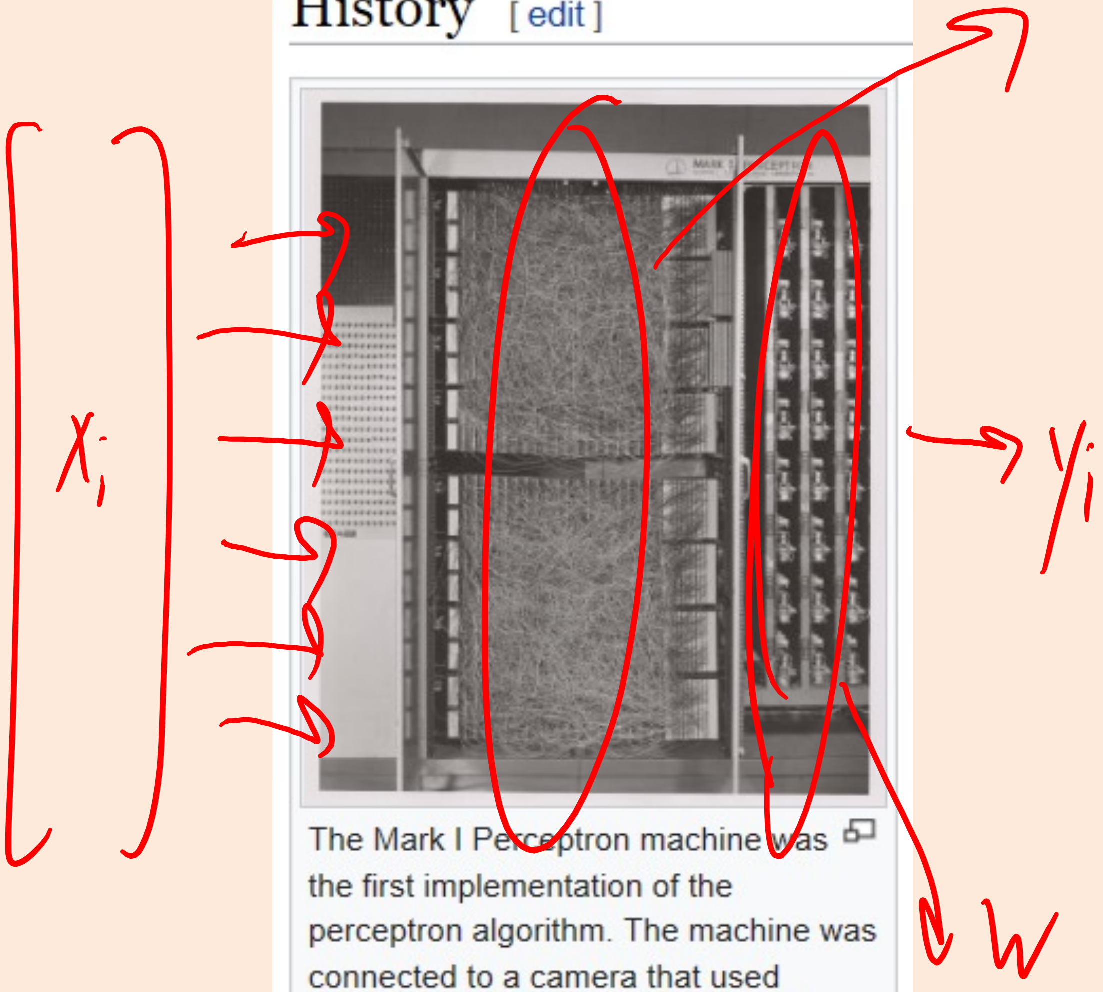
- Intuition:
  - Consider a case where $w^Tx_i < 0$ but $y_i = +1$.
  - In this case the update "adds more of x_i to w" so that w^Tx_i is larger.

$$(w^{t+1})^T x_i = (w^t + x_i)^T x_i = (w^t)^T x_i + x_i^T x_i = (\text{old prediction}) + \|x_i\|^2$$

  - If $y_i = -1$, you would be subtracting the squared norm.

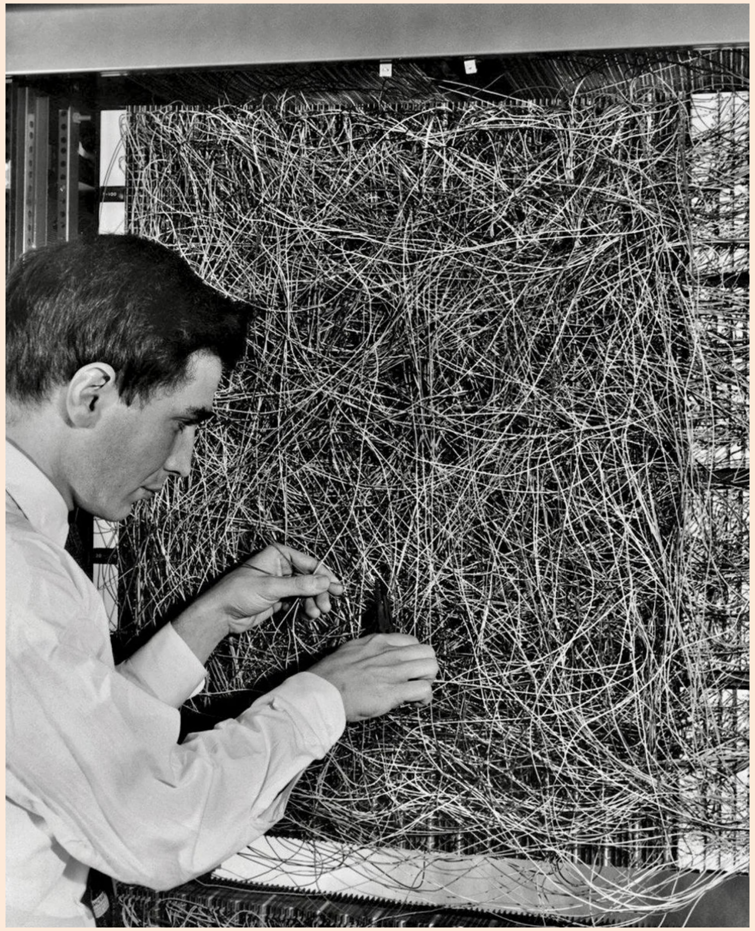
$$z_i = \left(x_1^2 \quad x_1 x_2 \quad x_3 \right)$$

History [edit]



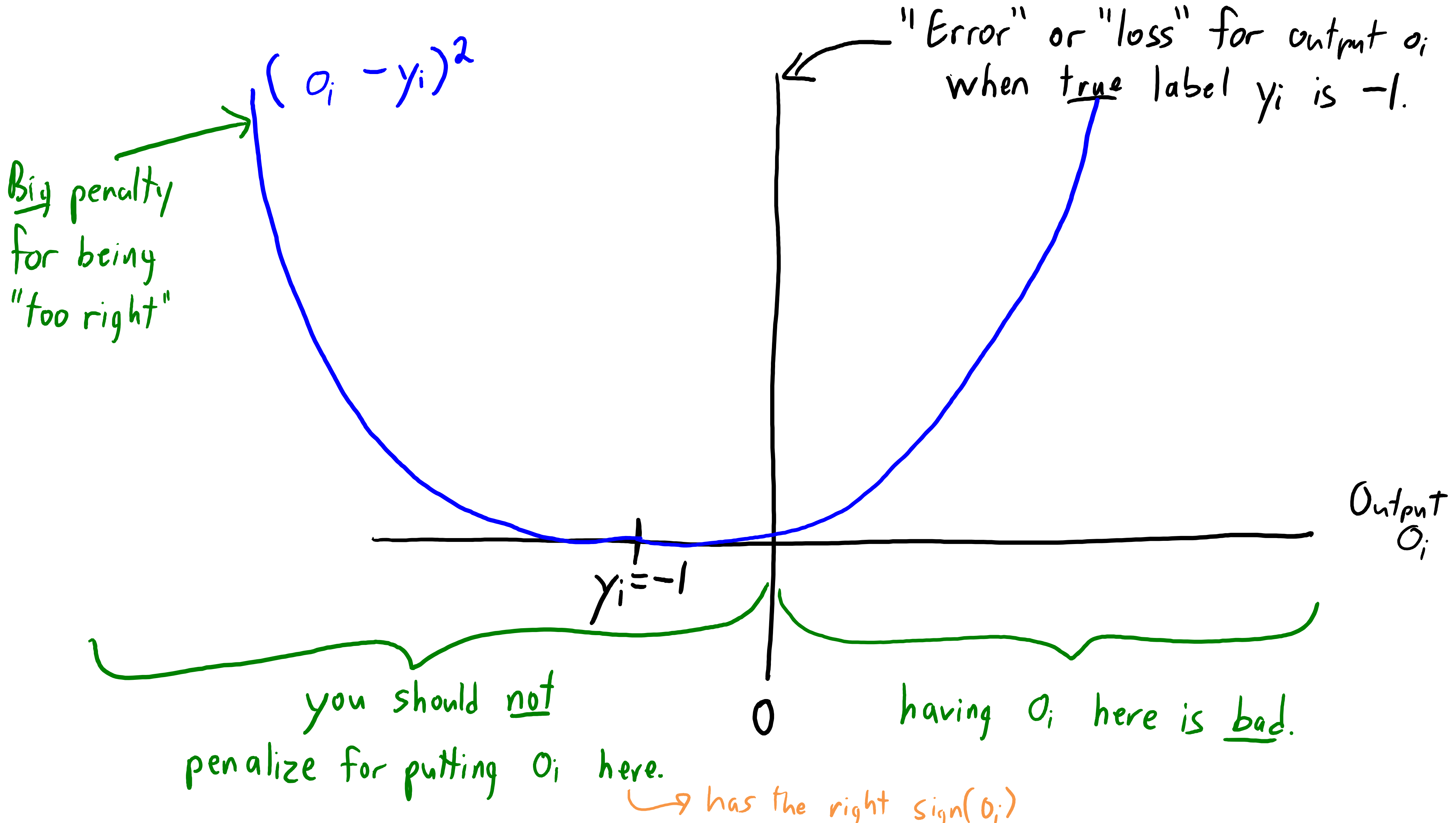
The Mark I Perceptron machine was the first implementation of the perceptron algorithm. The machine was connected to a camera that used 20×20 cadmium sulfide photocells to produce a 400-pixel image. The main visible feature is a patchboard that allowed experimentation with different combinations of input features. To the right of that are arrays of potentiometers that implemented the adaptive weights.[2]:213

Frank Rosenblatt



https://en.wikipedia.org/wiki/Perceptron

Geometry of why we want the 0-1 loss

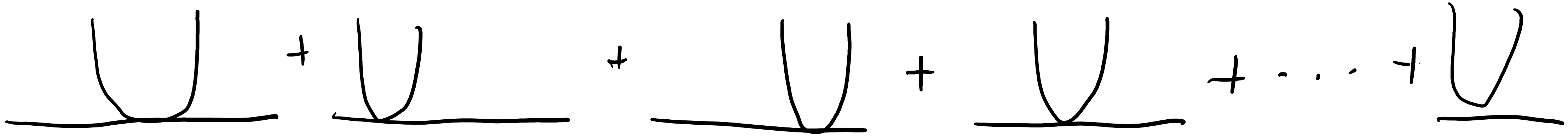

$(o_i - y_i)^2$
"Error" or "loss" for output o_i when true label y_i is -1.
Big penalty for being "too right"
Output o_i
$y_i = -1$
0
you should not penalize for putting o_i here.
has the right sign(o_i)
having o_i here is bad.

Thoughts on the previous (and next) slide

- We are now plotting the loss vs. the output o_i.
  - "Loss space", which is different than parameter space or data space.

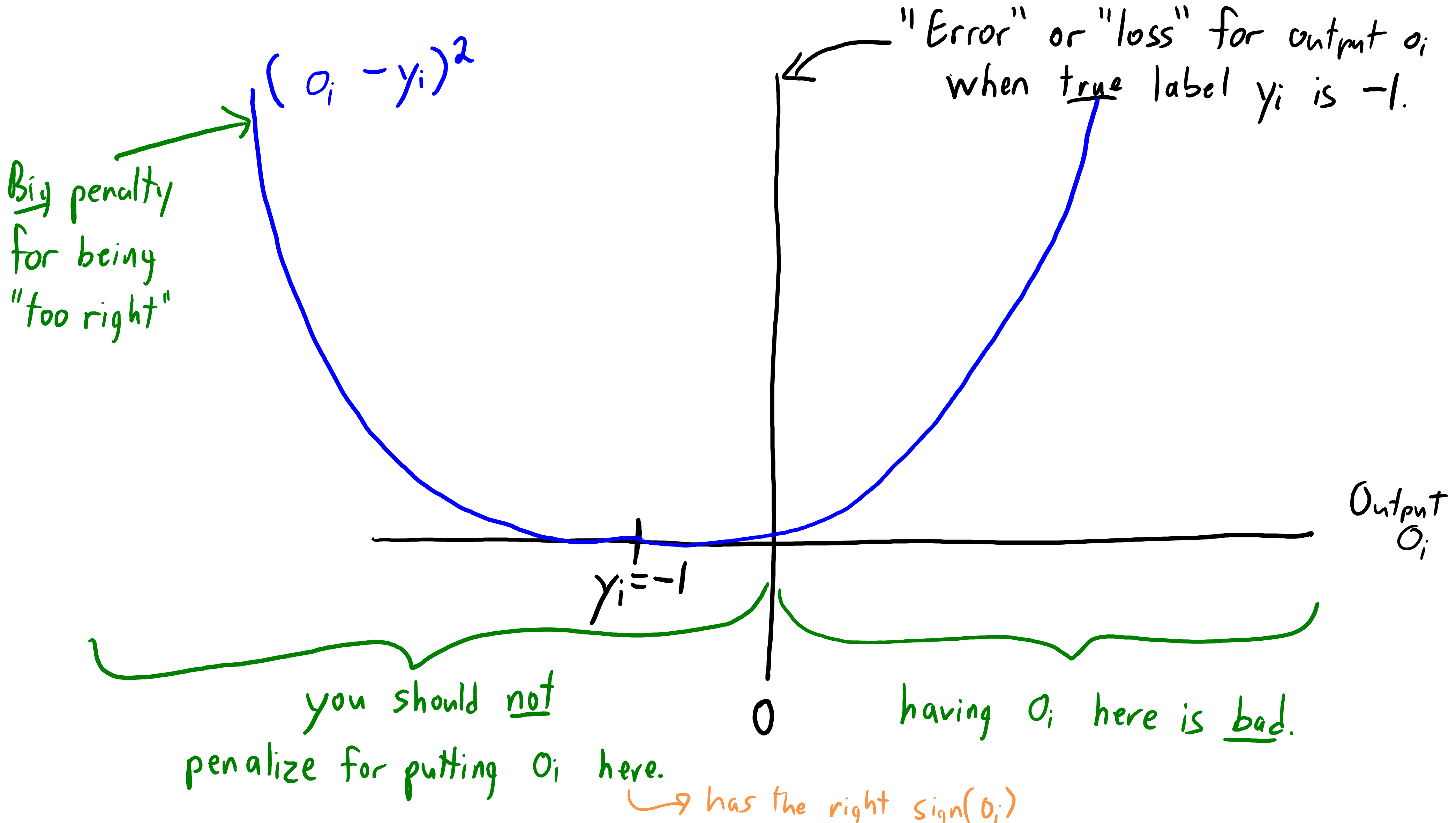
- We're plotting the individual loss for a particular training example.
  - In the figure the label is $y_i = -1$ (so loss is centered at -1).
    - It will be centered at +1 when $y_i = +1$.

  - The objective in least squares regression is a sum of 'n' of these losses:



- (The next slide is the same as the previous one)

Geometry of why we want the 0-1 loss


"Error" or "loss" for output o_i when true label y_i is -1.
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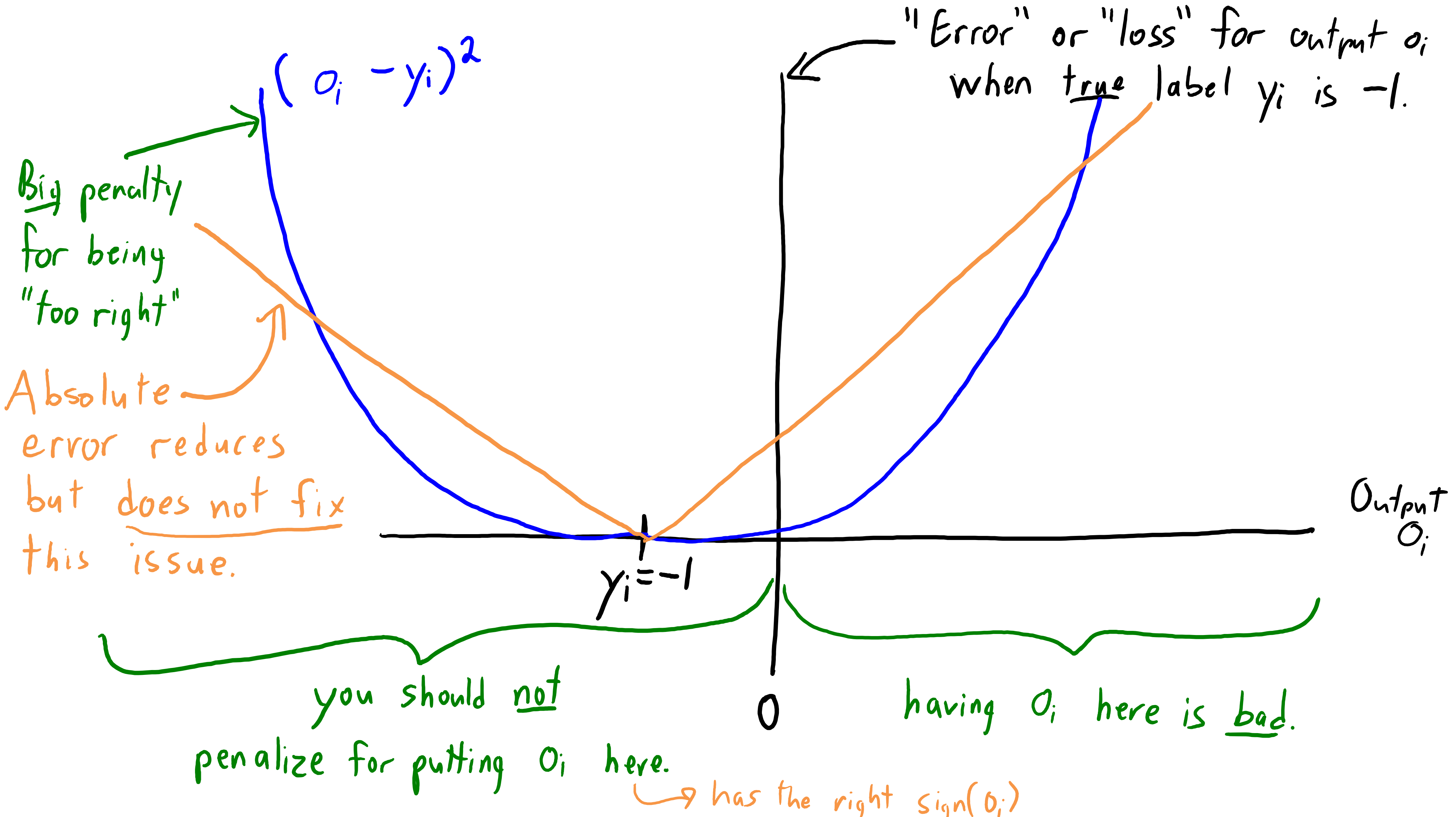
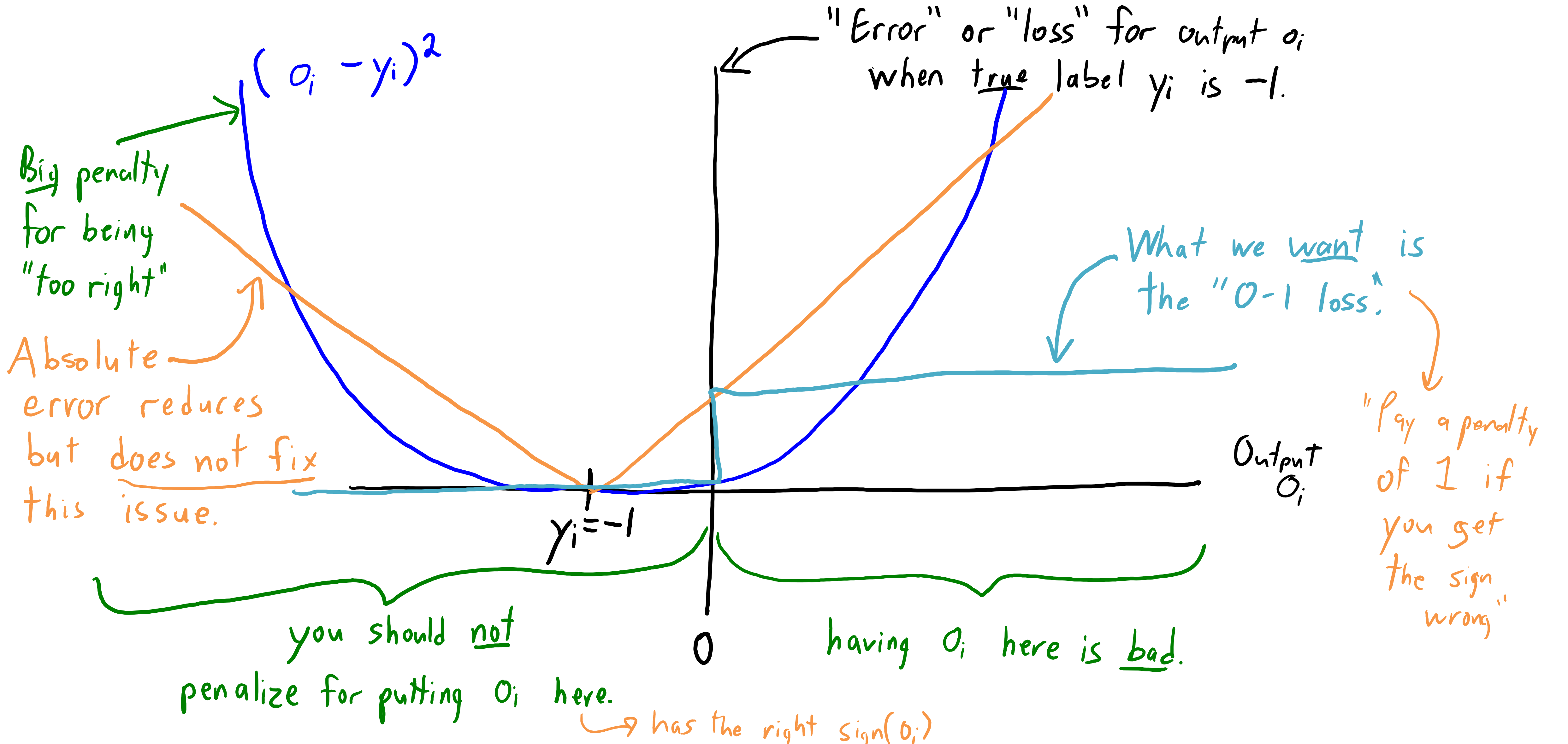
Geometry of why we want the 0-1 loss



Geometry of why we want the 0-1 loss



0-1 Loss Function

- Unfortunately the 0-1 loss is non-convex in ‘w’.
  - It is easy to minimize if a perfect classifier exists (perceptron).
  - Otherwise, finding the ‘w’ minimizing 0-1 loss is a hard problem.
  - Gradient is zero everywhere: don’t even know “which way to go”.
  - NOT the same type of problem we had with using the squared loss.
    - We can minimize the squared error, but it might give a bad model for classification.
- Motivates convex approximations to 0-1 loss.
  - The two most common are the “hinge” loss and the “logistic” loss.

Next Topic: Convex approx. to the 0-1 loss

Degenerate Convex Approximation to 0-1 Loss

- If $y_i = +1$, we get the label right if $o_i > 0$.
- If $y_i = -1$, we get the label right if $o_i < 0$, or equivalently $-o_i > 0$.
- So "classifying 'i' correctly" is equivalent to having $y_i o_i > 0$.

- One possible convex approximation to 0-1 loss:
  - Minimize how much this constraint is violated.

If $y_i o_i > 0$ then you get an "error" of 0.

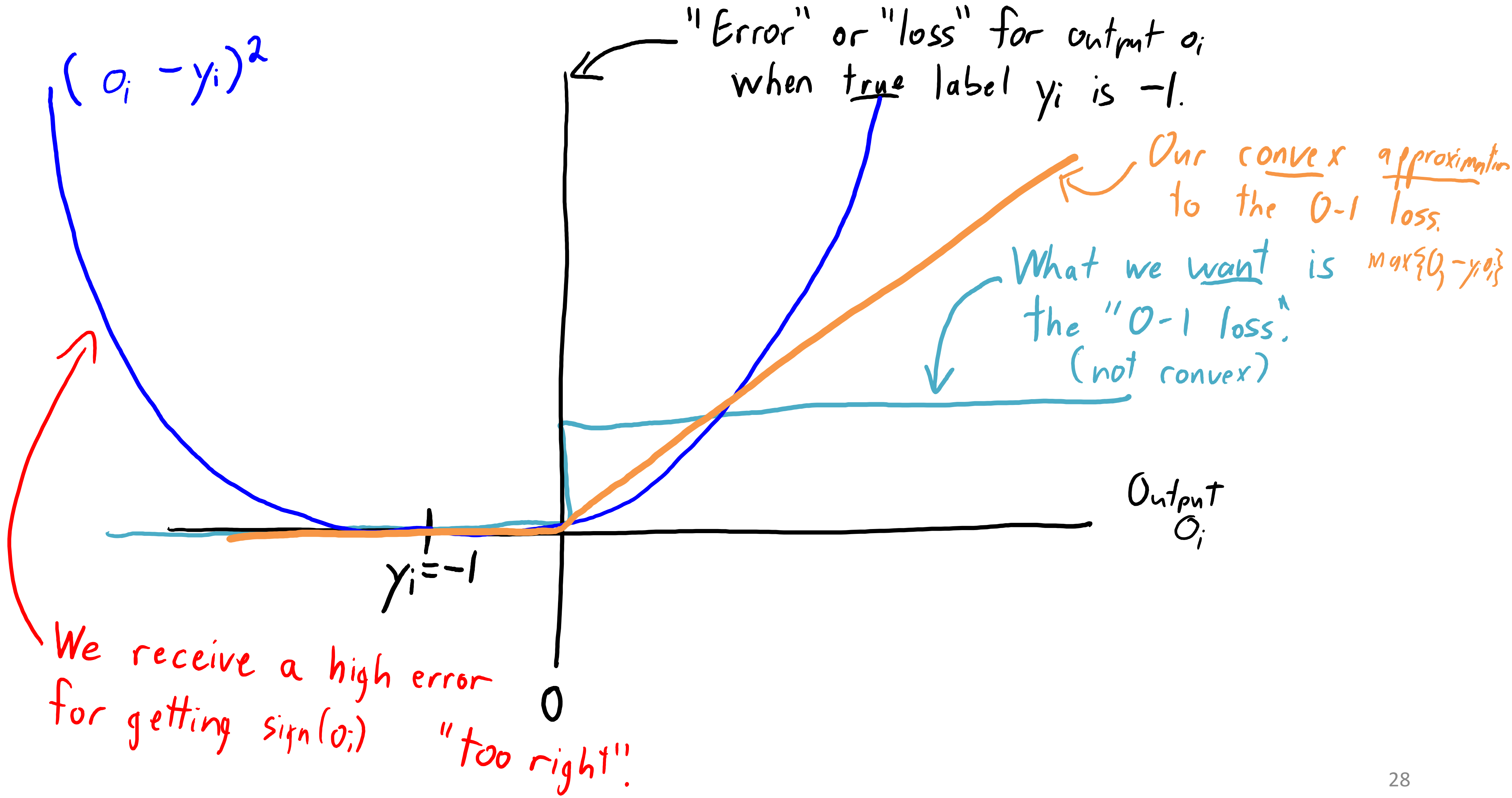
no penalty for correct classification

If $y_i o_i < 0$ then you get an "error" of $-y_i o_i$

penalty based on "how incorrect" o_i is.

$\rightarrow$ So the "error" is given by $\underbrace{\max\{0, -y_i o_i\}}_{\max\{\text{constant}, \text{linear}\} \Rightarrow \text{convex}}$

Hinge Loss: Convex Approximation to 0-1 Loss



Degenerate Convex Approximation to 0-1 Loss

- Our convex approximation of the error for one example is:

$$\max\{0, -y_i \underbrace{w^T x_i}_{\hat{y}_i}\}$$

- We could train by minimizing sum over all examples:

$$f(w) = \sum_{i=1}^{n} \max\{0, -y_i w^T x_i\}$$

- But this has a degenerate solution:
  - We have f(0) = 0, and this is the lowest possible value of ‘f’.
- There are two standard fixes: hinge loss and logistic loss.

Hinge Loss: Convex Approximation to 0-1 Loss

- We saw that we classify examples 'i' correctly if $y_i o_i > 0$.
  - Our convex approximation is the amount this inequality is violated.

- Consider replacing $y_i o_i > 0$ with $y_i o_i \geq 1$.

  (the "1" is arbitrary: we could make ||w|| bigger/smaller to use any positive constant)

- The violation of this constraint is now given by:

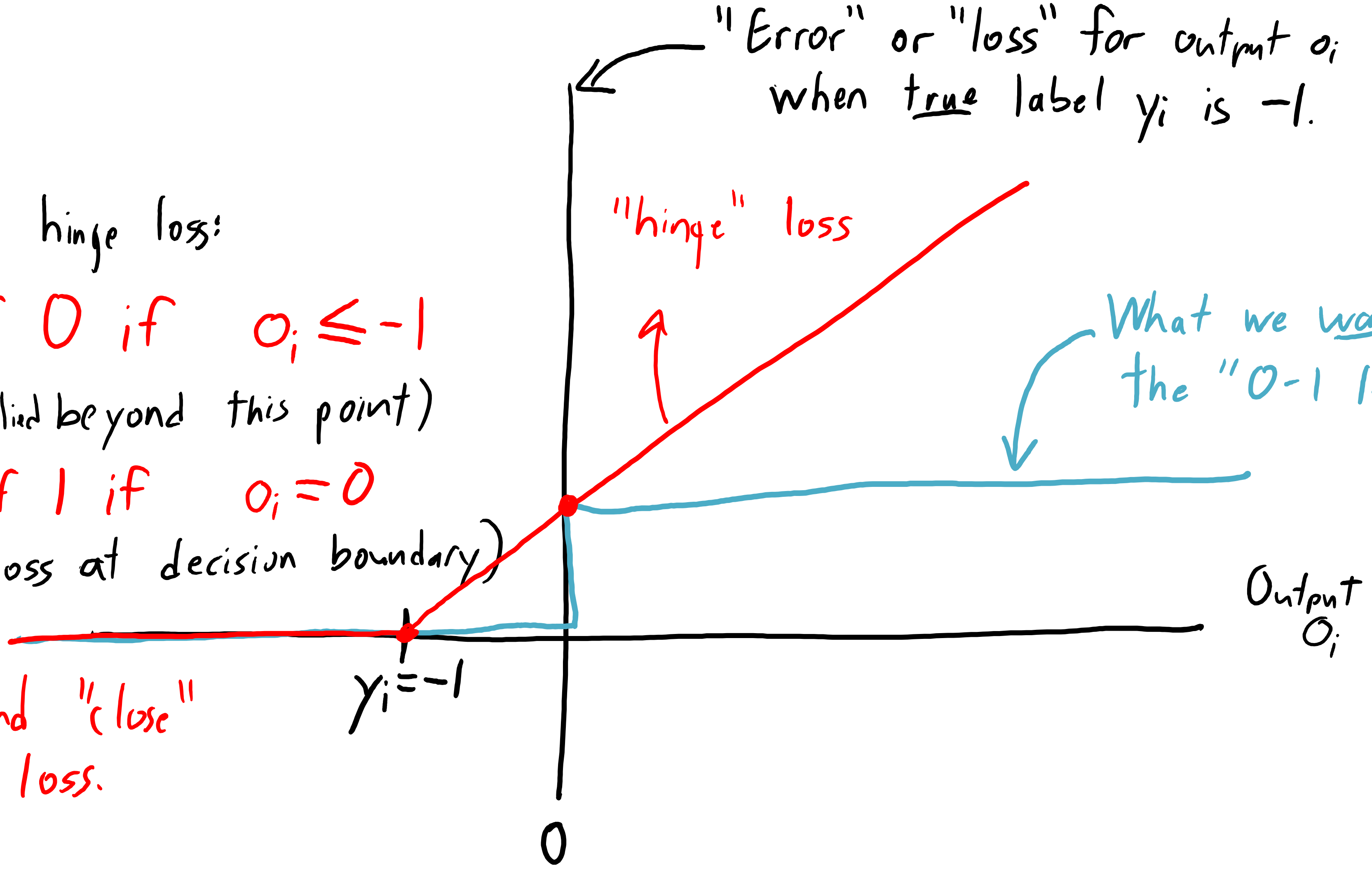
$$\max\{0, 1 - y_i o_i\}$$

- This is the called hinge loss.
  - It's convex: max(constant, linear).
  - It's not degenerate: w=0 now gives an error of 1 instead of 0.

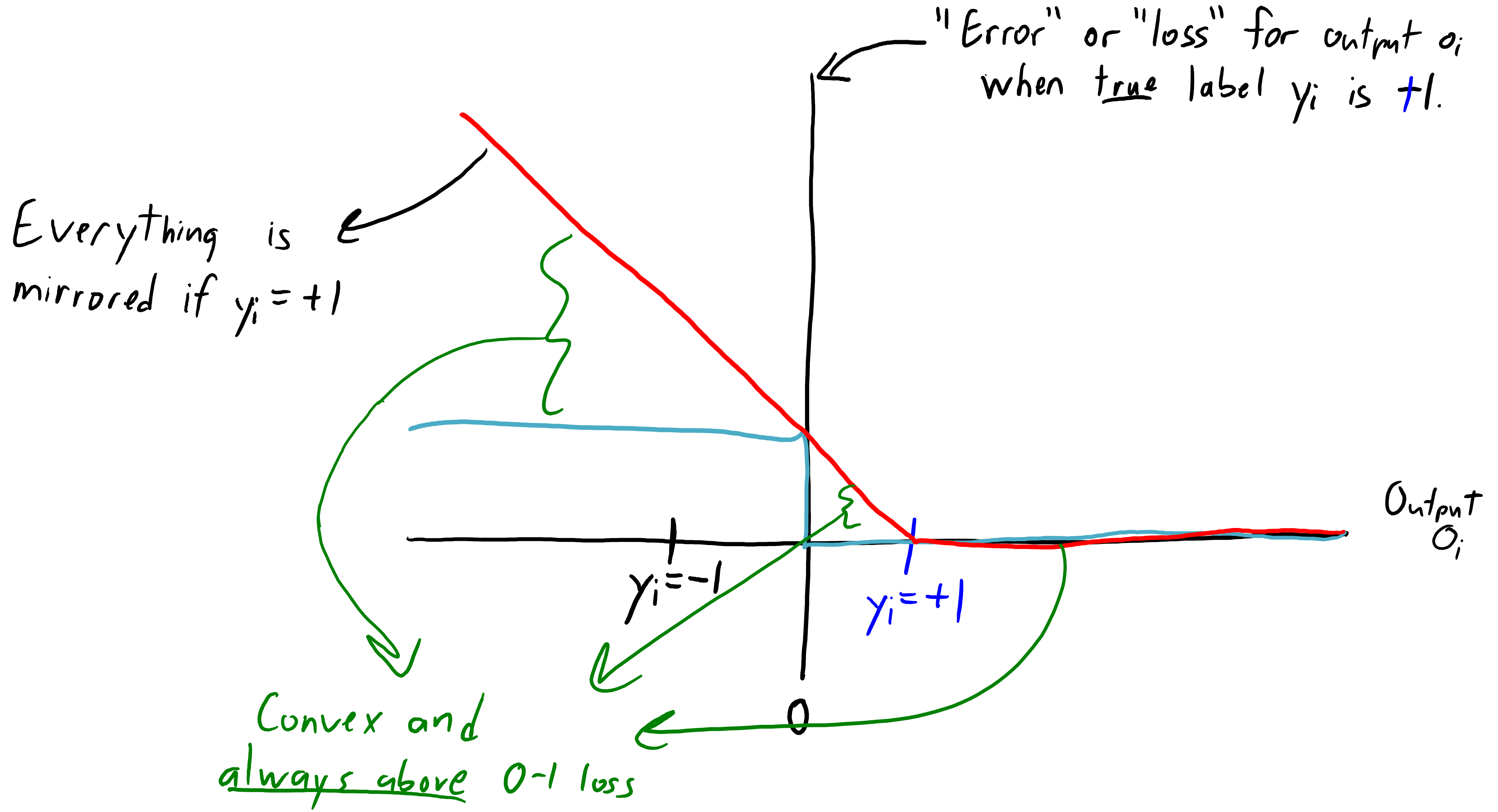
Hinge Loss: Convex Approximation to 0-1 Loss

Properties of the hinge loss:

1. Has error of 0 if $o_i \leq -1$
   (no penalty applied beyond this point)
2. Has a loss of 1 if $o_i = 0$
   (matches 0-1 loss at decision boundary)
3. Is convex and "close" to 0-1 loss.



Hinge Loss: Convex Approximation to 0-1 Loss



"Error" or "loss" for output o_i when true label y_i is +1.
Everything is mirrored if $y_i = +1$
Output O_i
$y_i = -1$
$y_i = +1$
0
Convex and always above 0-1 loss

Hinge Loss and Support Vector Machines (SVMs)

- Hinge loss for all 'n' training examples is given by:

$$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y_i \underbrace{w^T x_i}_{\hat{y}_i}\}$$

  - Convex upper bound on 0-1 loss.
    - If the hinge loss is 18.3, then number of training errors is at most 18.
    - So minimizing hinge loss indirectly tries to minimize training error.
    - Like perceptron, finds a perfect linear classifier if one exists.
- Support vector machine (SVM) is hinge loss with L2-regularization.

$$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\} + \frac{\lambda}{2}\|w\|^2$$

  - There exist specialized optimization algorithm for this problems.
  - SVMs can also be viewed as "maximizing the margin" (later).

'λ' vs 'C' as SVM Hyper-Parameter

- We have written SVM in terms of regularization parameter 'λ':

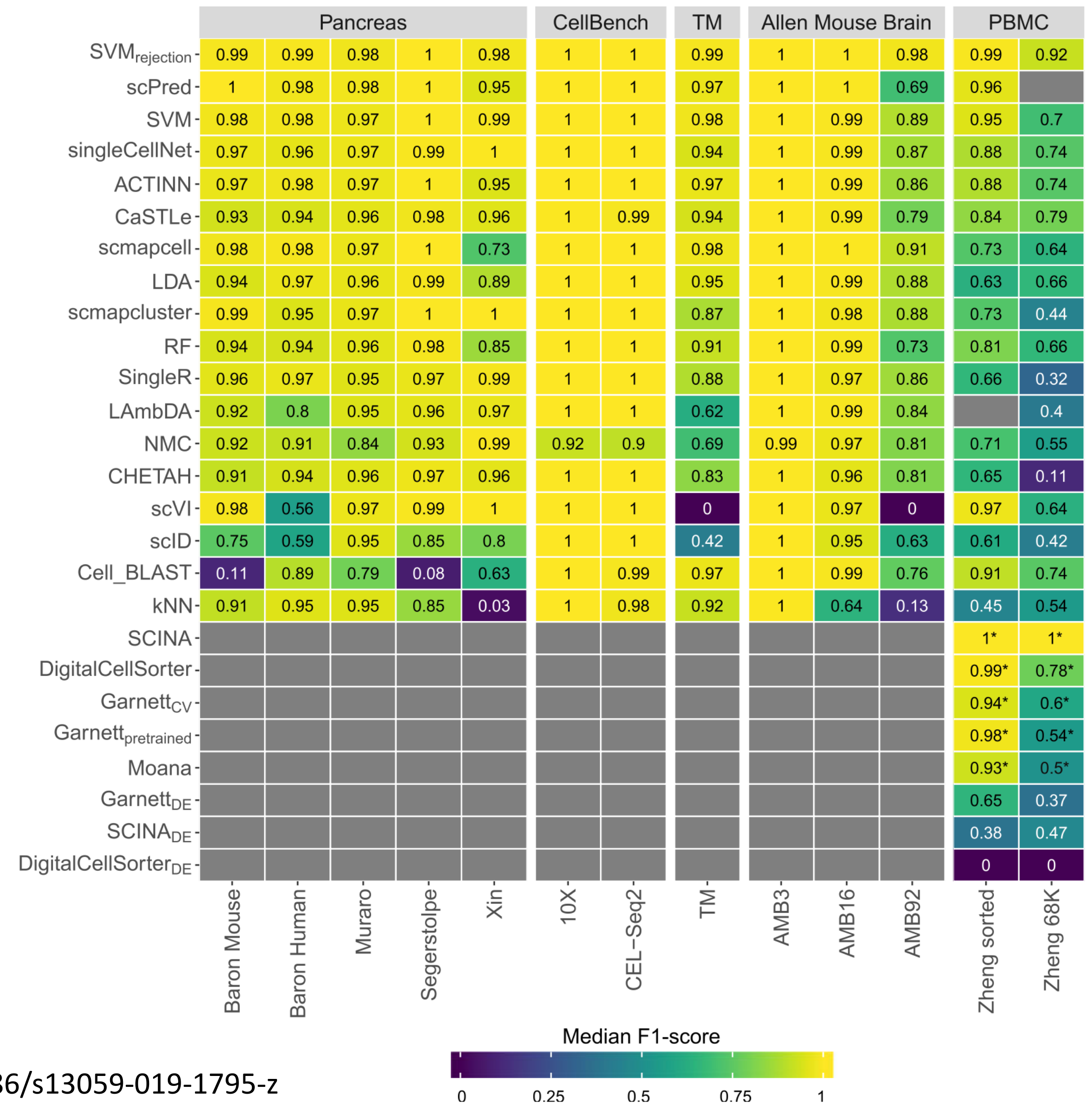
$$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\} + \frac{\lambda}{2}\|w\|^2$$

- Some software packages instead have regularization parameter 'C':

$$f(w) = C\sum_{i=1}^{n} \max\{0, 1 - y_i w^T x_i\} + \frac{1}{2}\|w\|^2$$

- In our notation, this corresponds to using λ = 1/C.
  - Equivalent to just multiplying f(w) by constant.
  - Note interpretation of 'C' is different: high regularization for small 'C'.
    - You can think of 'C' as "how much to focus on the classification error".

SVM performs the best in cell type annotations


Median F1-score
0
0.25
0.5
0.75
1

	Pancreas					CellBench		TM	Allen Mouse Brain			PBMC	
	Baron Mouse	Baron Human	Muraro	Segerstolpe	Xin	10X	CEL–Seq2	TM	AMB3	AMB16	AMB92	Zheng sorted	Zheng 68K
$SVM_{rejection}$	0.99	0.99	0.98	1	0.98	1	1	0.99	1	1	0.98	0.99	0.92
scPred	1	0.98	0.98	1	0.95	1	1	0.97	1	1	0.69	0.96	
SVM	0.98	0.98	0.97	1	0.99	1	1	0.98	1	0.99	0.89	0.95	0.7
singleCellNet	0.97	0.96	0.97	0.99	1	1	1	0.94	1	0.99	0.87	0.88	0.74
ACTINN	0.97	0.98	0.97	1	0.95	1	1	0.97	1	0.99	0.86	0.88	0.74
CaSTLe	0.93	0.94	0.96	0.98	0.96	1	0.99	0.94	1	0.99	0.79	0.84	0.79
scmapcell	0.98	0.98	0.97	1	0.73	1	1	0.98	1	1	0.91	0.73	0.64
LDA	0.94	0.97	0.96	0.99	0.89	1	1	0.95	1	0.99	0.88	0.63	0.66
scmapcluster	0.99	0.95	0.97	1	1	1	1	0.87	1	0.98	0.88	0.73	0.44
RF	0.94	0.94	0.96	0.98	0.85	1	1	0.91	1	0.99	0.73	0.81	0.66
SingleR	0.96	0.97	0.95	0.97	0.99	1	1	0.88	1	0.97	0.86	0.66	0.32
LAmbDA	0.92	0.8	0.95	0.96	0.97	1	1	0.62	1	0.99	0.84		0.4
NMC	0.92	0.91	0.84	0.93	0.99	0.92	0.9	0.69	0.99	0.97	0.81	0.71	0.55
CHETAH	0.91	0.94	0.96	0.97	0.96	1	1	0.83	1	0.96	0.81	0.65	0.11
scVI	0.98	0.56	0.97	0.99	1	1	1	0	1	0.97	0	0.97	0.64
scID	0.75	0.59	0.95	0.85	0.8	1	1	0.42	1	0.95	0.63	0.61	0.42
Cell_BLAST	0.11	0.89	0.79	0.08	0.63	1	0.99	0.97	1	0.99	0.76	0.91	0.74
kNN	0.91	0.95	0.95	0.85	0.03	1	0.98	0.92	1	0.64	0.13	0.45	0.54
SCINA												1*	1*
DigitalCellSorter												0.99*	0.78*
$Garnett_{CV}$												0.94*	0.6*
$Garnett_{pretrained}$												0.98*	0.54*
Moana												0.93*	0.5*
$Garnett_{DE}$												0.65	0.37
$SCINA_{DE}$												0.38	0.47
$DigitalCellSorter_{DE}$												0	0

https://genomebiology.biomedcentral.com/articles/10.1186/s13059-019-1795-z

Summary

- Ensemble feature selection reduces false positives or negatives.
- Binary classification using regression:
  - Encode using y_i in {-1,1}.
  - Use output $o_i = w^Tx_i$, and make predictions using $\text{sign}(o_i)$.
  - "Linear classifier" (a hyperplane splitting the space in half).
- Least squares is a weird error for classification.
- Perceptron algorithm: finds a perfect classifier (if one exists).
- 0-1 loss is the ideal loss, but is non-smooth and non-convex.
- Hinge loss is a convex upper bound on 0-1 loss.
  - SVMs add L2-regularization.

- Next time: loss functions used in many modern deep learning methods.

L1-Regularization as a Feature Selection Method

- Advantages:
  - Deals with conditional independence (if linear).
  - Sort of deals with collinearity:
    - Picks at least one of “mom” and “mom2”.
  - Very fast with specialized algorithms.
- Disadvantages:
  - Tends to give false positives (selects too many variables).
- Neither good nor bad:
  - Does not take small effects.
  - Says “gender” is relevant if we know “baby”.
  - Good for prediction if we want fast training and don’t care about having some irrelevant variables included.

"Elastic Net": L2- and L1-Regularization

- To address non-uniqueness, some authors use L2- and L1-:

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda_2}{2}\|w\|^2 + \lambda_1\|w\|_1$$

- Called "elastic net" regularization.
  - Solution is sparse and unique.
  - Slightly better with feature dependence:
    - Selects both "mom" and "mom2".
- Optimization is easier though still non-differentiable.

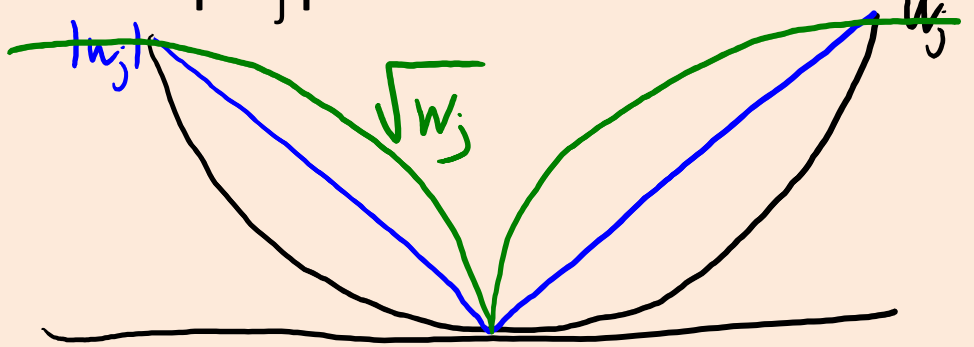
L1-Regularization Debiasing and Filtering

- To remove false positives, some authors add a debiasing step:
  - Fit ‘w’ using L1-regularization.
  - Grab the non-zero values of ‘w’ as the “relevant” variables.
  - Re-fit relevant ‘w’ using least squares or L2-regularized least squares.

- A related use of L1-regularization is as a filtering method:
  - Fit ‘w’ using L1-regularization.
  - Grab the non-zero values of ‘w’ as the “relevant” variables.
  - Run standard (slow) variable selection restricted to relevant variables.
    - Forward selection, exhaustive search, stochastic local search, etc.

Non-Convex Regularizers

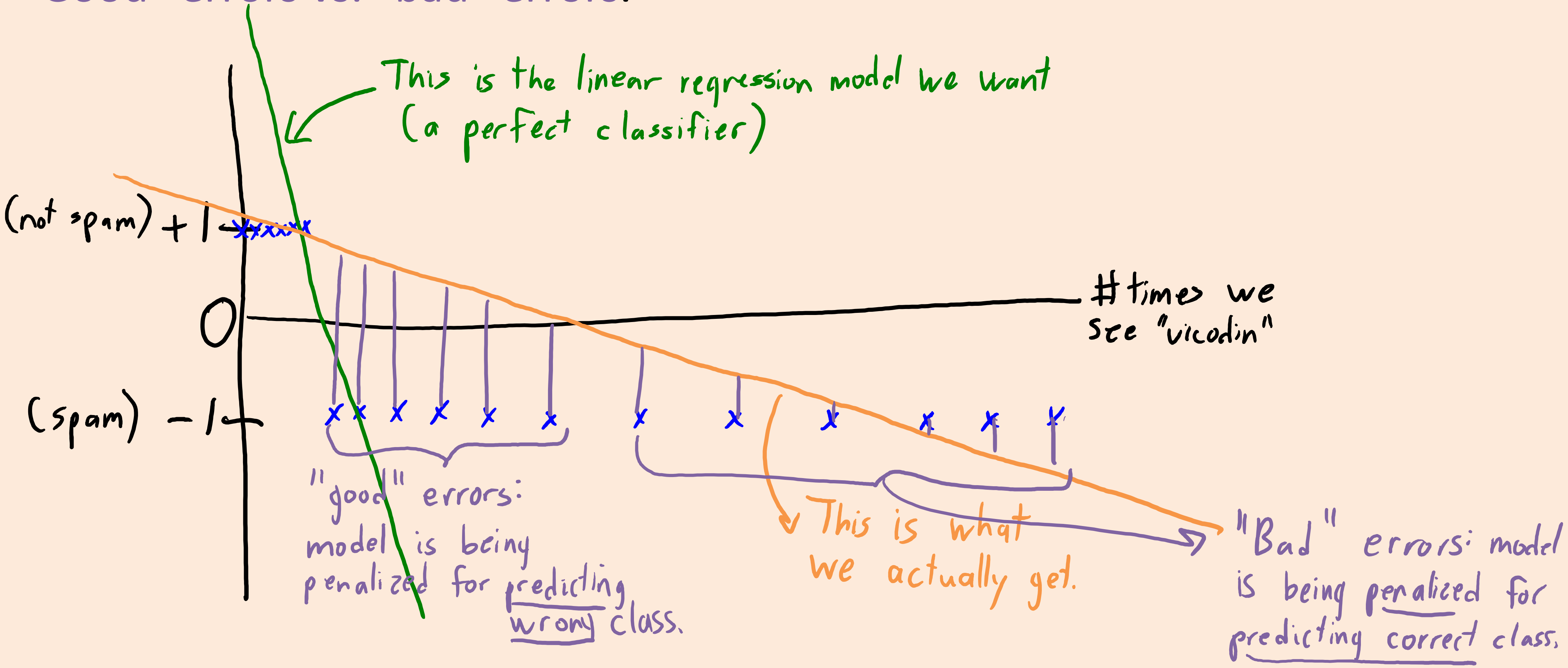
- Regularizing $|w_j|^2$ selects all features.
- Regularizing $|w_j|$ selects fewer, but still has many false positives.
- What if we regularize $|w_j|^{1/2}$ instead?



- Minimizing this objective would lead to fewer false positives.
  - Less need for debiasing, but it's not convex and hard to minimize.
- There are many non-convex regularizers with similar properties.
  - L1-regularization is (basically) the "most sparse" convex regularizer.

Can we just use least squares??

- What went wrong?
  - "Good" errors vs. "bad" errors.

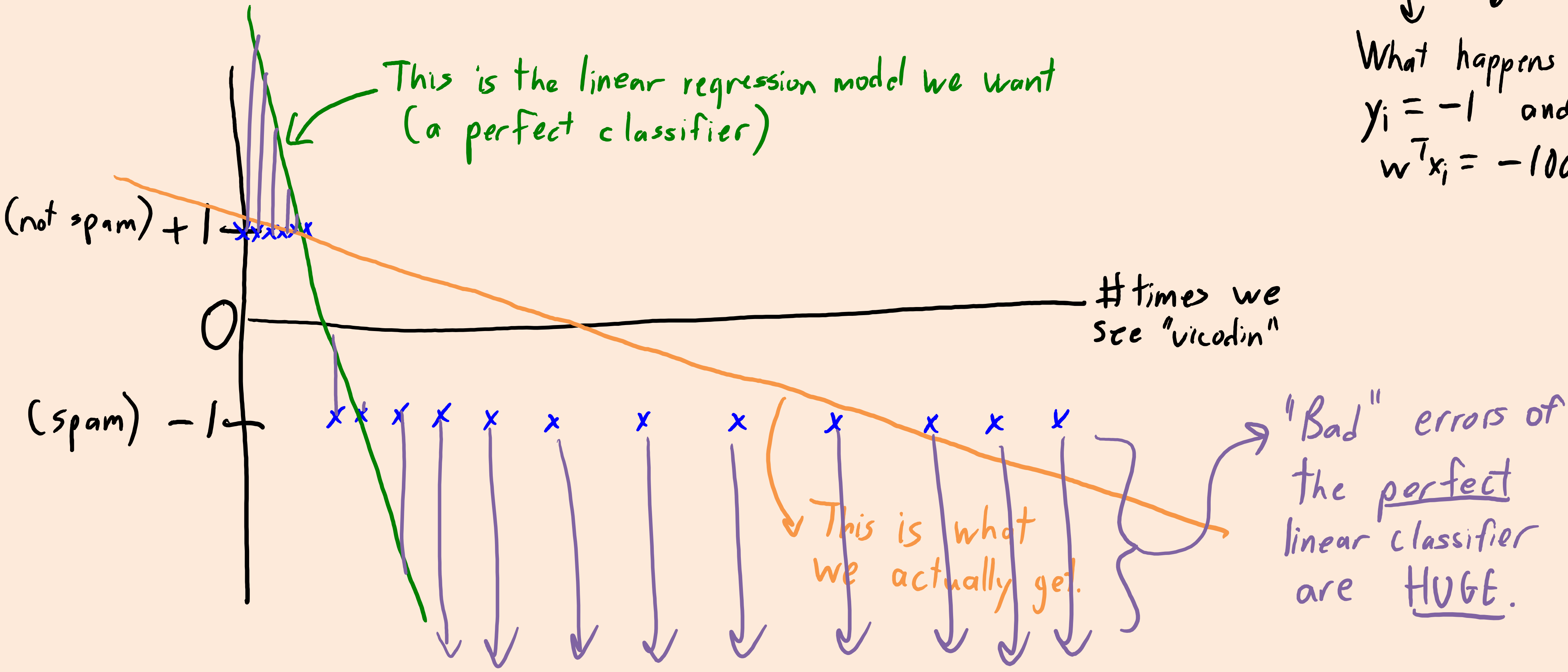


Can we just use least squares??

- What went wrong?
  - "Good" errors vs. "bad" errors.

$$f(w) = \sum_{i=1}^{n} (w^T x_i - y_i)^2$$

What happens if $y_i = -1$ and $w^T x_i = -1000$?



Online Classification with Perceptron

- Perceptron for online linear binary classification [Rosenblatt, 1957]
  - Start with $w_0 = 0$.
  - At time 't' we receive features x_t.
  - We predict $\hat{y}_t = \text{sign}(w_t^T x_t)$.
  - If $\hat{y}_t \neq y_t$, then set $w_{t+1} = w_t + y_t x_t$.
    - Otherwise, set $w_{t+1} = w_t$.

(Slides are old so above I'm using subscripts of 't' instead of superscripts.)

- Perceptron mistake bound [Novikoff, 1962]:
  - Assume data is linearly-separable with a "margin":
    - There exists w^* with $||w^*||=1$ such that $\text{sign}(x_t^T w^*) = \text{sign}(y_t)$ for all 't' and $|x^T w^*| \geq \gamma$. > 0
  - Then the number of total mistakes is bounded.
    - No requirement that data is IID.

Perceptron Mistake Bound

- Let's normalize each x_t so that $||x_t|| = 1$.
  - Length doesn't change label.
- Whenever we make a mistake, we have $\text{sign}(y_t) \neq \text{sign}(w_t^T x_t)$ and

$$\begin{aligned} \|w_{t+1}\|^2 &= \|w_t + y x_t\|^2 \\ &= \|w_t\|^2 + 2 \underbrace{y_t w_t^T x_t}_{<0} + 1 \\ &\leq \|w_t\|^2 + 1 \\ &\leq \|w_{t-1}\|^2 + 2 \\ &\leq \|w_{t-2}\|^2 + 3. \end{aligned}$$

- So after 'k' errors we have $||w_t||^2 \leq k$.

Perceptron Mistake Bound

- Let's consider a solution w*, so sign(y_t) = sign(x_t^Tw*).
  - And let's choose a w* with ||w*|| = 1,
- Whenever we make a mistake, we have:

$$\begin{aligned} \|w_{t+1}\| &= \|w_{t+1}\|\|w_*\| \\ &\geq w_{t+1}^T w_* \\ &= (w_t + y_t x_t)^T w_* \\ &= w_t^T w_* + y_t x_t^T w_* \\ &= w_t^T w_* + |x_t^T w_*| \\ &\geq w_t^T w_* + \gamma. \end{aligned}$$

  - Note: $w_t^T w_* \geq 0$ by induction (starts at 0, then at least as big as old value plus γ).
- So after 'k' mistakes we have $||w_t|| \geq \gamma k$.

Perceptron Mistake Bound

- So our two bounds are $||w_t|| \leq \text{sqrt}(k)$ and $||w_t|| \geq \gamma k$.

- This gives $\gamma k \leq \text{sqrt}(k)$, or a maximum of $1/\gamma^2$ mistakes.
  - Note that $\gamma > 0$ by assumption and is upper-bounded by one by $||x|| \leq 1$.
  - After this ‘k’, under our assumptions
    we’re guaranteed to have a perfect classifier.