CPSC 340: Machine Learning and Data Mining

More Linear Classifiers

Fall 2017

Admin

- Assignment 3:
  - Due Friday of next week.

- Midterm:
  - Can view your exam during instructor office hours next week, or after class this/next week.

Last Time: Classification using Regression

- Binary classification using sign of linear models:

Fit model $y_i \approx w^T x_i$ and predict using $\text{sign}(w^T x_i)$

$y_i \to +1$, -1

- Problems with existing errors:
  - If $y_i = +1$ and $w^T x_i = +100$, then squared error $(w^T x_i - y_i)^2$ is huge.
  - Hard to minimize training error ("0-1 loss") in terms of 'w'.

- Motivates convex approximations to 0-1 loss…

Degenerate Convex Approximation to 0-1 Loss

- If $y_i = +1$, we get the label right if $w^T x_i > 0$.
- If $y_i = -1$, we get the label right if $w^T x_i < 0$, or equivalently $-w^T x_i > 0$.
- So "classifying 'i' correctly" is equivalent to having $y_i w^T x_i > 0$.

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

If $y_i w^T x_i > 0$ then you get an "error" of 0.
If $y_i w^T x_i < 0$ then you get an "error" of $-y_i w^T x_i$

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

Degenerate Convex Approximation to 0-1 Loss

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

$$\max\{0, -y_i w^T x_i\}$$

- 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

- Consider replacing $y_i w^T x_i > 0$ with $y_i w^T x_i \geq 1$.

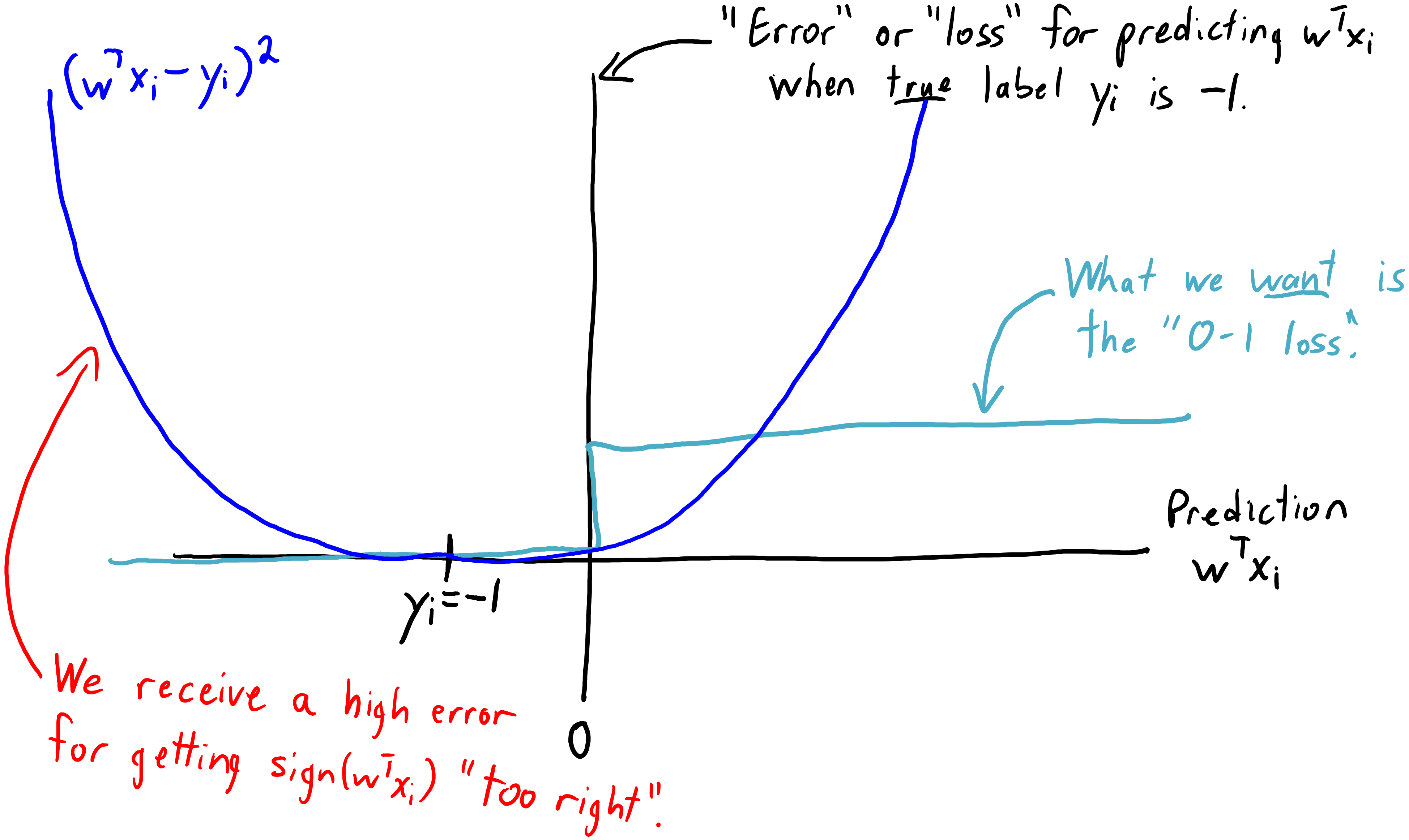
  (the "1" is arbitrary: we could make ||w|| bigger/smaller to use any positive constant)

- The violation of this constraint is now given by:

$$\max\{0, 1 - y_i w^T x_i\}$$

- 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.

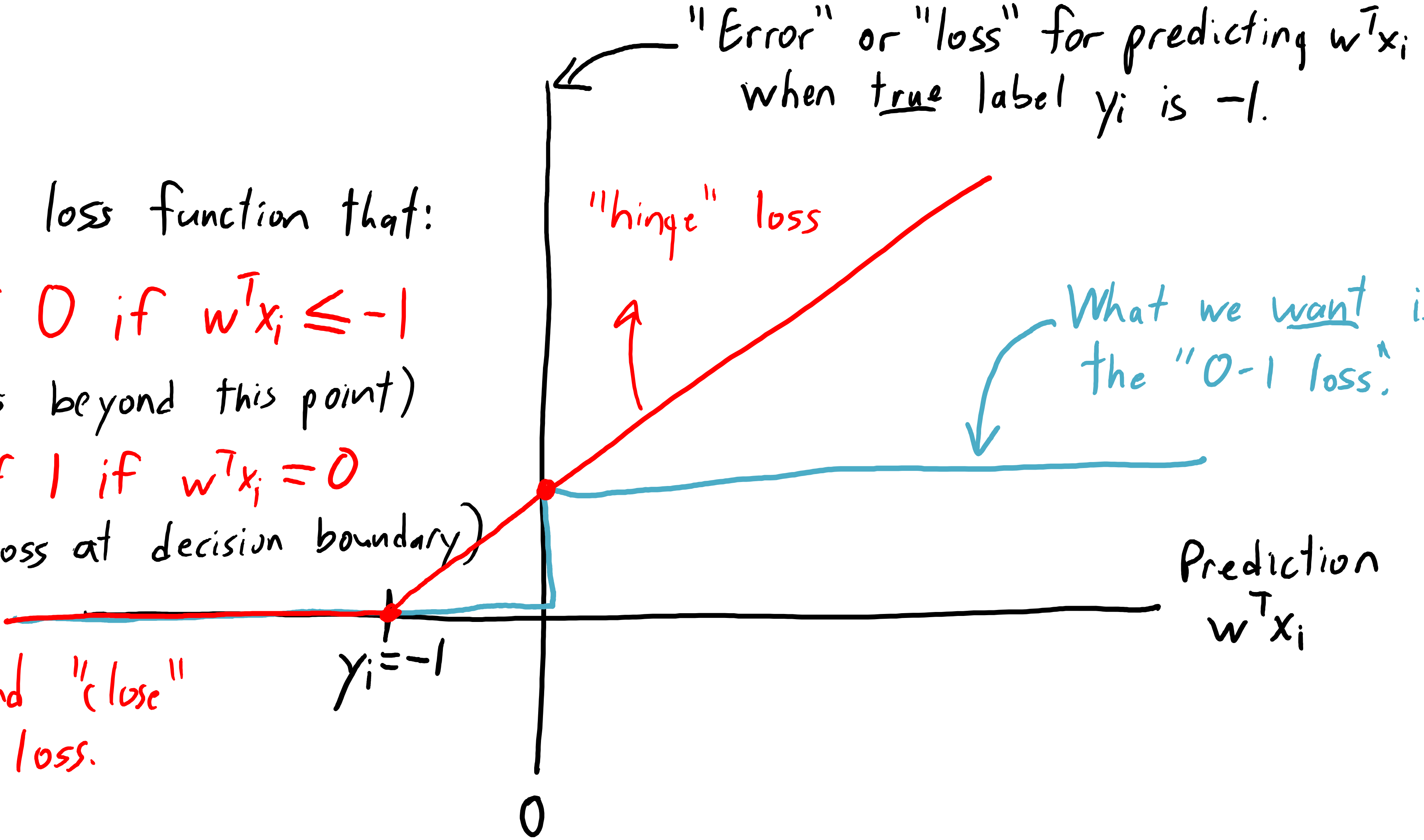
Hinge Loss: Convex Approximation to 0-1 Loss



Hinge Loss: Convex Approximation to 0-1 Loss

Let's choose a loss function that:

1. Has error of 0 if $w^T x_i \leq -1$
   (no "bad" errors beyond this point)
2. Has a loss of 1 if $w^T x_i = 0$
   (matches 0-1 loss at decision boundary)
3. Is convex and "close" to 0-1 loss.



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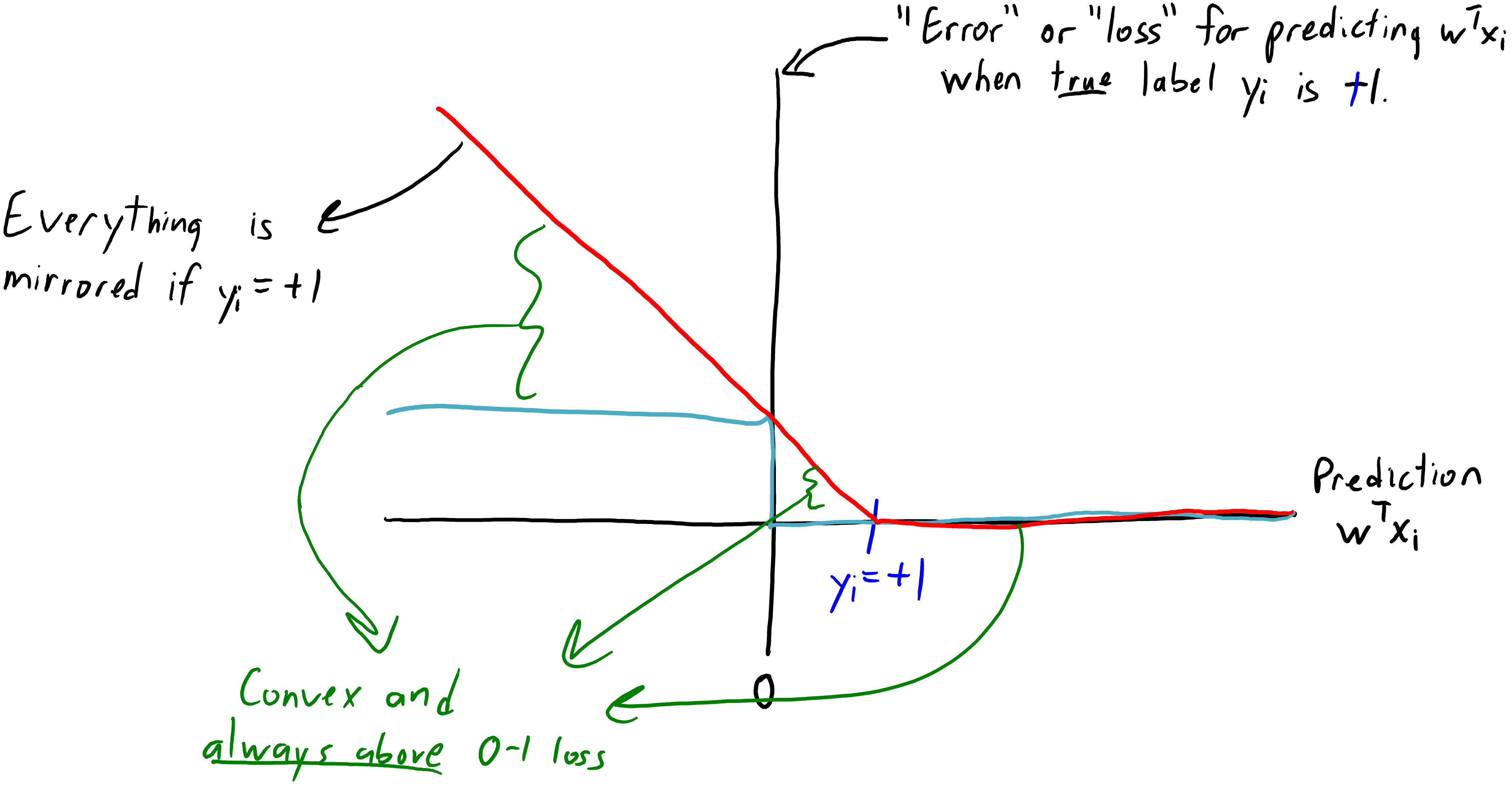


Hinge Loss

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

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

  - 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.
    - Finds a perfect linear classifier if one exists.
- Support vector machine (SVM) is hinge loss with L2-regularization.

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

- SVMs can also be viewed as "maximizing the margin" (later in lecture).

Logistic Loss

- We can smooth max in degenerate loss with log-sum-exp:

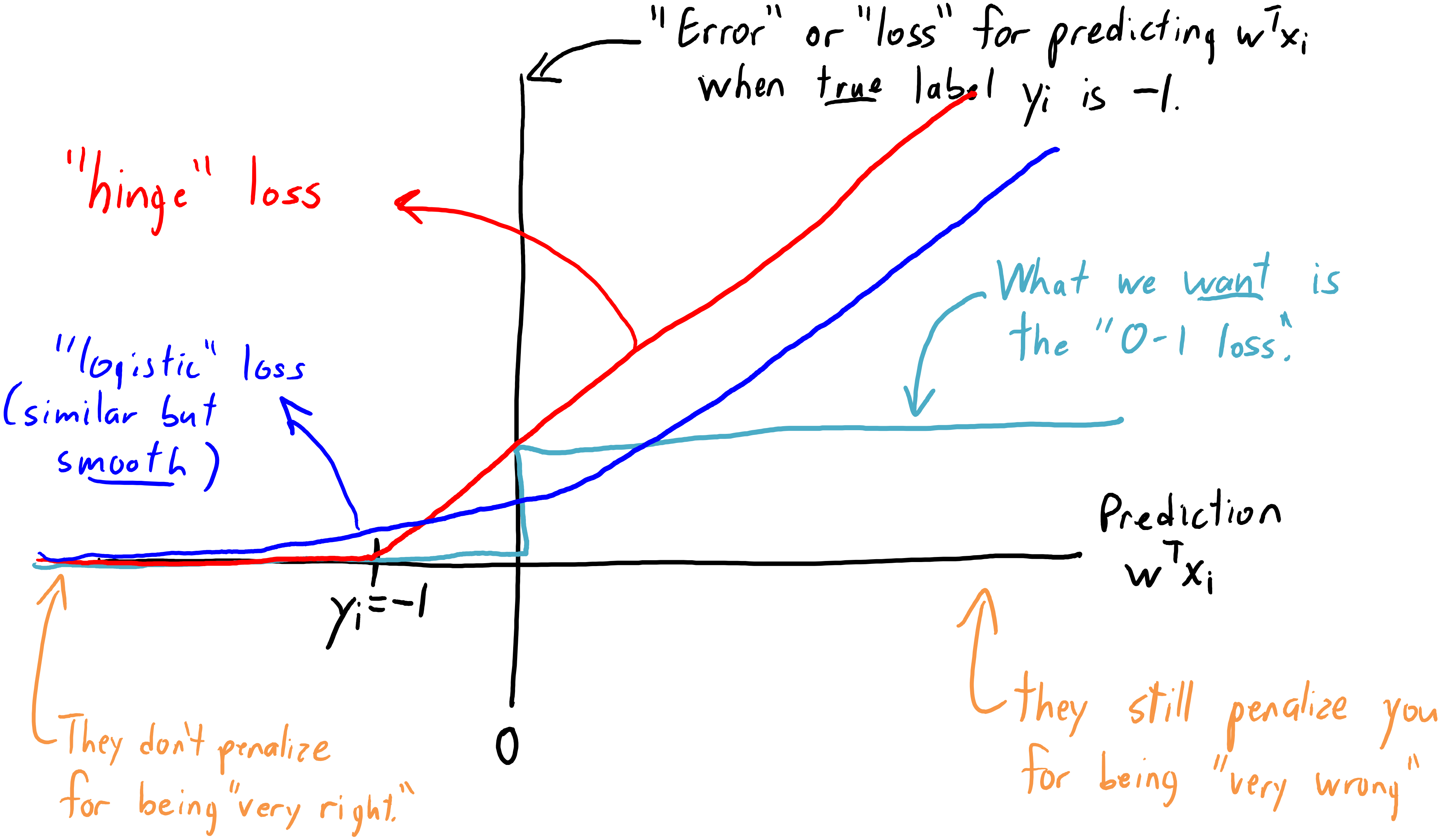
$$\max\{0, -y_i w^T x_i\} \approx \log(\underbrace{\exp(0)}_{1} + \exp(-y_i w^T x_i))$$

- Summing over all examples gives:

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

- This is the "logistic loss" and model is called "logistic regression".
  - It's not degenerate: w=0 now gives an error of log(2) instead of 0.
  - Convex and differentiable: minimize this with gradient descent.
  - You should also add regularization.
  - We'll see later that it has a probabilistic interpretation.

Convex Approximations to 0-1 Loss



Logistic Regression and SVMs

- Logistic regression and SVMs are used EVERYWHERE!
  - Fast training and testing.
    - Training on huge datasets using “stochastic” gradient descent (next week).
    - Testing is just computing $w^T x_i$.
  - Weights w_j are easy to understand.
    - It’s how much w_j changes the prediction and in what direction.
  - We can often get a good good test error.
    - With low-dimensional features using RBF basis and regularization.
    - With high-dimensional features and regularization.
  - Smoother predictions than random forests.

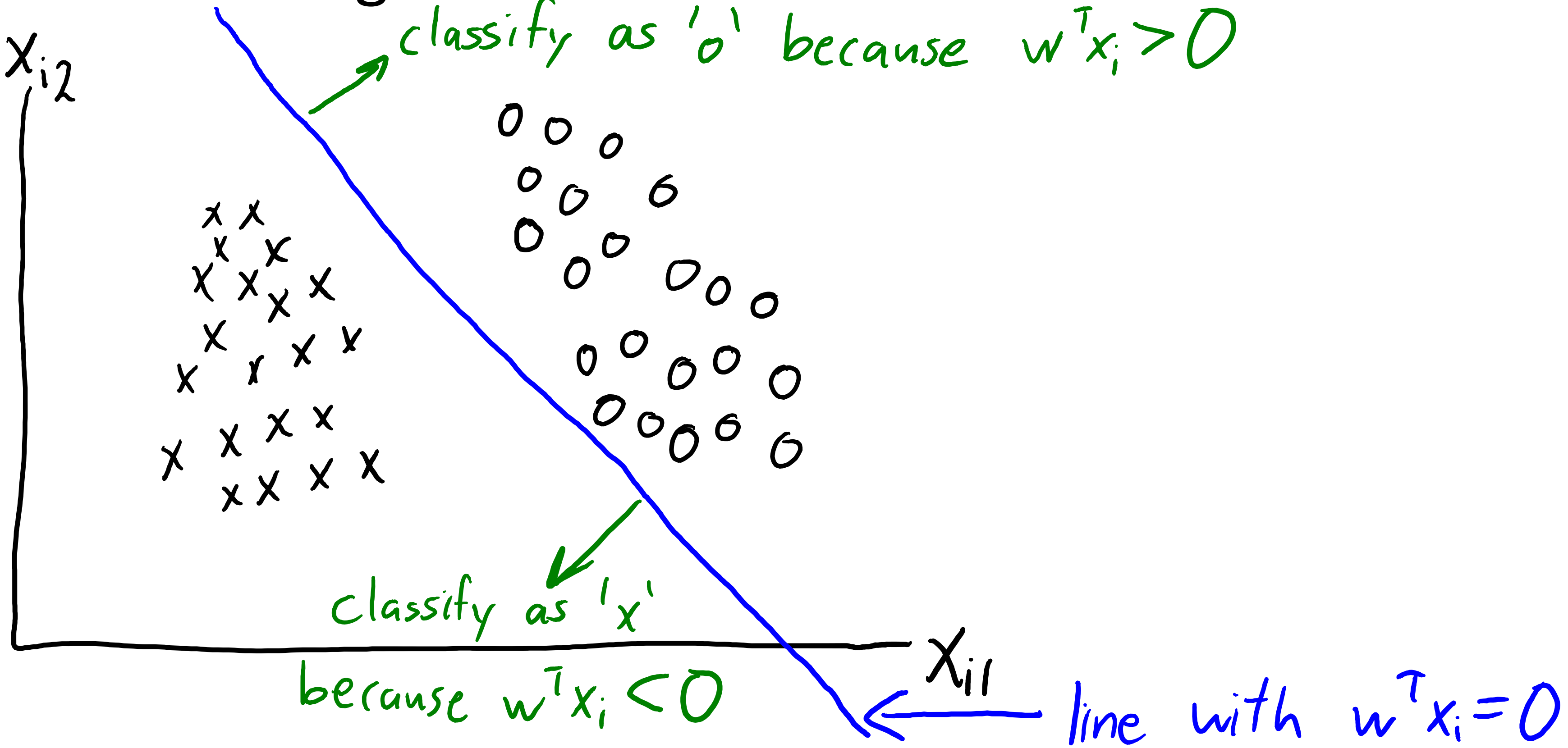
Comparison of “Black Box” Classifiers

- Fernandez-Delgado et al. [2014]:
  - “Do we Need Hundreds of Classifiers to Solve Real World Classification Problems?”

- Compared 179 classifiers on 121 datasets.
- Random forests are most likely to be the best classifier.
- Next best class of methods was SVMs (L2-regularization, RBFs).

Last Time: Linear Classifiers

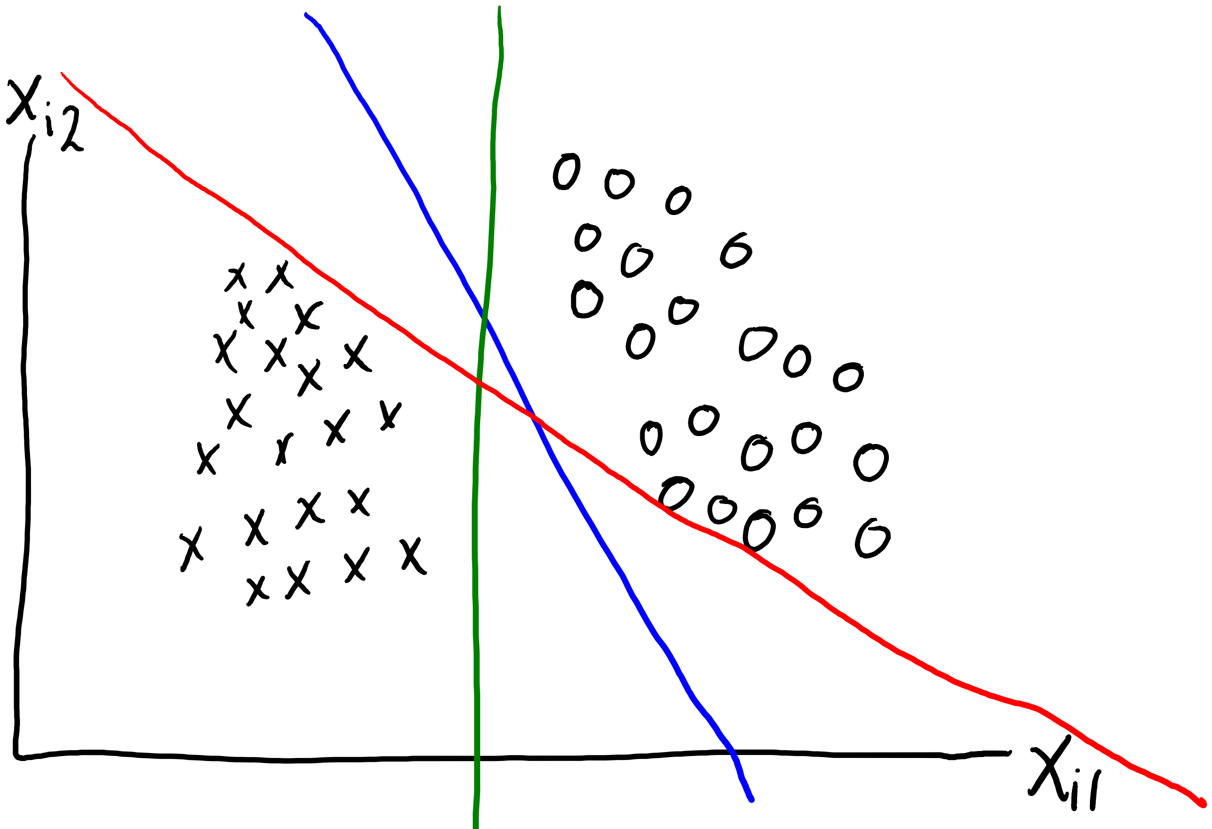
- 2D Visualization of linear regression for classification:



- "Linearly separable": a perfect linear classifier exists.

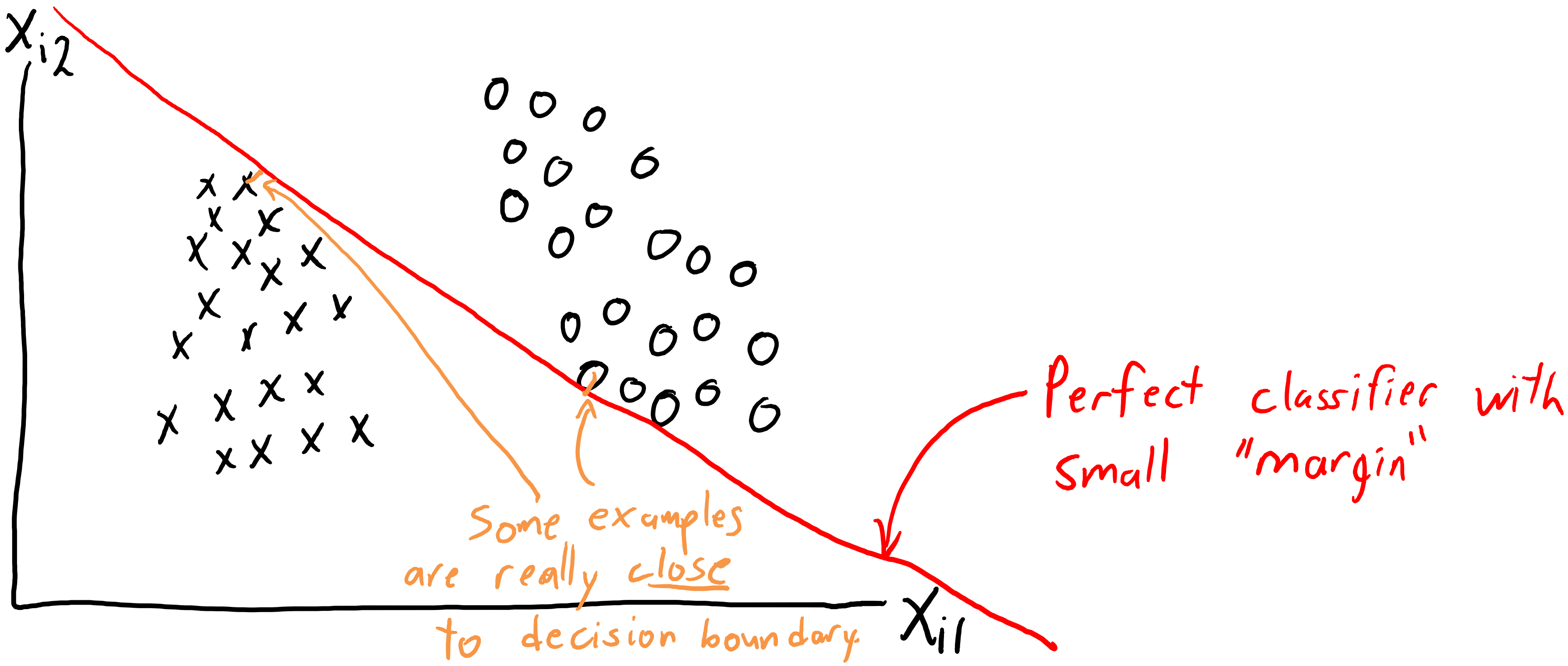
Maximum-Margin Classifier

- Consider a linearly-separable dataset.
  - Perceptron algorithm finds *some* classifier with zero error.
  - But are all zero-error classifiers equally good?



Maximum-Margin Classifier

- Consider a linearly-separable dataset.
  - Maximum-margin classifier: choose the farthest from both classes.



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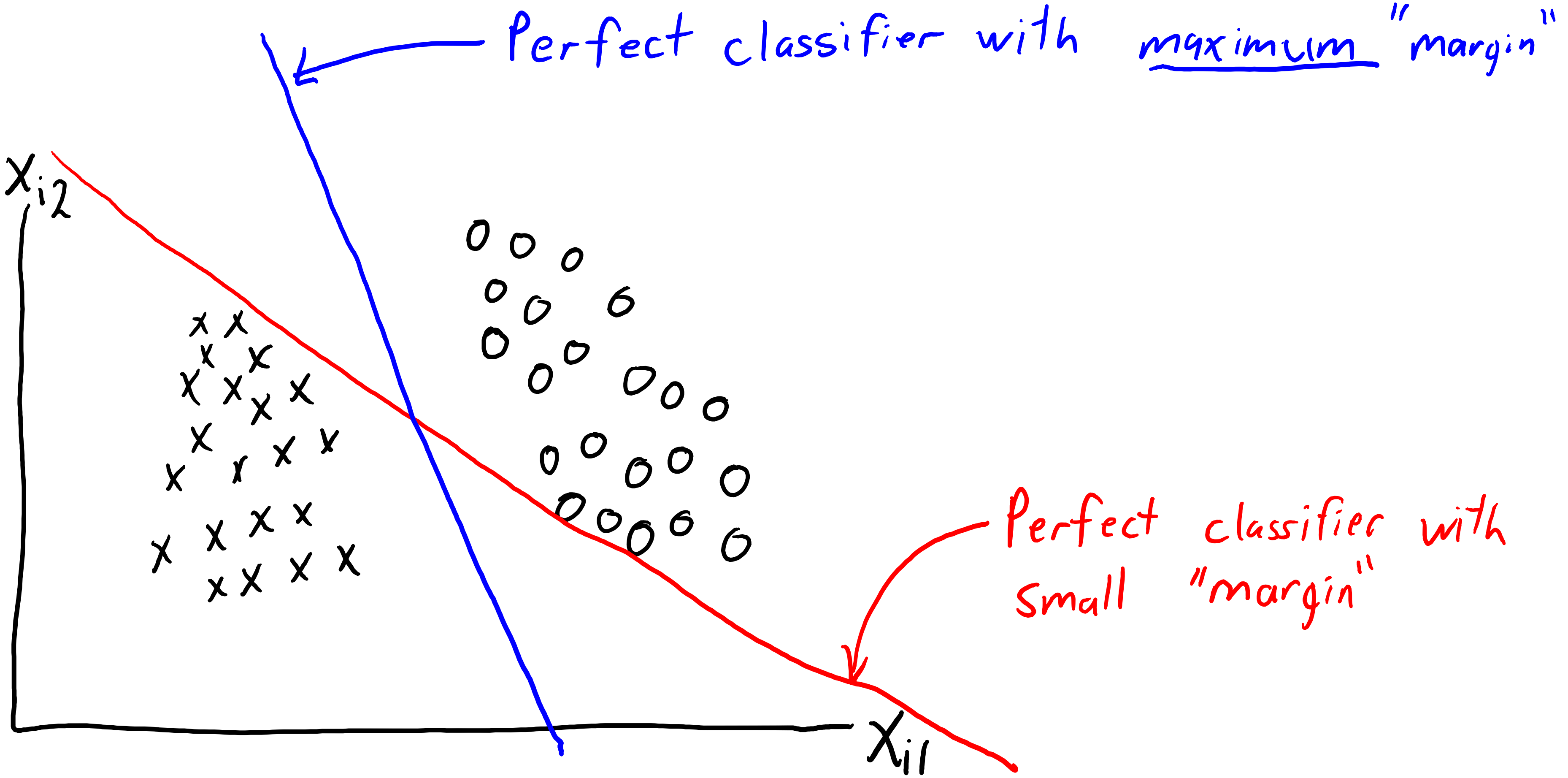

Maximum-Margin Classifier

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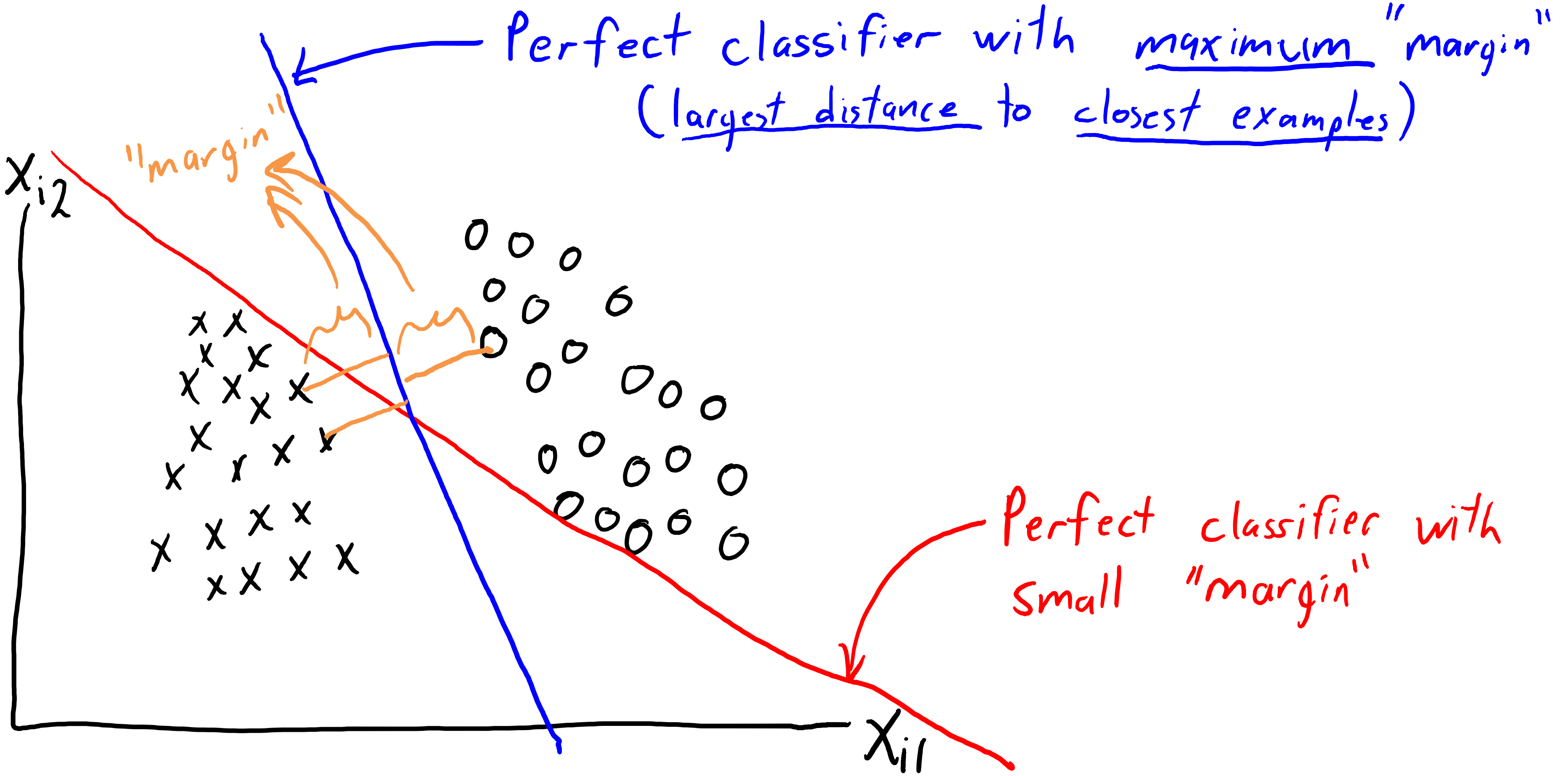
Why maximize margin?

If test data is close to training data, then max margin leaves more "room" before we make an error.



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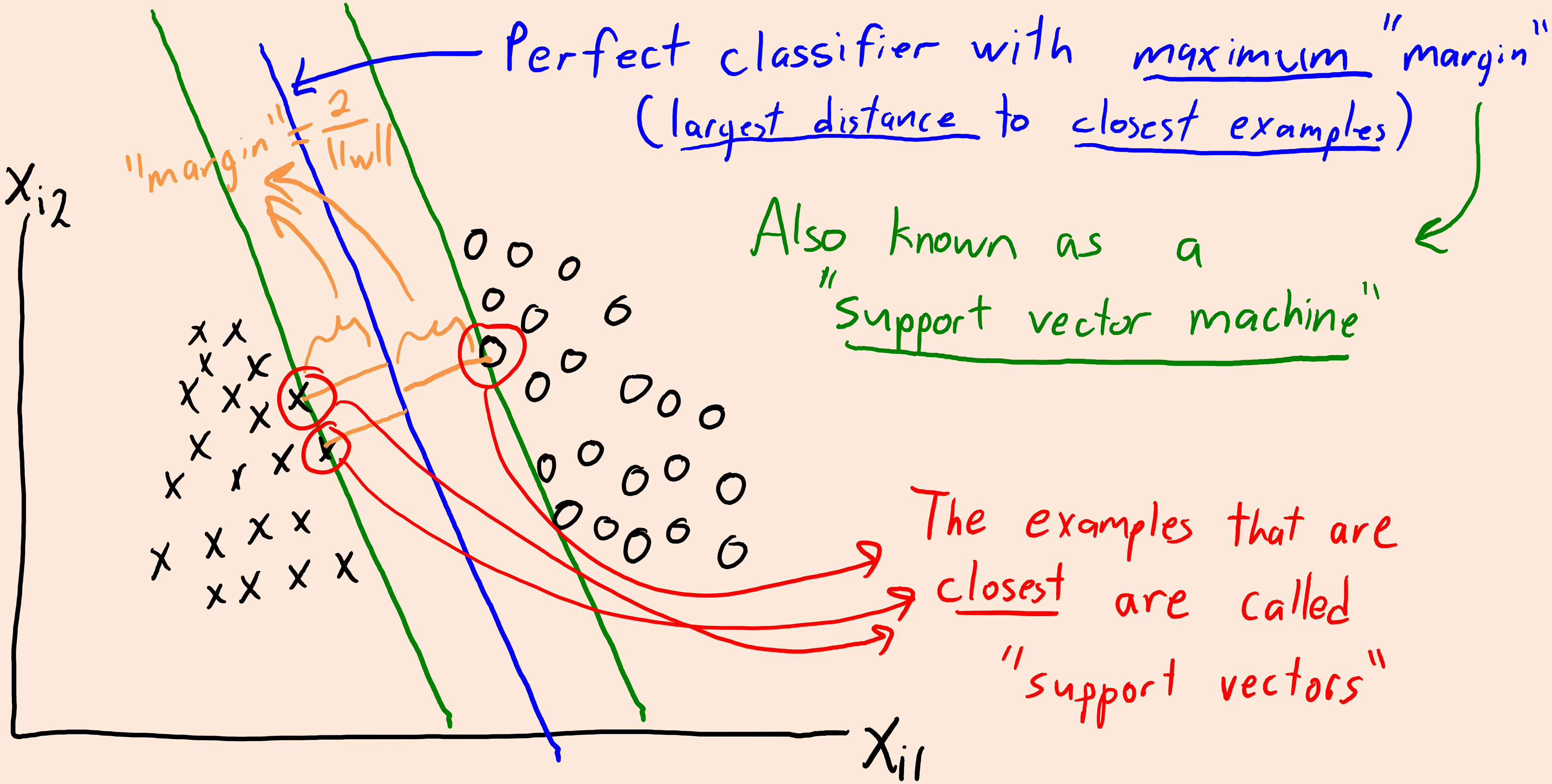

Maximum-Margin Classifier

- Consider a linearly-separable dataset.
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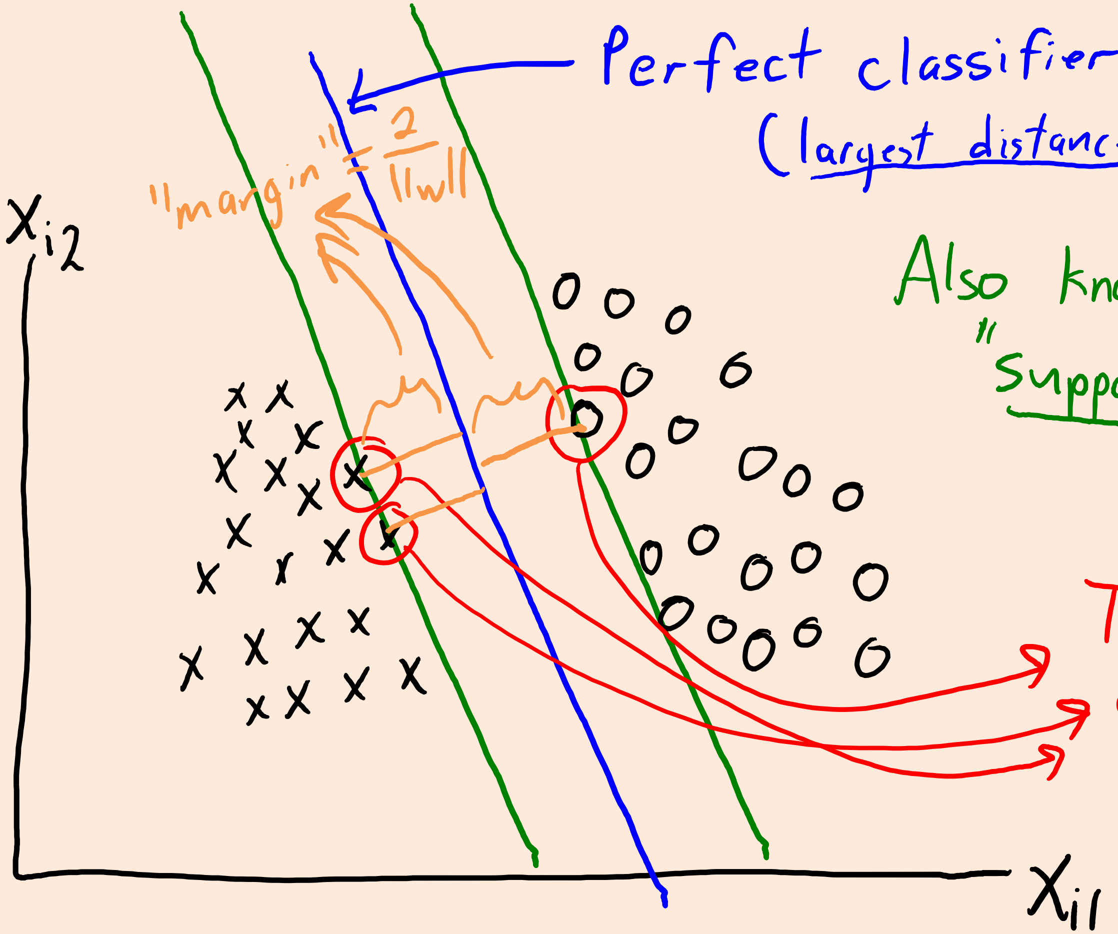
Perfect classifier with maximum "margin" (largest distance to closest examples)

Also known as a "support vector machine"

Final classifier only depends on support vectors



The examples that are closest are called "support vectors"

Maximum-Margin Classifier

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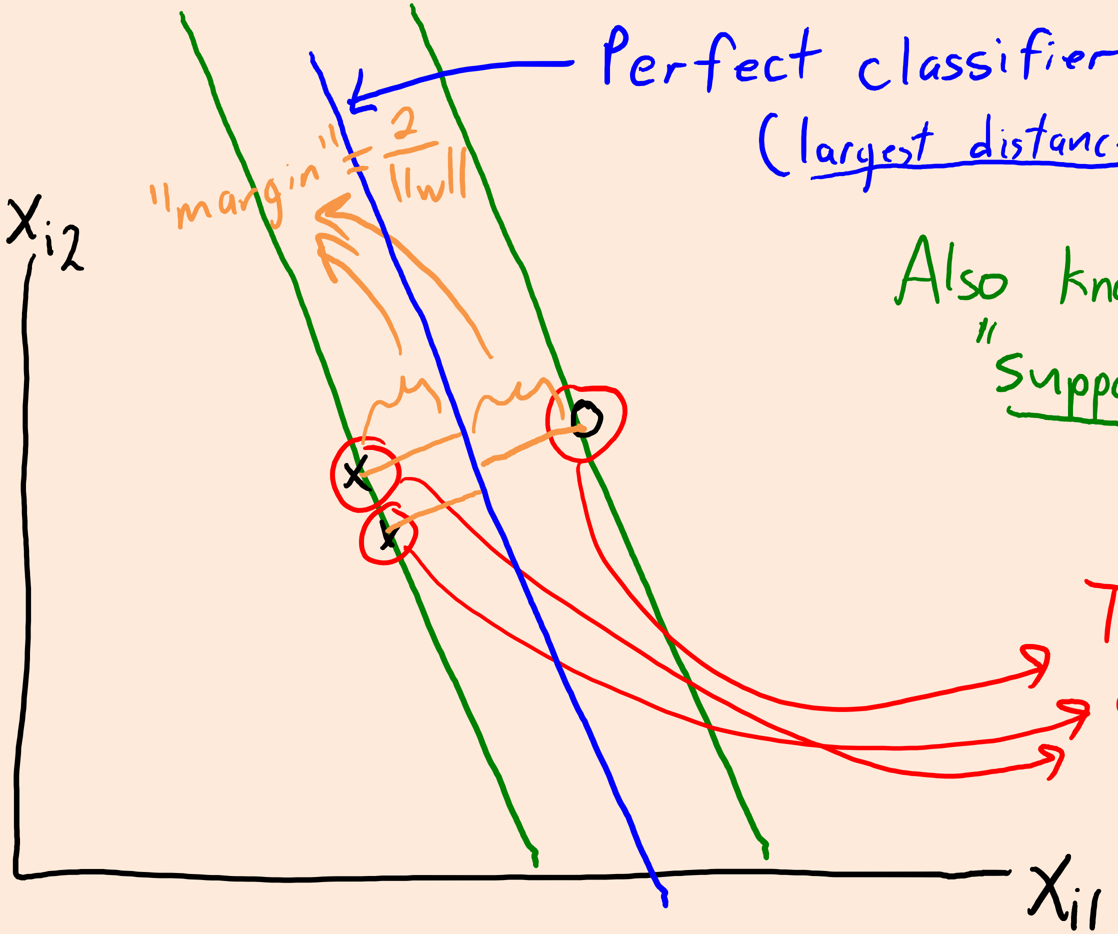


You could throw away the other examples and get the same classifier.

The examples that are closest are called "support vectors"

Support Vector Machines

- For linearly-separable data, SVM minimizes:

$$f(w) = \frac{1}{2}\|w\|^2$$ (equivalent to maximizing margin $\frac{2}{\|w\|}$)

  – Subject to the constraints that: (see Wikipedia/textbooks)

$$w^T x_i \geq 1 \quad \text{for } y_i = 1$$
$$w^T x_i \leq -1 \quad \text{for } y_i = -1$$

(classify all examples correctly)

- But most data is not linearly separable.
- For non-separable data, try to minimize violation of constraints:

If $w^T x_i \leq -1$ and $y_i = -1$ then "violation" should be zero.

If $w^T x_i \geq -1$ and $y_i = -1$ then we "<u>violate constraint</u>" by $1 + w^T x_i$

⋮

Constraint violation is the <u>hinge loss</u>.

Support Vector Machines

- Try to maximizing margin and also minimizing constraint violation:

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

Hinge loss for example 'i':

it's the amount we violate $y_i w^T x_i \geq 1$

"slack"

Original SVM objective: encourages large margin.

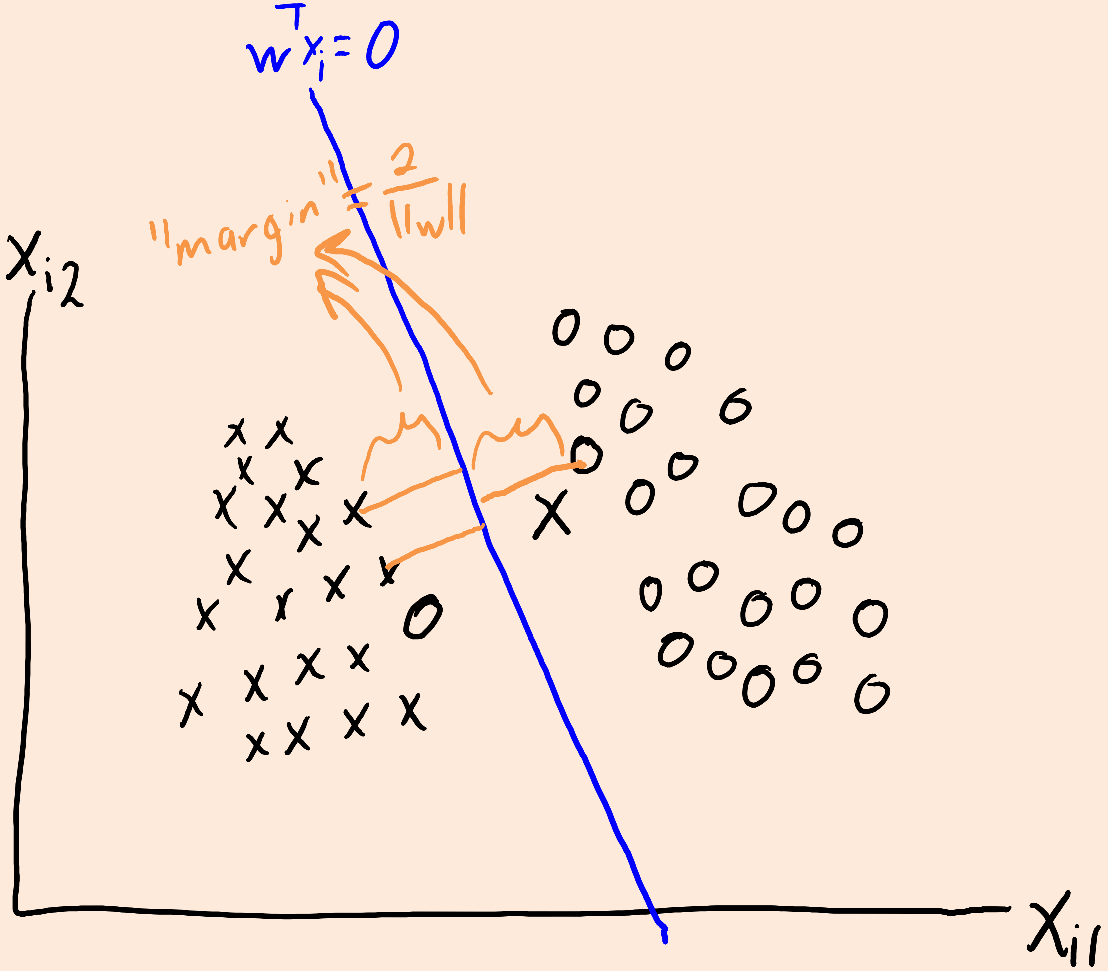
- We typically control margin/violation trade-off with parameter "λ":

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

- This is the standard SVM formulation (L2-regularized hinge).
  – Some formulations use λ = 1 and multiply hinge by 'C' (equivalent).

Support Vector Machines for Non-Separable

- Non-separable case:



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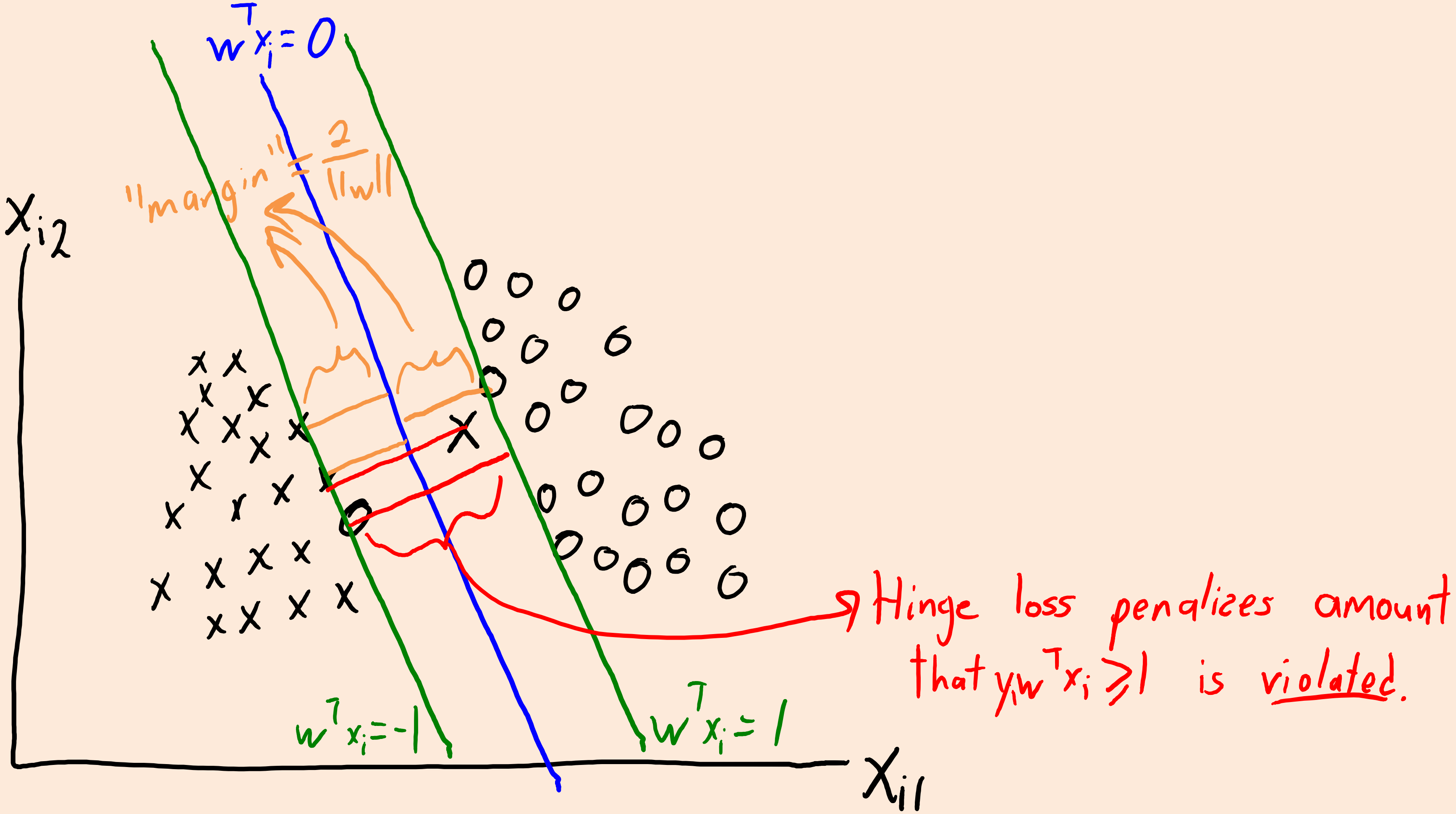


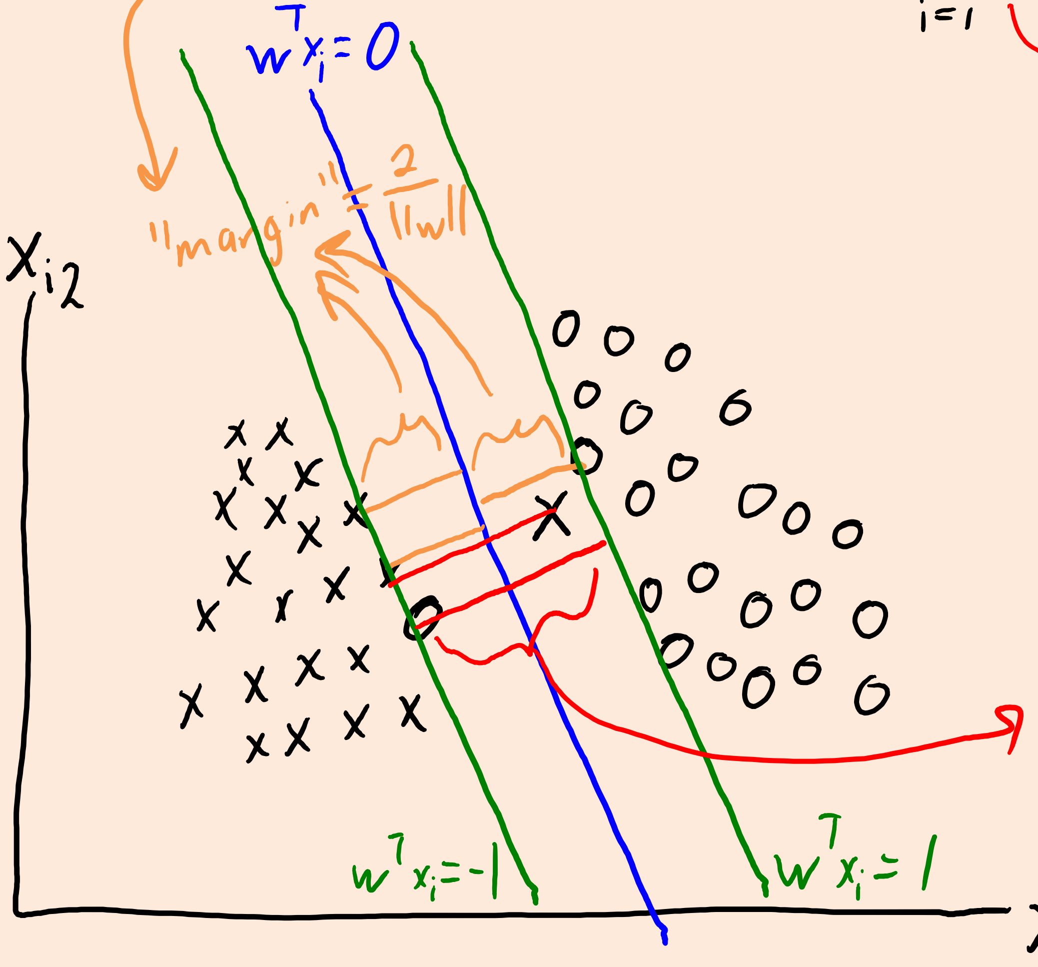
Support Vector Machines for Non-Separable

- Non-separable case:

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

Logistic regression can be viewed as smooth approximation to SVMs.

But, no concept of "support vectors" with logistic loss.



Hinge loss penalizes amount that $y_i w^T x_i \geq 1$ is violated.

λ controls trade-off between having large margin and classifying examples correctly.

Support Vector Machines for Non-Separable

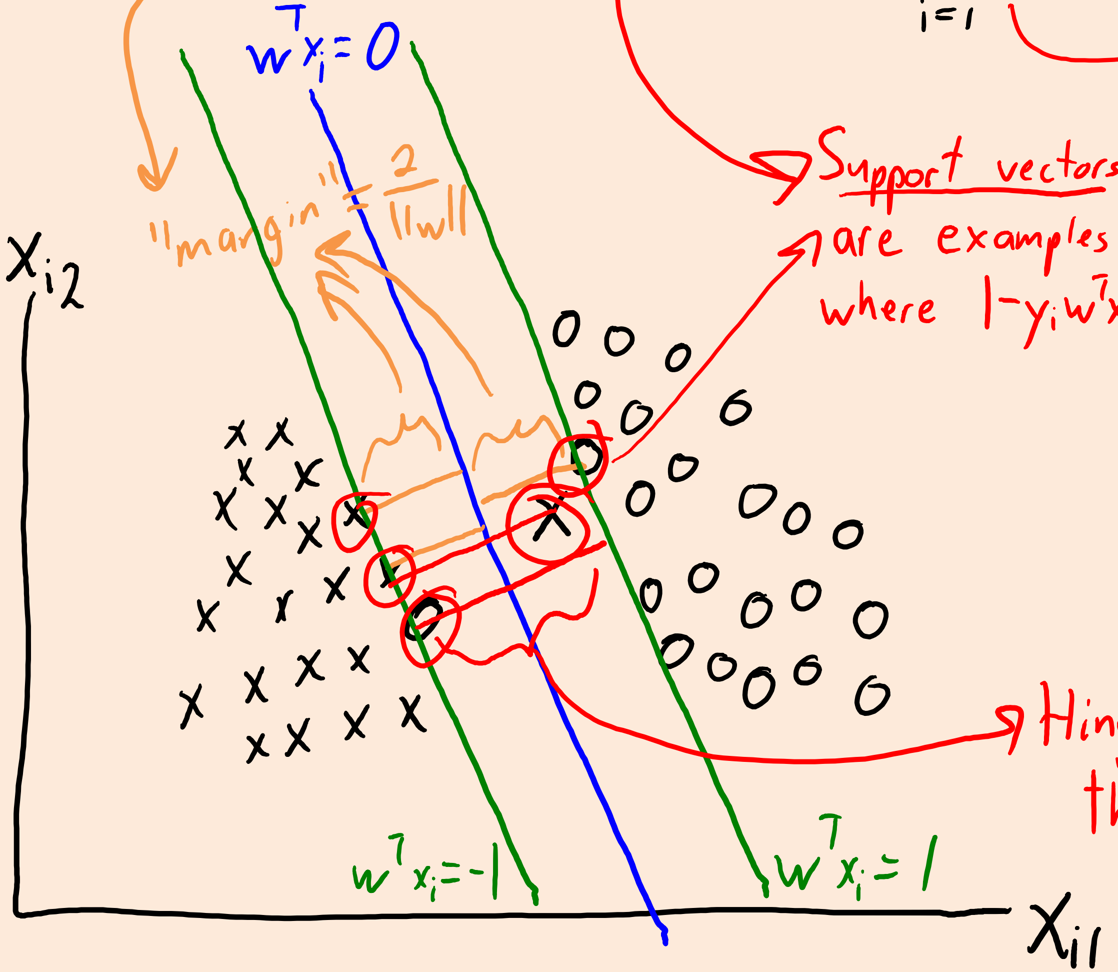
- Non-separable case:

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

Support vectors are examples 'i' where $1 - y_i w^T x_i \geq 0$

Hinge loss penalizes amount that $y_i w^T x_i \geq 1$ is violated.

λ controls trade-off between having large margin and classifying examples correctly.



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But, no concept of "support vectors" with logistic loss.

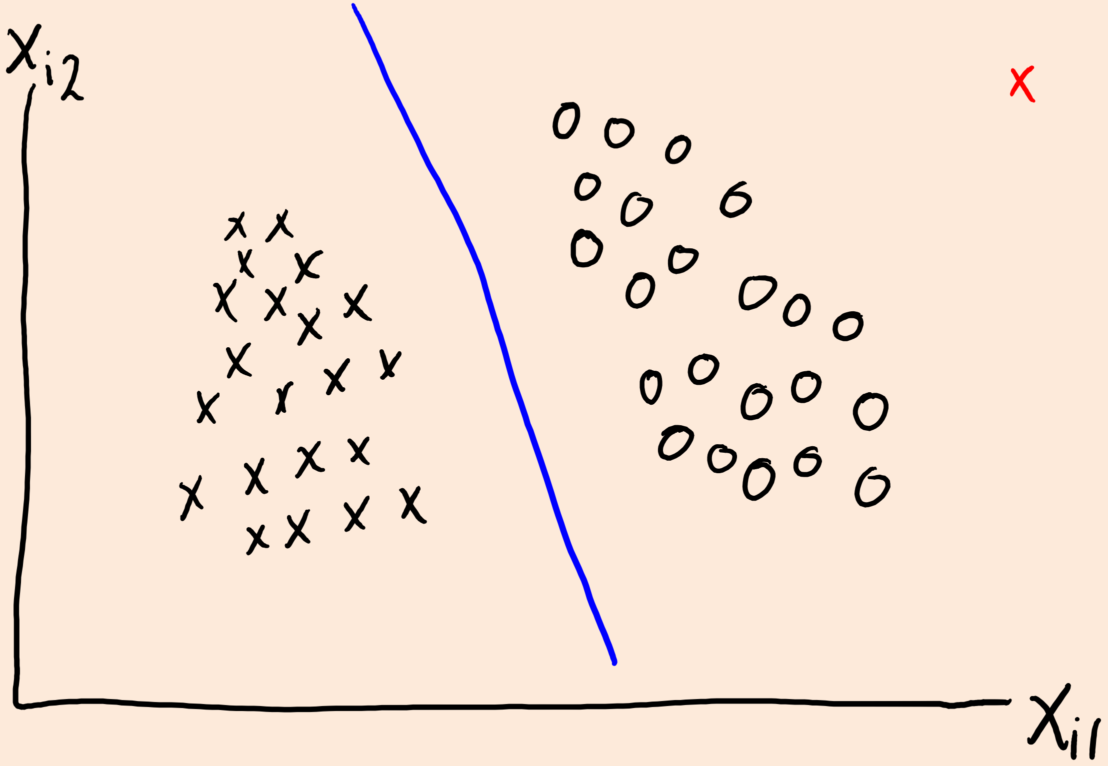
Summary

- Hinge loss is a convex upper bound on 0-1 loss.
  - SVMs add L2-regularization, can be viewed as "maximizing the margin".
- Logistic loss is a smooth convex approximation to the 0-1 loss.
  - "Logistic regression".
- SVMs and logistic regression are very widely-used.
  - A lot of ML consulting: "find good features, use L2-regularized logistic".
  - Both are just linear classifiers (a hyperplane dividing into two halfspaces).

- Next time:
  - A trick that lets you find gold and use polynomial basis with $d > 1$.

Robustness and Convex Approximations

- Because the hinge/logistic grow like absolute value for mistakes, they tend not to be affected by a small number of outliers.



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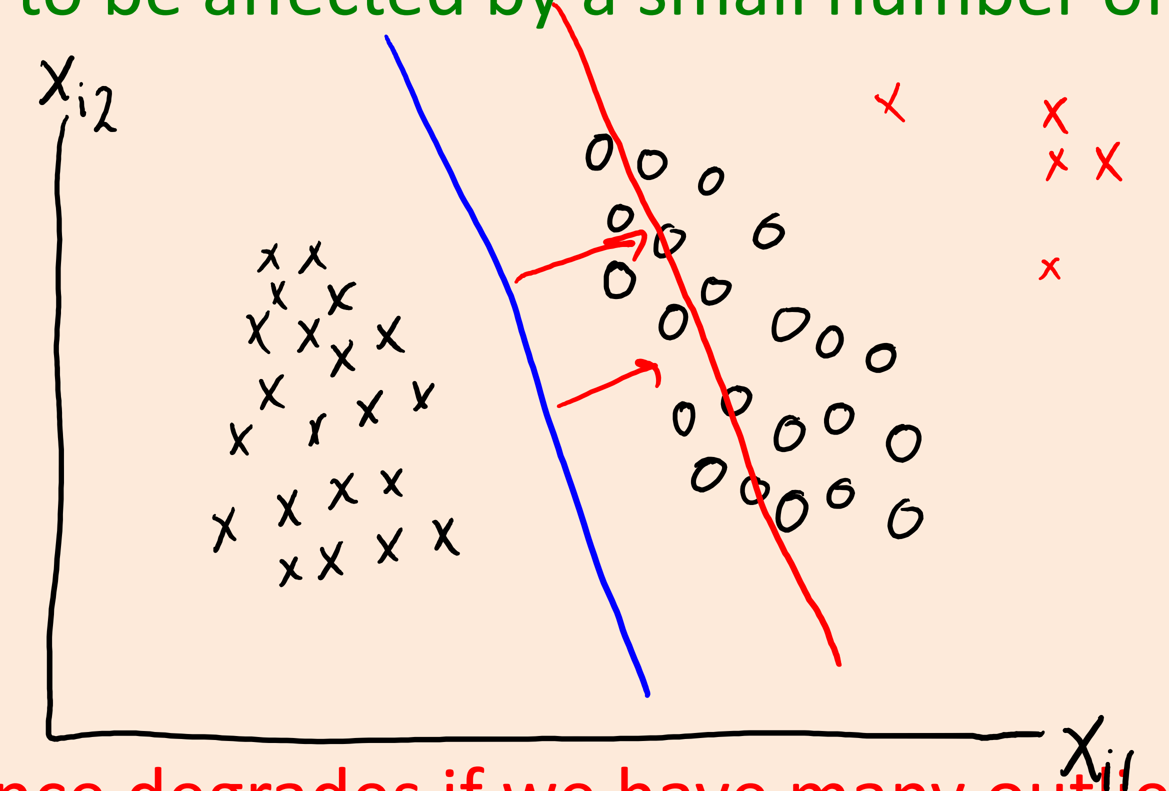
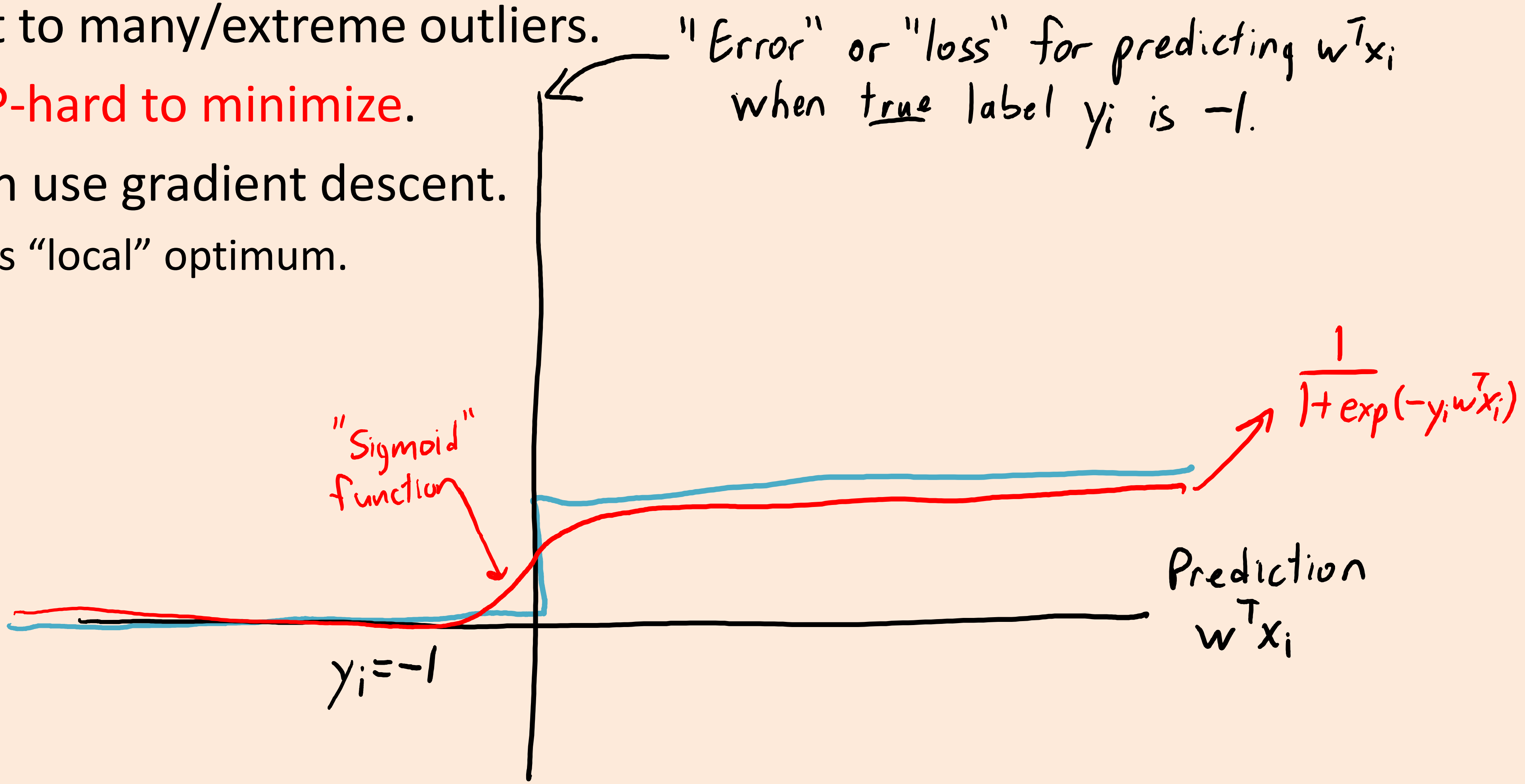


- But performance degrades if we have many outliers.

Non-Convex 0-1 Approximations

- There exists some smooth non-convex 0-1 approximations.
  - Robust to many/extreme outliers.
  - Still NP-hard to minimize.
  - But can use gradient descent.
    - Finds "local" optimum.



"Robust" Logistic Regression

- A recent idea: add a "fudge factor" v_i for each example.

$$f(w,v) = \sum_{i=1}^{n} \log(1 + \exp(-y_i w^T x_i + v_i))$$

- If $w^T x_i$ gets the sign wrong, we can "correct" the mis-classification by modifying v_i.
  - This makes the training error lower but doesn't directly help with test data, because we won't have the v_i for test data.
  - But having the v_i means the 'w' parameters don't need to focus as much on outliers (they can make $|v_i|$ big if sign($w^T x_i$) is very wrong).

"Robust" Logistic Regression

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- If $w^T x_i$ gets the sign wrong, we can "correct" the mis-classification by modifying v_i.
- A problem is that we can ignore the 'w' and get a tiny training error by just updating the v_i variables.
- But we want most v_i to be zero, so "robust logistic regression" puts an L1-regularizer on the v_i values:

$$f(w,v) = \sum_{i=1}^{n} \log(1+\exp(-y_i w^T x_i + v_i)) + \lambda\|v\|_1$$

- You would probably also want to regularize the 'w' with different λ.