Warm up: risk prediction with logistic regression

- Boss gives you a bunch of data on loans defaulting or not:

$$\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, \quad y_i \in \{-1, 1\}$$

- You model the data as: $$P(Y = y|x, w) = \frac{1}{1 + \exp(-y\, w^T x)}$$
- And compute the maximum likelihood estimator:

$$\widehat{w}_{MLE} = \arg\max_w \prod_{i=1}^n P(y_i|x_i, w)$$

For a new loan application x, boss recommends to give loan if your model says they will repay it with probability at least .95 (i.e. low risk):

Give loan to x if $\dfrac{1}{1 + \exp(-\widehat{w}_{MLE}^T x)} \geq .95$

- One year later only half of loans are paid back and the bank folds. What might have happened?

Projects

Proposal due Thursday 10/25

Guiding principles (for evaluation of project)

- Keep asking yourself "**why**" something works or not. Dig deeper than just evaluating the method and reporting a test error.
- Must use **real-world data** available NOW
- Must report **metrics**
- Must reference papers and/or books

- Study a real-world dataset
  - Evaluate multiple machine learning methods
  - Why does one work better than another? Form a hypothesis and test the hypothesis with a subset of the real data or, if necessary, synthetic data
- Study a method
  - Evaluate on multiple real-world datasets
  - Why does the method work better on one dataset versus another? Form a hypothesis…

Perceptron

Machine Learning – CSE546
Kevin Jamieson
University of Washington

October 23, 2018

Binary Classification

- **Learn:** f:**X —>**Y
  - **X** – features
  - Y – target classes

    $Y \in \{-1, 1\}$
- **Expected loss of f:**

$$\mathbb{E}_{XY}[\mathbf{1}\{f(X) \neq Y\}] = \mathbb{E}_X[\mathbb{E}_{Y|X}[\mathbf{1}\{f(x) \neq Y\}|X = x]]$$

$$\mathbb{E}_{Y|X}[\mathbf{1}\{f(x) \neq Y\}|X = x] = 1 - P(Y = f(x)|X = x)$$

- **Bayes optimal classifier:** $f(x) = \arg\max_y \mathbb{P}(Y = y|X = x)$

- **Loss function:**

$$\ell(f(x), y) = \mathbf{1}\{f(x) \neq y\}$$

Binary Classification

- **Learn**: f:**X** —>Y
  - **X** – features
  - Y – target classes

    $$Y \in \{-1, 1\}$$

- **Loss function:**

  $$\ell(f(x), y) = \mathbf{1}\{f(x) \neq y\}$$

- **Expected loss of f:**

$$\mathbb{E}_{XY}[\mathbf{1}\{f(X) \neq Y\}] = \mathbb{E}_X[\mathbb{E}_{Y|X}[\mathbf{1}\{f(x) \neq Y\}|X = x]]$$

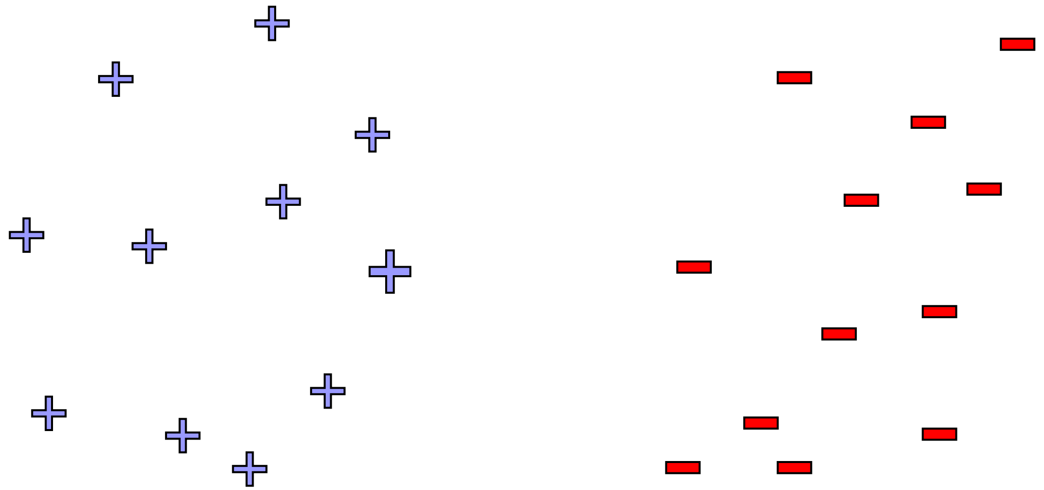
$$\mathbb{E}_{Y|X}[\mathbf{1}\{f(x) \neq Y\}|X = x] = 1 - P(Y = f(x)|X = x)$$

- **Bayes optimal classifier:** $$f(x) = \arg\max_y \mathbb{P}(Y = y|X = x)$$

- **Model of logistic regression:** $$P(Y = y|x, w) = \frac{1}{1 + \exp(-y\, w^T x)}$$

What if the model is wrong?

Binary Classification



Can we do classification without a model of $\mathbb{P}(Y = y|X = x)$?

The Perceptron Algorithm [Rosenblatt '58, '62]

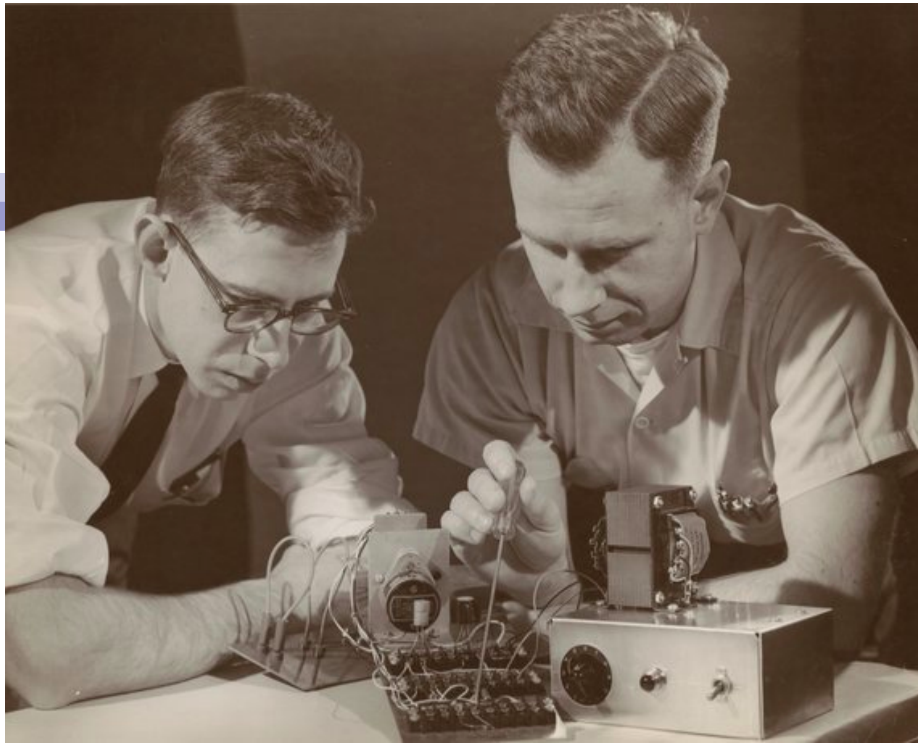
- Classification setting: y in {-1,+1}
- Linear model
  - Prediction:
- Training:
  - Initialize weight vector:
  - At each time step:
    - Observe features:
    - Make prediction:
    - Observe true class:
    - Update model:
      - If prediction is not equal to truth

The Perceptron Algorithm [Rosenblatt '58, '62]

- Classification setting: y in {-1,+1}
- Linear model
  - Prediction: $\text{sign}(w^T x_i + b)$

- Training:
  - Initialize weight vector: $w_0 = 0, b_0 = 0$
  - At each time step:
    - Observe features: x_k
    - Make prediction: $\text{sign}(x_k^T w_k + b_k)$
    - Observe true class: y_k
    - Update model:
      - If prediction is not equal to truth

$$\begin{bmatrix} w_{k+1} \\ b_{k+1} \end{bmatrix} = \begin{bmatrix} w_k \\ b_k \end{bmatrix} + y_k \begin{bmatrix} x_k \\ 1 \end{bmatrix}$$

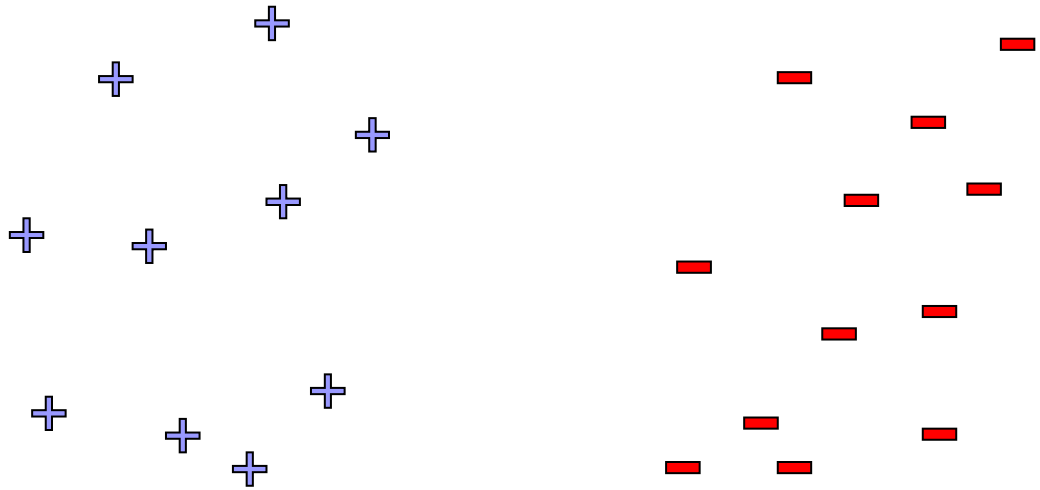


Rosenblatt 1957

"the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence."

The New York Times, 1958

Linear Separability



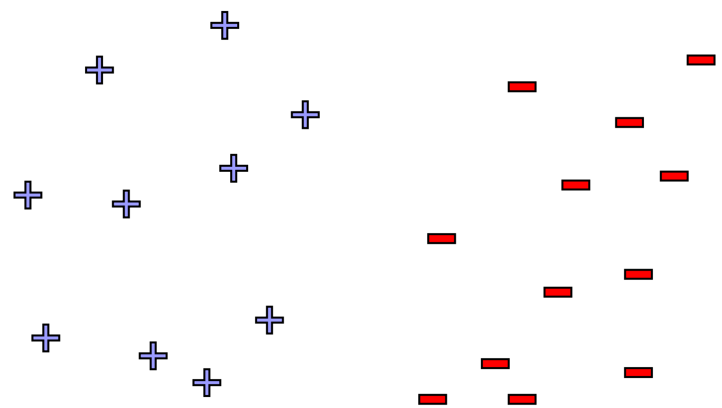
- Perceptron guaranteed to converge if
  - Data linearly separable:

Perceptron Analysis: Linearly Separable Case

- Theorem [Block, Novikoff]:
  - Given a sequence of labeled examples:
  - Each feature vector has bounded norm:
  - If dataset is linearly separable:
- Then the number of mistakes made by the online perceptron on any such sequence is bounded by

Beyond Linearly Separable Case

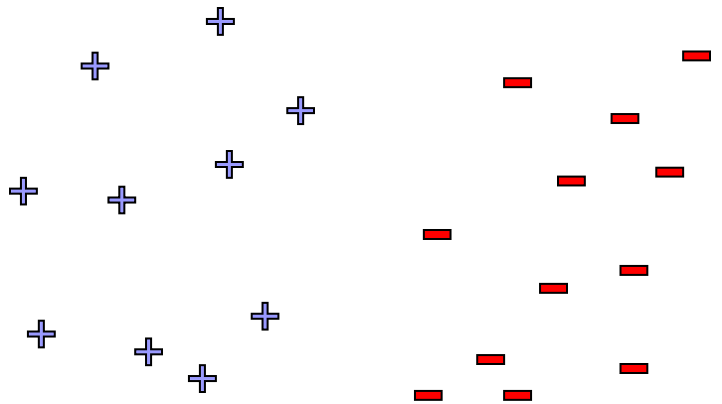
- Perceptron algorithm is super cool!
  - No assumption about data distribution!
    - Could be generated by an oblivious adversary, no need to be iid
  - Makes a fixed number of mistakes, and it's done for ever!
    - Even if you see infinite data



Beyond Linearly Separable Case

- Perceptron algorithm is super cool!
  - No assumption about data distribution!
    - Could be generated by an oblivious adversary, no need to be iid
  - Makes a fixed number of mistakes, and it's done for ever!
    - Even if you see infinite data

- Perceptron is useless in practice!
  - Real world not linearly separable
  - If data not separable, cycles forever and hard to detect
  - Even if separable may not give good generalization accuracy (small margin)



What is the Perceptron Doing???

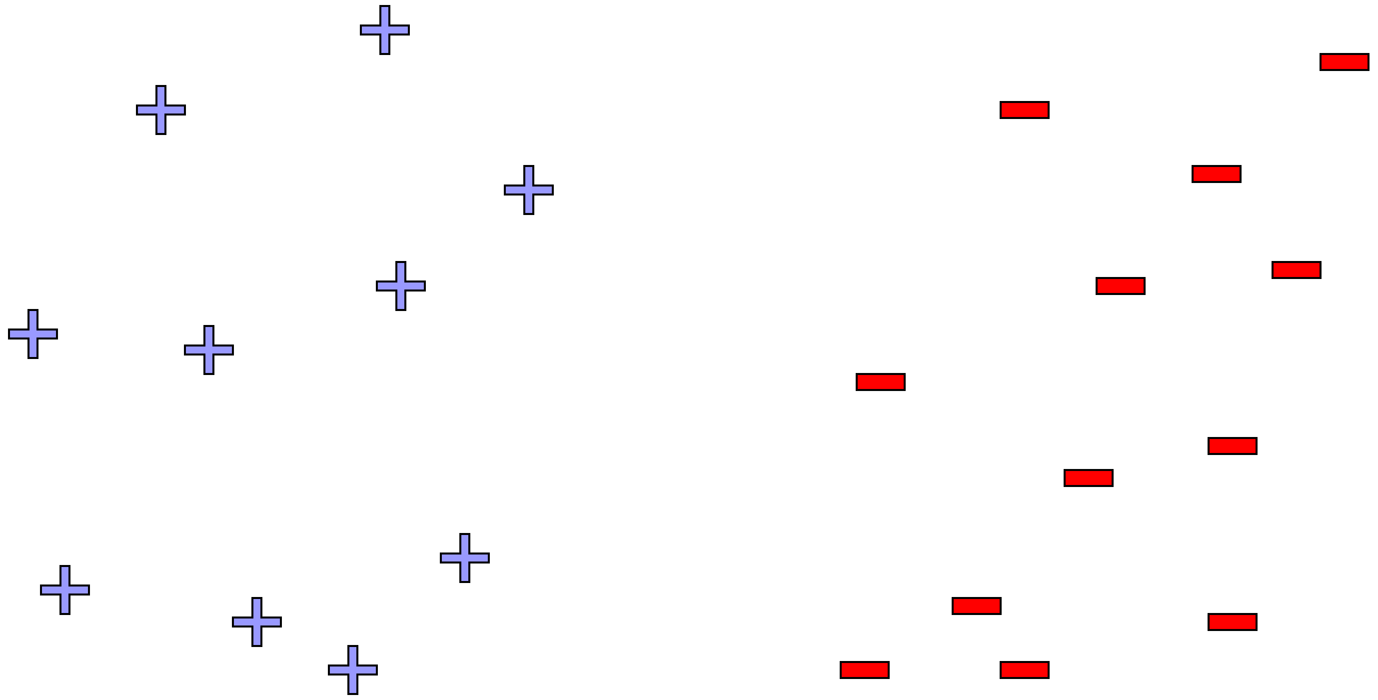
- When we discussed logistic regression:
  - Started from maximizing conditional log-likelihood
- When we discussed the Perceptron:
  - Started from description of an algorithm
- What is the Perceptron optimizing????

Support Vector Machines

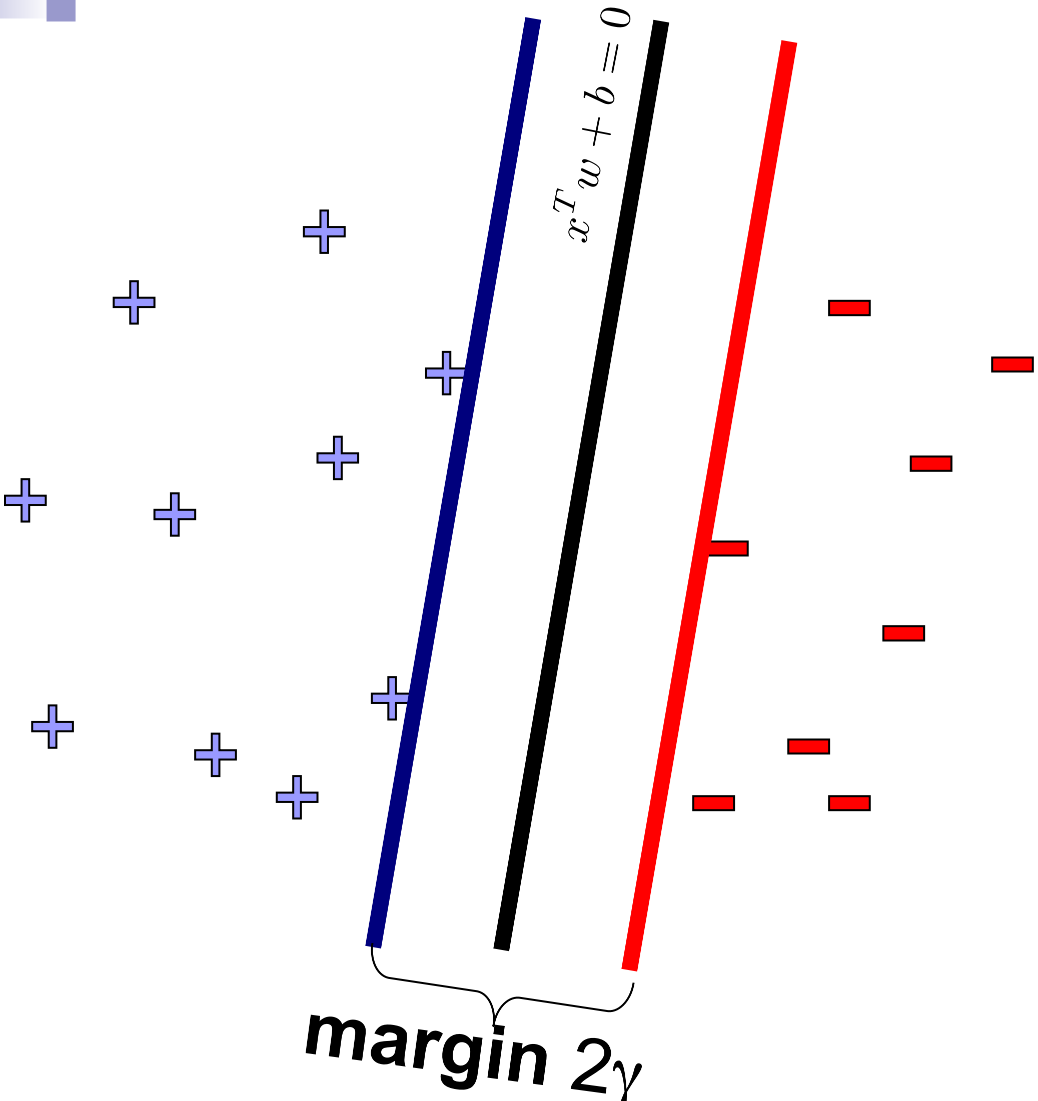
Machine Learning – CSE546
Kevin Jamieson
University of Washington

October 23, 2018

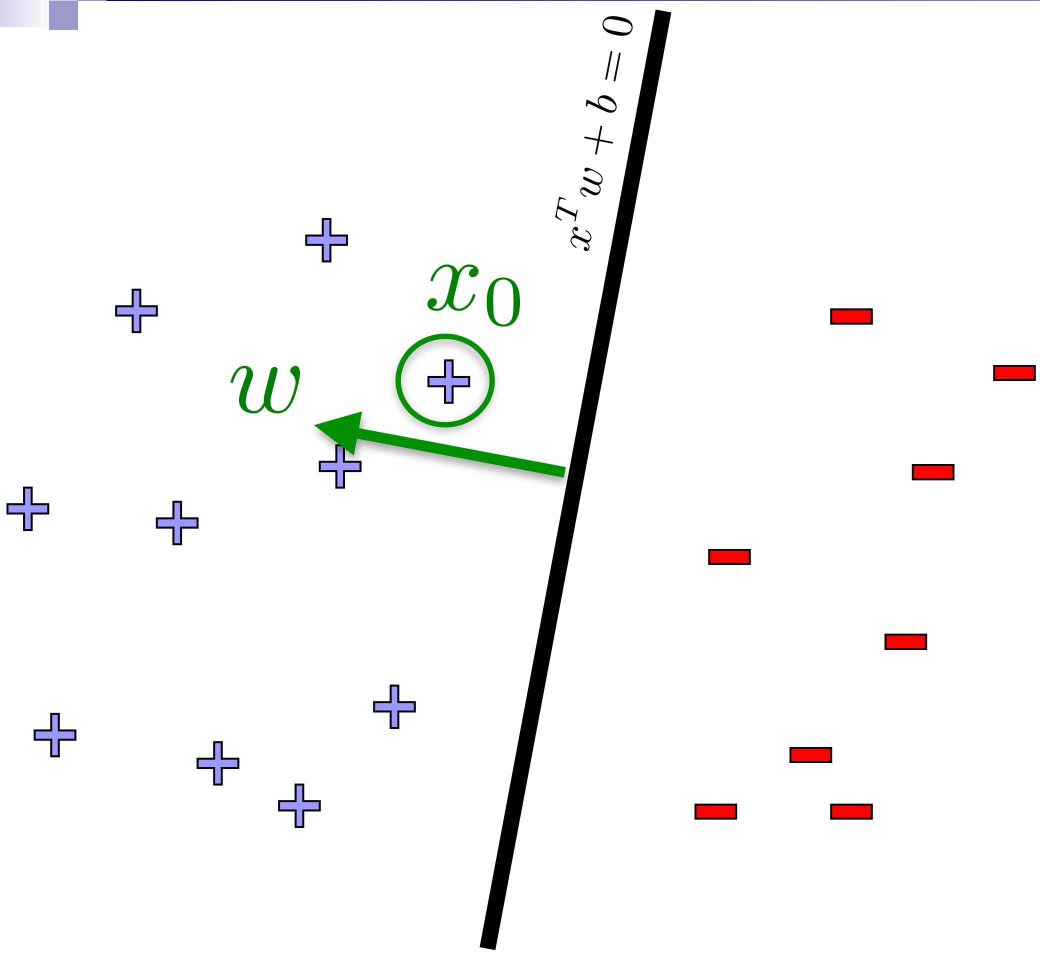
Linear classifiers – Which line is better?



Pick the one with the largest margin!

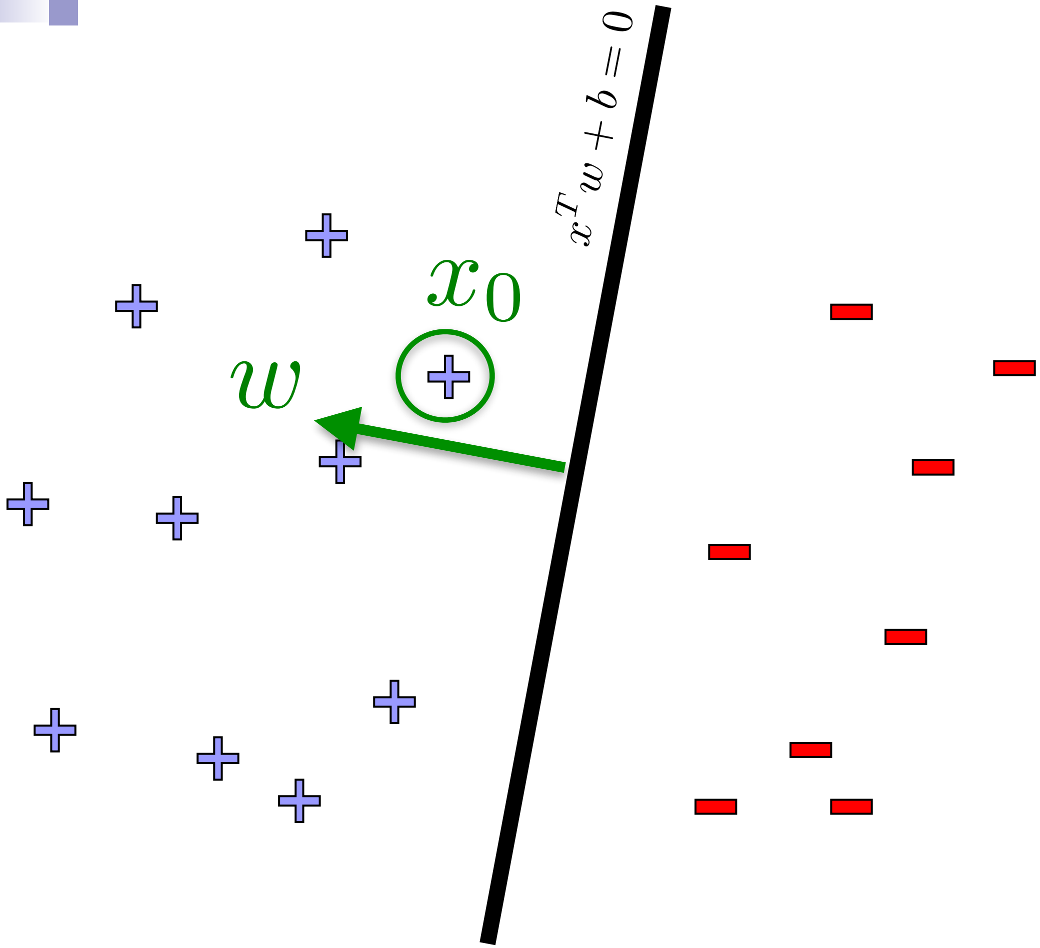


Pick the one with the largest margin!



Distance from x_0 to hyperplane defined by $x^T w + b = 0$?

Pick the one with the largest margin!



Distance from x_0 to hyperplane defined by $x^T w + b = 0$?

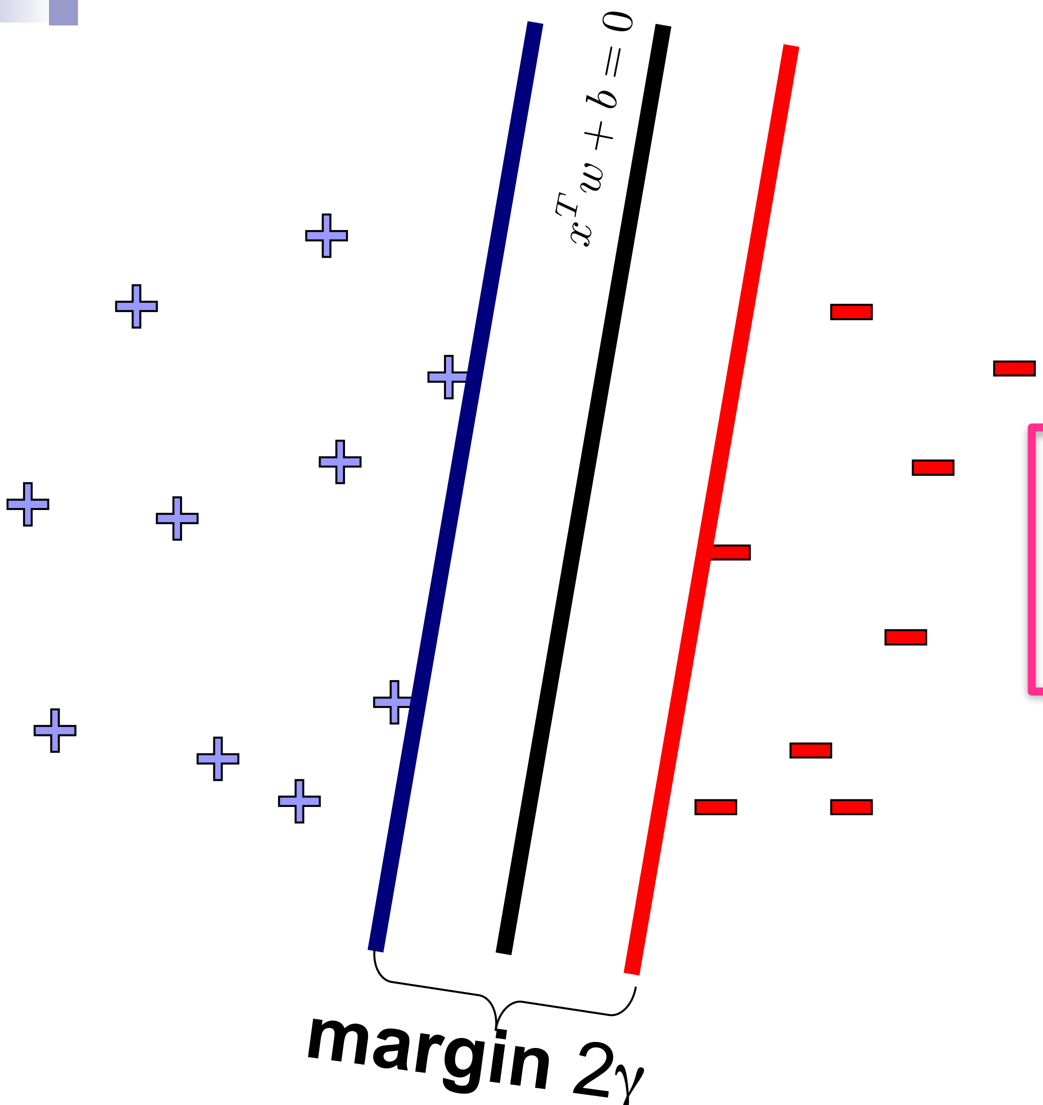
If $\widetilde{x}_0$ is the projection of x_0 onto the hyperplane then

$$||x_0 - \widetilde{x}_0||_2 = |(x_0^T - \widetilde{x}_0)^T \frac{w}{||w||_2}|$$

$$= \frac{1}{||w||_2} |x_0^T w - \widetilde{x}_0^T w|$$

$$= \frac{1}{||w||_2} |x_0^T w + b|$$

Pick the one with the largest margin!



Distance of x_0 from hyperplane x^Tw+b:

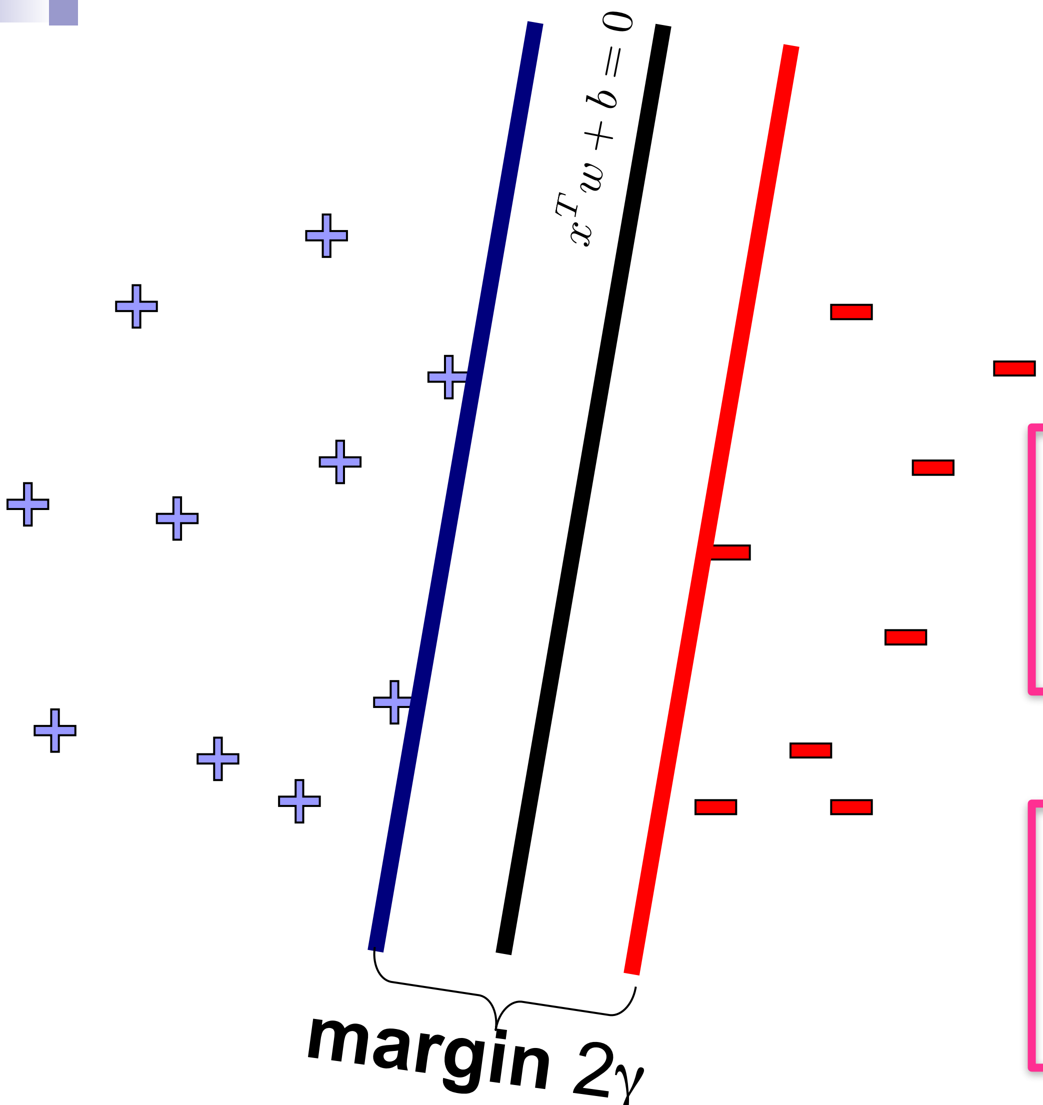
$$\frac{1}{||w||_2}(x_0^Tw+b)$$

Optimal Hyperplane

$$\max_{w,b} \gamma$$

$$\text{subject to } \frac{1}{||w||_2} y_i(x_i^Tw+b) \geq \gamma \quad \forall i$$

Pick the one with the largest margin!



Distance of x_0 from hyperplane $x^T w + b$:

$$\frac{1}{||w||_2}(x_0^T w + b)$$

Optimal Hyperplane

$$\max_{w,b} \gamma$$

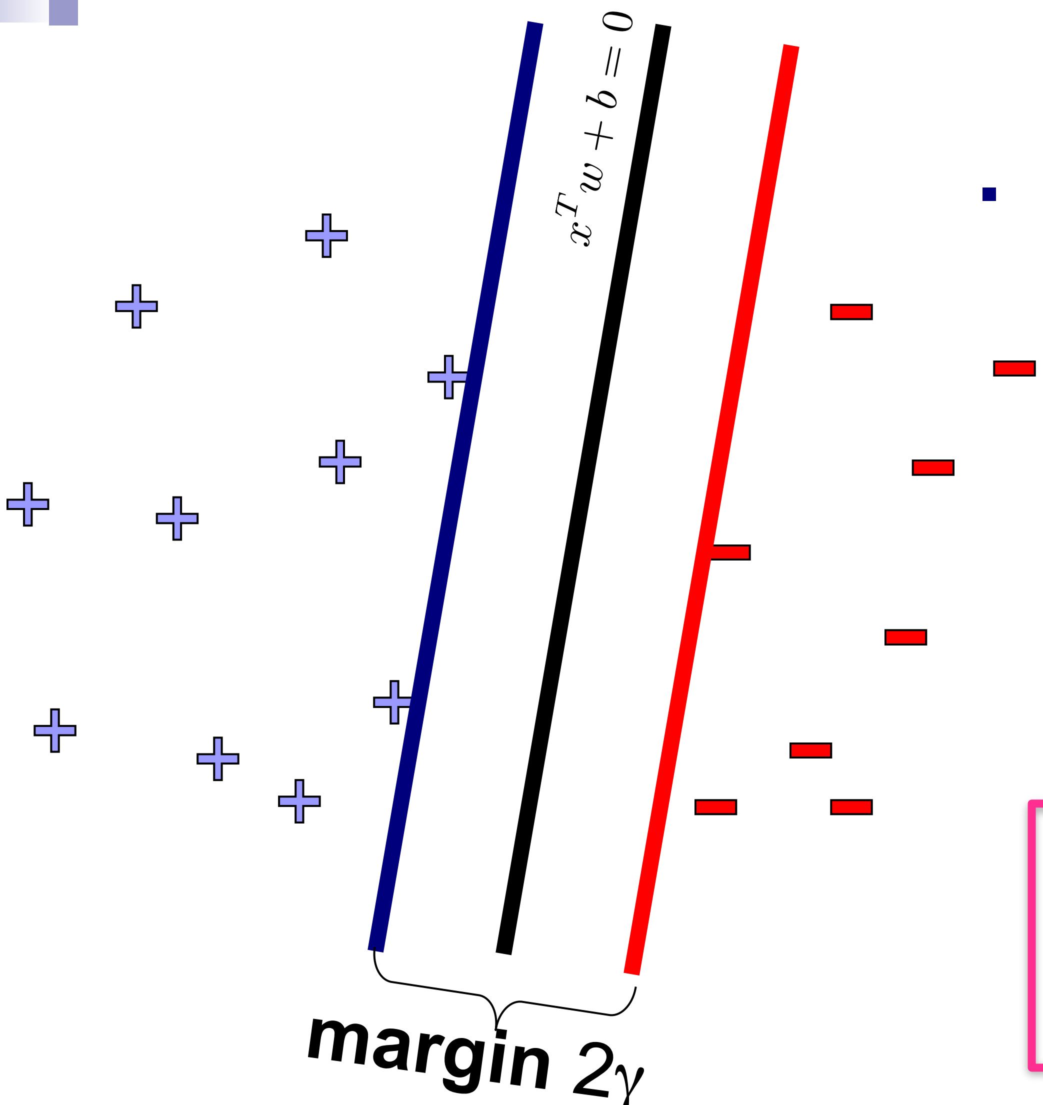
$$\text{subject to } \frac{1}{||w||_2} y_i (x_i^T w + b) \geq \gamma \quad \forall i$$

Optimal Hyperplane (reparameterized)

$$\min_{w,b} ||w||_2^2$$

$$\text{subject to } y_i (x_i^T w + b) \geq 1 \quad \forall i$$

Pick the one with the largest margin!

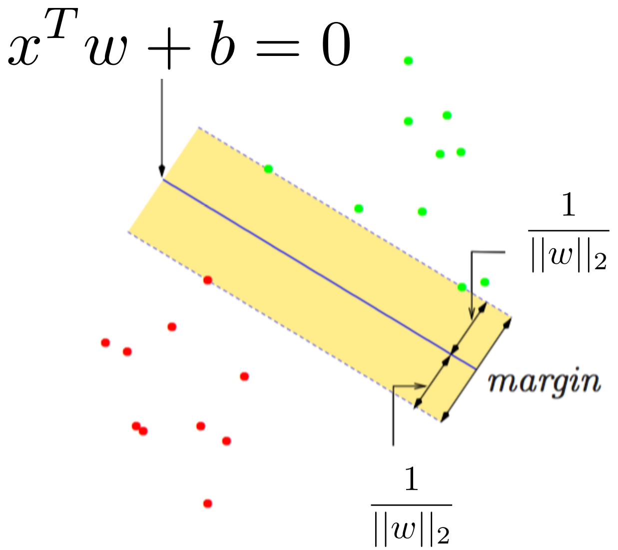


- Solve efficiently by many methods, e.g.,
  - quadratic programming (QP)
    - Well-studied solution algorithms
  - Stochastic gradient descent
  - Coordinate descent (in the dual)

Optimal Hyperplane (reparameterized)

$$\min_{w,b} ||w||_2^2$$
$$\text{subject to } y_i(x_i^T w + b) \geq 1 \quad \forall i$$

What if the data is still not linearly separable?

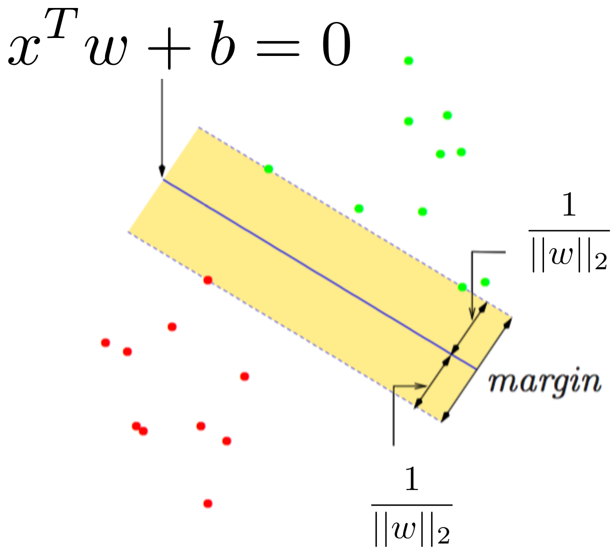


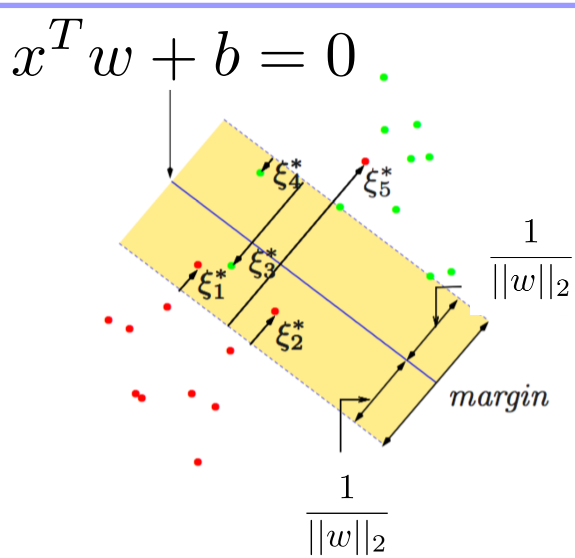
- If data is linearly separable

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 \quad \forall i$$

What if the data is still not linearly separable?





- If data is linearly separable

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 \quad \forall i$$

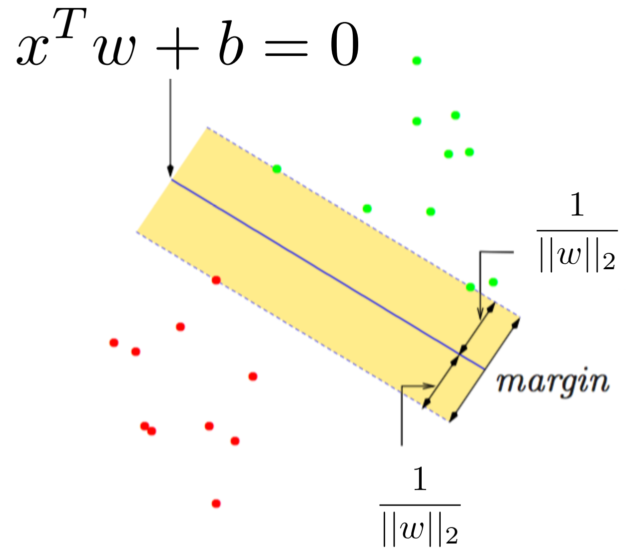
- If data is not linearly separable, some points don't satisfy margin constraint:

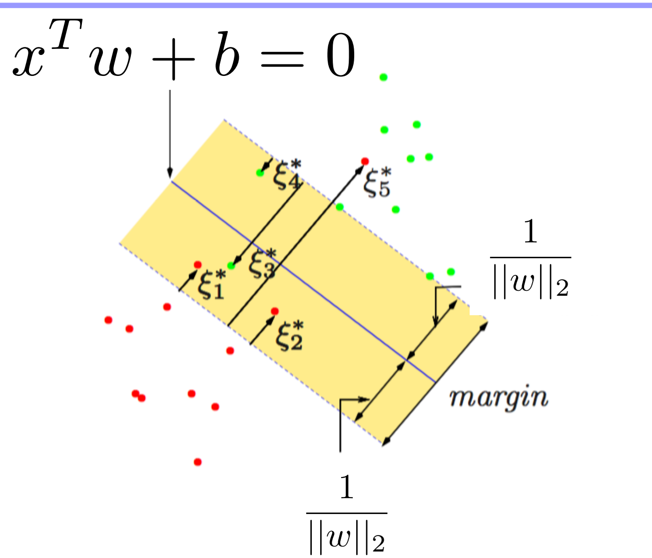
$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 - \xi_i \quad \forall i$$

$$\xi_i \geq 0, \sum_{j=1}^{n} \xi_j \leq \nu$$

What if the data is still not linearly separable?





- If data is linearly separable

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 \quad \forall i$$

- If data is not linearly separable, some points don't satisfy margin constraint:

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 - \xi_i \quad \forall i$$

$$\xi_i \geq 0, \sum_{j=1}^{n} \xi_j \leq \nu$$

- What are "support vectors?"

SVM as penalization method

- Original quadratic program with linear constraints:

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 - \xi_i \quad \forall i$$

$$\xi_i \geq 0, \sum_{j=1}^n \xi_j \leq \nu$$

SVM as penalization method

- Original quadratic program with linear constraints:

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 - \xi_i \quad \forall i$$

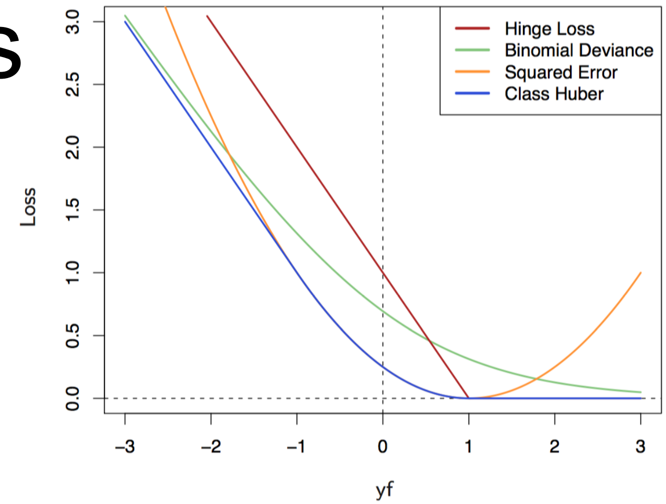
$$\xi_i \geq 0, \sum_{j=1}^n \xi_j \leq \nu$$

- Using same constrained convex optimization trick as for lasso:

For any $\nu \geq 0$ there exists a $\lambda \geq 0$ such that the solution the following solution is equivalent:

$$\boxed{\sum_{i=1}^n \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2}$$

Machine Learning Problems



- Have a bunch of iid data of the form:

$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- Learning a model's parameters:

$$\sum_{i=1}^n \ell_i(w)$$

Each $\ell_i(w)$ is convex.

Hinge Loss: $\ell_i(w) = \max\{0, 1 - y_i x_i^T w\}$

Logistic Loss: $\ell_i(w) = \log(1 + \exp(-y_i\, x_i^T w))$

Squared error Loss: $\ell_i(w) = (y_i - x_i^T w)^2$

How do we solve for *w*? The last two lectures!

Perceptron is optimizing what?

Perceptron update rule:

$$\begin{bmatrix} w_{k+1} \\ b_{k+1} \end{bmatrix} = \begin{bmatrix} w_k \\ b_k \end{bmatrix} + y_k \begin{bmatrix} x_k \\ 1 \end{bmatrix} \mathbf{1}\{y_i(b + x_i^T w) < 0\}$$

SVM objective:

$$\boxed{\sum_{i=1}^n \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2 \ = \sum_{i=1}^n \ell_i(w, b)}$$

$$\nabla_w \ell_i(w, b) =$$

Perceptron is optimizing what?

Perceptron update rule:

$$\begin{bmatrix} w_{k+1} \\ b_{k+1} \end{bmatrix} = \begin{bmatrix} w_k \\ b_k \end{bmatrix} + y_k \begin{bmatrix} x_k \\ 1 \end{bmatrix} \mathbf{1}\{y_i(b + x_i^T w) < 0\}$$

SVM objective:

$$\boxed{\sum_{i=1}^n \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2 \;=\; \sum_{i=1}^n \ell_i(w,b)}$$

$$\nabla_w \ell_i(w,b) = \begin{cases} -x_i y_i + \frac{2\lambda}{n} w & \text{if } y_i(b + x_i^T w) < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\nabla_b \ell_i(w,b) = \begin{cases} -y_i & \text{if } y_i(b + x_i^T w) < 1 \\ 0 & \text{otherwise} \end{cases}$$

Perceptron is just SGD on SVM with $\lambda = 0$, $\eta = 1$!

SVMs vs logistic regression

- We often want probabilities/confidences, logistic wins here?

SVMs vs logistic regression

- We often want probabilities/confidences, logistic wins here?
- No! Perform isotonic regression or non-parametric bootstrap for probability calibration. Predictor gives some score, how do we transform that score to a probability?

SVMs vs logistic regression

- We often want probabilities/confidences, logistic wins here?
- No! Perform isotonic regression or non-parametric bootstrap for probability calibration. Predictor gives some score, how do we transform that score to a probability?

- For classification loss, logistic and svm are comparable
- Multiclass setting:
  - Softmax naturally generalizes logistic regression
  - SVMs have
- What about good old least squares?

What about multiple classes?