Binary Classification / Perceptron

Nicholas Ruozzi

University of Texas at Dallas

Slides adapted from David Sontag and Vibhav Gogate

Reminders

- Homework 1 is available on eLearning and due in 2 weeks
  - Late homework will not be accepted
- Instructions for getting started with the course, e.g., joining Piazza, are on eLearning
- Office hours are happening this week
  - Prof. (blackboard) T 1:30pm-2:30pm, W 11:00am-12:00pm

Supervised Learning

- **Input:** $\left(x^{(1)}, y^{(1)}\right), \ldots, (x^{(M)}, y^{(M)})$
  - $x^{(m)}$ is the m^{th} data item and $y^{(m)}$ is the m^{th} **label**

- **Goal:** find a function f such that $f\left(x^{(m)}\right)$ is a "good approximation" to $y^{(m)}$
  - Can use it to predict y values for previously unseen x values

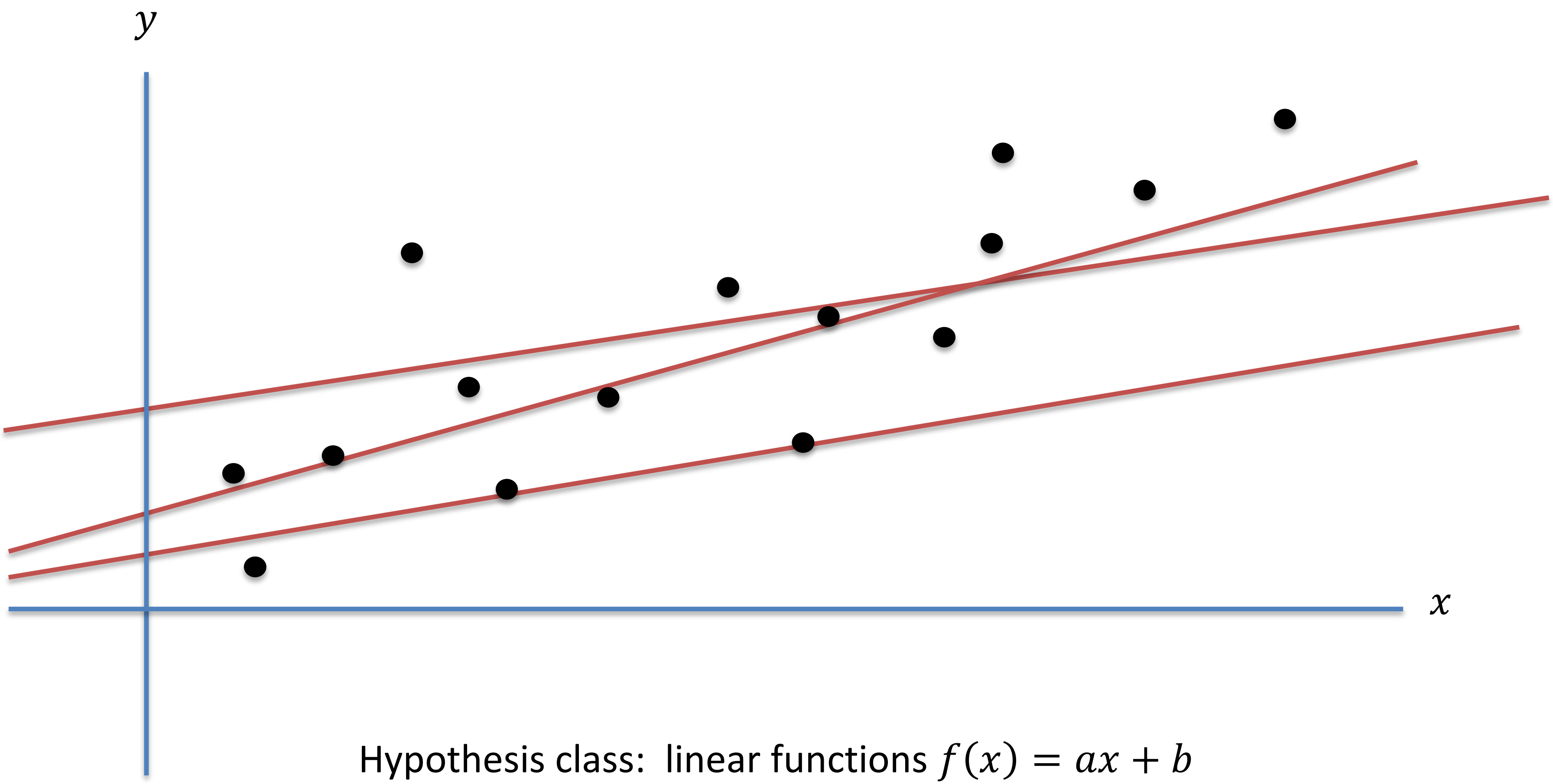
Supervised Learning

- Hypothesis space: set of allowable functions $f : X \to Y$

- Goal: find the "best" element of the hypothesis space

  - How do we measure the quality of f?

Regression



Hypothesis class: linear functions $f(x) = ax + b$

How do we measure the quality of the approximation?

Linear Regression

- In typical regression applications, measure the fit using a squared loss function

$$L(f) = \frac{1}{M}\sum_{m}\left(f\left(x^{(m)}\right) - y^{(m)}\right)^2$$

- Want to minimize the average loss on the training data

- For 2-D linear regression, the learning problem is then

$$\min_{a,b}\frac{1}{M}\sum_{m}\left(ax^{(m)} + b\ - y^{(m)}\right)^2$$

- For an unseen data point, x, the learning algorithm predicts $f(x)$

Supervised Learning

- **Select a hypothesis space** (elements of the space are represented by a collection of parameters)
- **Choose a loss function** (evaluates quality of the hypothesis as a function of its parameters)
- **Minimize loss function, e.g., using gradient descent** (minimization over the parameters)
- **Evaluate quality of the learned model using test data** – that is, data on which the model was not trained

Binary Classification

- Regression operates over a continuous set of outcomes
- Suppose that we want to learn a function $f : X \to \{0,1\}$
- As an example:

	$\boldsymbol{x_1}$	$\boldsymbol{x_2}$	x_3	y
1	0	0	1	0
2	0	1	0	1
3	1	1	0	1
4	1	1	1	0

How do we pick the hypothesis space?

How do we find the best f in this space?

Binary Classification

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How many functions with three binary inputs and one binary output are there?

Binary Classification

	x_1	x_2	x_3	y
	0	0	0	?
1	0	0	1	0
2	0	1	0	1
	0	1	1	?
	1	0	0	?
	1	0	1	?
3	1	1	0	1
4	1	1	1	0

2^8 possible functions

2^4 are consistent with the observations

How do we choose the best one?

What if the observations are noisy?

Challenges in ML

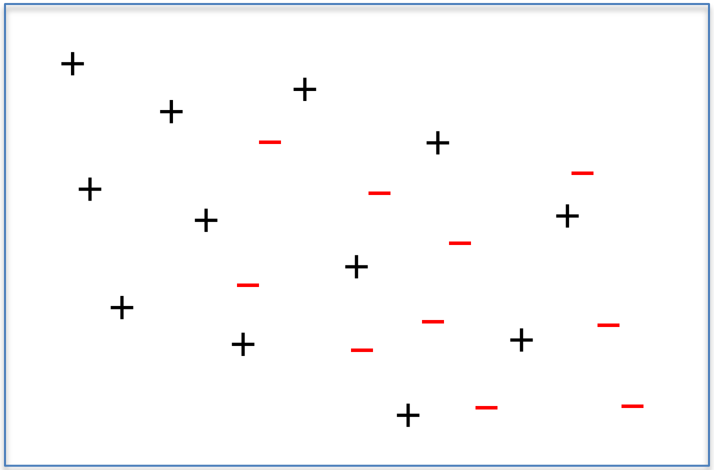
- How to choose the right hypothesis space?
  - Number of factors influence this decision: difficulty of learning over the chosen space, how expressive the space is, …
- How to evaluate the quality of our learned hypothesis?
  - Prefer "simpler" hypotheses (to prevent overfitting)
  - Want the outcome of learning to generalize to unseen data

Binary Classification

- Input $\left(x^{(1)}, y^{(1)}\right), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$

- We can think of the observations as points in $\mathbb{R}^n$ with an associated sign (either +/- corresponding to 0/1)

- An example with $n = 2$



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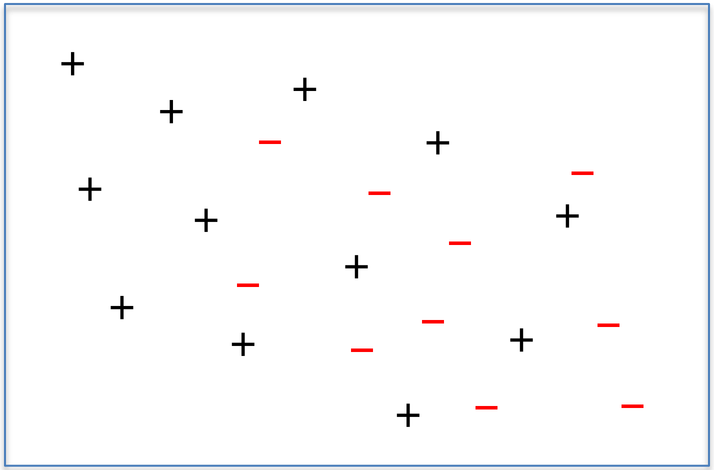
What is a good hypothesis space for this problem?



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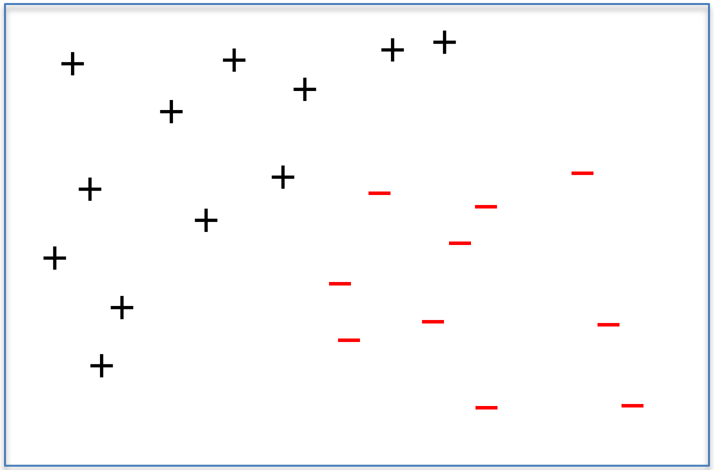

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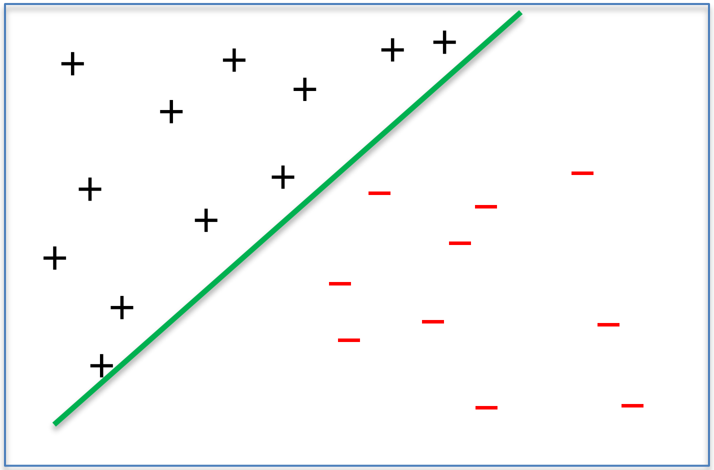
Binary Classification

- Input $\left(x^{(1)}, y^{(1)}\right), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$

- We can think of the observations as points in $\mathbb{R}^n$ with an associated sign (either +/- corresponding to 0/1)

- An example with $n = 2$

In this case, we say that the observations are linearly separable



Linear Separators

- In n dimensions, a hyperplane is a solution to the equation

$$w^T x + b = 0$$

with $w \in \mathbb{R}^n, b \in \mathbb{R}$

- Hyperplanes divide $\mathbb{R}^n$ into two distinct sets of points (called open halfspaces)

$$w^T x + b > 0$$

$$w^T x + b < 0$$

Binary Classification

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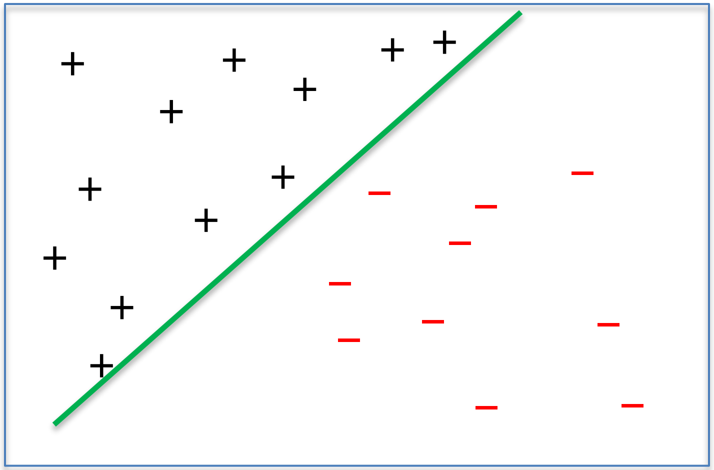

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The Linearly Separable Case

- Given $\left(x^{(1)}, y^{(1)}\right), \ldots$ with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$
- Hypothesis space: separating hyperplanes

$$f(x) = sign\ (w^T x + b)$$

- How should we choose the loss function?

The Linearly Separable Case

- Given $(x^{(1)}, y^{(1)}), \ldots$ with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$
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$$f(x) = sign\ (w^T x + b)$$

- How should we choose the loss function?
  - Count the number of misclassifications

$$loss = \sum_m \left| y^{(m)} - sign(w^T x^{(m)} + b) \right|$$

    - Tough to optimize, gradient contains no information

The Linearly Separable Case

- Given $\left(x^{(1)}, y^{(1)}\right)$, … with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$
- Hypothesis space: separating hyperplanes

$$f(x) = sign\ (w^T x + b)$$

- How should we choose the loss function?
  - Penalize misclassification linearly by the size of the violation

$$perceptron\ loss = \sum_m \max\left\{0, -y^{(m)}(w^T x^{(m)} + b)\right\}$$

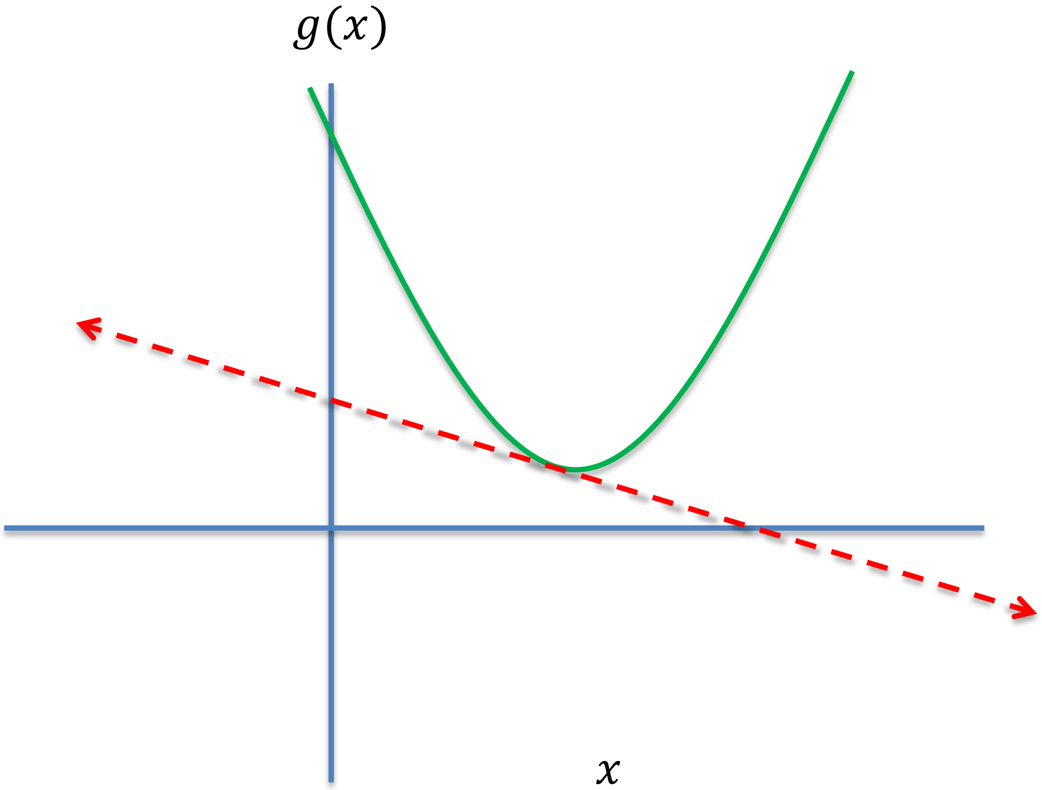
  - Modified hinge loss (convex but not differentiable)

The Perceptron Algorithm

- Try to minimize the perceptron loss using gradient descent
  - The perceptron loss isn't differentiable, how can we apply gradient descent?
  - Need a generalization of what it means to be the gradient of a **convex** function

Gradients of Convex Functions

- For a differentiable convex function $g(x)$ its gradients are **linear underestimators**



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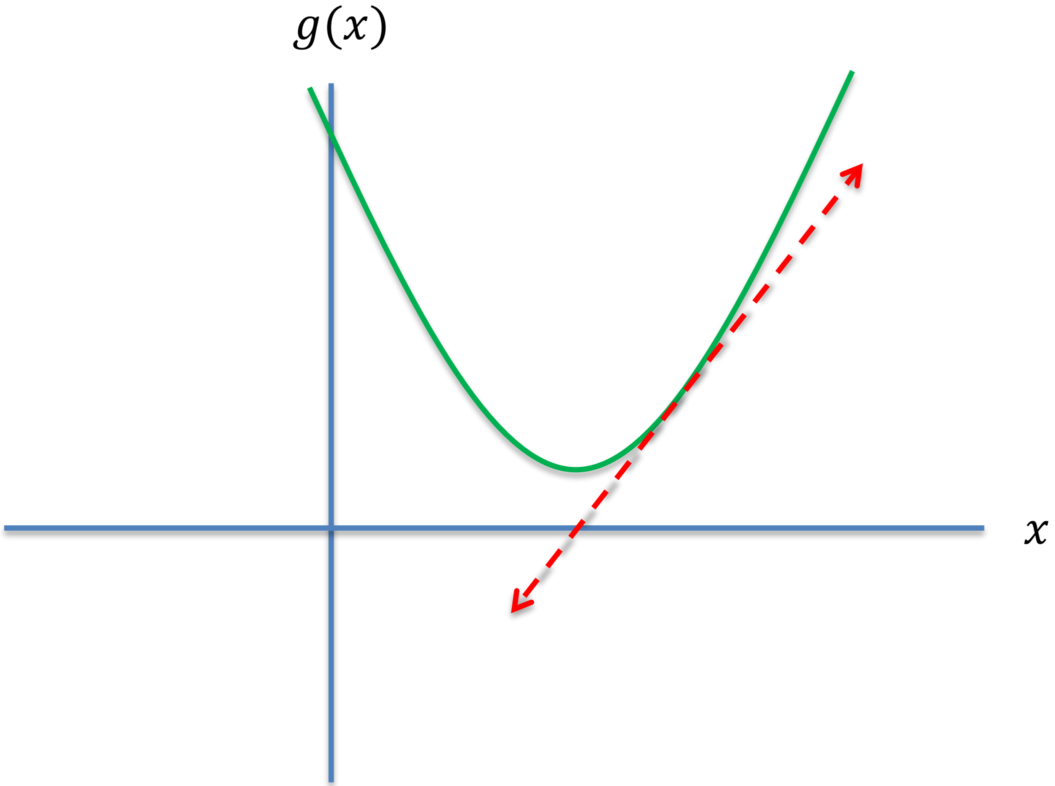
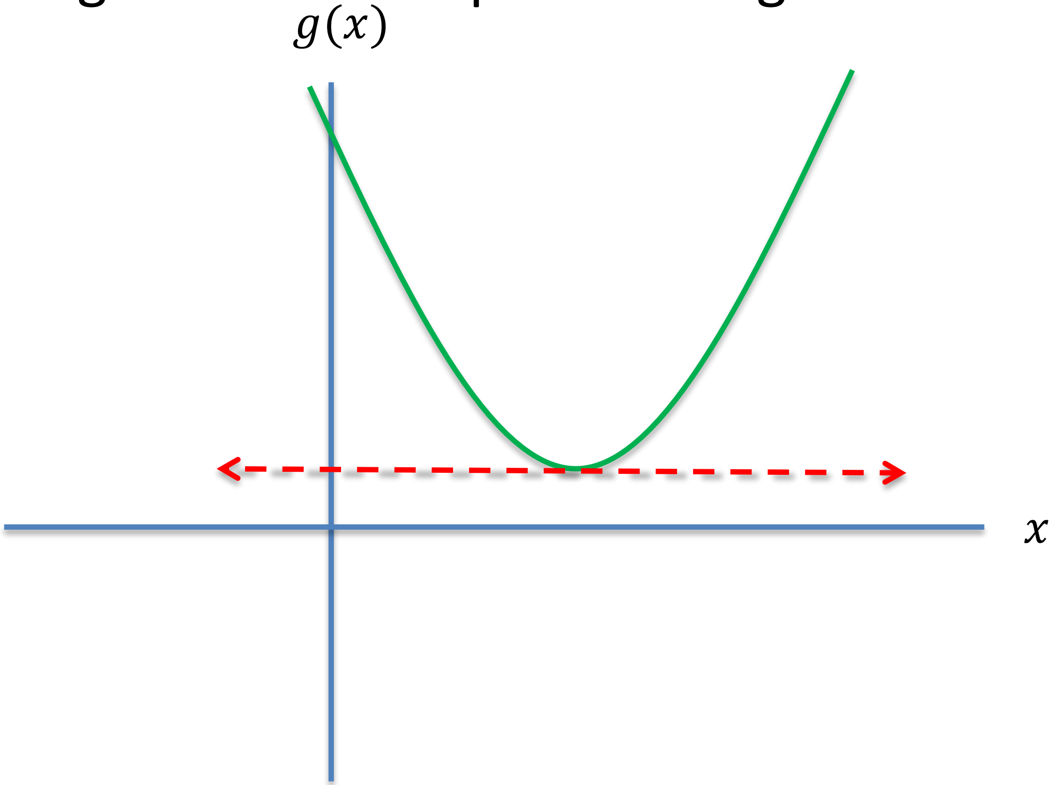


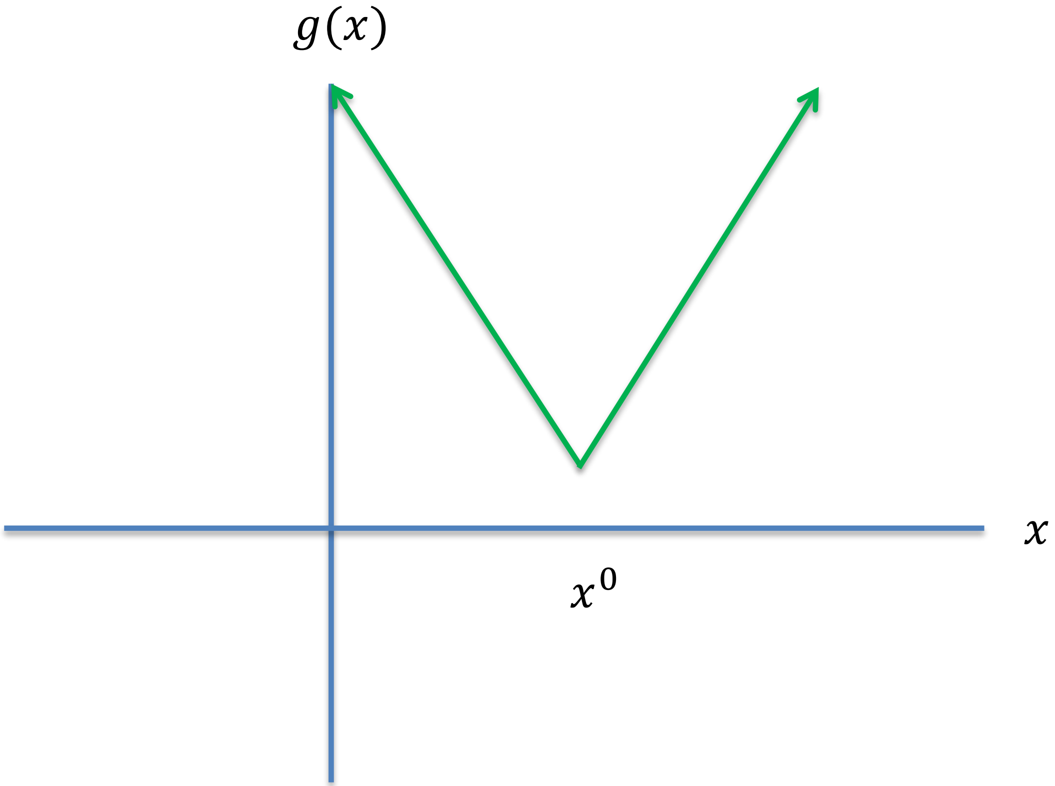
Gradients of Convex Functions

- For a differentiable convex function $g(x)$ its gradients are **linear underestimators**: zero gradient corresponds to a global optimum



Subgradients

- For a convex function $g(x)$, a subgradient at a point x^0 is given by any line, l, such that $l(x^0) = g(x^0)$ and $l(x) \leq g(x)$ for all x, i.e., it is a linear underestimator



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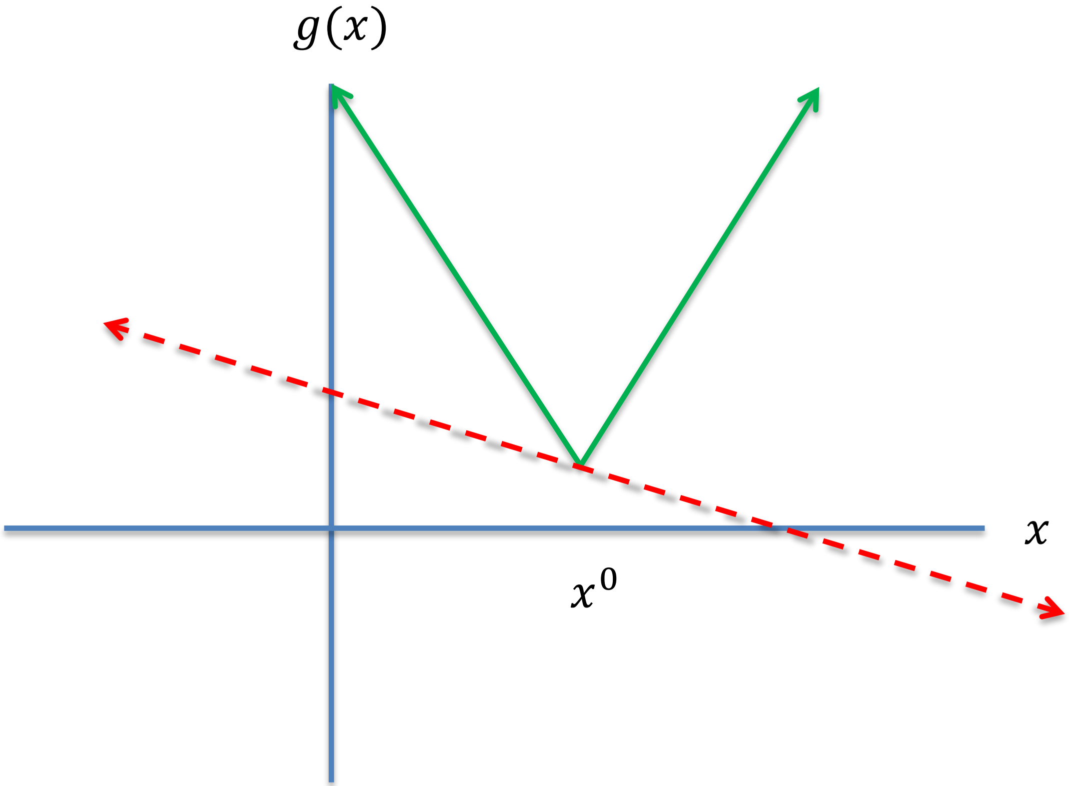

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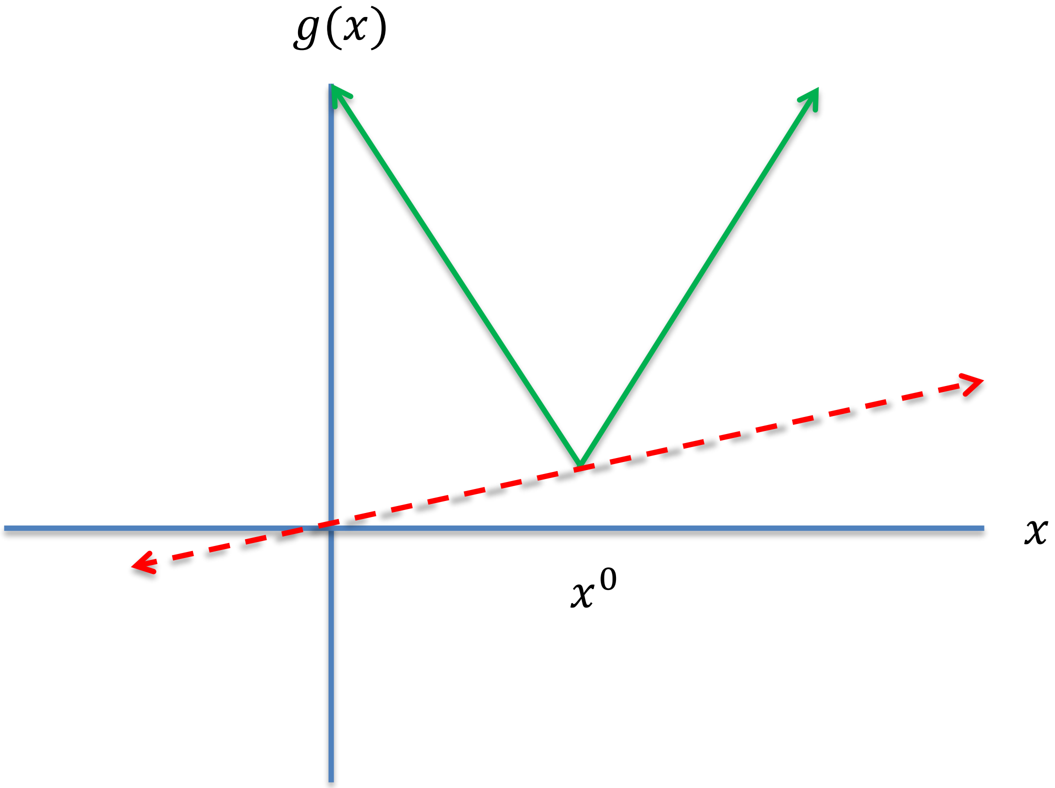

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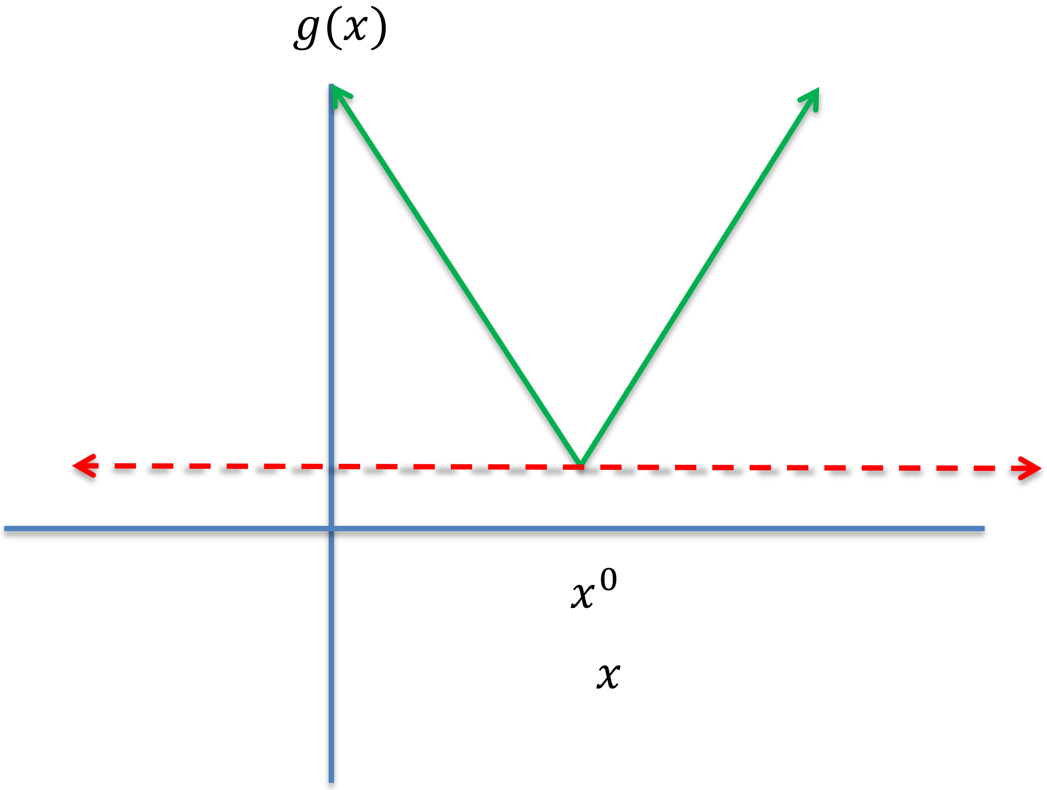
If $\vec{0}$ is a subgradient at x^0, then x^0 is a global minimum



Subgradients

- If a convex function is differentiable at a point x, then it has a unique subgradient at the point x given by the gradient

- If a convex function is not differentiable at a point x, it can have many subgradients

  - E.g., the set of subgradients of the convex function $|x|$ at the point $x = 0$ is given by the set of slopes $[-1,1]$

- Subgradients only guaranteed to exist for convex functions

The Perceptron Algorithm

$$perceptron\ loss = \sum_m \max\{0, -y^{(m)}(w^T x^{(m)} + b)\}$$

- Try to minimize the perceptron loss using (sub)gradient descent

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$$perceptron\ loss = \sum_m \max\{0, -y^{(m)}(w^T x^{(m)} + b)\}$$

- Try to minimize the perceptron loss using (sub)gradient descent

$$\nabla_w(perceptron\ loss) = -\sum_{m=1}^{M} \left(y^{(m)} x^{(m)} \cdot 1_{-y^{(m)} f_{w,b}(x^{(m)}) \geq 0}\right)$$

$$\nabla_b(perceptron\ loss) = -\sum_{m=1}^{M} \left(y^{(m)} \cdot 1_{-y^{(m)} f_{w,b}(x^{(m)}) \geq 0}\right)$$

The Perceptron Algorithm

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$$\nabla_b(perceptron\ loss) = -\sum_{m=1}^{M}\left(y^{(m)} \cdot 1_{-y^{(m)}f_{w,b}(x^{(m)})\geq 0}\right)$$

Is equal to zero if the m^{th} data point is correctly classified and one otherwise

The Perceptron Algorithm

- Try to minimize the perceptron loss using (sub)gradient descent

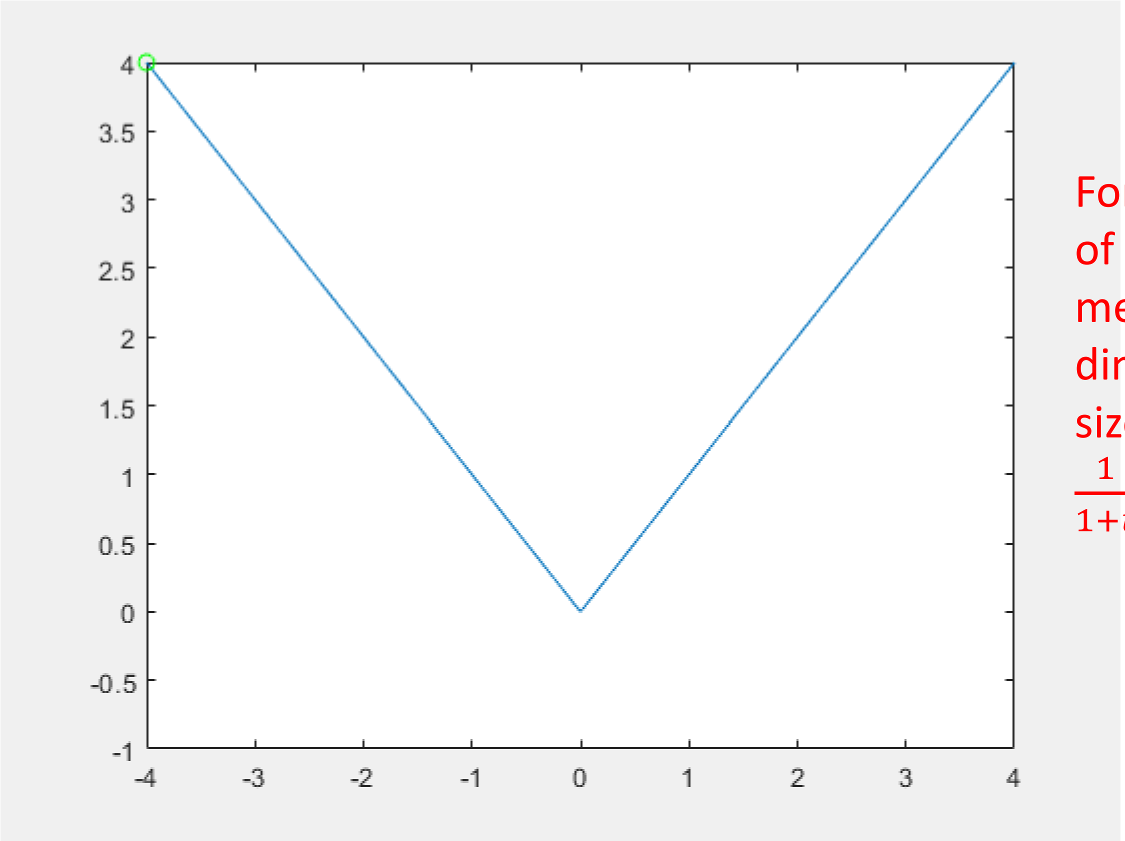
$$w^{(t+1)} = w^{(t)} + \gamma_t \sum_{m=1}^{M} \left(y^{(m)} x^{(m)} \cdot 1_{-y^{(m)} f_{w,b}\left(x^{(m)}\right) \geq 0} \right)$$

$$b^{(t+1)} = b^{(t)} + \gamma_t \sum_{m=1}^{M} \left(y^{(m)} \cdot 1_{-y^{(m)} f_{w,b}\left(x^{(m)}\right) \geq 0} \right)$$

- With step size γ_t (also called the learning rate)

Subgradient Descent

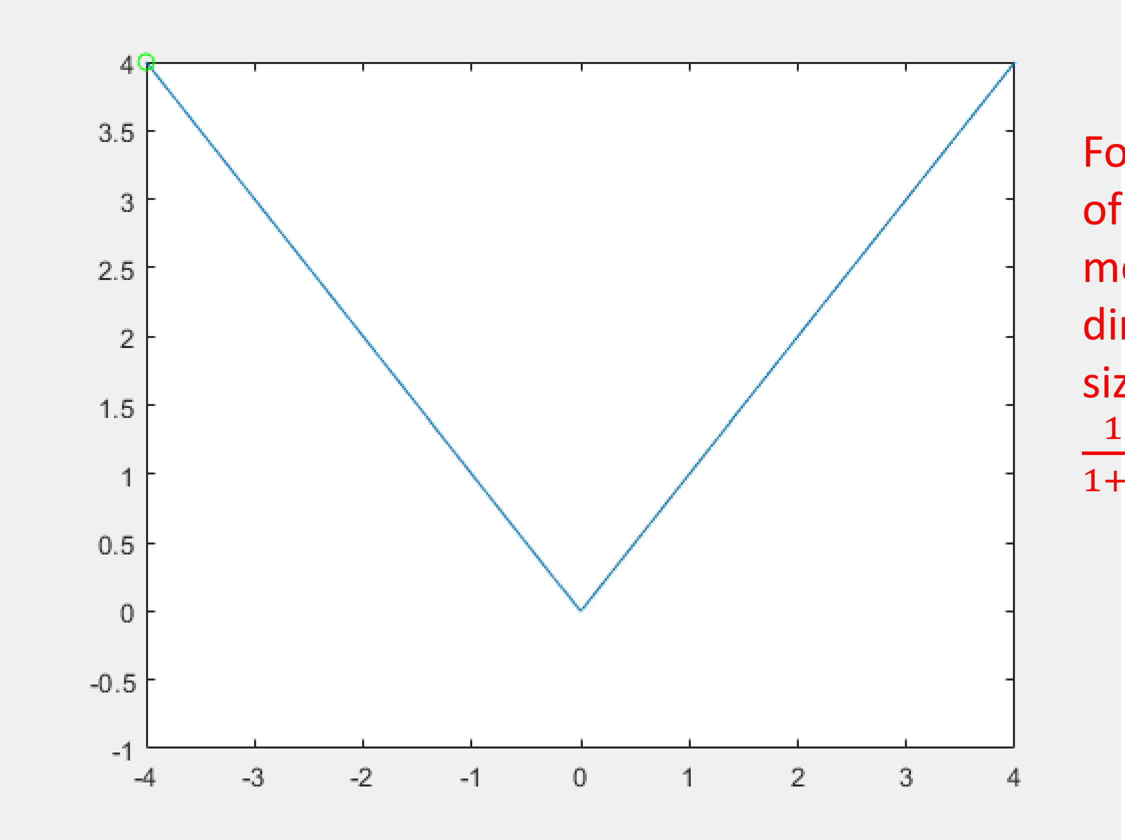
Fixed Step Size: .9



For convergence of subgradient methods, a diminishing step size, e.g., $\gamma_t = \frac{1}{1+t}$ is required

Subgradient Descent

Diminishing Step Size



For convergence of subgradient methods, a diminishing step size, e.g., $\gamma_t = \frac{1}{1+t}$ is required

Stochastic Gradient Descent

- Stochastic (sub)gradient descent used to make training practical

- Approximate the gradient of a sum by sampling a few indices (as few as one) uniformly at random and averaging

$$\nabla_x \left[\sum_{m=1}^{M} g_m(x) \right] \approx \frac{1}{K} \sum_{k=1}^{K} \nabla_x g_{m_k}(x)$$

here, each m_k is sampled uniformly at random from $\{1, \ldots, M\}$

- Stochastic gradient descent converges to the global optimum under certain assumptions on the step size

Stochastic Gradient Descent

- Setting $K = 1$, we pick a random observation m and perform the following update

if the $\boldsymbol{m^{th}}$ data point is misclassified:

$$w^{(t+1)} = w^{(t)} + \gamma_t y^{(m)} x^{(m)}$$

$$b^{(t+1)} = b^{(t)} + \gamma_t y^{(m)}$$

if the $\boldsymbol{m^{th}}$ data point is correctly classified:

$$w^{(t+1)} = w^{(t)}$$

$$b^{(t+1)} = b^{(t)}$$

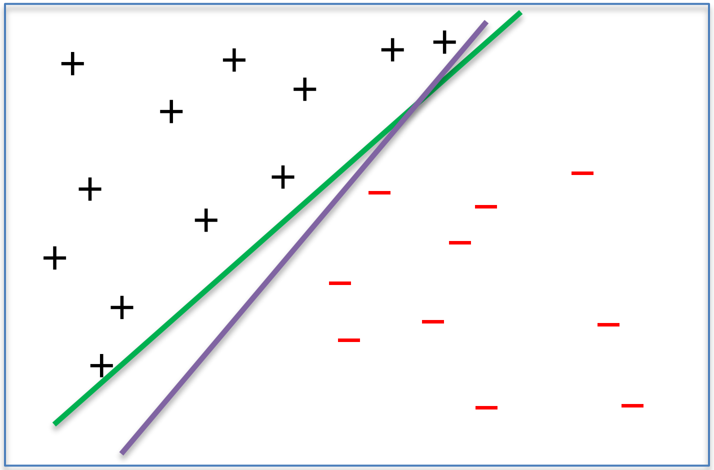
- Perceptron algorithm sometimes specified with $\gamma_t = 1$ for all t

Applications of Perceptron

- Spam email classification
  - Represent emails as vectors of counts of certain words (e.g., sir, madam, Nigerian, prince, money, etc.)
  - Apply the perceptron algorithm to the resulting vectors
  - To predict the label of an unseen email
    - Construct its vector representation, x'
    - Check whether or not $w^T x' + b$ is positive or negative

Perceptron Learning Drawbacks

- No convergence guarantees if the observations are not linearly separable
- Can overfit
  - There can be a number of perfect classifiers, but the perceptron algorithm doesn't have any mechanism for choosing between them

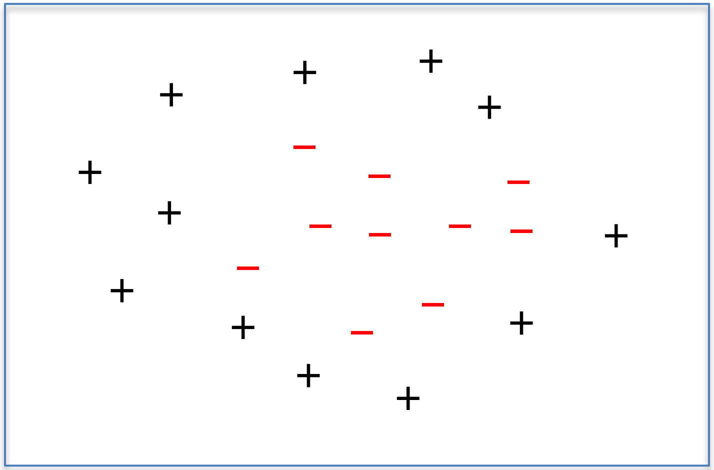


What If the Data Isn‘t Separable?

- Input $(x^{(1)}, y^{(1)}), \ldots, (x^{(M)}, y^{(M)})$ with $x^{(m)} \in \mathbb{R}^n$ and $y^{(m)} \in \{-1, +1\}$

- We can think of the observations as points in $\mathbb{R}^n$ with an associated sign (either +/- corresponding to 0/1)

- An example with $n = 2$



What is a good hypothesis space for this problem?

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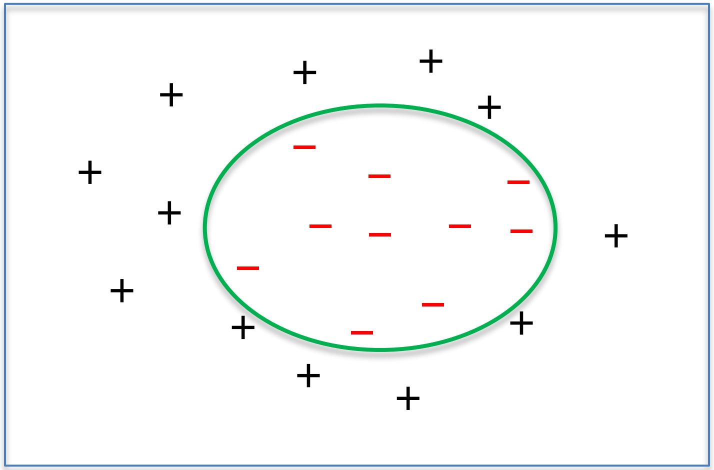
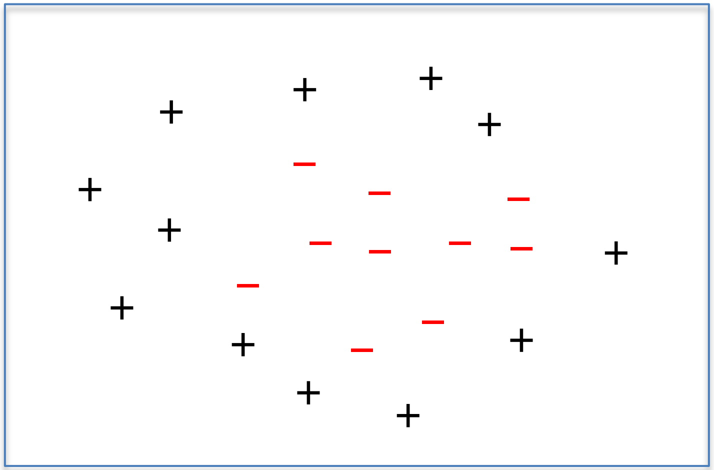


Adding Features

- Perceptron algorithm only works for linearly separable data



Can add features to make the data linearly separable in a higher dimensional space!

Essentially the same as higher order polynomials for linear regression!

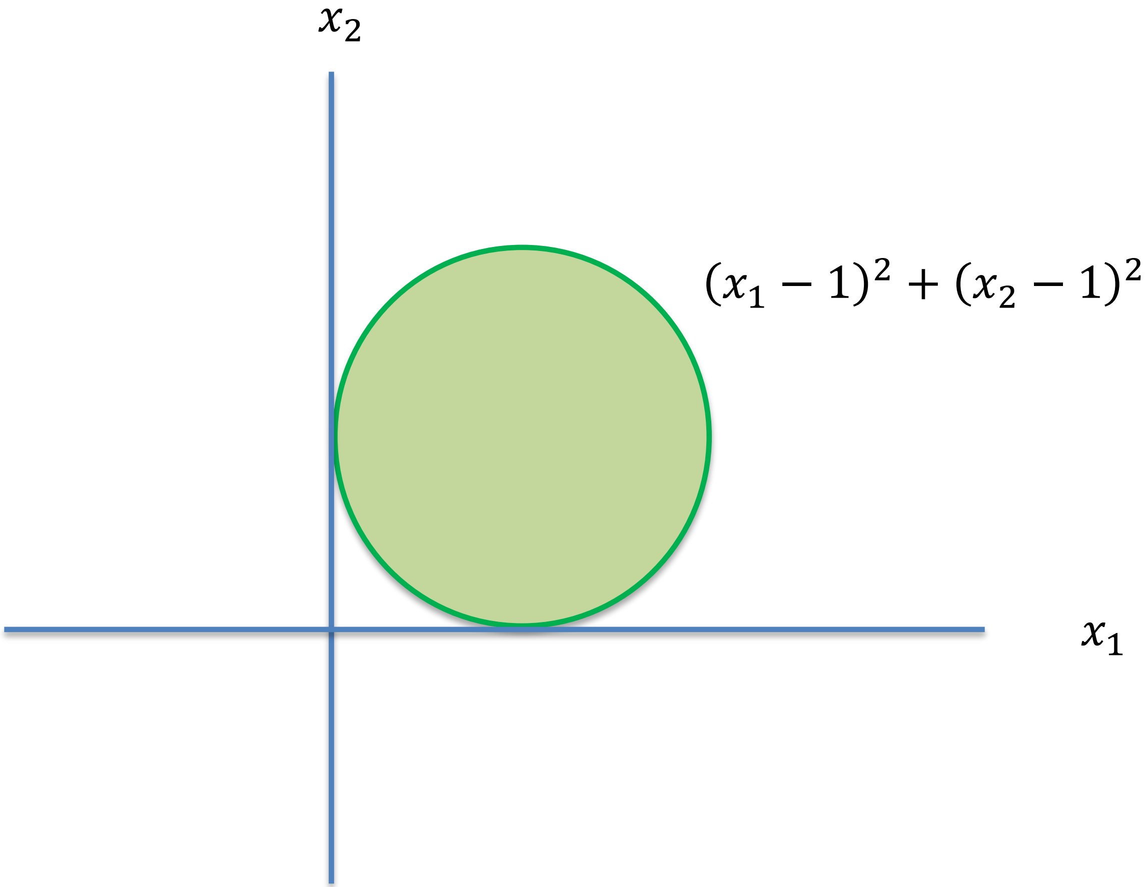
Adding Features

- The idea, choose a feature map $\phi: \mathbb{R}^n \to \mathbb{R}^k$
  - Given the observations $x^{(1)}, \ldots, x^{(M)}$, construct feature vectors $\phi\left(x^{(1)}\right), \ldots, \phi(x^{(M)})$
  - Use $\phi\left(x^{(1)}\right), \ldots, \phi\left(x^{(M)}\right)$ instead of $x^{(1)}, \ldots, x^{(M)}$ in the learning algorithm
  - Choose ϕ so that $\phi\left(x^{(1)}\right), \ldots, \phi\left(x^{(M)}\right)$ are linearly separable in $\mathbb{R}^k$
  - Learn linear separators of the form $w^T \phi(x)$ (instead of $w^T x$)
- Warning: more expressive features can lead to overfitting!

Adding Features: Examples

- $\phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$
  - This is just the input data, without modification
- $\phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ x_1^2 \\ x_2^2 \end{bmatrix}$
  - Corresponds to a second degree polynomial separator, or equivalently, elliptical separators in the original space

Adding Features



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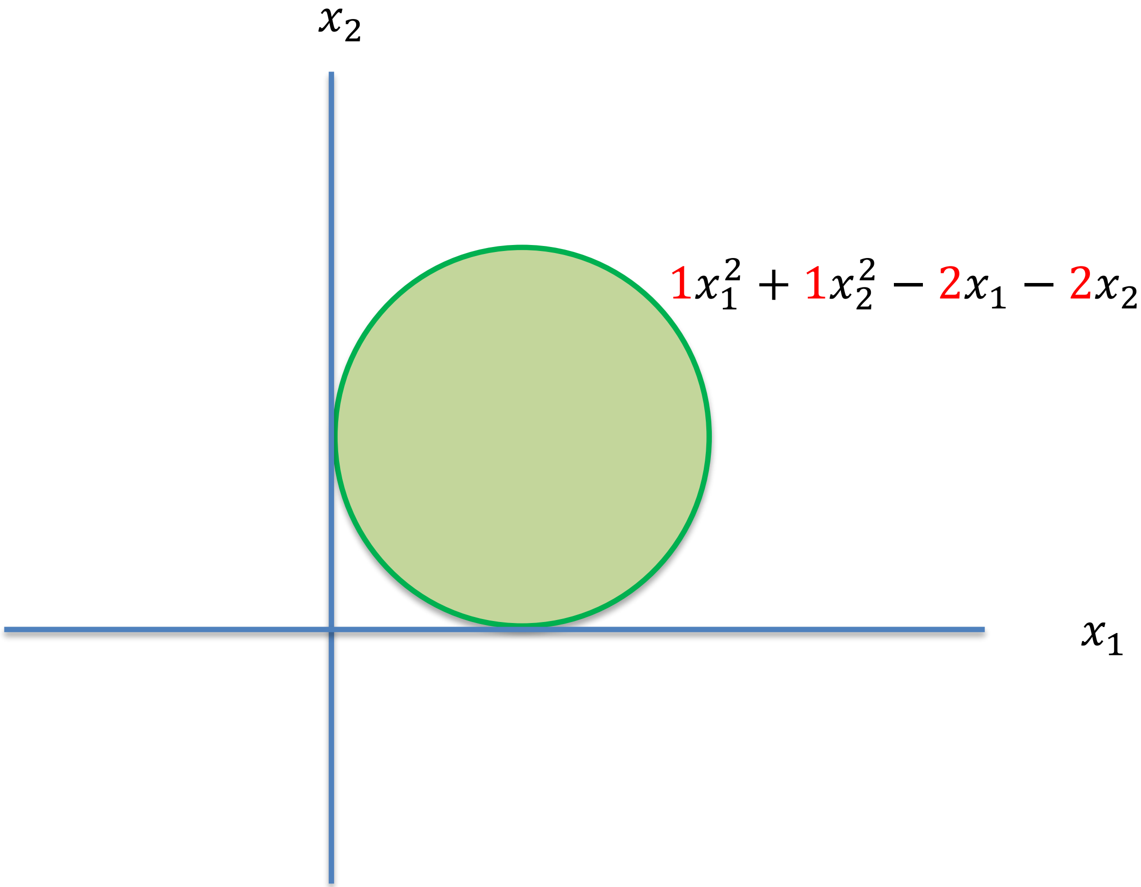
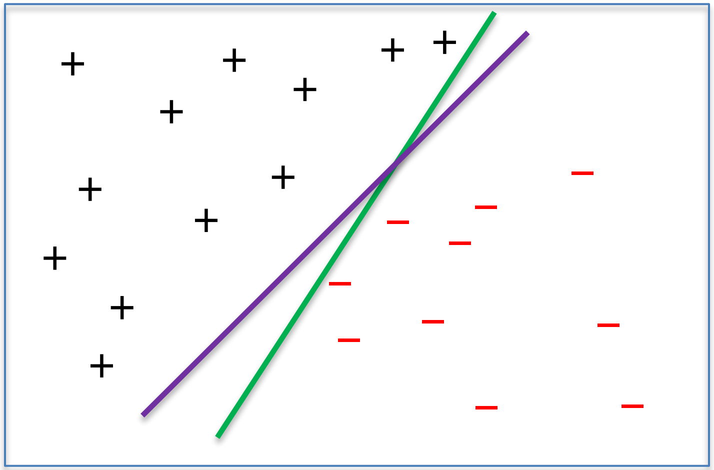


$$1x_1^2 + 1x_2^2 - 2x_1 - 2x_2 - 2 \leq 0$$

Support Vector Machines

- How can we decide between two perfect classifiers?



- What is the practical difference between these two solutions?