Machine Learning Department
School of Computer Science
Carnegie Mellon University

Linear Regression / Optimization for ML

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Lecture 7
Feb. 6, 2019

Q&A

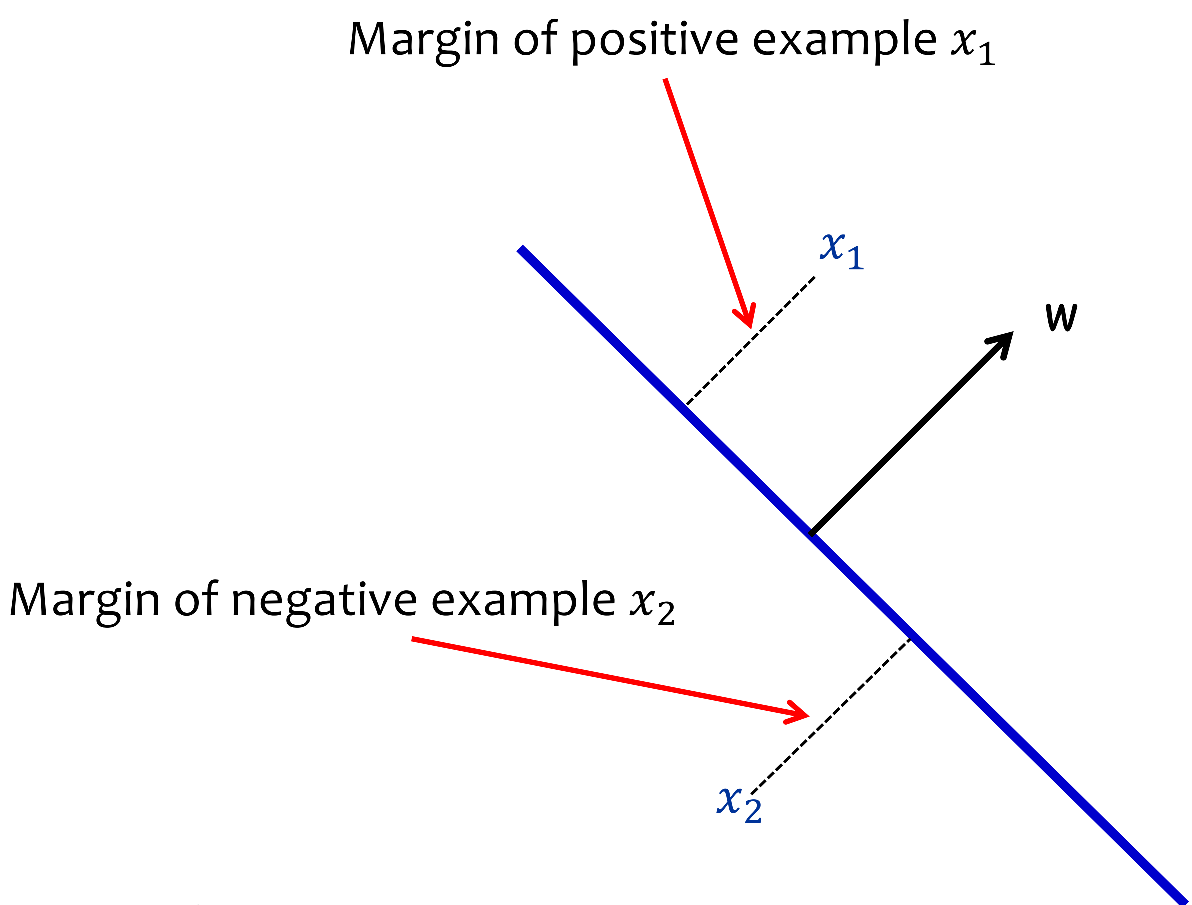
Reminders

- **Homework 2: Decision Trees**
  - Out: Wed, Jan 23
  - Due: Wed, Feb 6 at 11:59pm
- **Homework 3: KNN, Perceptron, Lin.Reg.**
  - Out: Wed, Feb 6
  - Due: Fri, Feb 15 at 11:59pm
- **Today's In-Class Poll**
  - http://p7.mlcourse.org

ANALYSIS OF PERCEPTRON

Geometric Margin

Definition: The margin of example x w.r.t. a linear sep. w is the distance from x to the plane $w \cdot x = 0$ (or the negative if on wrong side)



Slide from Nina Balcan

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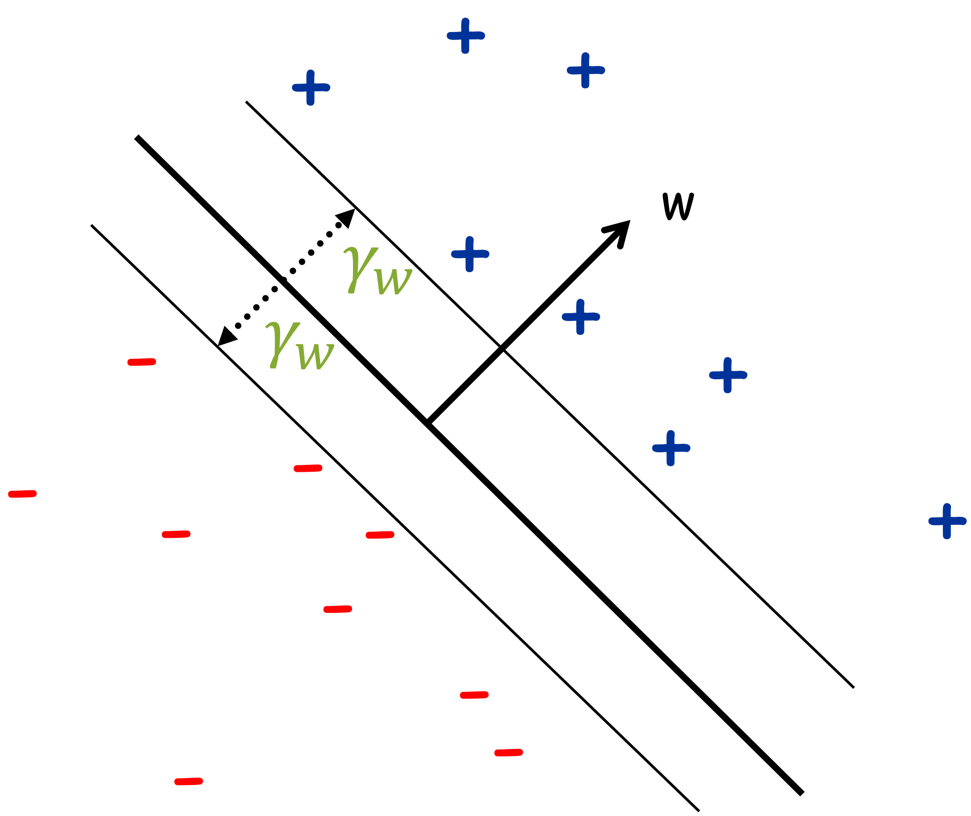
Definition: The margin γ_w of a set of examples S wrt a linear separator w is the smallest margin over points $x \in S$.



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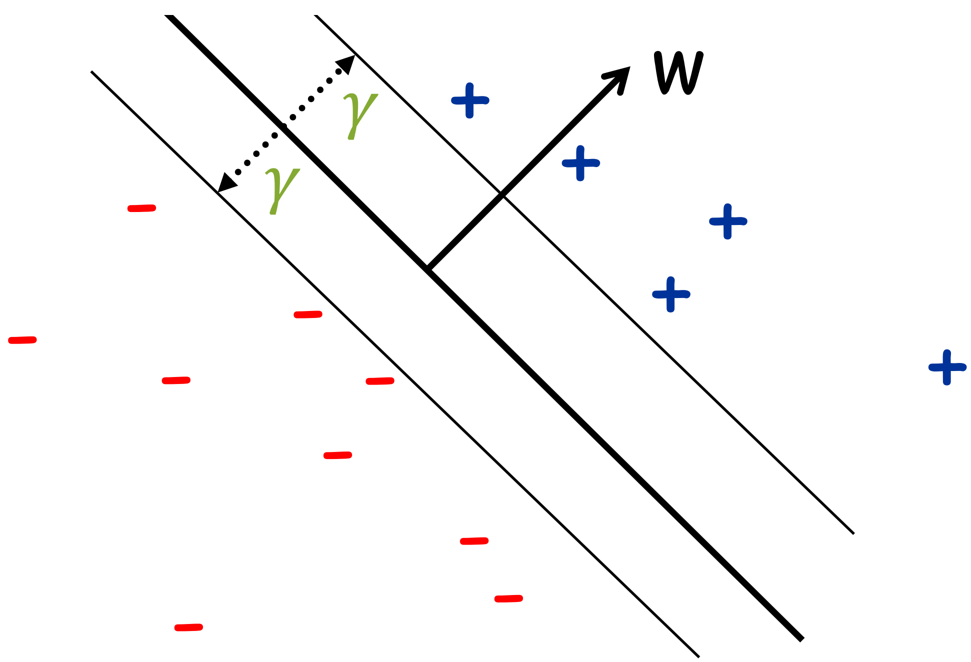
Definition: The margin γ_w of a set of examples S wrt a linear separator w is the smallest margin over points $x \in S$.

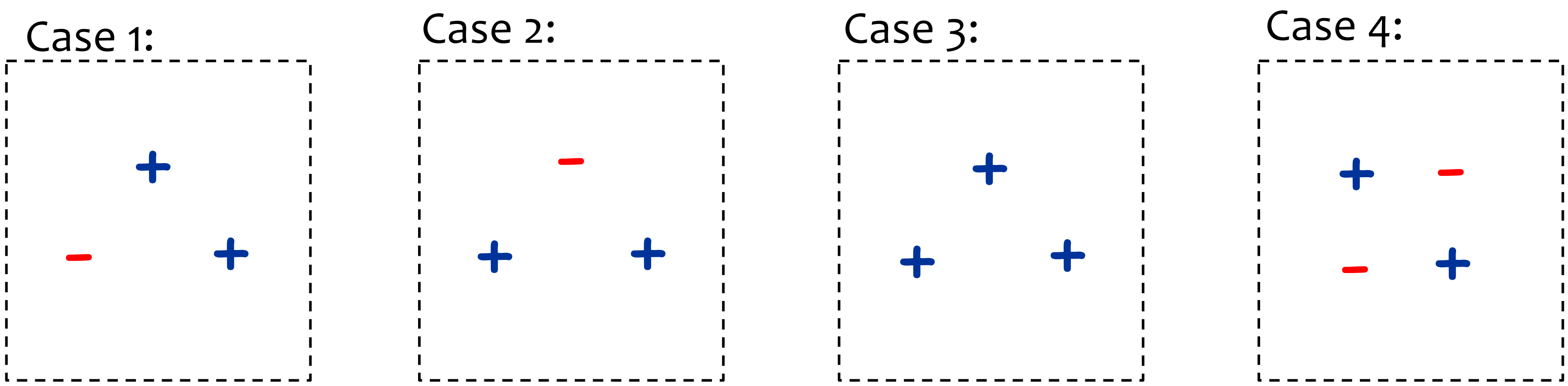
Definition: The margin γ of a set of examples S is the maximum γ_w over all linear separators w.



Slide from Nina Balcan

Linear Separability

***Def*:** For a **binary classification** problem, a set of examples S is **linearly separable** if there exists a linear decision boundary that can separate the points

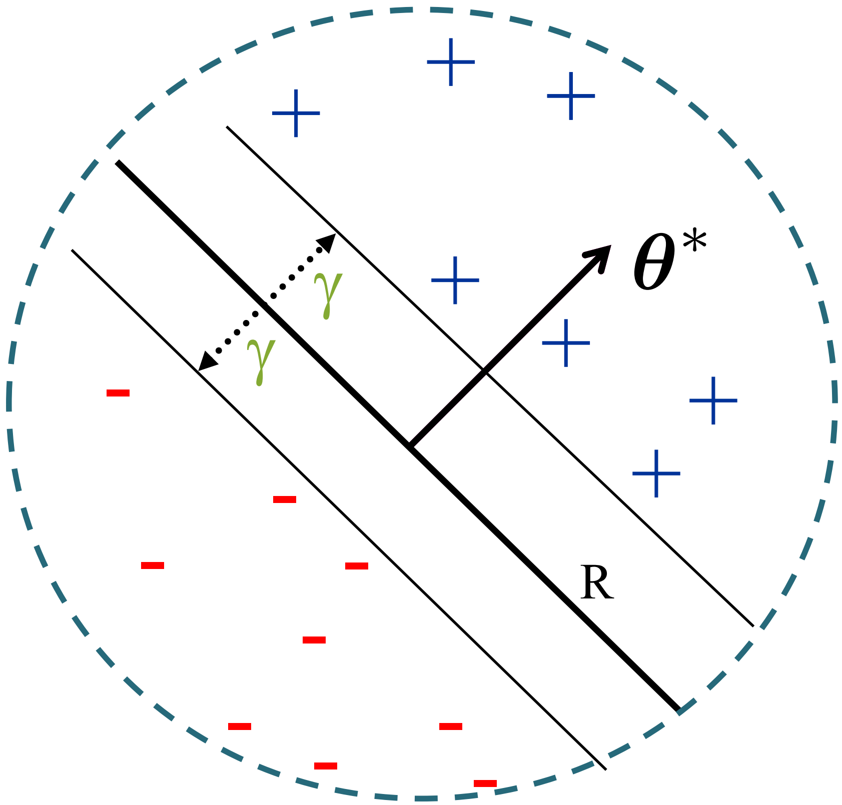


Analysis: Perceptron

Perceptron Mistake Bound

Guarantee: If data has margin γ and all points inside a ball of radius R, then Perceptron makes $\leq (R/\gamma)^2$ mistakes.

(Normalized margin: multiplying all points by 100, or dividing all points by 100, doesn't change the number of mistakes; algo is invariant to scaling.)



Slide adapted from Nina Balcan

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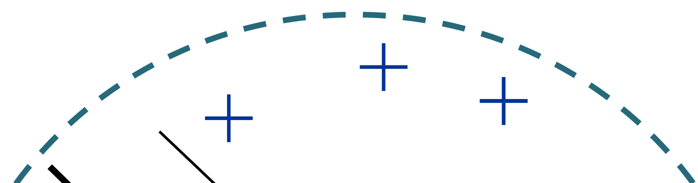

Def: We say that the (batch) perceptron algorithm has **converged** if it stops making mistakes on the training data (perfectly classifies the training data).

Main Takeaway: For **linearly separable** data, if the perceptron algorithm cycles repeatedly through the data, it will **converge** in a finite # of steps.

Slide adapted from Nina Balcan

Analysis: Perceptron

Perceptron Mistake Bound

Theorem 0.1 (Block (1962), Novikoff (1962)).
Given dataset: $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$.
Suppose:

1. *Finite size inputs:* $||x^{(i)}|| \leq R$
2. *Linearly separable data:* $\exists \boldsymbol{\theta}^*$ *s.t.* $||\boldsymbol{\theta}^*|| = 1$ *and* $y^{(i)}(\boldsymbol{\theta}^* \cdot \mathbf{x}^{(i)}) \geq \gamma, \forall i$

Then: The number of mistakes made by the Perceptron algorithm on this dataset is

$$k \leq (R/\gamma)^2$$

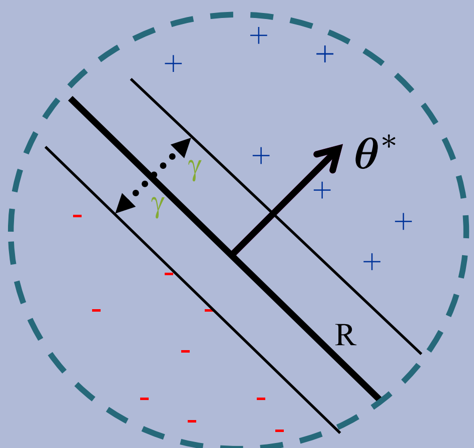

Figure from Nina Balcan

Analysis: Percept

Common Misunderstanding:
The **radius** is **centered at the origin**, not at the center of the points.

Perceptron Mistake Boun

Theorem 0.1 (Block (1962), Novikoff (19

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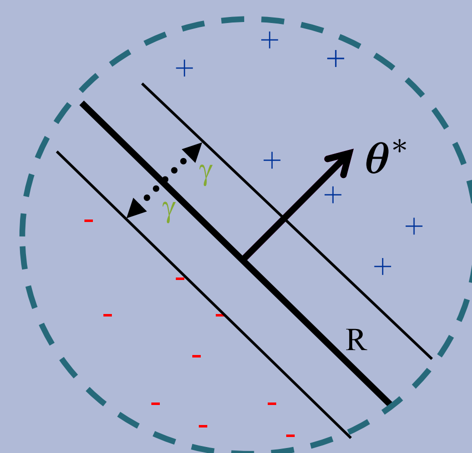


Figure from Nina Balcan

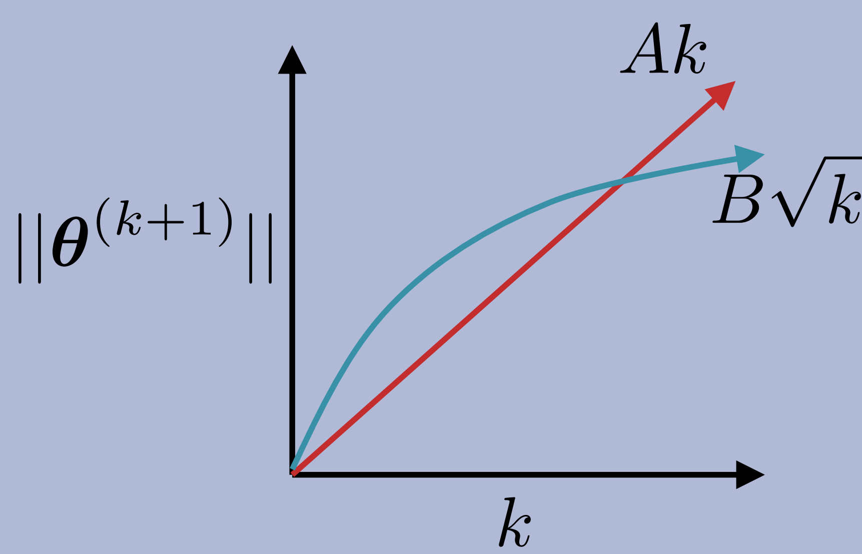
Analysis: Perceptron

Covered in Recitation

Proof of Perceptron Mistake Bound:

We will show that there exist constants A and B s.t.

$$Ak \leq ||\boldsymbol{\theta}^{(k+1)}|| \leq B\sqrt{k}$$



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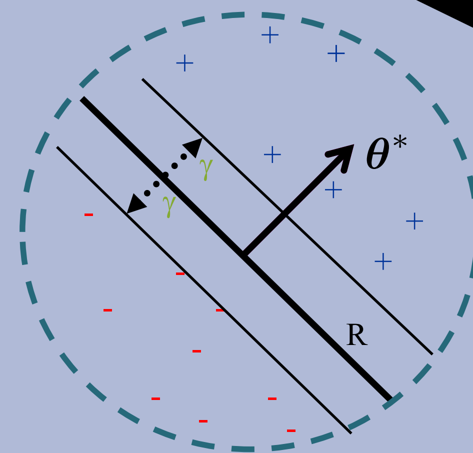


Algorithm 1 Perceptron Learning Algorithm (Online)

```
procedure PERCEPTRON(D = {(x^(1), y^(1)), (x^(2), y^(2)), ...})
    θ ← 0, k = 1                                  ▷ Initialize parameters
    for i ∈ {1, 2, ...} do                        ▷ For each example
        if y^(i)(θ^(k) · x^(i)) ≤ 0 then           ▷ If mistake
            θ^(k+1) ← θ^(k) + y^(i) x^(i)           ▷ Update parameters
            k ← k + 1
    return θ
```

Analysis: Perceptron

Covered in Recitation

Proof of Perceptron Mistake Bound:

Part 1: for some A, $Ak \leq ||\boldsymbol{\theta}^{(k+1)}||$

$$\boldsymbol{\theta}^{(k+1)} \cdot \boldsymbol{\theta}^* = (\boldsymbol{\theta}^{(k)} + y^{(i)}\mathbf{x}^{(i)})\boldsymbol{\theta}^*$$

by Perceptron algorithm update

$$= \boldsymbol{\theta}^{(k)} \cdot \boldsymbol{\theta}^* + y^{(i)}(\boldsymbol{\theta}^* \cdot \mathbf{x}^{(i)})$$

$$\geq \boldsymbol{\theta}^{(k)} \cdot \boldsymbol{\theta}^* + \gamma$$

by assumption

$$\Rightarrow \boldsymbol{\theta}^{(k+1)} \cdot \boldsymbol{\theta}^* \geq k\gamma$$

by induction on k since $\theta^{(1)} = \mathbf{0}$

$$\Rightarrow ||\boldsymbol{\theta}^{(k+1)}|| \geq k\gamma$$

since $||\mathbf{w}|| \times ||\mathbf{u}|| \geq \mathbf{w} \cdot \mathbf{u}$ and $||\theta^*|| = 1$

Cauchy-Schwartz inequality

Analysis: Perceptron

Covered in Recitation

Proof of Perceptron Mistake Bound:

Part 2: for some B, $||\boldsymbol{\theta}^{(k+1)}|| \leq B\sqrt{k}$

$$||\boldsymbol{\theta}^{(k+1)}||^2 = ||\boldsymbol{\theta}^{(k)} + y^{(i)}\mathbf{x}^{(i)}||^2$$

by Perceptron algorithm update

$$= ||\boldsymbol{\theta}^{(k)}||^2 + (y^{(i)})^2||\mathbf{x}^{(i)}||^2 + 2y^{(i)}(\boldsymbol{\theta}^{(k)} \cdot \mathbf{x}^{(i)})$$

$$\leq ||\boldsymbol{\theta}^{(k)}||^2 + (y^{(i)})^2||\mathbf{x}^{(i)}||^2$$

since kth mistake $\Rightarrow y^{(i)}(\boldsymbol{\theta}^{(k)} \cdot \mathbf{x}^{(i)}) \leq 0$

$$= ||\boldsymbol{\theta}^{(k)}||^2 + R^2$$

since $(y^{(i)})^2||\mathbf{x}^{(i)}||^2 = ||\mathbf{x}^{(i)}||^2 = R^2$ by assumption and $(y^{(i)})^2 = 1$

$$\Rightarrow ||\boldsymbol{\theta}^{(k+1)}||^2 \leq kR^2$$

by induction on k since $(\theta^{(1)})^2 = 0$

$$\Rightarrow ||\boldsymbol{\theta}^{(k+1)}|| \leq \sqrt{k}R$$

Analysis: Perceptron

Covered in Recitation

Proof of Perceptron Mistake Bound:

Part 3: Combining the bounds finishes the proof.

$$k\gamma \leq ||\boldsymbol{\theta}^{(k+1)}|| \leq \sqrt{k}R$$

$$\Rightarrow k \leq (R/\gamma)^2$$

The total number of mistakes must be less than this

Analysis: Perceptron

What if the data is *not* linearly separable?

1. Perceptron will **not converge** in this case (it can't!)
2. However, Freund & Schapire (1999) show that by projecting the points (hypothetically) into a higher dimensional space, we can achieve a similar bound on the number of mistakes made on **one pass** through the sequence of examples

Theorem 2. *Let* $\langle(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\rangle$ *be a sequence of labeled examples with* $\|\mathbf{x}_i\| \leq R$. *Let* $\mathbf{u}$ *be any vector with* $\|\mathbf{u}\| = 1$ *and let* $\gamma > 0$. *Define the deviation of each example as*

$$d_i = \max\{0, \gamma - y_i(\mathbf{u} \cdot \mathbf{x}_i)\},$$

and define $D = \sqrt{\sum_{i=1}^m d_i^2}$. *Then the number of mistakes of the online perceptron algorithm on this sequence is bounded by*

$$\left(\frac{R + D}{\gamma}\right)^2.$$

Perceptron Exercises

Question:

Unlike Decision Trees and K-Nearest Neighbors, the Perceptron algorithm ***does not suffer from overfitting*** *because it does not have any hyperparameters that could be over-tuned on the training data.*

A. *True*

B. *False*

C. *True and False*

Summary: Perceptron

- Perceptron is a **linear classifier**
- **Simple learning algorithm**: when a mistake is made, add / subtract the features
- Perceptron will converge if the data are **linearly separable**, it will **not** converge if the data are **linearly inseparable**
- For linearly separable and inseparable data, we can **bound the number of mistakes** (geometric argument)
- **Extensions** support nonlinear separators and structured prediction

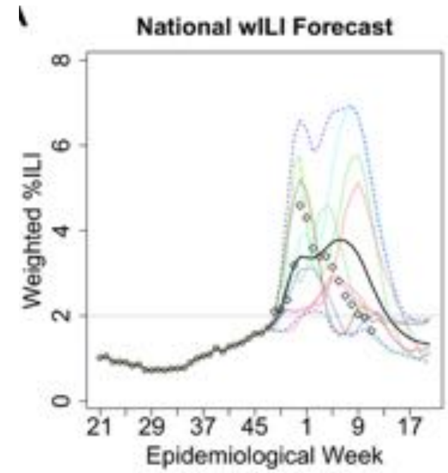
Perceptron Learning Objectives

You should be able to…

- Explain the difference between online learning and batch learning
- Implement the perceptron algorithm for binary classification [CIML]
- Determine whether the perceptron algorithm will converge based on properties of the dataset, and the limitations of the convergence guarantees
- Describe the inductive bias of perceptron and the limitations of linear models
- Draw the decision boundary of a linear model
- Identify whether a dataset is linearly separable or not
- Defend the use of a bias term in perceptron

LINEAR REGRESSION AS FUNCTION APPROXIMATION

Regression



Example Applications:

- Stock price prediction
- Forecasting epidemics
- Speech synthesis

- Generation of images (e.g. *Deep Dream*)

- Predicting the number of tourists on Machu Picchu on a given day

Regression Problems

Chalkboard

– Definition of Regression
– Linear functions
– Residuals
– Notation trick: fold in the intercept

Linear Regression as Function Approximation

Chalkboard

- Objective function: Mean squared error
- Hypothesis space: Linear Functions

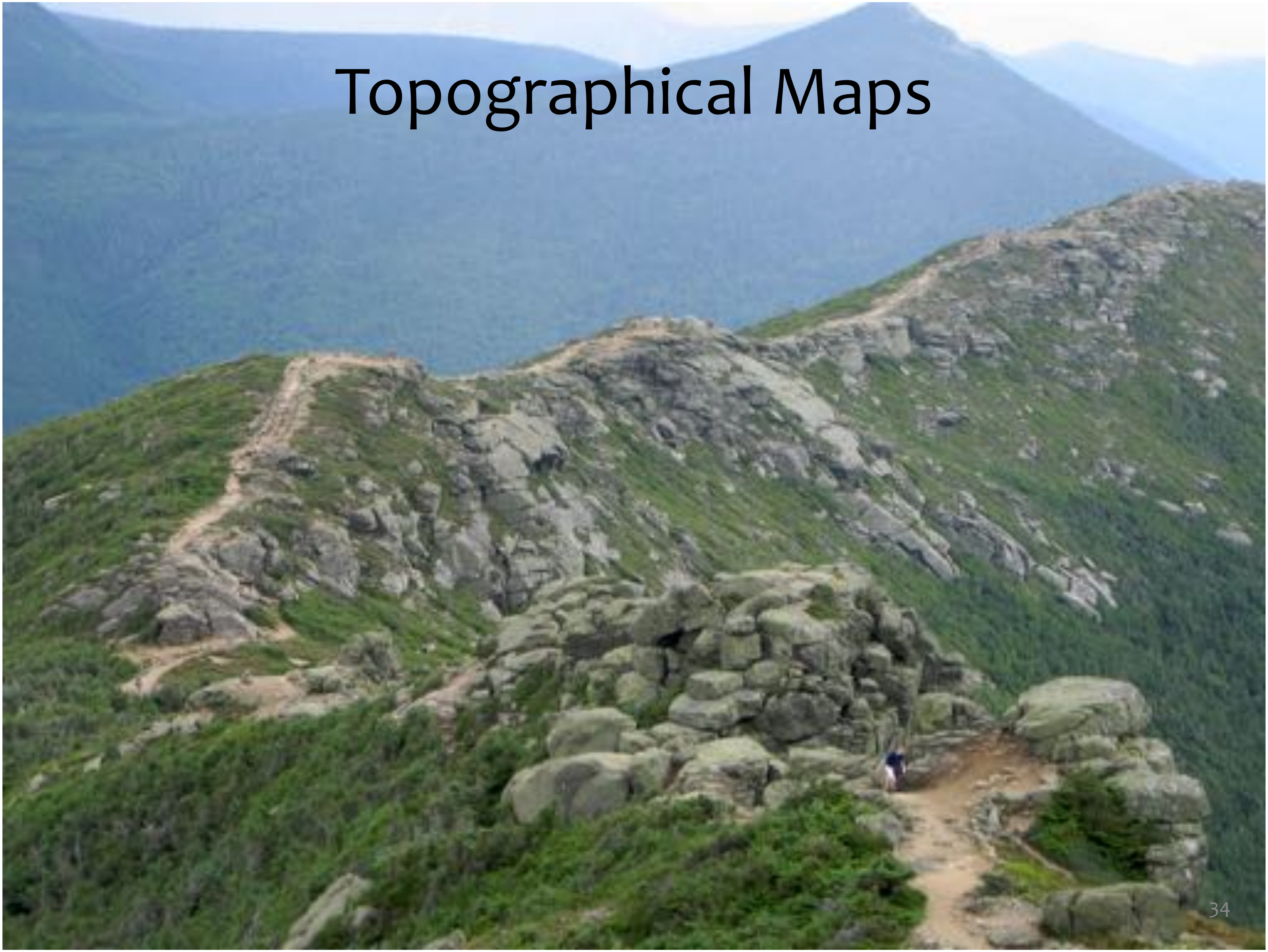
OPTIMIZATION IN CLOSED FORM

Optimization for ML

Not quite the same setting as other fields…

- Function we are optimizing might not be the true goal
  (e.g. likelihood vs generalization error)
- Precision might not matter
  (e.g. data is noisy, so optimal up to 1e-16 might not help)
- Stopping early can help generalization error
  (i.e. "early stopping" is a technique for regularization – discussed more next time)

Topographical Maps



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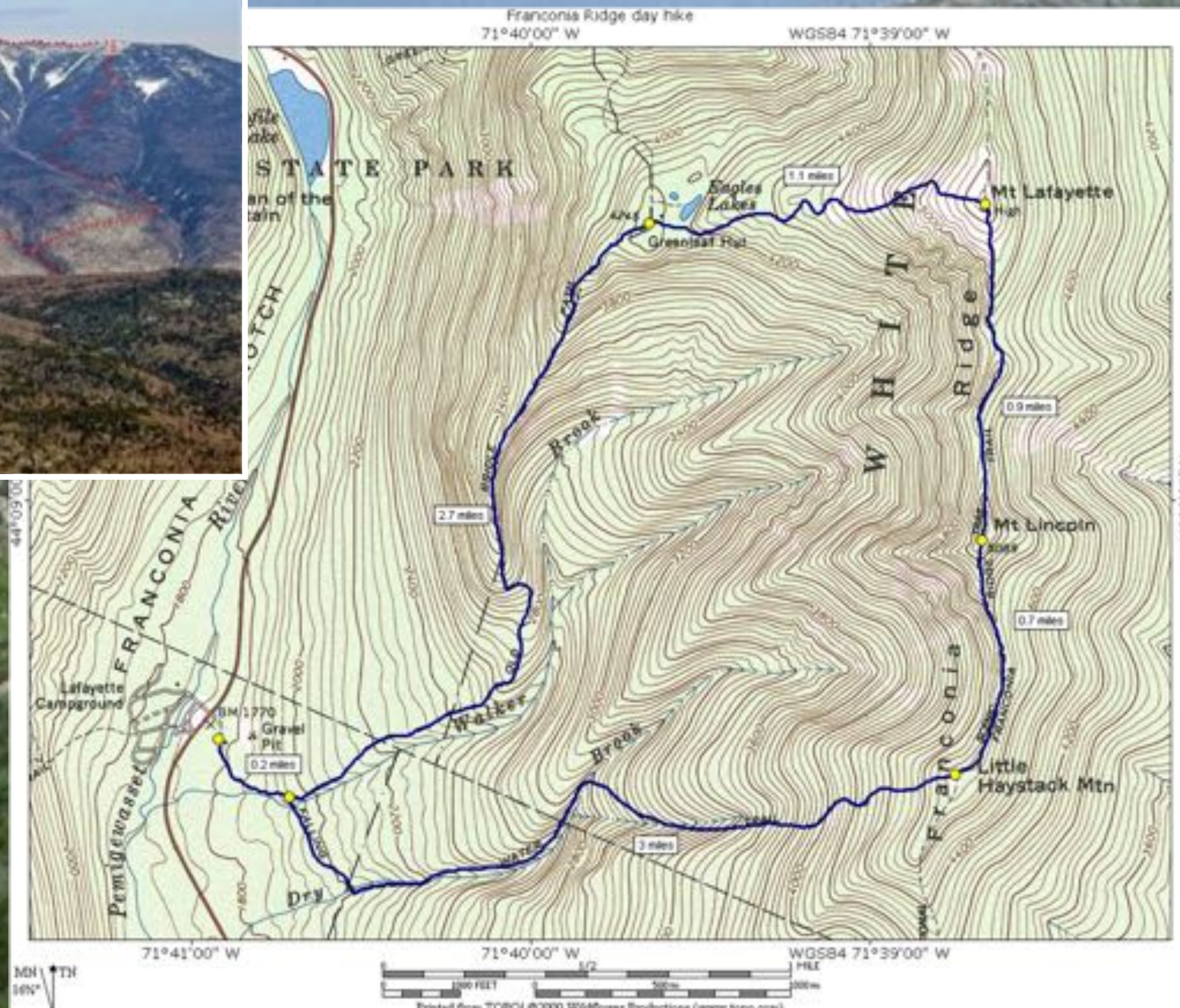


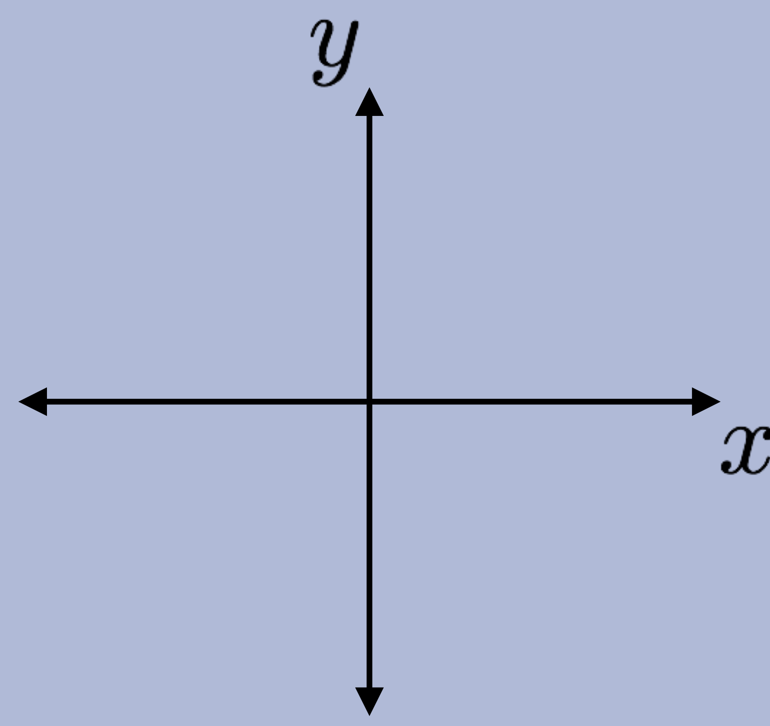
Calculus and Optimization

In-Class Exercise

Plot three functions:

1. $f(x) = x^3 - x$
2. $f'(x) = \frac{\partial y}{\partial x}$
3. $f''(x) = \frac{\partial^2 y}{\partial x^2}$

Answer Here:



Optimization for ML

Chalkboard

- Unconstrained optimization
- Convex, concave, nonconvex
- Derivatives
- Zero derivatives
- Gradient and Hessian

Optimization: Closed form solutions

Chalkboard

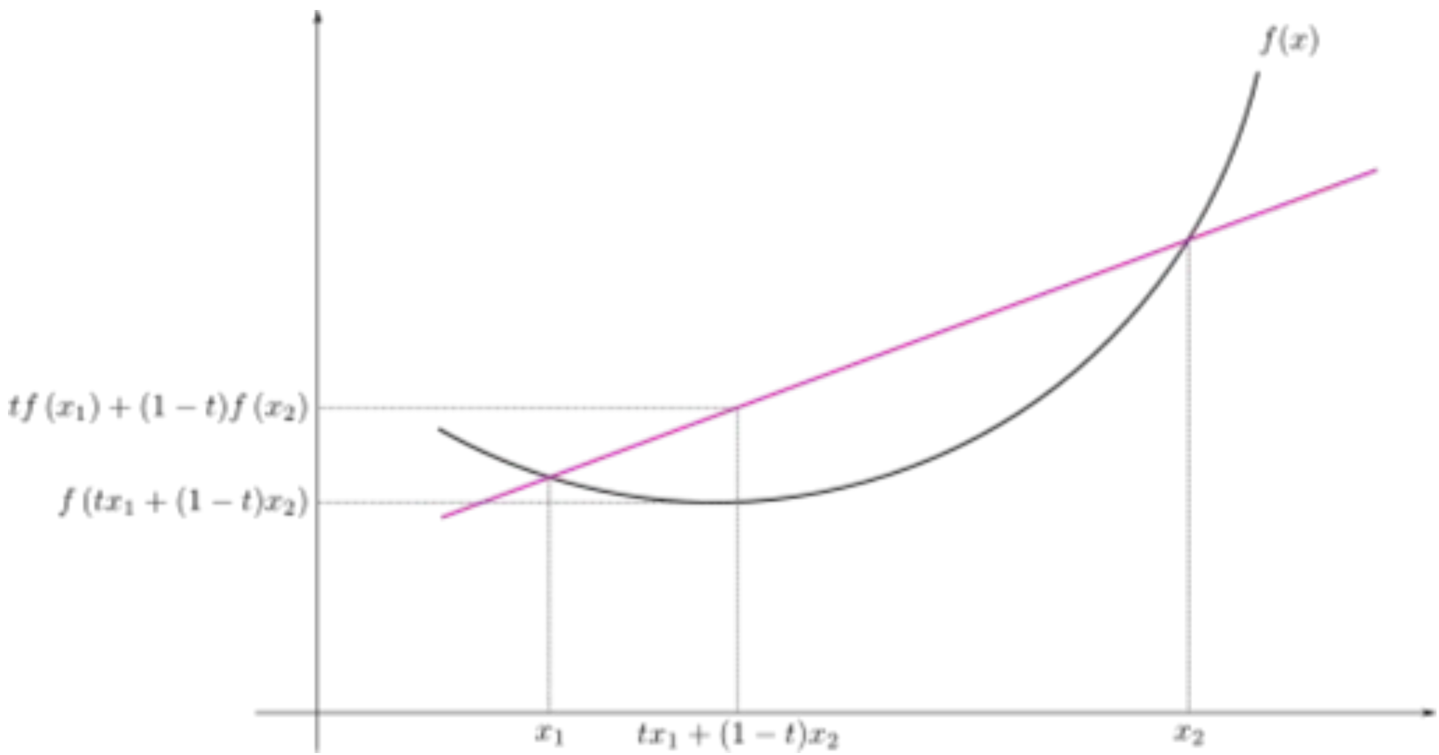
- Example: 1-D function
- Example: higher dimensions

Convexity

Function $f : \mathbb{R}^M \rightarrow \mathbb{R}$ is **convex**
if $\forall\ \mathbf{x}_1 \in \mathbb{R}^M, \mathbf{x}_2 \in \mathbb{R}^M, 0 \leq t \leq 1$:

$$f(t\mathbf{x}_1 + (1-t)\mathbf{x}_2) \leq tf(\mathbf{x}_1) + (1-t)f(\mathbf{x}_2)$$

There is only one local optimum if the function is *convex*



Slide adapted from William Cohen

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The **Mean Squared Error** function, which we will minimize for learning the parameters of Linear Regression, **is convex**!

Slide adapted from William Cohen

CLOSED FORM SOLUTION FOR LINEAR REGRESSION

Optimization for Linear Regression

Chalkboard

- Closed-form (Normal Equations)
- Computational complexity of Closed-form Solution
- Stability of Closed-form Solution

Function Approximation

Chalkboard

- The Big Picture