Caltech

Machine Learning & Data Mining

CMS/CS/CNS/EE 155

Lecture 2:

Perceptron & Gradient Descent

Announcements

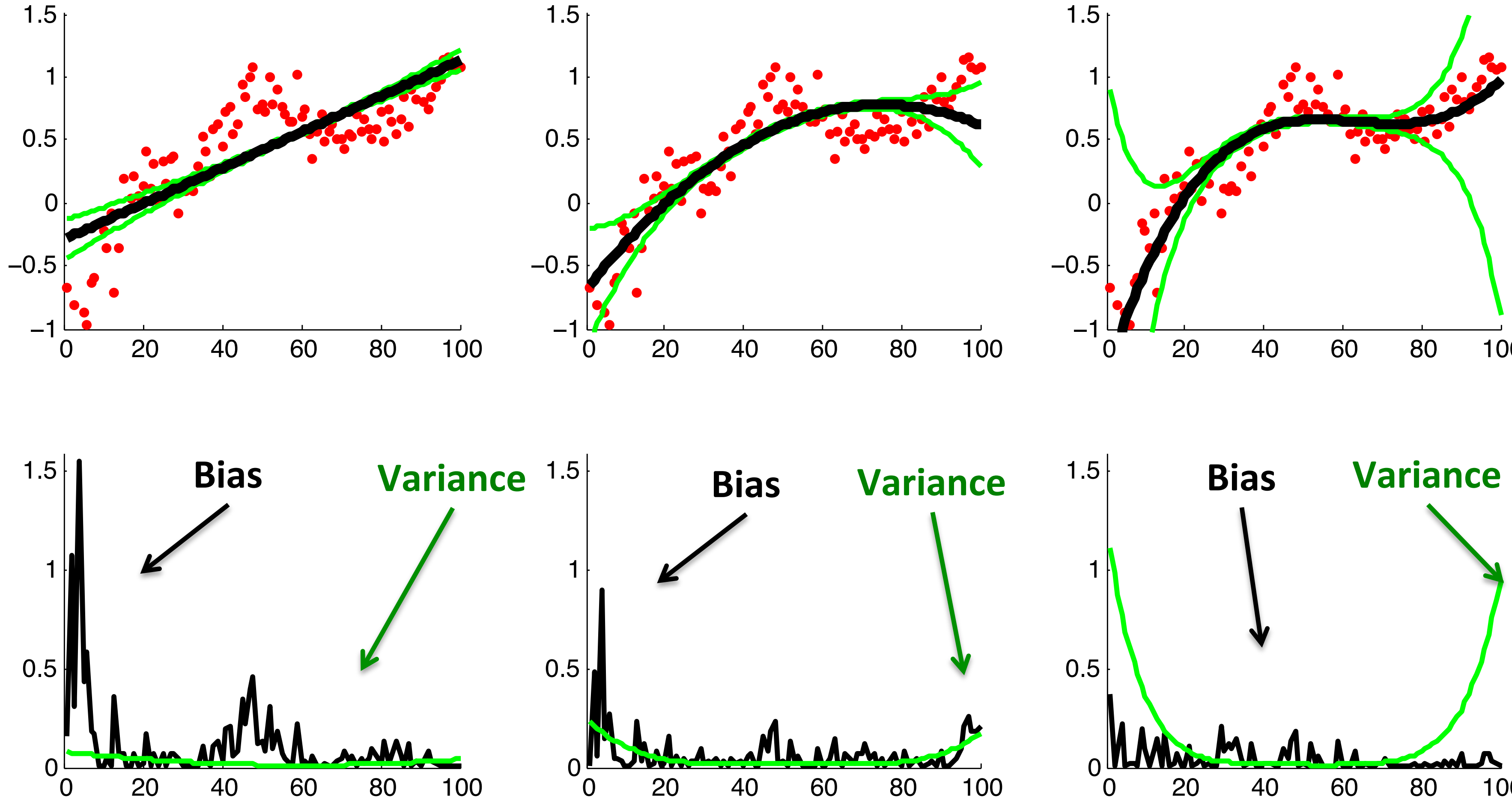
- Homework 1 is out
  - Due Tuesday Jan 12th at 2pm
  - Via Moodle
- Sign up for Moodle & Piazza if you haven't yet
  - Announcements are made via Piazza
- Recitation on Python Programming Tonight
  - 7:30pm in Annenberg 105

Recap: Basic Recipe

- Training Data: $S = \{(x_i, y_i)\}_{i=1}^{N}$ $\quad x \in R^D$, $y \in \{-1,+1\}$
- Model Class: $f(x \mid w,b) = w^T x - b$ **Linear Models**
- Loss Function: $L(a,b) = (a-b)^2$ **Squared Loss**
- Learning Objective: $\operatorname{argmin}_{w,b} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w,b)\big)$

Optimization Problem

Recap: Bias-Variance Trade-off



Recap: Complete Pipeline

$$S = \{(x_i, y_i)\}_{i=1}^{N}$$

Training Data

$$f(x \mid w, b) = w^T x - b$$

Model Class(es)

$$L(a,b) = (a-b)^2$$

Loss Function

$$\operatorname*{argmin}_{w,b} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$

Cross Validation & Model Selection

Profit!

Today

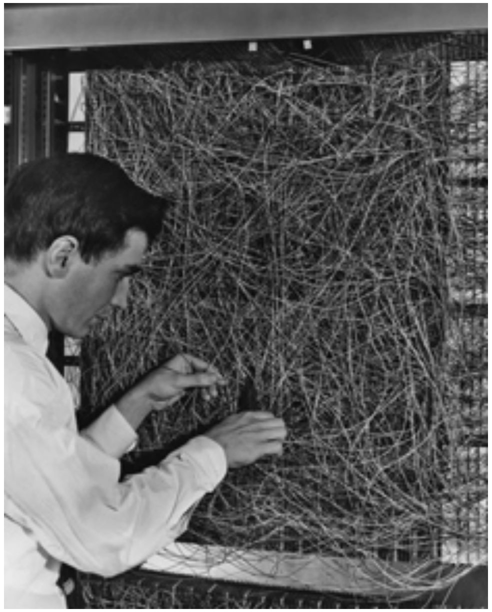
- **Two Basic Learning Approaches**

- Perceptron Algorithm

- Gradient Descent
  - Aka, actually solving the optimization problem

The Perceptron

- One of the earliest learning algorithms
  - 1957 by Frank Rosenblatt
- Still a great algorithm
  - Fast
  - Clean analysis
  - Precursor to Neural Networks



Frank Rosenblatt with the Mark 1 Perceptron Machine

Perceptron Learning Algorithm
(Linear Classification Model)

- $w^1 = 0, b^1 = 0$
- For t = 1 ….
  - Receive example (x,y)
  - If $f(x|w^t) = y$
    - $[w^{t+1}, b^{t+1}] = [w^t, b^t]$
  - Else
    - $w^{t+1} = w^t + yx$
    - $b^{t+1} = b^t + y$

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

Training Set:

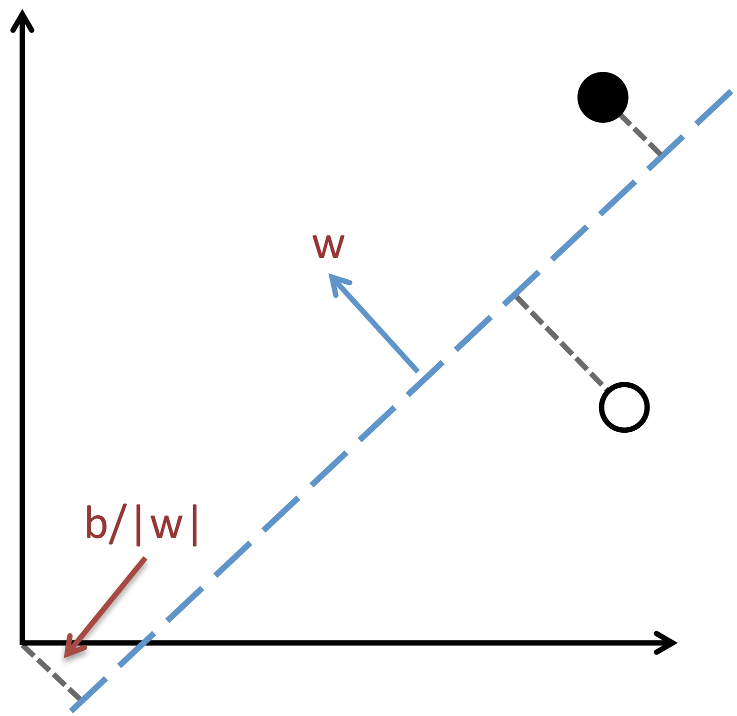
$$S = \{(x_i, y_i)\}_{i=1}^{N}$$

$$y \in \{+1, -1\}$$

Go through training set in arbitrary order (e.g., randomly)

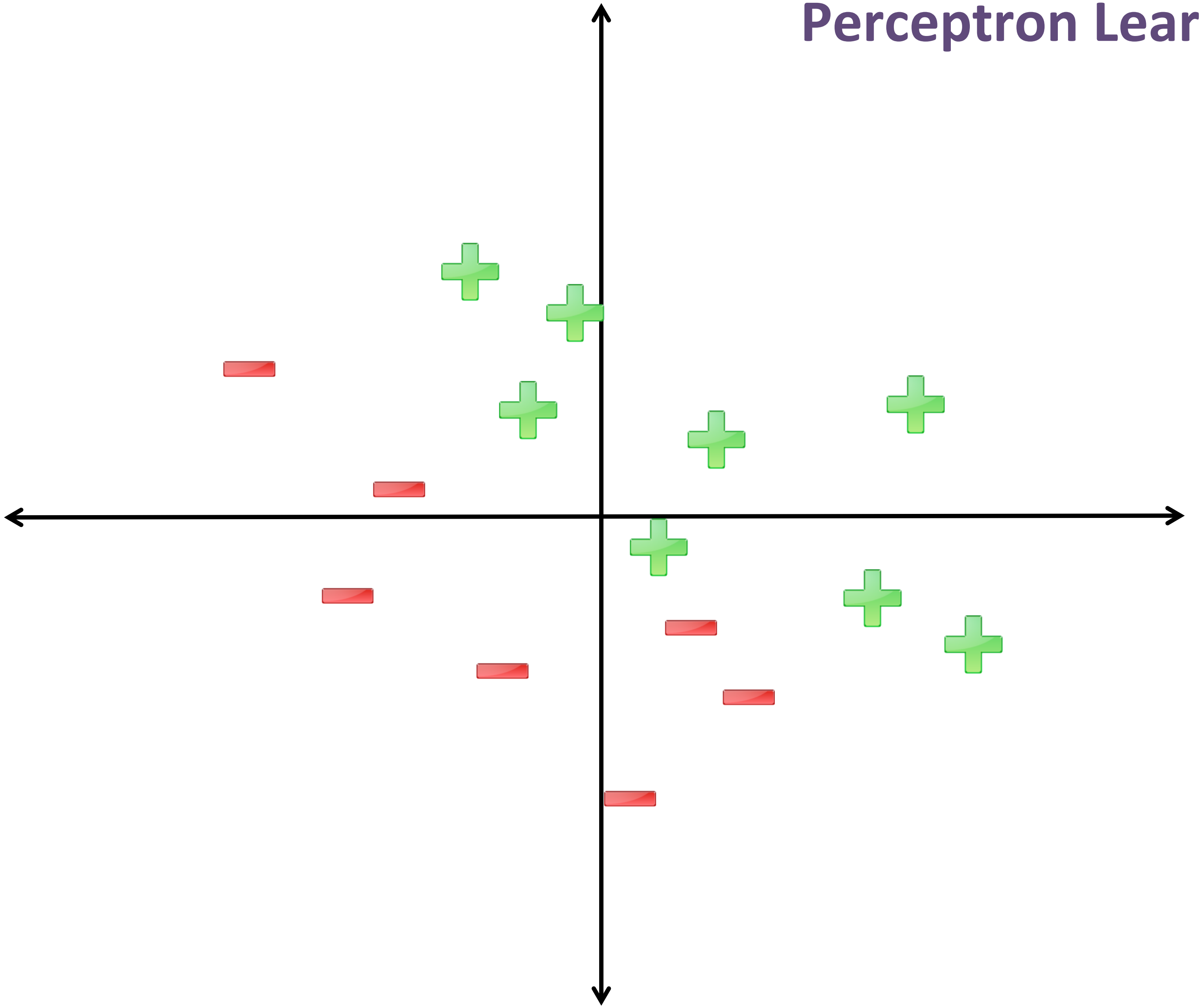
Aside: Hyperplane Distance

- Line is a 1D, Plane is 2D
- Hyperplane is many D
  - Includes Line and Plane
- Defined by (w,b)
- Distance: $$\frac{|w^T x - b|}{\|w\|}$$
- Signed Distance: $$\frac{w^T x - b}{\|w\|}$$



Linear Model = un-normalized signed distance!

Perceptron Learning



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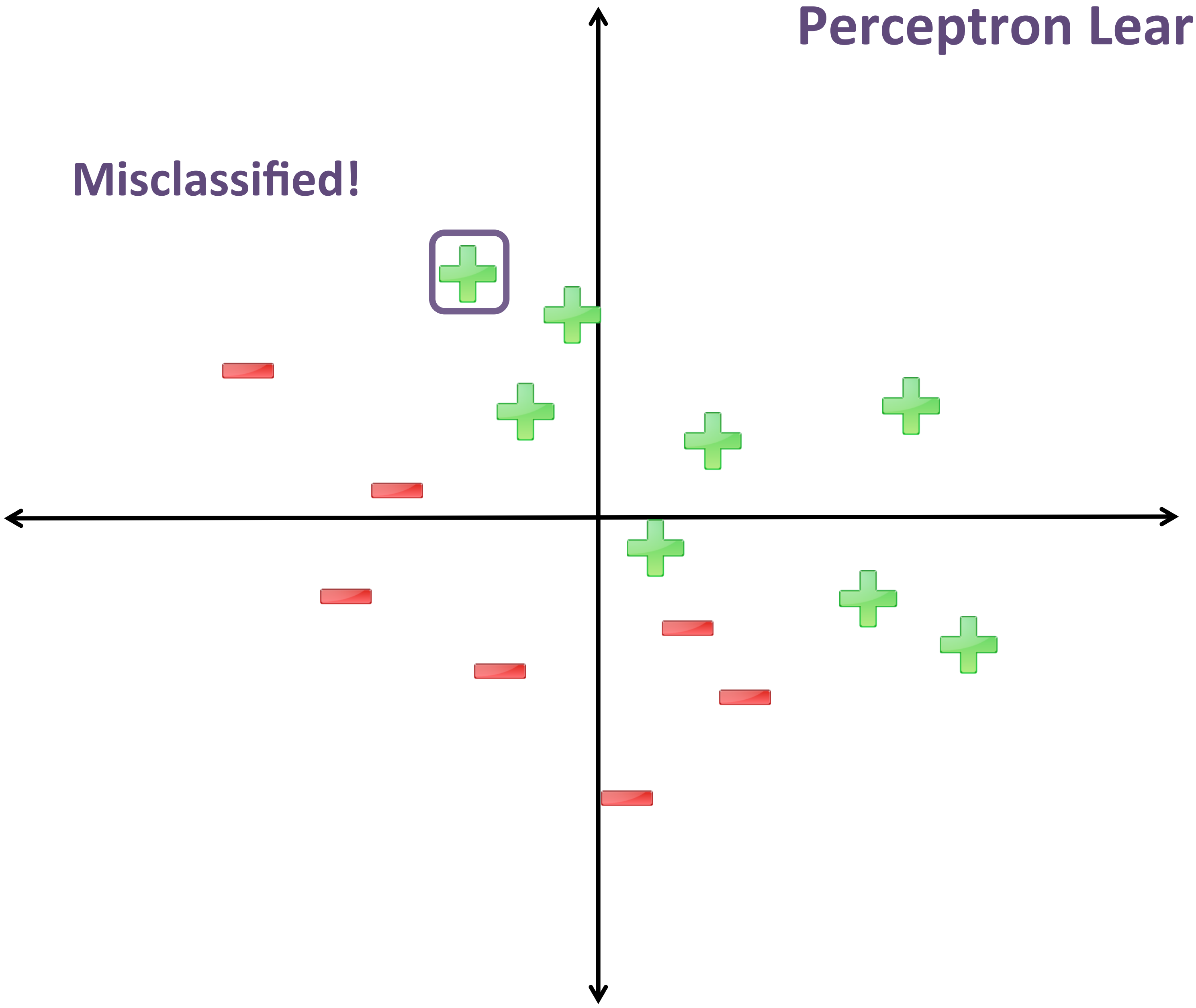

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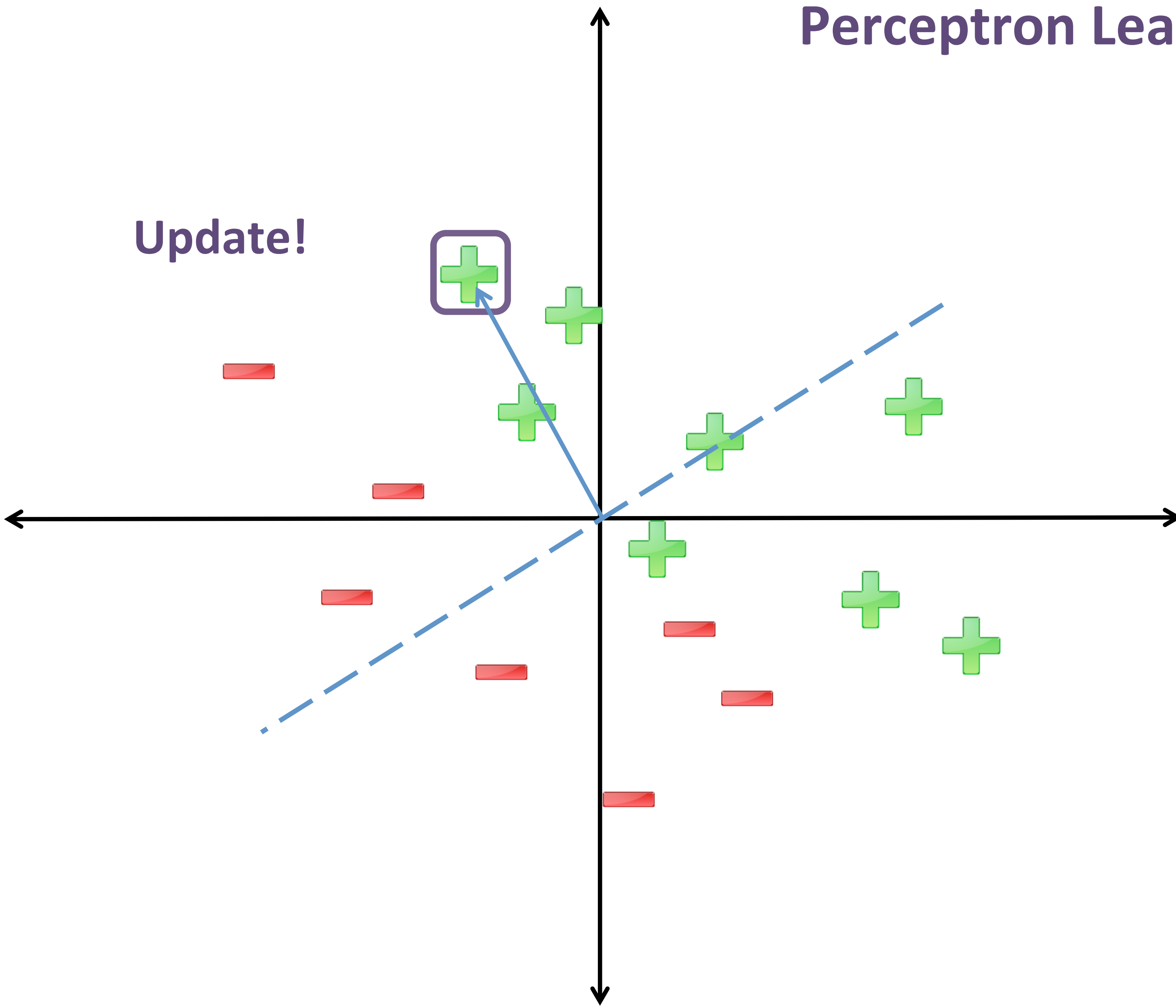

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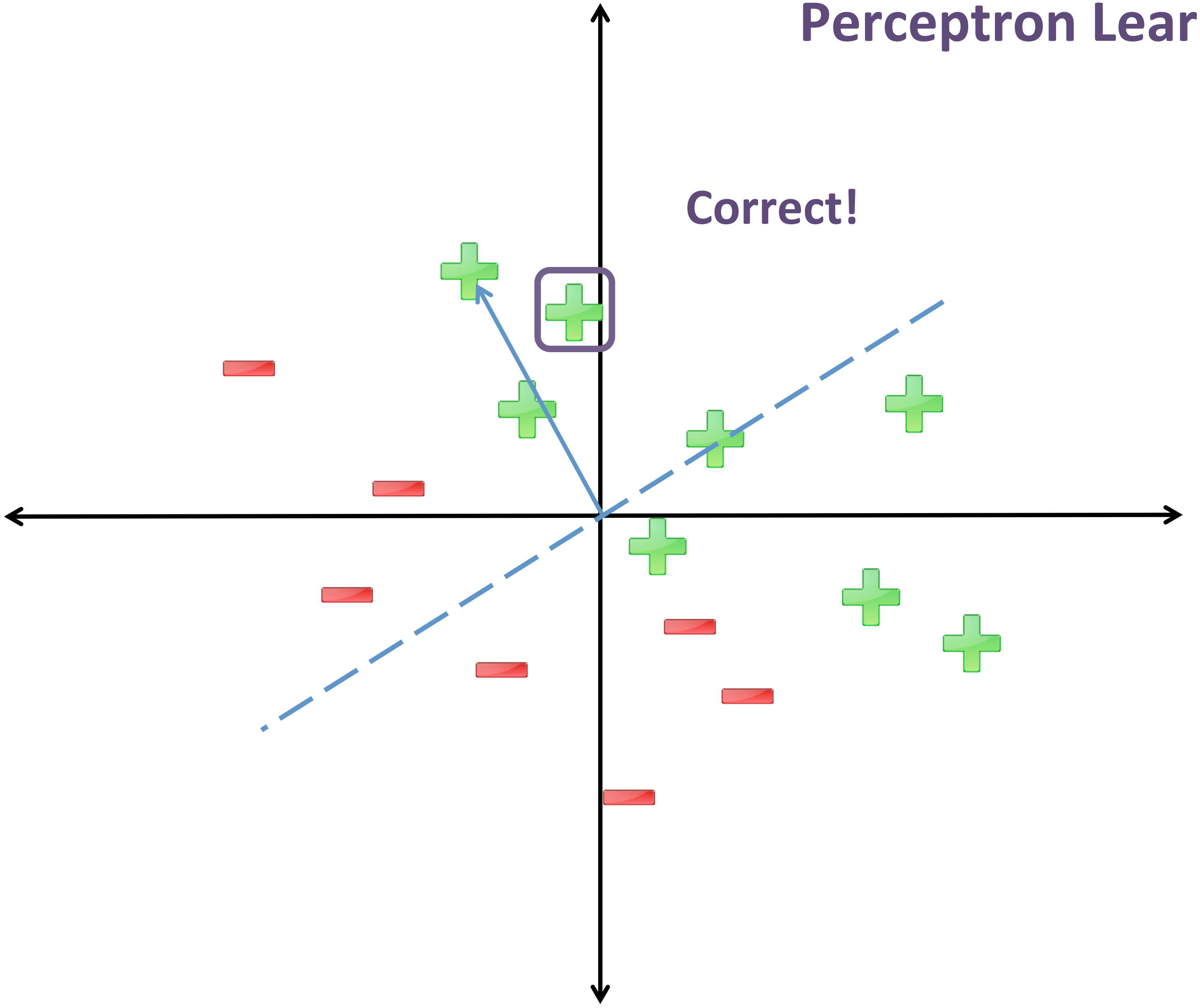

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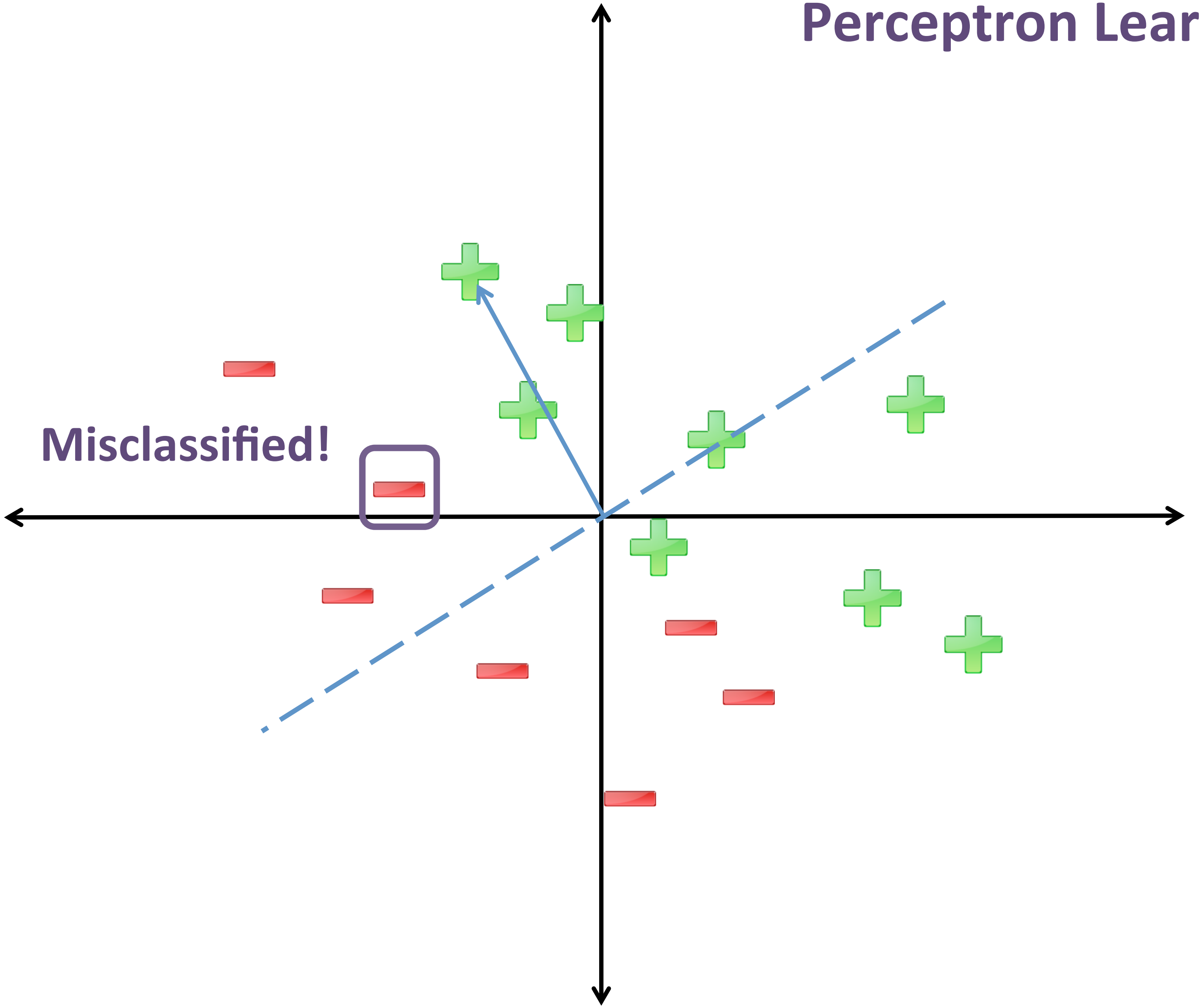

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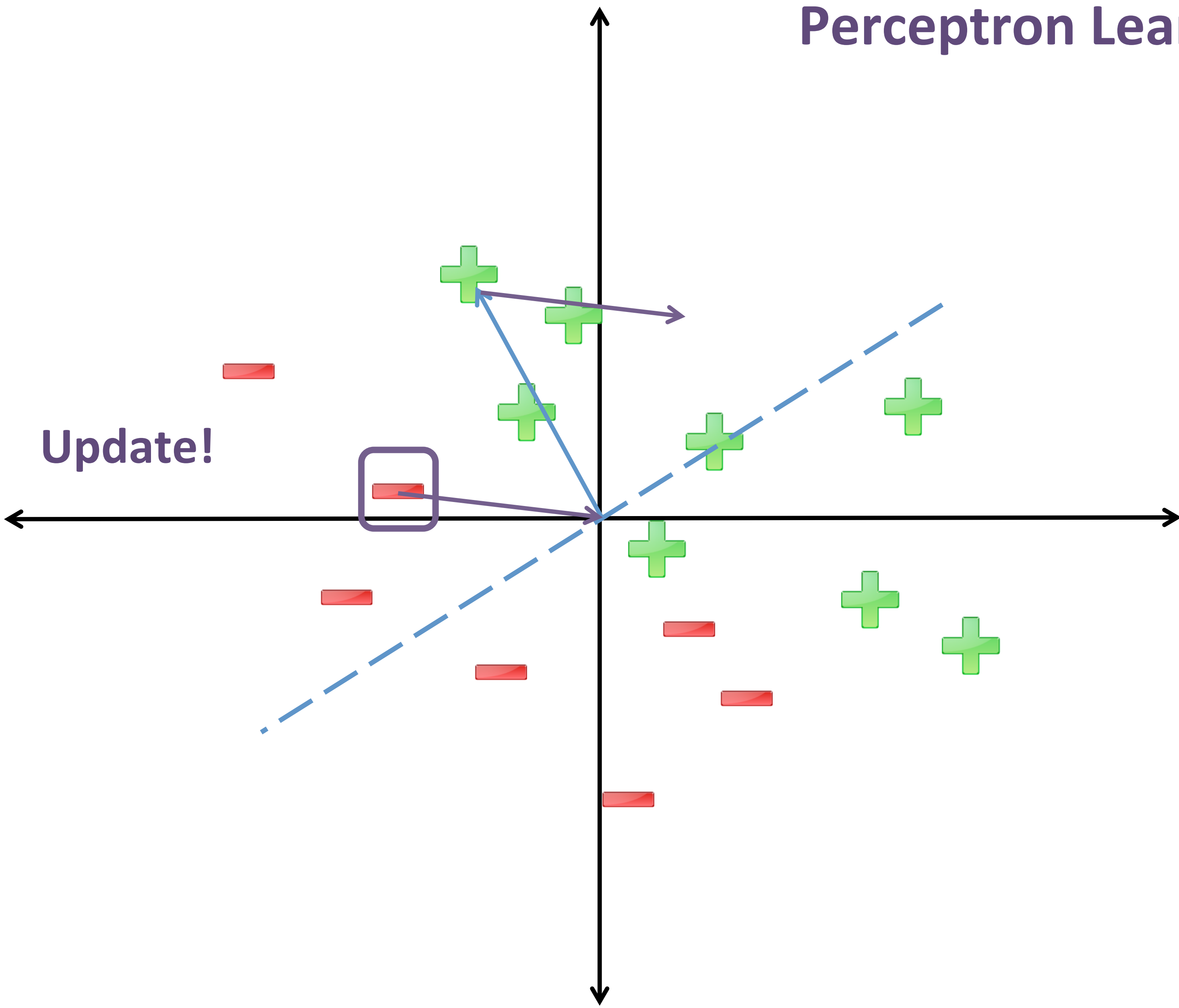

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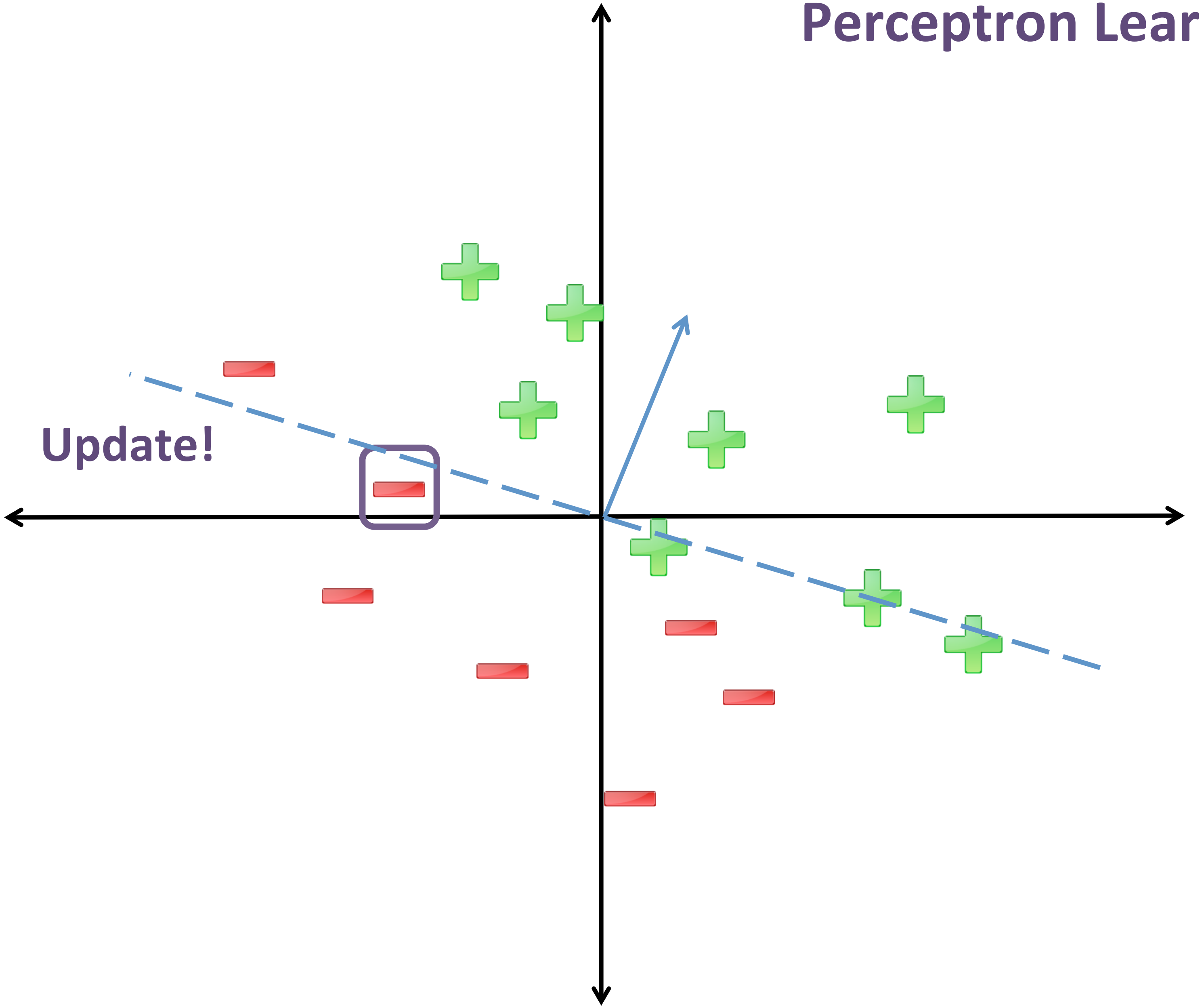

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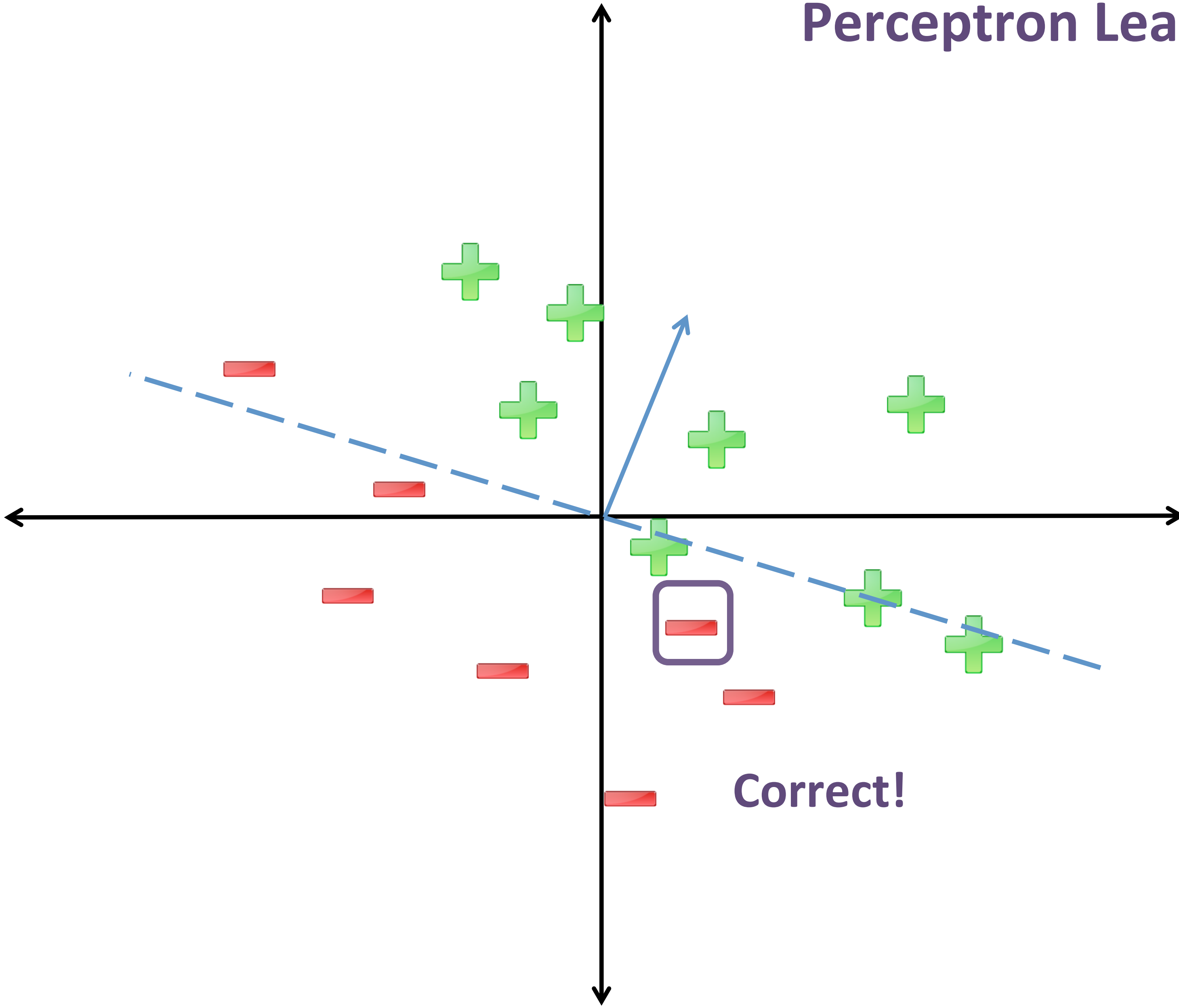
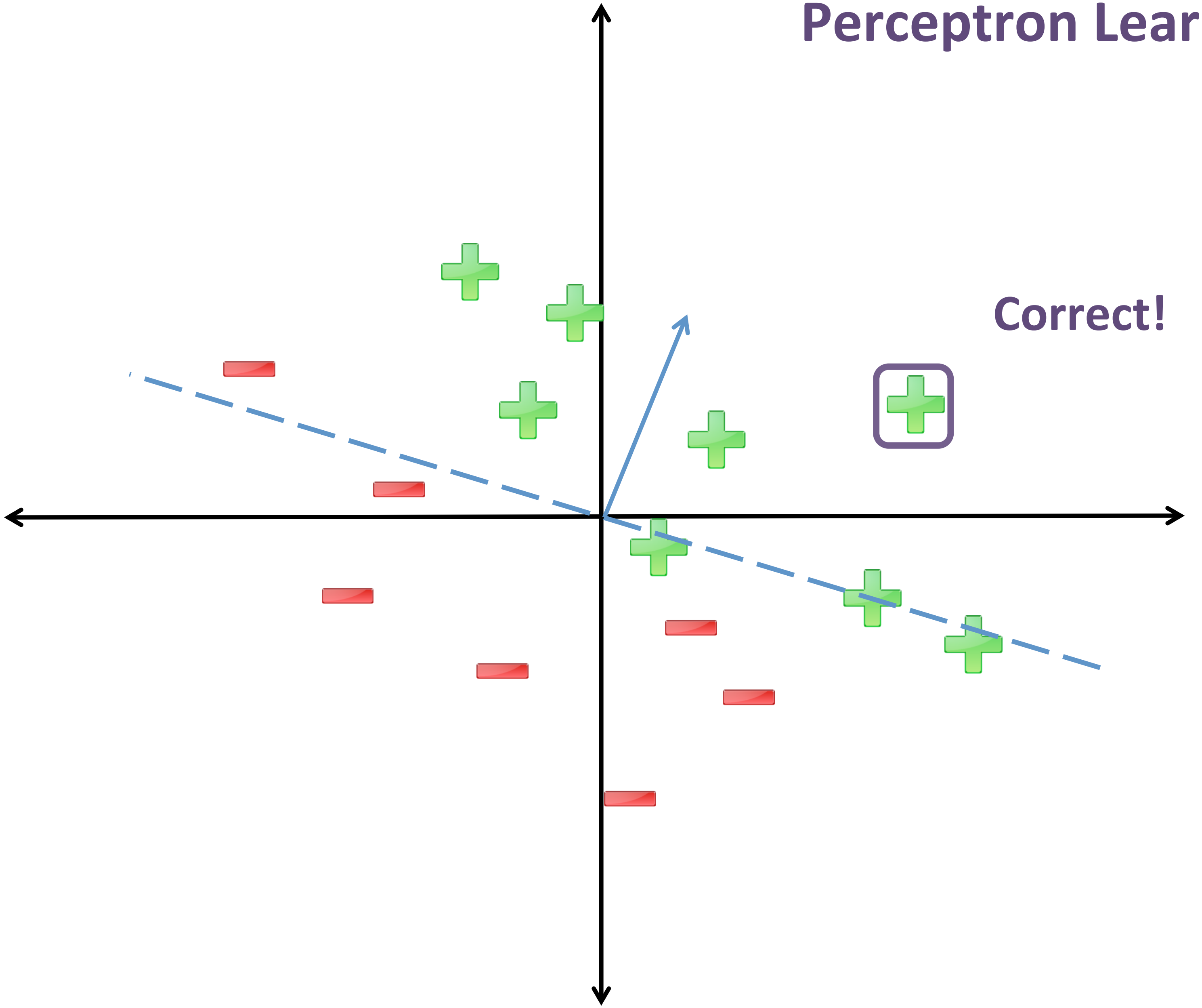


Correct!

Perceptron Learning



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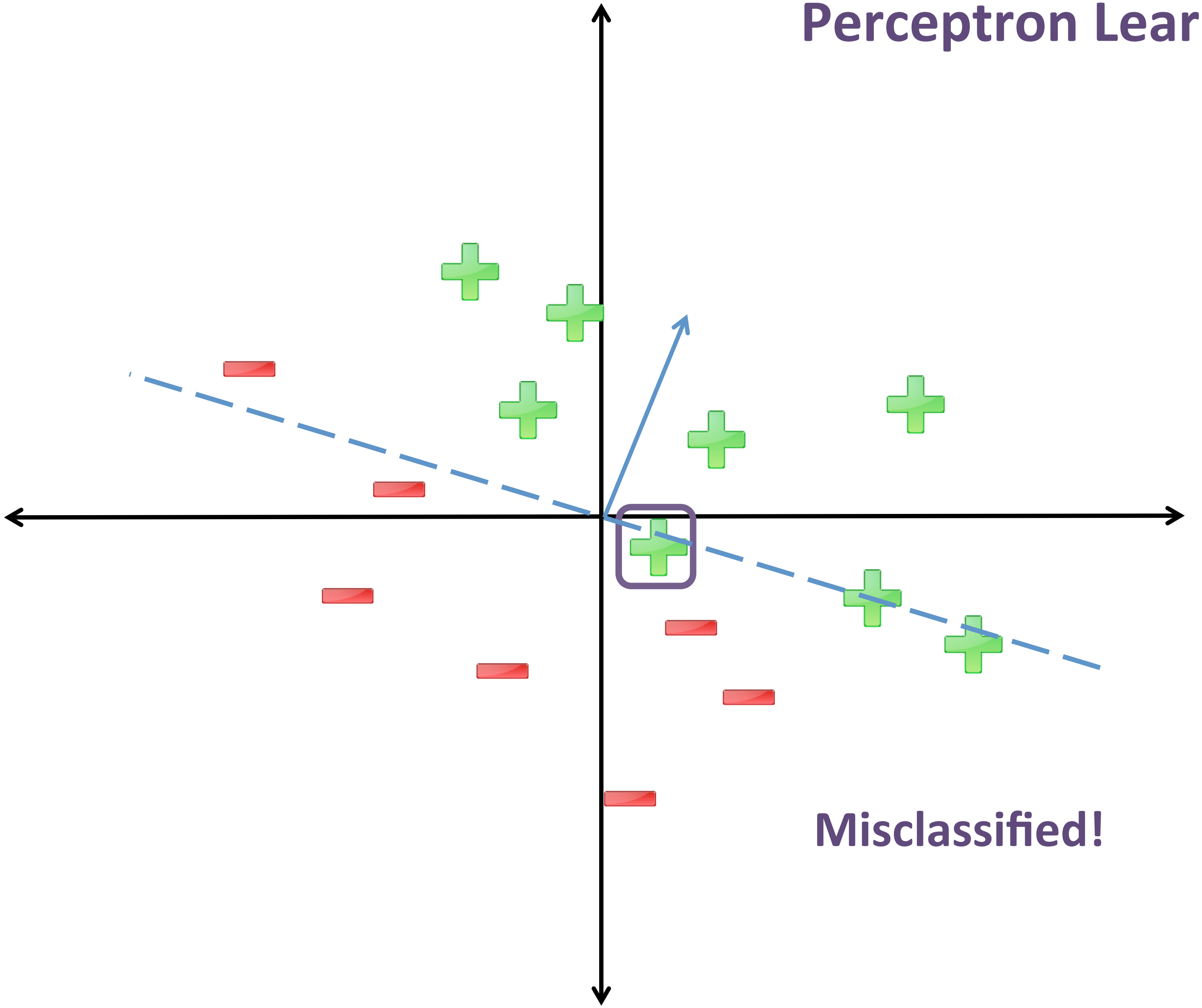
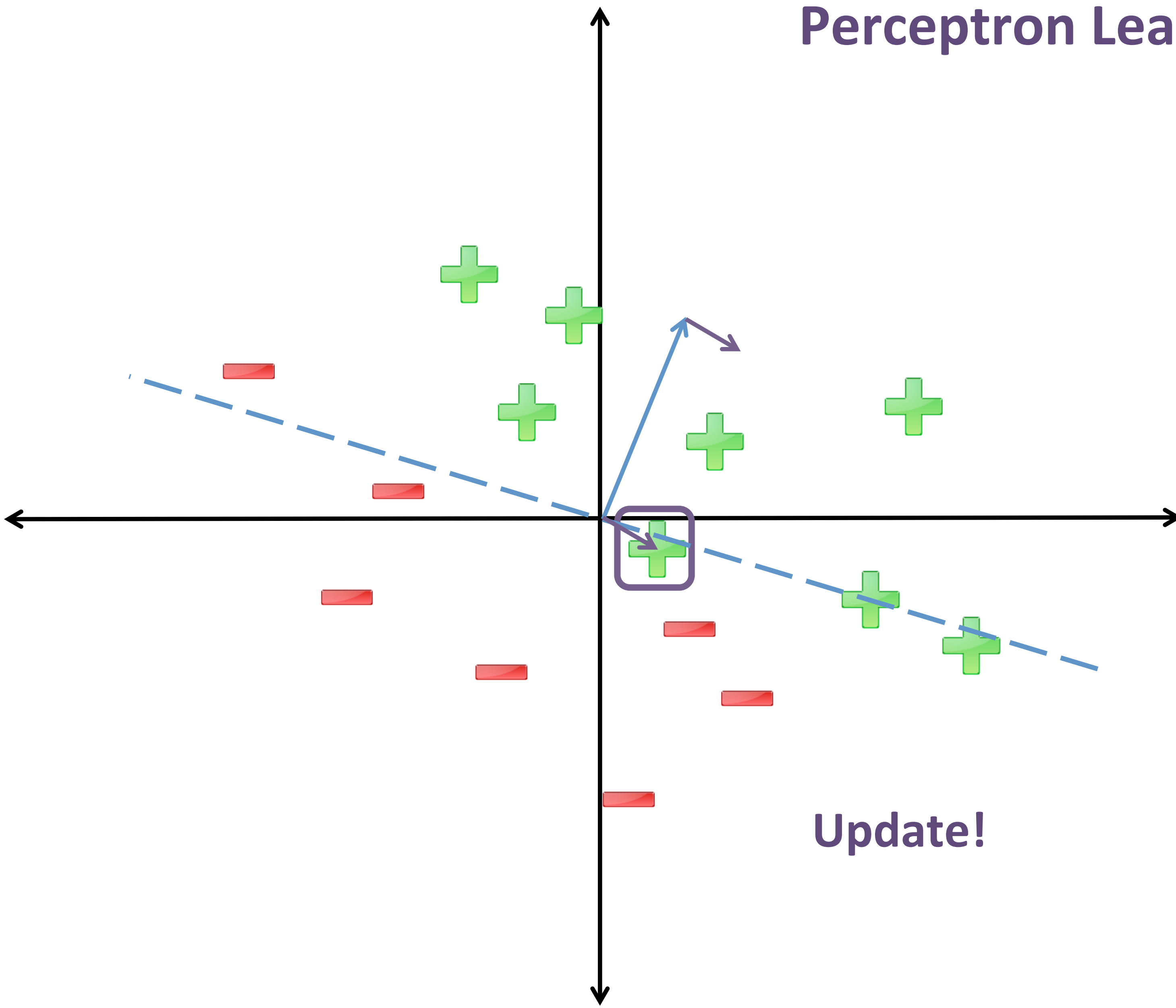


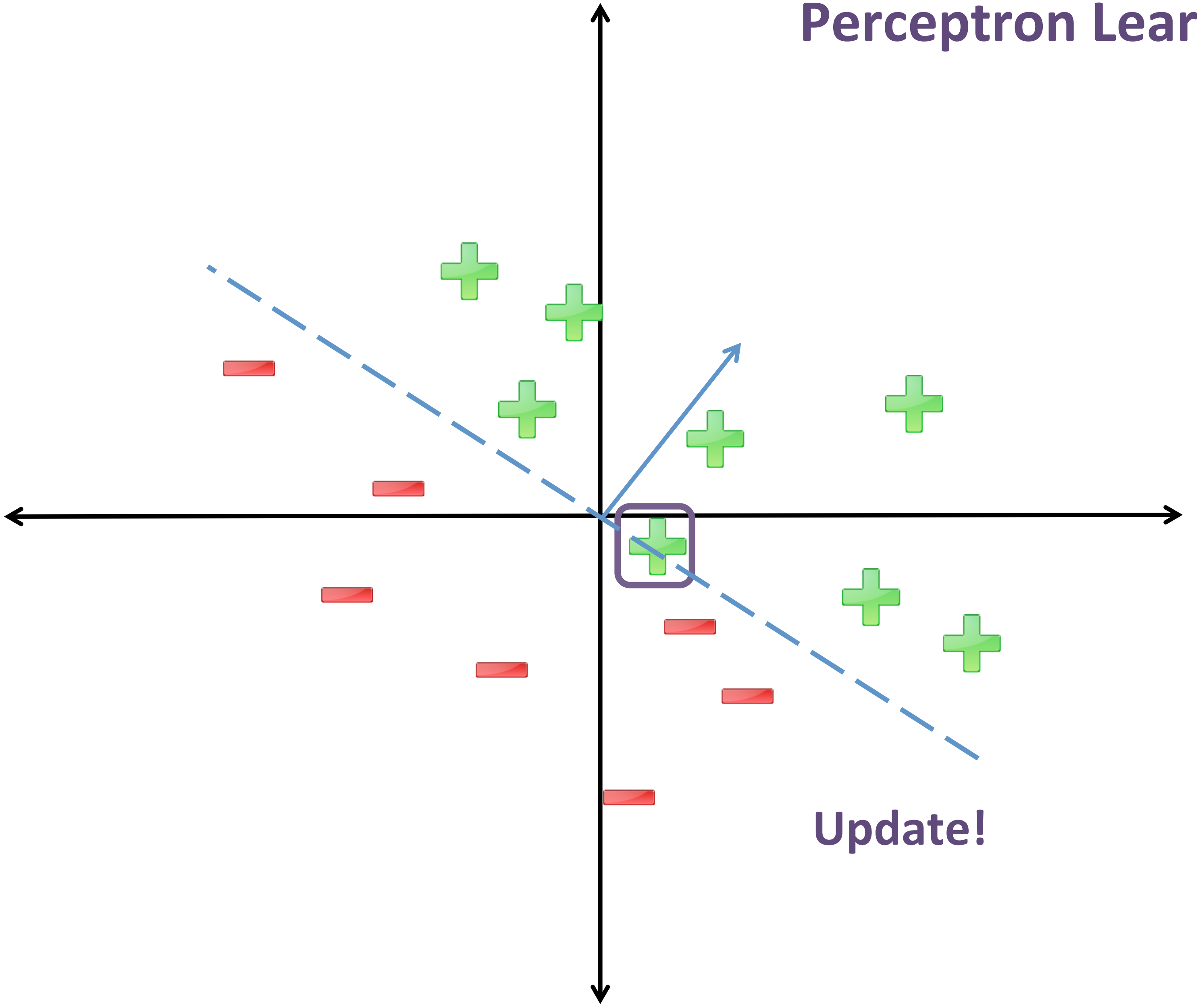
Misclassified!

Perceptron Learning



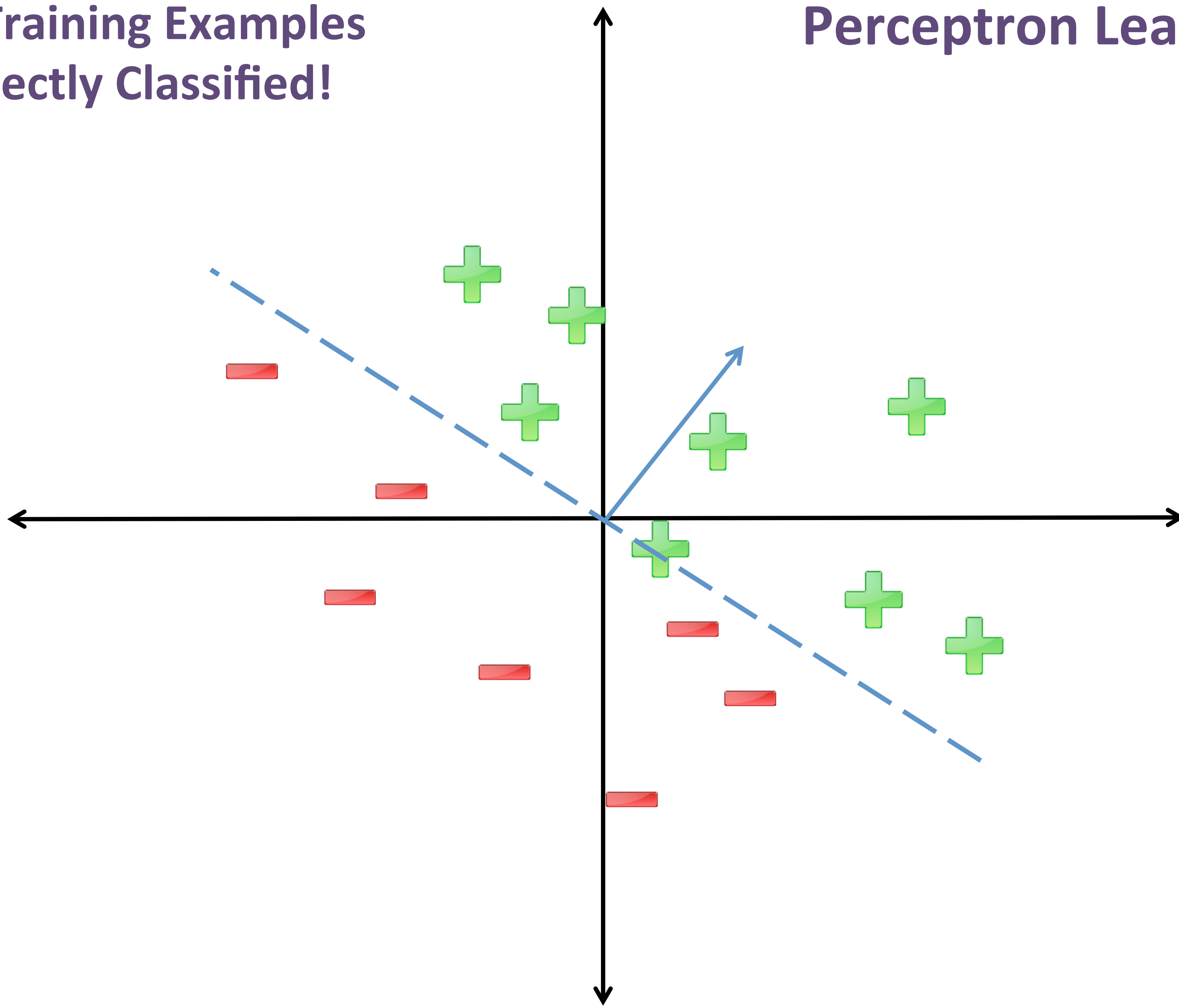
Update!

Perceptron Learning



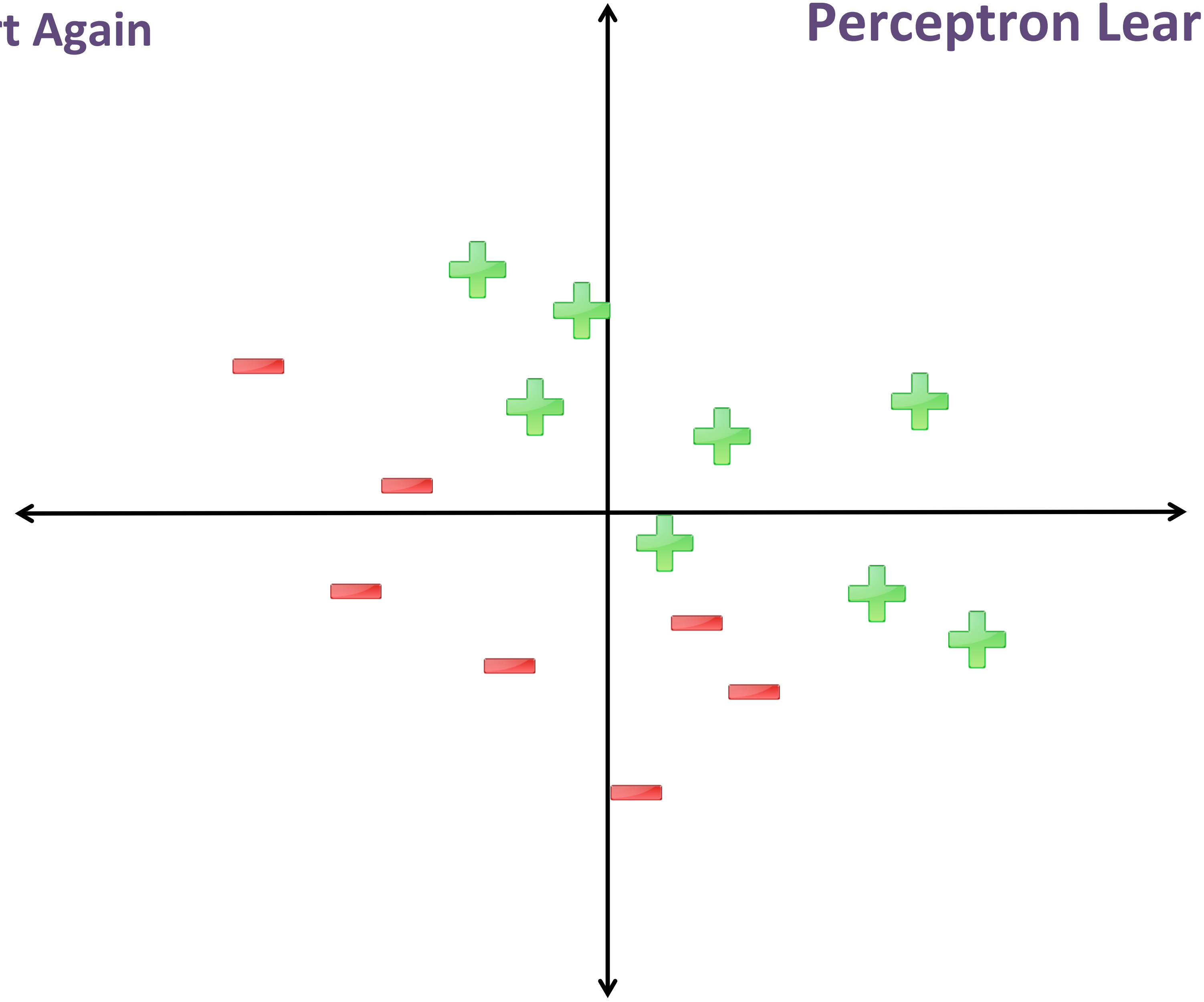
Perceptron Learning

All Training Examples Correctly Classified!



Start Again

Perceptron Learning



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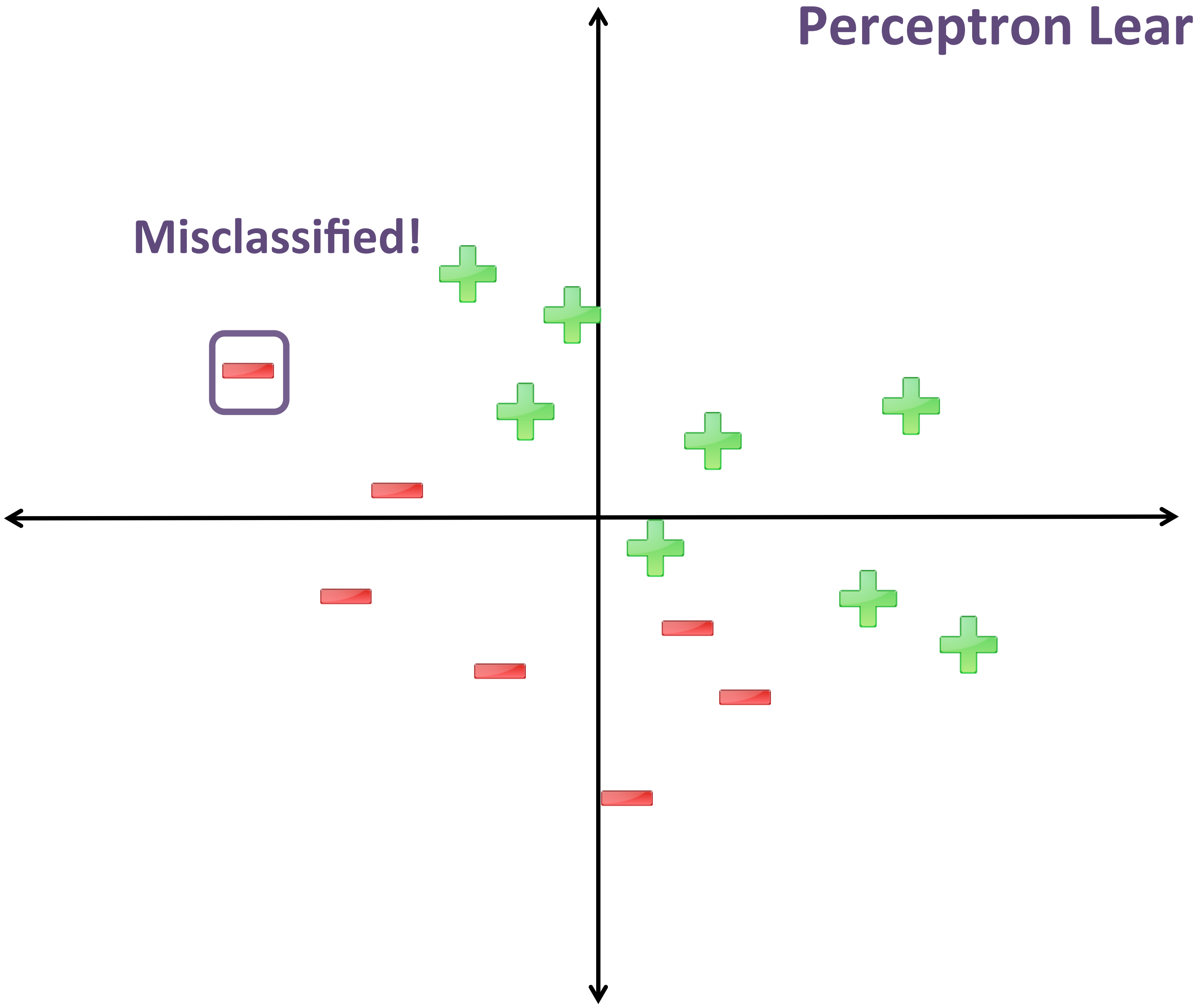

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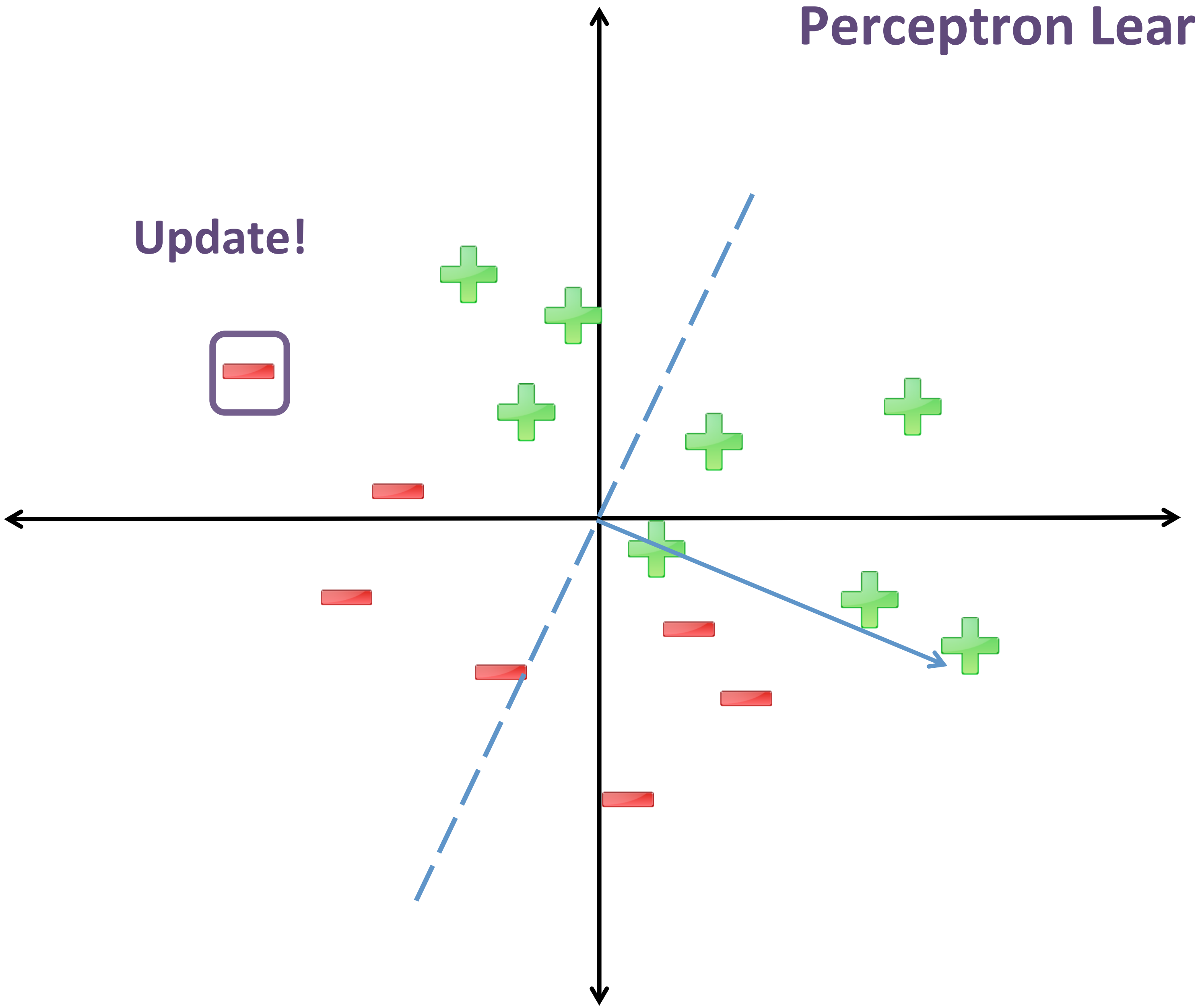

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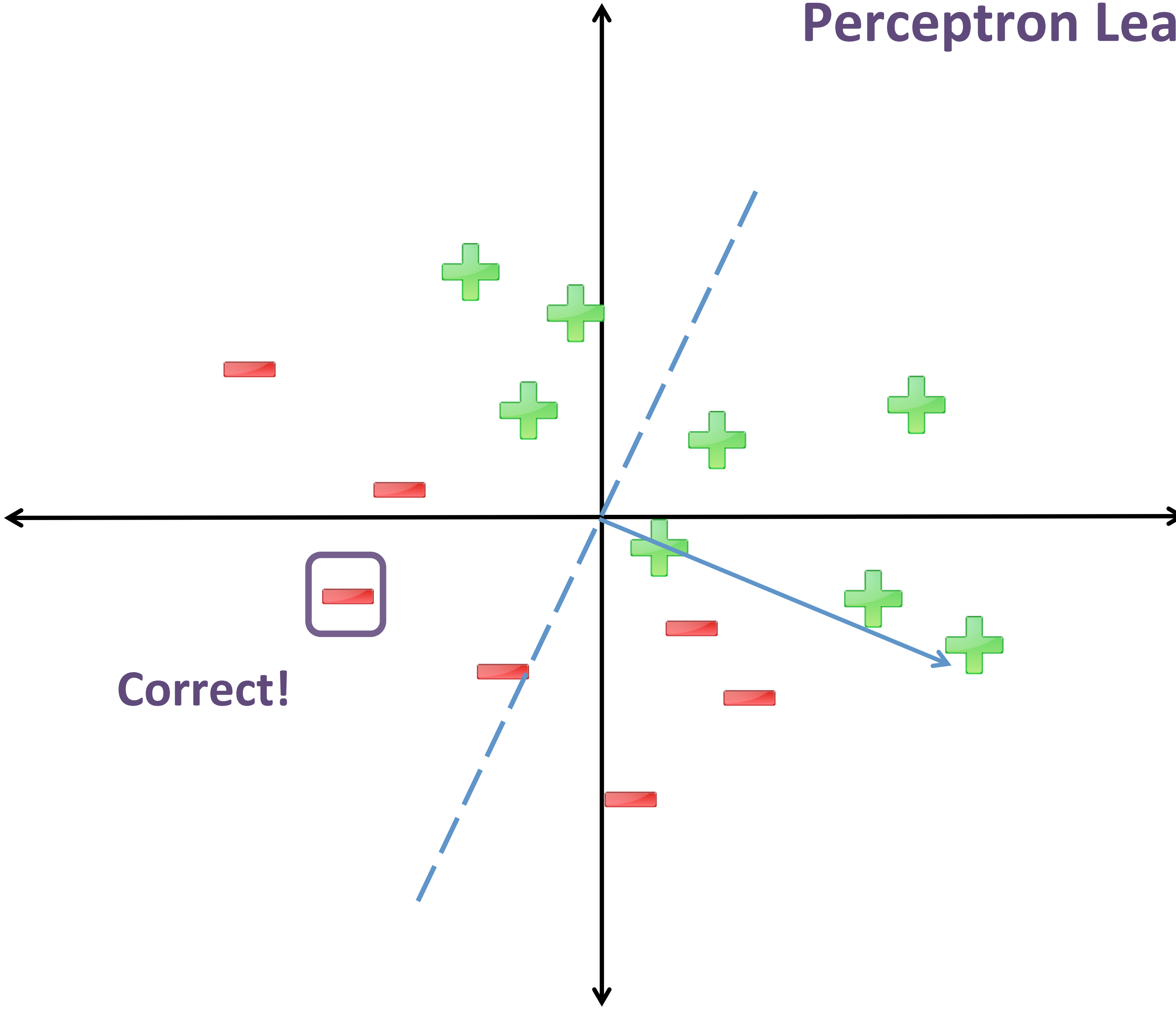

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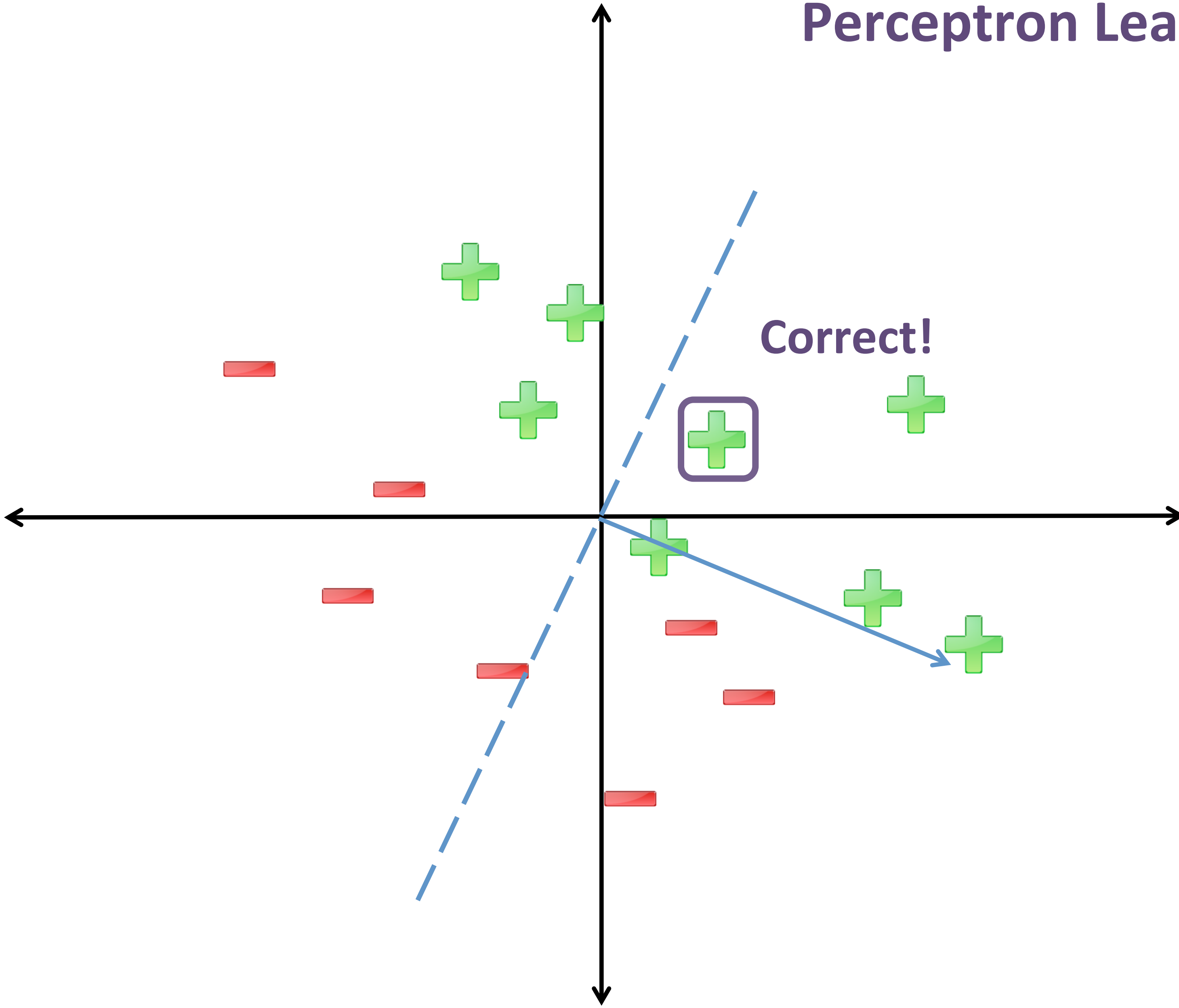

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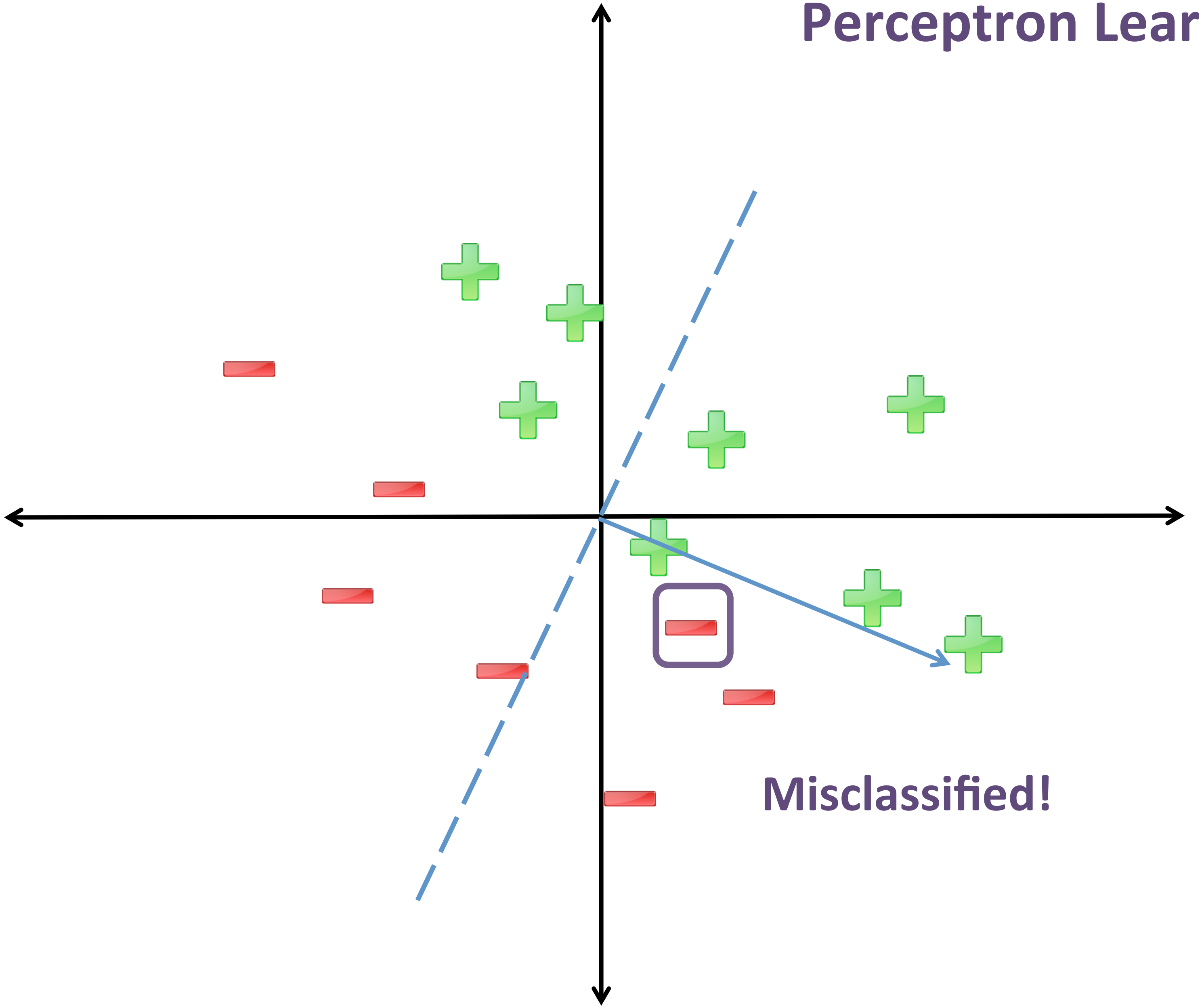

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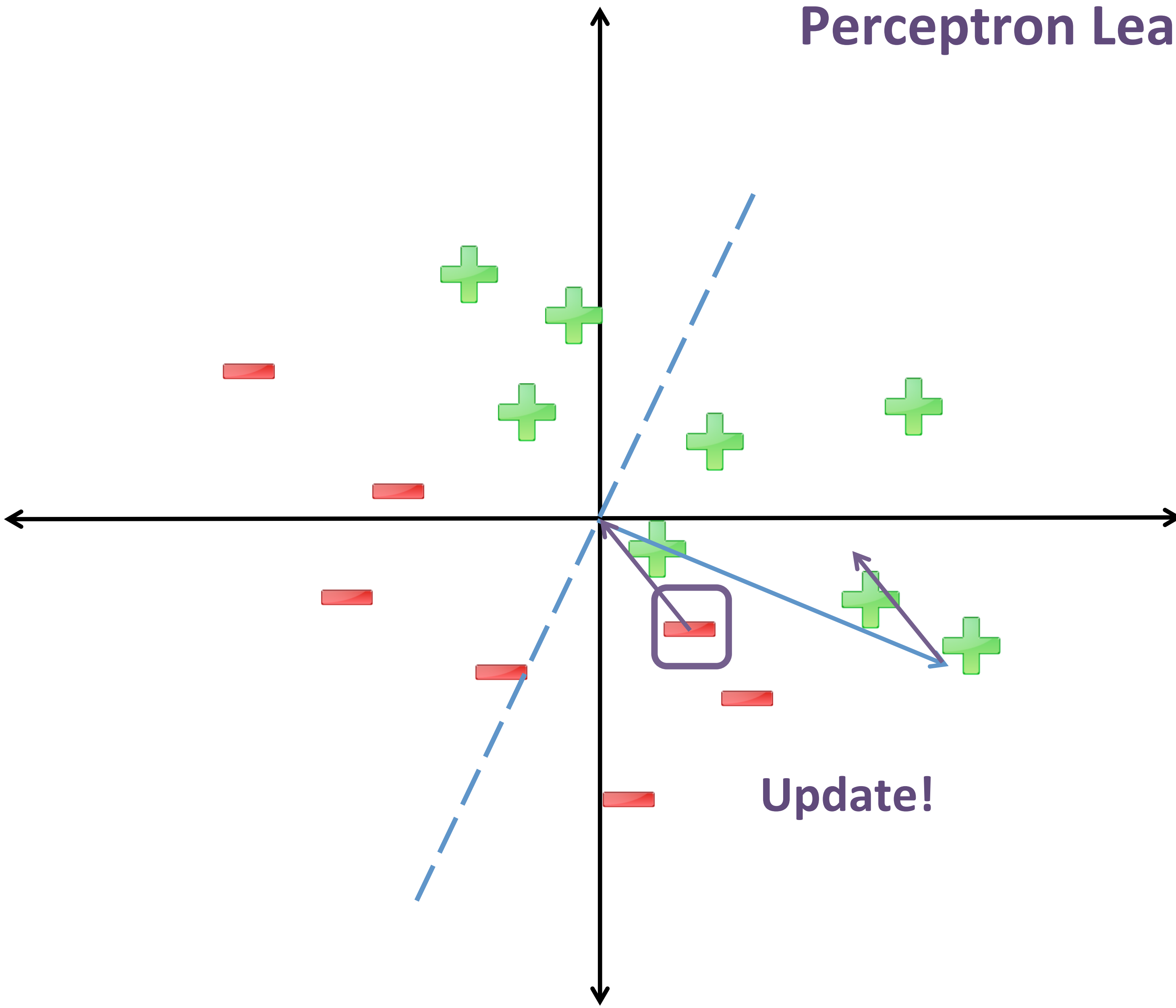
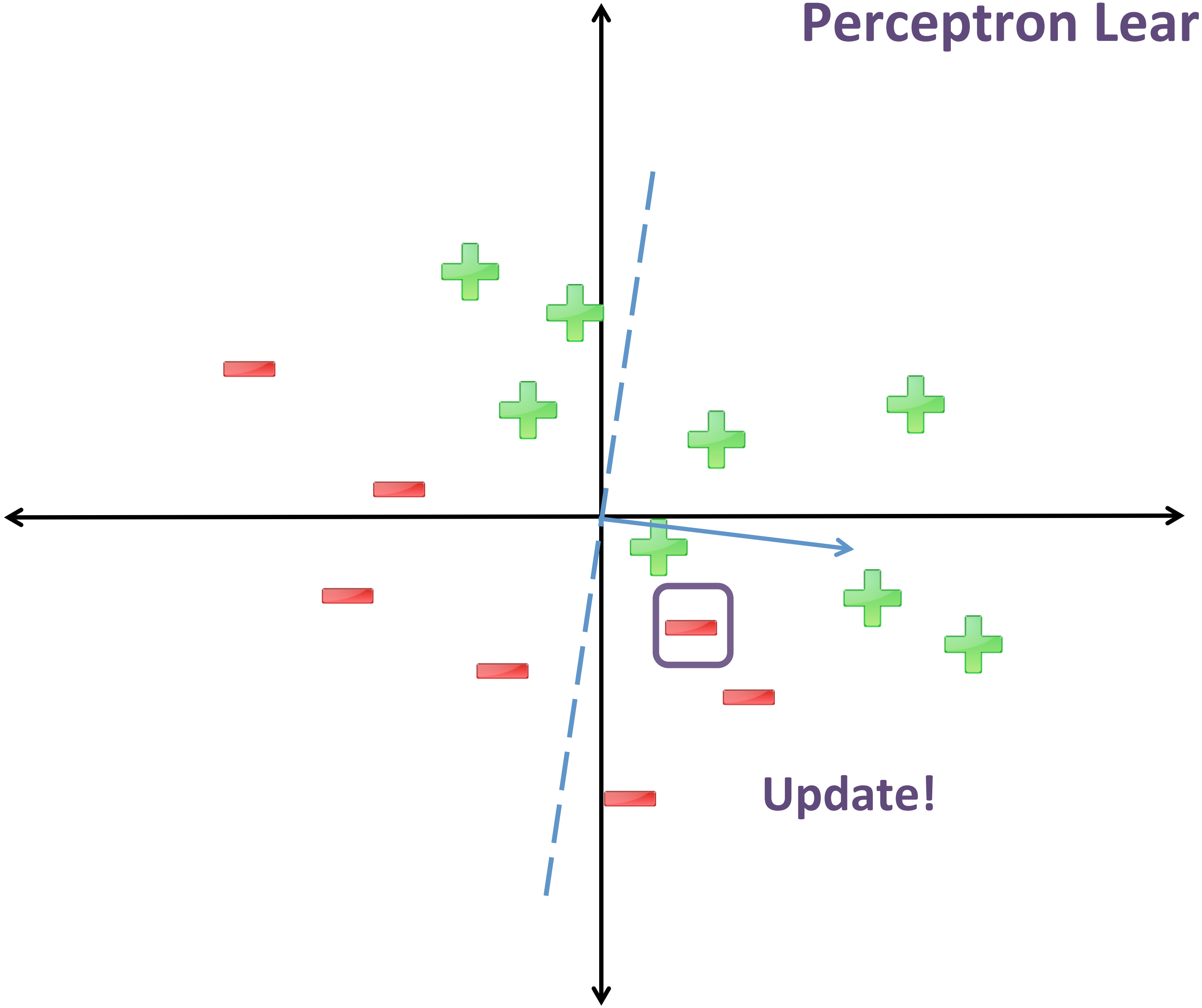


Update!

Perceptron Learning



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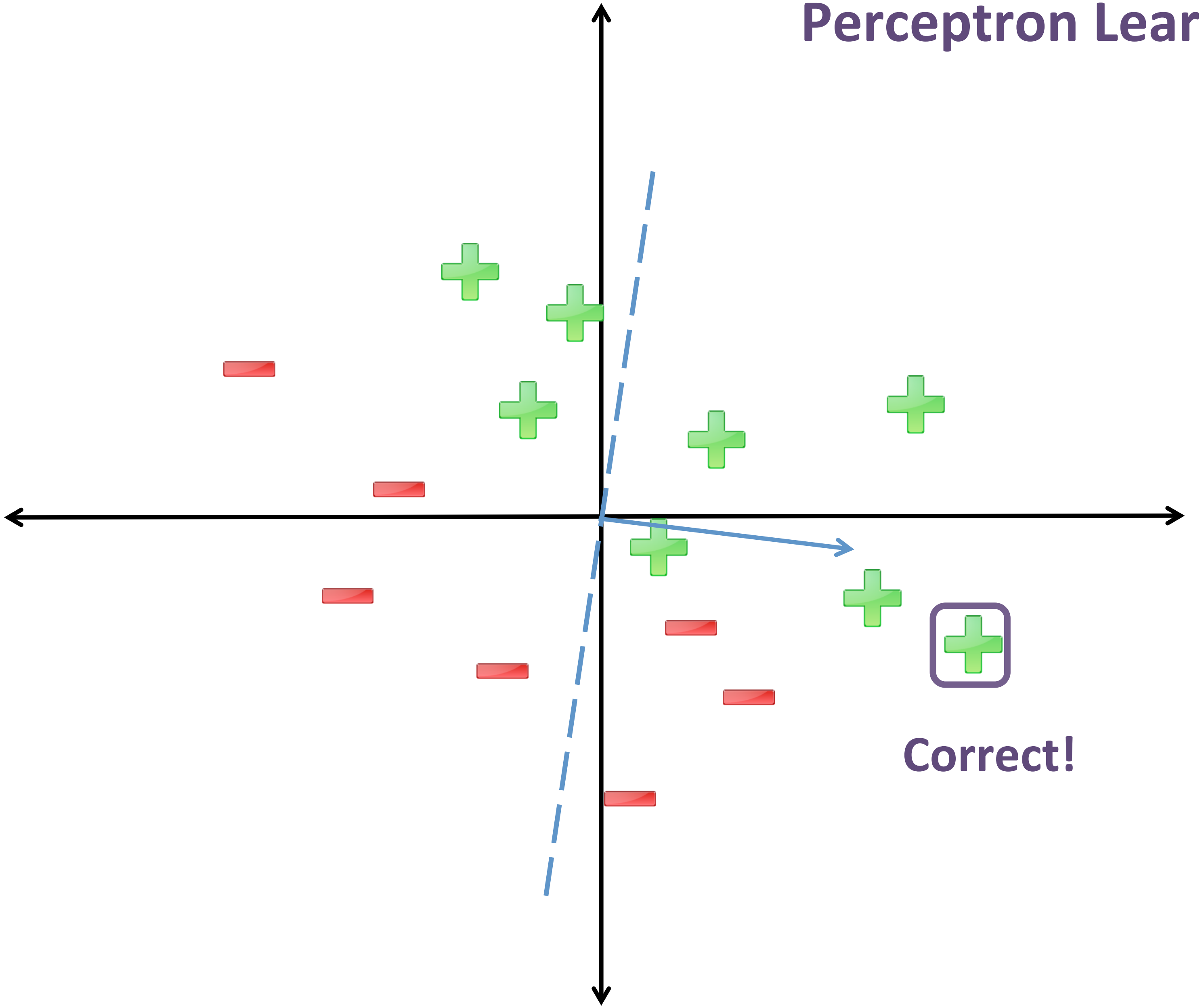

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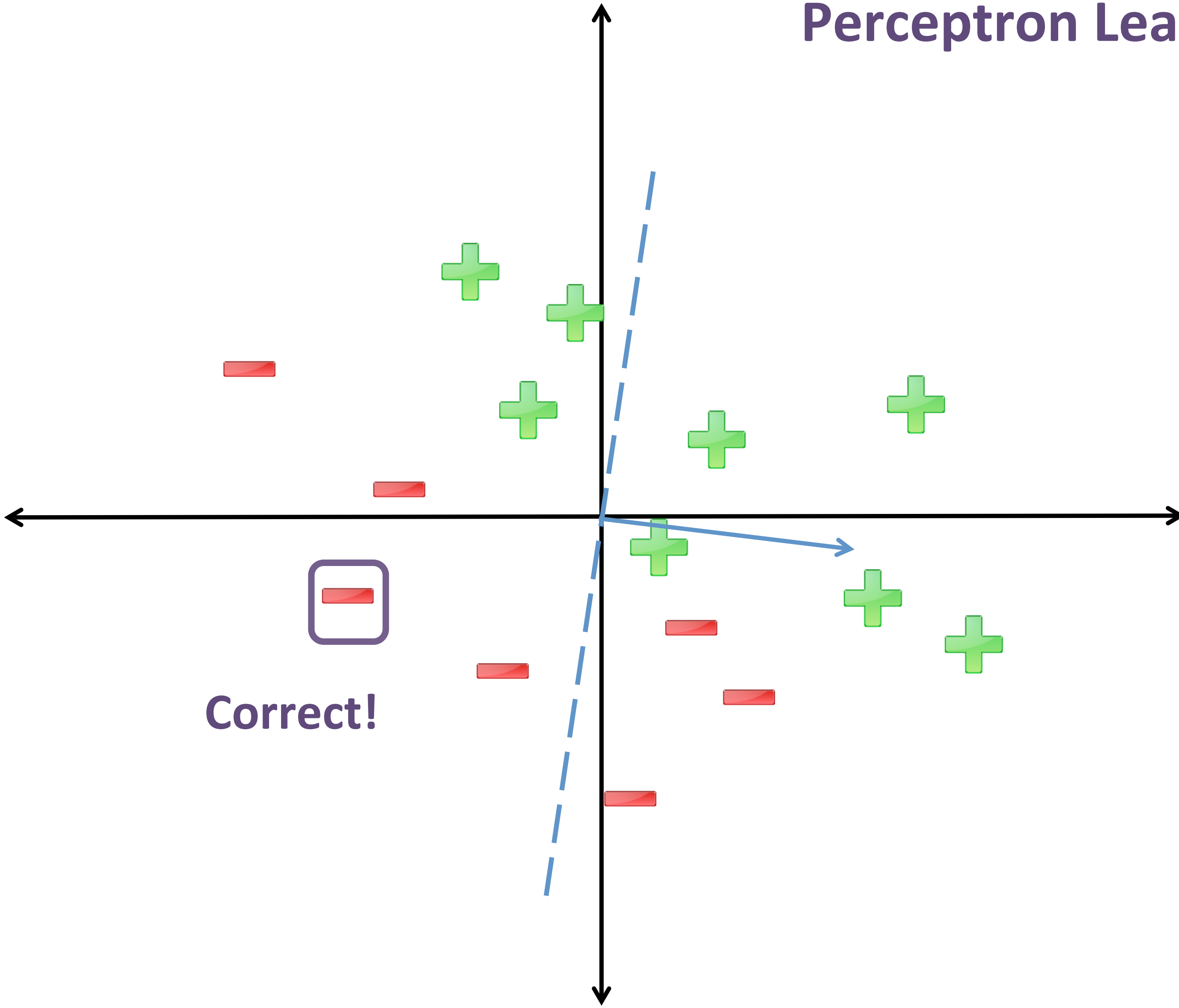

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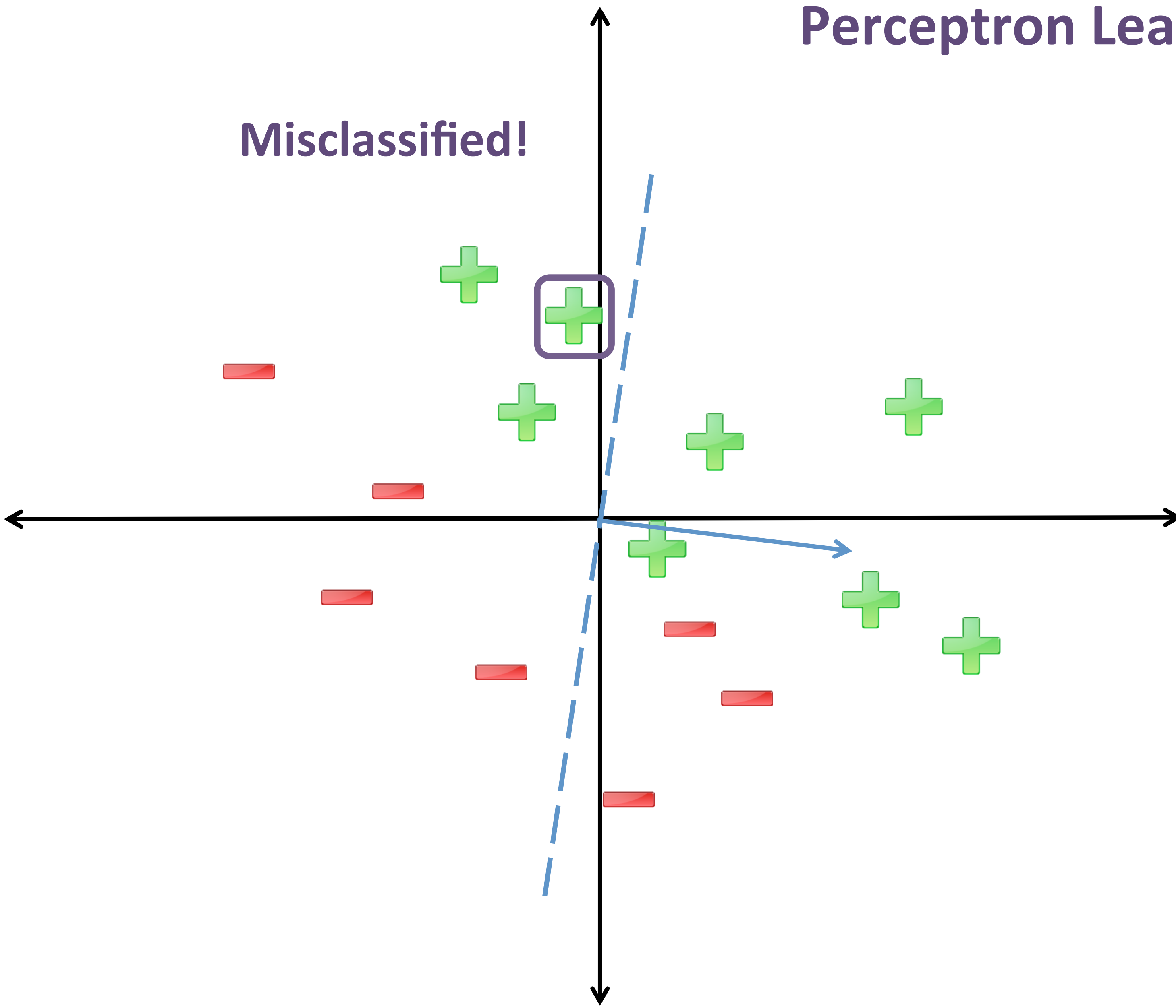
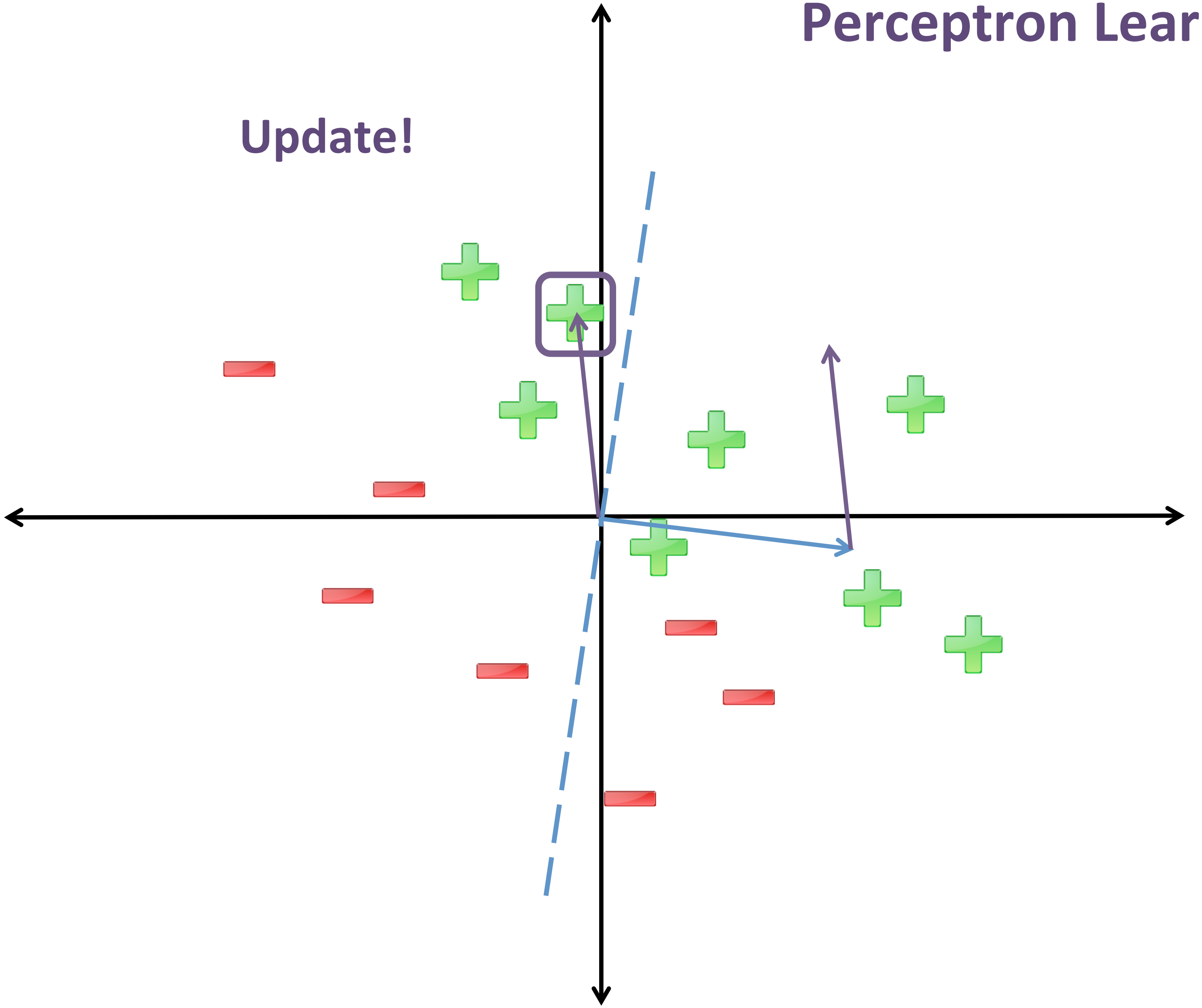


Perceptron Learning

Update!



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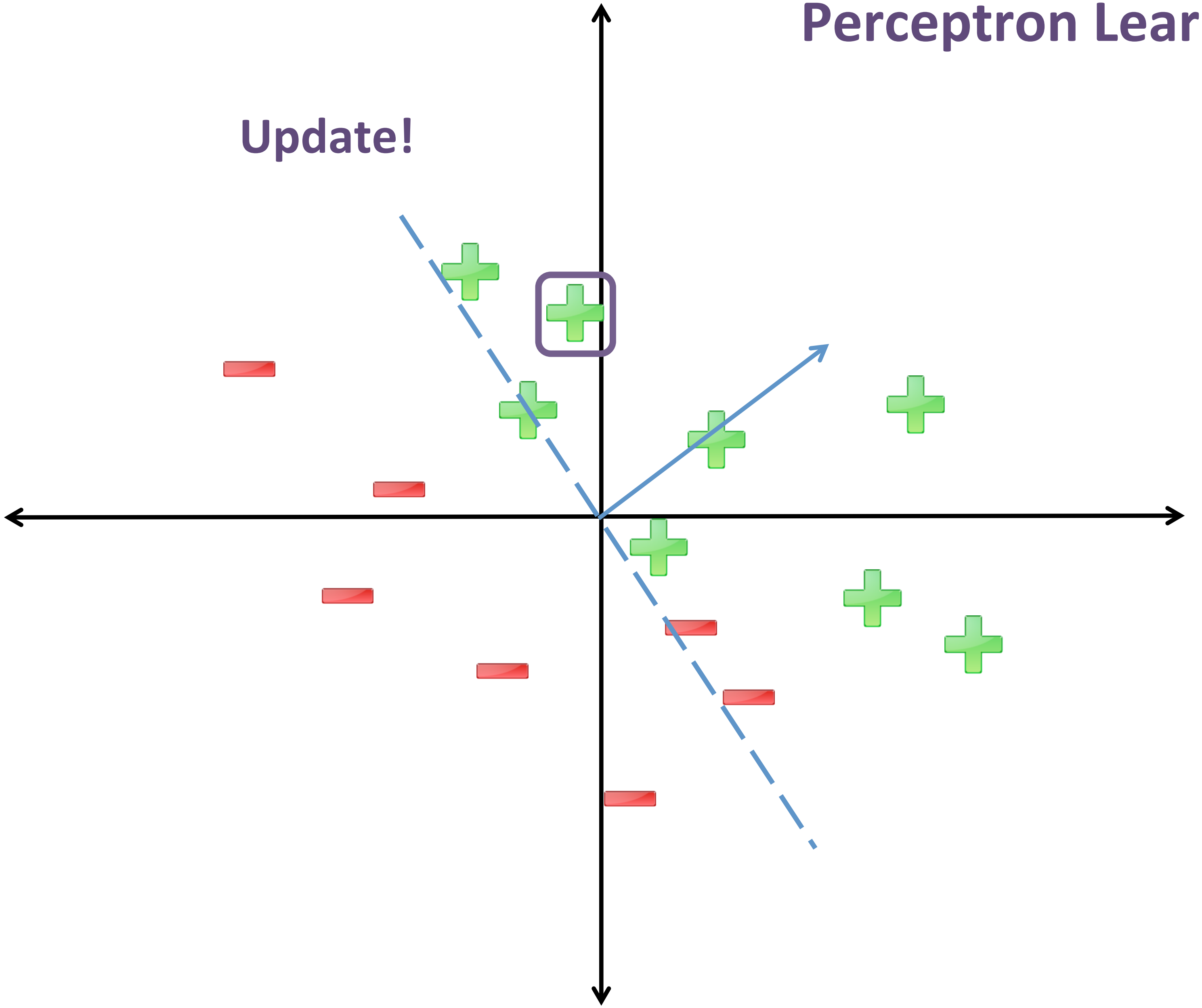

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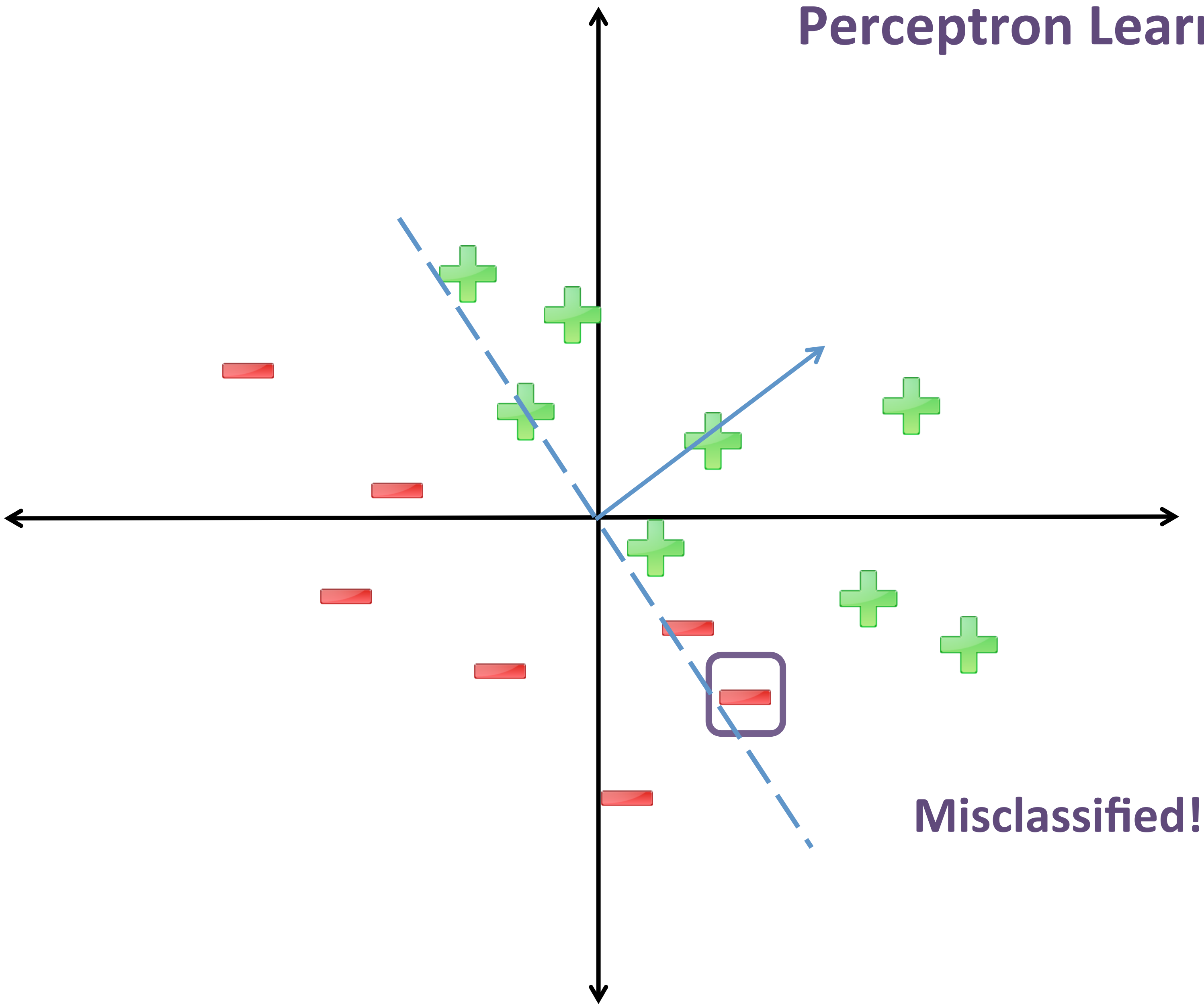

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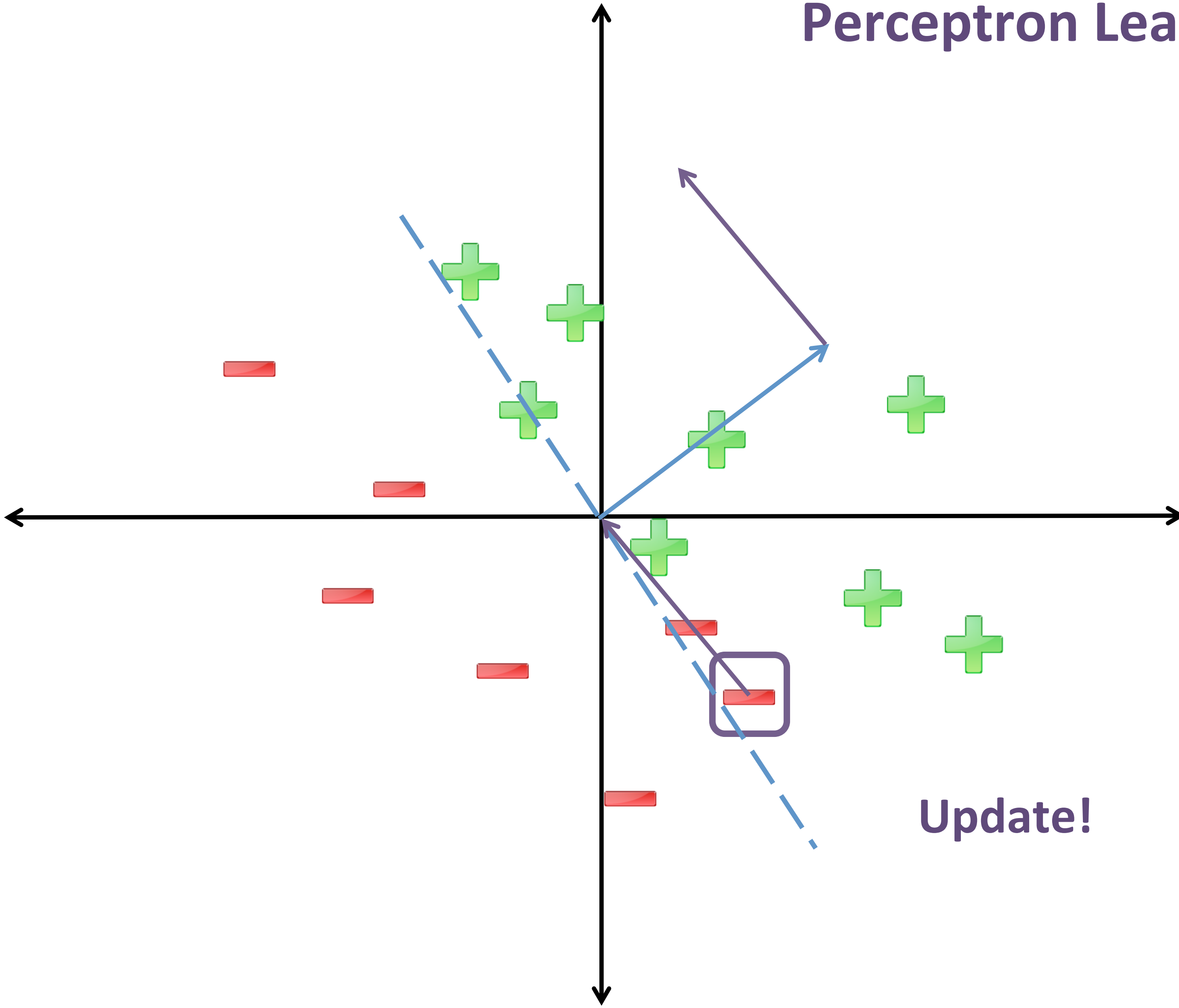

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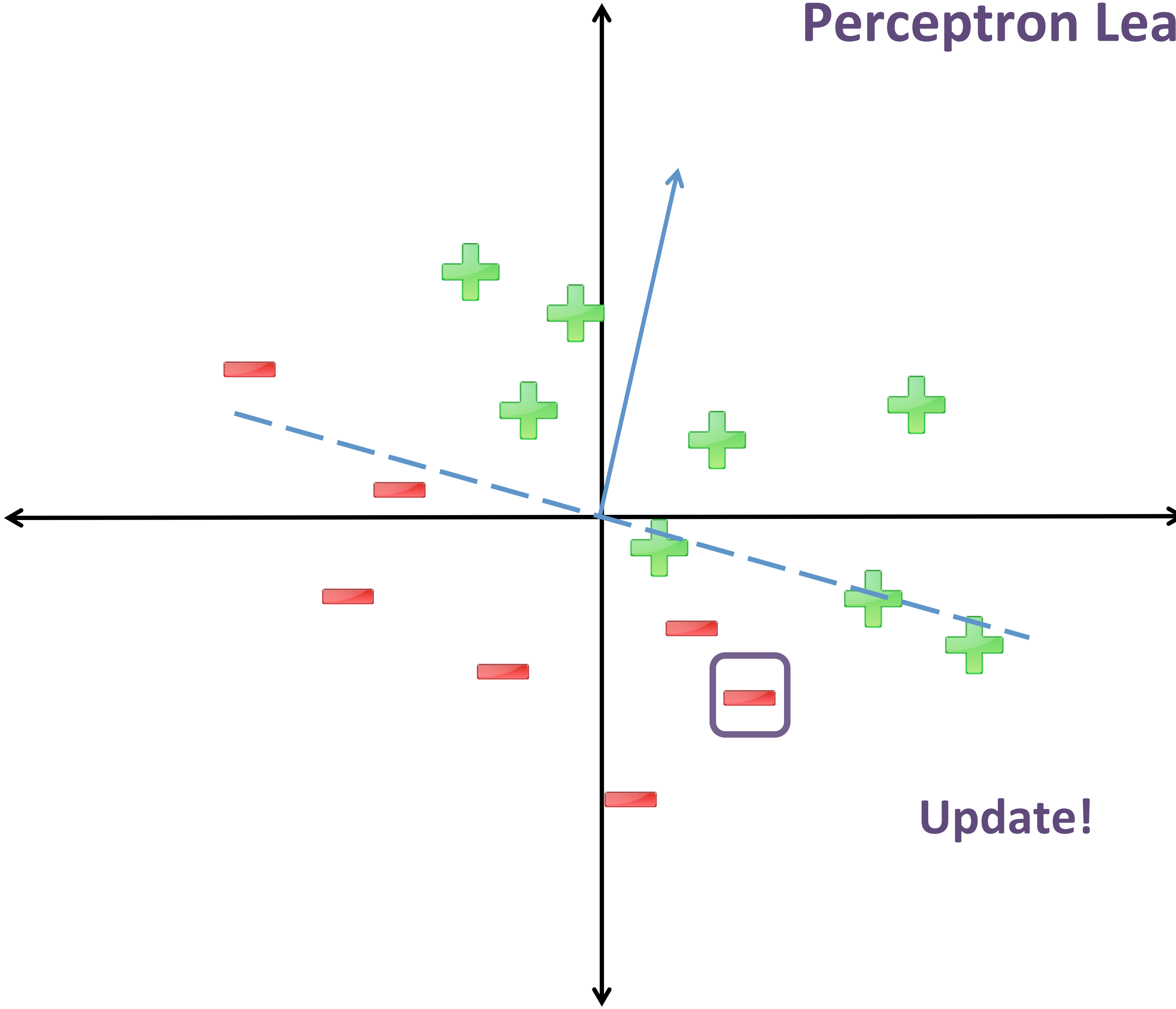

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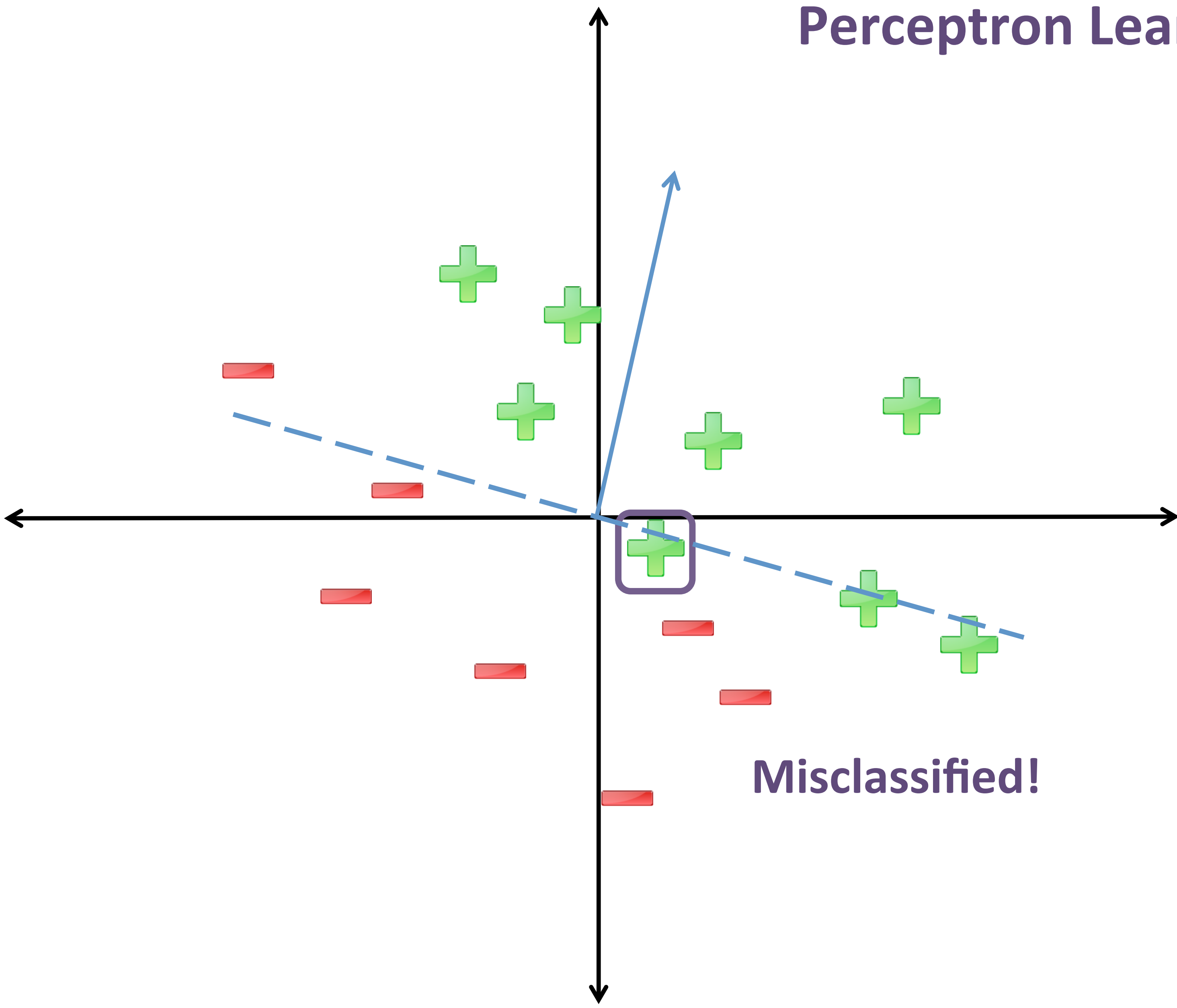

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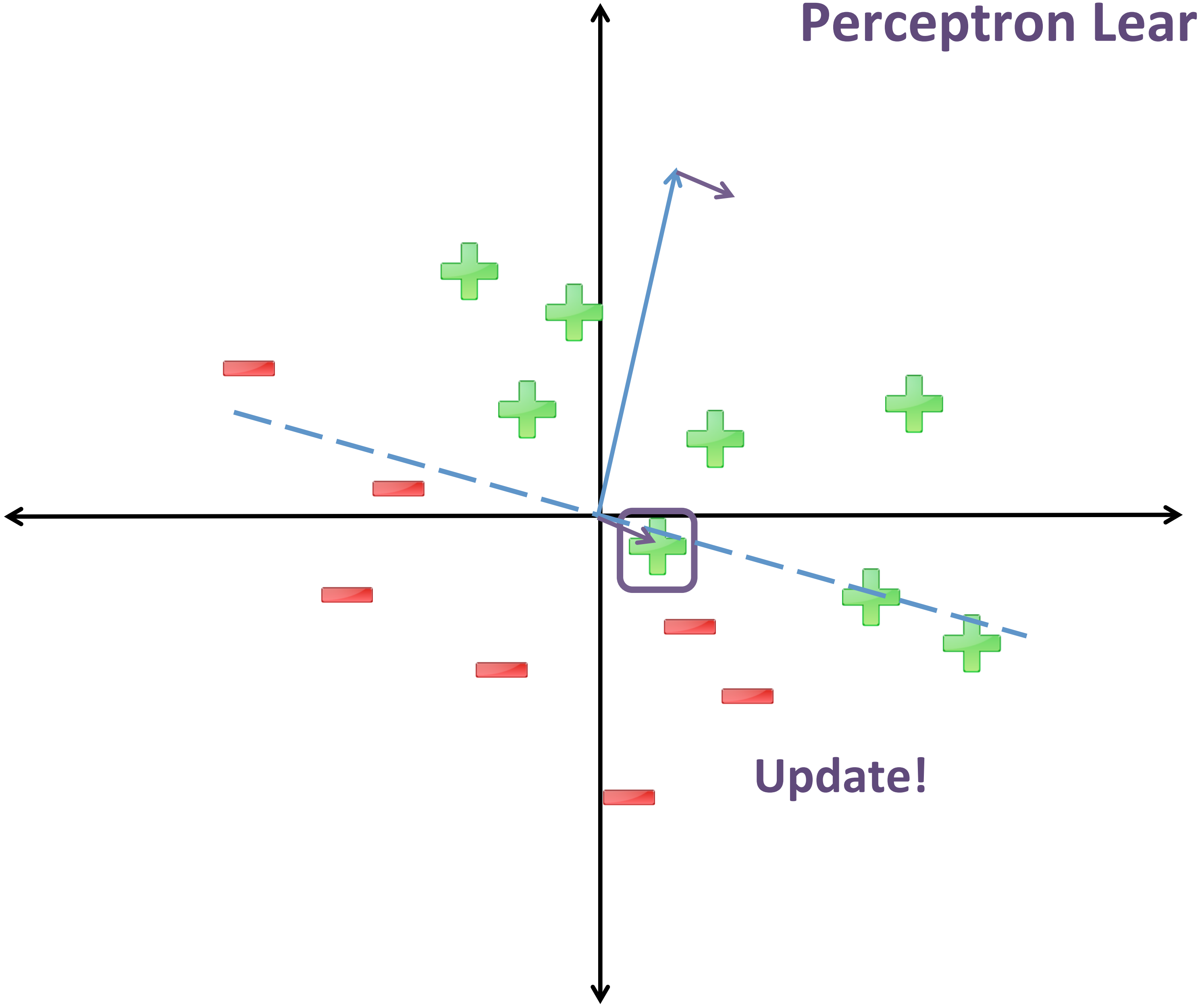

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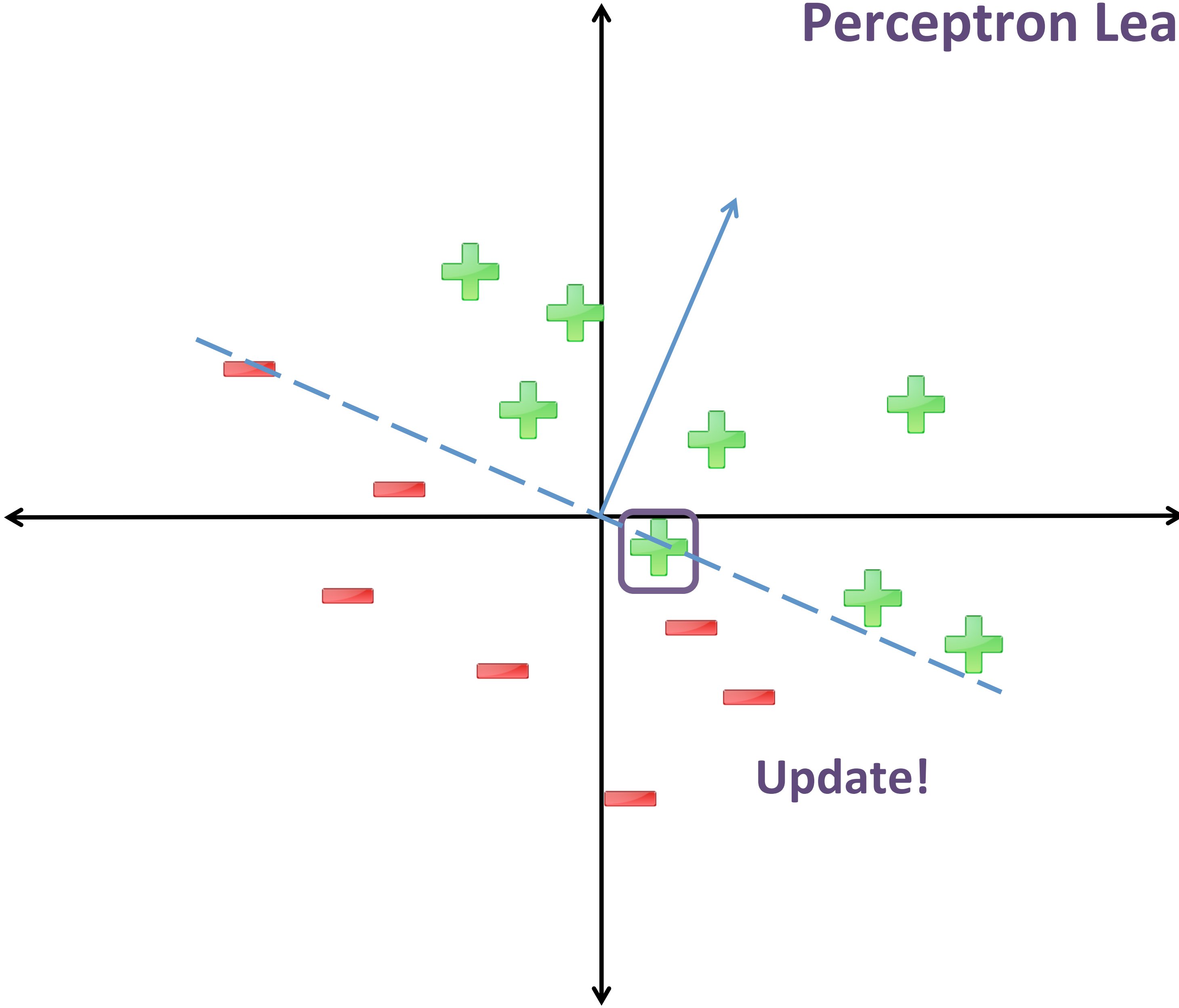

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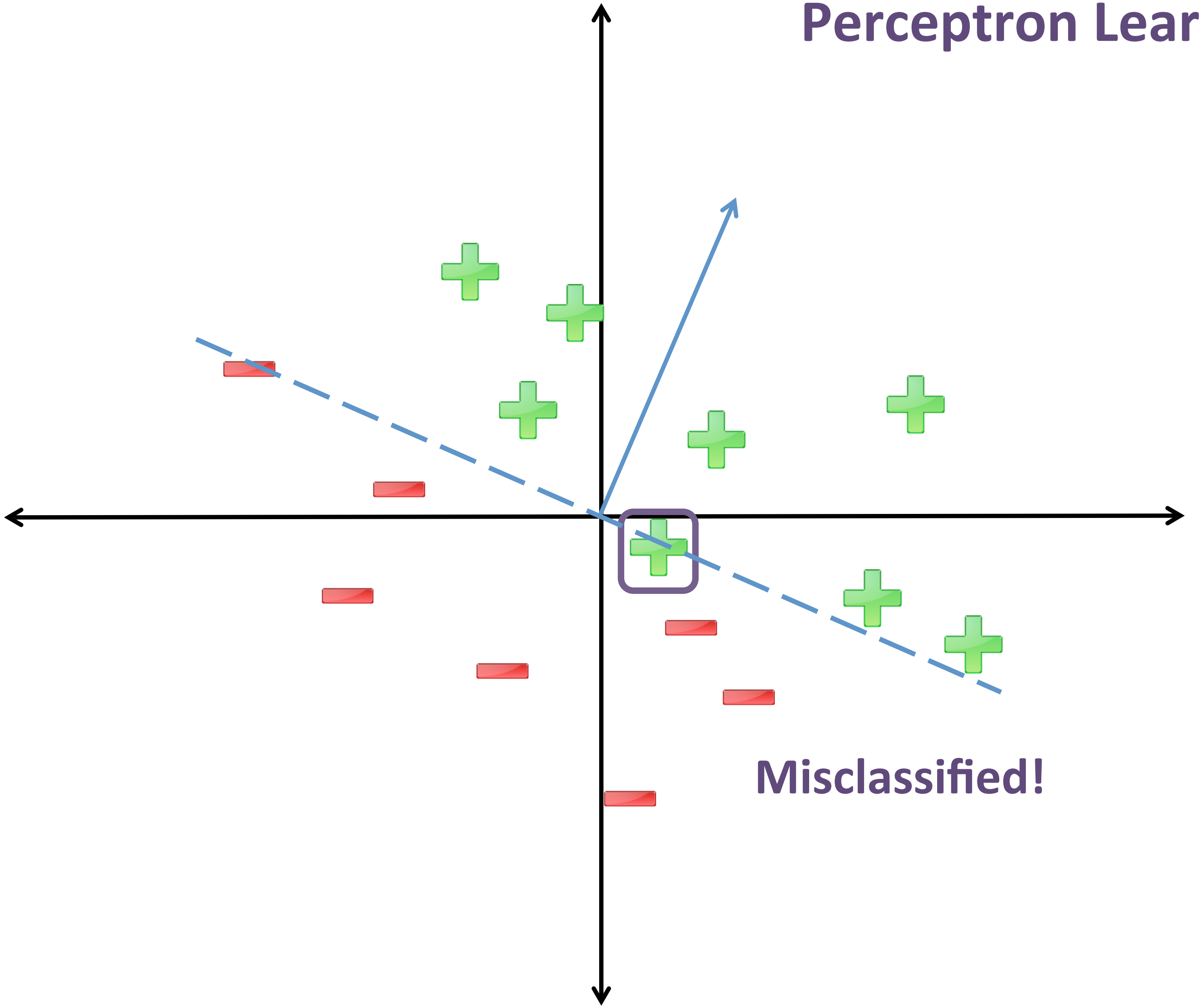

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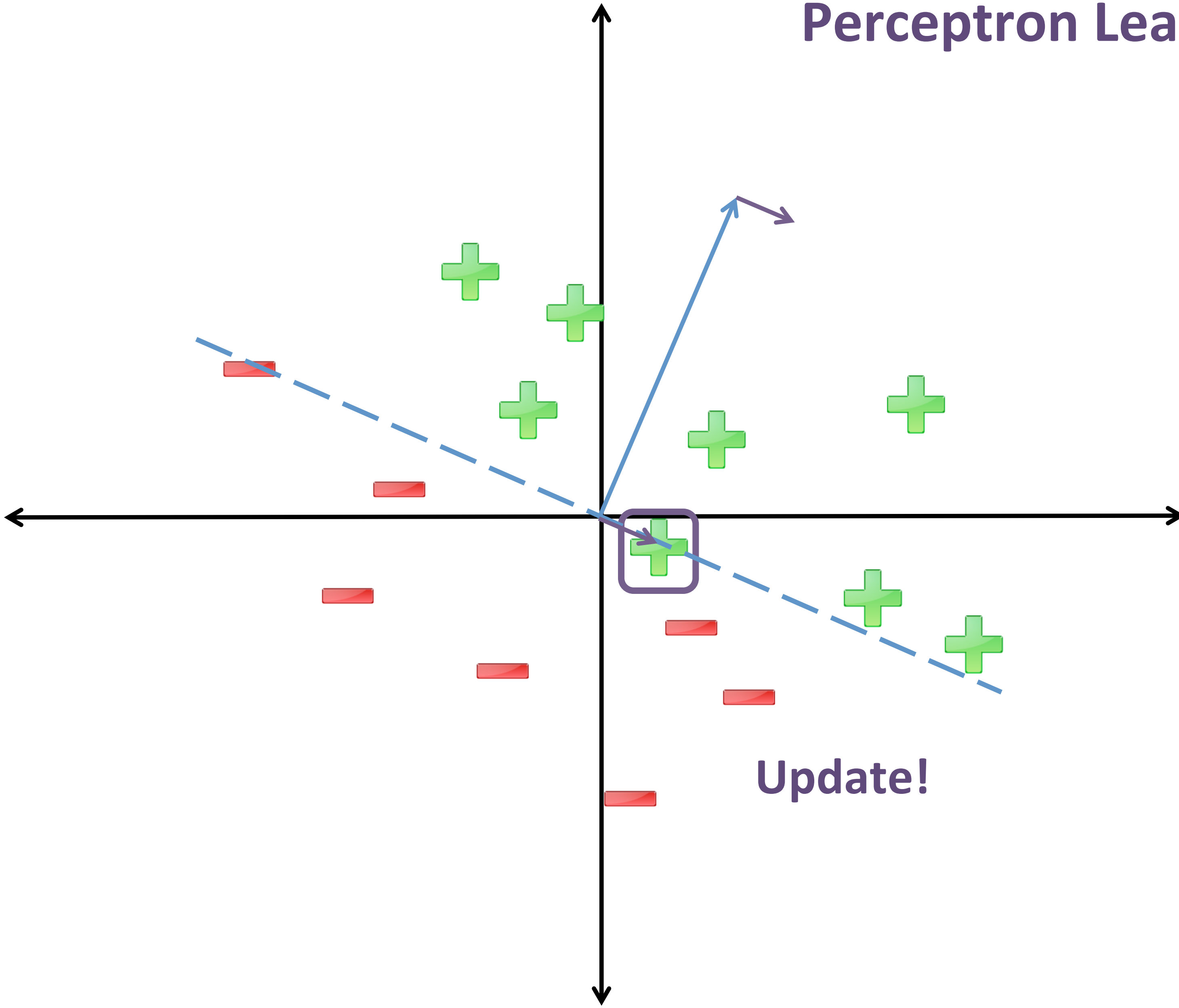

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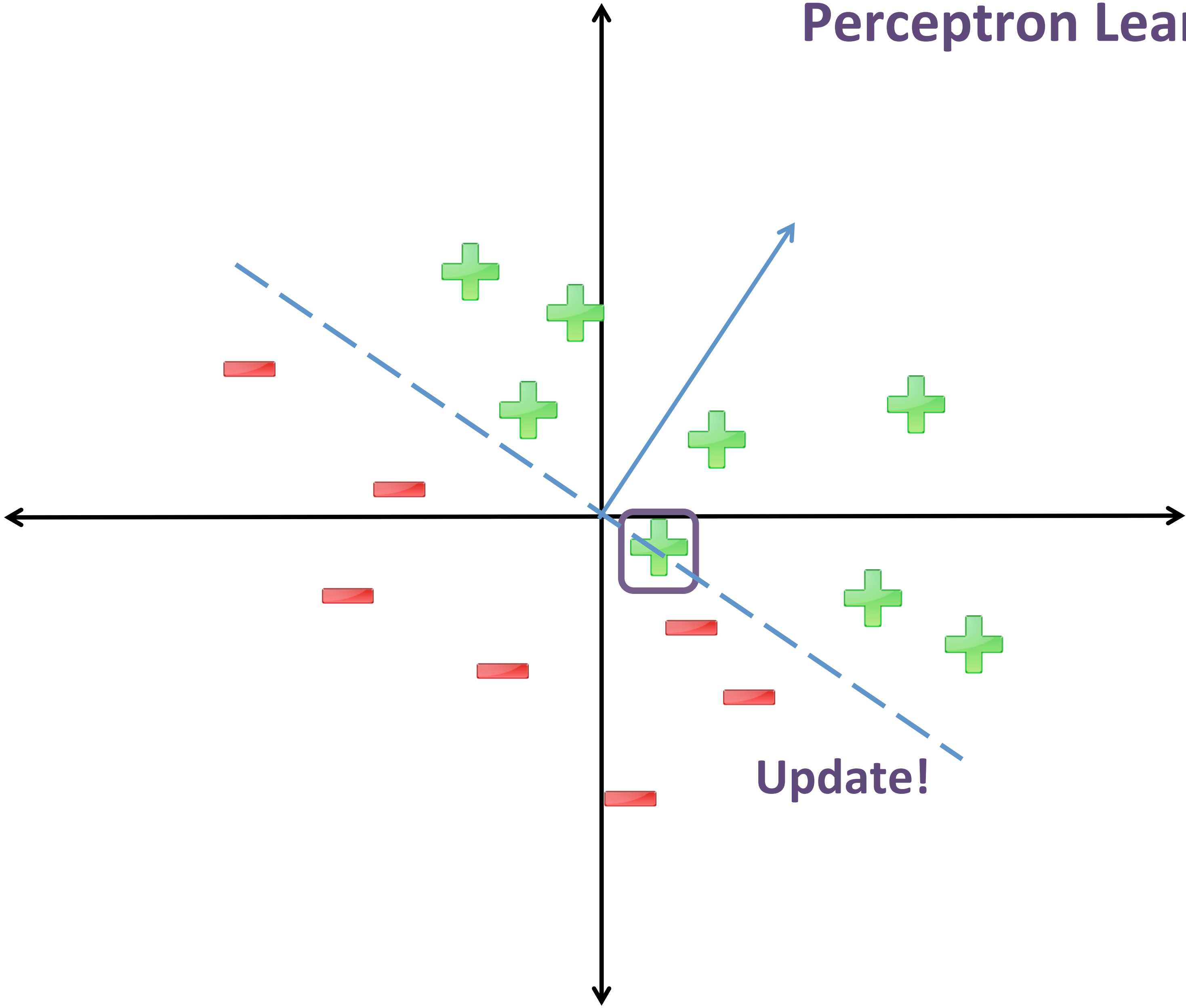
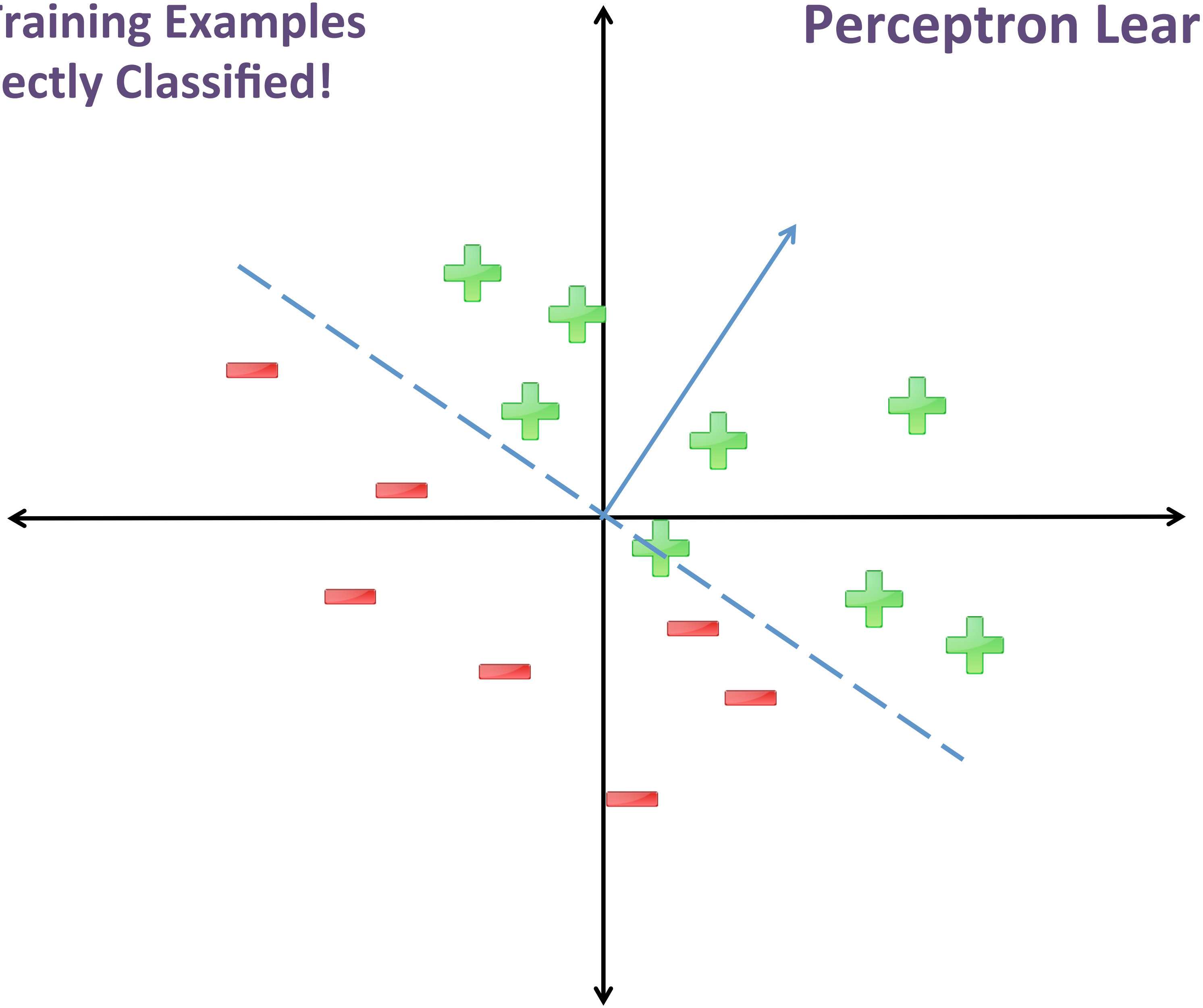


Perceptron Learning

All Training Examples Correctly Classified!



Recap: Perceptron Learning Algorithm
(Linear Classification Model)

- $w^1 = 0$, $b^1 = 0$
- For t = 1 ….
  - Receive example (x,y)
  - If $f(x|w^t) = y$
    - $[w^{t+1}, b^{t+1}] = [w^t, b^t]$
  - Else
    - $w^{t+1} = w^t + yx$
    - $b^{t+1} = b^t + y$

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

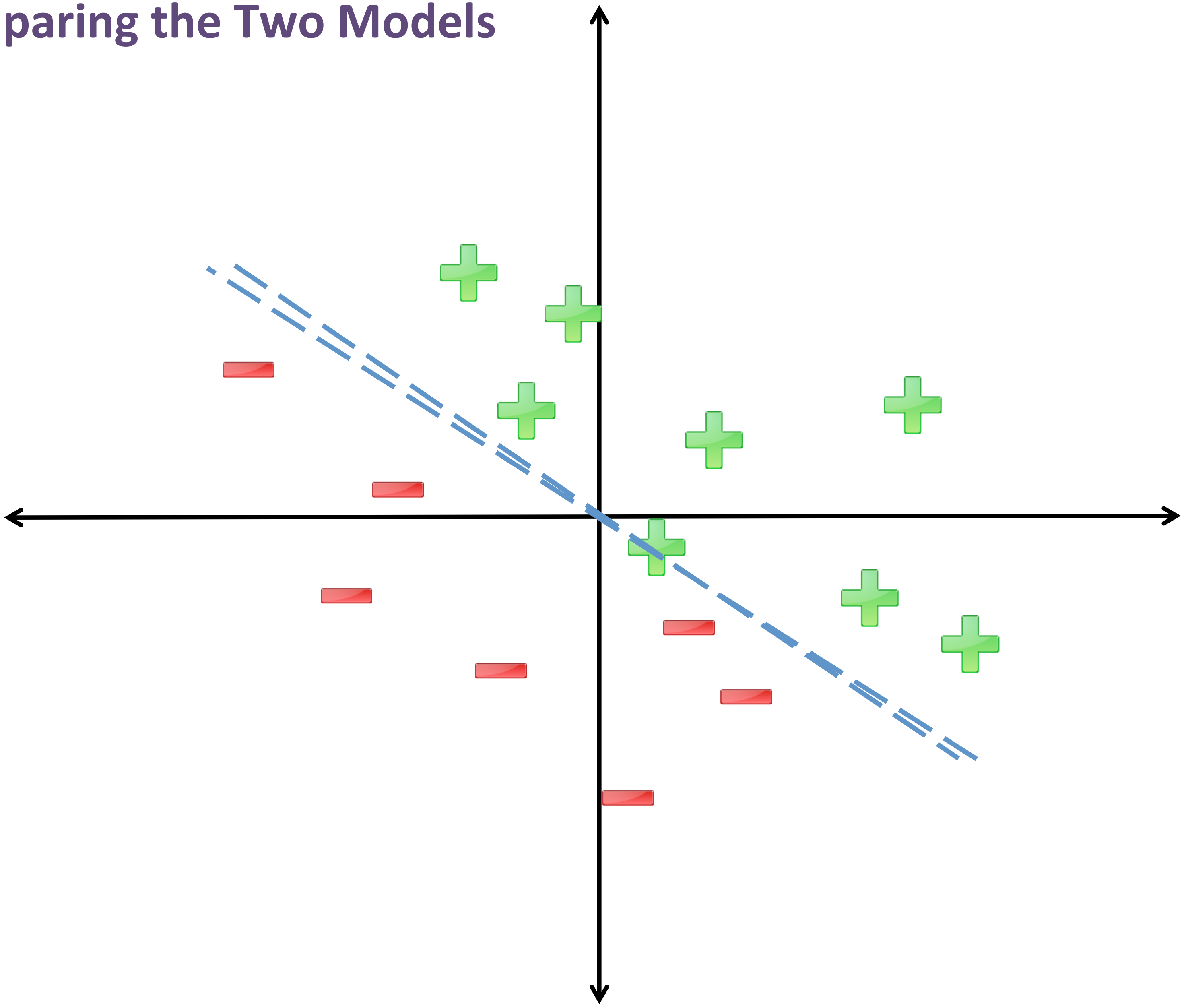
Training Set:

$$S = \left\{(x_i, y_i)\right\}_{i=1}^{N}$$

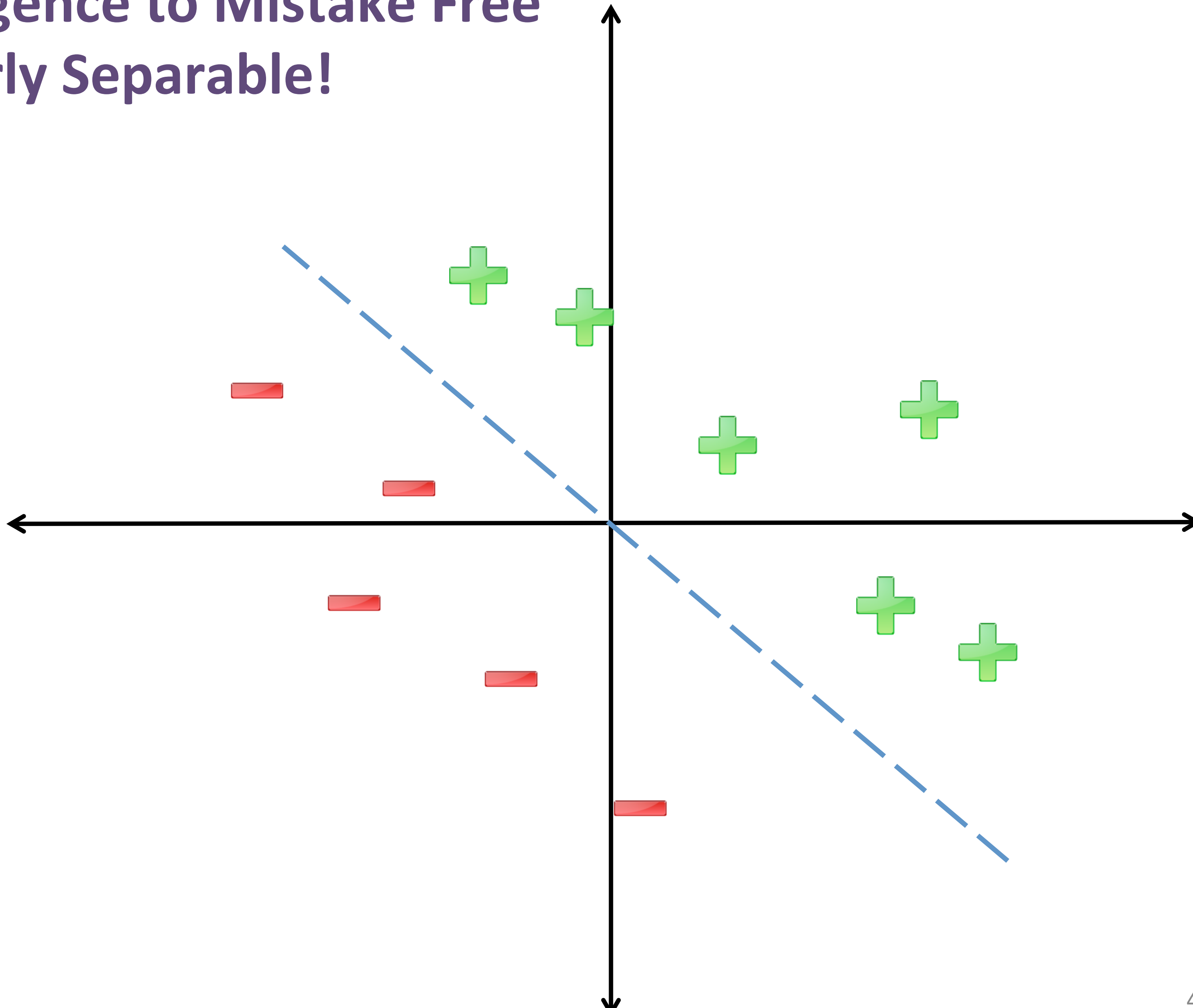
$$y \in \left\{+1, -1\right\}$$

Go through training set in arbitrary order (e.g., randomly)

Comparing the Two Models

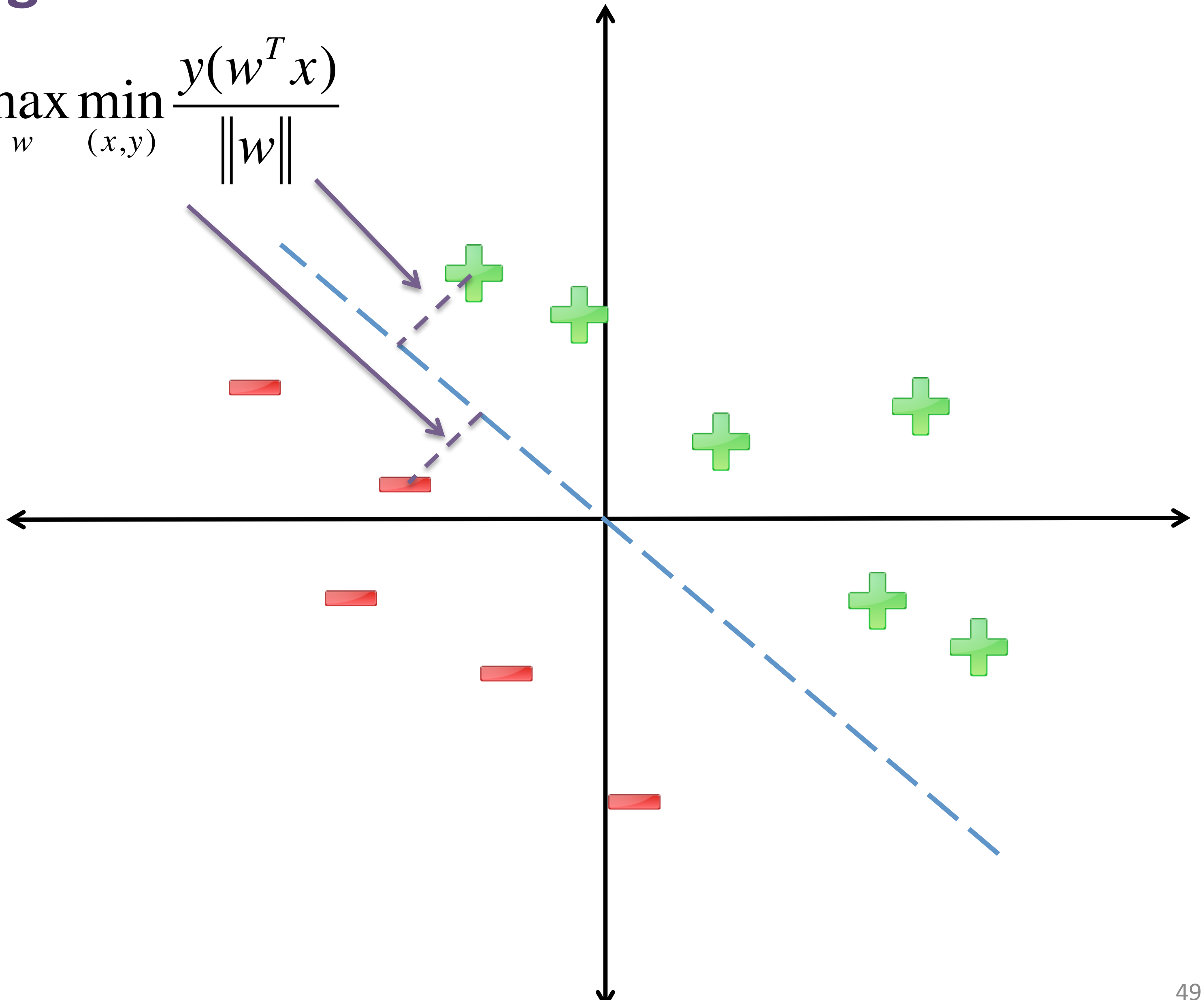


Convergence to Mistake Free = Linearly Separable!



Margin

$$\gamma = \max_{w} \min_{(x,y)} \frac{y(w^T x)}{\|w\|}$$



Linear Separability

- A classification problem is Linearly Separable:
  - Exists w with perfect classification accuracy

- Separable with Margin γ:

$$\gamma = \max_{w} \min_{(x,y)} \frac{y(w^T x)}{\|w\|}$$

- Linearly Separable: γ > 0

Perceptron Mistake Bound

Holds for any ordering of training examples!

"Radius" of Feature Space

$$R = \max_x \|x\|$$

#Mistakes Bounded By: $\dfrac{R^2}{\gamma^2}$

Margin

**If Linearly Separable

More Details: http://www.cs.nyu.edu/~mohri/pub/pmb.pdf

In the Real World…

- Most problems are NOT linearly separable!
- May never converge…
- So what to do?
- **Use validation set!**

Early Stopping via Validation

- Run Perceptron Learning on Training Set
- Evaluate current model on Validation Set
- Terminate when validation accuracy stops improving

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

Online Learning vs Batch Learning

- Online Learning:
  - Receive a stream of data (x,y)
  - Make incremental updates
  - Perceptron Learning is an instance of Online Learning

- Batch Learning
  - Train over all data simultaneously
  - Can use online learning algorithms for batch learning
  - E.g., stream the data to the learning algorithm

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

Recap: Perceptron

- One of the first machine learning algorithms
- **Benefits:**
  - Simple and fast
  - Clean analysis
- **Drawbacks:**
  - Might not converge to a very good model
  - What is the objective function?

(Stochastic) Gradient Descent

Back to Optimizing Objective Functions

- Training Data: $S = \{(x_i, y_i)\}_{i=1}^{N}$ $\quad x \in R^D$ $\quad y \in \{-1, +1\}$

- Model Class: $f(x \mid w, b) = w^T x - b$ **Linear Models**

- Loss Function: $L(a, b) = (a - b)^2$ **Squared Loss**

- Learning Objective: $\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$

Optimization Problem

Back to Optimizing Objective Functions

$$\underset{w,b}{\operatorname{argmin}} L(w,b \mid S) \equiv \sum_{i=1}^{N} L\left(y_i, f(x_i \mid w,b)\right)$$

- Typically, requires optimization algorithm.

- Simplest: **Gradient Descent**

- This Lecture: stick with squared loss
  - Talk about various loss functions next lecture

Gradient Review for Squared Loss

$$\partial_w L(w,b \mid S) = \partial_w \sum_{i=1}^{N} L\left(y_i, f(x_i \mid w,b)\right)$$

$$= \sum_{i=1}^{N} \partial_w L\left(y_i, f(x_i \mid w,b)\right)$$

Linearity of Differentiation

$$= \sum_{i=1}^{N} -2(y_i - f(x_i \mid w,b))\partial_w f(x_i \mid w,b)$$

$$L(a,b) = (a-b)^2$$

Chain Rule

$$= \sum_{i=1}^{N} -2(y_i - f(x_i \mid w,b))x_i$$

$$f(x \mid w,b) = w^T x - b$$

Gradient Descent

- Initialize: $w^1 = 0$, $b^1 = 0$
- For t = 1…

$$w^{t+1} = w^t - \eta^{t+1} \partial_w L(w^t, b^t \mid S)$$

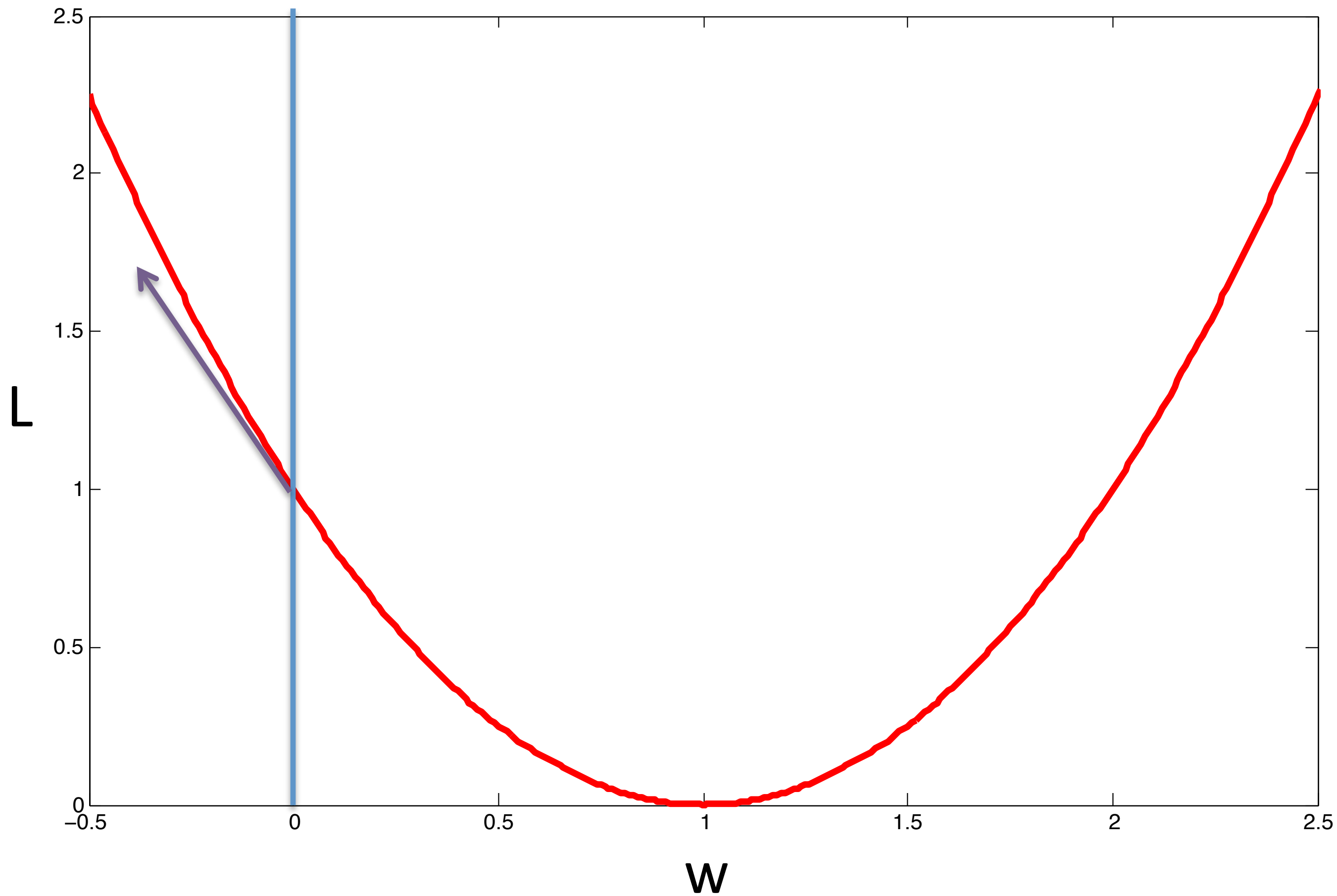
$$b^{t+1} = b^t - \eta^{t+1} \partial_b L(w^t, b^t \mid S)$$

"Step Size"

How to Choose Step Size?

$\eta = 1$

$$\partial_w L(w) = -2(1 - w)$$



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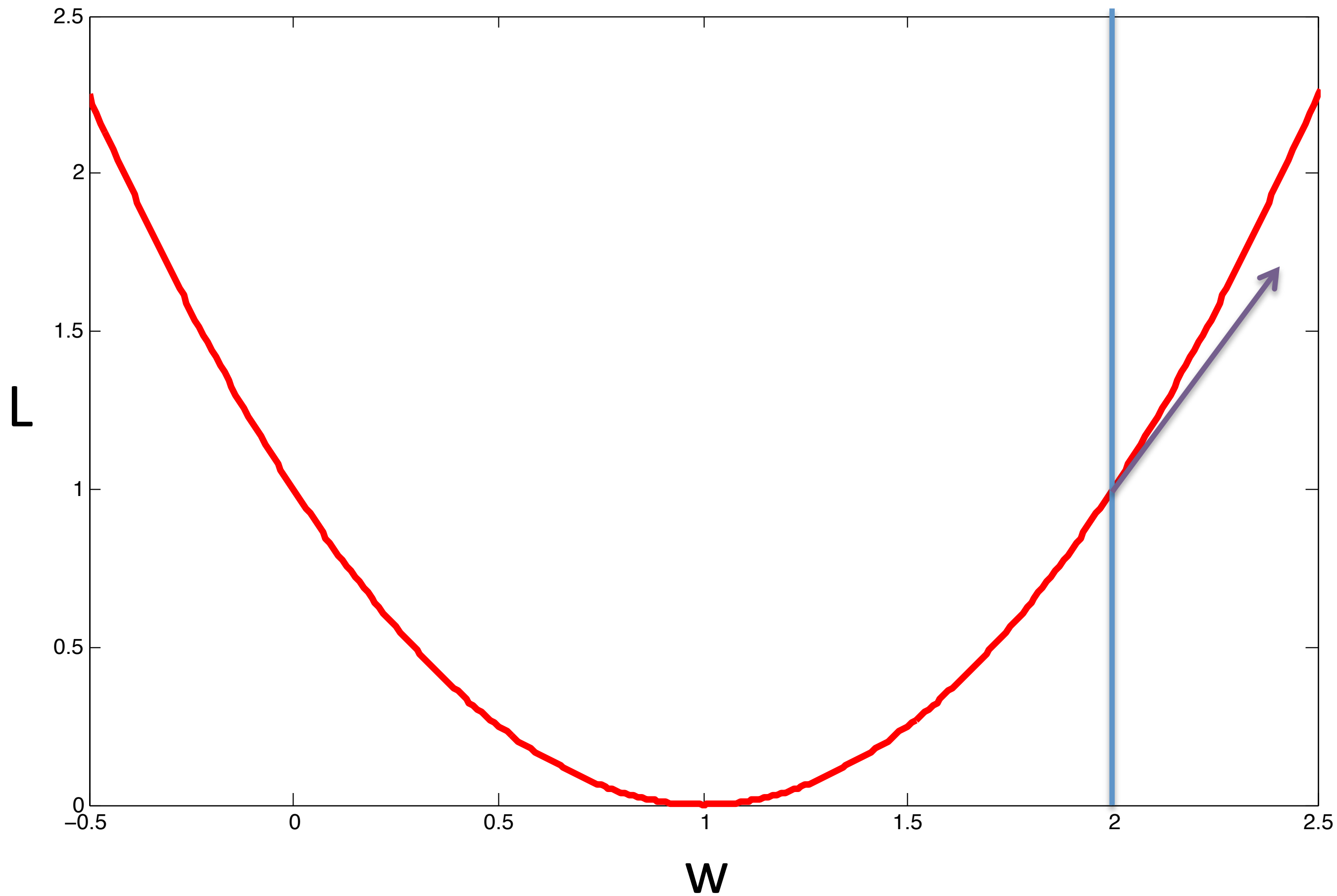

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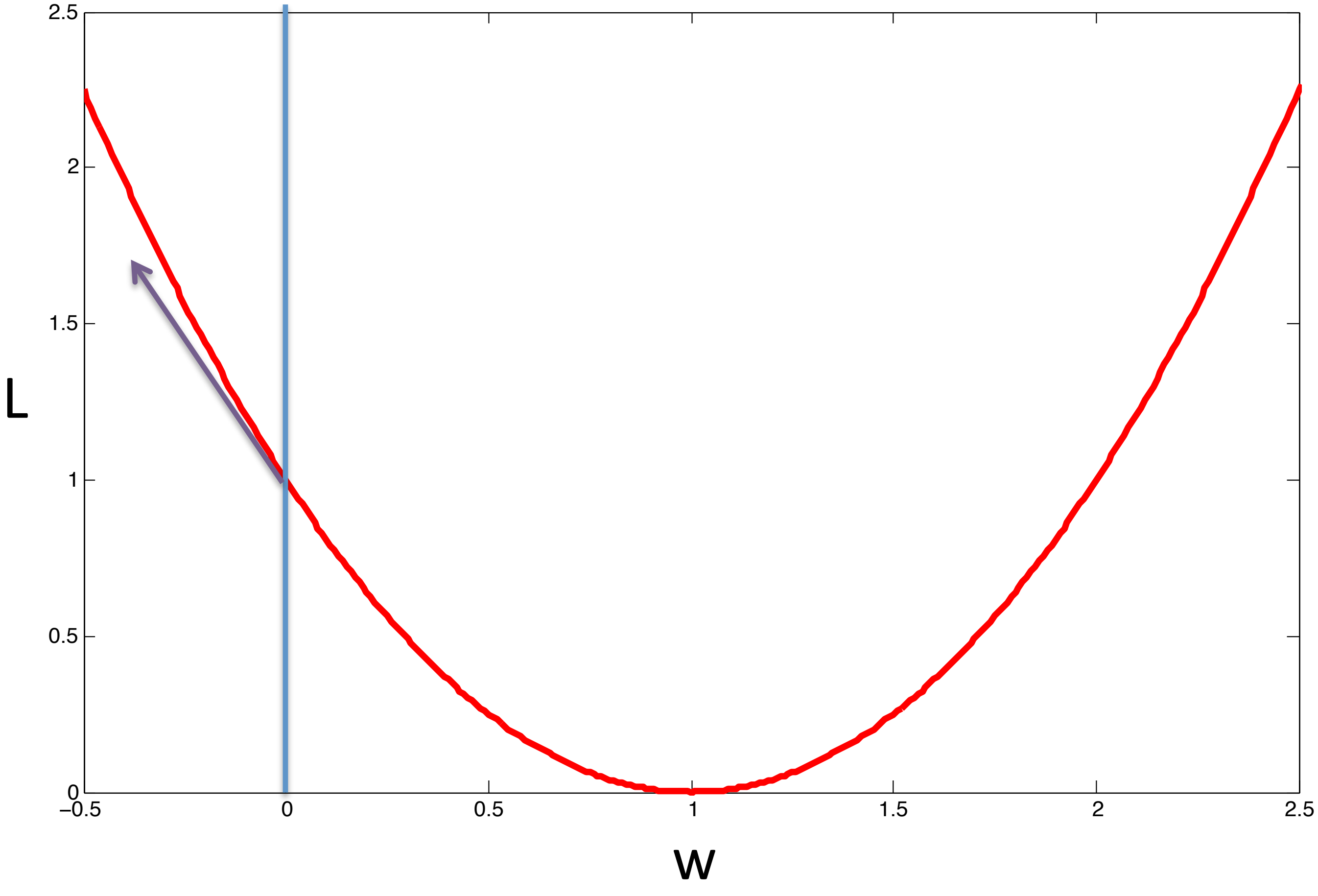

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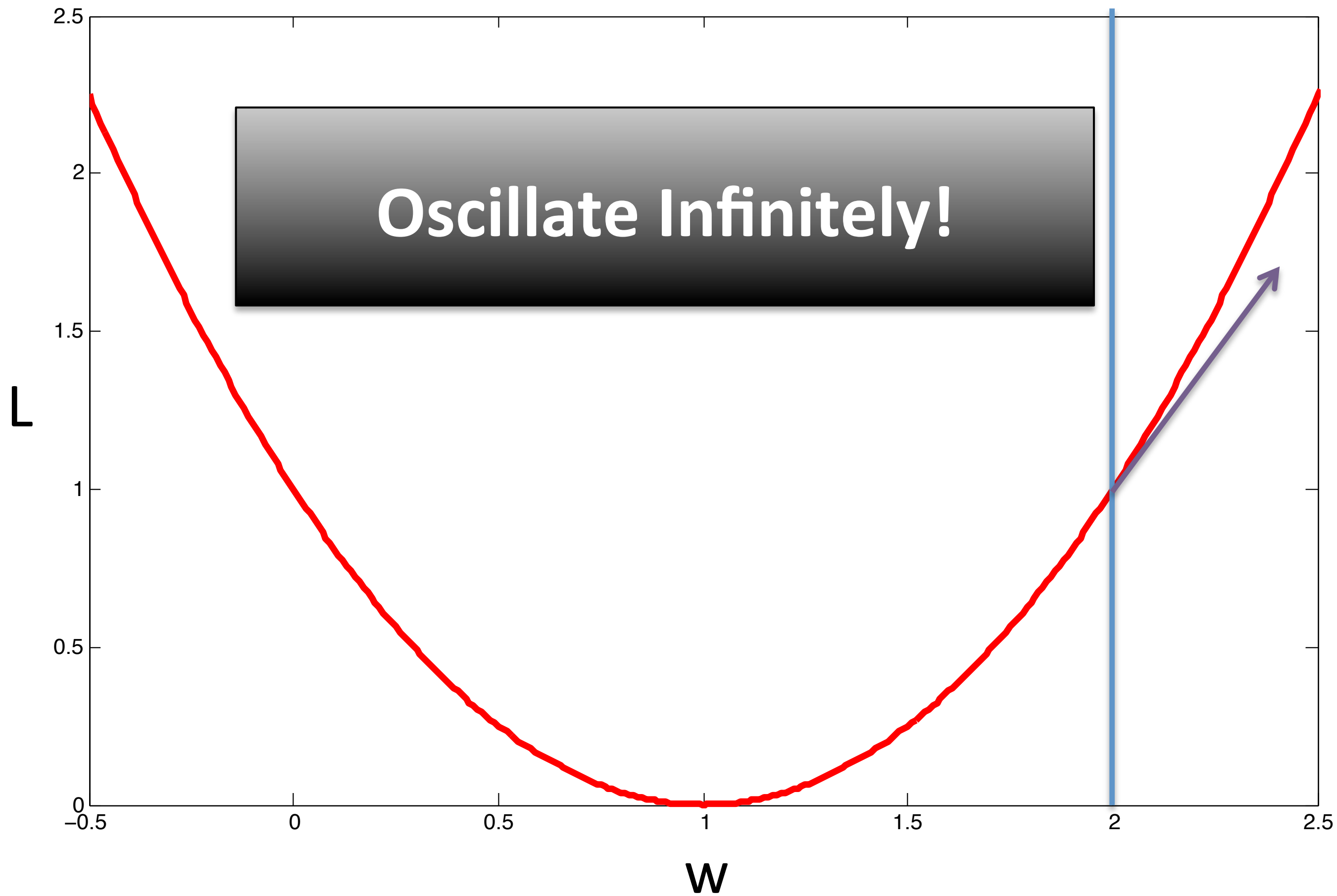
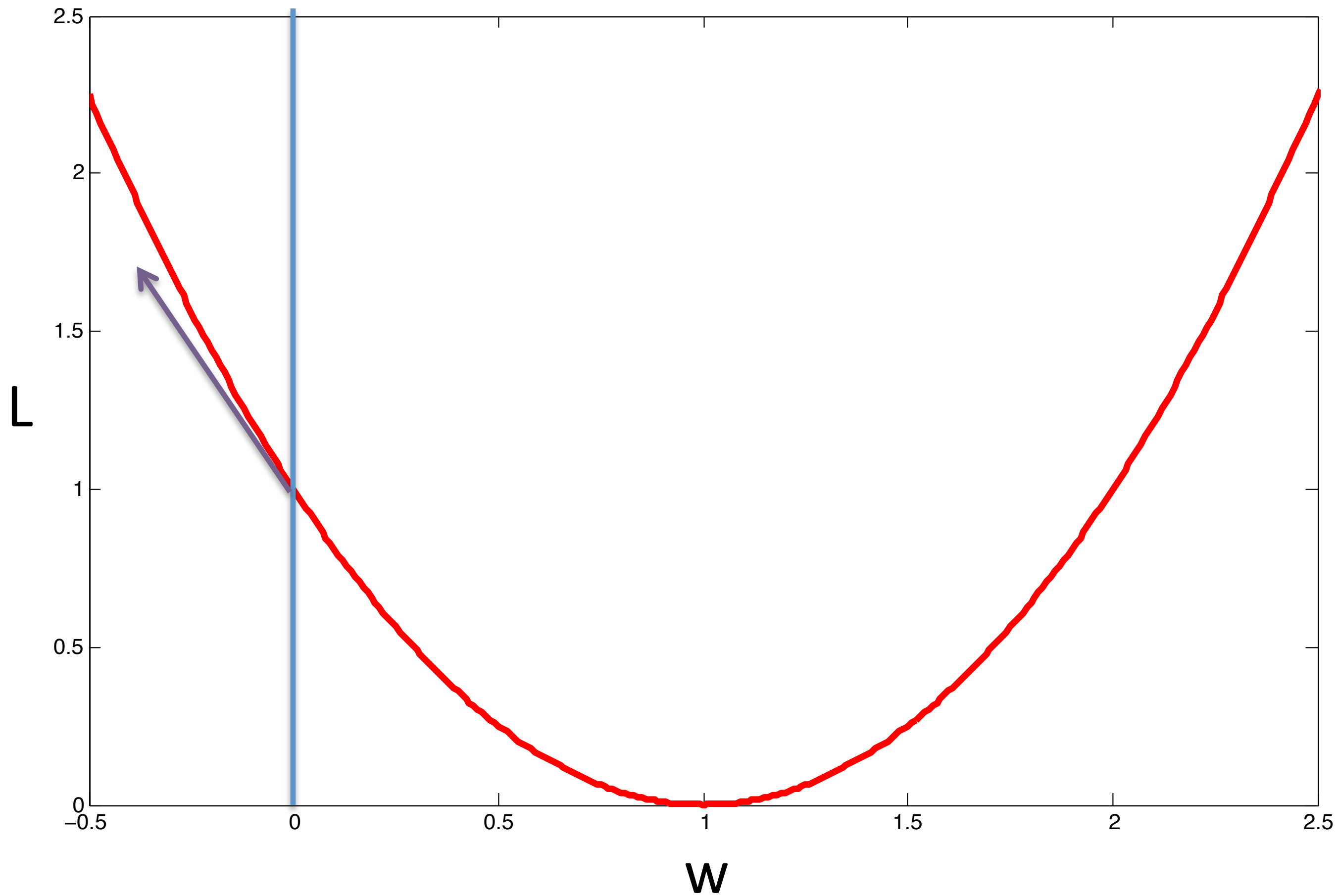


How to Choose Step Size?

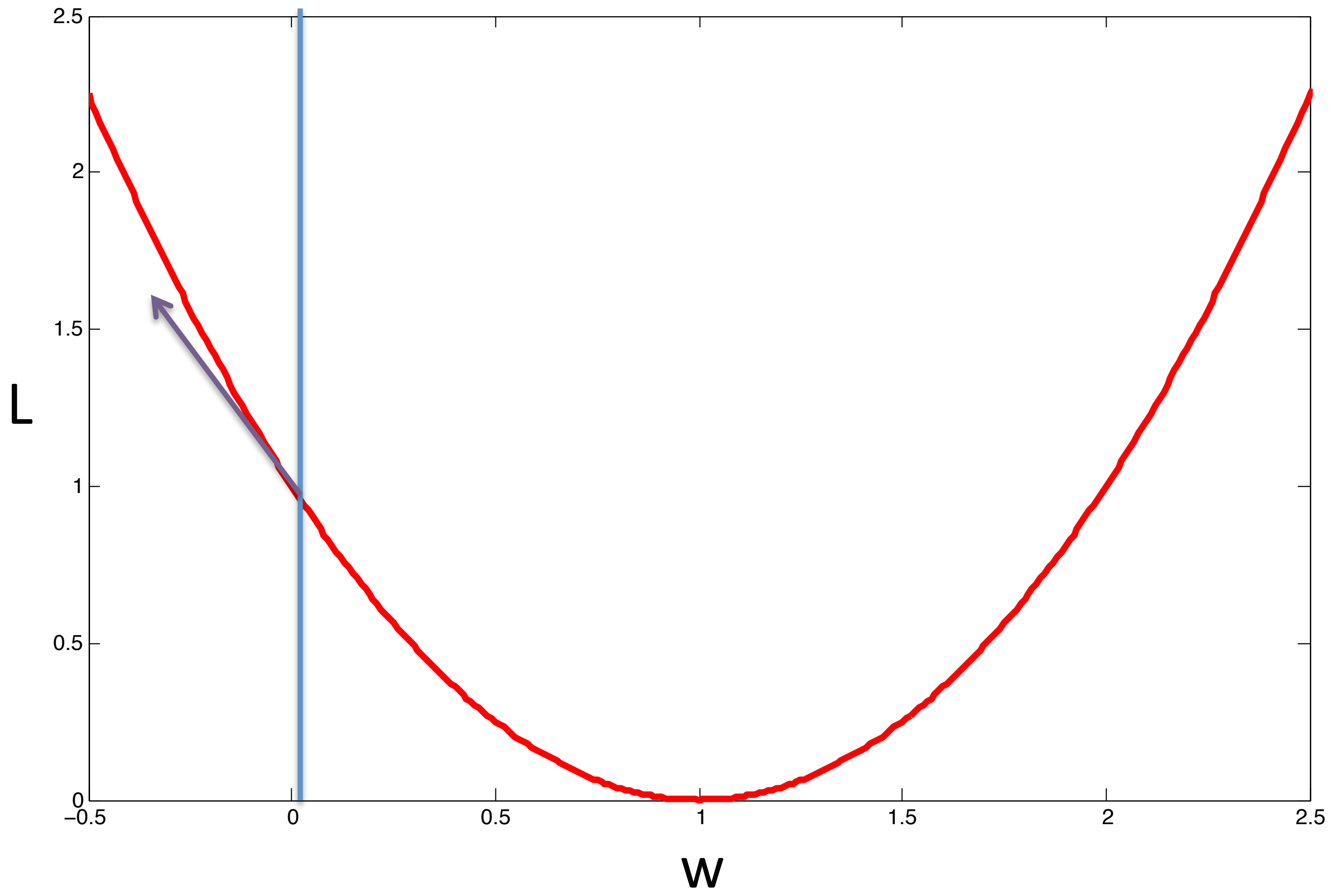
$\eta = 0.0001$

$\partial_w L(w) = -2(1-w)$



How to Choose Step Size?

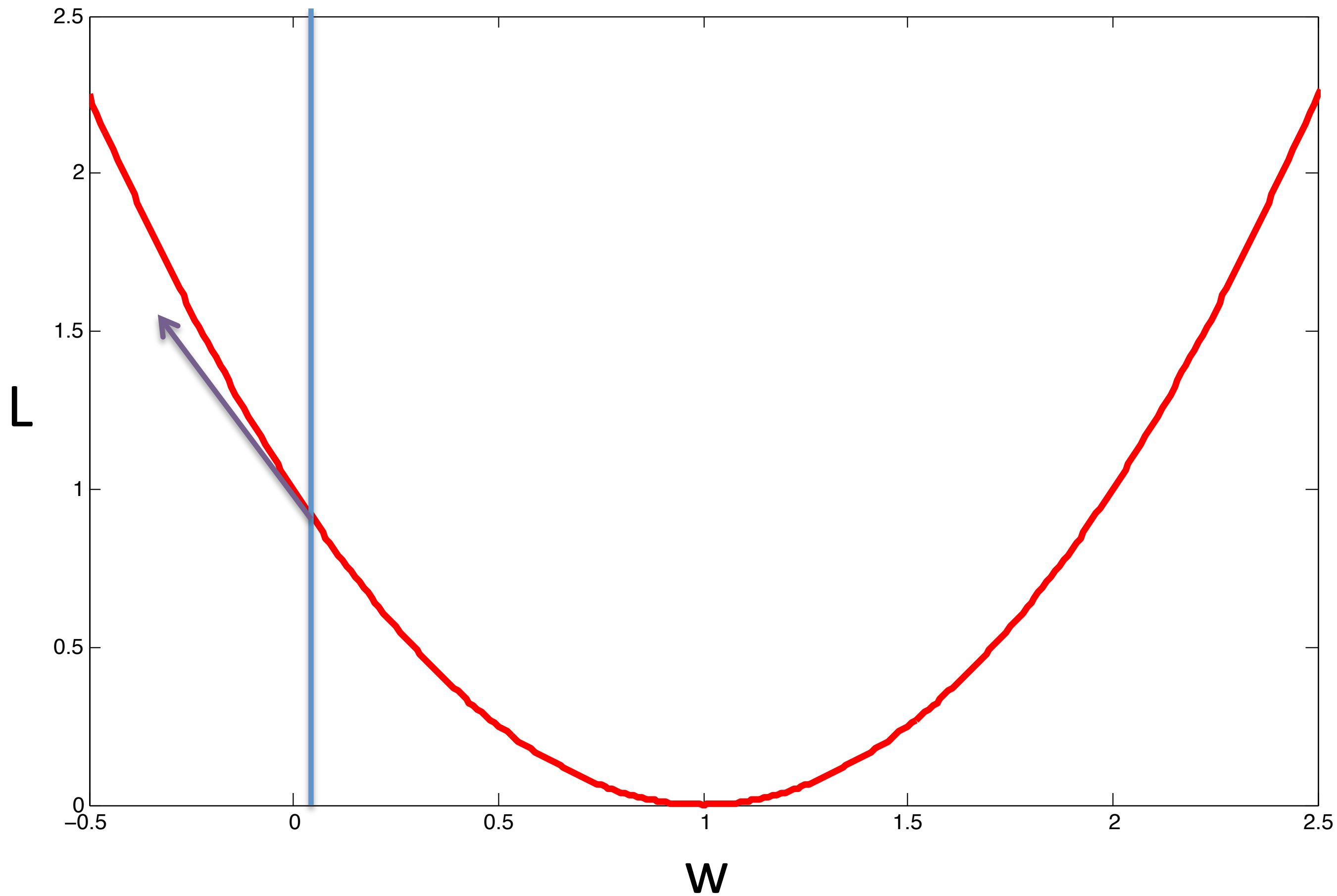
$\eta = 0.0001$ $\partial_w L(w) = -2(1-w)$



How to Choose Step Size?

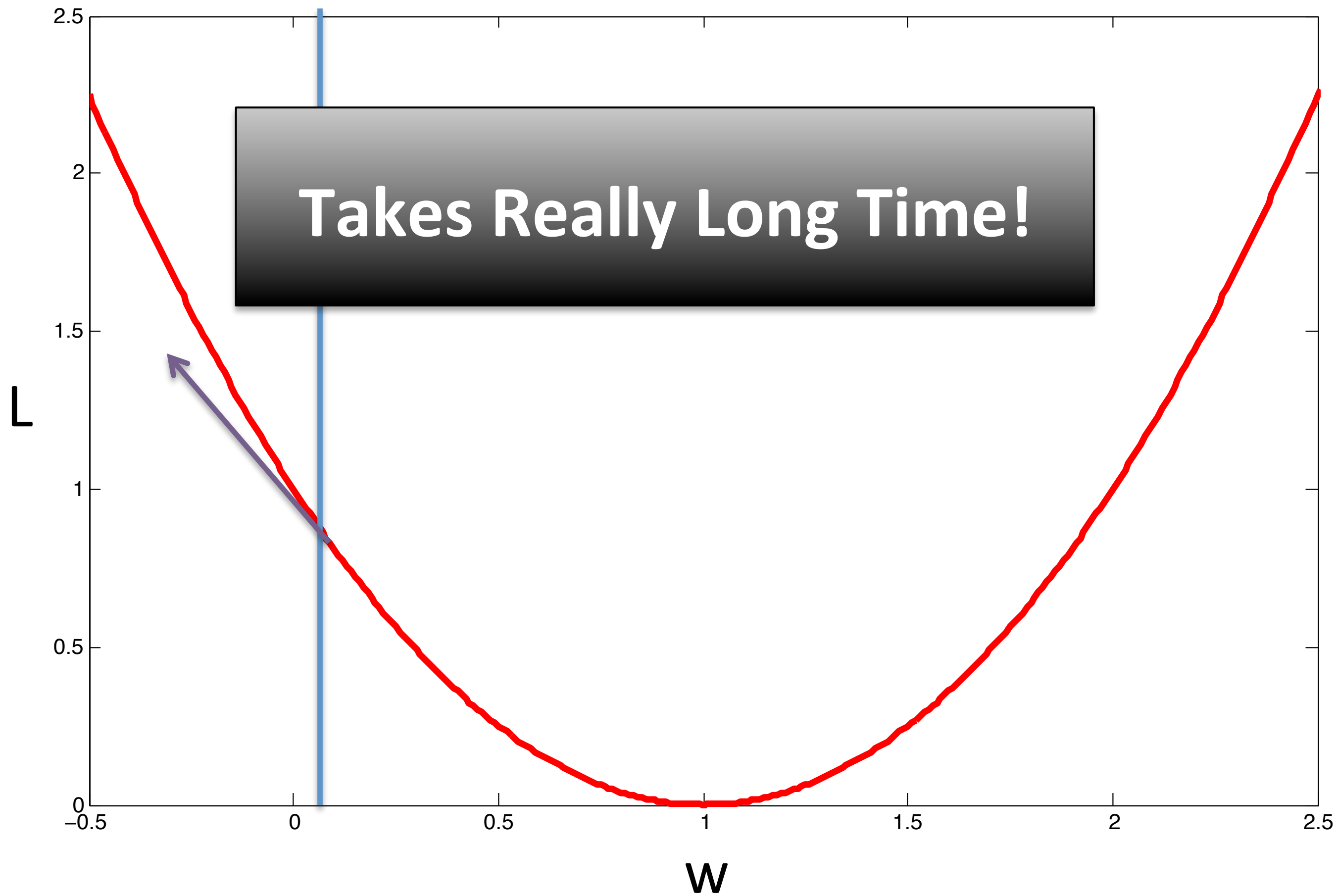
$\eta = 0.0001$

$\partial_w L(w) = -2(1-w)$



How to Choose Step Size?

$$\eta = 0.0001 \qquad \partial_w L(w) = -2(1-w)$$



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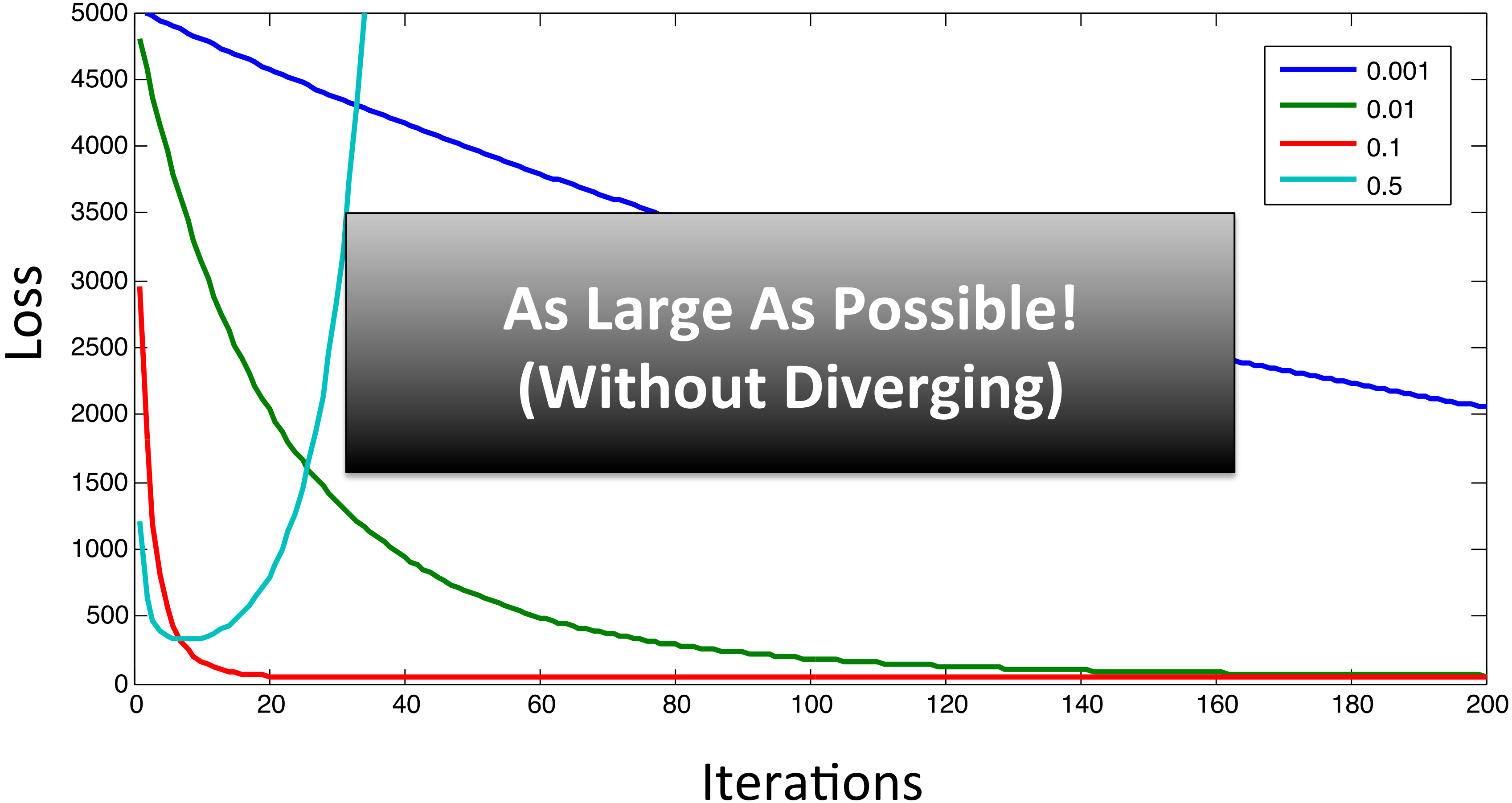


Note that the absolute scale is not meaningful
Focus on the relative magnitude differences

Being Scale Invariant

- Consider the following two gradient updates:

$$w^{t+1} = w^t - \eta^{t+1}\partial_w L(w^t, b^t \mid S)$$

$$w^{t+1} = w^t - \hat{\eta}^{t+1}\partial_w \hat{L}(w^t, b^t \mid S)$$

- Suppose: $\hat{L} = 1000L$
  - **How are the two step sizes related?**

$$\hat{\eta}^{t+1} = \eta / 1000$$

Practical Rules of Thumb

- Divide Loss Function by Number of Examples:

$$w^{t+1} = w^{t} - \left(\frac{\eta^{t+1}}{N}\right)\partial_w L(w^t, b^t \mid S)$$

- Start with large step size
  - If loss plateaus, divide step size by 2
  - (Can also use advanced optimization methods)
  - (Step size must decrease over time to guarantee convergence to global optimum)

Aside: Convexity

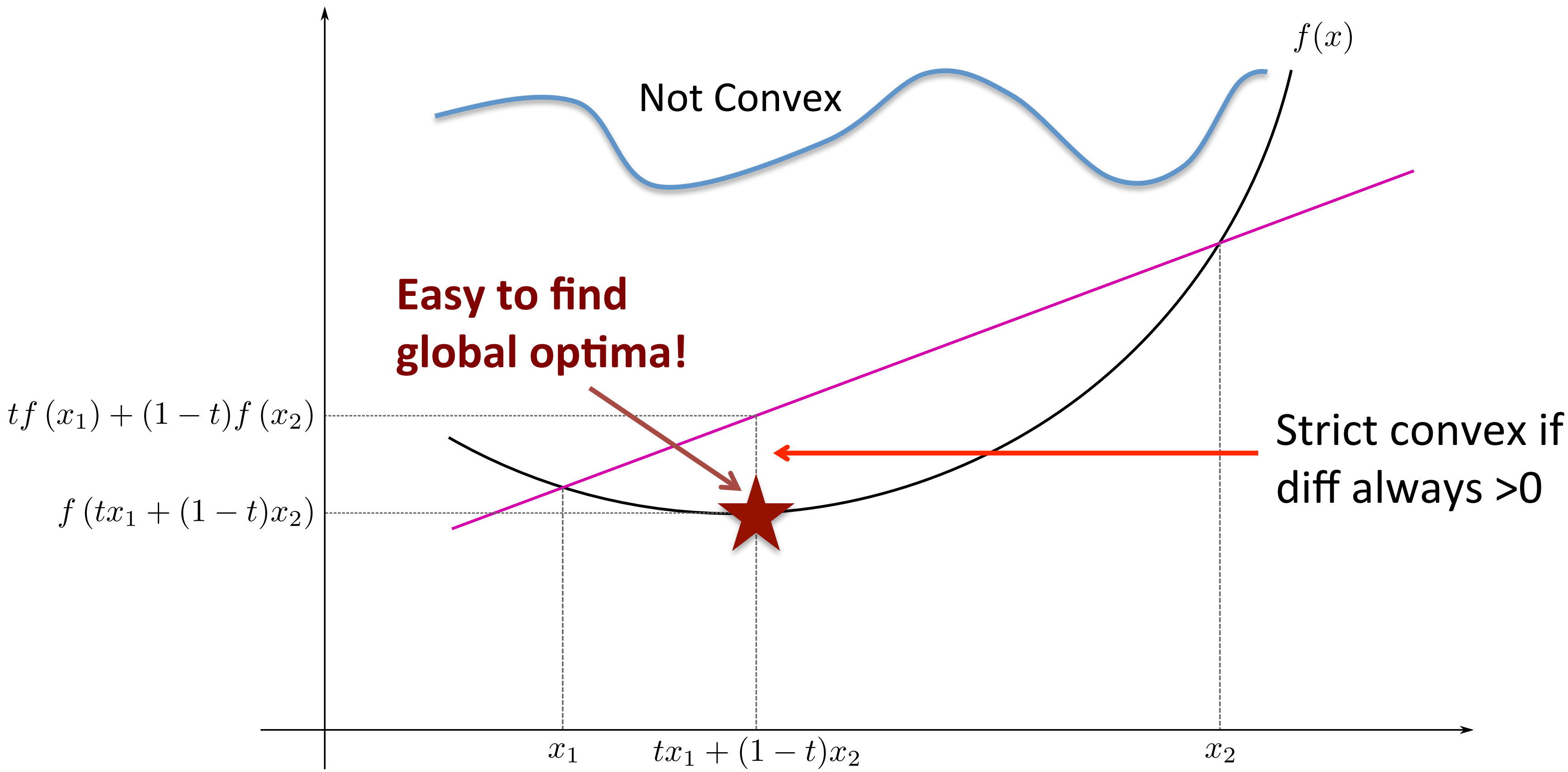
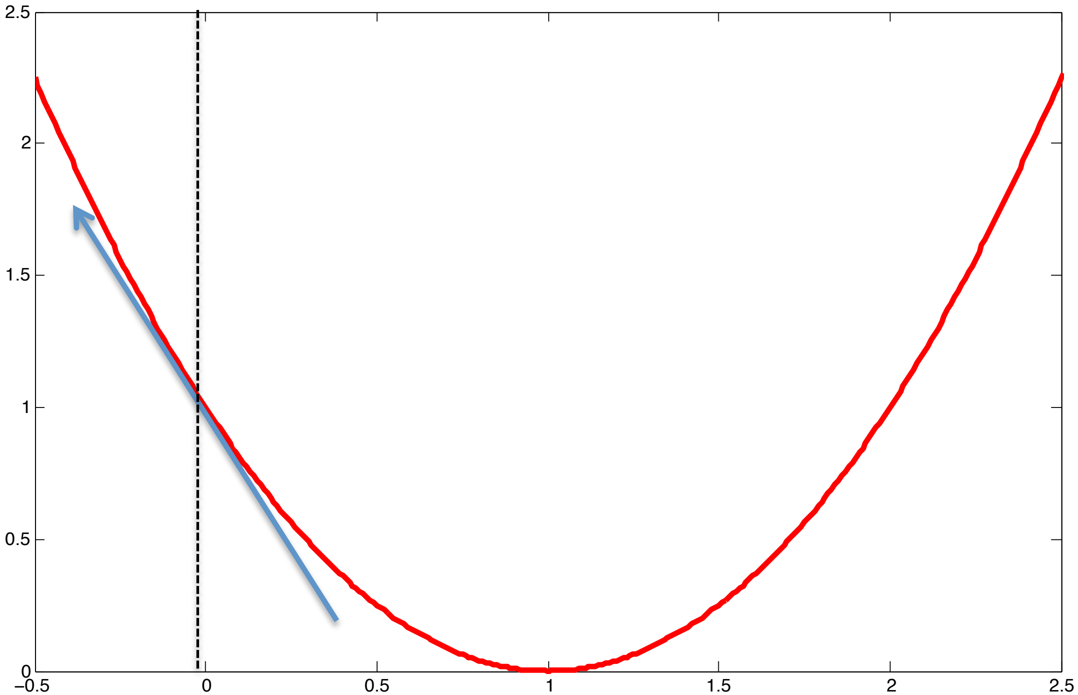


Image Source: http://en.wikipedia.org/wiki/Convex_function

Aside: Convexity

$$L(x_2) \geq L(x_1) + \nabla L(x_1)^T (x_2 - x_1)$$

Function is always above the locally linear extrapolation



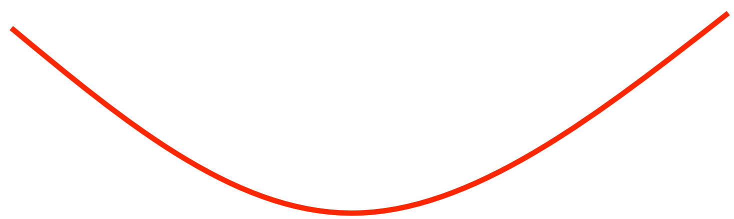
Aside: Convexity

- All local optima are global optima:

Gradient Descent will find optimum

Assuming step size chosen safely

- Strictly convex: unique global optimum:



- Almost all standard objectives are (strictly) convex:
  - Squared Loss, SVMs, LR, Ridge, Lasso
  - We will see non-convex objectives in 2^{nd} half of course

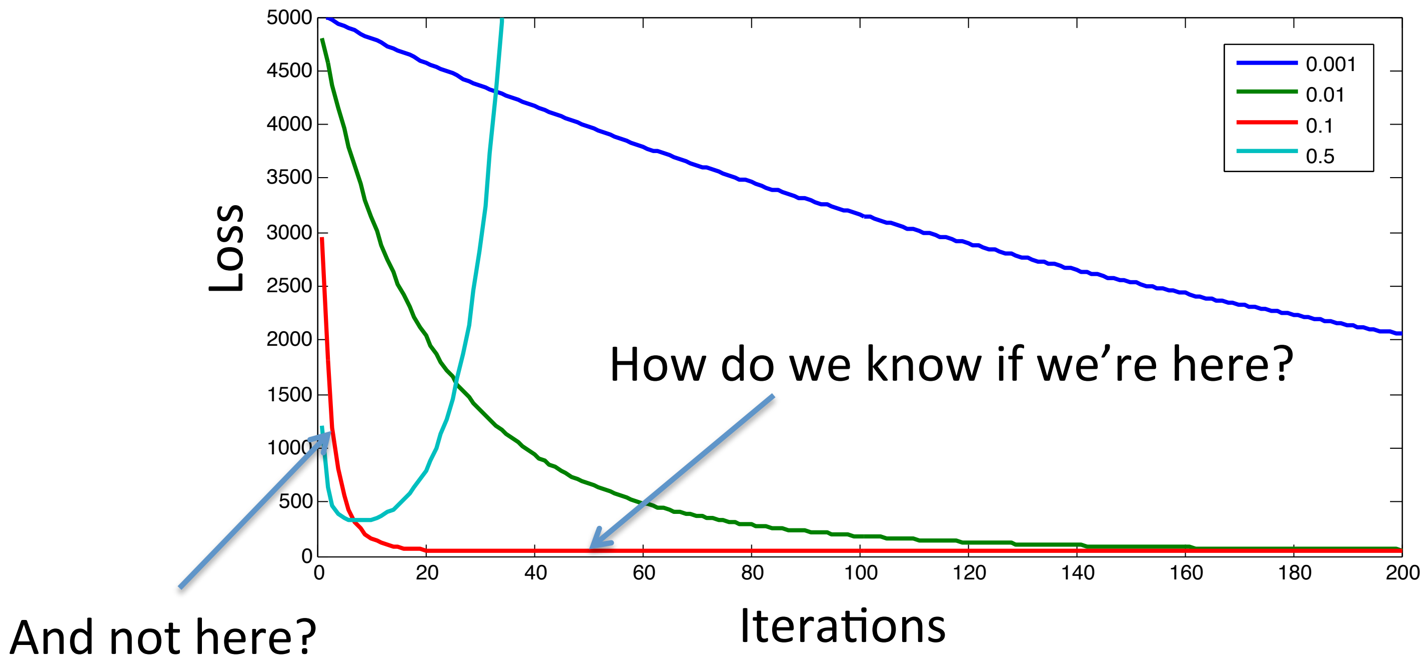
Convergence

- Assume L is convex
- How many iterations to achieve: $L(w) - L(w^*) \leq \varepsilon$
- If: $|L(a) - L(b)| \leq \rho \|a - b\|$ ← L is "ρ-Lipschitz"
  - Then $O(1/\varepsilon^2)$ iterations
- If: $|\nabla L(a) - \nabla L(b)| \leq \rho \|a - b\|$ ← L is "ρ-smooth"
  - Then $O(1/\varepsilon)$ iterations
- If: $L(a) \geq L(b) + \nabla L(b)^T (a - b) + \frac{\rho}{2} \|a - b\|^2$ ← L is "ρ-strongly convex"
  - Then $O(\log(1/\varepsilon))$ iterations

More Details: Bubeck Textbook Chapter 3

Convergence

- In general, takes infinite time to reach global optimum.
- But in general, we don't care!
  - As long as we're close enough to the global optimum



When to Stop?

- Convergence analyses = worst-case upper bounds
  - **What to do in practice?**
- Stop when progress is sufficiently small
  - E.g., relative reduction less than 0.001

Yisong prefers this option

- Stop after pre-specified #iterations
  - E.g., 100000
- Stop when validation error stops going down

Limitation of Gradient Descent

- Requires full pass over training set per iteration

$$\partial_w L(w,b \mid S) = \partial_w \sum_{i=1}^{N} L\left(y_i, f(x_i \mid w,b)\right)$$

- Very expensive if training set is huge

- **Do we need to do a full pass over the data?**

Stochastic Gradient Descent

- Suppose Loss Function Decomposes Additively

$$L(w,b) = \frac{1}{N}\sum_{i=1}^{N} L_i(w,b) = \mathrm{E}_i\left[L_i(w,b)\right]$$

Each L_i corresponds to a single data point

- Gradient = expected gradient of sub-functions

$$\partial_w L(w,b) = \partial_w \mathrm{E}_i\left[L_i(w,b)\right]$$

$$L_i(w,b) \equiv \left(y_i - f(x_i \mid w,b\right)^2$$

Stochastic Gradient Descent

- Suffices to take random gradient update
  - So long as it matches the true gradient in expectation
- Each iteration t:
  - Choose i at random

Expected Value is: $\partial_w L(w,b)$

$$w^{t+1} = w^t - \eta^{t+1}\partial_w L_i(w,b)$$

$$b^{t+1} = b^t - \eta^{t+1}\partial_b L_i(w,b)$$

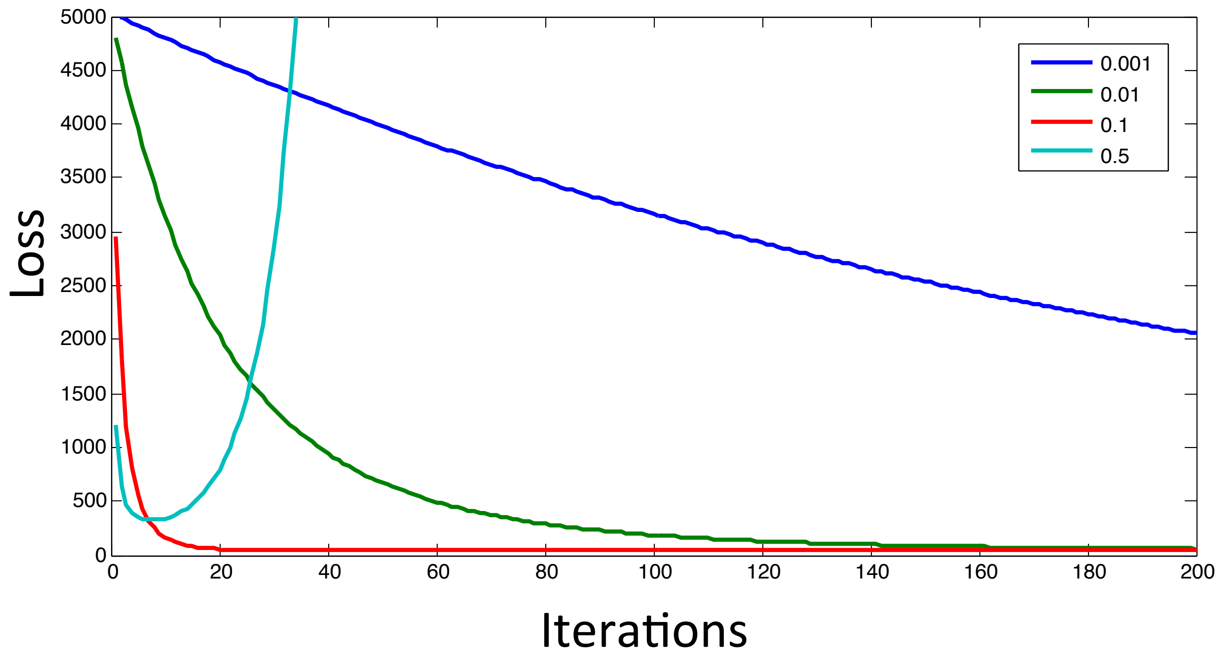
- **SGD is an online learning algorithm!**

Mini-Batch SGD

- Each L_i is a small batch of training examples
  - E.g,. 500-1000 examples
  - Can leverage vector operations
  - Decrease volatility of gradient updates
- Industry state-of-the-art
  - Everyone uses mini-batch SGD
  - Often parallelized
    - (e.g., different cores work on different mini-batches)

Checking for Convergence

- How to check for convergence?
  - Evaluating loss on entire training set seems expensive…



Checking for Convergence

- How to check for convergence?
  - Evaluating loss on entire training set seems expensive…
- Don’t check after every iteration
  - E.g., check every 1000 iterations
- Evaluate loss on a subset of training data
  - E.g., the previous 5000 examples.

Recap: Stochastic Gradient Descent

- Conceptually:
  - Decompose Loss Function Additively
  - Choose a Component Randomly
  - Gradient Update
- Benefits:
  - Avoid iterating entire dataset for every update
  - Gradient update is consistent (in expectation)
- Industry Standard

Perceptron Revisited

(What is the Objective Function?)

- $w^1 = 0, b^1 = 0$
- For t = 1 ….
  - Receive example (x,y)
  - If $f(x|w^t) = y$
    - $[w^{t+1}, b^{t+1}] = [w^t, b^t]$
  - Else
    - $w^{t+1} = w^t + yx$
    - $b^{t+1} = b^t + y$

$$f(x|w) = sign(w^T x - b)$$

Training Set:

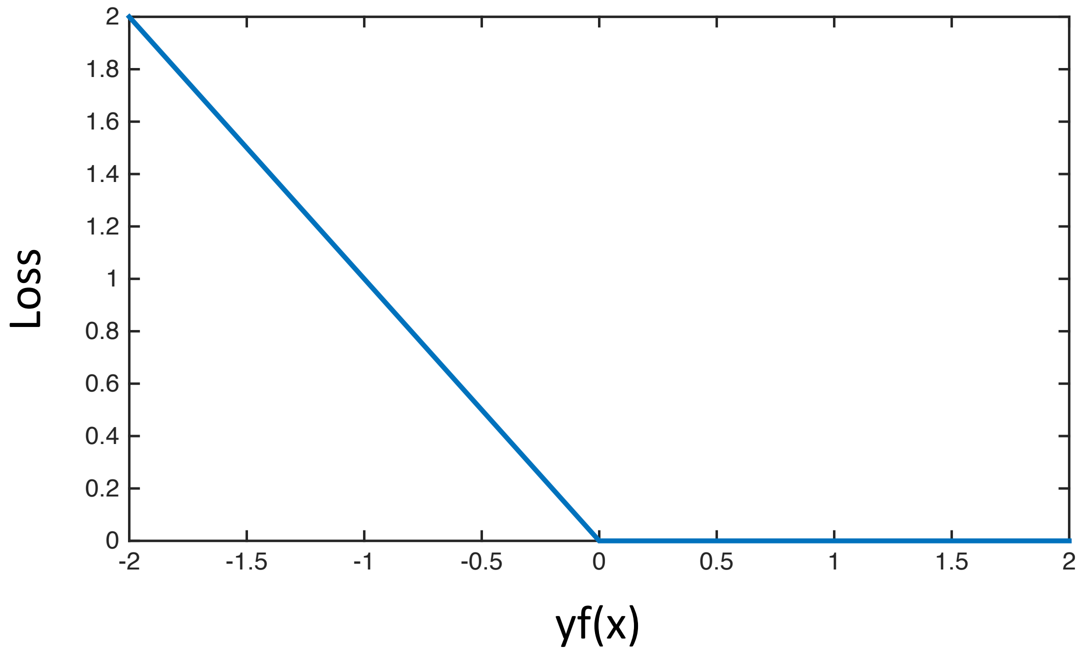
$$S = \{(x_i, y_i)\}_{i=1}^{N}$$

$$y \in \{+1, -1\}$$

Go through training set in arbitrary order (e.g., randomly)

Perceptron (Implicit) Objective

$$L_i(w,b) = \max\left\{0, -y_i f(x_i \mid w,b)\right\}$$



Recap: Complete Pipeline

$$S = \{(x_i, y_i)\}_{i=1}^{N}$$

Training Data

$$f(x \mid w, b) = w^T x - b$$

Model Class(es)

$$L(a,b) = (a-b)^2$$

Loss Function

$$\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$

Use SGD!

Cross Validation & Model Selection

Profit!

Next Week

- Different Loss Functions
  - Hinge Loss (SVM)
  - Log Loss (Logistic Regression)
- Non-linear model classes
  - Neural Nets
- Regularization
- **Recitation on Python Programming Tonight!**