Linear Models: (Sub)gradient Descent

CMSC 422

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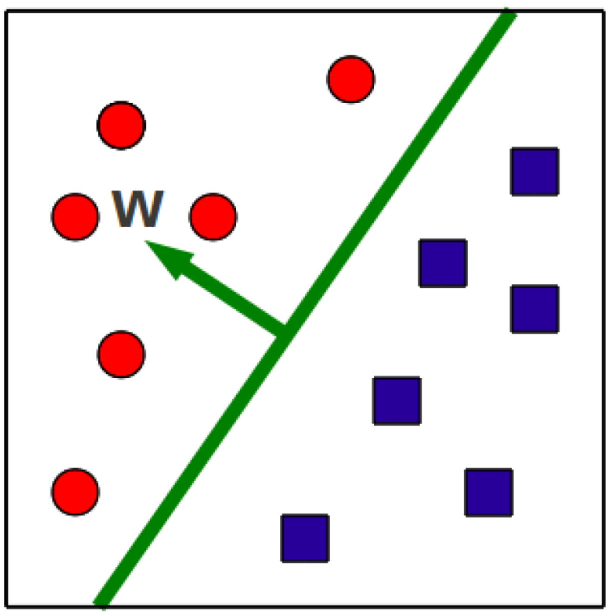
Recap: Linear Models

- General framework for binary classification
- Cast learning as optimization problem
- Optimization objective combines 2 terms
  - Loss function
  - Regularizer
- Does not assume data is linearly separable
- Lets us separate model definition from training algorithm **(Gradient Descent)**

Binary classification via hyperplanes



- A classifier is a hyperplane (w,b)
- At test time, we check on what side of the hyperplane examples fall

$$\hat{y} = sign(w^T x + b)$$

- This is a **linear classifier**
  - Because the prediction is a linear combination of feature values x

Casting Linear Classification as an Optimization Problem

Objective function

Loss function measures how well classifier fits training data

Regularizer prefers solutions that generalize well

$$\min_{\mathbf{w},b} L(\mathbf{w},b) = \min_{\mathbf{w},b} \sum_{n=1}^{N} \mathbb{I}(y_n(\mathbf{w}^T\mathbf{x}_n + b) < 0) + \lambda R(\mathbf{w},b)$$

$\mathbb{I}(.)$ Indicator function: 1 if (.) is true, 0 otherwise

The loss function above is called the 0-1 loss

Approximating the 0-1 loss with surrogate loss functions

- Examples (with b = 0)
  - Hinge loss $[1 - y_n \mathbf{w}^T \mathbf{x}_n]_+ = \max\{0, 1 - y_n \mathbf{w}^T \mathbf{x}_n\}$
  - Log loss $\log[1 + \exp(-y_n \mathbf{w}^T \mathbf{x}_n)]$
  - Exponential loss $\exp(-y_n \mathbf{w}^T \mathbf{x}_n)$

- All are convex upper-bounds on the 0-1 loss

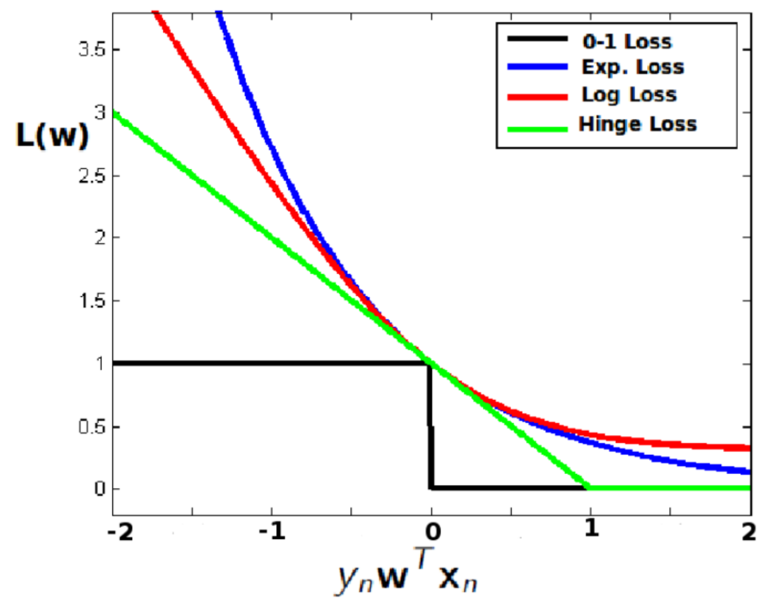
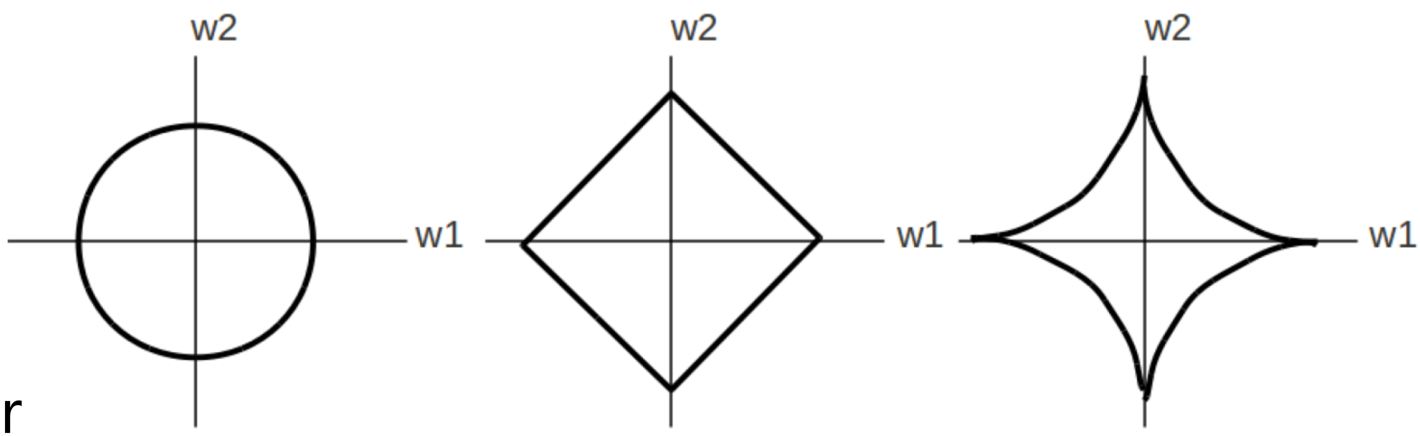


Figure credit: Piyush Rai

Norm-based Regularizers

- l_p norms can be used as regularizers

$$||\mathbf{w}||_2^2 = \sum_{d=1}^{D} w_d^2$$
$$||\mathbf{w}||_1 = \sum_{d=1}^{D} |w_d|$$
$$||\mathbf{w}||_p = (\sum_{d=1}^{D} w_d^p)^{1/p}$$



Contour plots for p = 2 p = 1 p < 1

Figure credit: Piyush Rai

Gradient descent

- A general solution for our optimization problem

$$\min_{\mathbf{w},b} L(\mathbf{w}, b) = \min_{\mathbf{w},b} \sum_{n=1}^{N} \mathbb{I}(y_n(\mathbf{w}^T \mathbf{x}_n + b) < 0) + \lambda R(\mathbf{w}, b)$$

- Idea: take iterative steps to update parameters in the direction of the gradient

Gradient descent algorithm

Objective function to minimize

Number of steps

Step size

Algorithm 22 $\textsc{GradientDescent}(\mathcal{F}, K, \eta_1, \dots)$

```
z^(0) ← ⟨0, 0, ..., 0⟩                        // initialize variable we are optimizing
for k = 1 ... K do
    g^(k) ← ∇_z F |_{z^(k-1)}                 // compute gradient at current location
    z^(k) ← z^(k-1) − η^(k) g^(k)             // take a step down the gradient
end for
return z^(K)
```

Illustrating gradient descent in 1-dimensional case

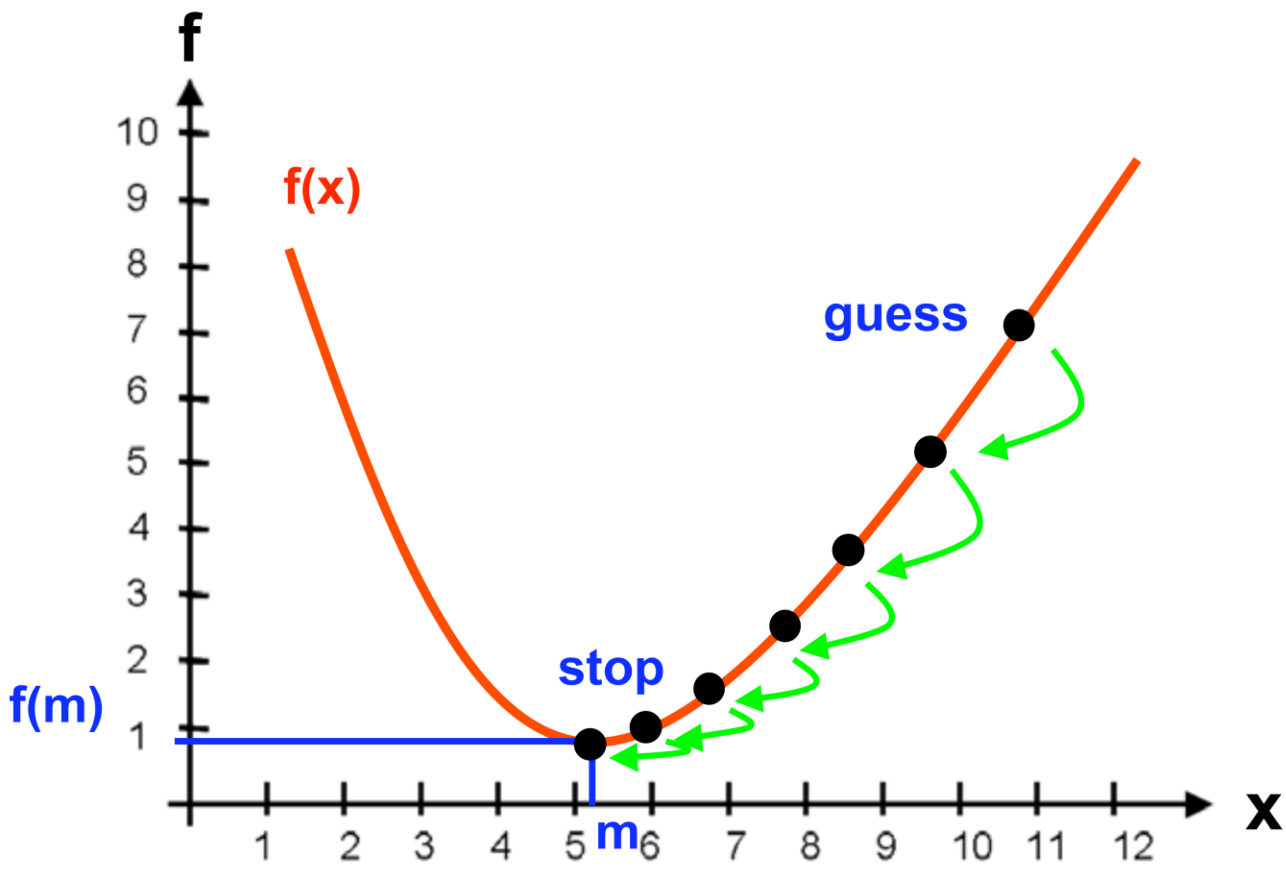


Figure credit: Piyush Rai

Impact of step size

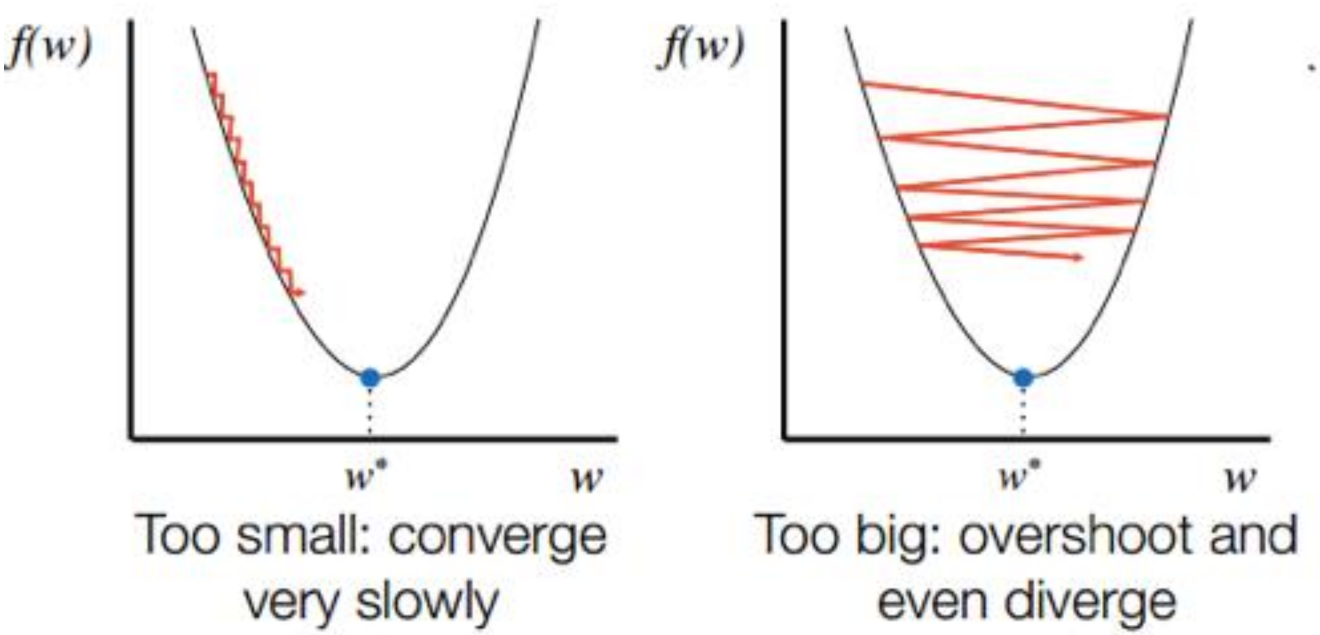
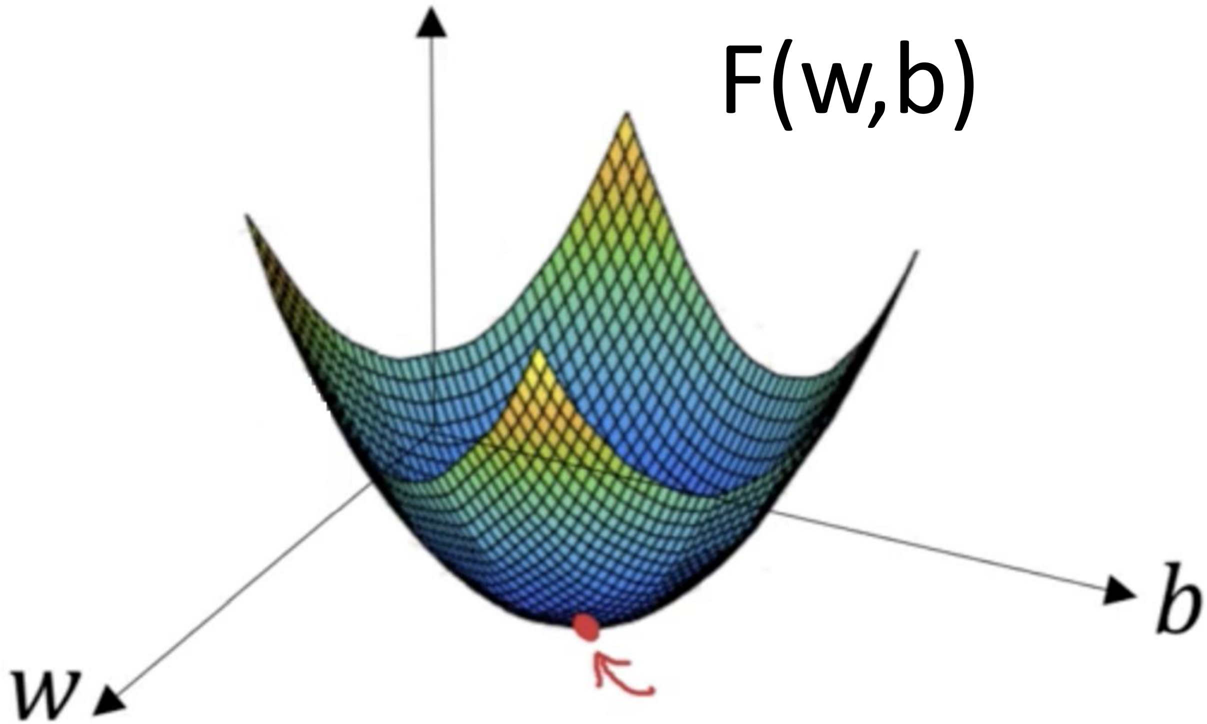


Image source: https://towardsdatascience.com/gradient-descent-in-a-nutshell-eaf8c18212f0

Illustrating gradient descent in 2-dimensional case



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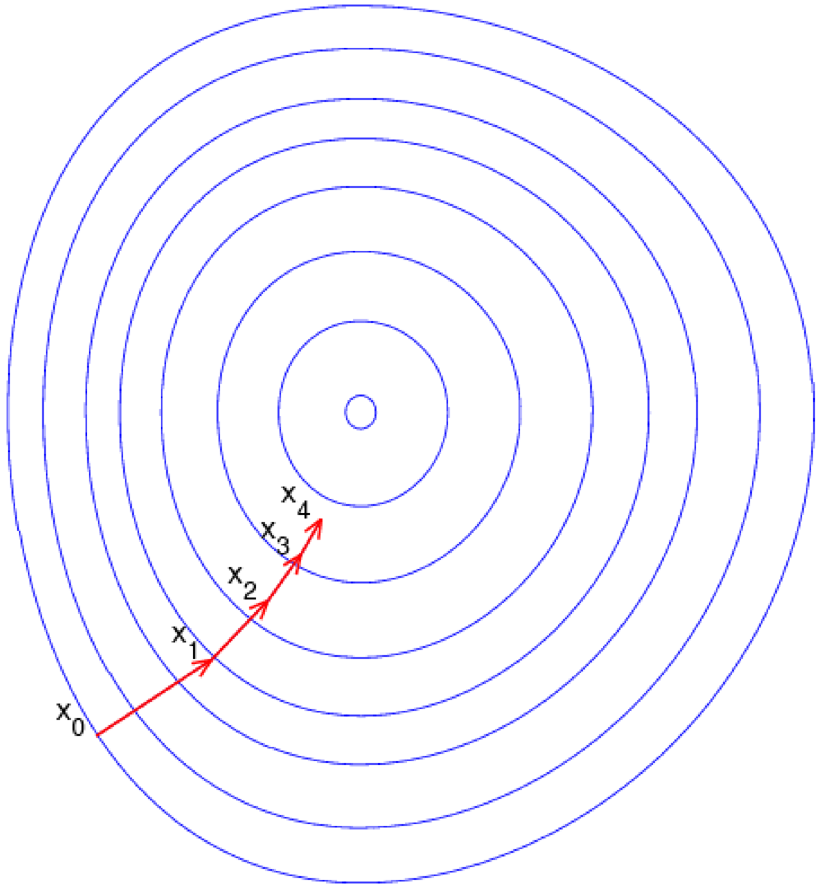
Illustrating gradient descent in 2-dimensional case



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Gradient descent algorithm

Objective function to minimize

Number of steps

Step size

Algorithm 22 $\textsc{GradientDescent}(\mathcal{F}, K, \eta_1, \ldots)$

$z^{(0)} \leftarrow \langle 0, 0, \ldots, 0 \rangle$ // initialize variable we are optimizing

for $k = 1 \ldots K$ **do**

  $g^{(k)} \leftarrow \nabla_z \mathcal{F}|_{z^{(k-1)}}$ // compute gradient at current location

  $z^{(k)} \leftarrow z^{(k-1)} - \eta^{(k)} g^{(k)}$ // take a step down the gradient

end for

return $z^{(K)}$

Gradient Descent

- 2 questions
  - When to stop?
    - When the gradient gets close to zero
    - When the objective stops changing much
    - When the parameters stop changing much
    - Early
    - When performance on held-out dev set plateaus
  - How to choose the step size?
    - Start with large steps, then take smaller steps

Now let's calculate gradients for multivariate objectives

- Consider the following learning objective

$$\mathcal{L}(\boldsymbol{w}, b) = \sum_n \exp\left[-y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b)\right] + \frac{\lambda}{2}||\boldsymbol{w}||^2$$

- What do we need to do to run gradient descent?

(1) Derivative with respect to b

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial}{\partial b} \sum_n \exp\left[- y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) \right] + \frac{\partial}{\partial b} \frac{\lambda}{2} \left|\left|\boldsymbol{w}\right|\right|^2 \tag{6.12}$$

$$= \sum_n \frac{\partial}{\partial b} \exp\left[- y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) \right] + 0 \tag{6.13}$$

$$= \sum_n \left(\frac{\partial}{\partial b} - y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) \right) \exp\left[- y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) \right] \tag{6.14}$$

$$= - \sum_n y_n \exp\left[- y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) \right] \tag{6.15}$$

(2) Gradient with respect to w

$$\nabla_w \mathcal{L} = \nabla_w \sum_n \exp\left[-y_n(\boldsymbol{w}\cdot\boldsymbol{x}_n + b)\right] + \nabla_w \frac{\lambda}{2}\,||\boldsymbol{w}||^2 \tag{6.16}$$

$$= \sum_n \left(\nabla_w - y_n(\boldsymbol{w}\cdot\boldsymbol{x}_n + b)\right)\exp\left[-y_n(\boldsymbol{w}\cdot\boldsymbol{x}_n + b)\right] + \lambda\boldsymbol{w} \tag{6.17}$$

$$= -\sum_n y_n\boldsymbol{x}_n \exp\left[-y_n(\boldsymbol{w}\cdot\boldsymbol{x}_n + b)\right] + \lambda\boldsymbol{w} \tag{6.18}$$

Subgradients

- Problem: some objective functions are not differentiable everywhere
  - Hinge loss, l1 norm

- Solution: subgradient optimization
  - Let’s ignore the problem, and just try to apply gradient descent anyway!!
  - we will just differentiate by parts…

Example: subgradient of hinge loss

For a given example n

$$\boldsymbol{\partial}_w \max\{0, 1 - y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b)\} \tag{6.22}$$

$$= \boldsymbol{\partial}_w \begin{cases} 0 & \text{if } y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) > 1 \\ y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) & \text{otherwise} \end{cases} \tag{6.23}$$

$$= \begin{cases} \mathbf{0} & \text{if } y_n(\boldsymbol{w} \cdot \boldsymbol{x}_n + b) > 1 \\ \text{-} y_n \boldsymbol{x}_n & \text{otherwise} \end{cases} \tag{6.25}$$

Subgradient Descent for Hinge Loss

Algorithm 23 HingeRegularizedGD($\mathbf{D}$, λ, $MaxIter$)

$\boldsymbol{w} \leftarrow \langle 0, 0, \dots 0 \rangle \quad , \quad b \leftarrow 0$ // initialize weights and bias

for $iter = 1 \dots MaxIter$ **do**

    $\boldsymbol{g} \leftarrow \langle 0, 0, \dots 0 \rangle \quad , \quad g \leftarrow 0$ // initialize gradient of weights and bias

    for all $(\boldsymbol{x}, y) \in \mathbf{D}$ **do**

        if $y(\boldsymbol{w} \cdot \boldsymbol{x} + b) \leq 1$ **then**

            $\boldsymbol{g} \leftarrow \boldsymbol{g} + y\,\boldsymbol{x}$ // update weight gradient

            $g \leftarrow g + y$ // update bias derivative

        end if

    end for

    $\boldsymbol{g} \leftarrow \boldsymbol{g} - \lambda \boldsymbol{w}$ // add in regularization term

    $\boldsymbol{w} \leftarrow \boldsymbol{w} + \eta \boldsymbol{g}$ // update weights

    $b \leftarrow b + \eta g$ // update bias

end for

return $\boldsymbol{w}, b$

What is the perceptron optimizing?

Algorithm 5 PerceptronTrain(**D**, *MaxIter*)

$w_d \leftarrow 0$, for all $d = 1 \dots D$ // initialize weights
$b \leftarrow 0$ // initialize bias
for $iter = 1 \dots MaxIter$ **do**
  for all $(x,y) \in \mathbf{D}$ **do**
    $a \leftarrow \sum_{d=1}^{D} w_d\, x_d + b$ // compute activation for this example
    if $ya \leq 0$ **then**
      $w_d \leftarrow w_d + y x_d$, for all $d = 1 \dots D$ // update weights
      $b \leftarrow b + y$ // update bias
    end if
  end for
end for
return $w_0, w_1, \dots, w_D, b$

- Loss function is a variant of the hinge loss

$$\max\{0, -y_n(\mathbf{w}^T \mathbf{x}_n + b)\}$$

Summary

- Gradient descent
  - A generic algorithm to minimize objective functions
  - Works well as long as functions are well behaved (ie convex)
  - Subgradient descent can be used at points where derivative is not defined
  - Choice of step size is important
- Can be used to find parameters of linear models
- Optional: alternatives to gradient descent
  - For some objectives, we can find closed form solutions (see CIML 7.6)