Big Data Computing

Master's Degree in Computer Science

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Recap from Last Lecture

- Logistic Regression is a powerful tool for predicting binary variables through probability of each class
- It fits a regression line between input (features) and output (logarithm of the odds), assuming probability takes the form of a sigmoid function
- Parameter estimation is typically done via MLE (i.e., by minimizing Cross-Entropy error)
- We need a more sophisticated learning algorithm! 🧐

LEARNING ALGORITHM

Picking the Best Hypothesis

- So far, we have defined:
  - The model (logistic function)
  - The error measure (cross-entropy)

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  - The error measure (cross-entropy)

To actually select the best hypothesis, we have to pick the vector of parameters $\boldsymbol{\theta}^*$ so that the error measure is minimized

$$\boxed{E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)}$$

Mean Squared Error vs. Cross-Entropy

In the case of linear regression we have a similar expression for the error measure, i.e., Mean Squared Error (MSE)

$$E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^T \mathbf{x_i} - y_i\right)^2$$

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Minimizing MSE through Ordinary Least Squares (OLS) leads to a closed-form solution often referred to as the OLS estimator for $\boldsymbol{\theta}^*$

$$\boxed{\hat{\boldsymbol{\theta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}}$$

Mean Squared Error vs. Cross-Entropy

The problem is that using Cross-Entropy as error measure we cannot find a closed-form solution to the minimization problem

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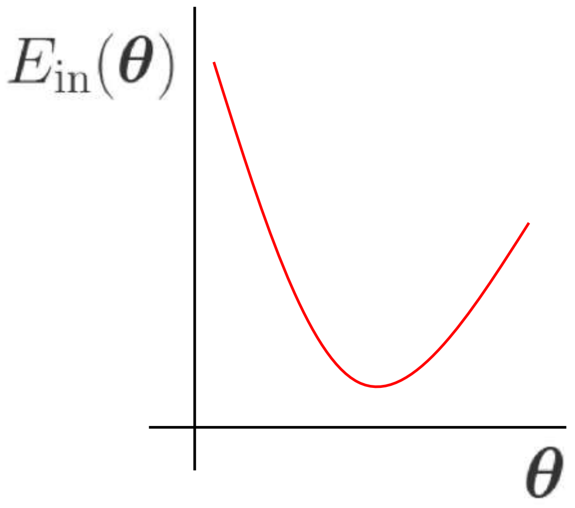
$$\Downarrow$$

Iterative Solution

(Batch) Gradient Descent

General iterative method for any nonlinear optimization



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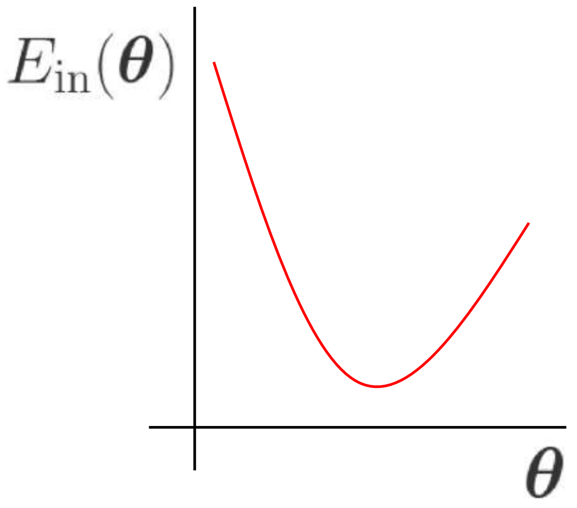

The method **guarantees the convergence to a local minimum**

(Under specific assumptions on the objective function and learning rate)

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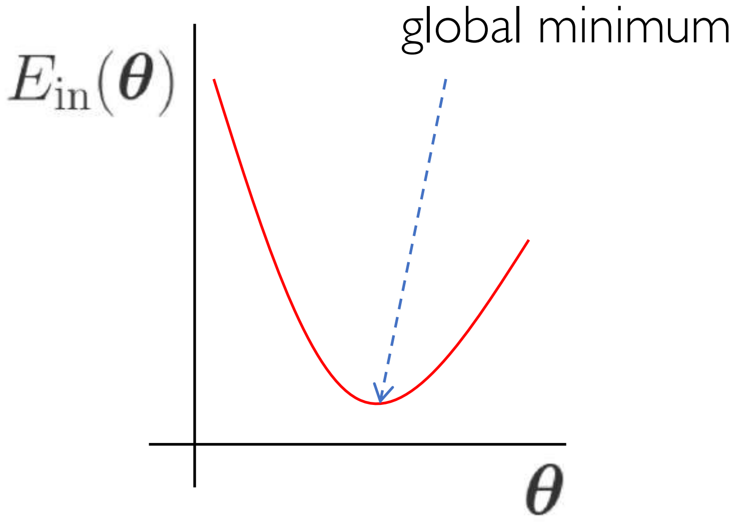

The method **guarantees the convergence to a local minimum**

(Under specific assumptions on the objective function and learning rate)

If the objective function is **convex** (like cross-entropy) then the local minimum is also the **global minimum**

Gradient Descent: The Main Idea

1. At $t = 0$ initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$

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Unit vector representing the direction of the steepest slope

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step

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Unit vector representing the direction of the steepest slope

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How do we determine the direction v?

Gradient Descent: The Direction v

- We already intuitively said that the direction **v** should be that of the "steepest" slope

Gradient Descent: The Direction v

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- Concretely, this means moving along the direction which mostly reduces the in-sample error function

$$\boxed{\Delta E_{\text{in}}(\boldsymbol{\theta}, t) = E_{\text{in}}(\boldsymbol{\theta}(t)) - E_{\text{in}}(\boldsymbol{\theta}(t-1))}$$

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We want ΔE_{in} to be as negative as possible, which means that we are actually reducing the error w.r.t. the previous iteration *t*-1

Gradient Descent: The Direction v

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Gradient Descent: The Direction v

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Let's first assume we are in the univariate case, i.e., $\boldsymbol{\theta} = \vartheta$ in R

$\boxed{f = E_{\text{in}}}$ $\boxed{x_0 = \boldsymbol{\theta}(t-1)}$ $\boxed{x = \boldsymbol{\theta}(t)}$

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$$\boxed{\delta f = \Delta E_{\text{in}} = f(x) - f(x_0)} \qquad \boxed{\delta x = x - x_0 = \boldsymbol{\theta}(t) - \boldsymbol{\theta}(t-1) = \eta \mathbf{v}}$$

Gradient Descent: The Direction v

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$$\boxed{f'(x_0) = \lim_{\delta x \to 0} \frac{f(x_0 + \delta x) - f(x_0)}{\delta x}}$$

$$\boxed{f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0} \approx \frac{\delta f}{\delta x}}$$

Gradient Descent: The Direction v

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$$\boxed{\delta f = f(x) - f(x_0) \approx f'(x_0)\delta x = f'(x_0)(x - x_0)}$$

Gradient Descent: The Direction v

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Gradient Descent: The Direction v

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$$f(x) = \underbrace{f(x_0) + f'(x_0)(x - x_0)}_{\text{First-order Taylor approximation}} \underbrace{+O((x - x_0)^2)}_{\text{Second-order error term}}$$

Gradient Descent: The Direction v

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To summarize and generalize to the multivariate case of **θ**:

$$\boxed{\delta f = f(x) - f(x_0) = \Delta E_{\text{in}} = \eta \underset{\uparrow}{\nabla} E_{\text{in}}(\boldsymbol{\theta}(t-1))^T \mathbf{v} + O(\eta^2)}$$

The greek letter *nabla* indicates the gradient

Gradient Descent: The Direction v

$$\Delta E_{\text{in}} = \eta \nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T \mathbf{v} + O(\eta^2)$$

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The unit vector v only contributes to the direction and not to the magnitude of the iterative step

Gradient Descent: The Direction v

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The unit vector v only contributes to the direction and not to the magnitude of the iterative step

The second-order approximation term is negligible

(when the step size is small)

Gradient Descent: The Direction v

$$\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))^T = \mathbf{u}$$

$$\Delta E_{\text{in}} = \eta \mathbf{u} \cdot \mathbf{v}$$

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$$-\eta||\mathbf{u}|| \leq \underbrace{\eta \mathbf{u} \cdot \mathbf{v}}_{\Delta E_{\text{in}}} \leq \eta||\mathbf{u}||$$

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The most positive ΔE_{in} when $\cos(\alpha) = 1$ (i.e., $\alpha = 0°$)

Both error and step vectors have the same direction

Gradient Descent: The Direction v

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$$\boxed{-\eta||\mathbf{u}||} \leq \underbrace{\eta \mathbf{u} \cdot \mathbf{v}}_{\Delta E_{\text{in}}} \leq \eta||\mathbf{u}||$$

The most negative ΔE_{in} when $\cos(\alpha) = -1$ (i.e., $\alpha = 180°$)

The error and step vectors have opposite direction

Gradient Descent: The Direction **v**

At each iteration t, we want the unit vector **v** which makes exactly **the most negative** ΔE_{in}

$$\eta \mathbf{u} \cdot \mathbf{v} = -\eta ||\mathbf{u}||$$

Gradient Descent: The Direction v

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$$\mathbf{u} \cdot \mathbf{v} = -||\mathbf{u}||$$

$$\mathbf{u}^T \cdot \mathbf{u} \cdot \mathbf{v} = -||\mathbf{u}||\mathbf{u}^T$$

$$\mathbf{v} = -\frac{||\mathbf{u}||\mathbf{u}^T}{||\mathbf{u}||^2} = -\frac{\mathbf{u}^T}{||\mathbf{u}||} = -\frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))}{||\nabla E_{\text{in}}(\boldsymbol{\theta}(t-1))||}$$

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Gradient Descent: The Step η

How the step magnitude η affects the convergence?

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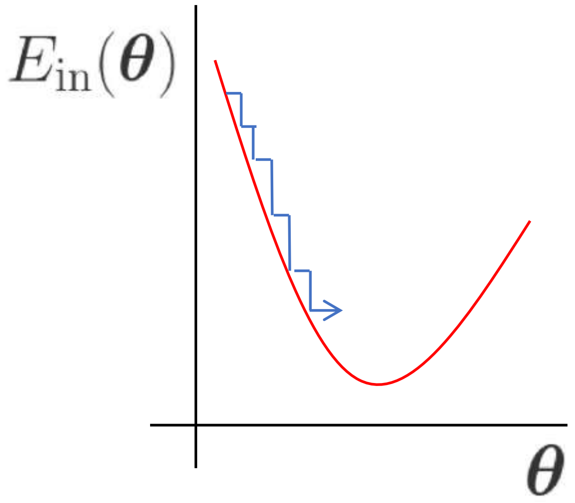
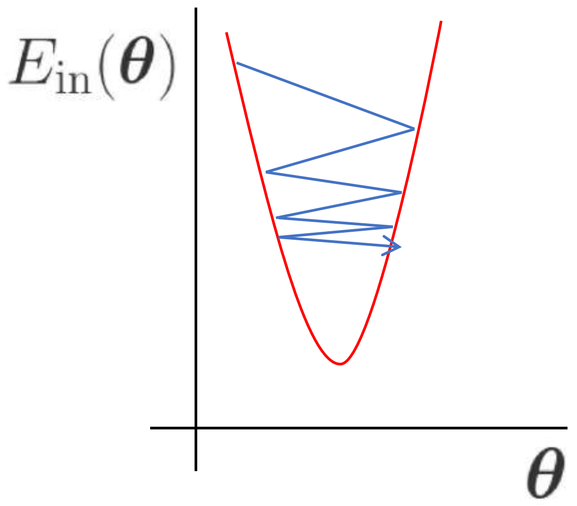


η too small

Gradient Descent: The Step η

How the step magnitude η affects the convergence?



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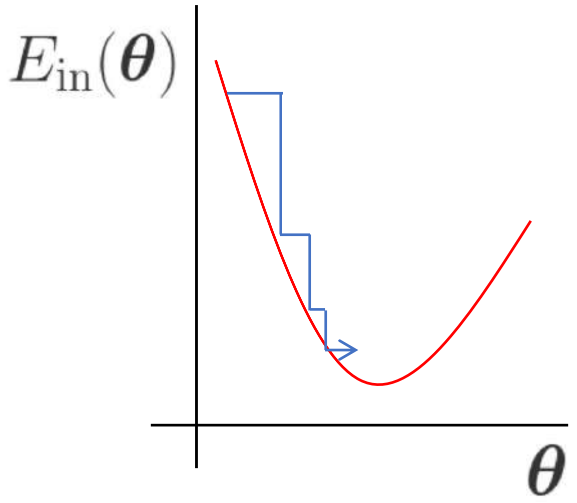

η variable

Gradient Descent: The Step η

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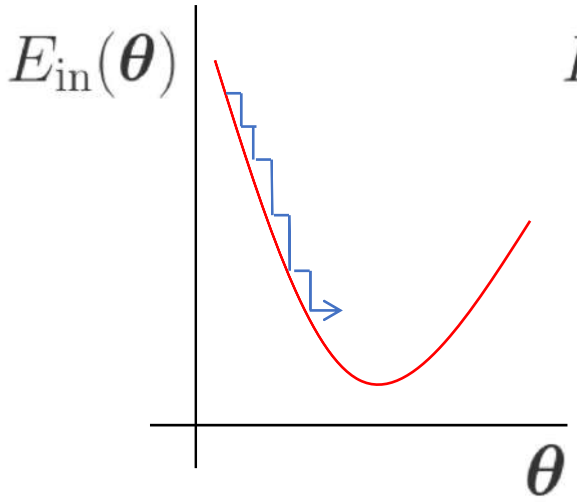

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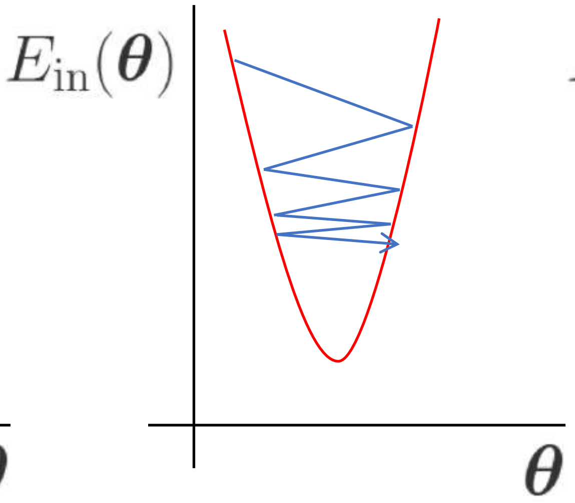

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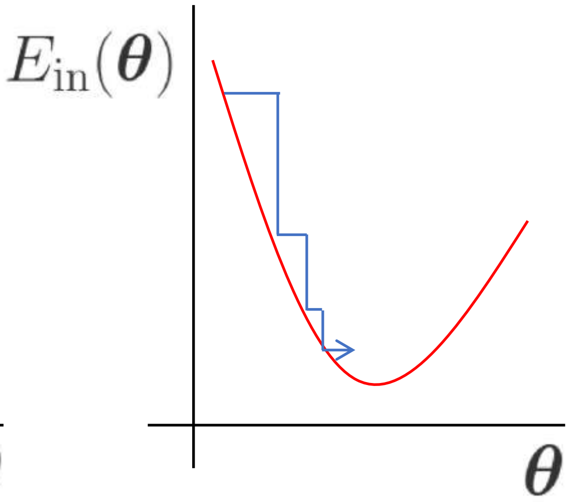

η variable

Rule of thumb

Dynamically change η proportionally to the gradient!

Gradient Descent: The Step η

Remember that at each iteration the update strategy is:

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta \mathbf{v}$$

$$\mathbf{v} = -\frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

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At each iteration *t*, the step η is fixed

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) - \eta \frac{\nabla E_{\text{in}}(\boldsymbol{\theta}(t))}{\|\nabla E_{\text{in}}(\boldsymbol{\theta}(t))\|}$$

Gradient Descent: The Step η

Instead of having a fixed η at each iteration, use a variable η_t as function of η

$$\boldsymbol{\theta}(t+1) = \boldsymbol{\theta}(t) + \eta_t \mathbf{v} \qquad \eta_t = \eta k$$

Gradient Descent: The Step η

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Let's take:
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Computing the Gradient of Cross-Entropy

$$\nabla E_{\text{in}}(\boldsymbol{\theta}) = \nabla \left[\frac{1}{m} \sum_{i=1}^{m} \ln(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1) \right]$$

Computing the Gradient of Cross-Entropy

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chain rule of derivative

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$$= \left[\frac{1}{m} \sum_{i=1}^{m} \nabla \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1\right) \right] = \left[\frac{1}{m} \sum_{i=1}^{m} \frac{1}{e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1} \nabla\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1\right) \right]$$

chain rule of derivative

$$= \frac{1}{m} \sum_{i=1}^{m} \frac{-y_i \mathbf{x}_i e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i}}{e^{-y_i \boldsymbol{\theta}^T \mathbf{x}_i} + 1}$$

Computing the Gradient of Cross-Entropy

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chain rule of derivative

$$= \frac{1}{m}\sum_{i=1}^{m}\frac{-y_i\mathbf{x}_i e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}}{e^{-y_i\boldsymbol{\theta}^T\mathbf{x}_i}+1} = \boxed{-\frac{1}{m}\sum_{i=1}^{m}\frac{y_i\mathbf{x}_i}{1+e^{y_i\boldsymbol{\theta}^T\mathbf{x}_i}}}$$

Gradient Descent: The Algorithm

1. At $t = 0$ initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$

Gradient Descent: The Algorithm

1. At $t = 0$ initialize the (guessed) vector of parameters $\boldsymbol{\theta}$ to $\boldsymbol{\theta}(0)$
2. For $t = 0, 1, 2, \ldots$ until stop:
   a. Compute the gradient of the cross-entropy error $\boxed{E_{\text{in}}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ln\left(e^{-y_i \boldsymbol{\theta}^T \mathbf{x_i}} + 1\right)}$

$$\boxed{\nabla E_{\text{in}}(\boldsymbol{\theta}(t)) = -\frac{1}{m} \sum_{i=1}^{m} \frac{y_i \mathbf{x}_i}{1 + e^{y_i \boldsymbol{\theta}(t)^T \mathbf{x}_i}}}$$

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3. Return the final vector of parameters $\boldsymbol{\theta}(\infty)$

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- If the function is convex we are guaranteed to reach the global minimum no matter what is the initial value of $\boldsymbol{\theta}(0)$
- In general, we may get to the local minimum nearest to $\boldsymbol{\theta}(0)$

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- GD can still be used to try to optimize non-convex objectives
- Problem: non-convex functions may have several local minima
- A bad initialization might cause GD to end up into a "bad" local minimum and miss "better" ones (or even the global if it exists)
- Solution (heuristic): repeating GD 100÷1,000 times each time with a different $\boldsymbol{\theta}(0)$ may reduce the chance the above issue occurs

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Gradient Descent: Stopping Criterion

- If the function is convex GD reaches the global minimum when $\nabla E_{in}(\boldsymbol{\theta}(t)) = 0$
- In general, we don't know if eventually the gradient gets to 0 therefore we can use several criteria of termination:
  - stop whenever the difference between two iterations is "small enough" → may converge "prematurely"
  - stop when the error equals to ε → may not converge if the target error is not achievable
  - stop after T iterations
  - combinations of the above in practice works…

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- Stochastic vs. Mini-Batch Gradient Descent (SGD vs. MBGD)
  - At each iteration, compute the gradient only from one instance (SGD) or a sample of *k* instances (MBGD) rather than the full dataset
- Regularization
  - Include the L1- or L2-norm of the vector of parameters $\boldsymbol{\theta}$ in the cross-entropy error to avoid overfitting

Take-Home Message of Today

- Gradient Descent (GD) is the standard method for solving optimization objectives (i.e., finding minimum/maximum of a function)
- It requires the function to be differentiable
- If the function is convex, it guarantees to converge to the global minimum
- If the function is quasi-convex, it must avoid getting stuck at a saddle point
- Many variants are currently used: Momentum, RMSProp, Adam, etc. (https://ruder.io/optimizing-gradient-descent/)