Stochastic Gradient Descent

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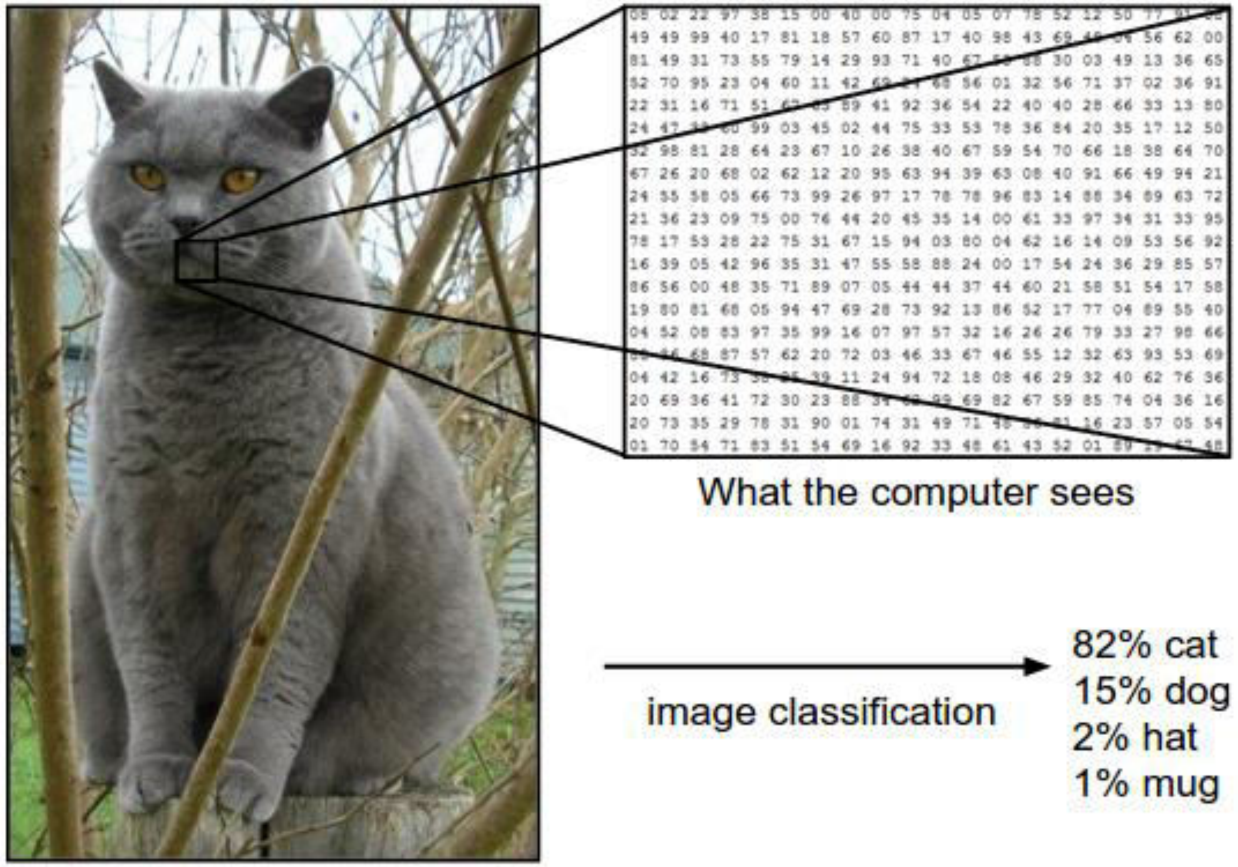
Image Classification



Linear model

- Score function
  - Maps raw data to class scores
- Loss function
  - Measures how well predicted classes agree with ground truth labels
    - Multiclass Support Vector Machine loss (SVM loss)
    - Softmax classifier (cross-entropy loss)
- Learning
  - Find parameters of score function that minimize loss function
    - Multiclass Support Vector Machine loss (SVM loss)

Recall: Linear model with SVM loss

- Score function
  - Maps raw data to class scores

$$f(x_i, W) = Wx_i$$

- Loss function
  - Measures how well predicted classes agree with ground truth labels

$$L = \frac{1}{N} \sum_i \sum_{j \neq y_i} [\max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + \Delta)] + \lambda \sum_k \sum_l W_{k,l}^2$$

SVM loss: equivalent formulation

- Loss function
  - Measures how well predicted classes agree with ground truth labels

$$L = \frac{1}{N}\sum_i \sum_{j \neq y_i} [\max(0, f(x_i;W)_j - f(x_i;W)_{y_i} + \Delta)] + \lambda \sum_k \sum_l W_{k,l}^2$$

Are Δ and λ independent parameters?

$$Set\, \Delta = 1$$

Today

- Learning model parameters with Stochastic Gradient Descent that minimize loss

- Later
  - Different score functions: deep networks
  - Same loss functions and learning algorithm

Outline

- Visualizing the loss function
- Optimization
  - Random search
  - Random local search
  - Gradient descent
    - Mini-batch gradient descent

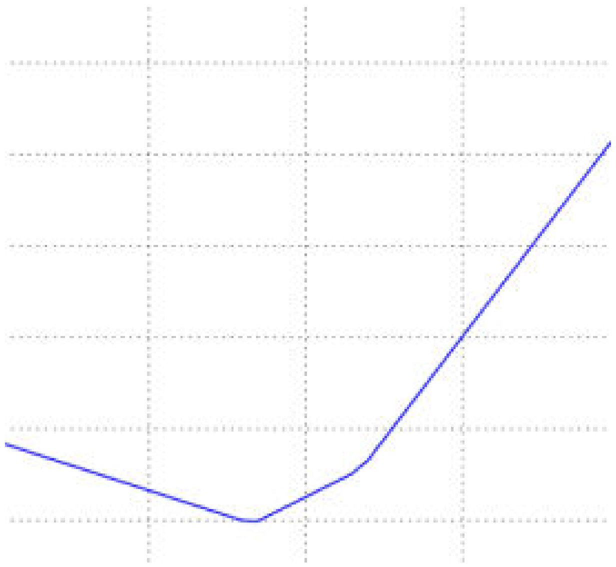
Visualizing SVM loss function

- Difficult to visualize fully
  - CIFAR-10 a linear classifier weight matrix is of size [10 x 3073] for a total of 30,730 parameters

- Can gain intuition by visualizing along rays (1 dimension) or planes (2 dimensions)

Visualizing in 1-D

- Generate random weight matrix W
- Generate random direction W_1
- Compute loss along this direction $L(W + aW_1)$

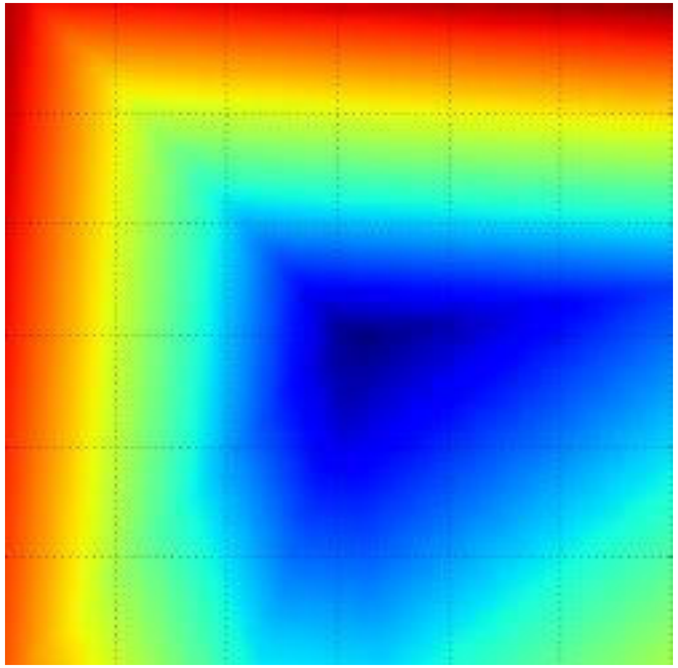


Loss for single example

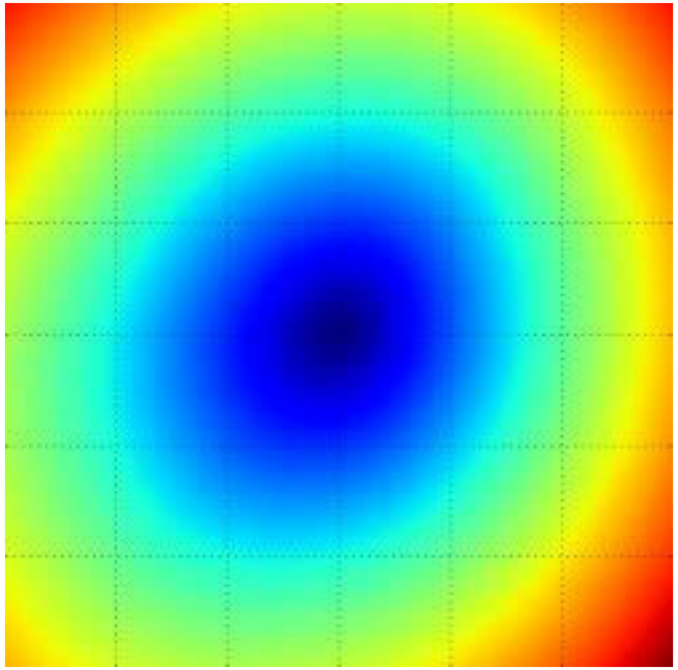
Where is the minima?

Visualizing in 2-D

- Compute loss along plane $L(W + aW_1 + bW_2)$



Loss for single example



Average loss for 100 examples
(convex function)

How do we find weights that minimize loss?

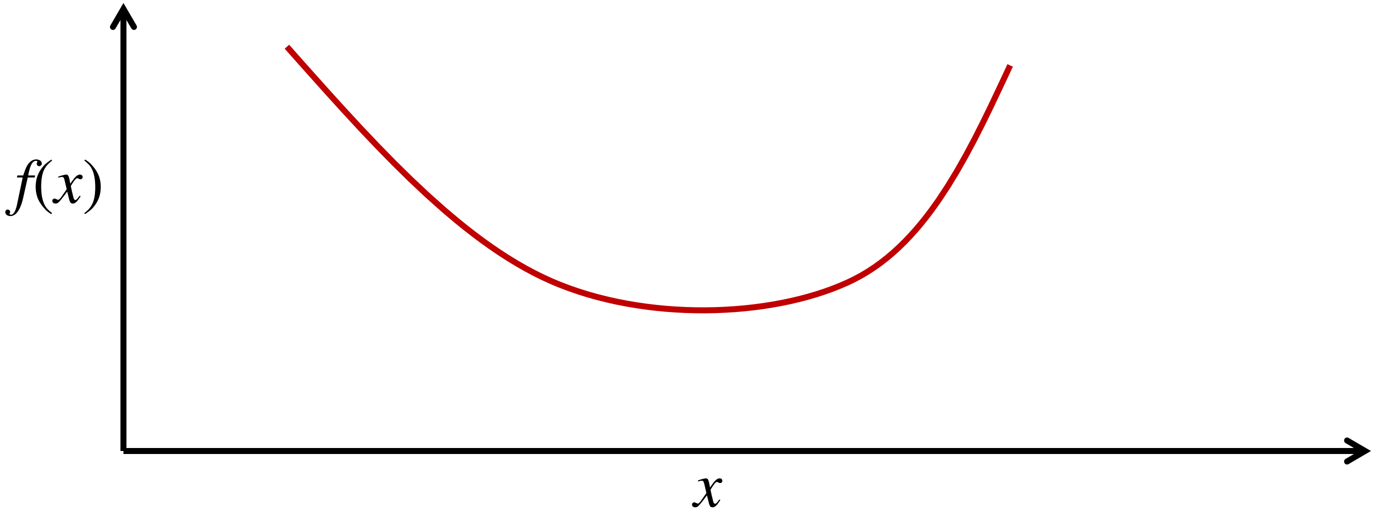
- Random search
  - Try many random weight matrices and pick the best one
  - Performance: poor

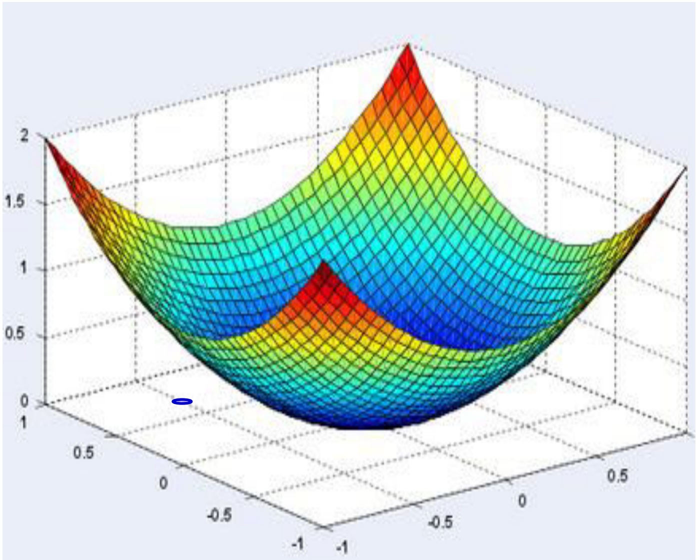
- Random local search
  - Start with random weight matrix
  - Try many local perturbations, pick the best one, and iterate
  - Performance: better but still quite poor

- Useful idea: iterative refinement of weight matrix

Optimization basics

The problem of optimization





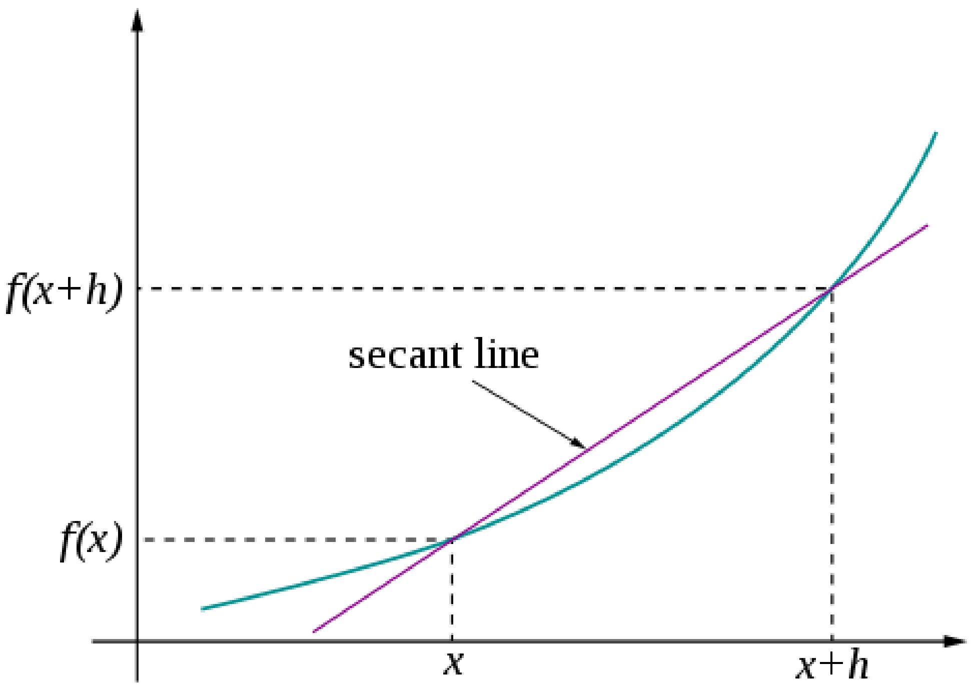
Find the value of $\boldsymbol{x}$ where $\mathbf{f}(\boldsymbol{x})$ is minimum

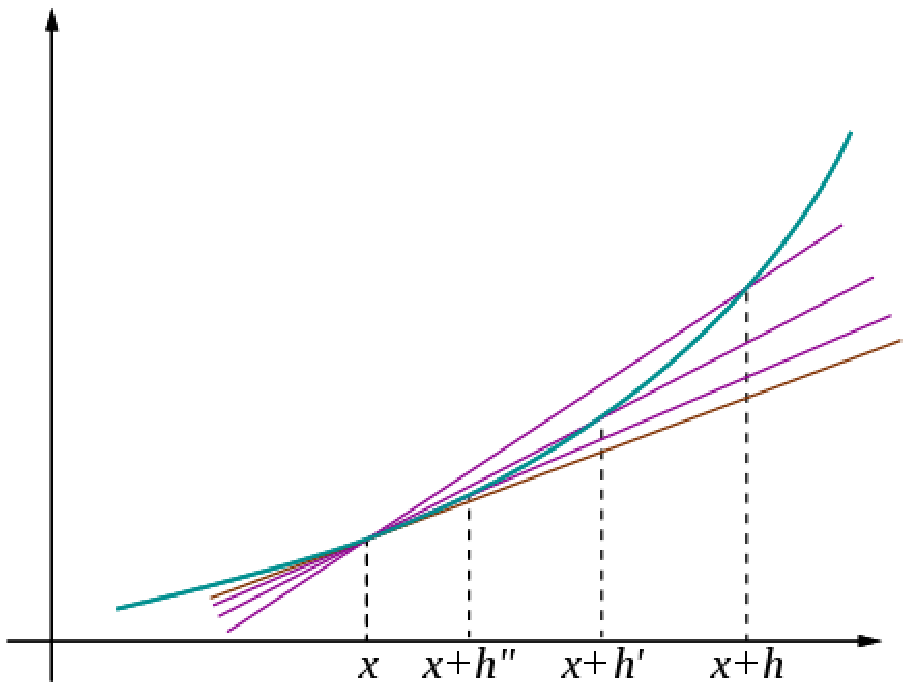
Our setting: $\boldsymbol{x}$ represents weights, $\mathbf{f}(\boldsymbol{x})$ represents loss function

In two stages

- Function of single variable
- Function of multiple variables

Derivative of a function of single variable





$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

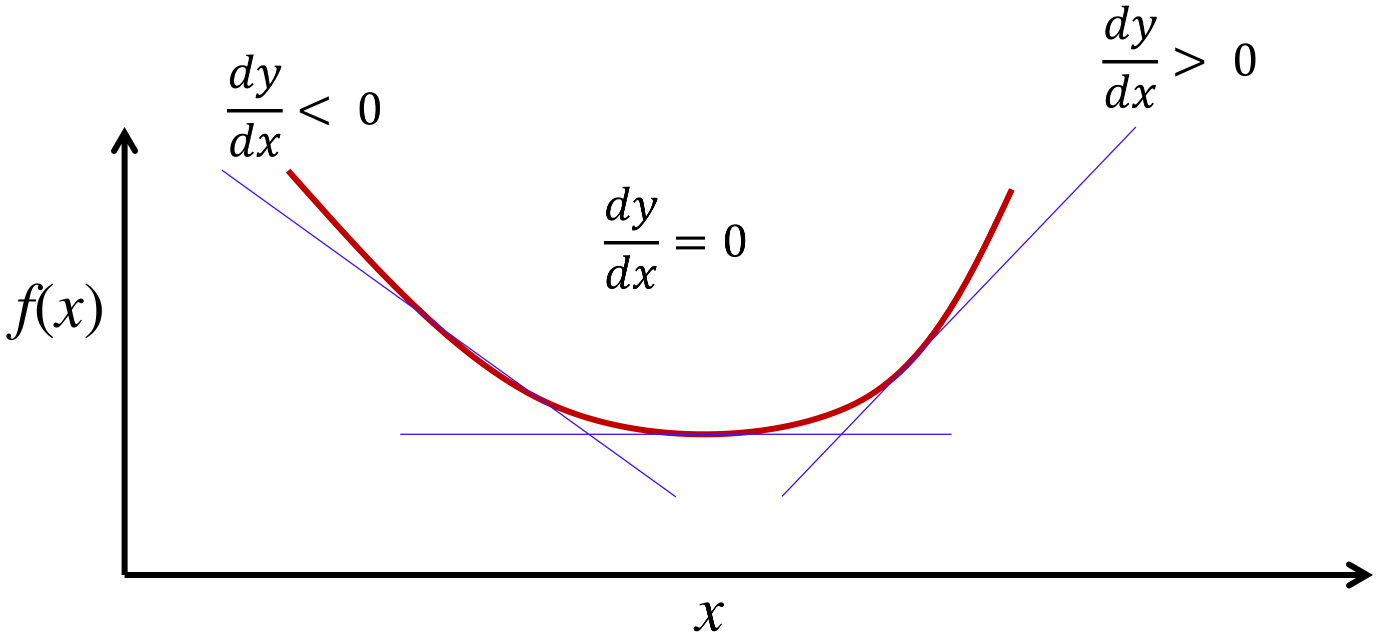
Derivatives

$$\frac{d}{dx}(x^2) = 2x$$

$$\frac{d}{dx}(e^x) = e^x$$

$$\frac{d}{dx}(ln\ x) = \frac{1}{x}\ if\, x > 0$$

Finding minima

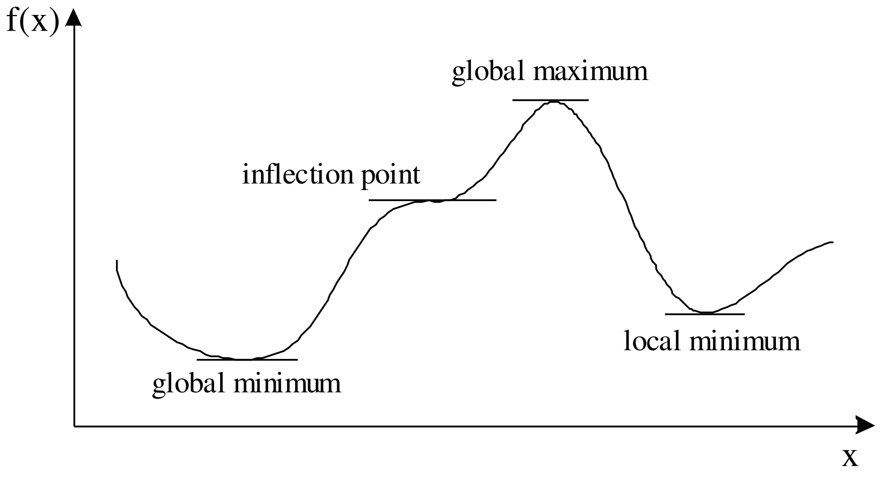


Increase x if derivative negative, decrease if positive

i.e., take step in direction opposite to sign of gradient

(key idea of gradient descent)

Doesn’t always work



- Theoretical and empirical evidence that gradient descent works quite well for deep networks

In two stages

- Function of single variable
- Function of multiple variables

Partial derivatives

The **partial derivative** of an n-ary function $f(x_1,\ldots,x_n)$ in the direction x_i at the point $(a_1,\ldots,a_n)$ is defined to be:

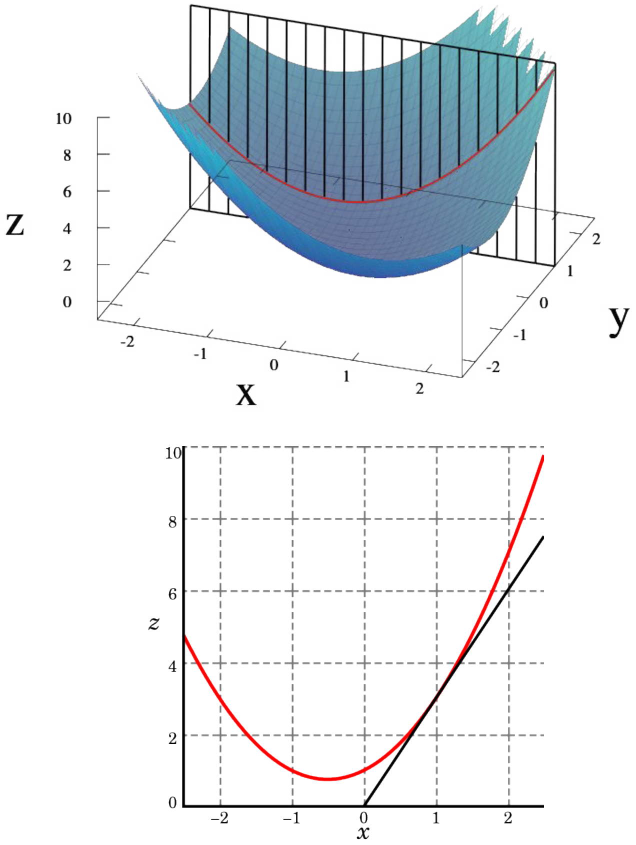
$$\frac{\partial f}{\partial x_i}(a_1,\ldots,a_n) = \lim_{h\to 0}\frac{f(a_1,\ldots,a_i+h,\ldots,a_n) - f(a_1,\ldots,a_i,\ldots,a_n)}{h}.$$

Partial derivative example

$$z = f(x, y) = x^2 + xy + y^2.$$

$$\frac{\partial z}{\partial x} = 2x + y.$$

At (1, 1), the slope is 3



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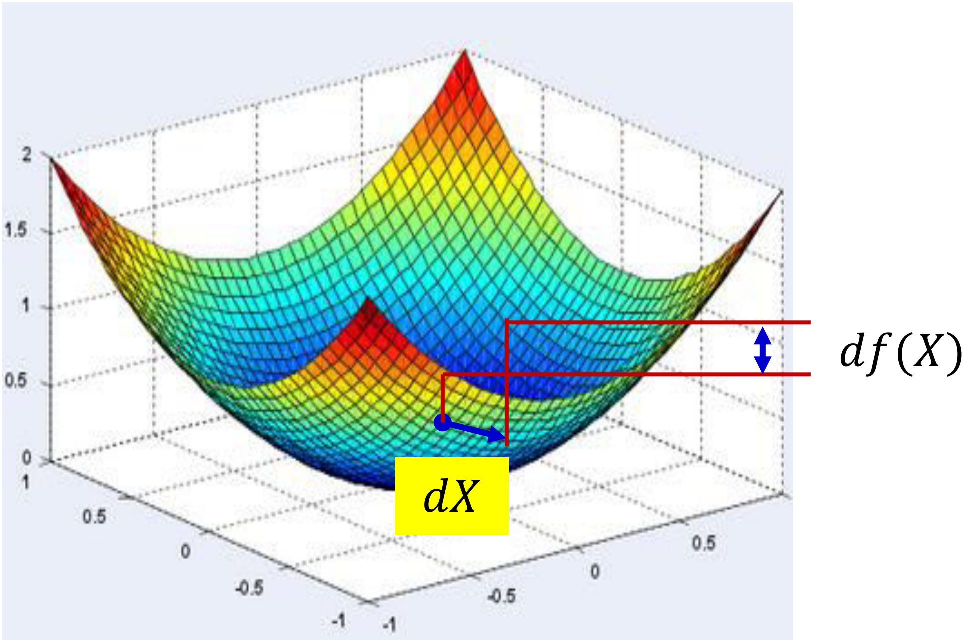
The gradient of a scalar function

- The *gradient* $\nabla f(X)$ of a scalar function $f(X)$ of a multi-variate input X is a multiplicative factor that gives us the change in $f(X)$ for tiny variations in X

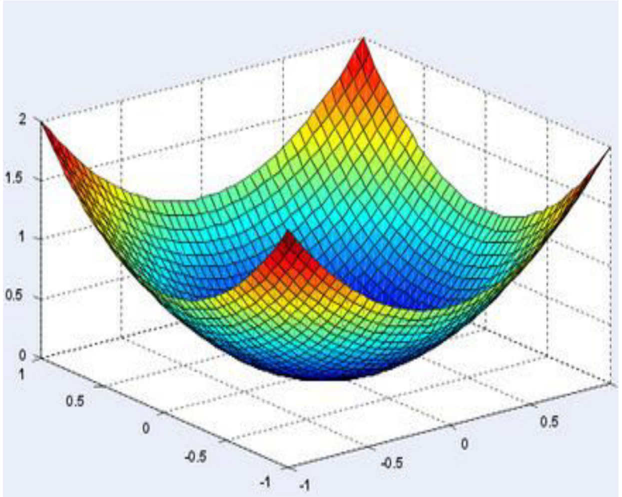
$$df(X) = \nabla f(X) dX$$



Gradients of scalar functions with multi-variate inputs

- Consider $f(X) = f(x_1, x_2, \ldots, x_n)$

- $\nabla f(X) = \begin{bmatrix} \frac{\partial f(X)}{\partial x_1} & \frac{\partial f(X)}{\partial x_2} & \cdots & \frac{\partial f(X)}{\partial x_n} \end{bmatrix}$



Computing gradients analytically

$$f(x,y) = xy \qquad \rightarrow \qquad \frac{\partial f}{\partial x} = y \qquad \frac{\partial f}{\partial y} = x$$

$$\nabla f = [\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}] = [y, x]$$

Derivatives measure sensitivity

$$x = 4, y = -3 \qquad f(x, y) = -12 \qquad \frac{\partial f}{\partial x} = -3$$

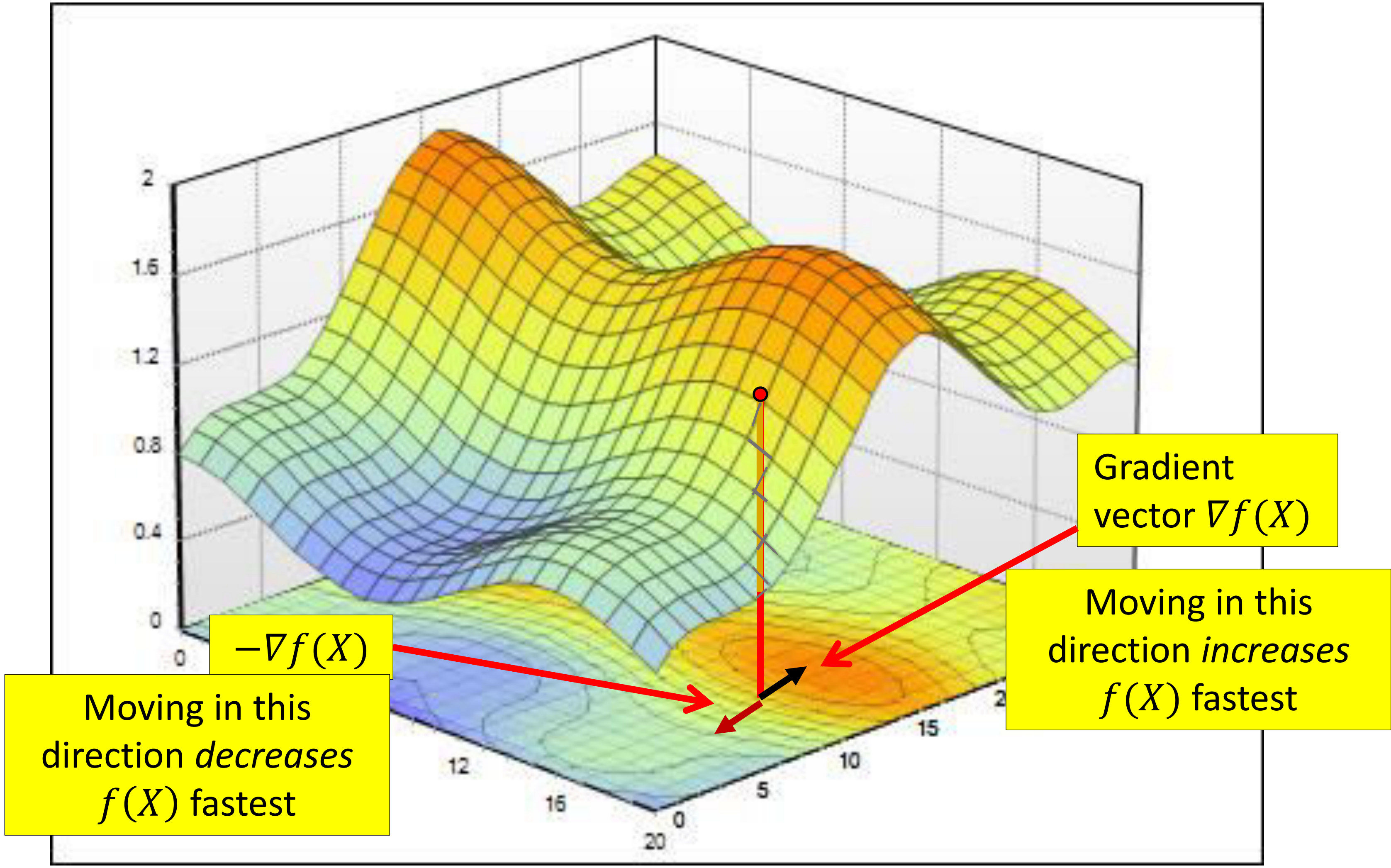
If we were to increase x by a tiny amount, the effect on the whole expression would be to decrease it (due to the negative sign), and by three times that amount.

Computing gradients analytically

$$f(x, y) = x + y \qquad \rightarrow \qquad \frac{\partial f}{\partial x} = 1 \qquad \frac{\partial f}{\partial y} = 1$$

Finding minima

Take step in direction opposite to sign of gradient



Gradient descent algorithm

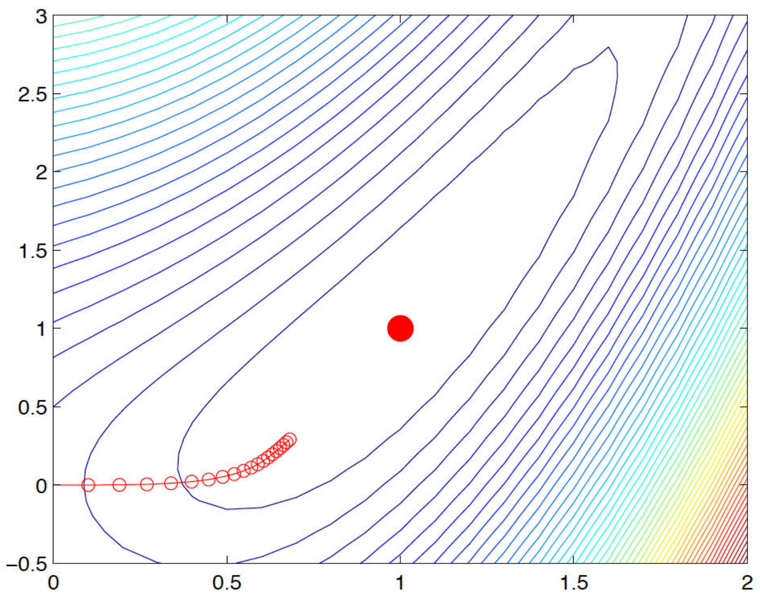
- Initialize:
  - x^0
  - $k = 0$
- While $\left|f\left(x^{k+1}\right) - f\left(x^k\right)\right| > \varepsilon$
  - $x^{k+1} = x^k - \eta^k \nabla f\left(x^k\right)^T$
  - $k = k + 1$

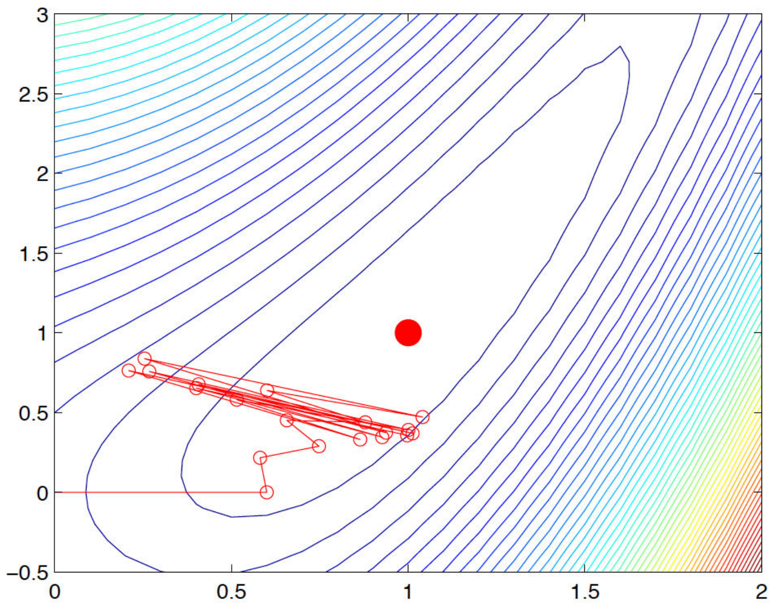
Average gradient across all training examples

$$f(x^k) = \frac{1}{N} \Sigma_{i=1}^{N} f_i(x^k)$$

$$\nabla f(x^k) = \frac{1}{N} \Sigma_{i=1}^{N} \nabla f_i(x^k)$$

Step size affects convergence of gradient descent





Murphy, Machine Learning, Fig 8.2

Gradient descent algorithm

- Initialize:
  - x^0
  - $k = 0$

- While $\left|f\left(x^{k+1}\right) - f\left(x^k\right)\right| > \varepsilon$
  - $x^{k+1} = x^k - \eta^k \nabla f\left(x^k\right)^T$
  - $k = k + 1$

Average gradient across all training examples

Challenge: Not scalable for very large data sets

Challenge to discuss later: How to choose step size?

Mini-batch gradient descent

- Initialize:
  - x^0
  - $k = 0$

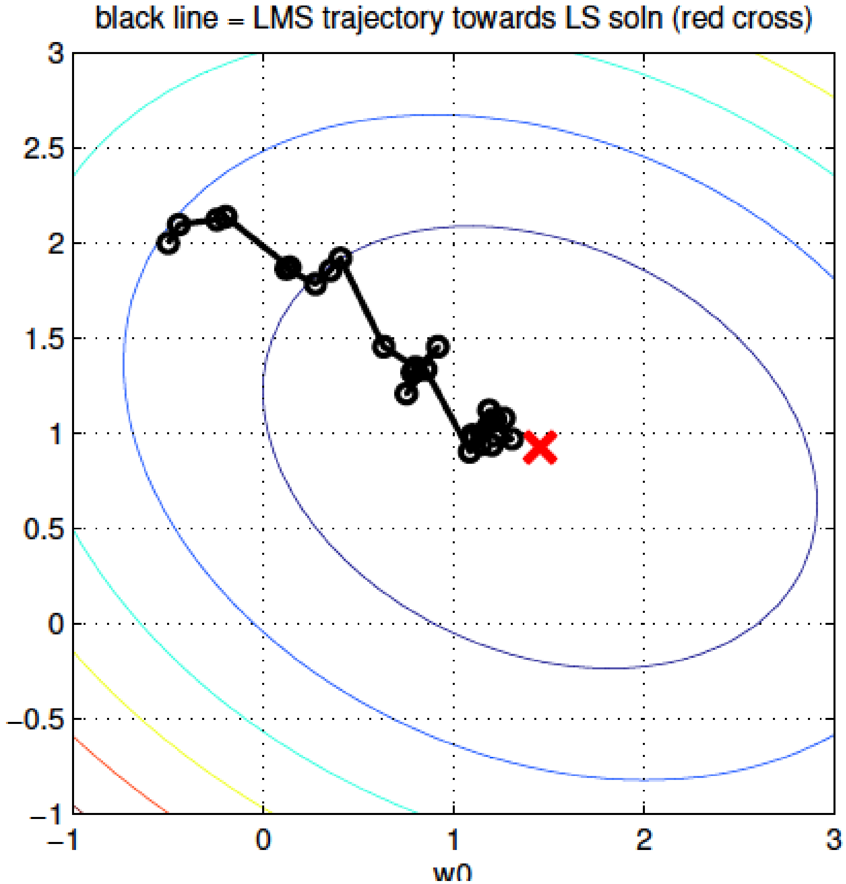
- While $\left|f\left(x^{k+1}\right) - f\left(x^k\right)\right| > \varepsilon$
  - $x^{k+1} = x^k - \eta^k \nabla f\left(x^k\right)^T$
  - $k = k + 1$

Average gradient over small batches of training examples (e.g., sample of 256 examples)

Faster convergence

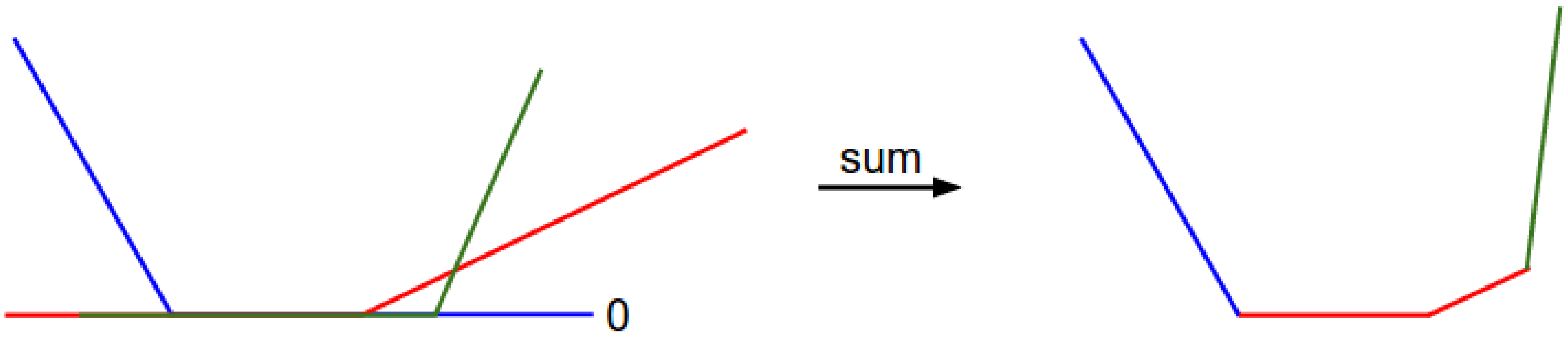
Special case: Stochastic or online gradient descent → use single training example in each update step

Stochastic gradient descent convergence



Murphy, Machine Learning, Fig 8.8

SVM loss visualization



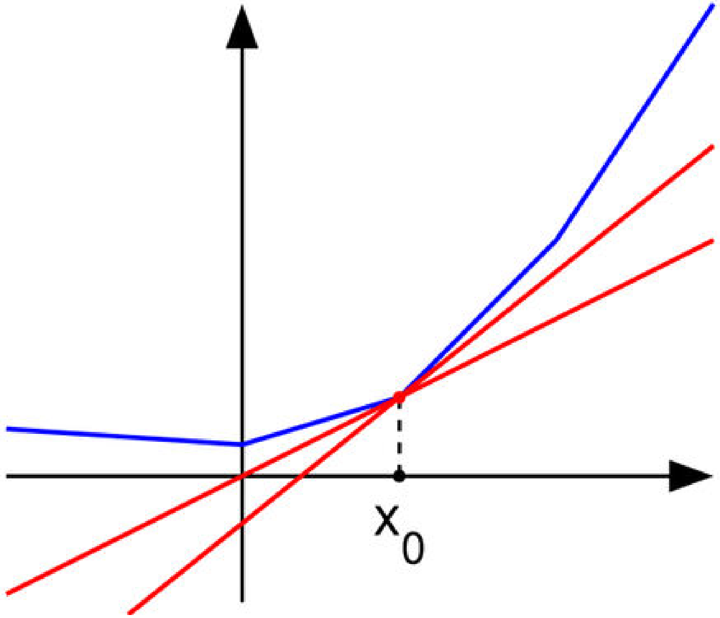
Challenge: Gradient does not exist

Computing subgradients analytically

The set of subderivatives at x_0 for a convex function is a nonempty closed interval [*a*, *b*], where *a* and *b* are the one-sided limits:

$$a = \lim_{x \to x_0^-} \frac{f(x) - f(x_0)}{x - x_0}$$

$$b = \lim_{x \to x_0^+} \frac{f(x) - f(x_0)}{x - x_0}$$



Computing subgradients analytically

$$f(x, y) = \max(x, y) \qquad \rightarrow \qquad \frac{\partial f}{\partial x} = \mathcal{I}(x >= y) \qquad \frac{\partial f}{\partial y} = \mathcal{I}(y >= x)$$

The (sub)gradient is 1 on the input that is larger and 0 on the other input

Subgradient of SVM loss

$$L_i = \sum_{j \neq y_i} \left[\max(0, w_j^T x_i - w_{y_i}^T x_i + \Delta) \right]$$

$$\nabla_{w_{y_i}} L_i = - \left(\sum_{j \neq y_i} \mathcal{I}(w_j^T x_i - w_{y_i}^T x_i + \Delta > 0) \right) x_i$$

Number of classes that didn't meet the desired margin

$$\nabla_{w_j} L_i = \mathcal{I}(w_j^T x_i - w_{y_i}^T x_i + \Delta > 0) x_i$$

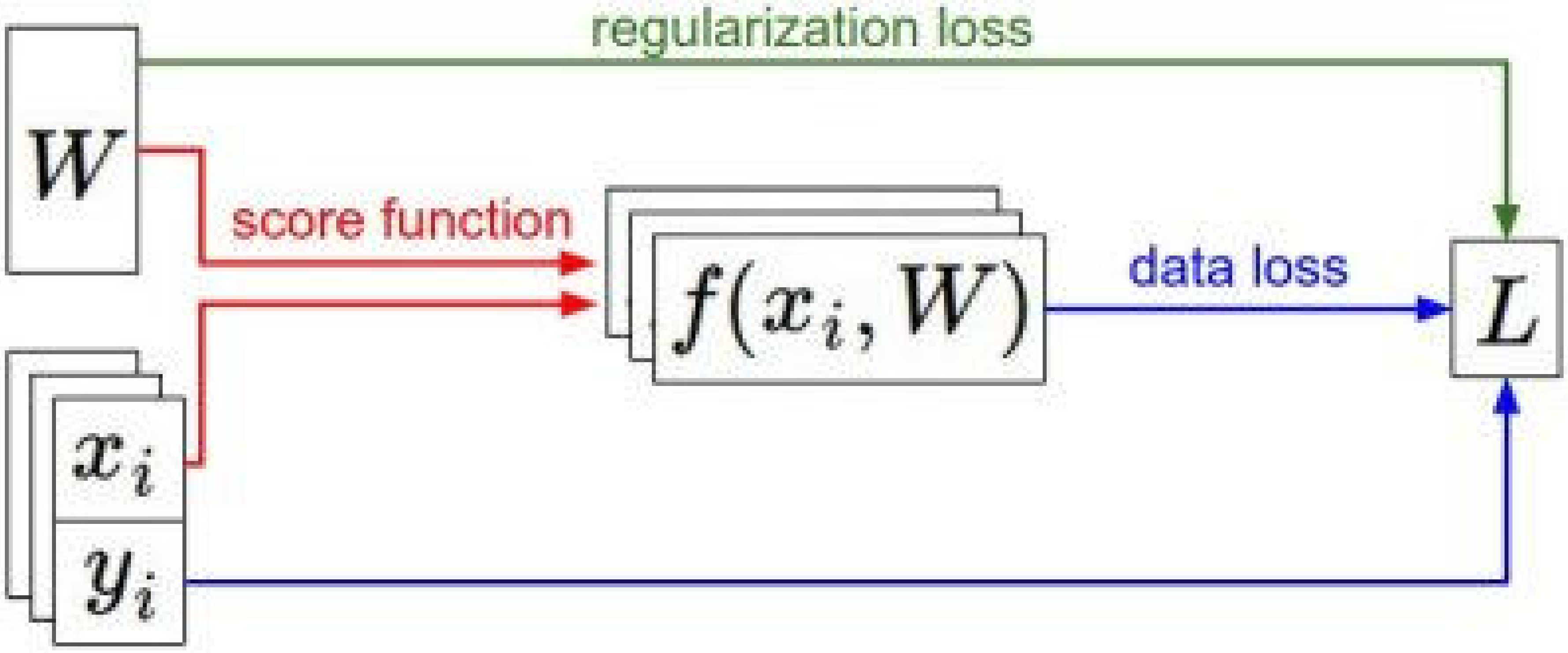
j-th class didn't meet the desired margin

Review derivatives

- Please review rules for computing derivatives and partial derivatives of functions, including the chain rule
  - https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives

- You will need to use them in HW1!

Summary



Acknowledgment

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http://cs231n.github.io/ and CMU 11-785