DSC 140B

Representation Learning

Lecture 21 | Part 1

Backpropagation

Gradient of a Network

- We want to compute the gradient $\nabla_{\vec{w}} H$.
  - That is, $\partial H / \partial W_{ij}^{(\ell)}$ and $\partial H / \partial b_i^{(\ell)}$ for all valid i, j, ℓ.
- A network is a composition of functions.
- We'll make good use of the **chain rule**.

Recall: The Chain Rule

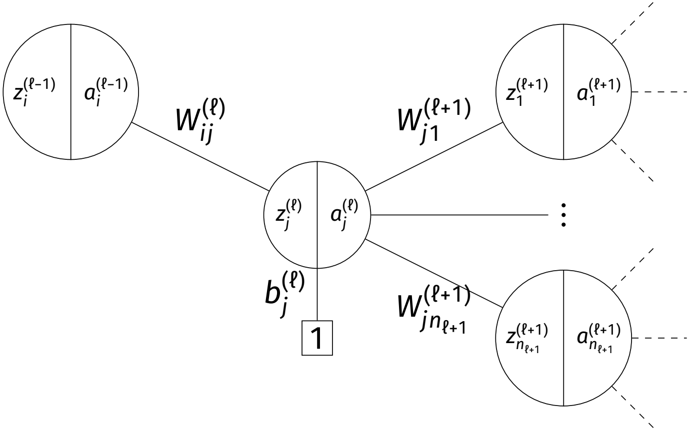
$$\frac{d}{dx} f(g(x)) = \frac{df}{dg}\frac{dg}{dx}$$

$$= f'(g(x))\, g'(x)$$

Some Notation

- We'll consider an arbitrary node in layer ℓ of a neural network.
- Let g be the activation function.
- n_ℓ denotes the number of nodes in layer ℓ.

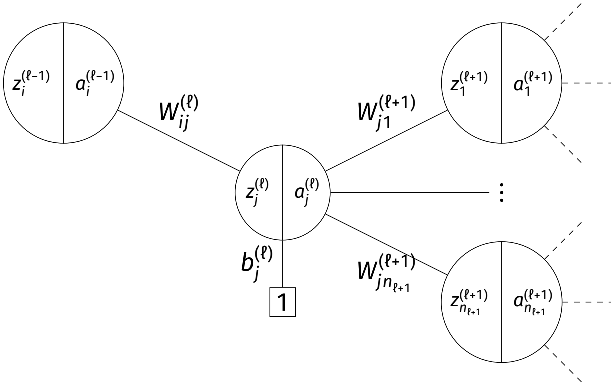
Arbitrary Node



- $\dfrac{\partial H}{\partial W_{ij}^{(\ell)}}$?
- $\dfrac{\partial H}{\partial b_j^{(\ell)}}$?

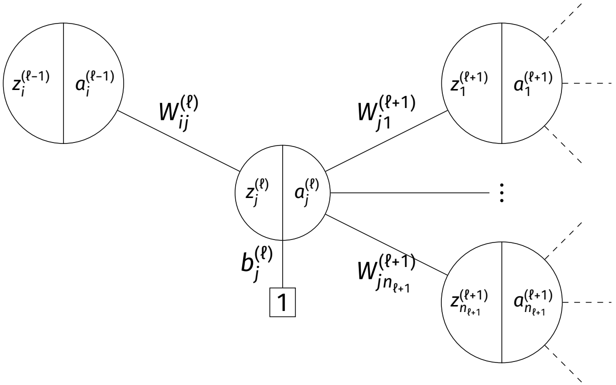
Claim #1

$$\frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$$



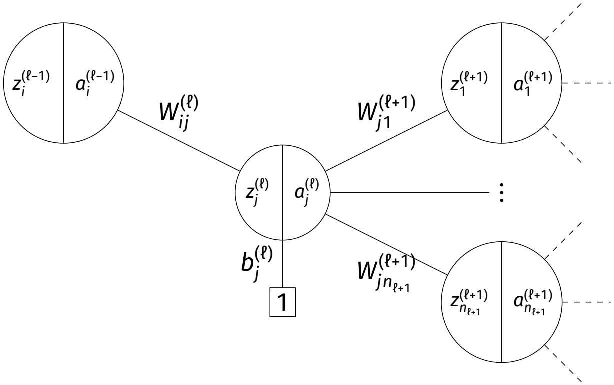
Claim #2

$$\frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell})$$



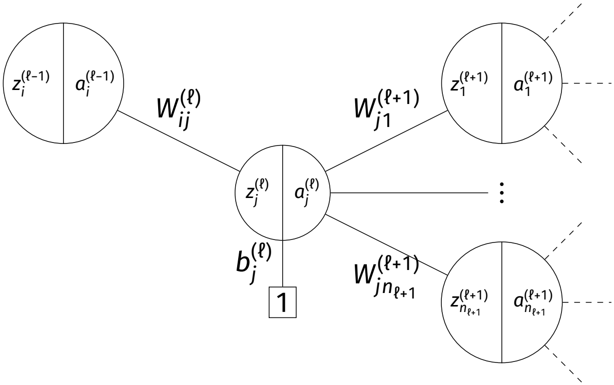
Claim #3

$$\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)}$$



Exercise

What is $\partial H / \partial b_j^{(\ell)}$?



General Formulas

- For any node in any neural network[1], we have the following recursive formulas:
  - $\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)}$
  - $\frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell})$
  - $\frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$
  - $\frac{\partial H}{\partial b_j^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}}$

[1] Fully-connected, feedforward network

Main Idea

The derivatives in layer ℓ depend on derivatives in layer $\ell + 1$.

Backpropagation

- **Idea:** compute the derivatives in last layers, first.
- That is:
  - Compute derivatives in last layer, ℓ; store them.
  - Use to compute derivatives in layer $\ell - 1$.
  - Use to compute derivatives in layer $\ell - 2$.
  - ...

Backpropagation

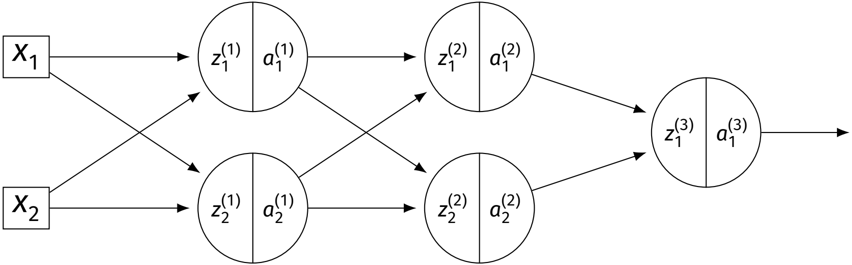
Given an input $\vec{x}$ and a current parameter vector $\vec{w}$:

1. Evaluate the network to compute $z_i^{(\ell)}$ and $a_i^{(\ell)}$ for all nodes.
2. For each layer ℓ from last to first:
   - Compute $\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)}$
   - Compute $\frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell})$
   - Compute $\frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$
   - Compute $\frac{\partial H}{\partial b_j^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}}$

Example

Compute the entries of the gradient given:

$$W^{(1)} = \begin{pmatrix} 2 & -3 \\ 2 & 1 \end{pmatrix} \quad W^{(2)} = \begin{pmatrix} 2 & 1 \\ 0 & 1 \end{pmatrix} \quad W^{(3)} = \begin{pmatrix} 3 \\ -2 \end{pmatrix} \quad \vec{x} = (2, 1)^T \quad g(z) = \text{ReLU}$$

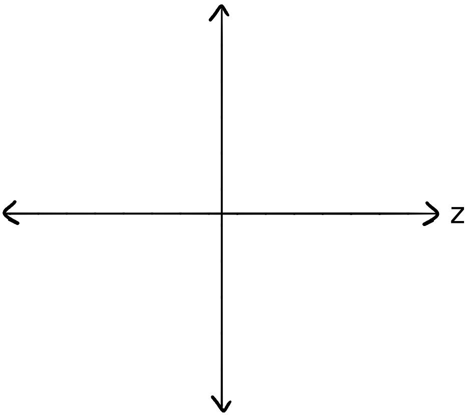


$$\frac{\partial H}{\partial a_j^{(\ell)}} = \sum_{k=1}^{n_{\ell+1}} \frac{\partial H}{\partial z_k^{(\ell+1)}} W_{jk}^{(\ell+1)} \qquad \frac{\partial H}{\partial z_j^{(\ell)}} = \frac{\partial H}{\partial a_j^{(\ell)}} g'(z_j^{\ell}) \qquad \frac{\partial H}{\partial W_{ij}^{(\ell)}} = \frac{\partial H}{\partial z_j^{(\ell)}} a_i^{(\ell-1)}$$

Aside: Derivative of ReLU

$$g(z) = \max\{0, z\}$$

$$g'(z) = \begin{cases} 0, & z < 0 \\ 1, & z > 0 \end{cases}$$



Summary: Backprop

- **Backprop** is an algorithm for efficiently computing the gradient of a neural network

- It is not an algorithm **you** need to carry out by hand: your NN library can do it for you.

DSC 140B
Representation Learning

Lecture 21 | Part 2

Gradient Descent for NN Training

Empirical Risk Minimization

0. Collect a training set, $\{(\vec{x}^{(i)}, y_i)\}$
1. Pick the form of the prediction function, H.
   - E.g., a neural network, H.
2. Pick a loss function.
3. Minimize the empirical risk w.r.t. that loss.

Minimizing Risk

- To minimize risk, we often use **vector calculus**.
  - Either set $\nabla_{\vec{w}} R(\vec{w}) = 0$ and solve...
  - Or use gradient descent: walk in opposite direction of $\nabla_{\vec{w}} R(\vec{w})$.

- Recall, $\nabla_{\vec{w}} R(\vec{w}) = (\partial R / \partial w_0, \partial R / \partial w_1, \ldots, \partial R / \partial w_d)^T$

In General

- Let ℓ be the loss function, let $H(\vec{x}; \vec{w})$ be the prediction function.

- The empirical risk:

$$R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- Using the chain rule:

$$\nabla_{\vec{w}} R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial \ell}{\partial H} \nabla_{\vec{w}} H(\vec{x}^{(i)}; \vec{w})$$

Training Neural Networks

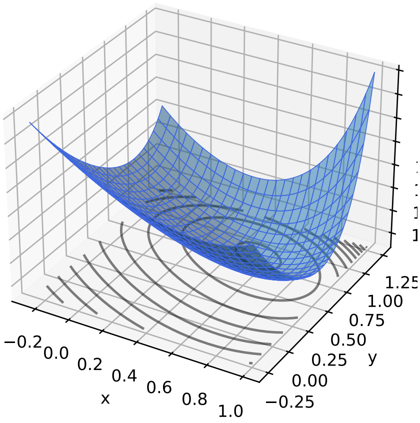
- For neural networks with nonlinear activations, the risk $R(\vec{w})$ is typically **complicated.**
- The mininimizer cannot be found directly.
- Instead, we use iterative methods, such as **gradient descent**.

Iterative Optimization

- To minimize a function $f(\vec{x})$, we may try to compute $\vec{\nabla} f(\vec{x})$; set to 0; solve.
- Often, there is **no closed-form solution**.
- How do we minimize f?

Example

- Consider $f(x, y) = e^{x^2+y^2} + (x-2)^2 + (y-3)^2$.



Example

- Try solving $\vec{\nabla} f(x, y) = 0$.

- The gradient is:

$$\vec{\nabla} f(x, y) = \begin{pmatrix} 2xe^{x^2+y^2} + 2(x-2) \\ 2ye^{x^2+y^2} + 2(y-3) \end{pmatrix}$$

- Can we solve the system?

$$2xe^{x^2+y^2} + 2(x-2) = 0$$
$$2ye^{x^2+y^2} + 2(y-3) = 0$$

Example

- Try solving $\vec{\nabla} f(x, y) = 0$.
- The gradient is:

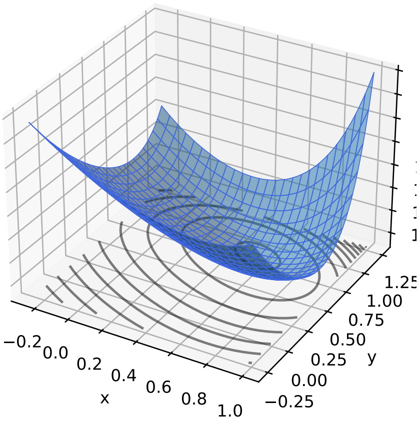
$$\vec{\nabla} f(x, y) = \begin{pmatrix} 2xe^{x^2+y^2} + 2(x-2) \\ 2ye^{x^2+y^2} + 2(y-3) \end{pmatrix}$$

- Can we solve the system? **Not in closed form.**

$$2xe^{x^2+y^2} + 2(x-2) = 0$$
$$2ye^{x^2+y^2} + 2(y-3) = 0$$

Idea

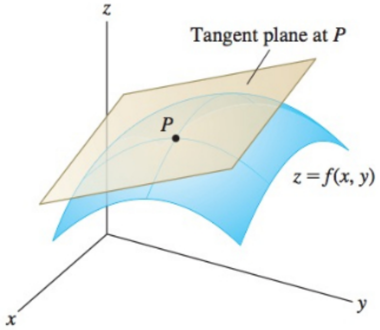
- Apply an iterative approach.
- Start at an arbitrary location.
- “Walk downhill”, towards minimum.



Which way is down?

- Consider a differentiable function $f(x, y)$.
- We are standing at $P = (x_0, y_0)$.
- In a small region around P, f looks like a plane.
- Slope of plane in x, y directions:

$$\frac{\partial f}{\partial x}(x_0, y_0) \quad \frac{\partial f}{\partial y}(x_0, y_0)$$



The Gradient

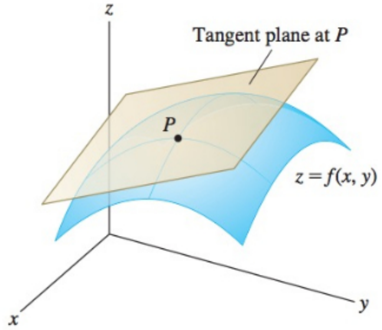
- Let $f : \mathbb{R}^d \to \mathbb{R}$ be differentiable. The **gradient** of f at $\vec{x}$ is defined:

$$\vec{\nabla} f(\vec{x}) = \left(\frac{\partial f}{\partial x_1}(\vec{x}), \frac{\partial f}{\partial x_2}(\vec{x}), \ldots, \frac{\partial f}{\partial x_d}(\vec{x}) \right)^T$$

- **Note:** $\vec{\nabla} f(\vec{x})$ is a **function** mapping $\mathbb{R}^d \to \mathbb{R}^d$.

Which way is down?

- $\vec{\nabla} f(x_0, y_0)$ points in direction of steepest **ascent** at (x_0, y_0).
- $-\vec{\nabla} f(x_0, y_0)$ points in direction of steepest **descent** at (x_0, y_0).



Gradient Properties

- The gradient is used in the linear approximation of f:

$$f(x_0 + \delta_x, y_0 + \delta_y) \approx f(x_0, y_0) + \vec{\delta} \cdot \vec{\nabla} f(x_0, y_0)$$

- Important properties:
  - $\vec{\nabla} f(\vec{x})$ points in direction of **steepest ascent** at $\vec{x}$.
  - $-\vec{\nabla} f(\vec{x})$ points in direction of **steepest descent** at $\vec{x}$.
  - In directions orthogonal to $\vec{\nabla} f(\vec{x})$, f does not change!
  - $\|\vec{\nabla} f(\vec{x})\|$ measures steepness of ascent

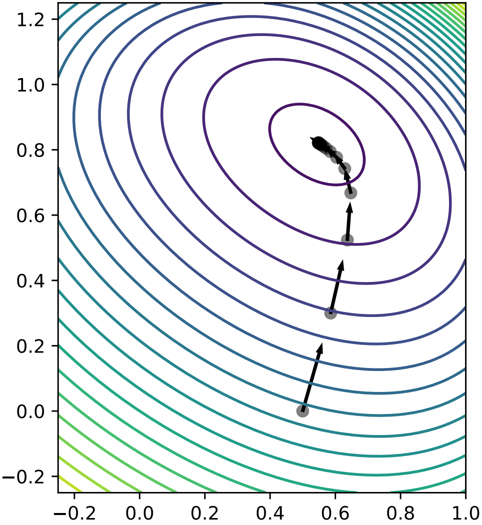
Gradient Descent

- Pick arbitrary starting point $\vec{x}^{(0)}$, **learning rate** parameter $\eta > 0$.

- Until convergence, repeat:
  - Compute gradient of f at $\vec{x}^{(i)}$; that is, compute $\vec{\nabla} f(\vec{x}^{(i)})$.
  - Update $\vec{x}^{(i+1)} = \vec{x}^{(i)} - \eta \vec{\nabla} f(\vec{x}^{(i)})$.

- When do we stop?
  - When difference between $\vec{x}^{(i)}$ and $\vec{x}^{(i+1)}$ is negligible.
  - I.e., when $\|\vec{x}^{(i)} - \vec{x}^{(i+1)}\|$ is small.

```python
def gradient_descent(
        gradient, x, learning_rate=.01,
        threshold=.1e-4
):
    while True:
        x_new = x - learning_rate * gradient(x)
        if np.linalg.norm(x - x_new) < threshold:
            break
        x = x_new
    return x
```


1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.2
0.0
0.2
0.4
0.6
0.8
1.0

Backprop Revisited

- The weights of a neural network can be trained using **gradient descent**.
- This requires the gradient to be calculated repeatedly; this is where **backprop** enters.
- Sometimes people use “backprop” to mean “backprop + SGD”, but this is not strictly correct.

Backprop Revisited

- Consider training a NN using the square loss:

$$
\begin{aligned}
\nabla_{\vec{w}} R(\vec{w}) &= \frac{1}{n} \sum_{i=1}^{n} \frac{\partial \ell}{\partial H} \nabla_{\vec{w}} H(\vec{x}^{(i)}; \vec{w}) \\
&= \frac{2}{n} \sum_{i=1}^{n} (H(\vec{x}^{(i)}) - y_i) \nabla_{\vec{w}} H(\vec{x}^{(i)}; \vec{w})
\end{aligned}
$$

Backprop Revisited

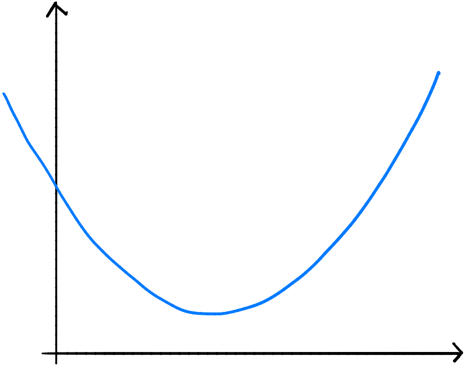
- Interpretation:

$$\nabla_{\vec{w}} R(\vec{w}) = \frac{2}{n} \sum_{i=1}^{n} \underbrace{\left(H(\vec{x}^{(i)}) - y_i\right)}_{\text{Error}} \underbrace{\nabla_{\vec{w}} H(\vec{x}^{(i)}; \vec{w})}_{\text{Blame}}$$

- When used in SGD, backprop “propagates error backward” in order to update weights.

Difficulty of Training NNs

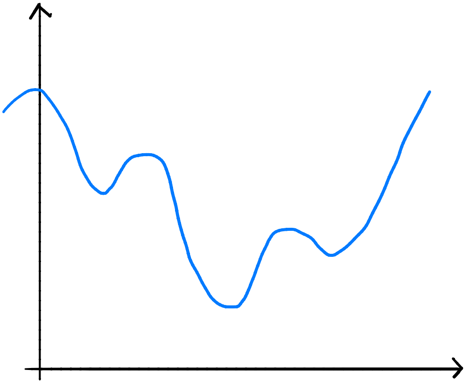
- Gradient descent is guaranteed to find optimum when objective function is **convex**.[2]



[2]Assuming it is properly initialized

Difficulty of Training NNs

- When activations are non-linear, neural network risk is **highly non-convex**:

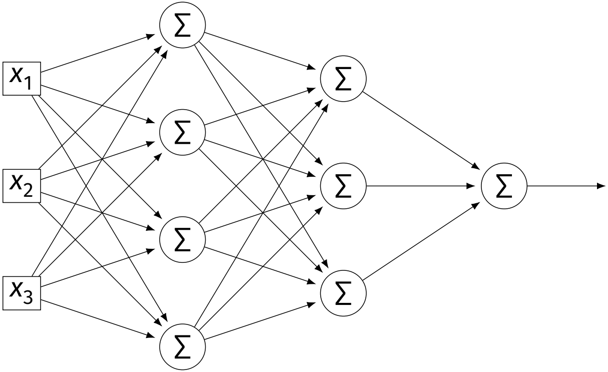


Non-Convexity

- When R is non-convex, GD can get "stuck" in local minima.
  - Solution depends on initialization.
- More sophisticated optimizers, using momentum, adaptation, better initialization, etc.
  - Adagrad, RMSprop, Adam, etc.

Difficulty of Training (Deep) NNs

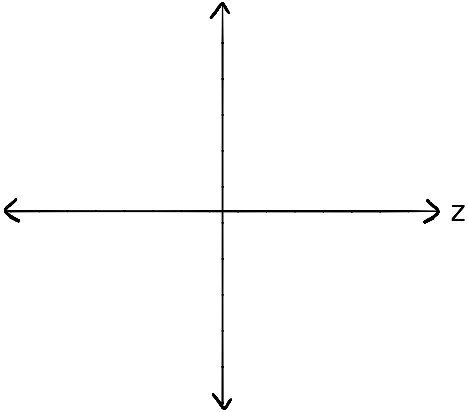
- Deep networks can suffer from the problem of **vanishing gradients**: if w is a weight at the "front" of the network, $\partial H / \partial w$ can be very small



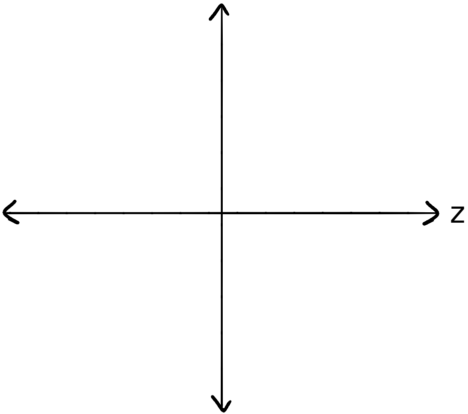
Vanishing Gradients

- If $\partial H / \partial w$ is always close to zero, w is updated **very slowly** by gradient descent.
- In short: early layers are slower to train.
- One mitigation: use ReLU instead of sigmoid.

Vanishing Gradients



Sigmoid



ReLU

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Representation Learning

Lecture 21 | Part 3

Stochastic Gradient Descent

Gradient Descent for Minimizing Risk

- In ML, we often want to minimize a **risk function**:

$$R(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

Observation

- The gradient of the risk function is a sum of gradients:

$$\vec{\nabla} R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \vec{\nabla} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- One term for each point in training data.

Problem

- In machine learning, the number of training points n can be **very large**.
- Computing the gradient can be **expensive** when n is large.
- Therefore, each step of gradient descent can be **expensive**.

Idea

- The (full) gradient of the risk uses all of the training data:

$$\nabla R(\vec{w}) = \frac{1}{n} \sum_{i=1}^{n} \nabla \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- It is an average of n gradients.
- **Idea:** instead of using all n points, randomly choose $\ll n$.

Stochastic Gradient

- Choose a random subset (**mini-batch**) B of the training data.

- Compute a **stochastic gradient**:

$$\nabla R(\vec{w}) \approx \sum_{i \in B} \vec{\nabla} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

Stochastic Gradient

$$\nabla R(\vec{w}) \approx \sum_{i \in B} \vec{\nabla} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

- **Good:** if $|B| \ll n$, this is much faster to compute.
- **Bad:** it is a (random) approximation of the full gradient, noisy.

Stochastic Gradient Descent (SGD) for ERM

- Pick arbitrary starting point $\vec{x}^{(0)}$, **learning rate** parameter $\eta > 0$, batch size $m \ll n$.
- Until convergence, repeat:
  - Randomly sample a batch B of m training data points (on each iteration).
  - Compute stochastic gradient of f at $\vec{x}^{(i)}$:

$$\vec{g} = \sum_{i \in B} \vec{\nabla} \ell(H(\vec{x}^{(i)}; \vec{w}), y_i)$$

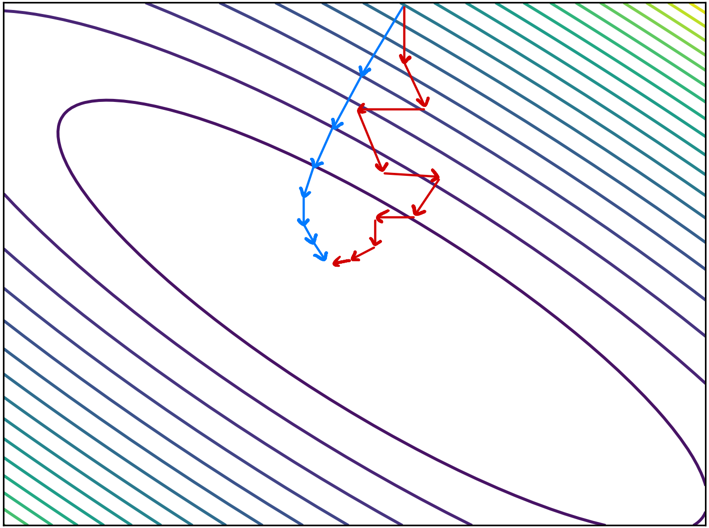
  - Update $\vec{x}^{(i+1)} = \vec{x}^{(i)} - \eta \vec{g}$

Idea

- In practice, a stochastic gradient often works well enough.
- It is better to take many noisy steps quickly than few exact steps slowly.

Batch Size

- Batch size m is a parameter of the algorithm.
- The larger m, the more reliable the stochastic gradient, but the more time it takes to compute.
- Extreme case when $m = 1$ will still work.



Usefulness of SGD

- SGD allows learning on **massive** data sets.
- Useful even when exact solutions available.
  - E.g., least squares regression / classification.

Training NNs in Practice

- There are several Python packages for training NNs:
  - PyTorch
  - Tensorflow / Keras

- This week’s discussion was a Tensorflow tutorial.