

**10707**

# **Deep Learning: Spring 2020**

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Lecture 5: Intro to  
optimization

# Supervised learning

**Empirical risk minimization approach:**  
minimize a **training** loss  $l$  over a class of **predictors**  $\mathcal{F}$ :

$$\hat{f} = \operatorname{argmin}_{f \in \mathcal{F}} \sum_{(x,y): \text{training samples}} l(f(x), y)$$

## Three pillars:

(1) How expressive is the class  $\mathcal{F}$ ? (**Representational power**)

(2) How do we minimize the training loss efficiently? (**Optimization**)

(3) How does  $\hat{f}$  perform on unseen samples? (**Generalization**)

# The world of continuous optimization

The typical training task in ML can be cast as:  $\min_{x \in \mathbb{R}^d} f(x)$

Usually, it is cheap to calculate  $f(x)$ ,  $\nabla f(x)$ , but (more) expensive to calculate higher-order derivatives.

Most algorithms we will look at are iterative: they progressively pick points  $x_1, x_2, \dots$  that are supposed to bring “improvement”.

Non-exhaustive coverage: entire field of optimization, with applications vastly beyond ML. We focus on deep-learning-relevant methods.

# The mother of all optimization algorithms: gradient descent

The simplest optimization algorithm: **Taylor expand** and find the direction of “**steepest**” descent. More precisely:

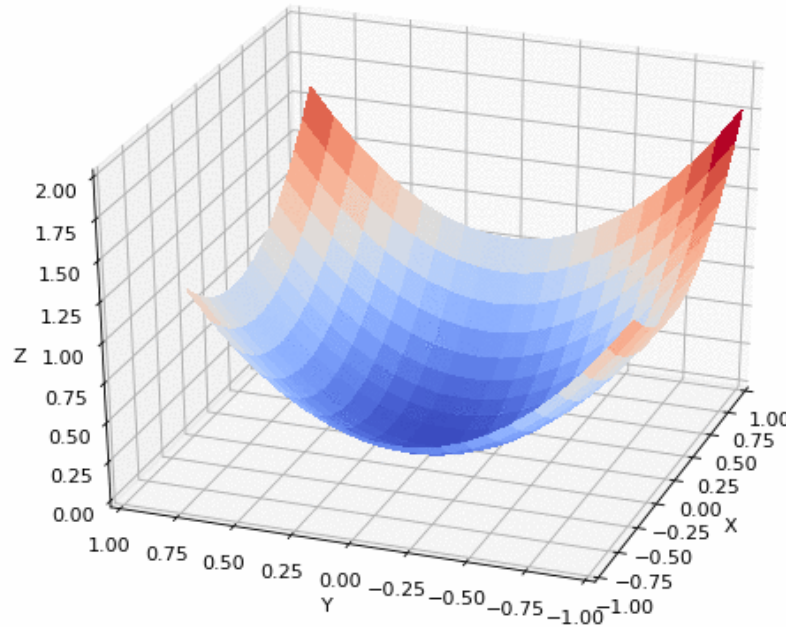
By Taylor’s theorem, we have  $f(x + \Delta) \approx f(x) + \Delta^T \nabla f(x) + O(||\Delta||^2)$

So, if we ignore higher-order effects, we have

$$\operatorname{argmin}_{\Delta, ||\Delta|| \leq \epsilon} \{ f(x + \Delta) - f(x) \} = -\epsilon \frac{\nabla f(x)}{||\nabla f(x)||}$$

i.e. we should move (appropriately scaled) opposite of the gradient

# Gradient descent, pictorially

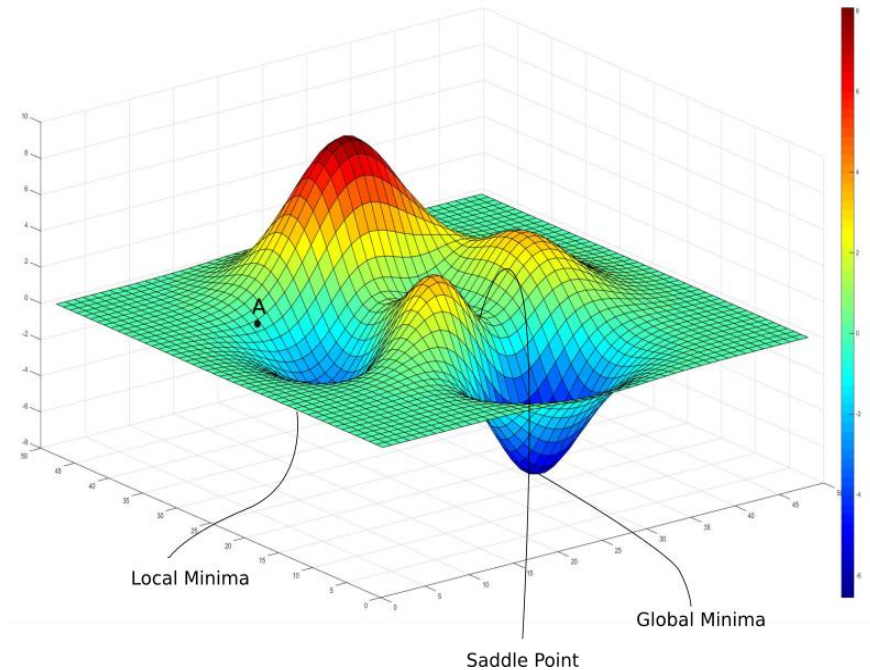


What can we hope for, in the case that  $||\Delta|| \rightarrow 0$ ?

We stop moving when  $\nabla f(\hat{x}) \approx 0$ : these are called **stationary points**.

**What kinds of stationary points are there?**

# Types of stationary points



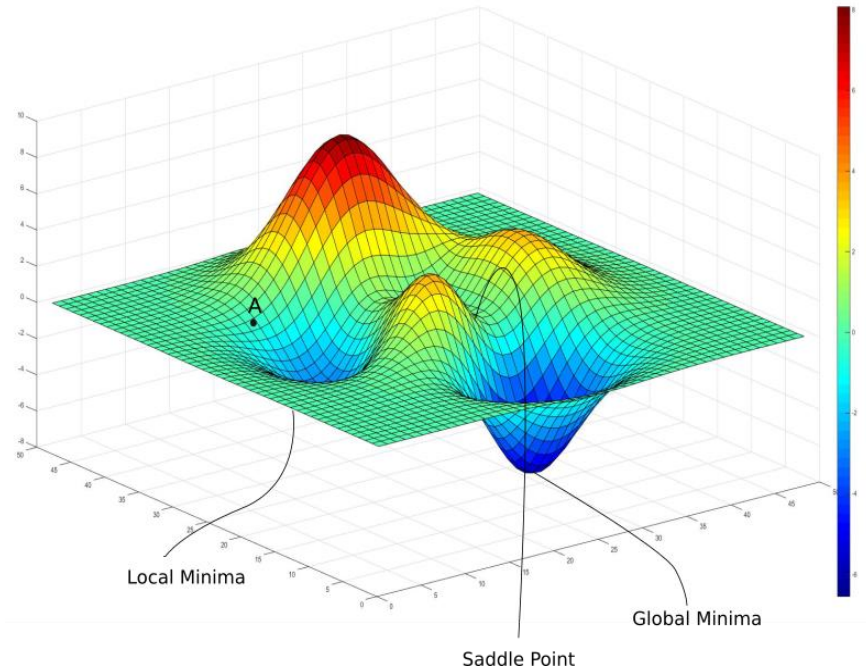
**Global minimum:** actual minimizer, namely  $f(\hat{x}) \leq f(x), \forall x \in \mathbb{R}^d$

**Local minimum:**  $f(\hat{x}) \leq f(x), \forall x$  s. t.  $\|x - \hat{x}\| \leq \epsilon$  for some  $\epsilon > 0$

**Local maximum:**  $f(\hat{x}) \geq f(x), \forall x$  s. t.  $\|x - \hat{x}\| \leq \epsilon$  for some  $\epsilon > 0$

**Saddle points:** stationary point that is \*not\* a local min/max.

# Types of stationary points



**Global minimum:** finding these in general is very hard (both in theory – NP-hard, as well as in practice)

**Local minimum:** seem to work quite well often. Some theoretical understanding of why in very restricted cases.

**Saddle points:** typically bad, arise from invariances in input. Want to avoid these. (Stay tuned.)

# Checking for local minima?

**Second order checks:** Hessian approximates a function to second order

**Taylor's thm:**  $f(x + \Delta) \approx f(x) + \Delta^T \nabla f(x) + \frac{1}{2} \Delta^T \nabla^2 f(x) \Delta + O(\|\Delta\|^3)$

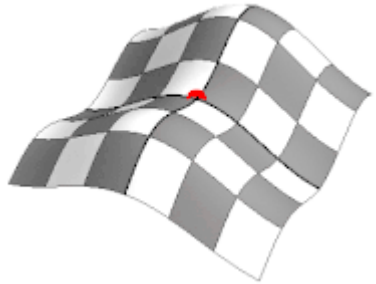
$$\approx f(x) + \frac{1}{2} \Delta^T \nabla^2 f(x) \Delta + O(\|\Delta\|^3)$$



If  $\nabla^2 f(x) \succ 0$ : for any direction  $\Delta$ , and small enough  $\|\Delta\|$

$$\Delta^T \nabla^2 f(x) \Delta + O(\|\Delta\|^3) \geq 0, \text{ so } f(x + \Delta) > f(x)$$

**Local minimum!** (Flipped for local maximum)



If  $\nabla^2 f(x)$  has both positive and negative eigenvalues:

**Saddle point** (not a local minimum/maximum)

**If neither of these attains, test is inconclusive!**



# The descent lemma: analyzing gradient descent

So far, we've only considered the limit  $||\Delta|| \rightarrow 0$ .

If  $||\Delta||$  is too large, the Taylor expansion will be invalid (and gradient descent can “jump over” local minima).

If  $||\Delta||$  is too small, the runtime of the algorithm will suffer.  
The descent lemma characterizes the “sweet spot”:

**Theorem (descent lemma):** Let  $f$  be twice differentiable, and  $||\nabla^2 f(x)||_2 \leq \beta$ . Then, setting  $\eta = 1/\beta$ , and calling  $x_t$  the iterates of gradient descent, namely  $x_{t+1} = x_t - \eta \nabla f(x_t)$ , we have:

$$f(x_t) - f(x_{t+1}) \geq \frac{1}{2\beta} ||\nabla f(x_t)||_2^2$$

# Using the descent lemma: Lyapunov functions

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Suppose  $f$  is lower bounded (e.g.  $f \geq 0$ ), and  $f(x_0) \leq M$

Suppose we want point  $x_t$ , s.t.  $\|\nabla f(x_t)\| \leq \epsilon$ .

**Lyapunov (potential) fn argument:** suppose  $\forall t \in [0, T], \|\nabla f(x_t)\| \geq \epsilon$

Then,  $f(x_T) \leq f(x_0) - T \frac{1}{2\beta} \epsilon^2 \leq M - T \frac{1}{2\beta} \epsilon^2$ . Also,  $f(x_T) \geq 0$ .

Putting these together, we get  $T \leq 2 M \beta / \epsilon^2$

# Proving the Descent Lemma

**Theorem (descent lemma):** Let  $f$  be twice differentiable, and  $\|\nabla^2 f(x)\|_2 \leq \beta$ . Then, setting  $\eta = 1/\beta$ , and calling  $x_t$  the iterates of gradient descent, we have:

$$f(x_t) - f(x_{t+1}) \geq \frac{1}{2\beta} \|\nabla f(x_t)\|_2^2$$

**Proof:** By Taylor expansion and the mean value theorem, we have

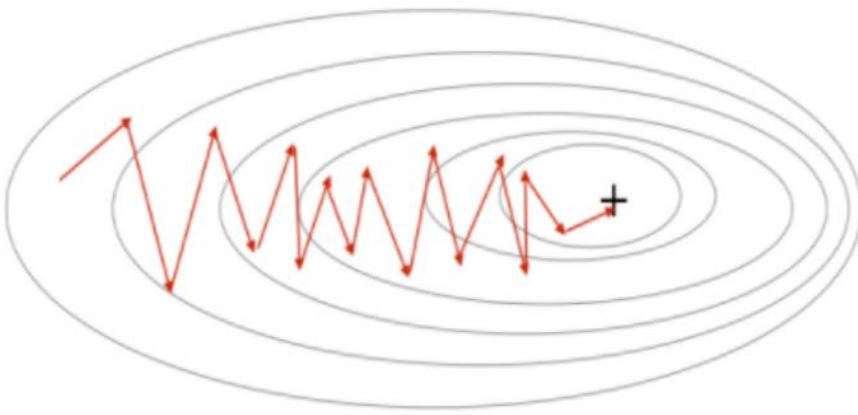
$$f(x + \Delta) = f(x) + \Delta^T \nabla f(x) + \frac{1}{2} \Delta^T \nabla^2 f(y) \Delta$$

Moreover,  $\Delta^T \nabla^2 f(y) \Delta \leq \|\nabla^2 f(y)\|_2 \|\Delta\|_2^2 \leq \beta \|\Delta\|_2^2$ . Plugging in  $\Delta = -\eta \nabla f(x_t)$ :

$$\begin{aligned} f(x_{t+1}) &\leq f(x_t) - \eta \|\nabla f(x_t)\|_2^2 + \frac{1}{2} \beta \eta^2 \|\nabla f(x_t)\|_2^2 \\ &= f(x_t) - 1/\beta \|\nabla f(x_t)\|_2^2 + \frac{1}{2} 1/\beta \|\nabla f(x_t)\|_2^2 \\ &= f(x_t) - 1/2\beta \|\nabla f(x_t)\|_2^2 \end{aligned}$$

# Understanding gradient descent locally

Let's consider  $f$ 's that are quadratic. (Close to local minima, this will be “true” due to Taylor). What quadratics are bad/good for gradient descent?



**Bad behavior:** gradients don't point towards minimizer – a lot of zig-zaging until we reach minimizer.

**Intuitively:** ellipsoidal contours (level sets) should be worse than spherical level sets.

**Question:** Let  $f(x) = \frac{1}{2}x^T A x$ , can we characterize convergence time of gradient descent more precisely? What does it depend on?

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**Thm:** Let  $A$  be a symmetric positive-definite matrix with minimum and maximum eigenvalues  $\lambda_{\min}$  and  $\lambda_{\max}$  and denote  $\kappa = \lambda_{\max} / \lambda_{\min}$  (**condition number**).

The iterates of gradient descent with  $\eta = \frac{2}{\lambda_{\max} + \lambda_{\min}}$  satisfy:

$$\|x_t\| \leq \left( \frac{\kappa - 1}{\kappa + 1} \right)^t \|x_0\|$$

$= \|x_t - 0\|$ , i.e. distance from optimum

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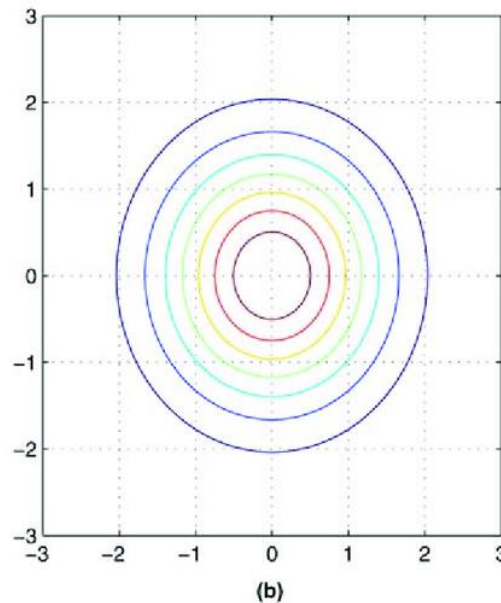
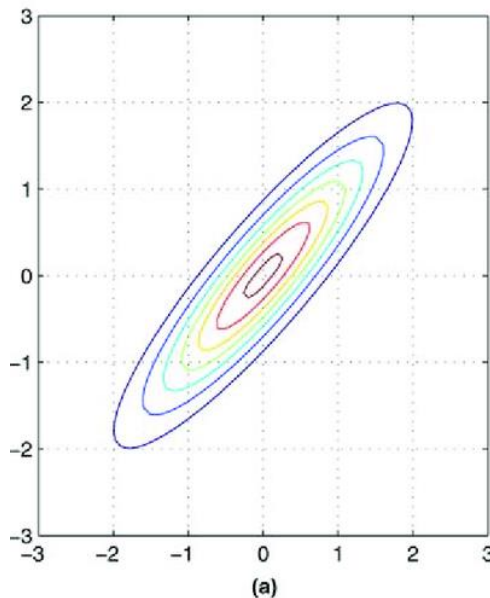
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$$\begin{aligned} \|x_t\| &\leq \left( \frac{\kappa - 1}{\kappa + 1} \right)^t \|x_0\| \\ &= \left( 1 - \frac{2}{\kappa + 1} \right)^t \|x_0\| \end{aligned}$$



*$\kappa$  large  $\Rightarrow$  slower convergence*



# Understanding gradient descent locally

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$$||x_t|| \leq \left( \frac{\kappa - 1}{\kappa + 1} \right)^t ||x_0||$$

**Proof:**

$$\begin{aligned} ||x_{t+1}|| &= ||x_t - \eta \nabla f(x_t)|| \\ &= ||x_t - \eta A x_t|| = ||(I - \eta A)x_t|| \leq ||I - \eta A||_2 ||x_t||_2 \\ &\leq \max(|1 - \eta \lambda_{\max}|, |1 - \eta \lambda_{\min}|) ||x_t||_2 \\ &= \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} ||x_t||_2 = \frac{\kappa - 1}{\kappa + 1} ||x_t||_2 \end{aligned}$$

# Fixes to the conditioning problem

What can we do for poorly conditioned problems?

Quadratic problem suggests solution: we can solve it in closed form!!

If  $f(x) = \frac{1}{2}x^T A x + b^T x + c$ , minimizer is  $A^{-1}b$ . (Just take derivatives, set to 0.)

What do we do for arbitrary  $f$ ? Approximate function to second order!!

By Taylor's thm:  $f(x + \Delta) \approx f(x) + \Delta^T \nabla f(x) + \frac{1}{2} \Delta^T \nabla^2 f(x) \Delta + O(\|\Delta\|^3)$

Ignoring 3<sup>rd</sup> and higher order terms, and using the above observation for quadratics:

$$\text{Set } x_{t+1} = x_t - \eta (\nabla^2 f(x_t))^{-1} \nabla f(x_t)$$

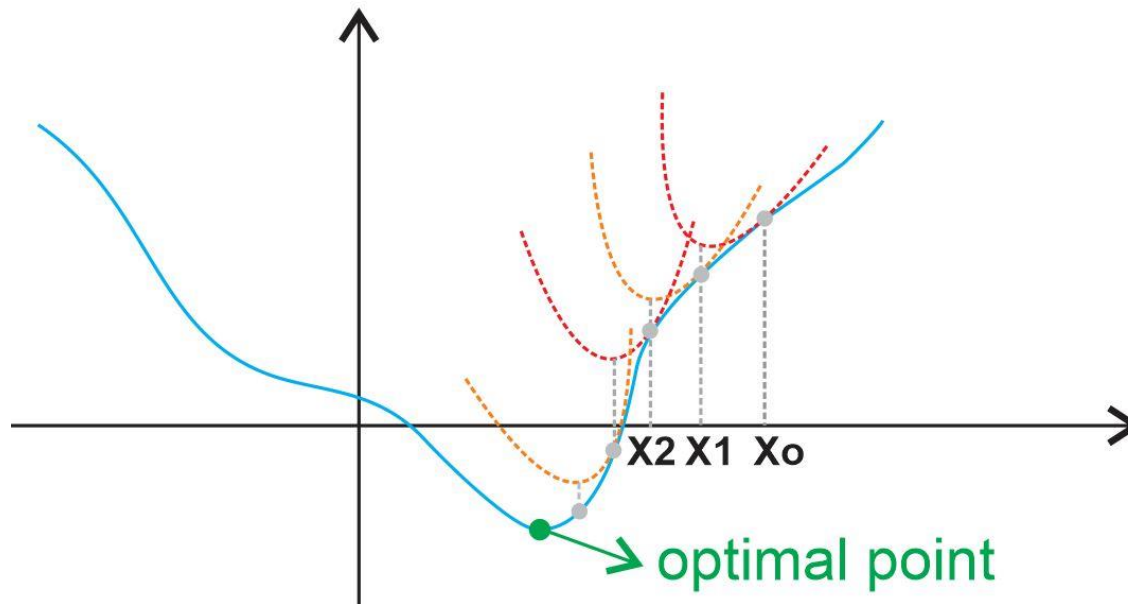
**Newton's method.**



# Fixes to the conditioning problem

$$\text{Set } x_{t+1} = x_t - \eta (\nabla^2 f(x_t))^{-1} \nabla f(x_t)$$

Newton's method.




**Problem:** need to invert a  $d \times d$  matrix  $\Rightarrow d^3$  runtime. Way too expensive.

# Momentum (Polyak '64)

**Alternative fix:** instead of using the gradient at the current step, use a linear combination of the gradients at prior steps. “Smooths” out zig-zagging, but not relying too much on current gradient.

*Linear combination of  
prior gradients + current one*


$$\begin{aligned}v_{t+1} &= -\nabla f(x_t) + \beta v_t \\x_{t+1} &= x_t + \eta v_{t+1}\end{aligned}$$


**Helps provably!** You'll show in homework that for the quadratic case we considered, i.e.  $f(x) = x^T A x$ :

$$\|x_t\| \leq \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^t \|x_0\|$$

# Momentum (Nesterov '83)

**Nesterov acceleration** is a *lookahead* variant of momentum, which has provable benefits for *\*any\** convex function. (And is in a certain precise sense, the optimal first-order optimization algorithm).

*Evaluate gradient at a  
“lookahead” point*


$$\begin{aligned}v_{t+1} &= -\nabla f(x_t + \beta v_t) + \beta v_t \\x_{t+1} &= x_t + \eta v_{t+1}\end{aligned}$$

**Magical!** There's been a mini cottage industry to “explain” Nesterov acceleration.

# Taking gradients of neural networks: backpropagation

The workhorse for training neural networks: an algorithm that for a network with  $V$  nodes and  $E$  edges calculates the gradient in **linear time**  $O(V+E)$ .

The name **backpropagation** was introduced by *Rumelhart, Hinton, Williams* '86, but so natural that it was rediscovered multiple times (as early as 60s). Algorithm seems to first be mentioned in *Werbos*' thesis '74 in the context of neural networks.

In **control theory**: Kelley '60, Bryson '61 [cast as **dynamic programming**];

In **theoretical computer science**: Baur-Strassen lemma '83 [in the context of **algebraic circuits**]

# Taking gradients of neural networks: backpropagation

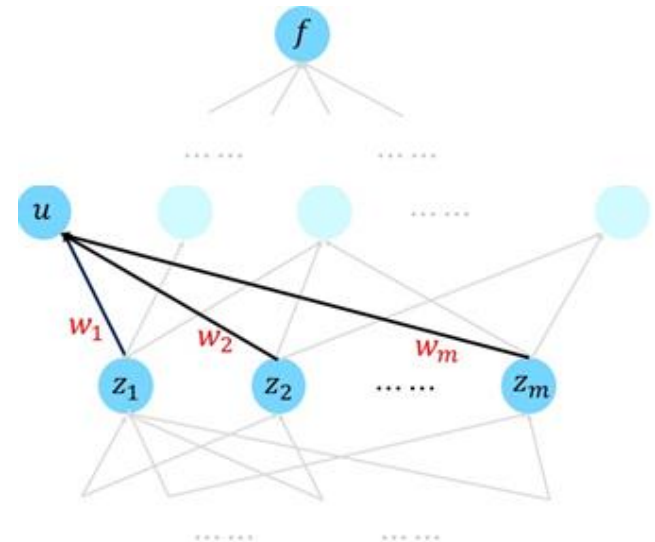
The main tool for deriving backprop: **chain rule**

Suppose  $f(y) = f(x_1(y), x_2(y), \dots, x_n(y))$

$$\text{Then, } \frac{\partial f}{\partial y} = \sum_{i=1}^n \frac{\partial f}{\partial x_i} \frac{\partial x_i}{\partial y}$$

**Observation 1:** It suffices to take derivatives with respect to node functions.

$$\begin{aligned} \frac{\partial f}{\partial w_1} &= \frac{\partial f}{\partial u} \frac{\partial u}{\partial w_1} = \frac{\partial f}{\partial u} \frac{\partial \sigma(\langle w, z \rangle + b)}{\partial w_1} \\ &= \frac{\partial f}{\partial u} \sigma'(u) z_1 \end{aligned}$$



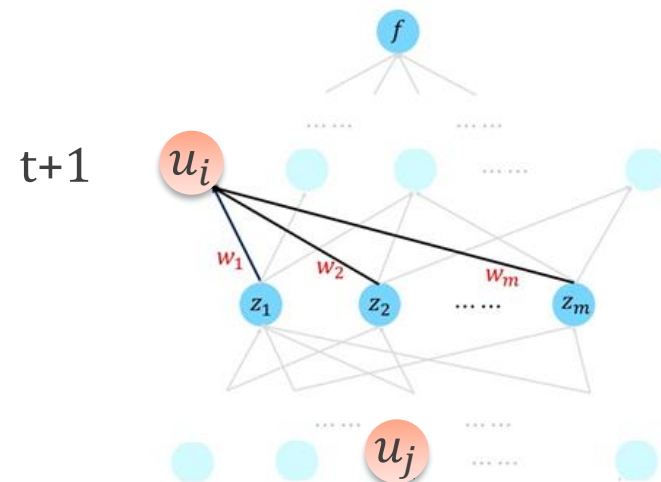
# Taking gradients of neural networks: backpropagation

**Observation 2:** The obvious forward propagation algorithm results in runtime of  $\Omega(V^2)$ . (Bad! We want  $O(V+E)$ )

Obvious algorithm? Calculate inductively  $\frac{\partial u_i}{\partial u_j}$ , for all pairs  $(u_i, u_j)$  where  $u_j$  is lower than  $u_i$  (obviously, this includes  $\frac{\partial f}{\partial u}$  which we want)

$$\frac{\partial u_i}{\partial u_j} = \sum_k \frac{\partial u_i}{\partial z_k} \frac{\partial z_k}{\partial u_j}$$

Easy as in prior slide      Have these by inductive hypothesis.



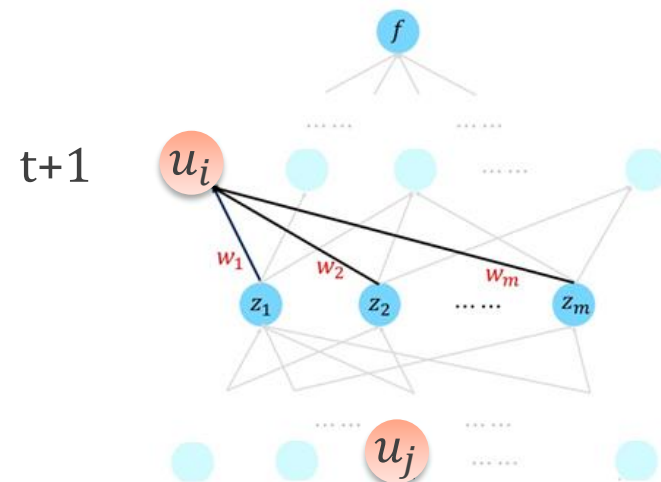
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*Bad – this will end up with  $\Omega(V^2)$  algorithm.*



# Taking gradients of neural networks: backpropagation

**Observation 3:** The better way to do this is in a backward fashion.

**Message passing algorithm [dynamic programming]:** each node  $u$  receives messages (real numbers) from its neighbors on top. Let their sum be  $S$ . The node passes to downward neighbors  $z$ :  $S \frac{\partial u}{\partial z}$ . Proceed from top to down.

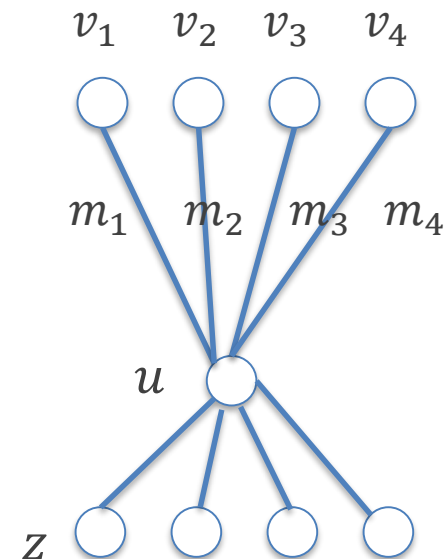
**Claim:** The sum of the messages that each node  $u$  computes  $S$  is equal to  $\frac{\partial f}{\partial u}$ .

**Proof:** By induction.

Suppose  $u$  is at layer  $t$ , and inductive hypothesis holds for layers  $t+1$  and above. Sum of messages to  $u$  satisfies:

$$S = \sum_k m_k = \sum_k \frac{\partial f}{\partial v_i} \frac{\partial v_i}{\partial u} = \frac{\partial f}{\partial u}$$

*Inductive hypothesis*      *Def. of messages*





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**Amount of work:** each node  $u$  needs to sum its upward neighbor messages (at most  $\deg(u)$  of them), and pass a message to its downward neighbors (at most  $\deg(u)$  of them).

Each downward message just takes an extra  $\frac{\partial u}{\partial z}$  calculation (easy const. time), so each node does  $O(\deg(u))$  amount of work.

Hence, **total amount of work** for all nodes is  $O(\sum_u \deg(u)) = O(E)$

**Amount of memory:** for calculating  $\frac{\partial u}{\partial z}$ , we need the activation values of intermediate nodes – so **memory**  $O(V)$ .

[**Important!** If recalculating these, runtime would be quadratic]

