10707
Deep Learning: Spring 2021

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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** $\mathcal{F}$:

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

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: $\min_{x \in \mathbb{R}^d} \quad f(x)$

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 $x_1, x_2, \ldots$ 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:

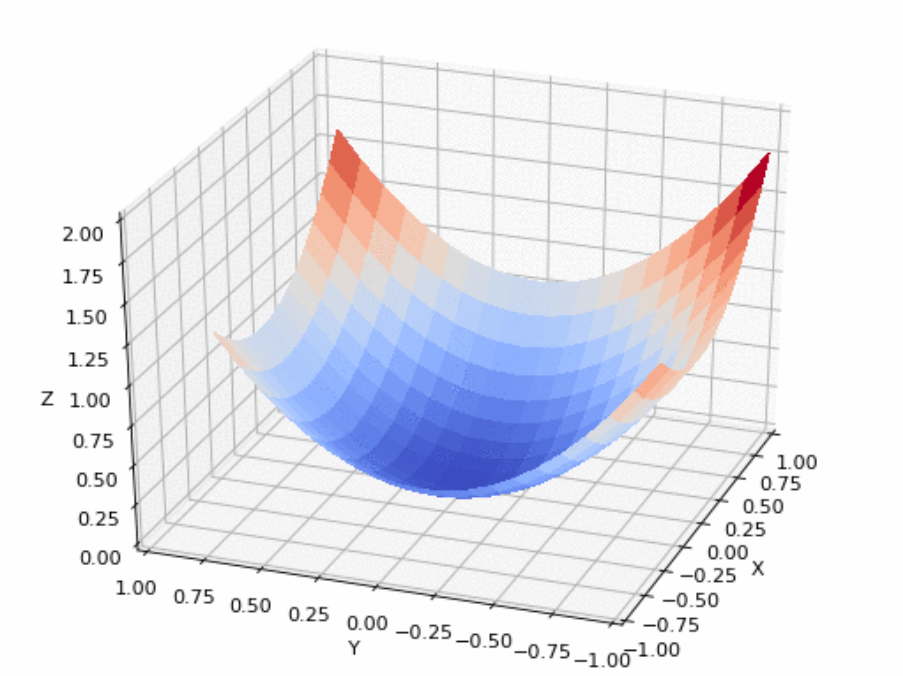
By Taylor's theorem, we have $f(x+\Delta) \approx f(x) + \Delta^T \nabla f(x) + O(||\Delta||^2)$

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

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

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

Gradient descent, pictorially

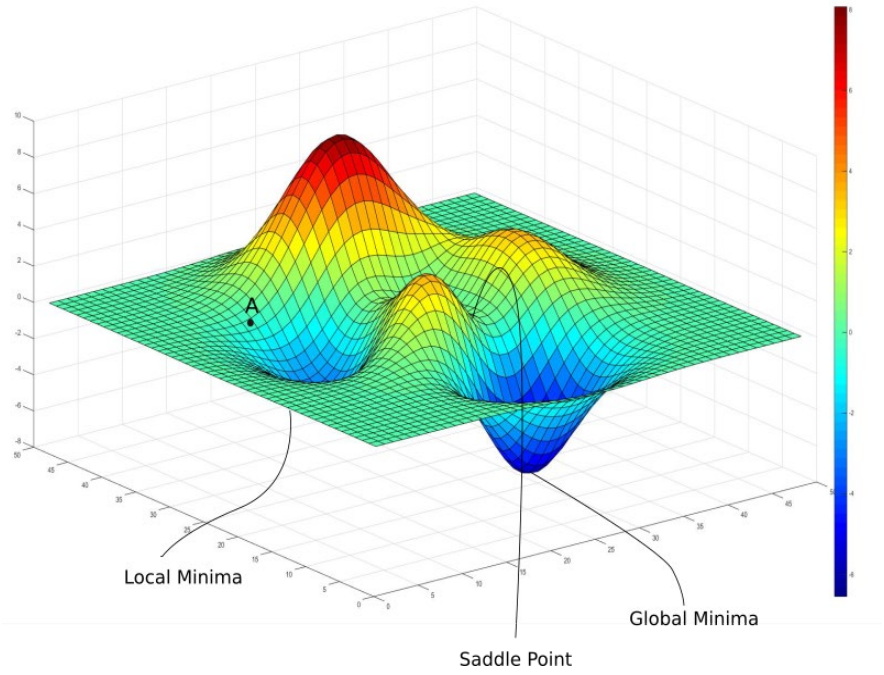


What can we hope for, in the case that $||\Delta|| \to 0$?

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

What kinds of stationary points are there?

Types of stationary points



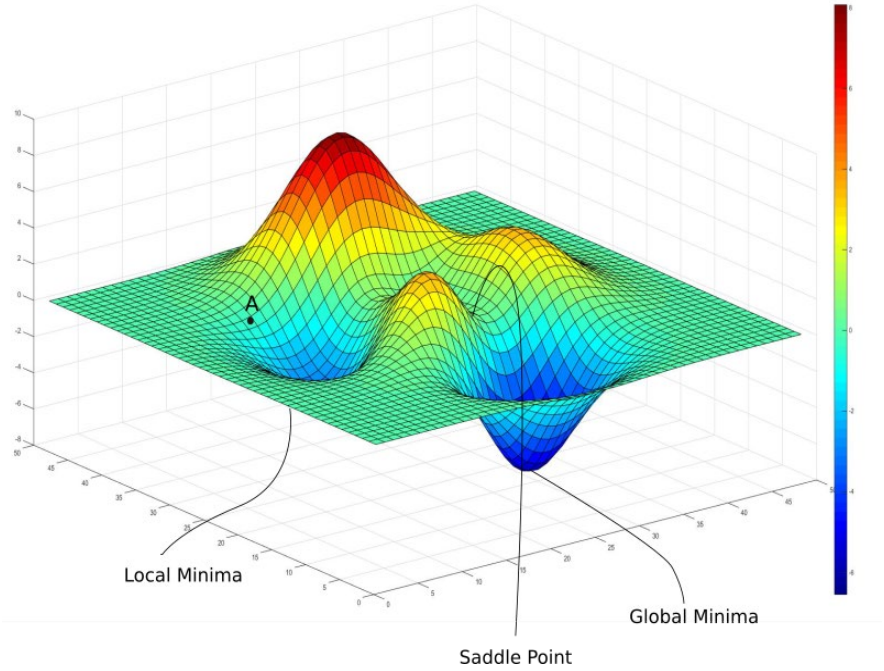
Global minimum: actual minimizer, namely $f(\hat{x}) \leq f(x), \forall x \in \mathbb{R}^d$

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

Local maximum: $f(\hat{x}) \geq f(x),\ \forall x \text{ s.t. } ||x - \hat{x}|| \leq \epsilon$ 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

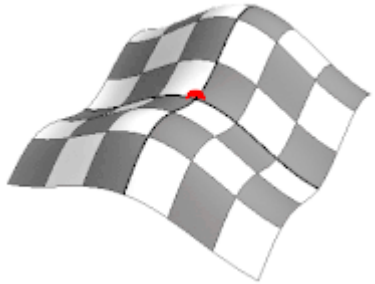
Taylor's thm: $f(x+\Delta) \approx f(x) + \Delta^T \nabla f(x) + \frac{1}{2}\Delta^T \nabla^2 f(x)\Delta + O(||\Delta||^3)$

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

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

$\Delta^T \nabla^2 f(x)\Delta + O(||\Delta||^3) \geq 0$, 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 $||\Delta|| \to 0$.

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:

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

Using the descent lemma: Lyapunov functions

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:

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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. $\big||\nabla f(x_t)\big|| \leq \epsilon$.

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

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 $T \leq 2M\beta/\epsilon^2$

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:

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

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 $\Delta = -\eta \nabla f(x_t)$:

$$f(x_{t+1}) \leq f(x_t) - \eta \big||\nabla f(x_t)|\big|^2 + \frac{1}{2}\beta\eta^2 \big||\nabla f(x_t)|\big|^2$$

$$= f(x_t) - 1/\beta \big||\nabla f(x_t)|\big|^2 + \frac{1}{2} 1/\beta \big||\nabla f(x_t)|\big|^2$$

$$= f(x_t) - 1/2\beta \big||\nabla f(x_t)|\big|^2$$

Choosing a learning rate in practice

The previous lemma was an instance of a **fixed** learning rate ($1/\beta$).
In fact, proof works up to "critical" value of $2/\beta$.

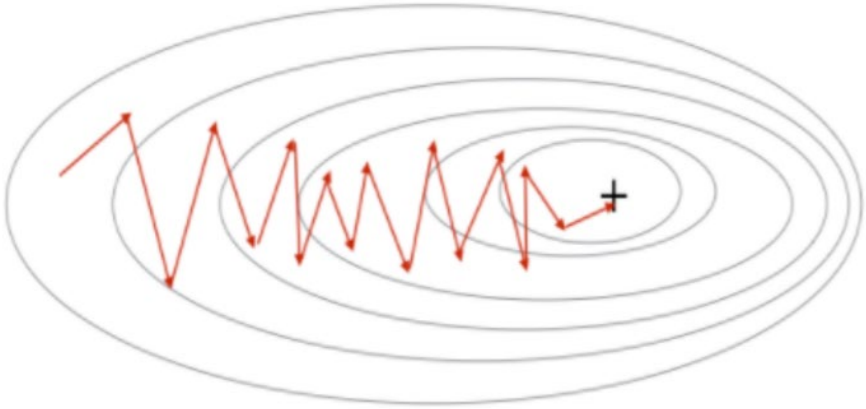
Fixed learning rates are common: typically grid search b/w 10^{-6} and 1.
Pick largest rate for which training doesn't diverge.
Frequently $\sim 10^{-2}$works ok.

Decaying learning schedules are also popular, e.g. : $\eta_t = \dfrac{\eta_0 \tau}{\max(t, \tau)}$

(i.e. set learning rate to η_0 for the first τ iteration, then decay like $1/t$)
Some intuitions for a decaying rate come from standard convex optimization.

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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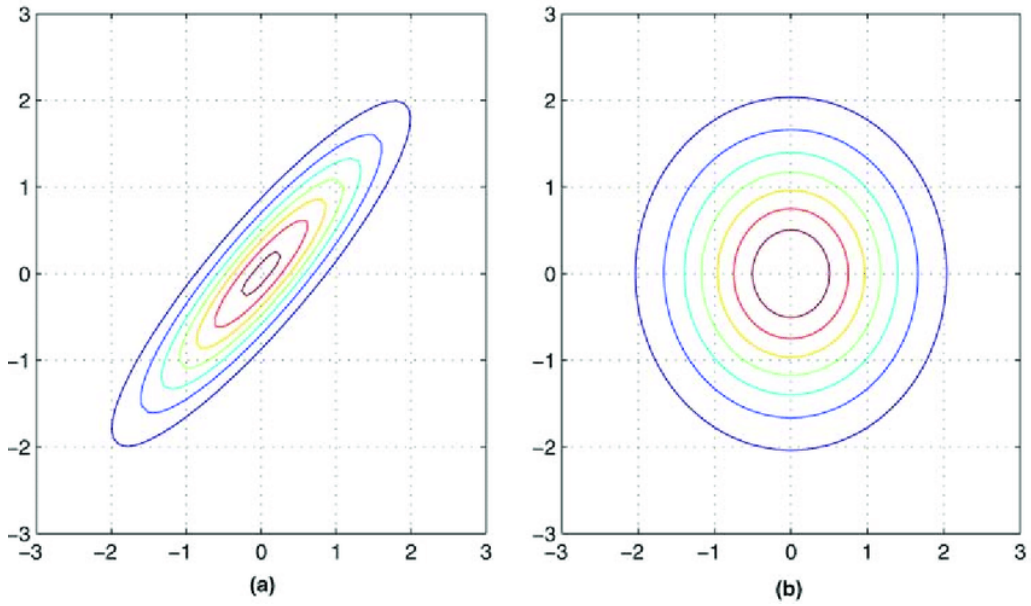

$$||x_t|| \leq \left(\frac{\kappa - 1}{\kappa + 1}\right)^t ||x_0||$$

$$= \left(1 - \frac{2}{\kappa + 1}\right)^t ||x_0||$$

κ large => slower convergence

Understanding gradient descent locally

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Proof:

$$||x_{t+1}|| = ||x_t - \eta \nabla f(x_t)||$$

$$= ||x_t - \eta A x_t|| = ||(I - \eta A) x_t|| \leq \left|\left|I - \eta A\right|\right|_2 \left|\left|x_t\right|\right|_2$$

$$\leq \max(|1 - \eta \lambda_{max}|, |1 - \eta \lambda_{\min}|) \left|\left|x_t\right|\right|_2$$

$$= \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \left|\left|x_t\right|\right|_2 = \frac{\kappa - 1}{\kappa + 1} \left|\left|x_t\right|\right|_2$$

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 3rd and higher order terms, and using the above observation for quadratics:

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

Newton's method.

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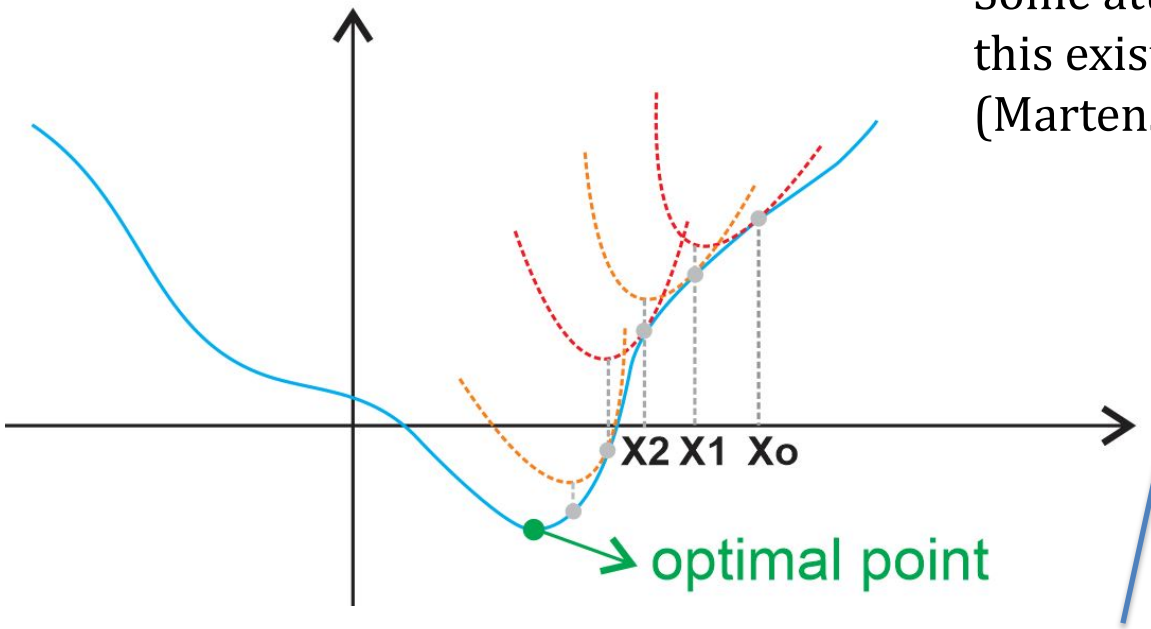


Some attempts to scale this exist. See K-FAC (Martens, Grosse '15)

Problem: need to invert a $d \times d$ matrix => 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, by not relying too much on current gradient.

Linear combination of prior gradients + current one

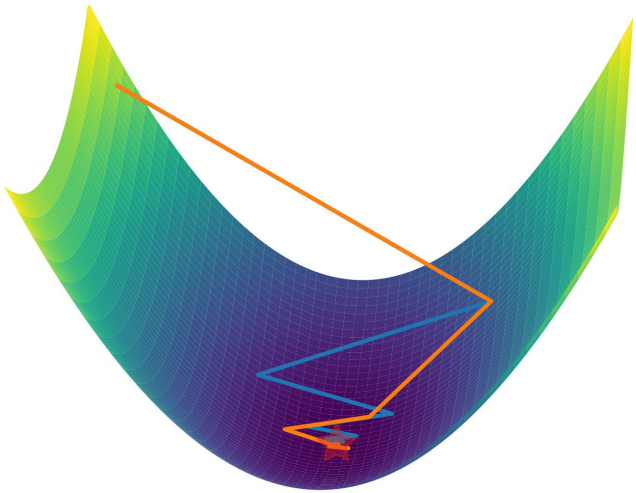
$$v_{t+1} = -\nabla f(x_t) + \beta v_t$$
$$x_{t+1} = x_t + \eta v_{t+1}$$

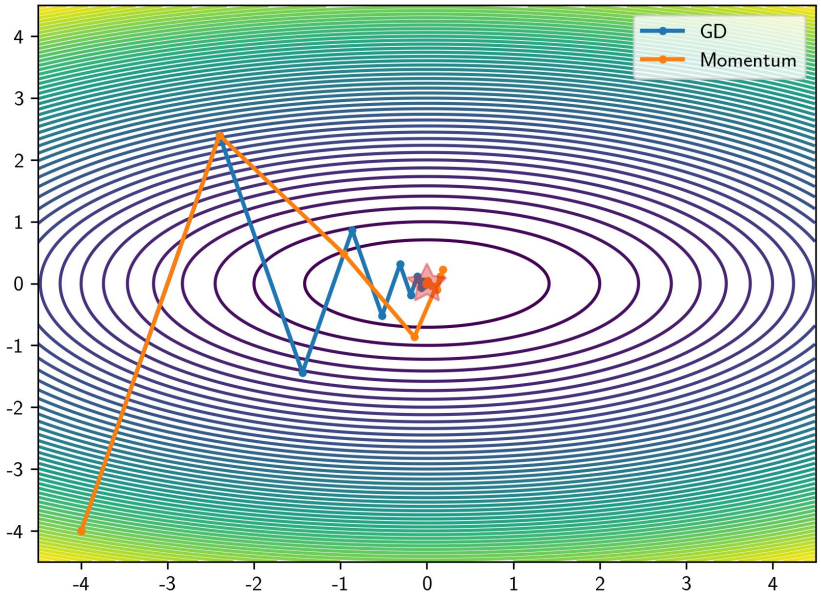
Helps provably! For quadratic case, i.e. $f(x) = x^T A\, x$, you can show:

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

It's common in practice to take β = 0.5, 0.9, 0.99.

Momentum (Polyak ‘64)





Momentum vs grad. descent

https://tangbinh.github.io/01/04/Optimizers.html

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

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

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**

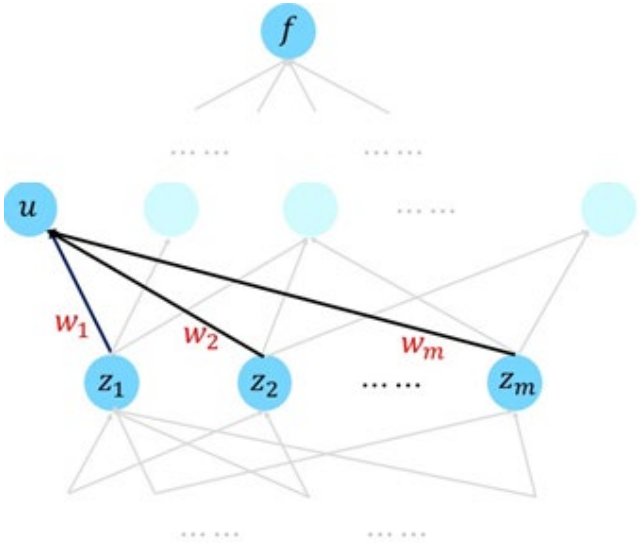
Suppose $f(y) = f(x_1(y), x_2(y), \ldots, x_n(y))$

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

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

$$\frac{\partial f}{\partial w_1} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial w_1} = \frac{\partial f}{\partial u}\frac{\partial \sigma(\langle w, z\rangle + b)}{\partial w_1}$$

$$= \frac{\partial f}{\partial u}\sigma'(u)z_1$$



Taking gradients of neural networks: backpropagation

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

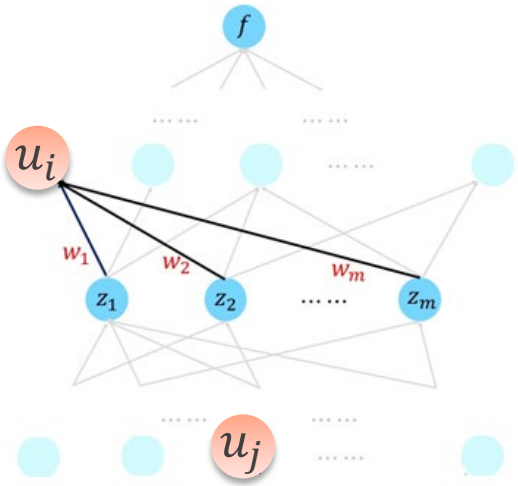
Obvious algorithm? Calculate inductively $\frac{\partial u_i}{\partial u_j}$, for all pairs (u_i, u_j) where u_j is lower than u_i (obviously, this includes $\frac{\partial f}{\partial u}$ which we want)

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

Easy as in prior slide

Have these by inductive hypothesis.

t+1



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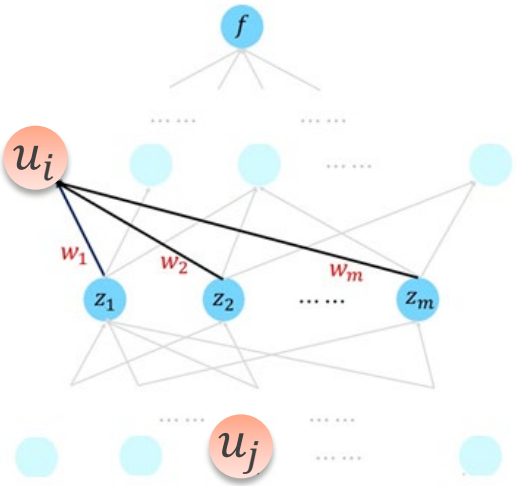


Bad *– this will end up with* $\Omega(V^2)$ *algorithm.*

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.

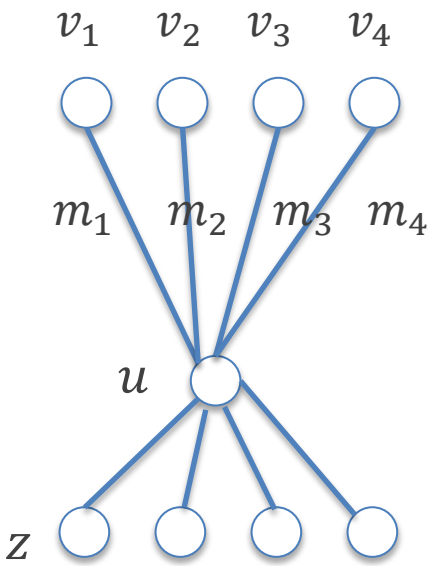
Claim: The sum S of the messages that each node u computes is equal to $\frac{\partial f}{\partial u}$.

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]