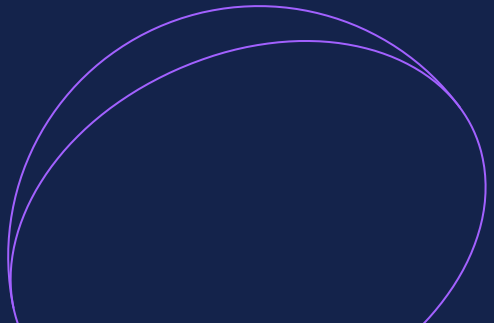
WELCOME TO THE

UCL x DeepMind lecture series

In this lecture series, leading research scientists from leading AI research lab, DeepMind, will give 12 lectures on an exciting selection of topics in Deep Learning, ranging from the fundamentals of training neural networks via advanced ideas around memory, attention, and generative modelling to the important topic of responsible innovation.

Please join us for a deep dive lecture series into Deep Learning!

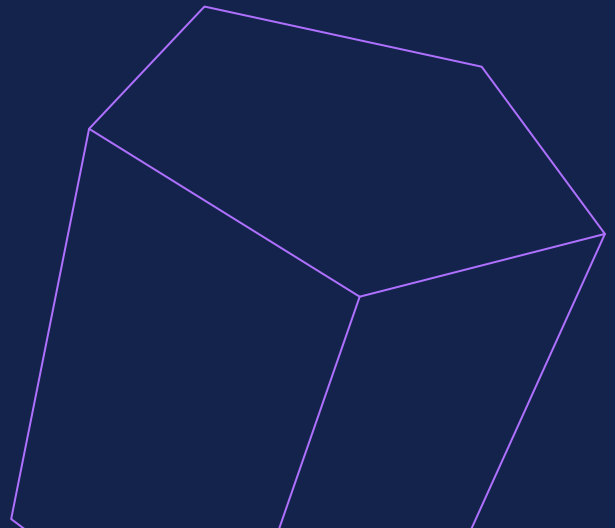
#UCLxDeepMind



General information

Exits:
At the back, the way you came in

Wifi:
UCL guest



TODAY'S SPEAKER

James Martens

James Martens is a research scientist at DeepMind working on the fundamentals of deep learning including optimization, initialization, and regularization. Before that he received his BMath from the University of Waterloo, and did his Masters and PhD at University of Toronto, co advised by Geoff Hinton and Rich Zemel. During his PhD he helped revive interest in deep neural network training by showing how deep networks could be effectively trained using pure optimization methods (which has now become the standard approach).

TODAY'S LECTURE

Optimization for Machine Learning

Optimization methods are the engines underlying neural networks that enable them to learn from data. In this lecture I will cover the fundamentals of gradient-based optimization methods, and their application to training neural networks. Major topics include gradient descent, momentum methods, 2nd-order methods, and stochastic methods. I will analyze these methods through the interpretive framework of local 2nd-order approximations.

DeepMind

Optimization for Machine Learning

James Martens

UCL x DeepMind Lectures

Plan for this Lecture

1. Intro and motivation
2. Gradient descent
3. Momentum methods
4. 2nd-order methods
5. Stochastic optimization

1 Intro and motivation

Motivation

- Optimization algorithms are the basic engine behind deep learning methods that enable models to learn from data by adapting their **parameters**

- They solve the problem of the minimization of an **objective function** that measures the mistakes made by the model
    - e.g. prediction error (classification), negative reward (reinforcement learning)

- Work by making a sequence of small incremental changes to model parameters that are each guaranteed to reduce the objective by some small amount

Basic notation

- Parameters:

$$\theta \in \mathrm{R}^n$$

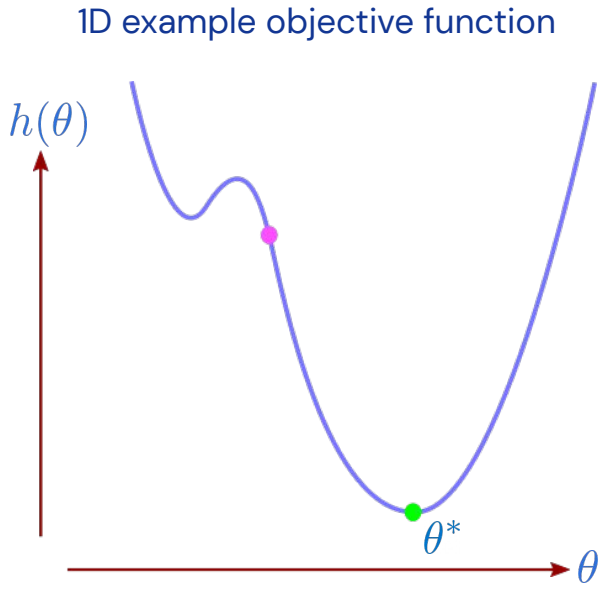
dimension

- Real-valued objective function :

$$h(\theta)$$

- Goal of optimization:

$$\theta^* = \arg\min_{\theta} h(\theta)$$



Example: neural network training objective

- The standard neural network training objective is given by:

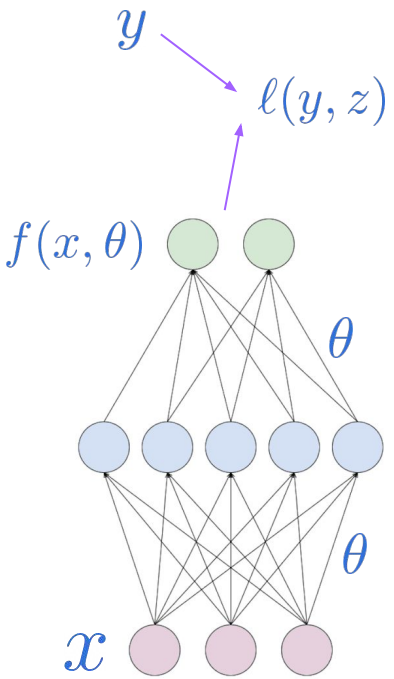
$$h(\theta) = \frac{1}{m} \sum_{i=1}^{m} \ell(y_i, f(x_i, \theta))$$

where:

$\ell(y, z)$ is a loss function measuring disagreement between y and z

and

$f(x, \theta)$ is a neural network function taking input x and outputing some prediction



2 Gradient descent

Gradient descent: definition

- Basic gradient descent iteration:

$$\theta_{k+1} = \theta_k - \alpha_k \nabla h(\theta_k)$$

Learning rate: α_k
(aka “step size”)

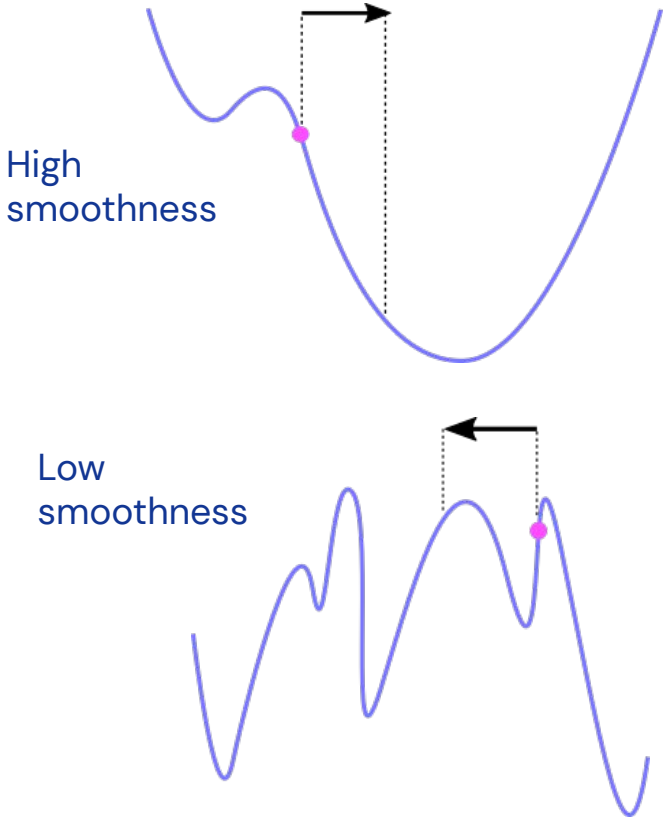
Gradient: $\nabla h(\theta) = \begin{bmatrix} \frac{\partial h(\theta)}{\partial [\theta]_1} \\ \frac{\partial h(\theta)}{\partial [\theta]_2} \\ \vdots \\ \frac{\partial h(\theta)}{\partial [\theta]_n} \end{bmatrix}$

Intuition: gradient descent is “steepest descent”

$$\theta_{k+1} = \theta_k - \alpha_k \nabla h(\theta_k)$$

- Gradient direction $\nabla h(\theta)$ gives *greatest* reduction in $h(\theta)$ per unit of change* in θ.

- If $h(\theta)$ is “sufficiently smooth”, and learning rate small, gradient will keep pointing down-hill over the region in which we take our step



Intuition: gradient descent is minimizing a local approximation

- 1st-order Taylor series for $h(\theta)$ around current θ is:

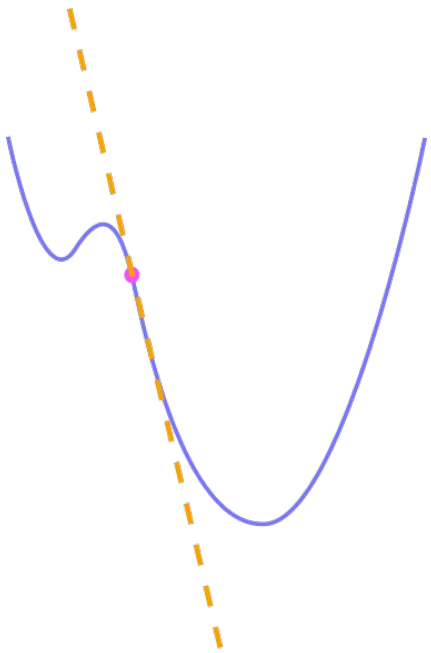
$$h(\theta + d) \approx h(\theta) + \nabla h(\theta)^\top d$$

- For small enough d this will be a reasonable approximation
- Gradient update computed by minimizing this within a sphere of radius r:

$$-\alpha \nabla h(\theta) = \arg\min_{d : \|d\| \leq r} \left(h(\theta) + \nabla h(\theta)^\top d \right)$$

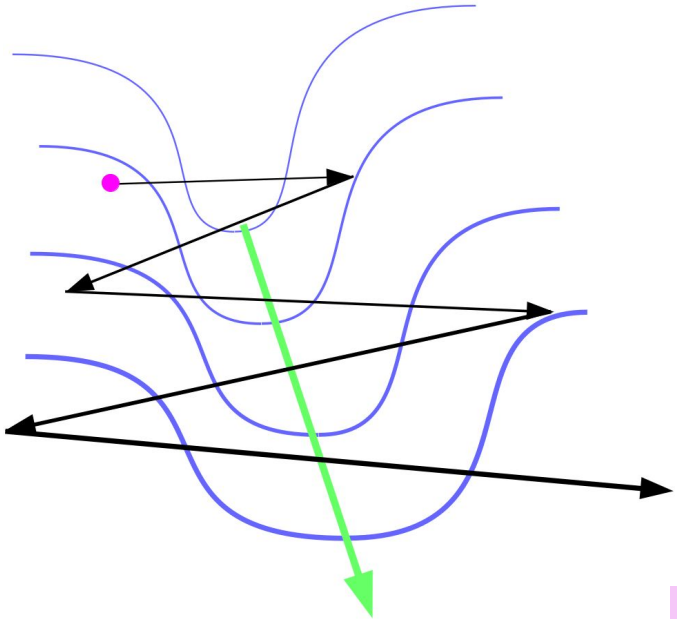
where

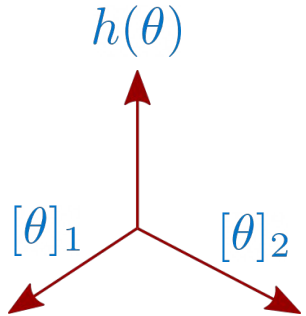
$$r = \alpha \|\nabla h(\theta)\|$$



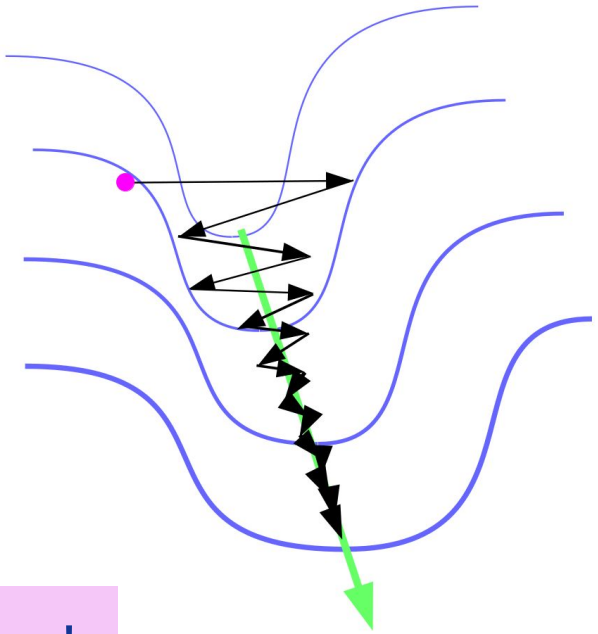
The problem with gradient descent visualized: the 2D "narrow valley" example

Large learning rate (α)





Small learning rate



No good choice !

Convergence theory: technical assumptions

- $h(\theta)$ has Lipschitz continuous derivatives (i.e. is "Lipschitz smooth"):

$$\|\nabla h(\theta) - \nabla h(\theta')\| \leq L\|\theta - \theta'\|$$ (an **upper bound** on the curvature)

- $h(\theta)$ is strongly convex (perhaps only near minimum):

$$h(\theta + d) \geq h(\theta) + \nabla h(\theta)^\top d + \frac{\mu}{2}\|d\|^2$$ (a **lower bound** on the curvature)

- And *for now:* Gradients are computed exactly (i.e. **not** stochastic)

Convergence theory: upper bounds

If previous conditions hold and we take $\alpha_k = \dfrac{2}{L+\mu}$:

$$h(\theta_k) - h(\theta^*) \leq \frac{L}{2}\left(\frac{\kappa - 1}{\kappa + 1}\right)^{2k} \|\theta_0 - \theta^*\|^2$$

minimizer

where $\kappa = L/\mu$.

Number of iterations to achieve $h(\theta_k) - h(\theta^*) \leq \epsilon$ is

$$k \in \mathcal{O}\left(\kappa \log \frac{1}{\epsilon}\right)$$

Convergence theory: useful in practice?

- Issues with bounds such as this one:
  - too pessimistic (they must cover worst-case examples)
  - some assumptions too strong (e.g. convexity)
  - other assumptions too weak (real problems have additional useful structure)
  - rely on crude measures of objective (e.g. condition numbers)
  - usually focused on asymptotic behavior
- The design/choice of an optimizer should always be informed by **practice** more than anything else. But theory can help guide the way and build intuitions.

3 Momentum methods

The momentum method

- Motivation:
  - the gradient has a tendency to flip back and forth as we take steps when the learning rate is large
  - e.g. the narrow valley example
- The key idea:
  - accelerate movement along directions that point consistently down-hill across many consecutive iterations (i.e. have low curvature)
- How?
  - treat current solution for θ like a “ball” rolling along a “surface” whose height is given by $h(\theta)$, subject the force of gravity

Credit: Devinsupertramp via youtube.com

Defining equations for momentum

- Classical Momentum:

$$v_{k+1} = \eta_k v_k - \nabla h(\theta_k) \qquad v_0 = 0$$

$$\theta_{k+1} = \theta_k + \alpha_k v_{k+1}$$

Learning rate: α_k

Momentum constant: η_k

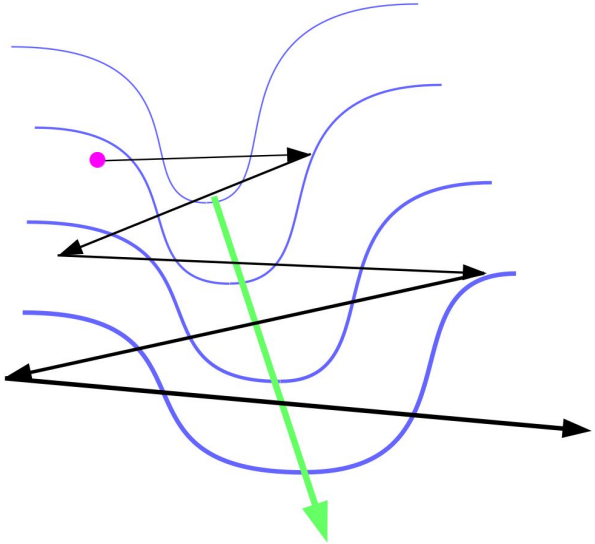
- Nesterov's variant:

$$v_{k+1} = \eta_k v_k - \nabla h(\theta_k + \alpha_k \eta_k v_k) \qquad v_0 = 0$$

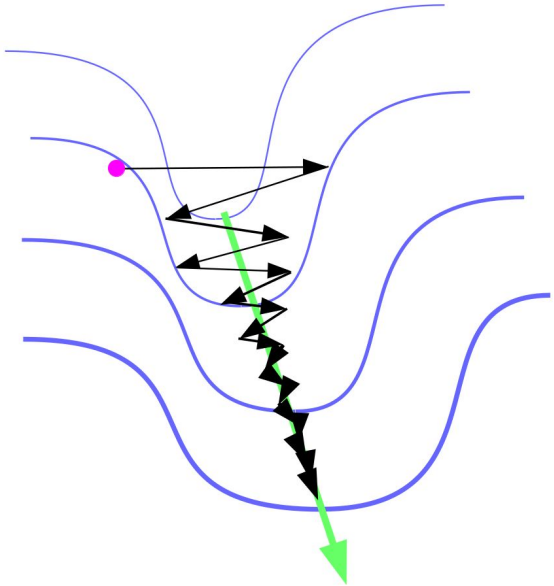
$$\theta_{k+1} = \theta_k + \alpha_k v_{k+1}$$

Narrow 2D valley example revisited

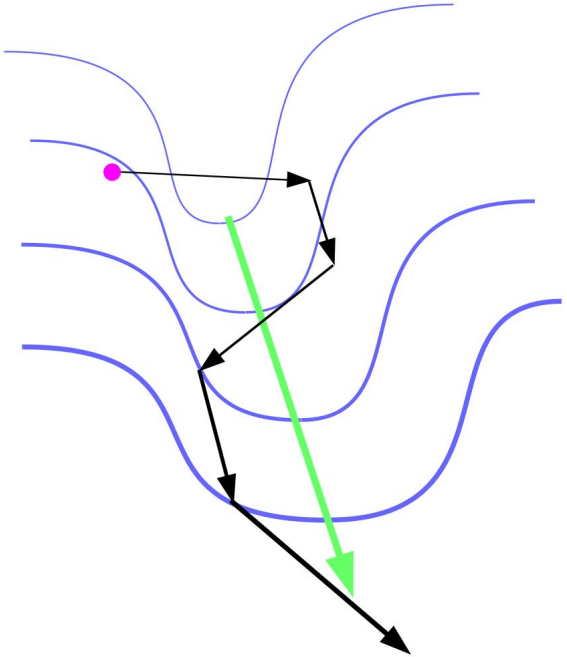
Gradient descent with large learning rate



Gradient descent with small learning rate



Momentum method



Upper bounds for Nesterov's momentum variant

Given objective $h(\theta)$ satisfying same technical conditions as before, and careful choice of α_k and η_k, Nesterov's momentum method satisfies:

$$h(\theta_k) - h(\theta^*) \leq L \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa}} \right)^k \|\theta_0 - \theta^*\|^2 \qquad \kappa = \frac{L}{\mu}$$

Number of iterations to achieve $h(\theta_k) - h(\theta^*) \leq \epsilon$:

$$k \in \mathcal{O}\left(\sqrt{\kappa} \log \frac{1}{\epsilon} \right)$$

Convergence theory: 1st-order methods and *lower bounds*

- A **first-order method** is one where updates are linear combinations of observed gradients. i.e.:

$$\theta_{k+1} - \theta_k = d \in \mathrm{Span}\{\nabla h(\theta_0), \nabla h(\theta_1), \ldots, \nabla h(\theta_k)\}$$

- Included:
  - gradient descent
  - momentum methods
  - conjugate gradients (CG)
- Not included:
  - preconditioned gradient descent / 2nd-order methods

Lower bounds (cont.)

Assume number of steps is greater than the dimension n (it usually is).
Then, there is example objective satisfying previous conditions for which:

$$h(\theta_k) - h(\theta^*) \geq \frac{\mu}{2}\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^{2k} \|\theta_0 - \theta^*\|^2 \qquad \kappa = L/\mu$$

Number of iterations to achieve $h(\theta_k) - h(\theta^*) \leq \epsilon$:

$$k \in \Omega\left(\sqrt{\kappa}\log\frac{1}{\epsilon}\right)$$

Comparison of iteration counts

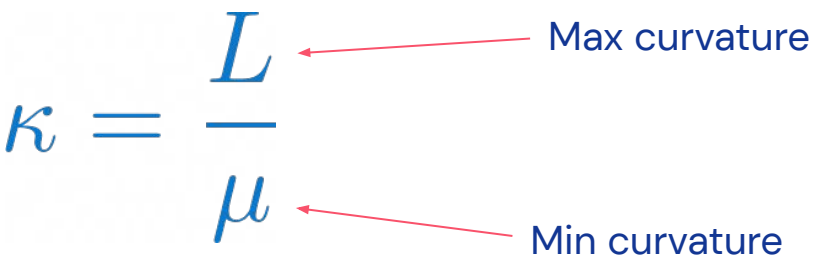
To achieve $h(\theta_k) - h(\theta^*) \leq \epsilon$ the number of iterations k satisfies:

- (Worst-case) lower bound for 1st-order methods: $k \in \Omega\left(\sqrt{\kappa}\log\frac{1}{\epsilon}\right)$
- Upper bound for gradient descent: $k \in \mathcal{O}\left(\kappa\log\frac{1}{\epsilon}\right)$
- Upper bound for GD w/ Nesterov's momentum: $k \in \mathcal{O}\left(\sqrt{\kappa}\log\frac{1}{\epsilon}\right)$

4 2nd-order methods

The problem with 1st-order methods

- For any 1st-order method, the number of steps needed to converge grows with “condition number”:



- This will be very large for some problems (e.g. certain deep architectures)
- 2nd-order methods can improve (or even eliminate) this dependency

Derivation of Newton's method

- Approximate $h(\theta)$ by its 2nd-order Taylor series around current θ:

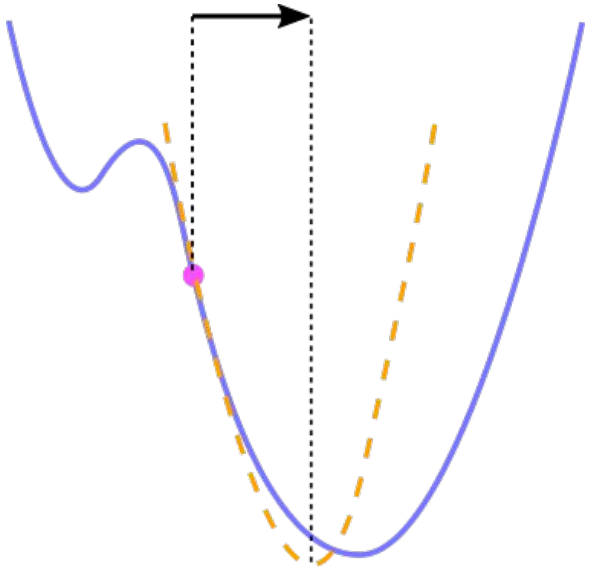
$$h(\theta + d) \approx h(\theta) + \nabla h(\theta)^\top d + \frac{1}{2} d^\top H(\theta) d$$

- Minimize this local approximation to obtain:

$$d = -H(\theta)^{-1} \nabla h(\theta)$$

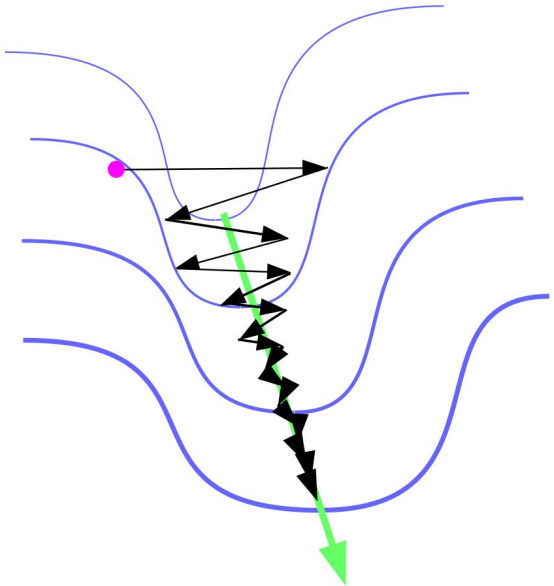
- Update current iterate with this:

$$\theta_{k+1} = \theta_k - H(\theta)^{-1} \nabla h(\theta_k)$$

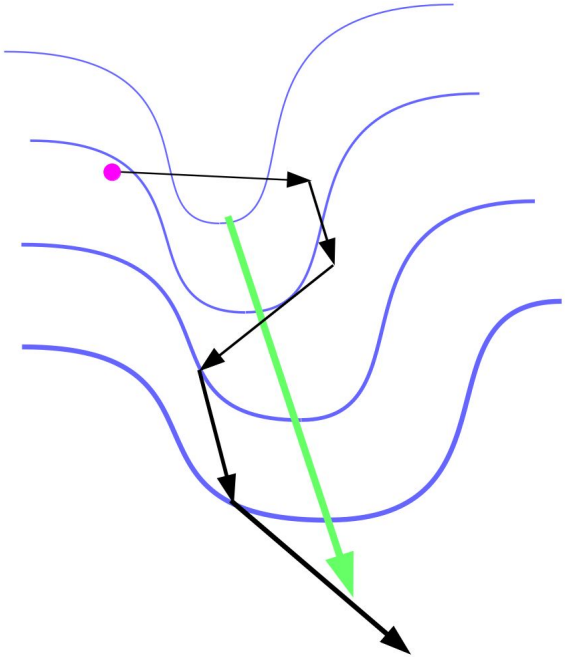


The 2D narrow valley example revisited (again)

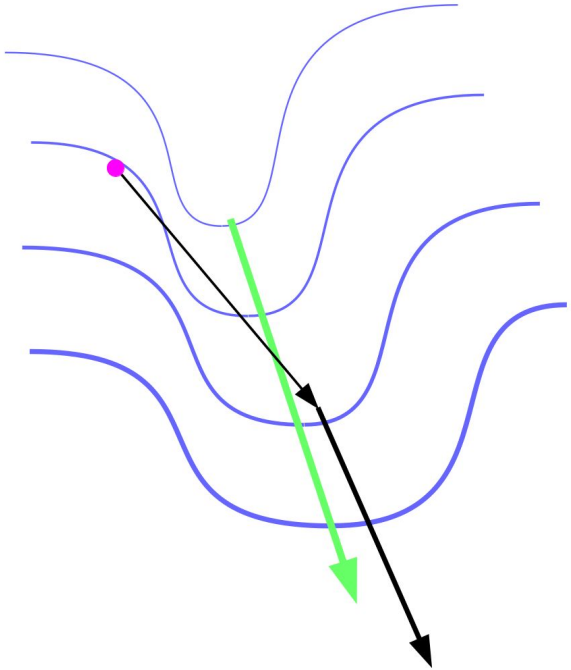
Gradient descent



Momentum method



2nd-order method



Comparison to gradient descent

- Maximum allowable global learning rate for GD to avoid divergence:

$$\alpha = 1/L$$

L is maximum curvature
aka “Lipschitz constant”

- Gradient descent implicitly minimizes a bad approximation of 2nd-order Taylor series:

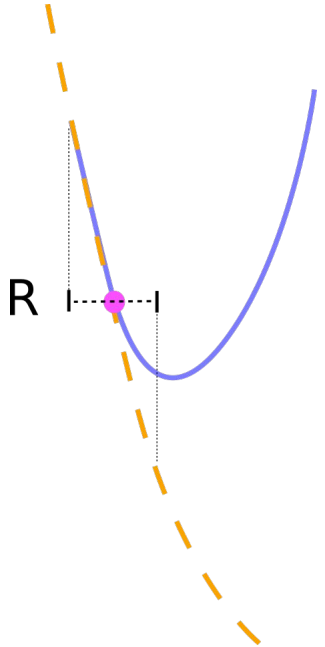
$$h(\theta + d) \approx h(\theta) + \nabla h(\theta)^\top d + \frac{1}{2} d^\top H(\theta) d$$

$$\approx h(\theta) + \nabla h(\theta)^\top d + \frac{1}{2} d^\top (LI) d$$

- LI is too pessimistic / conservative an approximation of $H(\theta)$! Treats all directions as having max curvature.

Breakdown of local quadratic approximation and how to deal with it

- Quadratic approximation of objective is only trustworthy in a local region around current θ
- Gradient descent (implicitly) approximates the curvature everywhere by its global max (and so doesn't have this problem)
- Newton's method uses $H(\theta)$, which may become an underestimate in the region we are taking our update step



Solution: Constrain update d to lie in a "trust region" R around, where approximation remains "good enough"

Trust-regions and “damping”

- If we take $R = \{d : \|d\|_2 \leq r\}$ then computing

$$\arg\min_{d \in R} \left(h(\theta) + \nabla h(\theta)^\top d + \frac{1}{2} d^\top H(\theta) d \right)$$

  is often equivalent to

$$-(H(\theta) + \lambda I)^{-1} \nabla h(\theta) = \arg\min_{d} \left(h(\theta) + \nabla h(\theta)^\top d + \frac{1}{2} d^\top (H(\theta) + \lambda I) d \right)$$

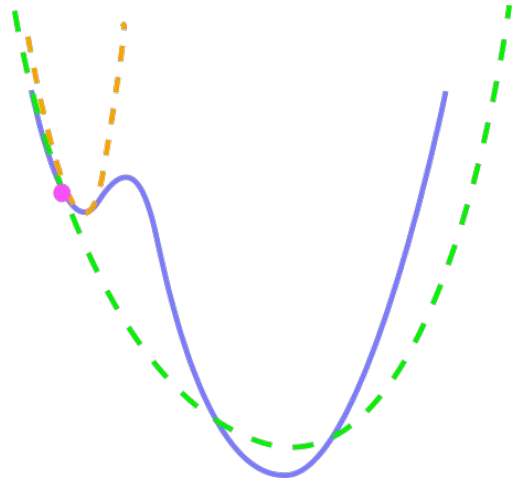
  for some λ.

- λ depends on r in a complicated way, but we can just work with λ directly

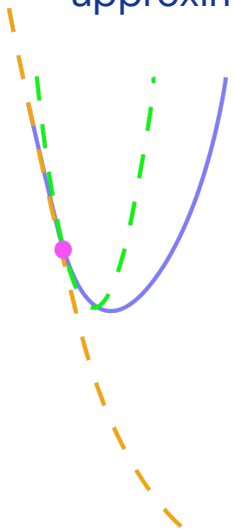
Alternative curvature matrices

$H(\theta)$ does not necessarily give the best quadratic approximation for optimization. Different replacements for $H(\theta)$ could produce:

A more global approximation



A more conservative approximation



Alternative curvature matrices (cont.)

- The most important family of related examples includes:
  - Generalized Gauss-Newton matrix (GGN)
  - Fisher information matrix
  - “Empirical Fisher”
- Nice properties:
  - always positive semi-definite (i.e. no negative curvature)
  - give parameterization invariant updates in small learning rate limit (unlike Newton’s method!)
  - work much better in practice for neural net optimization

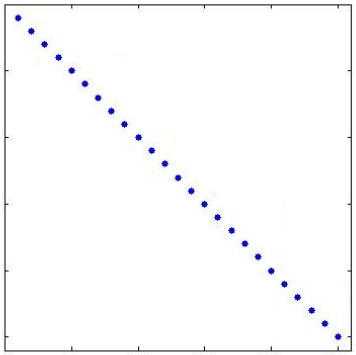
Barrier to application of 2nd-order methods for neural networks

- For neural networks, $\theta \in \mathbb{R}^n$ can have 10s of millions of dimensions
- We simply cannot compute and store an $n \times n$ matrix, let alone invert it!
- To use 2nd-order methods, we must simplify the curvature matrix's
  - computation,
  - storage,
  - and inversion

  This is typically done by approximating the matrix with a simpler form.

Diagonal approximations

The simplest approximation: include only the diagonal entries of curvature matrix (setting the rest to zero)



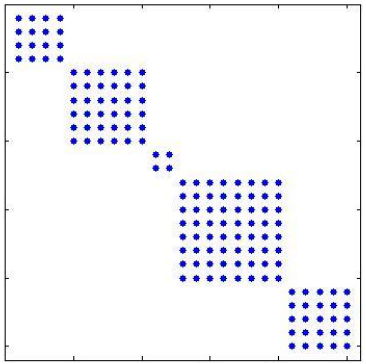
Properties:

- Inversion and storage cost: $\mathcal{O}(n)$
- Computational costs depends on form of original matrix (ranges from easy to hard)
- Unlikely to be accurate, but can compensate for basic scaling differences between parameters

Used (with a square root) in RMS-prop and Adam methods to approximate Empirical Fisher matrix

Block-diagonal approximations

Another option is to take only include certain diagonal blocks.



For neural nets, a block could correspond to:

- weights on connections going into a given unit
- weights on connections going out of a given unit
- all the weights for a given layer

Properties:

- Storage cost: $\mathcal{O}(bn)$ (assuming $b \times b$ block size)
- Inversion cost: $\mathcal{O}(b^2 n)$
- Similar difficulty to computing diagonal
- Can only be realistically applied for small block sizes

Well-known example developed for neural nets: TONGA

Kronecker-product approximations

- Block-diagonal approximation of GGN/Fisher where blocks correspond to network layers
- Approximate each block as Kronecker product of two small matrices:

$$A \otimes C = \begin{bmatrix} [A]_{1,1}C & \cdots & [A]_{1,k}C \\ \vdots & \ddots & \vdots \\ [A]_{k,1}C & \cdots & [A]_{k,k}C \end{bmatrix}$$

- Storage and computation cost: $\mathcal{O}(n)$*
- Cost to apply inverse: $\mathcal{O}(b^{0.5}n)$ (uses $(A \otimes C)^{-1} = A^{-1} \otimes C^{-1}$)
- Used in current most powerful neural net optimizer (K-FAC)

5 Stochastic methods

Motivation for stochastic methods

- Typical objectives in machine learning are an average over training cases of case-specific losses:

$$h(\theta) = \frac{1}{m} \sum_{i=1}^{m} h_i(\theta)$$

- m can be **very** big, and so computing the gradient gets expensive:

$$\nabla h(\theta) = \frac{1}{m} \sum_{i=1}^{m} \nabla h_i(\theta)$$

Mini-batching

- Fortunately there is often significant statistical overlap between $h_i(\theta)$'s
- Early in learning, when "coarse" features of the data are still being learned, most $\nabla h_i(\theta)$' s will look similar
- **Idea:** randomly subsample a "mini-batch" of training cases $S \subset \{1, 2, ..., m\}$ of size $b \ll m$, and estimate gradient as:

$$\widetilde{\nabla} h(\theta) = \frac{1}{b} \sum_{i \in S} \nabla h_i(\theta)$$

Stochastic gradient descent (SGD)

- Stochastic gradient descent (SGD) replaces $\nabla h(\theta)$ with its mini-batch estimate $\widetilde{\nabla} h(\theta)$, giving:

$$\theta_{k+1} = \theta_k - \alpha_k \widetilde{\nabla} h(\theta_k)$$

- To ensure convergence, need to do one of the following:
  - Decay learning rate: $\alpha_k = 1/k$
  - Use "Polyak averaging": $\bar{\theta}_k = \frac{1}{k+1} \sum_{i=0}^{k} \theta_i$ or $\bar{\theta}_k = (1-\beta)\theta_k + \beta \bar{\theta}_{k-1}$
  - Slowly increase the mini-batch size during optimization

Convergence of stochastic methods

- Stochastic methods converge slower than corresponding non-stochastic versions
- Asymptotic rate for SGD with Polyak averaging:

Gradient estimate covariance matrix

$$E[h(\theta_k)] - h(\theta^*) \in \frac{1}{2k} \operatorname{tr}\left(H(\theta^*)^{-1}\Sigma\right) + \mathcal{O}\left(\frac{1}{k^2}\right)$$

- Iterations to converge:

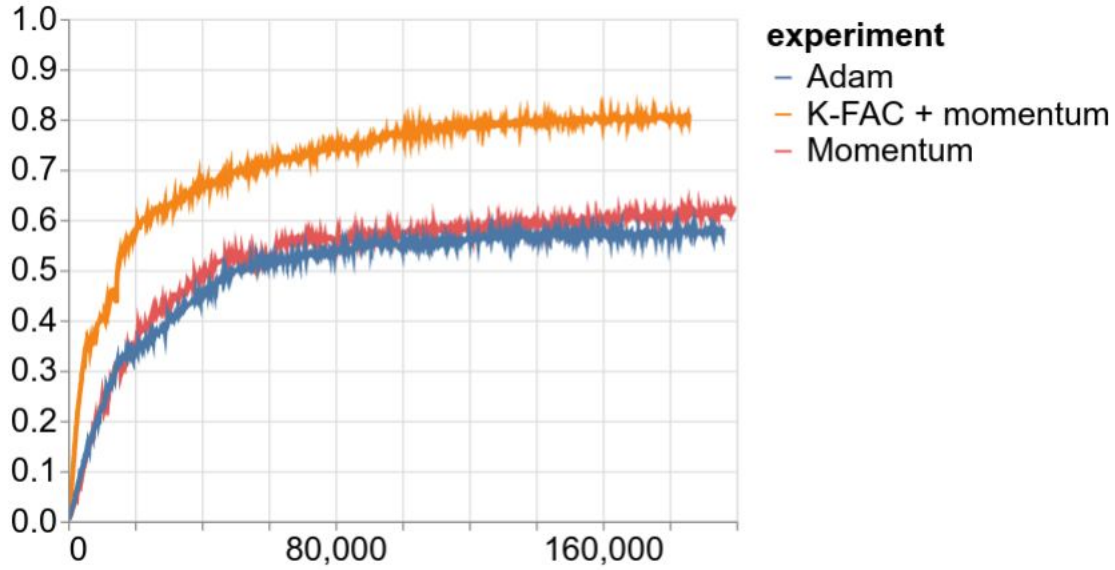
$$k \in \mathcal{O}\left(\operatorname{tr}\left(H(\theta^*)^{-1}\Sigma\right)\frac{1}{\epsilon}\right) \quad \text{vs} \quad k \in \mathcal{O}\left(\sqrt{\kappa}\log\frac{1}{\epsilon}\right)$$

no log!

Stochastic 2nd-order and momentum methods

- Mini-batch gradients estimates can be used with 2nd-order and momentums methods too
- Curvature matrices estimated stochastically using decayed averaging over multiple steps
- No stochastic optimization method that sees the same amount of data can have better **asymptotic** convergence speed than SGD with Polyak averaging
- *But…* **pre-asymptotic** performance usually matters more in practice. So stochastic 2nd-order and momentum methods can still be useful if:
    - the loss surface curvature is bad enough and/or
    - the mini-batch size is large enough

Experiments on deep convnets



Details

- Mini-batch size of 512
- Imagenet dataset
- 100 layer deep convolutional net without skips or batch norm
- Carefully initialized parameters

Conclusions / Summary

- Optimization methods:
  - enable learning in models by adapting parameters to minimize some objective
  - main engine behind neural networks
- 1st-order methods (gradient descent):
  - take steps in direction of “steepest descent”
  - run into issues when curvature varies strongly in different directions
- Momentum methods:
  - use principle of momentum to accelerate along directions of lower curvature
  - obtain “optimal” convergence rates for 1st-order methods

Conclusions / Summary

- 2nd-order methods:
  - improve convergence in problems with bad curvature, even more so than momentum methods
  - require use of trust-regions/damping to work well
  - also require the use of curvature matrix approximations to be practical in high dimensions (e.g. for neural networks)
- Stochastic methods:
  - use “mini-batches” of data to estimate gradients
  - asymptotic convergence is slower
  - pre-asymptotic convergence can be sped up using 2nd-order methods and/or momentum

Thank you

Questions

References and further reading

Solid introductory texts on optimization:

- *Numerical Optimization* (Nocedal & Wright)
- *Introductory Lectures on Convex Optimization: A Basic Course* (Nesterov)

Further reading for those interested in neural network optimization:

- *Optimization Methods for Large-Scale Machine Learning* (Bottou et al)
- *The Importance of Initialization and Momentum in Deep Learning* (Sutskever et al.)
- *New insights and perspectives on the natural gradient method* (Martens)
- *Optimizing Neural Networks with Kronecker-factored Approximate Curvature* (Martens & Grosse)
- *Which Algorithmic Choices Matter at Which Batch Sizes? Insights From a Noisy Quadratic Model* (Zhang et al.)