Optimisation

Jonathon Hare

Gradient descent and SGD (again), and mini-batch SGD

We'll start up by looking again at gradient descent algorithms and their behaviours...

Reminder: Gradient Descent

- Define total loss as $\mathcal{L} = \sum_{(\boldsymbol{x},y)\in\boldsymbol{D}} \ell(g(\boldsymbol{x},\boldsymbol{\theta}),y)$ for some loss function ℓ, dataset $\boldsymbol{D}$ and model g with learnable parameters $\boldsymbol{\theta}$.
- Define how many passes over the data to make (each one known as an Epoch)
- Define a learning rate λ

Gradient Descent updates the parameters $\boldsymbol{\theta}$ by moving them in the direction of the negative gradient with respect to the **total loss** $\mathcal{L}$ by the learning rate λ multiplied by the gradient: [1em] `for each Epoch:` $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda\nabla_{\boldsymbol{\theta}}\mathcal{L}$

Gradient Descent

- Gradient Descent has good statistical properties (very low variance)
- But is very data inefficient (particularly when data has many similarities)
- Doesn't scale to effectively infinite data (e.g. with augmentation)

Reminder: Stochastic Gradient Descent

- Define loss function ℓ, dataset $\boldsymbol{D}$ and model g with learnable parameters $\boldsymbol{\theta}$.
- Define how many passes over the data to make (each one known as an Epoch)
- Define a learning rate λ

Stochastic Gradient Descent updates the parameters $\boldsymbol{\theta}$ by moving them in the direction of the negative gradient with respect to the loss of a **single item** ℓ by the learning rate λ multiplied by the gradient: [1em] `for each Epoch:` `for each` $(\boldsymbol{x}, y) \in shuffle(\boldsymbol{D})$`:` $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda\nabla_{\boldsymbol{\theta}}\ell$

Stochastic Gradient Descent

- Stochastic Gradient Descent has poor statistical properties (very high variance)
- But is computationally inefficient (poor utilisation of resources - particularly with respect to vectorisation)

Mini-batch Stochastic Gradient Descent

- Define a batch size b
- Define batch loss as $\mathcal{L}_b = \sum_{(\boldsymbol{x},y)\in\boldsymbol{D}_b} \ell(g(\boldsymbol{x},\boldsymbol{\theta}),y)$ for some loss function ℓ and model g with learnable parameters $\boldsymbol{\theta}$. $\boldsymbol{D}_b$ is a subset of dataset $\boldsymbol{D}$ of cardinality b.
- Define how many passes over the data to make (each one known as an Epoch)
- Define a learning rate λ

Mini-batch Gradient Descent updates the parameters $\boldsymbol{\theta}$ by moving them in the direction of the negative gradient with respect to the loss of a **mini-batch** $\boldsymbol{D}_b$, $\mathcal{L}_b$ by the learning rate λ multiplied by the gradient: [1em] `for each Epoch:` shuffle & partition dataset $\boldsymbol{D}$ into an array of subsets of size b `for each` $\boldsymbol{D}_b \in partitioned(shuffle(\boldsymbol{D}$`)):` $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda \nabla_{\boldsymbol{\theta}} \mathcal{L}_b$

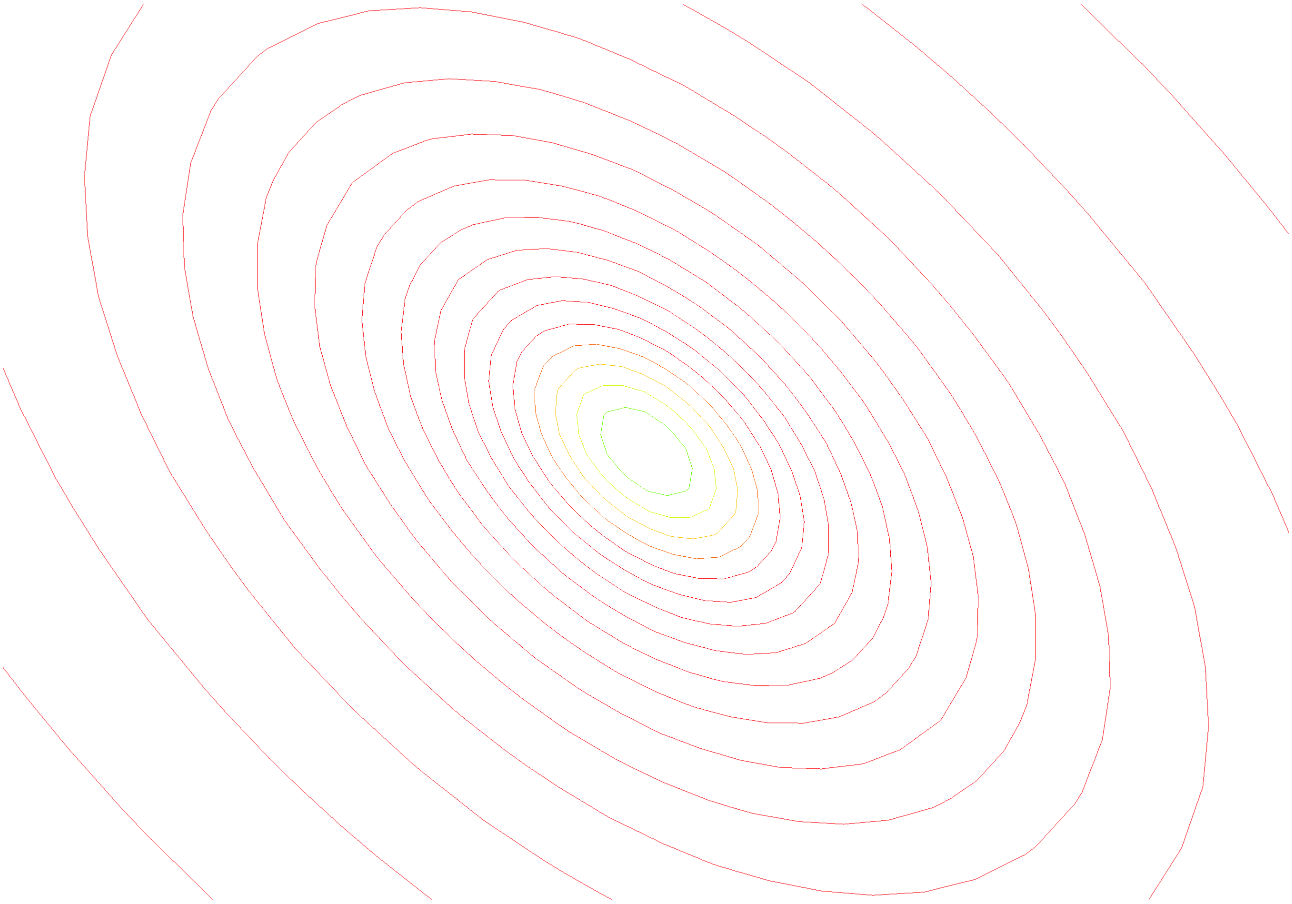
Mini-batch Stochastic Gradient Descent

- Mini-batch Stochastic Gradient Descent has reasonable statistical properties (much lower variance than SGD)
- Allows for computationally efficiency (good utilisation of resources)
- Ultimately we would normally want to make our batches as big as possible for lower variance gradient estimates, but:
    - Must still fit in RAM (e.g. on the GPU)
    - Must be able to maintain throughput (e.g. pre-processing on the CPU; data transfer time)

So, what about the learning rate?

- Choice of learning rate is extremely important
- But we have to reason about the ‘loss landscape’
    - Most convergence analysis of optimisation algorithms assumes a convex loss landscape
        - Easy to reason about
        - Can be shown that (S)GD will converge to the optimal solution for a variety of learning rates
        - Can give insights into potential problems in the non-convex case
    - Deep Learning is highly non-convex
        - Many local minima
        - Plateaus
        - Saddle points
        - Symmetries (permutation, etc)
        - Certainly no single global minima

*GD in the convex case: failure modes



Accelerated Gradient Methods

- Accelerated gradient methods use a *leaky* average of the gradient, rather than the instantaneous gradient estimate at each time step
- A physical analogy would be one of the momentum a ball picks up rolling down a hill...
- As you'll see, this helps address the *GD failure modes, but also helps avoid getting stuck in local minima

pause

Momentum I

It's common for the 'leaky' average (the 'velocity', v_t) to be a weighted average of the instantaneous gradient g_t and the past velocity[1]:

$$v_t = \beta v_{t-1} + g_t$$

where $\beta \in [0, 1]$ is the 'momentum'.

Momentum II

- The momentum method allows to accumulate velocity in directions of low curvature that persist across multiple iterations
- This leads to accelerated progress in low curvature directions compared to gradient descent

[1] There are quite a few variants of this; here we're following the PyTorch variant

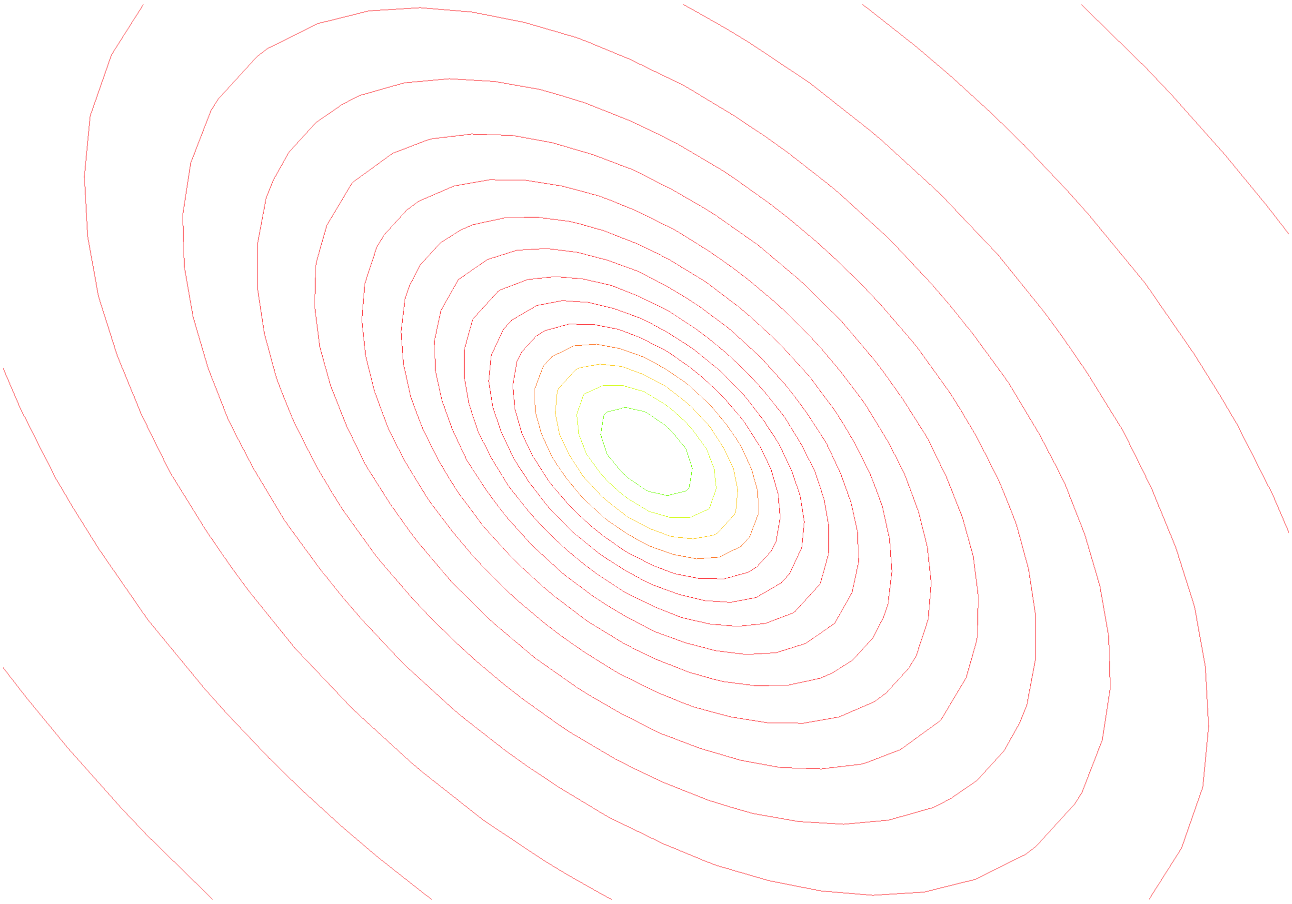
MB-SGD with Momentum

Learning with momentum on iteration t (batch at t denoted by $b(t)$) is given by:

$$\begin{aligned}\boldsymbol{v}_t &\leftarrow \beta\boldsymbol{v}_{t-1} + \nabla_{\boldsymbol{\theta}}\mathcal{L}_{b(t)}\\ \boldsymbol{\theta}_t &\leftarrow \boldsymbol{\theta}_{t-1} - \lambda\boldsymbol{v}_t\end{aligned}$$

Note $\beta = 0.9$ is a good choice for the momentum parameter.

SGD with Momentum - potentially better convex convergence



Learning rate schedules

- In practice you want to decay your learning rate over time
- Smaller steps will help you get closer to the minima
- But don't do it to early, else you might get stuck
- Something of an art form!
  - 'Grad Student Descent' or GDGS ('Gradient Descent by Grad Student')

Reduce LR on plateau

- Common Heuristic approach:
  - if the loss hasn't improved (within some tolerance) for k epochs
  - then drop the lr by a factor of 10
- Remarkably powerful!

Cyclic learning rates

- Worried about getting stuck in a non-optimal local minima?
- Cycle the learning rate up and down (possibly annealed), with a different lr on each batch
- See `https://arxiv.org/abs/1506.01186`

More advanced optimisers

- Adagrad
  - Decrease learning rate dynamically per weight.
  - Squared magnitude of the gradient (2nd moment) used to adjust how quickly progress is made - weights with large gradients are compensated with a smaller learning rate.
  - Particularly effective for sparse features.
- RMSProp
  - Modifies Adagrad to decouple learning rate from gradient magnitude scaling
  - Incorporates leaky averaging of squared gradient magnitudes
  - LR would typically follow a predefined schedule
- Adam
  - Essentially takes all the best ideas from RMSProp and SDG+Momentum
  - Bias corrected momentum and second moment estimation
  - Shown that it might still diverge (or be non optimal, even in convex settings)...
  - LR is still a hyperparameter (you might still schedule)

Take-away messages

- The loss landscape of a deep network is complex to understand (and is far from convex)
- If you're in a hurry to get results use Adam
- If you have time (or a Grad Student at hand), then use SGD (with momentum) and work on tuning the learning rate
- If you're implementing something from a paper, then follow what they did!