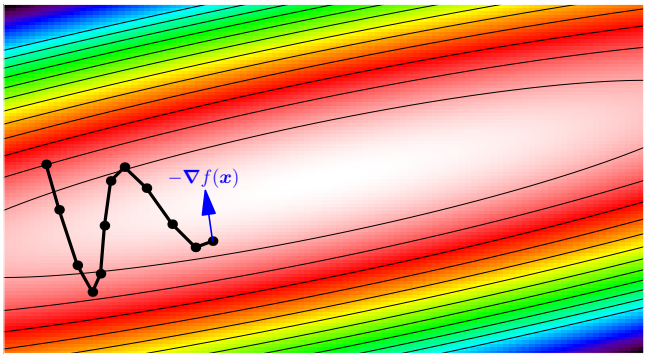
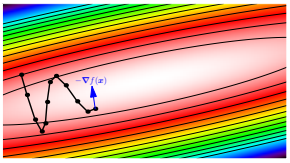
Advanced Machine Learning
Stochastic Gradient Descent



SGD, momentum, step size, ADAM

Outline

1. **SGD**
2. Momentum
3. Loss Landscapes



The Next Step

- In most machine learning problems we design a network and a loss function
- The rest requires simple optimisation
- Although Newton and Quasi-Newton methods ensure rapid convergence for many tasks this apparent advantage is delusionary
- Since the raise of deep learning, gradient descent and its variants have become dominant

Mini-Batch Learning

- Rather than computing the gradient of the loss function, e.g.

$$\nabla L_{\mathcal{D}}(\boldsymbol{w}) = \nabla \sum_{(\boldsymbol{x},y)\in\mathcal{D}} L\big(f(\boldsymbol{x}|\boldsymbol{w}),y\big)^2$$

- We often compute an approximation

$$\nabla L_{\mathcal{B}}(\boldsymbol{w}) = \nabla \sum_{(\boldsymbol{x},y)\in\mathcal{B}} L\big(f(\boldsymbol{x}|\boldsymbol{w}),y\big)^2$$

- where $\mathcal{B} \subset \mathcal{D}$ is a randomly sampled subset of the training set
- Usually $|\mathcal{B}| \ll |\mathcal{D}|$

Stochastic Gradient Descent

- Stochastic gradient descent (SGD) follows the gradient of mini-batches
- Computationally this is efficient because it is much quicker to compute $\nabla L_{\mathcal{B}}(\boldsymbol{w})$ than $\nabla L_{\mathcal{D}}(\boldsymbol{w})$
- The batch gradients add noise (are stochastic) as we are only sampling the dataset
- This noise might help escape local-minima (but I'm not sure there is compelling evidence for this)
- Taking many smaller steps of approximate gradients reduces the likelihood of divergence

Automatic Differentiation

- For gradient descent we need to compute the gradient
- For most of my life this was just a pain
- You guys have it easy, modern deep learning frameworks do this for you automatically
- This is a *game changer*! We are no longer afraid of large models
- We can differentiate through algorithms allowing us to training incredible sophisticated networks

Convergence

- Asymptotic convergence of gradient descent (and SGD) is slower than quasi-Newton methods
- But there are three reasons why we don't really care
  - For complex models we spend a lot of time before we are close to a quadratic minima where asymptotic convergence kicks in
  - These days we often use ReLUs (rectified linear units) which are non-analytic. The convergence we discussed depends on a Taylor expansion that assumes analyticity
  - We want to minimise the generalisation error, but are only minimising a poor surrogate, namely the training error

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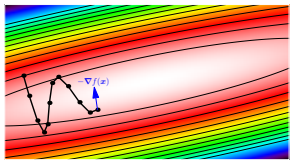
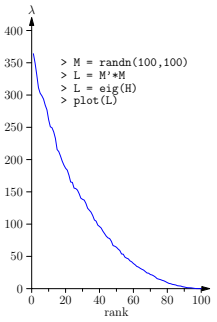


Step Size

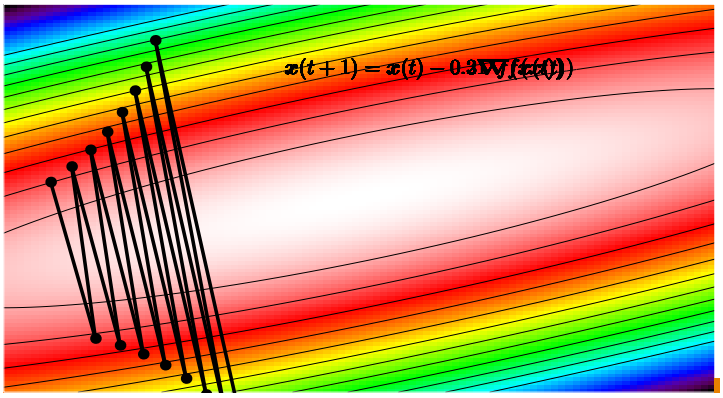
- The optimal step size depends on the gradient and the curvature (second derivative)
- For a quadratic minima the minimum is given by

$$x^* = x - \frac{f'(x)}{f''(x)}, \quad \boldsymbol{x}^* = \boldsymbol{x} - \mathbf{H}^{-1}\nabla f(\boldsymbol{x})$$

- In high dimensions the Hessian $\mathbf{H}$ will have a spectrum of eigenvalues
- This means there are different scales



Gradient Descent



Avoiding Divergence

- We saw in the last lecture that gradient descent can actually diverge from a local optimum if you have a too big step size
- If we use too large a step size we quickly get NaN errors
- If we only use SGD the step size is determined by the largest eigenvalue of the Hessian
- This seems impossibly slow, but weirdly straightforward SGD is often used in deep learning (although nearly always with momentum)

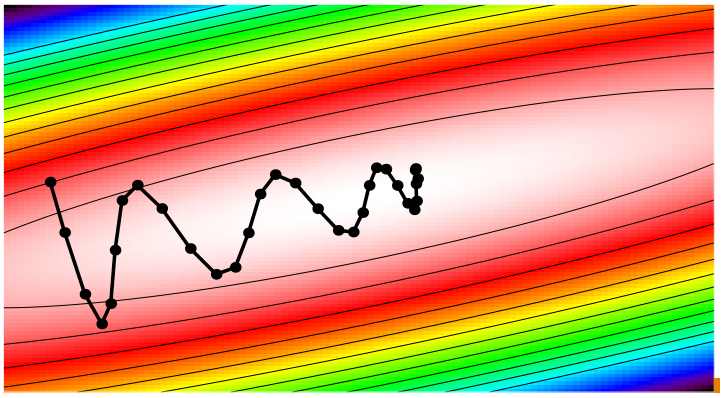
Momentum

- In high dimensions we zig-zag:
  - ⋆ stepping consistently in directions with low curvature
  - ⋆ jumping backwards and forwards past the minimum in directions with high curvature
- By introducing "momentum" we can increase our steps in low curvature directions and decrease it in high curvature directions

$$\boldsymbol{v}(t+1) = \gamma \boldsymbol{v}(t) - \eta \nabla f(\boldsymbol{x}(t))$$
$$\boldsymbol{x}(t+1) = \boldsymbol{x}(t) + \boldsymbol{v}(t+1)$$

$0 < \gamma < 1$ is a damping term

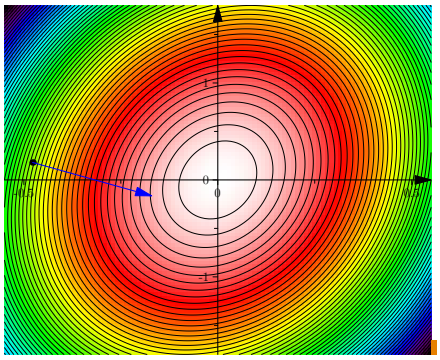
Gradient Descent with Momentum



Adaptive Methods

- A major difficulty of high dimensional optimisation is the existence of different scales
- That is, there are some directions were we have to move a lot (low curvature), while other directions we have to make small steps
- In adaptive methods we use a dynamic algorithm to rescale the step size of each parameter (weight)
- We can think of this as a "regularisation" that makes our basins of attraction more spherical

Rescaling Co-ordinates



AdaDelta

- We want to rescale the coordinates in proportion to the curvature in that direction
- To estimate the curvature we compute a running average of the squared gradients

$$S_i^g(t+1) = (1-\gamma)S_i^g(t) + \gamma\left(\frac{\partial L_{\mathcal{B}}(\boldsymbol{w}(t))}{\partial w_i(t)}\right)^2$$

- To estimate the relative scale of the weights we compute a running average of the squared weights

$$S_i^w(t+1) = (1-\gamma)S_i^w(t) + \gamma w_i(t)^2$$

AdaDelta

- The AdaDelta algorithm uses the update

$$w_i(t+1) = w_i(t) - \eta\sqrt{\frac{S_i^w(t+1)+\epsilon}{S_i^g(t+1)+\epsilon}}\frac{\partial L_{\mathcal{B}}(\boldsymbol{w}(t))}{\partial w_i(t)}$$

- Note that we can rescale the weights or rescale the gradients yet the update would be the same—this is one aspect of a covariant algorithm

- Because we are adaptively changing our step size we can use a single step size throughout the optimisation

Adding in Momentum

- AdaDelta doesn't use momentum (there is an argument this isn't so important as it has "regularised the landscape')'

- Nevertheless we can learn a momentum term

$$M_i(t+1) = (1-\beta)M_i(t) + \beta\frac{\partial L_{\mathcal{B}}(\boldsymbol{w}(t))}{\partial w_i(t)}$$

$$S_i(t+1) = (1-\gamma)S_i(t) + \gamma\left(\frac{\partial L_{\mathcal{B}}(\boldsymbol{w}(t))}{\partial w_i(t)}\right)^2$$

- These running averages have a lag time which we can remove

$$\hat{M}_i(t+1) = \frac{M_i(t+1)}{1-(1-\beta)^t} \qquad \hat{S}_i(t+1) = \frac{S(t+1)}{1-(1-\gamma)^t}$$

ADAM

- Adaptive Moment Estimation (Adam) adapts the scale of the parameters, but also uses momentum

- Update weights

$$w_i(t+1) = w_i(t) - \frac{\eta}{\sqrt{\hat{S}_i(t+1)+\epsilon}}\hat{M}_i(t+1)$$

- ADAM and its variants are very successful in deep learning

- It is very robust so often results in a network learning which might not learn under standard SGD (with momentum)

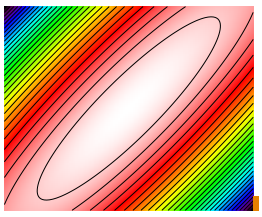
Covariant Equations

- Vector arithmetic, (matrix multiplication, addition, multiplying by a scale, computing gradients) has a covariant property that it is invariant to the coordinate system

- That is we can translate and rotate our coordinates and get the same result

- That is not true of element-wise multiplication of vectors

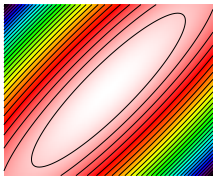
- Many ML algorithms do this (including ADAM and adaDelta), but they aren't invariant if we rotate our coordinates



Can't rescale coordinates

Correlated Weights

- Correlated weights will lead to skewed valleys
- Adaptive methods would be more efficient if they were rotationally invariant
- However, this would slow down the algorithm
- ADAM is a compromise between speed of implementation and effectiveness



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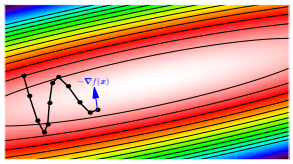
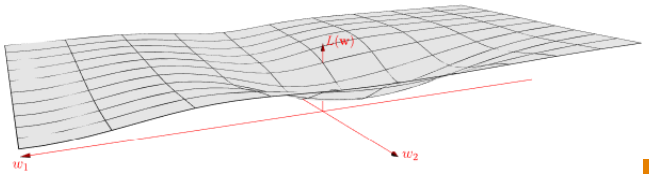


Loss Landscape

- A useful concept for understanding optimisation is the loss landscape
- For every value of the weights $\boldsymbol{w}$ there is some loss associated with it
- Note that this landscape is very high dimensional, so our intuition can be a bit misleading
- The landscape is also huge



Global and Local Minima

- Our objective is to minimise our loss
- This would mean finding the global minimum
- There are no algorithms that are guaranteed to find the global minimum
- The best we can hope is to find a local minimum by doing gradient descent
- In practice, our landscapes are so large that we are probably unable to find even a local minimum

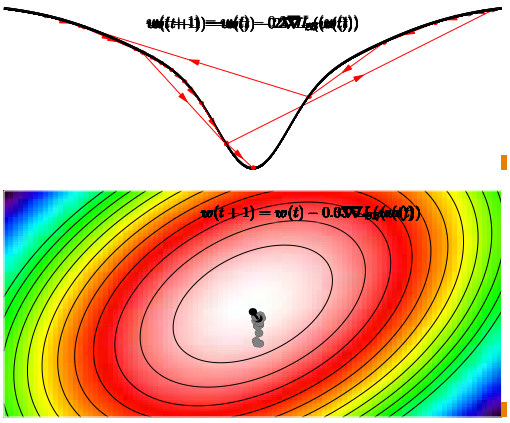
Noisy Optimisation

- Because we are using mini-batches we aren't actually following the correct gradients
- If we reduce our step size then our average gradient is closer to the true gradient
- Thus our optimisation is inherently noisy
- At least for deep learning there is no evidence that the weights stop changing even after learning for a huge amount of time

Valleys in Valleys in Valleys

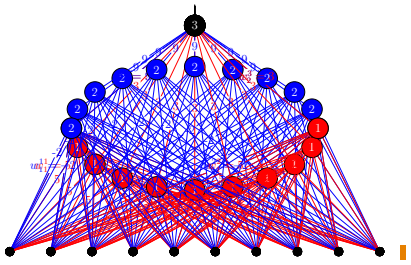
- My view of the loss landscape is that we have valleys inside bigger valleys insider bigger valleys, and so on
- If our noise is high (we use large step size), we can navigate away from local valleys and move towards the big valley
- But, we can't explore the small valleys
- Often when the rate of improvement slows down, practitioners will reduce their learning rate by a factor of 10 and the rate of improvement jumps up
- Some practitioners cycle through raising and lowering their learning rates which may speed up convergence

Reducing the Step Size



Symmetries

- When training neural networks (deep or shallow) there are typically many symmetries
- Examples come from exchanging the weights of neurons (or filters in CNNs) in two layers



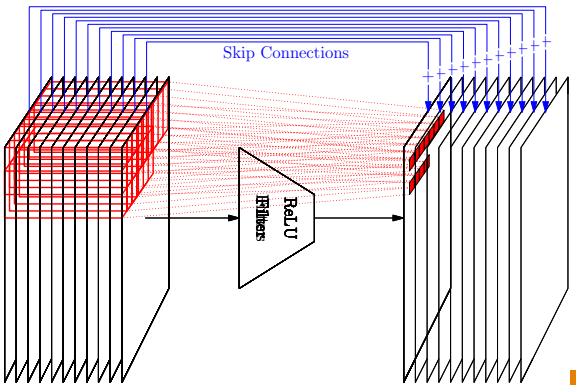
More Symmetries

- With n hidden nodes there are $n!$ symmetries
- Often if I multiply all the input and output weights to a node by -1 the network will be the same
- There are also continuous symmetries. For linear networks with two layers performing a mapping $\mathbf{W}_2\mathbf{W}_1$ then for any invertible matrix $\mathbf{U}$ (where $\mathbf{U}\mathbf{U}^{-1} = \mathbf{I}$)

$$\mathbf{W}_2\mathbf{W}_1 = \mathbf{W}_2\mathbf{I}\mathbf{W}_1 = \mathbf{W}_2(\mathbf{U}\mathbf{U}^{-1})\mathbf{W}_1 = (\mathbf{W}_2\mathbf{U})(\mathbf{U}^{-1}\mathbf{W}_1)$$

  so a network with weights $\mathbf{W}'_2 = \mathbf{W}_2\mathbf{U}$ and $\mathbf{W}'_1 = \mathbf{U}^{-1}\mathbf{W}_1$ will perform the same mapping
- There will be a huge space of equivalent networks

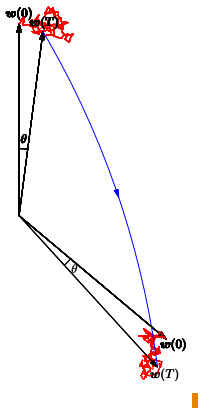
Skip Connections



- Breaks permutation symmetry. Used in Resnets, transformer, etc.

Symmetries

- The landscape potentially has a huge manifold with the same losses (neutral network)
- Find solution close to start
- We should think of optimisation more as a process of travelling than a process of arriving
- Of course even if we do minimise our loss we are not guaranteed to minimise our generalisation performance



Lessons

- SGD together with automatic differentiation has revolutionised machine learning
- There are a number of techniques to get the step size right: momentum, adaptive step size, ADAM
- Still need to understand that we are exploring a huge and complex loss landscape
- What works is problem specific (as always)