Appendix B — Optimizing Neural Networks

B.1 Strategies towards adaptive step-size

B.1.1 Running averages

We'll start by looking at the notion of a *running average*. It's a computational strategy for estimating a possibly weighted average of a sequence of data. Let our data sequence be $c_1, c_2, \ldots$; then we define a sequence of running average values, $C_0, C_1, C_2, \ldots$ using the equations

$$\begin{aligned} C_0 &= 0, \\ C_t &= \gamma_t \, C_{t-1} + (1 - \gamma_t) \, c_t, \end{aligned}$$

where $\gamma_t \in (0, 1)$. If γ_t is a constant, then this is a *moving* average, in which

$$\begin{aligned} C_T &= \gamma \, C_{T-1} + (1 - \gamma) \, c_T \\ &= \gamma \Big(\gamma \, C_{T-2} + (1 - \gamma) \, c_{T-1} \Big) + (1 - \gamma) \, c_T \\ &= \sum_{t=1}^{T} \gamma^{\,T-t} (1 - \gamma) \, c_t. \end{aligned}$$

So, you can see that inputs c_t closer to the end of the sequence have more effect on C_T than early inputs.

If, instead, we set $\gamma_t = \frac{t-1}{t}$, then we get the actual average.

> **? Study Question**
>
> Prove to yourself that the previous assertion holds.

B.1.2 Momentum

Now, we can use methods that are a bit like running averages to describe strategies for computing η. The simplest method is *momentum*, in which we try to "average" recent gradient updates, so that if they have been bouncing back and forth in some direction, we take out that component of the motion. For momentum, we have

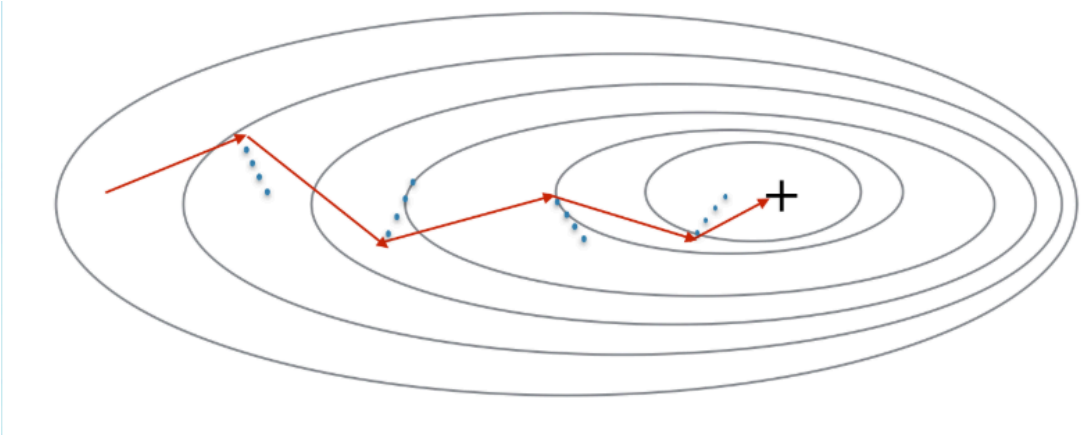
$$\begin{aligned} V_0 &= 0, \\ V_t &= \gamma \, V_{t-1} + \eta \, \nabla_W J(W_{t-1}), \\ W_t &= W_{t-1} - V_t. \end{aligned}$$

This doesn't quite look like an adaptive step size. But what we can see is that, if we let $\eta = \eta'(1-\gamma)$, then the rule looks exactly like doing an update with step size η' on a moving average of the gradients with parameter γ:

$$
\begin{aligned}
M_0 &= 0, \\
M_t &= \gamma\, M_{t-1} + (1-\gamma)\, \nabla_W J(W_{t-1}), \\
W_t &= W_{t-1} - \eta'\, M_t.
\end{aligned}
$$

> **? Study Question**
>
> Prove to yourself that these formulations are equivalent.

We will find that V_t will be bigger in dimensions that consistently have the same sign for ∇_W and smaller for those that don't. Of course we now have *two* parameters to set (η and γ), but the hope is that the algorithm will perform better overall, so it will be worth trying to find good values for them. Often γ is set to be something like 0.9.



Momentum

The red arrows show the update after each successive step of mini-batch gradient descent with momentum. The blue points show the direction of the gradient with respect to the mini-batch at each step. Momentum smooths the path taken towards the local minimum and leads to faster convergence.

> **? Study Question**
>
> If you set $\gamma = 0.1$, would momentum have more of an effect or less of an effect than if you set it to 0.9?

B.1.3 Adadelta

Another useful idea is this: we would like to take larger steps in parts of the space where $J(W)$ is nearly flat (because there's no risk of taking too big a step due to the gradient being large) and smaller steps when it is steep. We'll apply this idea to each weight independently, and end up with a method called *adadelta*, which is a

variant on *adagrad* (for adaptive gradient). Even though our weights are indexed by layer, input unit, and output unit, for simplicity here, just let W_j be any weight in the network (we will do the same thing for all of them).

$$
\begin{aligned}
g_{t,j} &= \nabla_W J(W_{t-1})_j, \\
G_{t,j} &= \gamma\, G_{t-1,j} + (1-\gamma)\, g_{t,j}^2, \\
W_{t,j} &= W_{t-1,j} - \frac{\eta}{\sqrt{G_{t,j}+\epsilon}}\, g_{t,j}.
\end{aligned}
$$

The sequence $G_{t,j}$ is a moving average of the square of the jth component of the gradient. We square it in order to be insensitive to the sign—we want to know whether the magnitude is big or small. Then, we perform a gradient update to weight j, but divide the step size by $\sqrt{G_{t,j}+\epsilon}$, which is larger when the surface is steeper in direction j at point W_{t-1} in weight space; this means that the step size will be smaller when it's steep and larger when it's flat.

B.1.4 Adam

Adam has become the default method of managing step sizes in neural networks.

Although, interestingly, it may actually violate the convergence conditions of SGD: arxiv.org/abs/1705.08292

It combines the ideas of momentum and adadelta. We start by writing moving averages of the gradient and squared gradient, which reflect estimates of the mean and variance of the gradient for weight j:

$$
\begin{aligned}
g_{t,j} &= \nabla_W J(W_{t-1})_j, \\
m_{t,j} &= B_1\, m_{t-1,j} + (1-B_1)\, g_{t,j}, \\
v_{t,j} &= B_2\, v_{t-1,j} + (1-B_2)\, g_{t,j}^2.
\end{aligned}
$$

A problem with these estimates is that, if we initialize $m_0 = v_0 = 0$, they will always be biased (slightly too small). So we will correct for that bias by defining

$$
\begin{aligned}
\hat{m}_{t,j} &= \frac{m_{t,j}}{1-B_1^t}, \\
\hat{v}_{t,j} &= \frac{v_{t,j}}{1-B_2^t}, \\
W_{t,j} &= W_{t-1,j} - \frac{\eta}{\sqrt{\hat{v}_{t,j}+\epsilon}}\, \hat{m}_{t,j}.
\end{aligned}
$$

Note that B_1^t is B_1 raised to the power t, and likewise for B_2^t. To justify these corrections, note that if we were to expand $m_{t,j}$ in terms of $m_{0,j}$ and $g_{0,j}, g_{1,j}, \ldots, g_{t,j}$, the coefficients would sum to 1. However, the coefficient behind $m_{0,j}$ is B_1^t and since $m_{0,j} = 0$, the sum of coefficients of nonzero terms is $1 - B_1^t$; hence the correction. The same justification holds for $v_{t,j}$.

> **? Study Question**

Define $\hat{m}_{t,j}$ directly as a moving average of $g_{t,j}$. What is the decay (γ parameter)?

Even though we now have a step size for each weight, and we have to update various quantities on each iteration of gradient descent, it's relatively easy to implement by maintaining a matrix for each quantity (m_t^ℓ, v_t^ℓ, g_t^ℓ, $g_t^{2\,\ell}$) in each layer of the network.

B.2 Batch Normalization Details

Let's think of the batch-normalization layer as taking Z^l as input and producing an output $\widehat{Z}^l$. But now, instead of thinking of Z^l as an $n^l \times 1$ vector, we have to explicitly think about handling a mini-batch of data of size K all at once, so Z^l will be an $n^l \times K$ matrix, and so will the output $\widehat{Z}^l$.

Our first step will be to compute the *batchwise* mean and standard deviation. Let μ^l be the $n^l \times 1$ vector where

$$\mu_i^l = \frac{1}{K} \sum_{j=1}^{K} Z_{ij}^l,$$

and let σ^l be the $n^l \times 1$ vector where

$$\sigma_i^l = \sqrt{\frac{1}{K} \sum_{j=1}^{K} \left(Z_{ij}^l - \mu_i^l\right)^2}.$$

The basic normalized version of our data would be a matrix, element (i, j) of which is

$$\overline{Z}_{ij}^l = \frac{Z_{ij}^l - \mu_i^l}{\sigma_i^l + \epsilon},$$

where ϵ is a very small constant to guard against division by zero.

However, if we let these be our $\widehat{Z}^l$ values, we really are forcing something too strong on our data—our goal was to normalize across the data batch, but not necessarily force the output values to have exactly mean 0 and standard deviation 1. So, we will give the layer the opportunity to shift and scale the outputs by adding new weights to the layer. These weights are G^l and B^l, each of which is an $n^l \times 1$ vector. Using the weights, we define the final output to be

$$\widehat{Z}_{ij}^l = G_i^l \overline{Z}_{ij}^l + B_i^l.$$

That's the forward pass. Whew!

Now, for the backward pass, we have to do two things: given $\frac{\partial L}{\partial \widehat{Z}^l}$,

- Compute $\frac{\partial L}{\partial Z^l}$ for back-propagation, and
- Compute $\frac{\partial L}{\partial G^l}$ and $\frac{\partial L}{\partial B^l}$ for gradient updates of the weights in this layer.

Schematically, we have

$$\frac{\partial L}{\partial B} = \frac{\partial L}{\partial \widehat{Z}} \frac{\partial \widehat{Z}}{\partial B}.$$

It's hard to think about these derivatives in matrix terms, so we'll see how it works for the components. B_i contributes to $\widehat{Z}_{ij}$ for all data points j in the batch. So,

$$\frac{\partial L}{\partial B_i} = \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}} \frac{\partial \widehat{Z}_{ij}}{\partial B_i} = \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}}.$$

Similarly, G_i contributes to $\widehat{Z}_{ij}$ for all data points j in the batch. Thus,

$$\frac{\partial L}{\partial G_i} = \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}} \frac{\partial \widehat{Z}_{ij}}{\partial G_i} = \sum_j \frac{\partial L}{\partial \widehat{Z}_{ij}} \overline{Z}_{ij}.$$

Now, let's figure out how to do backprop. We can start schematically:

$$\frac{\partial L}{\partial Z} = \frac{\partial L}{\partial \widehat{Z}} \frac{\partial \widehat{Z}}{\partial Z}.$$

And because dependencies only exist across the batch, but not across the unit outputs,

$$\frac{\partial L}{\partial Z_{ij}} = \sum_{k=1}^{K} \frac{\partial L}{\partial \widehat{Z}_{ik}} \frac{\partial \widehat{Z}_{ik}}{\partial Z_{ij}}.$$

The next step is to note that

$$\frac{\partial \widehat{Z}_{ik}}{\partial Z_{ij}} = \frac{\partial \widehat{Z}_{ik}}{\partial \overline{Z}_{ik}} \frac{\partial \overline{Z}_{ik}}{\partial Z_{ij}} = G_i \frac{\partial \overline{Z}_{ik}}{\partial Z_{ij}}.$$

And now that

$$\frac{\partial \overline{Z}_{ik}}{\partial Z_{ij}} = \left(\delta_{jk} - \frac{\partial \mu_i}{\partial Z_{ij}}\right) \frac{1}{\sigma_i} - \frac{Z_{ik} - \mu_i}{\sigma_i^2} \frac{\partial \sigma_i}{\partial Z_{ij}},$$

where $\delta_{jk} = 1$ if $j = k$ and 0 otherwise. We need two more pieces:

$$\frac{\partial \mu_i}{\partial Z_{ij}} = \frac{1}{K}, \qquad \frac{\partial \sigma_i}{\partial Z_{ij}} = \frac{Z_{ij} - \mu_i}{K\,\sigma_i}.$$

Putting the whole thing together, we get

$$\frac{\partial L}{\partial Z_{ij}} = \sum_{k=1}^{K} \frac{\partial L}{\partial \widehat{Z}_{ik}} G_i \frac{1}{K\,\sigma_i} \left(K\,\delta_{jk} - 1 - \frac{(Z_{ik} - \mu_i)(Z_{ij} - \mu_i)}{\sigma_i^2} \right).$$