# TTIC 31230, Fundamentals of Deep Learning

David McAllester An SGD Algorithm from Winter 2017

A Quenching SGD Algorithm

## Quenching

Steel is a mixture of iron and carbon. At temperatures below 727° C the carbon "freezes out" of the iron and we get iron grains separated by carbon sheets. But above 727° the carbon sheets "evaporate" into the iron and we get a homogeneous mixture of iron and carbon that is still a crystaline solid but with a different crystal structure (steel melts around 1510°). If we heat steel above 727° and then drop it in water the carbon does not have time to segregate out of the steel and we get "hardened steel" with a different lattice structure from slowly cooled grainy "soft steel". Hardened steel can be used as a cutting blade in a drill bit to drill into soft steel.

## Annealing and Tempering

Annealing is a process of gradually reducing the temperature. Gradual annealing produces soft grainy steel.

Tempering is a process of re-heating quenched steel to temperatures high enough to change its properties but below the original pre-quenching temperature. This can make the steel less brittle while preserving its hardness.

Acknowledgments to my eighth grade shop teacher.

## Is Quenching Desirable?

These slides describe an SGD algorithm that I designed at a time when I assumed that quenching was desirable — that one should design SGD to reach a local minimum as quickly as possible.

## A Quenching Algorithm

Suppose that we want to quench the parameters — to reach a local minimum as quickly as possible.

We must consider

- Gradient Estimation. The accuracy of  $\hat{g}$  as an estimate of g.
- Gradient Drift (second order structure). The fact that g changes as the parameters change.

## Analysis Plan

We will calculate a batch size  $B^*$  and learning rate  $\eta^*$  by optimizing an improvement guarantee for a single batch update.

We then use learning rate scaling to derive the learning rate  $\eta_B$  for a batch size  $B \ll B^*$ .

## Deriving Learning Rates

If we can calculate  $B^*$  and  $\eta^*$  for optimal loss reduction in a single batch we can calculate  $\eta_B$ .

$$\eta_B = B \ \eta_1$$

$$\eta^* = B^* \eta_1$$

$$\eta_1 = \frac{\eta^*}{B^*}$$

$$\eta_B = \frac{B}{B^*} \, \eta^*$$

## Calculating $B^*$ and $\eta^*$ in One Dimension

We will first calculate values  $B^*$  and  $\eta^*$  by optimizing the loss reduction over a single batch update in one dimension.

$$g = \hat{g} \pm \frac{2\hat{\sigma}}{\sqrt{B}}$$

$$\hat{\sigma} = \sqrt{E_{(x,y)\sim \text{Batch}} \left(\frac{d \operatorname{loss}(\beta, x, y)}{d\beta} - \hat{g}\right)^2}$$

# The Second Derivative of $loss(\beta)$

$$loss(\beta) = E_{(x,y) \sim Train} loss(\beta, x, y)$$

$$d^2 loss(\beta)/d\beta^2 \le L$$
 (Assumption)

$$loss(\beta - \Delta\beta) \le loss(\beta) - g\Delta\beta + \frac{1}{2}L\Delta\beta^2$$

$$loss(\beta - \eta \hat{g}) \le loss(\beta) - g(\eta \hat{g}) + \frac{1}{2}L(\eta \hat{g})^{2}$$

## A Progress Guarantee

$$loss(\beta - \eta \hat{g}) \le loss(\beta) - g(\eta \hat{g}) + \frac{1}{2}L(\eta \hat{g})^{2}$$

$$= loss(\beta) - \eta(\hat{g} - (\hat{g} - g))\hat{g} + \frac{1}{2}L\eta^2\hat{g}^2$$

$$\leq \log(\beta) - \eta \left(\hat{g} - \frac{2\hat{\sigma}}{\sqrt{B}}\right)\hat{g} + \frac{1}{2}L\eta^2\hat{g}^2$$

## Optimizing B and $\eta$

$$loss(\beta - \eta \hat{g}) \le loss(\beta) - \eta \left(\hat{g} - \frac{2\hat{\sigma}}{\sqrt{B}}\right) \hat{g} + \frac{1}{2}L\eta^2 \hat{g}^2$$

We optimize progress per gradient calculation by optimizing the right hand side divided by B. The derivation at the end of the slides gives

$$B^* = \frac{16\hat{\sigma}^2}{\hat{g}^2}, \quad \eta^* = \frac{1}{2L}$$

$$\eta_B = \frac{B}{B^*} \eta^* = \frac{B\hat{g}^2}{32\hat{\sigma}^2 L}$$

Recall this is all just in one dimension.

# Estimating $\hat{g}_{B^*}$ and $\hat{\sigma}_{B^*}$

$$\eta_B = \frac{B\hat{g}^2}{32\hat{\sigma}^2 L}$$

We are left with the problem that  $\hat{g}$  and  $\hat{\sigma}$  are defined in terms of batch size  $B^* >> B$ .

We can estimate  $\hat{g}_{B^*}$  and  $\hat{\sigma}_{B^*}$  using a running average with a time constant corresponding to  $B^*$ .

## Estimating $\hat{g}_{B^*}$

$$\hat{g}_{B^*} = \frac{1}{B^*} \sum_{(x,y) \sim \text{Batch}(B^*)} \frac{d \operatorname{Loss}(\beta, x, y)}{d\beta}$$

$$= \frac{1}{N} \sum_{s=t-N+1}^{t} \hat{g}^{s} \quad \text{with } N = \frac{B^{*}}{B} \text{ for batch size } B$$

$$\tilde{g}^{t+1} = \left(1 - \frac{B}{B^*}\right)\tilde{g}^t + \frac{B}{B^*}\hat{g}^{t+1}$$

We are still working in just one dimension.

# A Complete Calculation of $\eta$ (in One Dimension)

$$\tilde{g}^{t+1} = \left(1 - \frac{B}{B^*(t)}\right) \tilde{g}^t + \frac{B}{B^*(t)} \hat{g}^{t+1}$$

$$\tilde{s}^{t+1} = \left(1 - \frac{B}{B^*(t)}\right) \tilde{s}^t + \frac{B}{B^*(t)} (\hat{g}^{t+1})^2$$

$$\tilde{\sigma}^t = \sqrt{\tilde{s}^t - (\tilde{g}^t)^2}$$

$$B^*(t) = \begin{cases} K & \text{for } t \leq K \\ 16(\tilde{\sigma}^t)^2 / ((\tilde{g}^t)^2 + \epsilon) & \text{otherwise} \end{cases}$$

# A Complete Calculation of $\eta$ (in One Dimension)

$$\eta^t = \begin{cases} 0 & \text{for } t \leq K \\ \frac{(\tilde{g}^t)^2}{32(\tilde{\sigma}^t)^2 L} & \text{otherwise} \end{cases}$$

As  $t \to \infty$  we expect  $\tilde{g}^t \to 0$  and  $\tilde{\sigma}^t \to \sigma > 0$  which implies  $\eta^t \to 0$ .

## The High Dimensional Case

So far we have been considering just one dimension.

We now propose treating each dimension  $\Phi[i]$  of a high dimensional parameter vector  $\Phi$  independently using the one dimensional analysis.

We can calculate  $B^*[i]$  and  $\eta^*[i]$  for each individual parameter  $\Phi[i]$ .

Of course the actual batch size B will be the same for all parameters.

## A Complete Algorithm

$$\tilde{g}^{t+1}[i] = \left(1 - \frac{B}{B^*(t)[i]}\right) \tilde{g}^t[i] + \frac{B}{B^*(t)[i]} \hat{g}^{t+1}[i]$$

$$\tilde{s}^{t+1}[i] = \left(1 - \frac{B}{B^*(t)[i]}\right) \tilde{s}^t[i] + \frac{B}{B^*(t)[i]} \hat{g}^{t+1}[i]^2$$

$$\tilde{\sigma}^t[i] = \sqrt{\tilde{s}^t[i] - \tilde{g}^t[i]^2}$$

$$B^*(t)[i] = \begin{cases} K & \text{for } t \leq K \\ \lambda_B \tilde{\sigma}^t[i]^2 / (\tilde{g}^t[i]^2 + \epsilon) & \text{otherwise} \end{cases}$$

## A Complete Algorithm

$$\eta^{t}[i] = \begin{cases} 0 & \text{for } t \leq K \\ \frac{\lambda_{\eta} \tilde{g}^{t}[i]^{2}}{\tilde{\sigma}^{t}[i]^{2}} & \text{otherwise} \end{cases}$$

$$\Phi^{t+1}[i] = \Phi^{t}[i] - \eta^{t}[i]\hat{g}^{t}[i]$$

Here we have meta-parameters K,  $\lambda_B$ ,  $\epsilon$  and  $\lambda_{\eta}$ .

## Appendix: Optimizing B and $\eta$

$$loss(\beta - \eta \hat{g}) \le loss(\beta) - \eta \hat{g} \left( \hat{g} - \frac{2\hat{\sigma}}{\sqrt{B}} \right) + \frac{1}{2} L \eta^2 \hat{g}^2$$

Optimizing  $\eta$  we get

$$\hat{g}\left(\hat{g} - \frac{2\hat{\sigma}}{\sqrt{B}}\right) = L\eta\hat{g}^2$$

$$\eta^*(B) = \frac{1}{L} \left( 1 - \frac{2\hat{\sigma}}{\hat{q}\sqrt{B}} \right)$$

Inserting this into the guarantee gives

$$loss(\Phi - \eta \hat{g}) \le loss(\Phi) - \frac{L}{2} \eta^*(B)^2 \hat{g}^2$$

## Optimizing B

Optimizing progress per sample, or maximizing  $\eta^*(B)^2/B$ , we get

$$\frac{\eta^*(B)^2}{B} = \frac{1}{L^2} \left( \frac{1}{\sqrt{B}} - \frac{2\hat{\sigma}}{\hat{g}B} \right)^2$$

$$0 = -\frac{1}{2}B^{-\frac{3}{2}} + \frac{2\hat{\sigma}}{\hat{g}}B^{-2}$$

$$B^* = \frac{16\hat{\sigma}^2}{\hat{g}^2}$$

$$\eta^*(B^*) = \eta^* = \frac{1}{2L}$$
20

# Appendix II: A Formal Bound for the Vector Case

We will prove that minibatch SGD for a **sufficiently large batch size** (for gradient estimation) and a **sufficient small learning rate** (to avoid gradient drift) is guaranteed (with high probability) to reduce the loss.

This guarantee has two main requirements.

- A smoothness condition to limit gradient drift.
- A bound on the gradient norm allowing high confidence gradient estimation.

#### Smoothness: The Hessian

We can make a second order approximation to the loss.

$$\ell(\Phi + \Delta\Phi) \approx \ell(\Phi) + g^{\top} \Delta\Phi + \frac{1}{2} \Delta\Phi^{\top} H \Delta\Phi$$
$$g = \nabla_{\Phi} \ell(\Phi)$$
$$H = \nabla_{\Phi} \nabla_{\Phi} \ell(\Phi)$$

#### The Smoothness Condition

We will assume

$$||H\Delta\Phi|| \le L||\Delta\Phi||$$

We now have

$$\Delta \Phi^{\top} H \Delta \Phi \le L ||\Delta \Phi||^2$$

Using the second order mean value theorem one can prove

$$\ell(\Phi + \Delta\Phi) \le \ell(\Phi) + g^{\top} \Delta\Phi + \frac{1}{2} L||\Delta\Phi||^2$$

## A Concentration Inequality for Gradient Estimation

Consider a vector mean estimator where the vectors  $g_n$  are drawn IID.

$$g_n = \nabla_{\Phi} \ell_n(\Phi)$$
  $\hat{g} = \frac{1}{k} \sum_{n=1}^k g_n$   $g = E_n \nabla_{\Phi} \ell_n(\Phi)$ 

If with probability 1 over the draw of n we have  $|(g_n)_i - g_i| \le b$  for all i then with probability of at least  $1 - \delta$  over the draw of the sample

$$||\hat{g} - g|| \le \frac{\eta}{\sqrt{k}}$$
  $\eta = b \left( 1 + \sqrt{2\ln(1/\delta)} \right)$ 

Norkin and Wets "Law of Small Numbers as Concentration Inequalities ...", 2012, theorem 3.1

$$\ell(\Phi + \Delta\Phi) \leq \ell(\Phi) + g^{\top} \Delta\Phi + \frac{1}{2} L ||\Delta\Phi||^{2}$$

$$\ell(\Phi - \eta \widehat{g}) \leq \ell(\Phi) - \eta g^{\top} \widehat{g} + \frac{1}{2} L \eta^{2} ||\widehat{g}||^{2}$$

$$= \ell(\Phi) - \eta (\widehat{g} - (\widehat{g} - g))^{\top} \widehat{g} + \frac{1}{2} L \eta^{2} ||\widehat{g}||^{2}$$

$$= \ell(\Phi) - \eta ||\widehat{g}||^{2} + \eta (\widehat{g} - g)^{\top} \widehat{g} + \frac{1}{2} L \eta^{2} ||\widehat{g}||^{2}$$

$$\leq \ell(\Phi) - \eta ||\widehat{g}||^{2} + \eta \frac{\eta}{\sqrt{k}} ||\widehat{g}|| + \frac{1}{2} L \eta^{2} ||\widehat{g}||^{2}$$

$$= \ell(\Phi) - \eta ||\widehat{g}|| \left( ||\widehat{g}|| - \frac{\eta}{\sqrt{k}} \right) + \frac{1}{2} L \eta^{2} ||\widehat{g}||^{2}$$

## Optimizing $\eta$

Optimizing  $\eta$  we get

$$||\widehat{g}|| \left( ||\widehat{g}|| - \frac{\eta}{\sqrt{k}} \right) = -L\eta ||\widehat{g}||^2$$

$$\eta = \frac{1}{L} \left( 1 - \frac{\eta}{||\widehat{g}||\sqrt{k}} \right)$$

Inserting this into the guarantee gives

$$\ell(\Phi - \eta \widehat{g}) \le \ell(\Phi) - \frac{L}{2} \eta^2 ||\widehat{g}||^2$$

#### Optimizing k

Optimizing progress per sample, or maximizing  $\eta^2/k$ , we get.

$$\frac{\eta^2}{k} = \frac{1}{L^2} \left( \frac{1}{\sqrt{k}} - \frac{2\hat{\sigma}}{||\widehat{g}||k} \right)^2$$

$$0 = -\frac{1}{2} k^{-\frac{3}{2}} + \frac{2\hat{\sigma}}{||\widehat{g}||} k^{-2}$$

$$k = \left( \frac{22\hat{\sigma}}{||\widehat{g}||} \right)^2$$

$$\eta = \frac{1}{2L}$$

# $\mathbf{END}$