TTIC 31230, Fundamentals of Deep Learning

David McAllester, Winter 2018

Gradients as Dual Vectors

Hessian-Vector Products

Information Geometry

Coordinates

For a vector space we can make an arbitrary choice of basis vectors $b_1, \ldots, b_N$ that are linearly independent and span the space.

A basis defines coordinates $x[i]$ for each vector x.

$$x = x[1]b_1 + \cdots + x[N]b_N$$

The basis, and the induced coordinate system, is arbitrary.

Orthogonality is Coordinate-Relative

In two dimensions the vectors represented by $(1, 0)$ and $(0, 1)$ need not be orthogonal.

$(1, 0)$ represents b_1 and $(0, 1)$ represents b_2.

We only require that b_1 and b_2 are independent.

Hence inner product is coordinate-relative.

Inner Products in Taylor Expansions are Coordinate-Independent

$$f(\Phi + \Delta\Phi) \approx f(\Phi) + \left[\nabla_\Phi \, f(\Phi)\right](\Delta\Phi)$$

What is a Gradient?

The gradient $\nabla_\Phi f(\Phi)$ is the change in f per change in Φ.

More formally, $\nabla_\Phi f(\Phi)$ is a linear function from $\Delta\Phi$ to Δf.

$$f(\Phi + \Delta\Phi) \approx f(\Phi) + [\nabla_\Phi f(\Phi)](\Delta\Phi)$$

Coordinate-Free Definition of the Gradient

$$f(\Phi + \Delta\Phi) \approx f(\Phi) + \left[\nabla_\Phi f(\Phi)\right](\Delta\Phi)$$

$$f(\Phi + \epsilon\Delta\Phi) \approx f(\Phi) + \left[\nabla_\Phi f(\Phi)\right](\epsilon\Delta\Phi)$$

$$\frac{f(\Phi + \epsilon\Delta\Phi) - f(\Phi)}{\epsilon} \approx \left[\nabla_\Phi f(\Phi)\right](\Delta\Phi)$$

$$\left[\nabla_\Phi f(\Phi)\right](\Delta\Phi) \doteq \lim_{\epsilon \to 0} \frac{f(\Phi + \epsilon\Delta\Phi) - f(\Phi)}{\epsilon}$$

No coordinates required.

Dual Vectors

A dual vector is a linear function from vectors to scalars.

The gradient is a dual vector.

Coordinates

We calculate

$$[\nabla_\Phi f(\Phi)]\,\Delta\Phi$$

using coordinates.

$$[\nabla_\Phi f(\Phi)]\,\Delta\Phi \quad = \quad \sum_i \left[\frac{\partial f}{\partial \Phi[i]}\right] \Delta\Phi[i]$$

But this calculation is coordinate-independent.

$$[\nabla_\Phi\ f(\Phi)]\,(\Delta\Phi) \quad \equiv \quad \lim_{\epsilon\to 0}\ \frac{f(\Phi+\epsilon\Delta\Phi)-\ f(\Phi)}{\epsilon}$$

Strange Coordinate Systems

Consider any gradient $\nabla_\Phi f(\Phi)$ at any value of Φ.

For any such situation, and any vector $\Delta\Phi$ with $[\nabla_\Phi f(\Phi)]\,\Delta\Phi > 0$, and any learning rate $\eta > 0$, there exists a coordinate system in which $\eta\Phi.\text{grad}[c] = \Delta\Phi[c]$ and hence

$$\Phi_{t+1} = \Phi_t - \Delta\Phi$$

Note that gradient decent always yields $[\nabla_\Phi f(\Phi)]\,\Delta\Phi > 0$.

Proof

Define the basis vectors $b_1, \ldots, b_N$ by

$$b_1 \doteq \frac{\Delta\Phi}{\sqrt{\eta[\nabla_\Phi f(\Phi)]\Delta\Phi}} \qquad [\nabla_\Phi f(\Phi)]\ b_i = 0 \ \text{ for } i > 1$$

In this coordinate system we have

$$\Phi = \Phi[1]b_1 + \ldots + \Phi[N]b_n$$

$$\frac{\partial f(\Phi)}{\partial \Phi[1]} = \frac{\sqrt{[\nabla_\Phi f(\Phi)]\Delta\Phi}}{\sqrt{\eta}} \qquad \frac{\partial f(\Phi)}{\partial \Phi[j]} = 0 \quad \text{for } j > 0$$

$$\sum_i \Phi.\text{grad}[i]\Phi[i]b_i = \frac{\sqrt{[\nabla_\Phi f(\Phi)]\Delta\Phi}}{\sqrt{\eta}}\, b_1 = \frac{\Delta\Phi}{\eta}$$

Coordinate-Free Versions of SGD

Newton's Method

We can make a second order approximation to the loss function

$$f(\Phi + \Delta\Phi) \approx f(\Phi) + (\nabla_\Phi\, f(\Phi))\Delta\Phi + \frac{1}{2}\Delta\Phi^\top H \Delta\Phi$$

where H is the second derivative of f, the Hessian, equal to $\nabla_\Phi \nabla_\Phi\, f(\Phi)$.

Again, no coordinates are needed — we can define the operator ∇_Φ generally indpendent of coordinates.

$$\Delta\Phi_1^\top\; H\; \Delta\Phi_2 = (\nabla_\Phi\,((\nabla_\Phi\, f_t(\Phi)) \cdot \Delta\Phi_1)) \cdot \Delta\Phi_2$$

Newton's Method

We consider the first order expansion of the gradient.

$$\nabla_\Phi f(\Phi)\,|_{\Phi+\Delta\Phi} \approx (\nabla_\Phi f(\Phi)\,|_\Phi) + H\Delta\Phi$$

We approximate Φ^* by setting this gradient approximation to zero.

$$0 = \nabla_\Phi f(\Phi) + H\Delta\Phi$$

$$\Delta\Phi = -H^{-1}\,\nabla_\Phi f(\Phi)$$

This gives Newton's method (without coordinates)

$$\Phi \text{ -= } H^{-1}\,\nabla_\Phi f(\Phi)$$

Newton Updates

It seems safer to take smaller steps. So it is common to use

$$\Phi \;\texttt{-=}\; \eta\, H^{-1}\, \nabla_\Phi\, f(\Phi)$$

for $\eta \in (0, 1)$ where η is naturally dimensionless.

Most second order methods attempt to approximate making updates in the Newton direction.

The Gradient Covariance Martix

$$\Sigma \doteq E_t \, (\hat{g}_t - g)(\hat{g}_t - g)^\top$$

$$\Phi_{t+1} = \Phi_t - \eta \Sigma^{-1} \nabla_\Phi \text{Loss}(\Phi, x_t, y_y)$$

This is related to RMSProp.

Information Geometry and the Natural Gradient

We consider the case where loss is determined by a probability distribution. For example $-\log P(y)$.

The set of all distributions P forms a manifold.

For a given point (distribution) P we can consider the ball

$$B_\epsilon(P) = \{Q \mid KL(P, Q) \leq \epsilon\}$$

$$\Delta P = \underset{\Delta P \in B_\epsilon(P)}{\text{argmin}} \; f(P + \Delta P)$$

Distance Functions Define a Point-Wise Inner Product

For any smooth (doubly differentiable) function $d(x, y)$ with $d(x, y) \geq 0$ and $d(x, x) = 0$ we must have

$$\nabla_{\Delta x}\, d(x, x + \Delta x)|_{\Delta x=0} = 0$$

$$d(x, x + \Delta x) \approx \Delta x^{\top} H \Delta x$$

$$H \doteq \nabla_{\Delta x} \nabla_{\Delta x} d(x, x + \Delta x)|_{\Delta x=0}$$

The coordinate-independent gradient direction defined by $d(x, y)$ is then

$$H^{-1} \nabla_x f(x)$$

Information Geometry and Gradient Descent

For KL divergence H is diagonal with

$$\Delta P^\top H \Delta P = \sum_y \frac{\Delta P(y)^2}{P(y)}$$

Although KL is not symmetric, H happens to be the same for $KL(P, P + \Delta P)$ and $KL(P + \Delta P, P)$.

Hessian-Vector Products

$$H\Delta\Phi = \nabla_\Phi \left((\nabla_\Phi \ f^t(\Phi)) \cdot \Delta\Phi \right)$$

This is supported in PyTorch — in PyTorch Φ.grad is a variable while Φ.grad.data is a tensor.

Hessian-Vector Products

For backpropagation to be efficient it is important that the value of the graph is a scalar (like a loss). But note that for v fixed we have that

$$(\nabla_\Phi \, f^t(\Phi)) \cdot v$$

is a scalar and hence its gradient with respect to Φ, which is Hv, can be computed efficiently.

Complex-Step Differentiation

Consider a function $f : \mathbb{R} \to \mathbb{R}$ defined by a computer program.

For C code on a CPU we can run program the program on complex numbers simply by changing the data type of x.

James Lyness and Cleve Moler, Numerical Differentiation of Analytic Functions SIAM J. of Numerical Analysis, 1967.

Complex-Step Differentiation

Consider $f(x+i\epsilon)$ at real input x and consider the first order Taylor expansion.

$$f(x+i\epsilon) = f(x) + i(df/dx)\epsilon$$

Note that $f(x)$ and df/dx must both be real. Therefore

$$\mathrm{Im}(f(x+i\epsilon)) = \epsilon(df/dx)$$

$$\frac{df}{dx} = \frac{\mathrm{Im}(f(x+i\epsilon))}{\epsilon}$$

Complex-Step Differentiation

$$\frac{df}{dx} = \frac{\mathrm{Im}(f(x + i\epsilon))}{\epsilon}$$

This is vastly better than

$$\frac{df}{dx} \approx \frac{f(x + \epsilon) - f(x)}{\epsilon}$$

The point is that in complex arithmetic the real and imaginary parts have independent floating point representations.

In 64 bit floating point arithmetic ϵ can be taken to be 2^{-50}.

For $\epsilon = 2^{-50}$, division by ϵ simply changes the exponent of the floating point representation leaving the mantissa unchanged.

First Order Polynomial Arithmetic

Numerically, complex-step differentiation is equivalent to first order polynomial arithmetic.

$$(a + b\epsilon)(a' + b'\epsilon) = (a + a') + (ab' + a'b)\epsilon$$

Differentiation based on first order polynomial arithmetic is exact.

Equivalence to Polynomial Arithmetic

$$(a + ib\epsilon)(a' + ib'\epsilon) = (a + a' - bb'\epsilon^2) + i(ab' + a'b)\epsilon$$

$$\epsilon = 2^{-50}$$

Here the ϵ^2 term is below the precision of $a + a'$.

Numerically, complex-step arithmetic and first order polynomial arithmetic are the same.

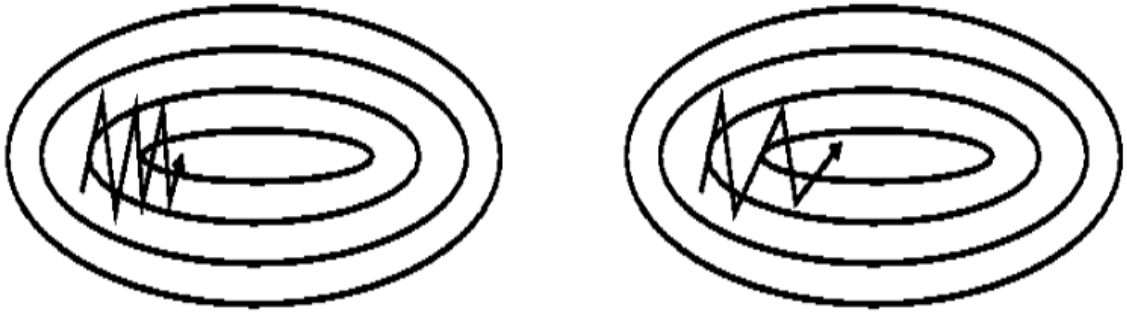
Hessian-Vector Products

We are interested in computing $H_t v$ for $v = (\eta \odot \hat{g})$.

$$H_t v = \frac{\mathrm{Im}(\nabla_\Phi f(\Phi)|_{\Phi + i\epsilon v})}{\epsilon}$$

$$\epsilon = 2^{-50}$$

Second Order SGD



Rudin's blog

Focusing on the Hessian.

Quasi-Newton Methods

It is often faster and more effective to approximate the Hessian.

Maintain an approximation $M \approx H^{-1}$.

Repeat:

- Φ **-=** $\eta M \nabla_\Phi f(\Phi)$ (η is often optimized in this step).
- Restimate M.

The restimation of M typically involves a finite difference

$$\left(\nabla_\Phi f(\Phi) \mid_{\Phi_{t+1}}\right) - \left(\nabla_\Phi f(\Phi) \mid_{\Phi_t}\right)$$

As a numerical approximation of $H\Delta\Phi$.

Quasi-Newton Methods

Conjugate Gradient

BFGS

Limited Memory BFGS

Issues with Quasi-Newton Methods

In SGD the gradients are random even when Φ does not change.

We cannot use

$$\left(\nabla_\Phi \, f_{t+1}(\Phi)|_{\Phi_{t+1}}\right) - \left(\nabla_\Phi \, f_t(\Phi) \, |_{\Phi_t}\right)$$

as an estimate of $H\Delta\Phi$.

Issues

- **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.

- **Convergence.** To converge to a local optimum the learning rate must be gradually reduced toward zero.

The Classical Convergence Theorem

$$\Phi_{t+1} \;=\; \Phi_t - \eta_t \nabla_\Phi \,\mathrm{loss}(\Phi, x_t, y_t)$$

For sufficiently smooth loss functions, and holding the coordinate system constant through time, and for

$$\eta_t > 0 \quad \text{and} \quad \lim_{t\to\infty} \eta_t = 0 \quad \text{and} \quad \sum_t \eta_t = \infty,$$

the loss value of SGD converges.

Structure From Motion

See the Videos
https://www.youtube.com/watch?v=i7ierVkXYa8
http://www.mada.org.il/brain/Shape/shape.html

The Levenberg-Marquart Algorithm (Bundle Adjustment)

$$\text{Loss} = E_{(x,y)\sim\text{Train}} \frac{1}{2}||f_\Phi(x) - y||^2$$

$$f_{\Phi+\Delta\Phi}(x_t) \approx f_\Phi(x_t) + J_t\Delta\Phi$$

$$J_t = \nabla_\Phi \, f_\Phi(x_t)$$

$$\hat{g}_t = (f_\Phi(x_t) - y_t)J_t \quad = r_t J_t$$

$$r_t = f_\Phi(x_t) - y_t$$

The Levenberg-Marquart Algorithm

$$\text{Loss}(\Phi + \Delta\Phi) \approx E_t \ \frac{1}{2}||r_t + J_t\Delta\Phi||^2$$

Minimizing this squared error over the choice of $\Delta\Phi$ is a least squares regression problem.

$$0 = E_t \ (r_t + J_t\Delta\Phi)J_t$$

$$0 = (E_t \ r_t J_t) + E_t \ J_t^\top J_t\Delta\Phi$$

$$(E_t \ J_t^\top J_t)\Delta\Phi = -E_t \ \hat{g}_t$$

$$\Delta\Phi = -(E_t \ J_t^\top J_t)^{-1}(E_t \ \hat{g}_t)$$

A General Loss Function

$$\text{Loss}_t(f(\Phi + \Delta\Phi)) \approx L_t + \hat{g}_t^\top \Delta\Phi + (J_t \Delta\Phi)^\top H_t \; J_t \Delta\Phi$$

$$J_t \doteq \nabla_\Phi \; f(\Phi)$$

$$H_t \doteq \nabla_f \nabla_f \; \text{Loss}_t(f)$$

Setting the gradient to zero and solving for $\Delta\Phi$:

$$\Delta\Phi_t = -(E_t \;\; J_t^\top H_t \; J_t)^{-1} \hat{g}_t$$

The Levenberg-Marquart Algorithm for Log Loss

$$\Phi_{t+1} = \Phi_t - \eta(E_t \;\; J_t^\top H_t \; J_t)^{-1} \hat{g}_t$$

$$\begin{aligned}
\text{Loss}(\Phi, x, y) &= -\log Q_{f_\Phi(x)}(y) \\
Q_f(y) &= \underset{y}{\text{softmax}}\, f(y) \\
H_t &= E_{y \sim Q_{f_t}} (\delta_y - Q_{f_t})(\delta_y - Q_{f_t})^\top \\
&= \text{Diag}(Q_{f_t}) - Q_{f_t} Q_{f_t}^T
\end{aligned}$$

END