

Lecture 3 Part 2: Finite-difference Approximations

MIT 18.S096 Matrix Calculus For Machine Learning and Beyond

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1 Finite-difference approximation for vector-to-scalar functions

This part largely follows from Section 8.1 of Numerical Optimization by Nocedal and Wright.

There are so many assumptions (colored in red)!

1.1 Truncation error

Consider a twice continuously differentiable function $f: \mathbb{R}^n \rightarrow \mathbb{R}$. Let $x, p \in \mathbb{R}^n$. Then, by Taylor's theorem,

$$f(x+p) = f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x+tp) p \quad \text{for some } t \in (0, 1).$$

Note that this is actually pretty interesting because $\nabla^2 f(x+tp)$ is the Hessian of a point on the line that interpolates x and p .

Continuing on:

$$\begin{aligned} f(x+p) &= f(x) + \nabla f(x)^T p + \frac{1}{2} p^T \nabla^2 f(x+tp) p \\ f(x+p) - f(x) - \nabla f(x)^T p &= \frac{1}{2} p^T \nabla^2 f(x+tp) p \\ \|f(x+p) - f(x) - \nabla f(x)^T p\| &= \left\| \frac{1}{2} p^T \nabla^2 f(x+tp) p \right\| \\ \|f(x+p) - f(x) - \nabla f(x)^T p\| &\leq \frac{1}{2} \|p^T\| \|\nabla^2 f(x+tp)\| \|p\|. \end{aligned}$$

Let L be the bound on $\|\nabla^2 f(\cdot)\|$ in the region of interest. Obtain

$$\|f(x+p) - f(x) - \nabla f(x)^T p\| \leq (L/2) \|p\|^2.$$

If we choose p to be εe_i , then $\nabla f(x)^T p = \varepsilon (\partial f / \partial x_i)$ and $\|p\|^2 = \varepsilon^2$. Obtain

$$\begin{aligned} -(L/2)\varepsilon^2 &\leq f(x + \varepsilon e_i) - f(x) - \varepsilon \frac{\partial f}{\partial x_i}(x) \leq (L/2)\varepsilon^2 \\ -f(x + \varepsilon e_i) + f(x) - (L/2)\varepsilon^2 &\leq -\varepsilon \frac{\partial f}{\partial x_i}(x) \leq -f(x + \varepsilon e_i) + f(x) + (L/2)\varepsilon^2 \\ \frac{f(x + \varepsilon e_i) - f(x)}{\varepsilon} + (L/2)\varepsilon &\geq \frac{\partial f}{\partial x_i}(x) \geq \frac{f(x + \varepsilon e_i) - f(x)}{\varepsilon} - (L/2)\varepsilon \\ \frac{\partial f}{\partial x_i}(x) &= \frac{f(x + \varepsilon e_i) - f(x)}{\varepsilon} + \delta_\varepsilon \quad \text{where } |\delta_\varepsilon| \leq (L/2)\varepsilon. \end{aligned}$$

δ_ε is commonly referred to as the *truncation error*. This becomes *forward difference* formula if we ignore the δ_ε term, which becomes smaller and smaller as $\varepsilon \rightarrow 0$.

1.2 Round-off error

For simplicity, **assume that the relative error in the computed f is bounded by \mathbf{u}** (\mathbf{u} is about 10^{-16} in double-precision representation) (I don't really know when this assumption is reasonable.):

$$\begin{aligned} |\text{comp}(f(x) - f(x))| &\leq \mathbf{u}L_f \\ |\text{comp}(f(x + \varepsilon e_i) - f(x + \varepsilon e_i))| &\leq \mathbf{u}L_f, \end{aligned}$$

where $\text{comp}(\cdot)$ denotes the computed value, and L_f is a bound on the value of $|f(\cdot)|$ in the region of interest. If we use the computed values in the forward difference formula

$$\frac{\partial f}{\partial x_i}(x) = \frac{f(x + \varepsilon e_i) - f(x)}{\varepsilon} + \delta_\varepsilon,$$

we get

$$|\delta_\varepsilon| \leq \underbrace{(L/2)\varepsilon}_{\text{truncation error}} + \underbrace{2\mathbf{u}L_f/\varepsilon}_{\text{round-off error}}.$$

Notice how the truncation error decreases as $\varepsilon \rightarrow 0$, while the round-off error blows up as $\varepsilon \rightarrow 0$.

Taking the derivative of this expression with respect to ε and setting it to zero, we obtain

$$\varepsilon^* = \sqrt{\frac{4L_f\mathbf{u}}{L}}.$$

Assuming that $4L_f/L \approx 1$, we get

$$\varepsilon^* = \sqrt{\mathbf{u}},$$

which is what's used in most packages. In PyTorch, $\mathbf{u} = 1 \times 10^{-6}$.

2 Finite-difference approximation for matrix-to-matrix functions

Let v be a generic vector (could be a scalar, a vector or a matrix). Then, in the differential notation, we have

$$f(v + dv) - f(v) = f'(v)[dv] + \text{higher-order terms}.$$

When dv is very small, we have

$$f(v + dv) - f(v) \approx f'(v)[dv].$$

$f'(v)[\cdot]$ would typically be something that we derive by hand or autograd – we can check the correctness of this derivation by first choosing a small dv and then comparing $f(v + dv) - f(v)$ and $f'(v)[dv]$ – their difference should be small.

How should we measure their difference? Ratio of norms:

$$\frac{\|\text{estimated} - \text{truth}\|}{\|\text{truth}\|}$$

For matrices, we would use the Frobenius norm.

$f(v + dv) - f(v)$ is called the *forward* difference. We also could have chosen $f(v) - f(v - dv)$, the *backward* difference. But it turns out that the *central* difference usually works the best:

$$f\left(v + \frac{1}{2}dv\right) - f\left(v - \frac{1}{2}dv\right).$$