

is to compare the derivatives computed by your implementation of automatic differentiation to the derivatives computed by a **finite differences**. Because

$$f'(x) = \lim_{\epsilon \rightarrow 0} \frac{f(x + \epsilon) - f(x)}{\epsilon}, \quad (11.5)$$

we can approximate the derivative by using a small, finite ϵ :

$$f'(x) \approx \frac{f(x + \epsilon) - f(x)}{\epsilon}. \quad (11.6)$$

We can improve the accuracy of the approximation by using the **centered difference**:

$$f'(x) \approx \frac{f(x + \frac{1}{2}\epsilon) - f(x - \frac{1}{2}\epsilon)}{\epsilon}. \quad (11.7)$$

The perturbation size ϵ must be chosen to be large enough to ensure that the perturbation is not rounded down too much by finite-precision numerical computations.

Usually, we will want to test the gradient or Jacobian of a vector-valued function $g : \mathbb{R}^m \rightarrow \mathbb{R}^n$. Unfortunately, finite differencing only allows us to take a single derivative at a time. We can either run finite differencing mn times to evaluate all of the partial derivatives of g , or we can apply the test to a new function that uses random projections at both the input and output of g . For example, we can apply our test of the implementation of the derivatives to $f(x)$ where $f(x) = \mathbf{u}^T g(\mathbf{v}x)$, where \mathbf{u} and \mathbf{v} are randomly chosen vectors. Computing $f'(x)$ correctly requires being able to back-propagate through g correctly, yet is efficient to do with finite differences because f has only a single input and a single output. It is usually a good idea to repeat this test for more than one value of \mathbf{u} and \mathbf{v} to reduce the chance that the test overlooks mistakes that are orthogonal to the random projection.

If one has access to numerical computation on complex numbers, then there is a very efficient way to numerically estimate the gradient by using complex numbers as input to the function (Squire and Trapp, 1998). The method is based on the observation that

$$f(x + i\epsilon) = f(x) + i\epsilon f'(x) + O(\epsilon^2) \quad (11.8)$$

$$\text{real}(f(x + i\epsilon)) = f(x) + O(\epsilon^2), \quad \text{imag}\left(\frac{f(x + i\epsilon) - f(x)}{\epsilon}\right) = f'(x) + O(\epsilon^2), \quad (11.9)$$

where $i = \sqrt{-1}$. Unlike in the real-valued case above, there is no cancellation effect due to taking the difference between the value of f at different points. This allows the use of tiny values of ϵ like $\epsilon = 10^{-150}$, which make the $O(\epsilon^2)$ error insignificant for all practical purposes.