Appendix D

Discretization of the Derivative Operator

In this appendix, we consider the problem of evaluating the derivative of a function known at a finite number of points on an equally spaced grid. This is the case for examples when the variable is age or time. We report here a simple way to obtain an approximate derivative of arbitrary order and refer the reader to texts on numerical analysis for an analysis of the error. The equations given here will reproduce, with appropriate choices of the parameters, well known formulas (like the Richardson extrapolation, Press et al., 1987).

Let $f(x)$ be a function whose values are known on an integer grid (so x is always an integer in the following). Our problem is to evaluate the derivative of some order at the point x. The starting point is to assume that f can be represented by a polynomial of degree k:

$$f(x+n) = f(x) + \sum_{j=1}^{k} \frac{n^j}{j!} f^{(j)}(x), \tag{D.1}$$

where the k derivatives $f^{(j)}(x)$ in this expression are unknown. The idea here is that, if we evaluate equation D.1 at k different points, we obtain a linear system that we can solve for $f^{(j)}(x)$.

Let $\mathbf{n}$ be a set of k integers that excludes 0, for example, $\mathbf{n} = \{-2, -1, 1, 2\}$. We then rewrite equation D.1 as

$$f(x+n_i) - f(x) = \sum_{j=1}^{k} A_{ij} f^{(j)}(x) \quad i = 1, \ldots k,$$

where the matrix A has elements $A_{ij} \equiv \frac{n_i^j}{j!}$. By inverting this linear system, we obtain the intuitively pleasing formula:

$$f^{(j)}(x) = \sum_{i=1}^{k} A_{ji}^{-1} [f(x+n_i) - f(x)]. \tag{D.2}$$

This is just the statement of the fact that the derivative of order j at a point is a weighted combination of the values of the function at nearby points: the points $f(x+n_i)$ receive a weight A_{ji}^{-1}, while $f(x)$ receives a weight $-\sum_{i=1}^{k} A_{ji}^{-1}$, so that the sum of the weights is zero.

With reasonable choices of the set of integers $\mathbf{n}$, equation D.2 is sufficient to recover the standard formulas for numerical derivatives. For example, choosing $k = 4$ and $\mathbf{n} = \{-2, -1, 1, 2\}$, we obtain, for $j = 2$, the classic five-point central second derivative formula, which is fourth-order accurate:

$$f^{(2)}(x) \approx \frac{1}{12} \left(f(x-2) - 8f(x-1) + 8f(x+1) - f(x+2) \right).$$

While choosing a set $\mathbf{n}$ that is symmetric around the origin is always recommended, a nonsymmetric $\mathbf{n}$ is needed when the function is defined over a finite segment, and we need to evaluate the derivative near the end points. For example, if we know the values of the function at the integers $0, 1, \ldots 10$ and we want the derivative at $x = 0$ using a five-point formula (that is, $k = 4$), the boundary at 0 forces us to choose $\mathbf{n} = \{1, 2, 3, 4\}$. Following the criterion that the set $\mathbf{n}$ should be as symmetric as possible, for the evaluation of the second derivative at $x = 1$, we will make the choice $\mathbf{n} = \{-1, 1, 2, 3\}$. Therefore, if we denote by $\mathbf{f}$ the vector whose elements are the values of the function f on an integer grid, its derivative of order j is the vector $D^j\mathbf{f}$, where D^j is a square matrix whose rows contain the weights that can be computed according to equation D.2. The matrix D^j is a k-band matrix: except for the first and last few rows, where we cannot use a symmetric choice of n, the elements along the band are equal to each other. In addition, we know from equation D.2 that each row sums up to 0, that is, $\sum_{ij} D^j_{ik} = 0$. This property is just a reflection of the fact that any differential operator of degree at least one annihilates the constant function, that is, $D^j\mathbf{f} = 0$, if $\mathbf{f}$ is a constant vector.

For example, using $k = 4$ and $j = 1$ we have

$$D^1 = \left|\begin{array}{cccccccccccc}
-2.0833 & 4 & -3 & 1.333 & -0.25 & 0 & 0\;0\;0\;0\;0\;0 & 0 & 0 & 0 & 0 & 0 \\
-0.25 & -0.8333 & 1.5 & -0.5 & 0.083 & 0 & 0\;0\;0\;0\;0\;0 & 0 & 0 & 0 & 0 & 0 \\
0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 & 0 & 0\;0\;0\;0\;0\;0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 & 0\;0\;0\;0\;0\;0 & 0 & 0 & 0 & 0 & 0 \\
. & . & . & . & . & . & .\;.\;.\;.\;.\;. & . & . & . & . & . \\
0 & 0 & 0 & 0 & 0 & 0 & 0\;0\;0\;0\;0\;0 & 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 \\
0 & 0 & 0 & 0 & 0 & 0 & 0\;0\;0\;0\;0\;0 & -0.083 & 0.5 & -1.5 & 0.8333 & 0.25 \\
0 & 0 & 0 & 0 & 0 & 0 & 0\;0\;0\;0\;0\;0 & 0.25 & -1.333 & 3 & -4 & 2.0833
\end{array}\right|.$$

The matrix D^1 is nearly antisymmetric (i.e., is antisymmetric except for the “border” effects). This is not an accident: it follows from simple properties of differential operators that D^j will be almost antisymmetric for j odd and almost symmetric for j even.