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MATHEMATISCH-NATURWISSENSCHAFTLICHE FAKULTÄT II
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Introduction to Algorithmic Differentiation

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Exercise Set 1

Consider the following function of $x = (x_1, x_2, x_3, x_4) \in \mathbb{R}^4_{+0}$

$$f(x) = (x_2 + x_1)^2 \frac{1}{4x_4} \frac{u^3(u - \cos u \sin u)}{(u \cos u - \sin u)^2} + (x_2 - x_1)^2 \frac{1}{4x_4} \frac{u(u + \cos u \sin u)}{\sin^2 u}$$

with

$$u = \frac{x_3 x_4}{2}$$

Exercise 1.1. Any operation that is provided natively in a simple programming language (C++/Python ...) or a desktop scientific calculator is called an elementary operation. Identify the elementary operations required to compute $f(x)$ and make a table for the elementary partial derivatives.

Exercise 1.2. A computational graph is a directed acyclic graph where the vertices represent the results of elementary operations and the edges point from the operands to the result. The edges are annotated with the elementary partial derivatives. Sketch a computational graph with minimal number of vertices for the computation of $f(x)$.

Exercise 1.3. Write a computational procedure for $f(x)$ using the computational graph, let each vertex be denoted by a variable v_i $i \in \{-3, -2, \ldots, N_{\text{vertices}}\}$ such that

$$v_{-3} = x_1 \quad v_{-2} = x_2 \quad v_{-1} = x_3 \quad v_0 = x_4 \quad \text{and} \quad v_{N_{\text{vertices}}} = y = f(x)$$

Exercise 1.4. Assume the vector $(\dot{v}_{-3}, \ldots, \dot{v}_0)$ to be a cartesian basis vector. In the computational graph go over all the vertices one by one in vertex order starting from v_1. For incoming edges to the vertex v_i such that $v_j \xrightarrow{q_1} v_i$ and $v_k \xrightarrow{q_2} v_i$ assign $\dot{v}_i = q_1 \cdot \dot{v}_j + q_2 \cdot \dot{v}_k$. Inline this procedure with the one in Exercise 1.3, so that $\dot{v}_i$ is computed right after v_i was computed. Write up the inlined procedure. Comment on the value $\dot{v}_{N_{\text{vertices}}}$.

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Exercise 1.5. Differentiate $f(x)$ symbolically (Maple/Mathematica/By Hand) and observe the blow up in expression length. Count the number of operations required to compute the derivative numerically after symbolic differentiation.

Exercise 1.6. Count the number of operations required to execute the procedures from Exercise 1.4. Write a finite difference procedure to compute the directional derivative of $f(x)$ along the cartesian basis vectors. Compare the number of operations required by the finite difference procedure and procedure from Exercise 1.4 so that all gradient components are computed.

Exercise 1.7. Implement these procedures in a program (C++/ Python/ Ruby/ FreePascal/ Perl) and compare the results. Plot the difference between the finite difference gradient for varying ρ and the vector obtained after running the procedure from Exercise 1.4 with each cartesian basis at $x = \left(0, \frac{1}{\sqrt{3}}, \pi, \frac{3}{2}\right)$. *Hint: Use logarithmic scales to plot ρ on the x-axis and the euclidean norm of the difference vector on the y axis. ρ may be varied between* 0.1 *and* 10^{-16}.

Exercise 1.8. Assume the vector $(\dot{v}_{-3}, \ldots, \dot{v}_0)$ to be a cartesian basis vector. Assume all other $\dot{v}_i = 0, \forall i \in \{1 \ldots, N_{\text{vertices}}\}$. Traverse the computational graph starting from the vertex that has $\dot{v}_i = 1 (i \in \{-3, \ldots, 0\})$. For each outgoing edge $v_i \xrightarrow{q} v_j$ add the vertex v_j in a list and assign $\dot{v}_j$ += $q \cdot \dot{v}_i$. Mark the edges as traversed. Remove the next vertex from the list that has the largest number of outgoing edges and repeat the above process until the list is empty. Take care that the vertex you remove from the list has no untraversed incoming path from the starting vertex. If so traverse that path as detailed above first. Comment on the value of $\dot{v}_{N_{\text{vertices}}}$. Compare the number of operations required with that of the procedure in Exercise 1.4 and with the finite difference gradients for computing all gradient components.

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