Generalized Dual Numbers and Higher-Order Automatic Differentiation

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Algebraic Foundations

Definition (Generalized Dual Numbers)**.** *Let $n \in \mathbb{N}$ be the number of variables and $m \in \mathbb{N}$ the order of the Taylor expansion of a function. Define a set of symbols $\{\varepsilon_1, \dots, \varepsilon_n\}$ with the following properties:*

$$\varepsilon_i^{m+1} = 0, \quad \varepsilon_i^j \neq 0 \text{ for } 1 \leq j \leq m, \quad \text{and } \varepsilon_i \varepsilon_j = \varepsilon_j \varepsilon_i.$$

Let $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$ be a multi-index with $|\alpha| = \sum_i \alpha_i$, and define $\varepsilon^\alpha := \varepsilon_1^{\alpha_1} \cdots \varepsilon_n^{\alpha_n}$. Then a generalized dual number is of the form:

$$X := f_0 + \sum_{1 \leq |\alpha| \leq m} f_\alpha \, \varepsilon^\alpha, \quad f_\alpha \in \mathbb{R}.$$

Theorem (Taylor Expansion via Generalized Dual Numbers)**.** *Let $f : \mathbb{R}^n \to \mathbb{R}$ be a smooth function. Then:*

$$f\big(\mathbf{x} + \varepsilon\big) = f(\mathbf{x}) + \sum_{1 \leq |\alpha| \leq m} \frac{1}{\alpha!} \, \partial^\alpha f(\mathbf{x}) \, \varepsilon^\alpha,$$

where $\partial^\alpha := \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}$.

Proof (Sketch). *Follows from the multidimensional Taylor expansion of the function f around the point $\mathbf{x}$, where the symbols ε_i act as formal differential elements (analogous to symbolic differentiation), with nilpotency $\varepsilon_i^{m+1} = 0$ causing truncation of the series.*

Proposition (Practical Application)**.** *By wrapping the function f within the generalized dual algebra, all partial derivatives up to order m can be computed simultaneously in a single evaluation.*

[1]

[1]Truncated Taylor Algebra: https://darioizzo.github.io/audi/theory_algebra.html

Approximate Integration via Multivariate Taylor Polynomials

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a sufficiently smooth function on the hyper-rectangle $\mathbf{A} = (A_1, \ldots, A_n)$, $\mathbf{B} = (B_1, \ldots, B_n)$. Partition the domain into boxes by subdividing each dimension i into N_i intervals of length $h_i = \frac{B_i - A_i}{N_i}$, with centers $\mathbf{c_j}$.

Around each center, approximate f by its Taylor polynomial of order m:

$$f(\mathbf{x}) \approx \sum_{|\alpha| \leq m} \frac{D^\alpha f(\mathbf{c_j})}{\alpha!} (\mathbf{x} - \mathbf{c_j})^\alpha.$$

Integrating each monomial over the box yields a separable product of one-dimensional integrals:

$$\int_{\text{box}_\mathbf{j}} (\mathbf{x} - \mathbf{c_j})^\alpha d\mathbf{x} = \prod_{i=1}^{n} \frac{(h_i/2)^{\alpha_i+1} - (-h_i/2)^{\alpha_i+1}}{\alpha_i + 1}.$$

Summing over all boxes and multi-indices gives the approximate integral:

$$\int_{\mathbf{A}}^{\mathbf{B}} f(\mathbf{x}) d\mathbf{x} \approx \sum_{\mathbf{j}} \sum_{|\alpha| \leq m} \frac{D^\alpha f(\mathbf{c_j})}{\alpha!} \prod_{i=1}^{n} \frac{(h_i/2)^{\alpha_i+1} - (-h_i/2)^{\alpha_i+1}}{\alpha_i + 1}.$$

This method efficiently exploits local Taylor expansions for numerical integration in multiple dimensions.