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Multivariate polynomial interpolation and meshfree differentiation via undetermined coefficients

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ABSTRACT

Using undetermined coefficients, we develop a meshfree method to approximate partial derivatives of a multivariate real function from data on a finite set of possibly disordered base points satisfying a natural condition which always holds true in the one dimensional case. The method yields a generalization of Lagrange's interpolation polynomial and a recursive formula different from Neville's algorithm.

1. Introduction

Elementary methods to estimate derivatives of a real analytic function f on $\mathbb{R}$ are found in most texts on numerical analysis. One such method used when data $\{f(p_i)\}_{i=0}^{m} \subset \mathbb{R}$ is given on a set of base points $\sigma = \{p_i\}_{i=0}^{m} \subset \mathbb{R}$, consists in first introducing the family of polynomials

$$l_i(p;\sigma) = \prod_{p_j \in \sigma \setminus p_i} \frac{p - p_j}{p_i - p_j} \quad (i = 0, \ldots, m) \tag{1}$$

from which is then constructed the Lagrange polynomial

$$L_f(p;\sigma) = \sum_{i=0}^{m} f(p_i)\, l_i(p;\sigma) \tag{2}$$

(of degree at most m) which interpolates $\{(p_i, f(p_i))\}_{i=0}^{m}$. The derivative

$$L^{(\alpha)}(p;\sigma) = \sum_{i=0}^{m} f(p_i)\, l_i^{(\alpha)}(p;\sigma)$$

for any given integer $\alpha \in \{0, \ldots, m\}$ is often a satisfactory polynomial approximation of $f^{(\alpha)}(p)$ where, to ease notation, by $f^{(0)}(p)$ we mean $f(p)$ (see, for example [1–3]). We will show that this is equivalent to the method of

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undetermined coefficients (see for example [4, p. 291]) where, for any given $\alpha \in \{0, \ldots, m\}$, the polynomial derivatives $l_0^{(\alpha)}(p;\sigma), \ldots, l_m^{(\alpha)}(p;\sigma)$ satisfy the system

$$\sum_{i=0}^{m} (p_i - p)^{\alpha'} l_i^{(\alpha)}(p;\sigma) = \alpha!\delta_\alpha^{\alpha'} \quad (\alpha' = 0, \ldots, m) \tag{3}$$

with

$$\delta_\alpha^{\alpha'} = \begin{cases} 1 & \text{if } \alpha = \alpha' \\ 0 & \text{otherwise.} \end{cases}$$

Condition (3) is the one dimensional version of (18) introduced later for $\sigma \subset \mathbb{R}^d$ ($d \in \mathbb{N}$). As in higher dimensions, a synthesis of Lagrange interpolation and the method of undetermined coefficients is easier to attain by studying the solutions $l_i^{(\alpha)}(p;\sigma)$ of (3) instead of analyzing the αth derivative of the polynomial $l_i(p;\sigma)$ given by (1). Furthermore, applying the multidimensional version of (3) to the Taylor series of a multivariate function yields the error in approximating the derivative of the function by the corresponding derivative of its Lagrange interpolation.

In the literature one finds methods to estimate derivatives by replacing $l_i(p;\sigma)$ in (2) with predetermined basis functions (e.g. [5,6]). Furthermore, if one seeks partial derivatives only at the points of $\sigma \subset \mathbb{R}^d$, pseudospectral methods can be applied to the multidimensional version of (2) where $f(x_i)$ and $l_i(p;\sigma)$ are replaced respectively by constants and radial basis functions (e.g. [7,8]). In place of the modern approach based on well chosen basis functions, we use the method of undetermined coefficients in a multidimensional setting. This method has never been fully developed in the literature. It yields a multivariate Lagrange-like polynomial which interpolates the data. In the process we obtain a recursive formula which, in the one dimensional case, is written as

$$L_f^{(\alpha)}(p;\sigma) = L_f^{(\alpha)}(p;\sigma \setminus p_m) + \left(f(p_m) - L_f(p_m;\sigma \setminus p_m)\right) l_m^{(\alpha)}(p;\sigma)$$

where $l_m(p;\sigma)$ is given by (1) for $i = m$. When $\alpha = 0$ this recursive formula, which differs from Neville's well known algorithm (e.g. [9, p. 72]), follows easily from the uniqueness of the Lagrange interpolation polynomial $L_f(p;\sigma)$ in conjunction with the property $l_m(p_j;\sigma) = \delta_m^j \forall p_j \in \sigma$. Subject to a natural condition on σ (see (17)), which is always valid in the one dimensional case, we establish these same properties in the multivariate case and so obtain our recursive result.

One also finds in the literature methods to approximate a multivariate function f and its derivatives by way of triangulation-based algorithms. In [10,11] for example, base points $\sigma = \{(x_i, y_i)\}_{i=0}^m \subset \mathbb{R}^2$ serve as vertices for a triangulation and f is approximated in the vicinity of a given point $(x_i, y_i) \in \sigma$ by way of a polynomial of the form

$$G(x,y) = f(x_i,y_i) + a(x-x_i) + b(y-y_i) + c(x-x_i)^2 + d(x-x_i)(y-y_i) + e(y-y_i)^2$$

where $f(x_i, y_i)$ is part of the data. The real constants a, b, c, d, e are estimated by a least squares method weighted so as to give those points of σ near (x_i, y_i) more relevance. The coefficients a and b are then taken as approximations for the derivatives $f_x(x_i, y_i)$ and $f_y(x_i, y_i)$, respectively. Our method based on undetermined coefficients is free of weights assigned (somewhat arbitrarily) at the points of $\sigma \setminus (x_i, y_i)$ and provides error estimates.

As our tables will show, given sufficient data, approximating partial derivatives by undetermined coefficients is accurate and can yield useful error bounds. It provides, for example, a meshfree method other than SPH (smoothed particle hydrodynamics) to approximate gradients and Laplacians in partial differential equations associated with fluid dynamics (see for example [12,13] and the references therein). The lack of numerical precision inherent to SPH is compounded by the complexity of the few theoretical error bounds found in the literature [14–17]. By contrast, replacing the problematic convolution in SPH with the method of undetermined coefficients based on (18) yields theoretical error bounds and significantly better numerical results for the gradient and Laplacian. It also avoids situations of current concern to researchers in SPH when particles (i.e. base points) are near a boundary. On the negative side, our method is more time consuming. When data is limited, we can pass to a higher dimension so as to apply our techniques to level sets. Data associated with a set of nodes in $\mathbb{R}^n$ is viewed as points on a surface in $\mathbb{R}^{n+1}$. We assume that this surface is a level set for some real function G on $\mathbb{R}^{n+1}$ for which both the implicit function theorem and Taylor's theorem hold. We obtain good interpolation results by our method provided G is polynomial-like in the sense that its Taylor series converges rapidly to G. Furthermore, the method is not subject to condition (17).

2. Preliminaries

For any fixed $d \in \mathbb{N}$, a multi-index consists of an element $\alpha = (a_1, a_2, \ldots, a_d)$ of the d-dimensional product space $\mathbb{N}^{\star d}$ where $\mathbb{N}^\star$ is the class of nonnegative integers. The *length* of α is given by

$$|\alpha| = a_1 + a_2 + \cdots + a_d$$

and when $a_1 = a_2 = \cdots = a_d = 0$ we denote α by α_0 or simply 0. The following is reminiscent of the manner in which the positive rationals are ordered (see also [18]).