# Numerical differentiation on scattered data through multivariate polynomial interpolation

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## Abstract

We discuss a pointwise numerical differentiation formula on multivariate scattered data, based on the coefficients of local polynomial interpolation at Discrete Leja Points, written in Taylor's formula monomial basis. Error bounds for the approximation of partial derivatives of any order compatible with the function regularity are provided, as well as sensitivity estimates to functional perturbations, in terms of the inverse Vandermonde coefficients that are active in the differentiation process. Numerical tests are presented showing the accuracy of approximation.

## Introduction

Let us denote by $\Pi_d(\mathbb{R}^s)$ the space of $s$-variate polynomials with total degree not exceeding $d$, by $B_h(\overline{\mathbf{x}})$ the Euclidean ball of radius $h$ centered at $\overline{\mathbf{x}}$, by $D^\alpha = \partial_{x_1}^{\alpha_1}\dots\partial_{x_s}^{\alpha_s}$ the differentiation operator with multi-index $\alpha = (\alpha_1,\dots,\alpha_s)$ of length $|\alpha| = \alpha_1+\dots+\alpha_s$, and by $C^{d,1}(\Omega)$ the space of $C^d$ functions with Lipschitz-continuous derivatives of length $d$ on a convex $\Omega$, equipped with the seminorm

$$\sup\left\{\frac{|D^\alpha f(\mathbf{u}) - D^\alpha f(\mathbf{v})|}{\|\mathbf{u}-\mathbf{v}\|_2} : \mathbf{u},\mathbf{v}\in\Omega,\ \mathbf{u}\neq\mathbf{v},\ |\alpha| = d\right\}.$$

Moreover, we consider the graded lexicographical ordering of muti-indices and we adopt the usual notation with multi-indices where factorials and powers are interpreted as componentwise products, e.g. $\alpha! = \alpha_1!\dots\alpha_s!$ and $\mathbf{x}^\alpha = x_1^{\alpha_1}\dots x_s^{\alpha_s}$.

## Error bounds and sensitivity estimates

**Theorem 1** *Let $\Omega\subset\mathbb{R}^s$ be a convex body, $\overline{\mathbf{x}}\in\Omega$, $f\in C^{d,1}(\Omega)$, and $p_d[\mathbf{y},X]\in\Pi_d(\mathbb{R}^s)$ the interpolating polynomial at a unisolvent subset $X = \{\mathbf{x}_1,\dots,\mathbf{x}_m\}\subset\mathcal{N}_h = B_h(\overline{\mathbf{x}})\cap\Omega$, where $m = \binom{s+d}{s} = \dim(\Pi_d(\mathbb{R}^s))$ and $\mathbf{y} = [y_i]_{i=1,\dots,m} = [f(\mathbf{x}_i)]_{i=1,\dots,m}$. Moreover, let $\widetilde{\mathbf{y}} = [\widetilde{y}_i]_{i=1,\dots,m}$ be a vector of perturbed sample of $f$ at $X$, where $\|\mathbf{y}-\widetilde{\mathbf{y}}\|_\infty\le\varepsilon$.*
*Then the following pointwise differentiation error estimate holds*

$$|D^\nu f(\overline{\mathbf{x}}) - D^\nu p_d[\widetilde{\mathbf{y}},X](\overline{\mathbf{x}})| \le \lambda_{\nu,h}(\overline{\mathbf{x}})\left(\frac{s^d}{(d-1)!}\|f\|_{C^{d,1}(\mathcal{N}_h)}h^{d+1}+\varepsilon\right),\quad |\nu|\le d,$$

$$\lambda_{\nu,h}(\overline{\mathbf{x}}) = \nu!h^{-|\nu|}\|\rho_{\nu,h}(\overline{\mathbf{x}})\|_1,$$

*where $\rho_{\nu,h}(\overline{\mathbf{x}})$ denotes the row indexed by $\nu$ of the inverse Vandermonde matrix $(V_{d,h}(X))^{-1}$, with $V_{d,h}(X) = \left[\left(\frac{\mathbf{x}_i-\overline{\mathbf{x}}}{h}\right)^\alpha\right]$, $1\le i\le m$, $|\alpha|\le d$.*

- It is worth observing that the approximate derivative of $f$ with multi-index $\nu$ can be computed conveniently as

$$D^\nu p_d[\mathbf{y},X](\overline{\mathbf{x}}) = \nu!h^{-|\nu|}c_\nu\approx D^\nu f(\overline{\mathbf{x}}),$$

  where $c_\nu$ is the interpolation coefficient corresponding to $\left(\frac{\mathbf{x}-\overline{\mathbf{x}}}{h}\right)^\nu$, i.e. the component indexed by $\nu$ of the vector $\mathbf{c}$ that solves the linear system $V_{d,h}(X)\,\mathbf{c} = \mathbf{y}$.
- It is also worth observing that $\lambda_{\nu,h}(\overline{\mathbf{x}})$ is the "stability constant" of pointwise differentiation via local polynomial interpolation, namely the value at $\overline{\mathbf{x}}$ of the "stability function" $\lambda_{\nu,h}(\mathbf{x})$.

## Conclusion

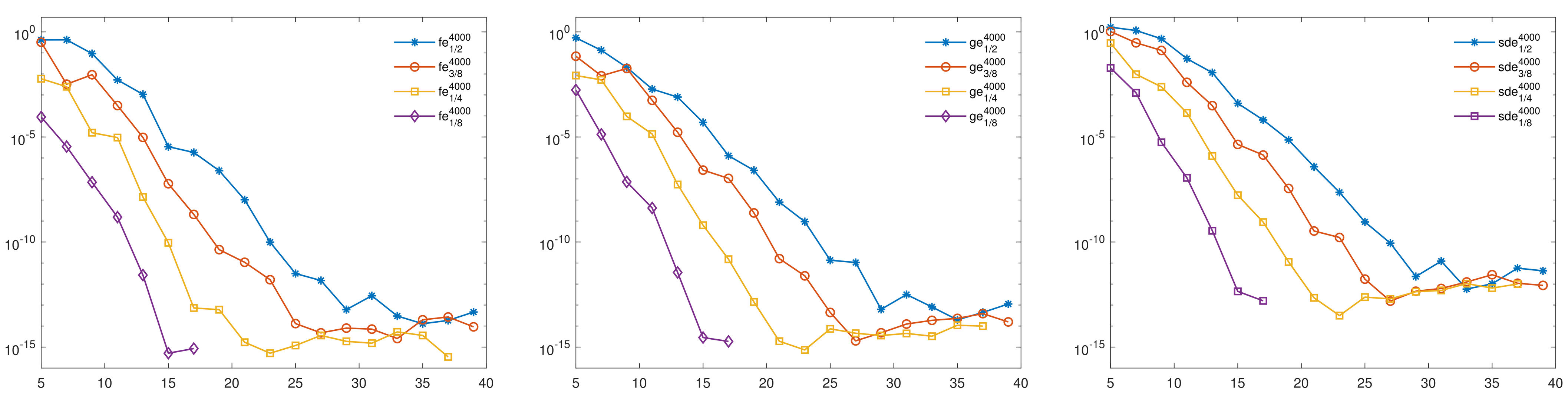
- The key tools behind the good accuracy of the method on the interior of the domain $\Omega$ are:
  1. The local scaling of the shifted monomial basis, to reduce the conditioning of the Vandermonde matrix.
  2. The connection to Taylor's formula via this basis.
  3. The extraction of Discrete Leja Points from the scattered sampling set via basic numerical linear algebra.
- The worsening of the accuracy at the boundary and at the vertex of $\Omega$, can be ascribed to the fact that the stability functions $\lambda_{\nu,h}(\mathbf{x})$ increase rapidly near the boundary of the local interpolation domains $B_h(\overline{\mathbf{x}})\cap\Omega$.

## Numerical results

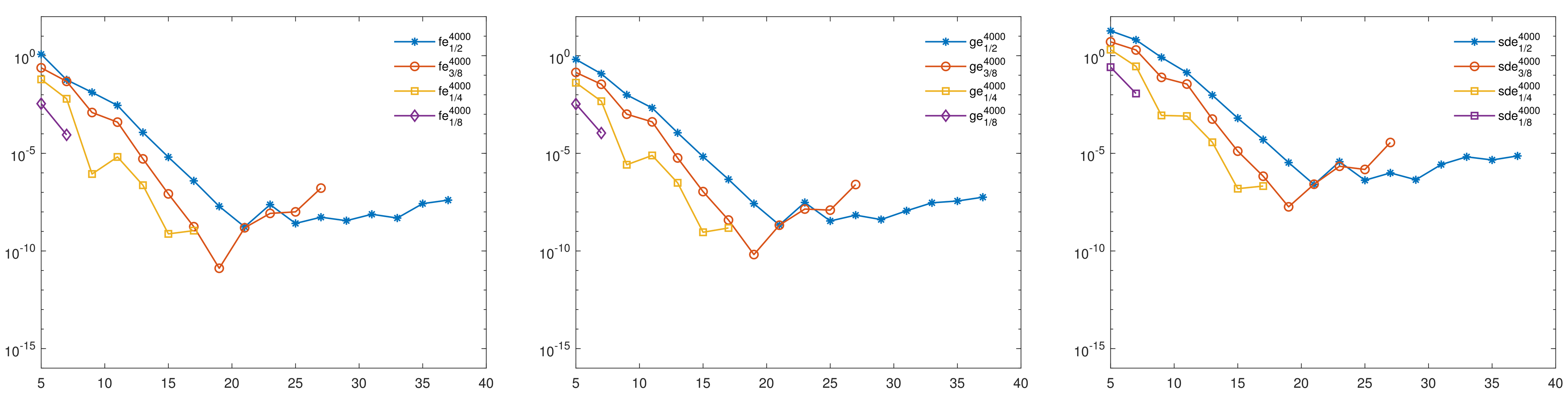
We provide some numerical tests on the approximation of function, gradient and second order derivative values. We fix $s=2$, $\Omega=[0,1]^2$ and we take $\overline{\mathbf{x}}$ at the center and on a corner of $\Omega$. We use Halton points and we focus on the scattered points in the ball $B_r(\overline{\mathbf{x}})$ centered at $\overline{\mathbf{x}}$ for different radii $r = \frac{1}{2},\frac{3}{8},\frac{1}{4},\frac{1}{8}$, from which we extract an interpolation subset $\sigma$ of $m = \binom{d+2}{2}$ Discrete Leja Points at a sequence of degrees $d$.
For simplicity, we set $p := p[\mathbf{y},\sigma]$ and, to measure the error of approximation, we compute the relative errors

$$fe = \frac{|f(\overline{\mathbf{x}})-p(\overline{\mathbf{x}})|}{|f(\overline{\mathbf{x}})|},\quad ge = \frac{\|\nabla f(\overline{\mathbf{x}})-\nabla p(\overline{\mathbf{x}})\|_2}{\|\nabla f(\overline{\mathbf{x}})\|_2},\quad sde = \frac{\|(f_{xx}(\overline{\mathbf{x}}),f_{xy}(\overline{\mathbf{x}}),f_{yy}(\overline{\mathbf{x}}))-(p_{xx}(\overline{\mathbf{x}}),p_{xy}(\overline{\mathbf{x}}),p_{yy}(\overline{\mathbf{x}}))\|_2}{\|(f_{xx}(\overline{\mathbf{x}}),f_{xy}(\overline{\mathbf{x}}),f_{yy}(\overline{\mathbf{x}}))\|_2},$$

by using the bivariate test function $f_1(x,y) = 2\cos(10x)\sin(10y)+\sin(10xy)$.



Relative errors $fe$, $ge$ and $sde$ for the function $f_1$ by using 4000 Halton points with $\overline{\mathbf{x}} = (0.5, 0.5)$.



Relative errors $fe$, $ge$ and $sde$ for the function $f_1$ by using 4000 Halton points with $\overline{\mathbf{x}} = (1, 1)$.

**Remark 0.1** *Similar results can be obtained using uniform random points and different positions of the point $\overline{\mathbf{x}}$ in the interior of $\Omega$, while the accuracy of approximation gets worse taking $\overline{\mathbf{x}}$ at the boundary and at the vertex of $\Omega$. We stress also that the method is not restricted to dimension 2 and the accuracy of derivative approximation for the 3D case is quite similar to the 2D case.*

## References

[1] F. Dell'Accio, F. Di Tommaso & N. Siar (2021). On the numerical computation of bivariate Lagrange polynomials. Applied Mathematics Letters, 112, 106845.

[2] L. Bos, S. De Marchi, A. Sommariva & M. Vianello (2010). Computing multivariate Fekete and Leja points by numerical linear algebra. SIAM Journal on Numerical Analysis, 48(5), 1984-1999.

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