

# NUMERICAL DIFFERENTIATION IN MULTIPLE DIMENSIONS *via Polynomial Interpolation*

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Derek Li

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## Abstract

Numerical differentiation by polynomial interpolation and the related methods of derivative approximation with finite differences are a foundational aspect of scientific computing. In this study, we present a method for deriving finite difference formulas of arbitrary orders of accuracy using polynomial interpolation. This is implemented as a symbolic routine in MATLAB. These formulas are classified by the number of interpolation points  $n$ , the order of differentiation  $k$ , the location where the derivative is evaluated, denoted the pivot, and the order of accuracy  $e$ , related as  $n = k + e$ . We assemble these finite difference expressions into a *centric* differentiation matrix that applies central formulas when possible and pseudo-central formulas near the boundaries, all of the same accuracy order.

This provides a commodious numerical differentiation module that, to the author's knowledge, has no built-in counterpart in MATLAB or Python.<sup>1</sup> This may be referred to as *directional differentiation*. As the order of accuracy describes asymptotic behavior, we show by an example that as different partial functions may converge at different rates, and that computer memory is finite, practically for multidimensional functions, the asymptotic convergence may not be observed or observable.

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## 1. POLYNOMIAL INTERPOLATION

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Numerical differentiation is instrumental when the function of interest is not known by definition, such as in physical experiments where discrete measurements are made, or when deriving the derivative analytically is difficult. A general approach is to interpolate the available function values with an *interpolant* functions, whose derivatives are then evaluated at desired points as estimates of the original. Polynomial interpolants are easily constructed and differentiated, with the *Interpolation Error Theorem* warranting error orders for differentiable functions. The expressions derived for the derivatives are known as *finite difference formulas*.

In this section, we pose the 1D problem, the solution to which translates directly to multiple dimensions, as treated later. To pose the problem, we assume function values are taken at a set of grid points uniformly spaced by  $h$ . To approximate the derivative at some grid point  $x_i$ , we utilize some  $n$  consecutive neighboring points, including itself, to interpolate a polynomial of  $n - 1^{\text{th}}$  degree. We then evaluate the derivative of the polynomial at  $x_i$ .

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<sup>1</sup>The Julia language has a package *FiniteDiff* which computes first and second derivatives with finite differences at various orders of accuracy.

The expression derived for the derivative at this point is independent of the specific abscissa value and applies, as a formula to all situations where we have the same relative selection of neighboring points. This is simply because for a shifted abscissa  $x' = x + h$ ,

$$\frac{df}{dx'} = \frac{df}{dx}$$

at the corresponding abscissa values.

Thus our problem is formulated as interpolating a polynomial through  $n$  uniformly spaced abscissa, which we conveniently choose to be

$$\vec{x} = (0 \quad h \quad 2h \quad \dots \quad (n-1)h) \quad (1)$$

With corresponding ordinate values of function  $f(x)$  as

$$\vec{y} = (y_0 \quad y_1 \quad y_2 \quad \dots \quad y_{n-1}). \quad (2)$$

Evaluating the derivative of the polynomial at different abscissa locations, the location of evaluation called the *pivot*, yields different finite difference formulas that use different neighboring ordinate values relative to the pivot, which are nonetheless of the same order of accuracy, as they originate from the same underlying polynomial.

$$P(x) = a_0 + a_1x + a_2x^2 \dots a_{n-1}x^{n-1} \equiv \vec{a} \cdot \vec{x}^p \quad (3)$$

The interpolant polynomial is of degree  $n - 1$ , whose coefficients are determined from the fitted points. This constitutes a linear system of equations, where a row of the matrix corresponds to a distinct abscissa and the columns contain consecutive powers of different abscissas. This matrix is known as the *Vandermonde* matrix.

$$V\vec{x} \equiv \begin{bmatrix} 1 & x_0 & x_0^2 & \dots & x_0^{n-1} \\ 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ \vdots & \vdots & \dots & \vdots & \\ 1 & x_{n-1} & x_{n-1}^2 & \dots & x_{n-1}^{n-1} \end{bmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} \quad (4)$$

$$= \begin{bmatrix} 1 & h & h^2 & \dots & h^{n-1} \\ 1 & 2h & (2h)^2 & \dots & (2h)^{n-1} \\ \vdots & \vdots & \dots & \vdots & \\ 1 & (n-1)h & [(n-1)h]^2 & \dots & [(n-1)h]^{n-1} \end{bmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{n-1} \end{pmatrix} \quad (5)$$

$$= \vec{y} \quad (6)$$

For distinct abscissa values, the Vandermonde matrix is non-singular, so  $\vec{a}$  is uniquely defined by the abscissa and ordinate values. This is proved by assuming the fundamental theorem of algebra<sup>2</sup>, which states that a single variate polynomial of degree  $n \in \mathbb{N}$  has exactly  $n$  roots, which may be repeated, real or complex. Suppose to the contrary that given pairwise distinct

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<sup>2</sup>Proof idea from Martin Sleziak [1].

values  $x_0, x_1, \dots, x_{n-1}$ , the Vandermonde matrix is singular, that is  $\exists \vec{b} = (b_0, b_1, \dots, b_{n-1})$  such that

$$b_0 \begin{pmatrix} x_0^0 \\ x_1^0 \\ \vdots \\ x_{n-1}^0 \end{pmatrix} + b_1 \begin{pmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{pmatrix} + \dots + b_{n-1} \begin{pmatrix} x_0^{n-1} \\ x_1^{n-1} \\ \vdots \\ x_{n-1}^{n-1} \end{pmatrix} = \mathbf{0}.$$

The abscissa  $x_i$  from each of the  $n$  rows in this linear system is then a root of the  $n - 1^{\text{th}}$  degree polynomial

$$P(x) = b_0 + b_1x + b_2x^2 + \dots + b_{n-1}x^{n-1}$$

Which is a contradiction with the fundamental theorem unless  $P$  is the trivial polynomial, that is 0. This assures us that  $\vec{a}$  can be determined by elementary operations.

The generalized linear system (4) allows for deriving polynomial interpolants, thereby finite difference formulas, for customized non-uniformly spaced points, useful in various situations. In this study, we proceed with uniformly sampled points which possess a form amenable to unified treatment.

The derivation of the coefficients can be executed by a program capable of performing arithmetical operations symbolically. The MATLAB *Symbolic Toolbox* is employed to solve the above system of linear equations symbolically in  $h$  and  $\vec{y}$ .

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## 2. POLYNOMIAL DIFFERENTIATION

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The solution to (5), which we've shown is well-defined, gives the formula of the polynomial. We now need only to differentiate the polynomial to an arbitrary order and evaluate the derivative at different pivot positions. This task can be handled by symbolic computing with the ability of differentiating polynomials and substitution. For example, using three points, we obtain the following polynomial.

$$P(x) = y_0 - \frac{3y_0 - 4y_1 + y_2}{2h}x + \frac{y_0 - 2y_1 + y_2}{2h^2}x^2$$

Symbolically differentiating this expression and evaluating the derivative at  $x = 0, h, 2h$  yields the following finite difference formulas, the second of which is the commonly used simple central difference.

$$\begin{aligned} \hat{f}'(0) &= \frac{-3y_0 + 4y_1 - y_2}{2h} \\ \hat{f}'(h) &= \frac{-y_0 + y_2}{2h} \\ \hat{f}'(2h) &= \frac{y_0 - 4y_1 + 3y_2}{2h} \end{aligned}$$

Here  $\hat{f}'$  is the estimate of the derivative. This is conveniently organized into a matrix

$$\hat{f}' = h^{-1} \begin{bmatrix} -\frac{3}{2} & 2 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & -2 & \frac{3}{2} \end{bmatrix} \begin{pmatrix} y_0 \\ y_1 \\ y_2 \end{pmatrix} \equiv F\vec{y}.$$

The matrix  $F$  collects the coefficients of the finite difference formulas, excluding the factor  $h^{-1}$ . Computationally, these can be acquired by first evaluating the derivative of the polynomial at the desired pivot, and then differentiating with respect to the ordinate  $y_i$ , which can only exist as a monomial.<sup>3</sup> Mathematically, if we have a three-point grid and wish to perform numerical differentiation, the multiplication  $h^{-1}F\vec{y}$  produces the estimated derivatives at the grid points. Thus  $F$  here is an example of a *differentiation matrix*, whose product with the ordinate vector, scaled by the proper power of step size, yields the derivative.

This is readily generalized to using an arbitrary number of points for interpolation, the result of which would be a collection of finite difference formulas  $F$ . Similarly, we can obtain higher order derivatives, say  $k^{\text{th}}$  order, by differentiating the polynomial  $k$  times and then evaluating. It can be easily seen with Cramer's rule that for the  $k^{\text{th}}$  derivative, the differentiation matrix, when applied, should be scaled by the power  $h^{-k}$ .

The procedure hitherto described of interpolating a polynomial and evaluating its derivative at different pivot locations to obtain finite difference formulas is implemented in script *polydiff.m*. The complexity of this algorithm cannot be customarily estimated for the operations performed are symbolic rather than on floating point numbers. Indeed, the runtime for the collection of formulas of order greater than 4 is highly non-trivial. Thus, these formulas were pre-computed and stored as a native MATLAB array that is loaded with the differentiation module, up to using 41 points of interpolation. If a higher order formula is requested, it will be computed and memoized.

Now, estimates of a first derivative can be obtained with using different numbers of points to interpolate, using at least 2. The difference between using different degrees of polynomial interpolants is the asymptotic order of accuracy, denoted  $O(h^p)$ , where  $p \in \mathbb{N}$ . This states that  $\exists \alpha \in \mathbb{R}$  so that

$$\lim_{h \rightarrow 0} \hat{f}'(x_i) - f'(x_i) = \alpha h^p. \quad (7)$$

Here,  $p$  is denoted the *order of accuracy* of a finite difference formula. We note that this is an asymptotic definition which may only materialize at small enough step sizes  $h$ . In general, the subsequent relation exists.

**PROPOSITION.** *For a function  $f$  that can be differentiated  $n$  times in some closed neighborhood, a finite difference formula obtained through a polynomial interpolant of  $n$  distinct points therein, of an order of differentiation  $k$ , and order of accuracy  $e$  obeys the following relation*

$$n = k + e.$$

It would be delightful to prove this relation. Albeit, it will not be given here. The author has verified it against the commonly used finite difference formulas with stated order of accuracy. It has also been conformed to empirically, as shall be seen shortly, for employed test cases. This relation and our earlier discussion offer us an elegant classification of finite difference formulas. A finite difference formula is defined by the number of distinct grid points  $n$  used to interpolate a polynomial function, the order of differentiation  $k$ , the pivot, or location where the derivative of the polynomial is evaluated, which, collectively, determine the order of accuracy.

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<sup>3</sup>This is apparent inspecting Cramer's rule.

Finally, we return to our question of applying finite difference formulas for numerical differentiation. For each grid point, we may elect to use some selection of neighboring points, not all the grid points, for interpolation. We'd like to apply finite difference formulas of the same order of accuracy. For these conditions, we define the differentiation matrix below.

**DEFINITION.** For a set of  $n$  uniformly spaced abscissas, the **centric** differentiation matrix  $D$  of accuracy order  $e$  is a  $n \times n$  matrix whose rows consist of coefficients in finite difference formulas.

Specifically, for  $2 \nmid e$ ,  $\forall \lfloor \frac{e}{2} \rfloor \leq i \leq n - \lfloor \frac{e}{2} \rfloor + 1$ , the  $i^{\text{th}}$  row of  $\vec{d}_i$  has coefficients centered at index  $i$  corresponding to the central formula of accuracy order  $e$ , while all other elements of  $\vec{d}_i$  is 0. For any other  $i$ , we use a formula of the same accuracy order that incorporates all the ordinates in the direction with fewer available data points, that is to either its right or its left, depending on the number of remaining points to the boundary.

For  $2|e$ , arbitrarily, we construct  $D$  using as the central formula the central difference expression of accuracy order  $e$  evaluated at pivot  $e/2 + 1$ . For an index where there is insufficient number of neighboring points in either direction, we similarly use a formula that incorporates all the available points in the deficient direction.

This definition is unclear on its own, and may not be so interesting to the reader. Thus we illustrate with an example. Below is the centric differentiation matrix of order  $e = 4$  for the first derivative on a grid of 10 points, computed by our companion code *centricMatrix.m*.

$$\begin{bmatrix} -2.0833 & 4.0000 & -3.0000 & 1.3333 & -0.2500 & 0 & 0 & 0 & 0 & 0 \\ -0.2500 & -0.8333 & 1.5000 & -0.5000 & 0.0833 & 0 & 0 & 0 & 0 & 0 \\ 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.0833 & -0.6667 & 0 & 0.6667 & -0.0833 \\ 0 & 0 & 0 & 0 & 0 & -0.0833 & 0.5000 & -1.5000 & 0.8333 & 0.2500 \\ 0 & 0 & 0 & 0 & 0 & 0.2500 & -1.3333 & 3.0000 & -4.0000 & 2.0833 \end{bmatrix}$$

This is a sparse matrix whose middle rows are a banded matrix with the  $(0.0833, -0.6667, 0, 0.6667, -0.0833)$  entry repeated which corresponds to the central formula of 5<sup>th</sup> order. These rows correspond to grid points with sufficient neighboring points on both sides, here 2 each, to apply the central formula. The first two and last two rows lack one or two points to the left and right respectively to apply the central formula. Thus for the second and second to last row, we use pseudo-centered formulas where one point is utilized on one side and three on the other. At the very boundaries, only a forward or backward formula can be applied that uses all points to the right or left.

Differentiation is performed by the multiplication

$$\hat{f}' = h^{-1} D \vec{y}$$

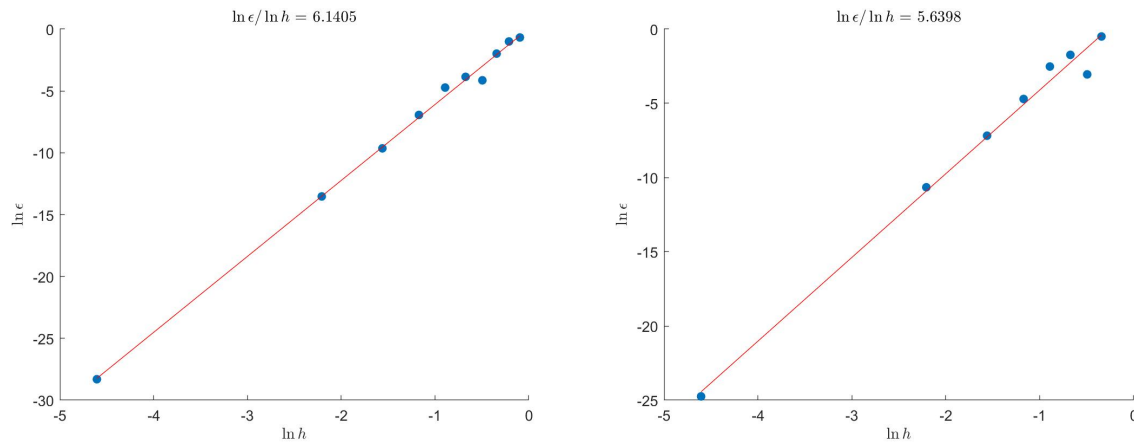


Figure 1. Empirical error order of first derivative. Figure 2. Empirical error order of second derivative.

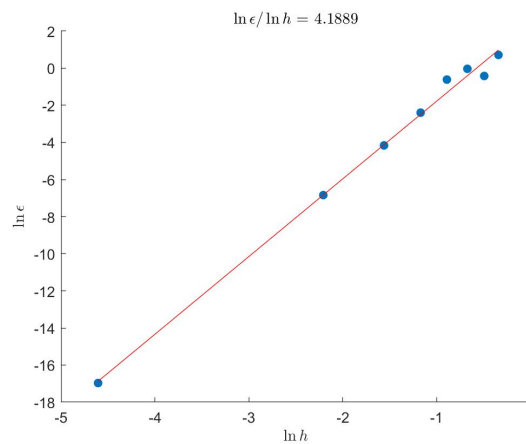


Figure 3. Empirical error order of third derivative.

Which computes the first derivative at all the grid points, all to the same theoretical order of accuracy. The motivation for preferring central formulas to construct the differentiation matrix is the idea that for differentiable functions, the behavior of change at a point is described by a two-sided locale, given sufficient resolution. This can be assessed more critically.

Given here are several sample graphs showing the asymptotic convergence to the theoretical order of accuracy. (Figure 1-3) We've chosen  $f(x) = e^{\sin x}$  as the testing function, whose derivative is  $e^{\sin x} \cos x$ . Centric differentiation matrices of 6<sup>th</sup>, 5<sup>th</sup>, and 4<sup>th</sup> orders of accuracy for 1<sup>st</sup>, 2<sup>nd</sup>, and 3<sup>rd</sup> derivatives. Here the error is defined as the mean absolute error of the derivatives estimated at all grid points used, which span  $[0, 2\pi]$ . The empirical orders of accuracy are printed, which agree generally with our expectation, though as seen for the second derivative, may not always be precise practically, depending on our choice of step sizes and our means of measuring error.

These graphs were produced by *orderAccuracy.m*.

### 3. DIRECTIONAL DIFFERENTIATION IN MULTIPLE DIMENSIONS

Succeeding our treatment of differentiation in one dimension, we can now fulfill the titular promise of this paper—generalization into multiple dimensions. For a multivariate vector function, the derivative is defined by component of the ordinate and by direction of differentiation of the abscissa. Derivatives in all directions in the abscissa space can then be derived from the partial derivatives with respect to the standard basis vectors.

The procedure for computing partial derivatives is as thus. For a vector function  $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$ , with abscissa  $\vec{x} = (x_1, x_2, \dots, x_n)$ , to compute  $\frac{\partial F_j}{\partial x_i}$  at an arbitrary  $\vec{x} = \vec{a} \equiv (a_1, a_2, \dots, a_n)$ , consider the partial function  $y(x_i) = F_j(a_1, a_2, \dots, x_i, \dots, a_n)$ , with all other  $x_k \neq x_i$  held constant at  $\vec{a}$ . Discretize this 1D function uniformly as  $\vec{x}_i$  and  $\vec{y}_i$ ; we thus have

$$\left. \frac{\partial F_j}{\partial x_i} \right|_{(a_1, a_2, \dots, \vec{x}_i, \dots, a_n)} \approx h^{-1} D \vec{y}_i.$$

Hereby the problem is reduced to one dimension, where  $\hat{x}_i$  is the direction of differentiation and  $\vec{x}_i$  and  $\vec{y}_i$  are the discretized abscissas and ordinates of a ray of grid points along that direction. We may then iterate through all  $x_d \forall d \neq i$  to compute  $\frac{\partial F_j}{\partial x_i}$  for all points on the grid. Applied to all components of the ordinate and all directions of the abscissa, this yields all the partial derivatives.

The procedure may be referred to as *directional differentiation*, for only the functions values along the direction of differentiation are used by the finite difference formulas. More complex schemes of multidimensional differentiation can be devised assuming local differentiability of the function, that is, differentiability in all directions. We may, for instance, interpolate a multivariate polynomial using non-colinear or non-coplanar points. Then, ordinate values not along the direction of differentiation may contribute to the estimated derivative, enforcing more continuity in the derivative. This condition of differentiability may be relevant in various practical situations, though the simplest method of differentiation in multiple dimensions which assumes least of differentiability is as we have stated it.

Higher order derivatives are analogously obtained. This method also extends to directional derivatives along any constant direction, where the rays of grid points are correspondingly obtained, which may be of different lengths. This may demand some ingenuity to program, a practical alternative of which is to apply the chain rule to construct the directional derivative. The chain rule however assumes differentiability, so does not warrant the same order of accuracy directly as using the rays of points along the direction.

$$\left. \frac{\partial^q F_j}{\partial x_i^q} \right|_{(a_1, a_2, \dots, \vec{x}_i, \dots, a_n)} \approx h^{-q} D^{(q)} \vec{y}_i \quad (8)$$

We note that mixed derivatives are obtained effectively by differentiating the derivative field along another direction of differentiation, so do not operate on the same ray of points. For this, the derivative field along the first direction is obtained and then differentiated with respect to the new direction. We will consider the order of accuracy for multidimensional differentiation later, but we observe here that the accuracy order of mixed partial derivatives is a special ques-

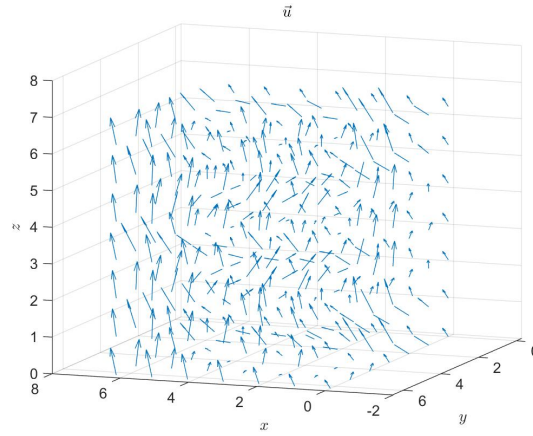


Figure 4. Low-resolution plot of synthetic field

tion, for it is not reducible to a 1D problem—the accuracy order of the second differentiation depends on that of the first.

Since at this stage, no symbolic operations are involved in differentiation, we may give an account of the complexity of the algorithm. Differentiation of a ray of data, that is, the 1D problem, consumes  $O(k + e)$  operations, which is the number of neighboring points involved in interpolation, per data point, so  $O(n(k + e))$  for  $n$  total data points. For a vector grid of  $n_1, n_2, \dots, n_m$  dimension, the runtime complexity of computing the partial derivative of one of its components for the entire grid is  $O(\prod_{i=1}^m n_i(k + e))$ , equal to  $O(n^m(k + e))$  for a symmetric grid. Such accounting is reasonable given that the finite differencing operation performed at each grid point is of order  $O(k + e)$ . Complexity is multiplied by the dimension of the abscissa and the dimension of the ordinate for a full computation of the  $k^{\text{th}}$  partial derivatives of accuracy order  $e$ .

Directional differentiation is implemented for vector fields  $F : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  in *VelocityField.diff()*, *VelocityField.gradient()*, and *VelocityField.vorticity()*, which we now utilize for a case study.<sup>4</sup>

## 4. A PERIODIC FIELD

$$\vec{u} = (\sin(y \cos z), \cos(x \sin z), e^{\sin(xy)}) \quad (9)$$

We invent an infinitely differentiable vector field, which owns a certain periodicity in its structure. It can be instantiated with various resolutions, that is, spacing between vectors which will correspond to step size during differentiation. Plotted is a sample on  $[0, 2\pi]$  with uniform increments of  $\pi/3$  in all three dimensions, a coarsely resolved sample. (Figure 4)

The analytical solutions of the first-derivative quantities are derived directly from the field's definition. We observe that each component of the field is independent of the variation of its

<sup>4</sup>*VelocityField.m* is a data structure I'm developing for manipulating 3D vector fields interpreted as fluidic velocity fields. Its functions of numerical differentiation is implemented by the polynomial differentiation method we've described [2].



corresponding abscissa dimension; hence the null divergence.

$$\nabla \vec{u} = \begin{bmatrix} 0 & \cos z \cos(y \cos z) & -y \sin z \cos(y \cos z) \\ -\sin z \sin(x \sin z) & 0 & -x \cos z \sin(x \sin z) \\ y \cos(xy) e^{\sin(xy)} & x \cos(xy) e^{\sin(xy)} & 0 \end{bmatrix} \quad (10)$$

$$\nabla \times \vec{u} = \begin{pmatrix} x \cos(xy) e^{\sin(xy)} + x \cos z \sin(x \sin z) \\ -y \sin z \cos(y \cos z) - y \cos(xy) e^{\sin(xy)} \\ -\sin z \sin(x \sin z) - \cos z \cos(y \cos z) \end{pmatrix} \quad (11)$$

$$\nabla \cdot \vec{u} = 0 \quad (12)$$

## 4.1. ACCURACY OF PARTIAL DERIVATIVES

Were we to compute the partial derivative of one component along a ray of grid points, say  $u_x(x_0, y, z_0)$ , the problem reduces to the 1D case, where the order of accuracy agrees with the degree of the interpolant polynomial, given differentiability of this synthetic field. Theoretically, since a partial derivative at an abscissa is the derivative of the corresponding partial function, the order of accuracy for a partial derivative at any point on the 3D grid still corresponds to the degree of the interpolant polynomial. For instance, if we apply a third-order accurate finite difference formula to operate on each ray, the global order of accuracy for computing a partial derivative is also third-order.<sup>5</sup>

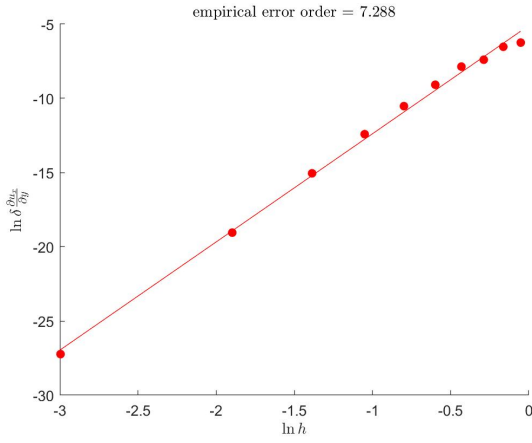
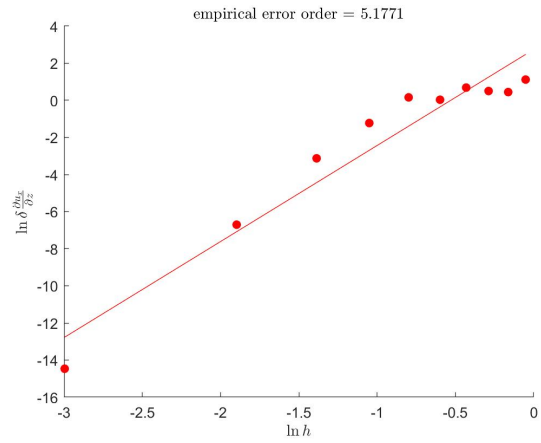
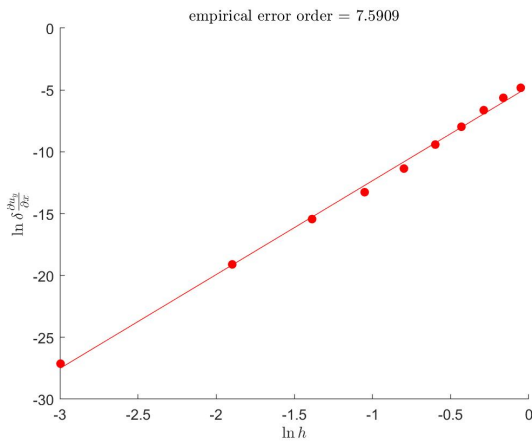
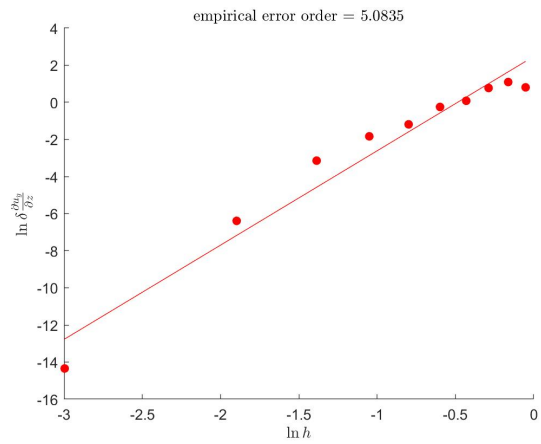
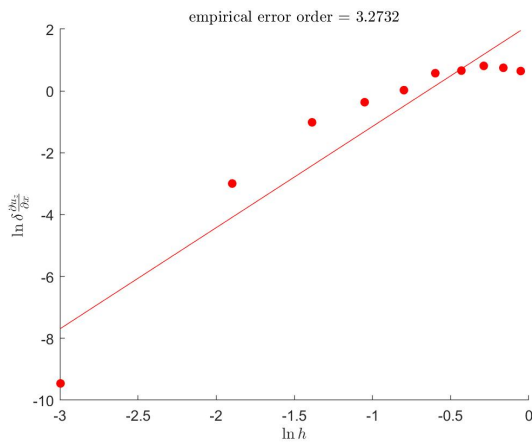
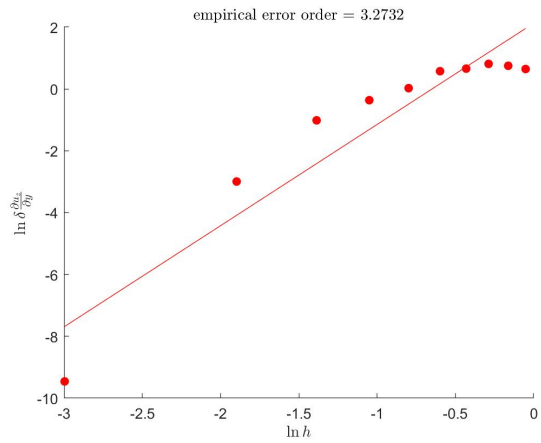
Nevertheless, as the partial function  $u_x(x_0, y, z_0)$  varies with  $x_0$  and  $z_0$ , the rate of error's decrease varies amongst  $u_x(x, y, z)$ . Since the order of accuracy refers to *asymptotic* behavior of error as  $h \rightarrow 0$ , the characteristic decrease of error as a power function may or may not manifest depending on our choice of step sizes used.<sup>6</sup> With many rays, thereby many partial functions, approaching asymptotic behavior at different rates, a problem is posed that, depending on the method by which error is measured, the theoretical order of accuracy may or may not be observed.

We shall substantiate these statements now with our vector field. Below are the log-error plots of the non-zero partial derivatives generated with a 7<sup>th</sup> order accurate centric matrix. (Figures 5-10) The error here is measured by computing the mean absolute error<sup>7</sup> of the estimated partial derivative over all 3D grid points, normalized by the mean theoretical value of that partial derivative over all grid points. This is a reasonable way of measuring error: using the mean error scaled by the mean theoretical, which crudely corresponds to the percentage error.

We see that only in two of the dimensions does the empirical order of error matches the theoretical, namely for  $\frac{\partial u_x}{\partial y}$  and  $\frac{\partial u_y}{\partial x}$ .<sup>8</sup> These two partial derivatives, we observe from (9), originate from basic sine and cosine oscillations whose derivative is not difficult to approximate. The other four partial derivatives, nonetheless, involve more complex variations that are composite, so generate more chaotic oscillations.

<sup>5</sup>We note that in the 1D case, as for the 3D, the asymptotic error bound  $O(h^p)$  pertains to the derivative estimation error at each grid point.

<sup>6</sup>This is also true for univariate functions. Given a hyper variational function, say one whose characteristic pat-

Figure 5. Error of  $\frac{\partial u_x}{\partial y}$ Figure 6. Error of  $\frac{\partial u_x}{\partial z}$ Figure 7. Error of  $\frac{\partial u_y}{\partial x}$ Figure 8. Error of  $\frac{\partial u_y}{\partial z}$ Figure 9. Error of  $\frac{\partial u_z}{\partial x}$ Figure 10. Error of  $\frac{\partial u_z}{\partial y}$ 

If we pick any of the irregular derivatives and compute error along a specific ray, we obtain the expected order of accuracy by diminishing the step size. In Figure 11, we have computed

tern of change is captured at sub-machine precision, the order of accuracy cannot be observed.

<sup>7</sup>All error discussed in this paper is absolute error, or the norm, when the error is a vector.

<sup>8</sup>These graphs, as well as the later one for vorticity, were generated by the script *orderAccuracy3D.m*.

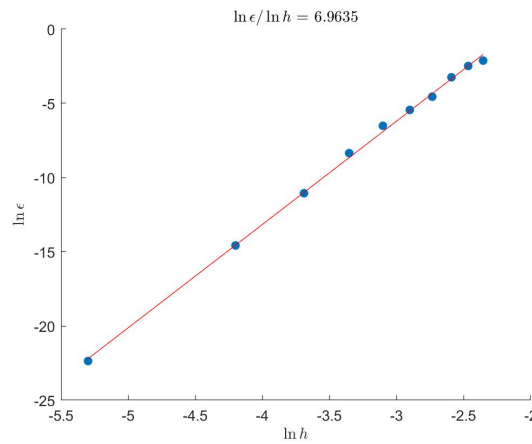


Figure 11. Irregular 3D error profile of  $\frac{\partial u_z}{\partial y}$  becomes regular reduced to 1D.

the error of  $\frac{\partial u_z}{\partial y}$  along a ray with  $x = 2\pi$ , which causes quick oscillations.<sup>9</sup> The minimum step size employed here is about 2.5 orders smaller than that used in 3D. We might hope to procure a similar trend as well using these minuter step sizes. This, however, is practically infeasible and reveals a limitation of numerical differentiation in multiple dimensions. Our field spans from 0 to  $2\pi$  in each dimension, so the amount of memory required for the construction of a field scales inverse-cubically with the size of the step. The step size with  $\ln h = -4$  corresponds to a  $348 \times 348 \times 348$  array, requiring more than 3 gigabytes of memory in MATLAB. Decreasing the step size by an order of ten requires 27 gigabytes, implausible on a typical personal computer. Thus, though the theoretical order of accuracy is still attained at high enough resolution, practically there might be no way to approach the asymptote.<sup>10</sup> Thus, for an  $O(h^p)$  accurate difference, it is more likely for multidimensional data that halving the step size will not produce the diminution of error by the factor of a desired power  $2^p$ , depending on the nature of the data. Other irregular partial derivatives shown in the previous graphs were analogously verified, showing the same effect.

## 4.2. ACCURACY OF CURL

Having realized now that the partial derivatives involved in the gradient approach asymptotic behavior at different rates, we combine them in the computation of  $\nabla \times \vec{u}$ , known as the vorticity when  $\vec{u}$  is a valid velocity field of a fluid. We expect that  $\nabla \times \vec{u}$  to not reach asymptotic behavior, illustrated by a lower order of empirical accuracy.

Error is measured here as the mean magnitude of difference between the computed and theoretical curls, normalized by the mean theoretical curl magnitude in the 3D region. Still we have applied a 7<sup>th</sup> order centric differentiation matrix and measure an empirical order around 4. (Figure 12) This is intermediate between the error orders of the partial derivatives, so appears reasonable given that the quicker decaying errors ameliorate the slower decaying ones in the average. We expect the theoretical order to evince with more minute step sizes, but again are

<sup>9</sup>This figure was made with the same script *orderAccuracy.m* as used earlier for the 1D problem.

<sup>10</sup>Another practical constraint, though not significant here, is that when the variation of the function is ultra-minute, values of error and step size might be in the range of machine precision, thus inaccurate for determining the order of accuracy.

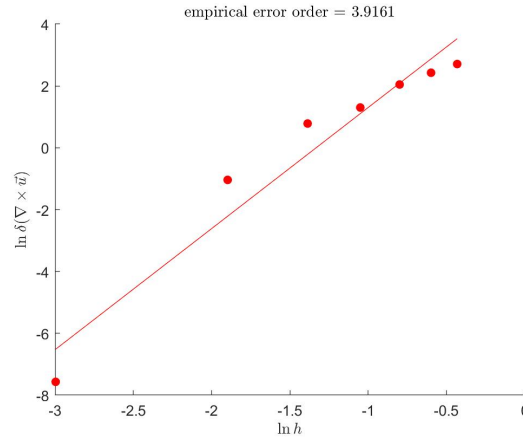
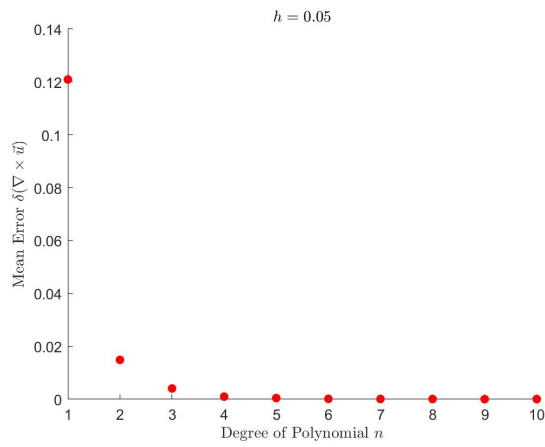
Figure 12. Empirical order of accuracy of  $\nabla \times \vec{u}$ 

Figure 12. Variation of error with accuracy order for high-resolution data.

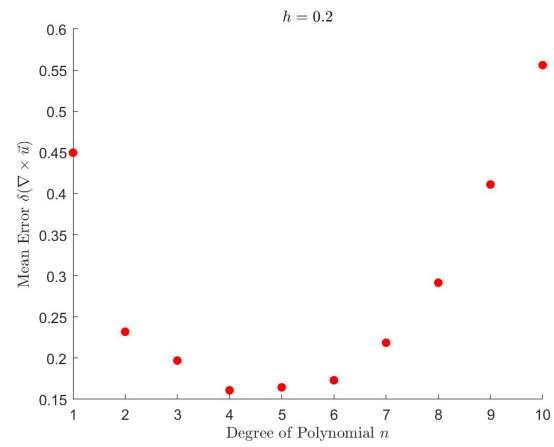


Figure 13. Variation of error with accuracy order for low-resolution data.

unable to obtain it due to limited computing power.

Here we also construct a plot for the error of curl approximation with respect to different orders of accuracy. A vector field of the given resolution is created, on which finite differences of various orders are then applied to compute the vorticity. When the step size is small, an apparently exponential drop of mean error is observed, due presumably to the increasing power of  $h$  in  $O(h^p)$ . Nonetheless, we recognize the problem of “overfitting” at low resolutions where a high degree polynomial interpolant introduces spurious patterns of change between given points.

These graphs were produced in *vort\_polyorder.m*.

## 5. CONCLUSION AND CRITIQUE

Differentiation by polynomial interpolation is a traditional method of numerical analysis that has been well-studied. The case study we have entertained here of deriving finite difference expressions and organizing them as a centric differentiation matrices is probably more for the student’s edification than of any scholarly contribution. Implementing these as a computation module, nonetheless, may have practical value of allowing for automated generation of finite

differences that can be applied in related problems.

Numerical differentiation in higher dimensions is an intriguing and extended field of study not fully reducible to 1D scenarios. The order of accuracy for mixed partial derivatives is one prominent problem to be addressed.

Of practical significance, We have also observed, through application of directional differentiation, that convergence patterns expected from 1D may not be as easily produced given limited computer memory and the added complexity of variation in multiple dimensions. The characteristic dependence of memory usage on the number of grid points per dimension  $n$  is  $O(n^m)$ , where  $m$  is the number of dimensions.

Importantly though, practical factors inevitably involved in experimental studies utilizing numerical differentiation were not discussed. Perhaps the most significant factor, noise is not considered in this study, the treatment of which is indispensable in analysis of experimental data. Typical treatment of noise may be applying a smoother to the noisy data prior to differentiation. Nonetheless, the averaging involved in smoothing may destroy local features of change. More advanced techniques such as smoothing polynomials or smoothing splines can be applied in such situations [3]. A more thorough study of the finite difference approximation of derivatives needs to consider and address the effect of noise.

Maybe the absence of a module for finite differences in MATLAB and Python bespeaks the presence of superior techniques, a candidate of which is spectral differentiation. Toward the prospect of studying these, I close our discourse presently.

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## 6. REFERENCES

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