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Truncation Error for Simplex Propagation
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Abstract
Cube propagation has been suggested as an alternative to Jacobian integration for estimating the volume change under a deformation in three dimensions [Pai et al., 2013]. Cube propagation estimates the change in volume by approximating a three-dimensional volume as a mesh of tetrahedra, which covers the interior of the volume and approximates the boundary as piece-wise triangular surface patches, and then estimate the change in volume under deformation of the volume as the sum of the change of volumes of the tetrahedra. This is an instance of the more general simplex counting, and in this technical report we derive the truncation error for simplex counting in 2 and 3 dimensions. In the appendix, we give a short review of numerical quadrature in 1 and 3 dimensions.

1 Introduction
We consider a \(d\)-dimensional simplex in \(\mathbb{R}^d\) being deformed by a smooth deformation field \(g : \mathbb{R}^d \to \mathbb{R}^d\):

\[ u = g(x), \] (1)

Given a simplex of interest \(\Gamma \subset \mathbb{R}^d\) and the determinant of the Jacobian of the transformation \(J(x) = \lvert \partial g(x) \rvert\), the volume of the transformed region \(\text{vol}(g(\Gamma))\) is given as

\[ \text{vol}(g(\Gamma)) = \int_{\Gamma} J(x) \, dx. \] (2)

Analytical solutions to this integral does not exist for most functions, and instead numerical techniques must be used. We will in the following consider the error of approximation of integrating the area of the deformed grid. In the appendix is given a review of numerical methods for estimating integrals in 1 and 3 dimensions together with their truncation error. In the following we will derive the truncation error for \(d = 1, 2, 3\).

1.1 Simplex counting for \(d = 1\)
In 1 dimension, \(g : \mathbb{R} \to \mathbb{R}\), and the volume reduces to the length of the deformed interval. Using numerical quadrature, we may estimate the integral of a function by sampling it in \(x_i, i = 0 \ldots N\). For simplicity we will assume regular sampling such that \(x_{i+1} - x_i = h = \frac{1}{N}.\) The following schemes are often used [Holmes, 2007],

\[ \int_{x_0}^{x_N} J(x) \, dx = \begin{cases} h \sum_{i=0}^{N-1} J(x_i) + \mathcal{O}(h), & \text{Left Box,} \\ 2h \sum_{i=0}^{N/2} J(x_{1+2i}) + \mathcal{O}(h^2), & \text{Midpoint,} \\ \frac{h}{4} \sum_{i=0}^{N-1} (J(x_i) + J(x_{i+1})) + \mathcal{O}(h^2), & \text{Trapezoidal,} \\ \frac{h}{6} \sum_{i=0}^{N/2} (J(x_{i-1}) + 4J(x_i) + J(x_{i+1})) + \mathcal{O}(h^4), & \text{Simpson.} \end{cases} \] (3)

Note that the Midpoint and Simpson rule are only defined for even \(N\), and that all orders of approximation are reduced by a factor \(h\), since each sum has \(N = \frac{1}{h}\) elements, thus, all orders are divided by \(h\).

Alternatively, the length of the deformed line may be estimated as the sum of deformation of each piece \((g(x_i), g(x_{i+1}))\) as

\[ \text{vol}(g(\Gamma)) = \sum_{i=0}^{N-1} g(x_{i+1}) - g(x_i) = g(x_N) - g(x_0). \] (4)
This we denote simplex counting and for 1 dimensions it is exact. Along the same lines of thought, the relative expansion may be evaluated as,

$$\text{vol}(g(\Omega)) - \text{vol}(\Omega) = (g(x_N) - g(x_0)) - (x_N - x_0) = (g(x_N) - x_N) - (g(x_0) - x_0).$$

Thus, we may equally well consider the change of length as the difference in the change of the end-points.

### 1.2 Simplex counting for $d = 2$

In 2 dimensions, $g : \mathbb{R}^2 \rightarrow \mathbb{R}^2$, and volume reduces to area. An example of a deformation is shown in Figure 1. The 1-dimensional integration rules (3) generalize for higher dimensions by applying them per integral, i.e.,

$$\int_{x_0}^{x_N} \int_{y_0}^{y_M} F(x, y) \, dy \, dx = \int_{x_0}^{x_N} f(x) \, dx,$$

where $f(x) = \int_{y_0}^{y_M} F(x, y) \, dy$. For future reference, we impose a regular sampling in the $y$ parameter as $y_i, i = 0 \ldots M$ such that $y_{i+1} - y_i = k = \frac{1}{M}$. It is worth noting that the error of approximation will, in most cases, be dominated by the last integration, since the inner integration(s) for each of the above rules will have been multiplied by the sampling distance in orthogonal directions one or more times.

An alternative estimate of the volume of the deformed grid is obtained by summing the volume of the deformed simplexes. We form simplexes in 2 dimensions as $(g(x_{i,j}), g(x_{i+1,j}), g(x_{i+1,j+1}))$ and $(g(x_{i,j}), g(x_{i,j+1}), g(x_{i+1,j+1}))$ as illustrated by the red, green and blue lines in Figure 1(a). The area of the deformed grid is thus,

$$\text{vol}(g(\Omega)) = \sum_{i=0}^{N-1} \sum_{j=0}^{M-1} \text{area}(g(x_{i,j}), g(x_{i+1,j}), g(x_{i+1,j+1})) + \text{area}(g(x_{i,j}), g(x_{i,j+1}), g(x_{i+1,j+1})).$$

where the area of a triangle defined by 3 points $a, b, c \in \mathbb{R}^2$ is given as

$$\text{area}(a, b, c) = \frac{1}{2} \left| \begin{array}{ccc} a & b & c \\ 1 & 1 & 1 \end{array} \right|.$$

Along the same lines of thought, the relative expansion may be evaluated as the sum of the triangles on the
boundary, e.g., \((x_{1,1}, g(x_{1,1}), g(x_{2,1}))\) and \((x_{1,1}, x_{2,1}, g(x_{2,1}))\), such that
\[
\text{vol}(g(\Omega)) - \text{vol}(\Omega) = \sum_{i=0}^{N-1} \text{area}(x_{i,1}, g(x_{i,1}), g(x_{i+1,1})) + \text{area}(x_{i,1}, x_{i+1,1}, g(x_{i+1,1})) \\
+ \sum_{i=0}^{N-1} \text{area}(x_{i,N}, g(x_{i,N}), g(x_{i+1,N})) + \text{area}(x_{i,N}, x_{i+1,N}, g(x_{i+1,N})) \\
+ \sum_{j=0}^{M-1} \text{area}(x_{1,j}, g(x_{1,j}), g(x_{1,j+1})) + \text{area}(x_{1,j}, x_{1,j+1}, g(x_{1,j+1})) \\
+ \sum_{j=0}^{M-1} \text{area}(x_{M,j}, g(x_{M,j}), g(x_{M,j+1})) + \text{area}(x_{M,j}, x_{M,j+1}, g(x_{M,j+1})) + R. 
\] (9)

In contrast to the 1-dimensional case, this has a non-zero remainder term. The situation is illustrated in Figure 2. Given 4 points on a star shaped object, the error by simplex counting is found as follows: Consider 2 consecutive
\[
\text{vol}(g(\Omega)) - \text{vol}(\Omega) = \sum_{i=0}^{N-1} \text{area}(x_{i,1}, g(x_{i,1}), g(x_{i+1,1})) + \text{area}(x_{i,1}, x_{i+1,1}, g(x_{i+1,1})) \\
+ \sum_{i=0}^{N-1} \text{area}(x_{i,N}, g(x_{i,N}), g(x_{i+1,N})) + \text{area}(x_{i,N}, x_{i+1,N}, g(x_{i+1,N})) \\
+ \sum_{j=0}^{M-1} \text{area}(x_{1,j}, g(x_{1,j}), g(x_{1,j+1})) + \text{area}(x_{1,j}, x_{1,j+1}, g(x_{1,j+1})) \\
+ \sum_{j=0}^{M-1} \text{area}(x_{M,j}, g(x_{M,j}), g(x_{M,j+1})) + \text{area}(x_{M,j}, x_{M,j+1}, g(x_{M,j+1})) + R. 
\]

By construction,
\[
\text{vol}(g(\Omega)) - \text{vol}(\Omega) = \sum_{i=0}^{N-1} \text{area}(x_{i,1}, g(x_{i,1}), g(x_{i+1,1})) + \text{area}(x_{i,1}, x_{i+1,1}, g(x_{i+1,1})) \\
+ \sum_{i=0}^{N-1} \text{area}(x_{i,N}, g(x_{i,N}), g(x_{i+1,N})) + \text{area}(x_{i,N}, x_{i+1,N}, g(x_{i+1,N})) \\
+ \sum_{j=0}^{M-1} \text{area}(x_{1,j}, g(x_{1,j}), g(x_{1,j+1})) + \text{area}(x_{1,j}, x_{1,j+1}, g(x_{1,j+1})) \\
+ \sum_{j=0}^{M-1} \text{area}(x_{M,j}, g(x_{M,j}), g(x_{M,j+1})) + \text{area}(x_{M,j}, x_{M,j+1}, g(x_{M,j+1})) + R. 
\]

In contrast to the 1-dimensional case, this has a non-zero remainder term. The situation is illustrated in Figure 2. Given 4 points on a star shaped object, the error by simplex counting is found as follows: Consider 2 consecutive points \(u_i = g(x_i)\) and \(u_{i+1} = g(x_{i+1})\) as points on the abscissa of a local cartesian coordinate system and choose one of the two possible orthogonal directions as the ordinate. Since the object is star shaped, the curve between the two points is a function in this local cartesian coordinate system. Denote the abscissa \(u\), the points \(u_i\) and \(u_{i+1}\), and the curve \(f(u)\), and scale the abscissa such that \(h = u_{i+1} - u_i = \|u_{i+1} - u_i\|\). Thus, the area between straight line between \(u_i\) and \(u_{i+1}\) and \(g(x)\) from \(x_i\) to \(x_{i+1}\) is equal to \(\int_0^h f(u)\, du\). Consider an analytical function,
\[
f(u) = f(0) + uf'(0) + \frac{u^2}{2} f''(0) + O(u^3). \]
(10)

Since by construction, \(f(0) = f(h) = 0\), and therefore we concluded that \(f(0) = 0\), and \(f'(0) = -\frac{h}{2} f''(0) + O(h^2)\). Finally we integrate \(f\) on the interval and find,
\[
\int_0^h f(u)\, du = \int_0^h u(-\frac{h}{2} f''(0) + O(h^2)) + \frac{u^2}{2} f''(0) + O(u^3)\, du = -\frac{h^3}{12} f''(0) + O(h^4). \]
(11)

Thus we conclude that the order of convergence is \(O(h^3)\) similarly to the trapezoidal rule. For the sum of the areas over a grid, the error by the inner interfaces will cancel out leaving only the error of the outer boundary. Hence, the area of a deformed grid approximated by simplex counting converges as \(\frac{1}{2} O(h^3) = O(h^2)\), where \(h \approx \text{const.} / N\) and \(N\) is the number of points on the boundary. This convergence result is valid even when the total object is not star-shaped. The only requirement is that the object is sampled sufficiently fine for \(f\) to be a function between \(u_i\) and \(u_{i+1}\).

We have performed an empirical comparison of the error of approximation of area for the deformation shown in Figure 1 for various number of sample points. This is shown in Figure 3. As can be seen, box counting has the lowest order of convergence, and midpoint, trapezoidal and the two simplex counting methods have similar order of convergence, although simplex counting consistently outperforms the midpoint and trapezoidal methods. The Simpson rule has the best order of convergence.

A note is in order w.r.t. the difference between the convergence of the integral of the Jacobian and simplex counting. Consider \(g\) to be a polynomial function of degree \(n\), then the Jacobian will be a polynomial of degree \(2(n - 1) = 2n - 2\). Hence, the trapezoidal rule for estimating the deformed area by Jacobian integration is an approximation of an integral that has a degree twice that of simplex counting. Higher degree often implies higher
derivatives, hence in order to obtain the same precision with Jacobian integration, we should expect that a finer grid is required, as confirmed by the Figure 3, where simplex counting is a constant factor more precise than Jacobian integration using the trapezoidal rule.

1.3 Simplex counting for \( d = 3 \)

In 3 dimensions, \( g : \mathbb{R}^3 \rightarrow \mathbb{R}^3 \). The 1-dimensional integration rules (3) generalize for higher dimensions by applying them per integral, i.e.,

\[
\int_{x_0}^{x_N} \int_{y_0}^{y_M} \int_{z_0}^{z_L} F(x, y, z) \, dz \, dy \, dx = \int_{x_0}^{x_N} \int_{y_0}^{y_M} \int_{z_0}^{z_L} f(x, y) \, dy \, dx = \int_{x_0}^{x_N} f(x) \, dx, \tag{12}
\]

where \( F(x, y) = \int_{z_0}^{z_L} F(x, y, z) \, dz \) and \( f(x) = \int_{y_0}^{y_M} F(x, y) \, dy \). For future reference, we impose a regular sampling in the \( z \) parameter as \( z_i = \frac{l}{L} \) such that \( z_{i+1} = z_i + \frac{l}{L} \). As for the 2 dimensional case, we note that the error of approximation will, in most cases, be dominated by the last integration, since the inner integration(s) for each of the above rules will have been multiplied by the sampling distance in orthogonal directions one or more times.

As for the lower dimensional cases, we will approximate the volume of the deformed shape by sum of the volume of deformed tetrahedra. The error of this approximation will be the area between the outer surface triangles and \( g \). Consider a surface triangle spanned by the 3 points \( g(x_{i,j}), g(x_{i+1,j}), \) and \( g(x_{i,j+1}) \). We may choose a local coordinate system whose ordinate is perpendicular to the triangle and define a local orthogonal coordinate system, \((u, v)\), in the triangle plane such that difference between the triangular plane and the surface \( g \) is given as \( f(u, v) \) and such that \( x_{i,j} \mapsto (0, 0), x_{i+1,j} \mapsto (h, 0), \) and \( x_{i,j+1} \mapsto (0, k) \) and the jacobian of the transformation is sinus the angle between the vectors \( g(x_{i+1,j}) - g(x_{i,j}) \) and \( g(x_{i,j+1}) - g(x_{i,j}) \). In the following we will denote this Jacobian for \( c_i \).

Writing

\[
f(u, v) = f(0, 0) + uf_u(0, 0) + v f_v(0, 0) + \frac{u^2}{2} f_{uu}(0) + uv f_{uv}(0) + \frac{v^2}{2} f_{vv}(0) + \mathcal{O}(u^3 + u^2 v + uv^2 + v^3), \tag{13}
\]

where \( f_u = \frac{\partial f}{\partial u} \) etc.. Since by construction \( f(0, 0) = f(h, 0) = f(0, k) = 0 \), we conclude that \( f(0, 0) = 0, f_u(0, 0) = -\frac{h}{2} f_{uu}(0) + \mathcal{O}(h^2), \) and \( f_v(0, 0) = -\frac{k}{2} f_{vv}(0) + \mathcal{O}(k^2) \). Thus integrating on the triangle spanned by
(0, 0), (h, 0), and (k, 0), we find the area between the triangle and the function \( f \) in \( g \)'s coordinate system to be
\[
c_i \int_0^k \int_0^{h(1-v/k)} f(u,v) \, du \, dv
\]
\[
= c_i \int_0^k \int_0^{h(1-v/k)} u(-\frac{h}{2} f_{uu}(0) + \mathcal{O}(h^2)) + v(\frac{k}{2} f_{uv}(0) + \mathcal{O}(k^2)) \, du \, dv
\]
\[
+ c_i \int_0^k \int_0^{h(1-v/k)} \frac{u^2}{2} f_{uu}(0) + uv f_{uv}(0) + \frac{v^2}{2} f_{vv}(0) + \mathcal{O}(u^3 + u^2v + uv^2 + v^3) \, du \, dv
\]
\[
= \frac{c_i}{21} (-h^3 k f_{uu}(0,0) + h^3 k^2 f_{uv}(0,0) - h k^3 f_{vv}(0,0)) + \mathcal{O}\left(\sum_{i=0}^4 h^4 k^{4-i}\right).
\]
Thus we conclude that the error of approximation for simplex counting in 3 dimensions is \( \mathcal{O}\left(h k \sum_{i=0}^2 h^i k^{2-i}\right) \) per surface triangle. Summing over in the order of \( \frac{\text{no of surface points}}{h} \) we find that the total error of approximation is \( \mathcal{O}\left(\sum_{i=0}^2 h^i k^{2-i}\right) \). The constants \( c_i \) will vary slightly as the sample points of \( g \) change, however not in a manner influencing the error of approximation.

### A. Review of Numerical Quadrature

In this appendix, we review rules for integration by numerical quadrature for 1 and 3 dimensional functions. The general problem is, given discrete set of points on a domain and a scalar, analytical function, find approximation to the integral of that function.

#### A.1 Case \( f : \mathbb{R} \rightarrow \mathbb{R} \)

To derive truncation error we utilize [Holmes, 2007, Table 1.4],
\[
\int_{x_0}^{x_1} f(x) \, dx = \begin{cases} \hspace{1cm} h f(x_0) + R_{LB}, & \text{Left Box,} \\ h f(x_\frac{1}{2}) + R_{MP}, & \text{Midpoint,} \\ \frac{h}{2} (f(x_0) + f(x_1)) + R_{T}, & \text{Trapezoidal,} \end{cases}
\]
where \( h = x_0 - x_1 \) is a constant, and \( R_* \) are remainder terms. To evaluate the remainder term of \( R_{LB} \), we consider the truncated Taylor series \( f_1(x_0 + \Delta x) = f(x_0) + \Delta x f'(x_0) + \mathcal{O}(\Delta x^2) \) for \( \Delta x \in [0, h] \), and where the Landau notation is used such that there exists a \( \delta > 0 \) for which \( \mathcal{O}(G(h)) \leq |G(h)| \) for \( |h| < \delta \). The integral of \( f_1(x_0 + \Delta x) \) over \( \Delta x \) is
\[
\int_0^h f_1(x_0 + \xi) \, d\xi = \int_0^h f(x_0) + \xi f'(x_0) \, d\xi
\]
\[
= h f(x_0) + \frac{1}{2} h^2 f'(x_0) + \mathcal{O}(h^3)
\]
\[
= h f(x_0) + \mathcal{O}(h^2).
\]
To ensure that \( \mathcal{O}(h^2) \) is the dominating term for \( 0 < h < 1 \), we consider the general difference between an \( n \)-degree polynomial \( p(x) \) and a continuous function \( y(x) \) with \( n + 1 \) continuous derivatives and, where \( y(x_i) = p(x_i) \) at \( x_0 < x_1 < \cdots < x_n \). This difference may be found to be,
\[
y(x) - p(x) = \frac{y^{(n+1)}(\eta)}{(n+1)!} \prod_{i=0}^n (x - x_i),
\]
for some point \( \eta \in [x_0, x_n] \). Thus, the difference between the integral of \( f \) and \( f_1 \) is
\[
\int_{x_0}^{x_1} f(x) - f_1(x) \, dx = \int_{x_0}^{x_1} \frac{f''(\eta)}{2} (x - x_0)(x - x_1) \, dx
\]
\[
= \frac{f''(\eta)}{12} (x_0 - x_1)^3
\]
\[
= -\frac{f''(\eta)}{12} h^3
\]
\[
= \mathcal{O}(h^3),
\]
and we conclude that this error is insignificant, when compared to \(O(h^2)\), hence we compare (18) with the Left Box rule and conclude that \(R_{LB} = O(h^2)\). Similarly, for the Midpoint method we have,

\[
\int_{-h/2}^{h/2} f_1(x_{1/2} + \xi) \, d\xi = \int_{-h/2}^{h/2} f(x_{1/2}) + \xi f'(x_{1/2}) \, d\xi = h f(x_{1/2}).
\]

(25)

In this case, the dominating part of the remainder is found by (23) and comparing (25) with the Midpoint rule, we conclude that \(R_{MP} = O(h^3)\). The remainder term for the Trapezoidal rule is derived by polynomial interpolation. A Lagrange polynomial of degree \(n\) and with zero crossings at \(x_0 < x_1 < \cdots < x_n\) and with values \(y_i = L_n(x_i)\) is given as

\[
L_n(x) = \sum_{i=0}^{n} y_i l_{i,n}(x)
\]

(26)

\[
l_{i,n}(x) = \prod_{m=0,1,\ldots,i-1,i+1,\ldots,n} \frac{x - x_m}{x_i - x_m}
\]

(27)

The Trapezoidal rule is a Lagrange polynomial of degree 1 for the points \(x_0 < x_1\), since

\[
\int_{x_0}^{x_1} L_1(x) \, dx = f(x_0) \int_{x_0}^{x_1} l_{0,1}(x) \, dx + f(x_1) \int_{x_0}^{x_1} l_{1,1}(x) \, dx
\]

(28)

\[
= f(x_0) \int_{x_0}^{x_1} \frac{x - x_1}{x_0 - x_1} \, dx + f(x_1) \int_{x_0}^{x_1} \frac{x - x_0}{x_1 - x_0} \, dx
\]

(29)

\[
= f(x_0) \frac{x_1 - x_0}{2} + f(x_1) \frac{x_1 - x_0}{2} = \frac{h}{2} (f(x_0) + f(x_1)).
\]

(30)

Since the Lagrange polynomial is of degree 1, the difference between the integral of \(f\) and \(L_1\) is found to be \(O(h^3)\) in a manner similarly (23). Hence, comparing (31) with the Trapezoidal rule we conclude that \(R_T = O(h^3)\).

A.2 Case \(f : \mathbb{R}^3 \to \mathbb{R}\)

We will now extend the numerical quadrature rules examine in Subsection A.1 to scalar fields in 3 dimensions. Consider the integral of \(f(x, y, z)\) on the domain, \(\Omega = [x_0, x_1] \times [y_0, y_1] \times [z_0, z_1]\). We will extend the quadrature rules by integrating the domain axis by axis as,

\[
\int_{\Omega} f(x, y, z) \, dx dy dz = \int_{z_0}^{z_1} f(z) \, dz,
\]

(32)

where

\[
f(z) = \int_{y_0}^{y_1} f(y, z) \, dy,
\]

(33)

and

\[
f(y, z) = \int_{x_0}^{x_1} f(x, y, z) \, dx,
\]

(34)

where we have overloaded the symbol \(f\). Applying the Left Box rule implies that

\[
f(y, z) = h_x f(x_0, y, z) + O(h_x^2),
\]

(35)

where \(h_x = x_1 - x_0\). Therefore,

\[
f(z) = \int_{y_0}^{y_1} h_x f(x_0, y, z) + O(h_x^2) \, dy
\]

(36)

\[
= h_y h_x f(x_0, y_0, z) + O(h_y h_x^2 + h_y^2)
\]

(37)

\[
= h_y h_x f(x_0, y_0, z) + O(h_x^2)
\]

(38)
where \( h_y = y_1 - y_0 \), and finally,

\[
\int_{\Omega} f(x, y, z) \, dxdydz = h_z h_y h_x f(x_0, y_0, z_0) + \mathcal{O}(h_z^2),
\]

(39)

where \( h_z = z_1 - z_0 \). Thus, the order of the remainder depends on the order of integration, and we conclude that integrating in the order, with decreasing \( h \) implies the smallest bound on the remainder in terms of \( h \). In any case, we conclude that the remainder for this generalisation of the Left Box rule to 3 dimensions is of order \( \mathcal{O}(h^2) \).

Using identical arguments we derive the Midpoint and Trapezoidal rules in 3 dimensions as,

\[
\int_{x_0}^{x_1} f(x) \, dx = \begin{cases} 
  h_z h_y h_x f(x_0, y_0, z_0) + \mathcal{O}(h_z^2), & \text{Left Box,} \\
  h_z h_y h_x f(x_1/2, y_1/2, z_1/2) + \mathcal{O}(h_z^2), & \text{Midpoint,} \\
  \frac{h_z h_y h_x}{8} \left( \sum_{i=0}^{1} \sum_{j=0}^{1} \sum_{k=0}^{1} f(x_i, y_j, z_k) \right) + \mathcal{O}(h_z^3), & \text{Trapezoidal.}
\end{cases}
\]

(40)

This concludes our review.

References
