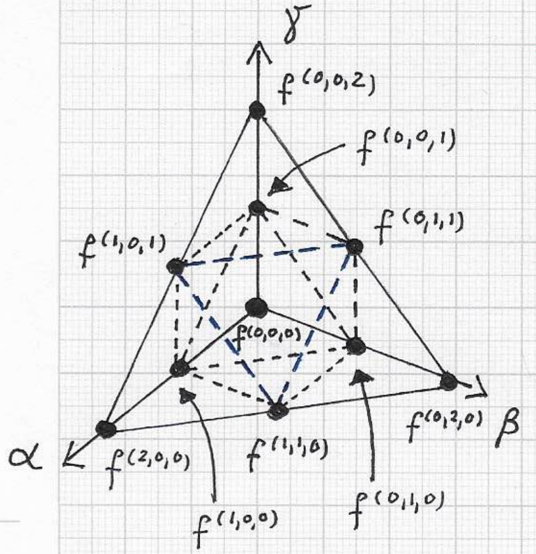
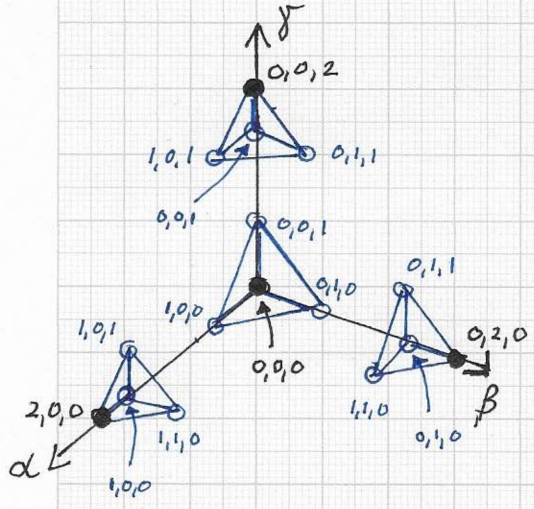
Stratovan

■ FRACTIONAL CALCULUS AND FEATURES – Cont'd.

• *Fractional derivatives:*



Stencil of data used to define non-integer-order partial derivatives $f^{(\alpha,\beta,\gamma)}$ over a 3D, volumetric domain – (α,β,γ)-space



Exploded view of stencil; shown are four tetrahedra and the four index triples p,q,r defining their vertices / vertex data

• Note: The use of simplicial elements (triangles, tetrahedra, simplices) and cube elements (squares, cubes, hypercubes) implies a simple, "natural," way of data interpolation: linear, bilinear, trilinear, "multi-linear" interpolation. This class of data interpolation ensures that the resulting interpolating function's values are bounded by the minimal and maximal values of the data given at an element's corners; undesirable "under-" and "overshoots" are impossible. Neverthless, it is not known what type of interpolation is "ideal" when interpolating integer-order partial derivatives for a specific classification problem.

The figures (left) illustrate the stencil of ten integer-order partial derivatives (finite difference approximations) $f^{(p,q,r)}$, $p+q+r \leq 2$, $p,q,r \geq 0$, and a possible way to establish edge connections between the points $(p,q,r)^T$ in 3D (α,β,γ)-space. In the lower figure we refer to $f^{(p,q,r)}$ and its associated point $(p,q,r)^T$ via "p,q,r".

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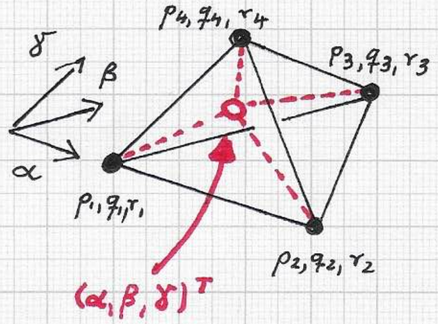
■ FRACTIONAL CALCULUS AND FEATURES — Cont'd.

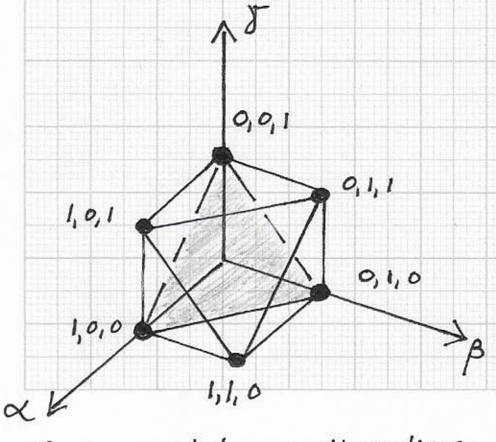
• Fractional derivatives:



Data needed to perform linear interpolation over tetrahedron; one must compute weight w_i for the derivatives at the corners. For example, the weight w_1 for $f^{(p_1, q_1, r_1)}$ is the barycentric coordinate value

$$w_1 = \mathrm{vol}\left((\alpha,\beta,\gamma)^T, (p_2,q_2,r_2)^T, (p_3,q_3,r_3)^T, (p_4,q_4,r_4)^T\right) / \mathrm{vol}\left((p_1,q_1,r_1)^T, (p_2,q_2,r_2)^T, (p_3,q_3,r_3)^T, (p_4,q_4,r_4)^T\right).$$

("vol" refers to volume.)



Convex polytope with vertices $(p,q,r)^T$, $p+q+r \geq 1$, $p+q+r \leq 2$; must decompose into tetrahedra

The prototypical building block for grid-based piecewise linear interpolation of integer-order partial derivatives is linear interpolation of four data $f^{(p_i, q_i, r_i)}$, $i=1...4$, over this data's associated tetrahedron (Left figure). The value of the non-integer-order derivative at point $(\alpha, \beta, \gamma)^T$ is

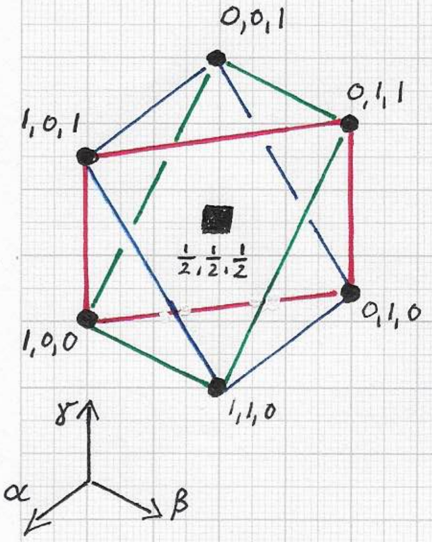
$$f^{(\alpha,\beta,\gamma)} = \sum_{i=1}^{4} w_i f^{(p_i, q_i, r_i)},$$

where $f^{(p_i, q_i, r_i)}$ is an integer-order partial derivative and w_i is the i-th barycentric coordinate of the point $(\alpha, \beta, \gamma)^T$ represented relative to the four corners $(p_i, q_i, r_i)^T$, $i=1...4$, of the tetrahedron containing $(\alpha, \beta, \gamma)^T$. (The second figure shown on the last page shows four tetrahedra that can be subjected to this approach to linear interpolation.)

The left figure shows the integer-order derivatives $f^{(p,q,r)}$, where $1 \leq p+q+r \leq 2$, $p, q, r \geq 0$. The edges in the figure define triangles bounding an (α,β,γ)-space volume that must be decomposed into tetrahedra for linear interpolation.

■ FRACTIONAL CALCULUS AND FEATURES – Cont'd.

• Fractional derivatives:



"Octahedral volume" bounded by eight triangles and decomposed into eight tetrahedra, using the additional point $(\frac{1}{2},\frac{1}{2},\frac{1}{2})^T$ and associated derivative approximation $f^{(\frac{1}{2},\frac{1}{2},\frac{1}{2})}$.

$f_{RED}^{(1/2,1/2,1/2)}$ = bilinInterpol $(f^{(1,0,0)}, f^{(0,1,0)}, f^{(1,0,1)}, f^{(0,1,1)})$

$f_{GREEN}^{(1/2,1/2,1/2)}$ = ...

$f_{BLUE}^{(1/2,1/2,1/2)}$ = ...

$\Rightarrow f^{(1/2,1/2,1/2)}$ = average

The polytope defined by the six points $(p,q,r)^T$, $1 \le p+q+r \le 2 \wedge p,q,r \ge 0$, together with the 12 edges as shown in the left figure is an octahedron (with eight triangular faces). A simple way to decompose this octahedron into eight tetrahedra is the following: Connect the six vertices of the octahedron to a "center point" $(\frac{1}{2},\frac{1}{2},\frac{1}{2})^T$; the vertices of a triangle face of the octahedron, when connected via an edge to the "center point", define three vertices of a tetrahedron – with $(\frac{1}{2},\frac{1}{2},\frac{1}{2})^T$ being the fourth vertex; eight tetrahedra result. For the eventual interpolation of the given integer-order partial derivatives $f^{(p,q,r)}$ over these eight tetrahedra one must determine a "meaningful" value of $f^{(\frac{1}{2},\frac{1}{2},\frac{1}{2})}$ associated with the point $(\frac{1}{2},\frac{1}{2},\frac{1}{2})^T$ in (α,β,γ)-space. Considering the left figure again, one can perform three bilinear interpolations in the colored rectangles (**red**, **green** and blue) and use the average as value of the non-integer-order derivative $f^{(\frac{1}{2},\frac{1}{2},\frac{1}{2})}$.

$\Rightarrow$ Perform linear interpolation of derivatives over each tetrahedron.

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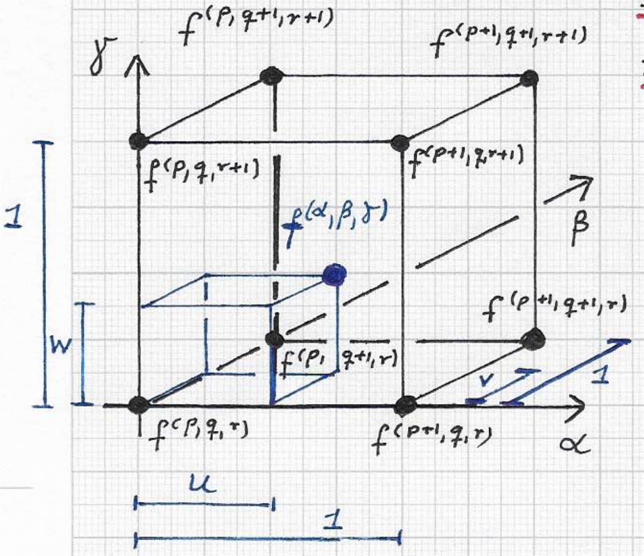
FRACTIONAL CALCULUS AND FEATURES – Cont'd.

• Fractional derivatives:



Data stencil and grid geometry defined by integer-order partial derivatives $f^{(p,q,r)}, \dots, f^{(p+1,q+1,r+1)}$ and unit cube (hyper-cube) grid cells; non-integer-order partial derivative value $f^{(\alpha,\beta,\gamma)}$ at location $(\alpha,\beta,\gamma)^T$ determined by given partial derivative data at corners of cube containing point (α,β,γ). Local coordinates $u, v, w \in [0,1]$ can be used to perform corner data interpolation.

• **Note:** As our driving application concerns the processing and analysis of 3D scan data and material classification, trivariate derivatives $f^{(\alpha,\beta,\gamma)}$ are of greatest interest; thus we discuss it in depth. Further, since image/scan data processing uses nearly exclusively given image/scan density/intensity values and derived first and second partial derivatives, we also focus on the computation of low-order derivatives $f^{(\alpha,\beta,\gamma)}$, i.e., the case $\alpha+\beta+\gamma \leq 2$. But: The ability to compute $f^{(\alpha,\beta,\gamma)}$ for real-valued parameter α, β, γ provides the possibility to compute "MANY" non-integer-order partial derivatives.

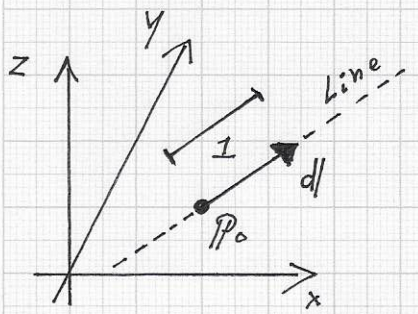
Trilinear interpolation can be used to compute a value for $f^{(\alpha,\beta,\gamma)}$, given eight integer-order derivatives $f^{(p,q,r)}, \dots, f^{(p+1,q+1,r+1)}$ at the vertices of the cube containing the point $(\alpha,\beta,\gamma)^T$. Using local coordinates $u = \alpha - p$, $v = \beta - q$ and $w = \gamma - r$, $f^{(\alpha,\beta,\gamma)}$ is computed as:

FRACTIONAL CALCULUS AND FEATURES – Cont'd.

• Fractional derivatives:

$$
\begin{aligned}
f^{(\alpha,\beta,\gamma)} = & (1-u)(1-v)(1-w)\, f^{(p,q,r)} \\
& + u\,(1-v)(1-w)\, f^{(p+1,q,r)} \\
& + (1-u)\, v\, (1-w)\, f^{(p,q+1,r)} \\
& + u\, v\, (1-w)\, f^{(p+1,q+1,r)} \\
& + (1-u)(1-v)\, w\, f^{(p,q,r+1)} \\
& + u\,(1-v)\, w\, f^{(p+1,q,r+1)} \\
& + (1-u)\, v\, w\, f^{(p,q+1,r+1)} \\
& + u\, v\, w\, f^{(p+1,q+1,r+1)} .
\end{aligned}
$$

Again, the value of $f^{(\alpha,\beta,\gamma)}$ is bounded by the minimal and maximal values of the eight derivative values at the cube's vertices — since trilinear interpolation is "repeated linear interpolation in the α-, β- and γ- directions.



Directional derivative of function $f(x,y,z)$; gradient of f is grad $f = \nabla f = (f^{(1,0,0)}, f^{(0,1,0)}, f^{(0,0,1)})$; derivative $D^{(1)}$ at point $p_0 = (x_0, y_0, z_0)^T$ in unit direction $dl = (dx, dy, dz)^T$ given as

$$D^{(1)} = D^{(1)}_{dl}(p_0) = \nabla f(p_0) \cdot dl$$

⇒ Can use $D^{(0)}, D^{(1)}, D^{(2)}, \ldots$ to characterize uni-directional derivative behavior.

• **Note:** It is also possible to consider directional, univariate derivative behavior in 2D/3D images/scans. The (first) directional derivative $D^{(1)}_{dl}(p_0)$ of a function f at point p_0 in direction dl, where $\|dl\| = 1$, is

$$D^{(1)}_{dl}(p_0) = (f^{(1,0)}, f^{(0,1)}) \begin{pmatrix} dx \\ dy \end{pmatrix} \text{ and}$$

$$D^{(1)}_{dl}(p_0) = (f^{(1,0,0)}, f^{(0,1,0)}, f^{(0,0,1)}) \begin{pmatrix} dx \\ dy \\ dz \end{pmatrix},$$

evaluated at $p_0 = (x_0, y_0, [z_0])^T$ for the functions $f(x,y)$ and $f(x,y,z)$, respectively.