Gradient and smoothing stencils with isotropic discretization error

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Abstract

Gradient stencils with isotropic $\mathcal{O}(h^2)$ and $\mathcal{O}(h^4)$ discretization error are constructed by considering their effect on common, rotationally invariant building blocks of field-theoretic Lagrangians in three dimensions. The same approach is then used to derive low-pass filters with isotropic $\mathcal{O}(h^4)$ and $\mathcal{O}(h^6)$ error.

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I. INTRODUCTION

Stencils, finite difference approximations of differential operators on a regular lattice, are a staple of numerical analysis. In [1], it was pointed out that the traditional measure of their quality, the order n of the leading discretization error ($\mathcal{O}(h^n)$ for lattice spacing h) is insufficient when the number of dimensions > 1. Different stencils then exist for a given n, generally with different, direction-dependent discretization errors. This anisotropy causes distortions, like preferred axes of growth or wave propagation.

The authors of [1] proceeded to derive a number of stencils with isotropic error, including $\mathcal{O}(h^2)$ discretizations of the Laplacian ∇^2, the Bilaplacian $(\nabla^2)^2$ and the gradient of the Laplacian $\partial_x(\nabla^2)$ in three dimensions. Notably absent are improved stencils for first order derivatives. One reason is presumably that in simple cases, their use can be avoided using Green's first identity, i.e. integration by parts,

$$\int_U \left(\psi\nabla^2\varphi + \nabla\varphi\cdot\nabla\psi\right) dV = \oint_{\partial U} \psi\left(\nabla\varphi\cdot\vec{n}\right) dS \tag{1}$$

where φ and ψ are scalar functions defined on the spatial region U with boundary ∂U. Given suitable (e.g. periodic or vanishing) boundary conditions, the surface integral vanishes. Any terms in an action integral on the form $\nabla\varphi\cdot\nabla\psi$ can therefore be replaced with the equivalent $-\psi\nabla^2\varphi$, as was done e.g. in [2][3][4].

Unfortunately, this simple trick does not work in more complicated cases, like the non-linear vector-scalar interaction terms on the form $f(\phi)\left(\mathcal{A}_\mu\partial_\nu\phi - \mathcal{A}_\nu\partial_\mu\phi\right)^2$ found in gauged sigma models. To study the dynamics of models containing such terms, one must turn to numerics, and to prevent the introduction of directional artifacts, one must confront the question: how can the first order derivative be discretized in such a way that the resulting errors are isotropic?

The obvious idea, using a weighted average of rotated one-dimensional operators, is incomplete; different weights can be chosen to minimize different errors. The issue has been studied in detail in the context of aeroacoustic simulations, where there is a special need to minimize dispersion and dissipation errors. Even in such a specific context, plenty of arbitrariness remains. You can choose to minimize dispersion over a certain spectral range, along certain directions (e.g. the diagonals between coordinate axes) and/or over some spatial average [5][6].

Here I will follow a different approach, closer in spirit to [1]: write down the most general stencil of order n, apply it to common rotationally invariant building blocks of field theories in three spatial dimensions, compare with the equivalent analytical expressions, and impose the requirement that the errors be rotationally invariant too, at least to $\mathcal{O}(h^n)$.

II. IMPROVED DERIVATIVE STENCILS

A. $\mathcal{O}(h^2)$ stencil

Given a differential operator D of order p and a stencil S_{ijk} with extension $2r+1$, i.e. with each index running from $-r$ to r, follow [1] and impose the requirement that

$$\sum_{ijk} S_{ijk} P_q(x+ih, y+jh, z+kh) = D P_q(x,y,z) \tag{2}$$

for any polynomial

$$P_q(x,y,z) = \sum_{i,j,k=0..q}^{i+j+k\leq q} a_{ijk} x^i y^j z^k \tag{3}$$

where a_{ijk} are arbitrary constant coefficients and $q = p+n-1$. This is a necessary and sufficient condition for S_{ijk} to be an $\mathcal{O}(h^n)$ approximation of D. Since we are interested in $p=1$, our test polynomials will all be $q=n$.

As a warmup, consider a compact (i.e. $r=1$) stencil. From the one-dimensional case, we know that it can be at most an $\mathcal{O}(h^2)$ approximation to the first derivative, so we write

$$\begin{aligned} P_2(x,y,z) &= a_{000} + a_{001} z + a_{002} z^2 \\ &+ a_{010} y + a_{011} yz + a_{020} y^2 \\ &+ a_{100} x + a_{101} xz + a_{110} xy \\ &+ a_{200} x^2 \end{aligned} \tag{4}$$

and demand that it behave like a derivative w.r.t. x:

$$\sum_{i,j,k=-1}^{1} S_{ijk} P_2(x+ih, y+jh, z+kh) = \partial_x P_2(x,y,z) \tag{5}$$

As such, it must also satisfy the symmetry conditions

$$S_{ikj} = S_{i-jk} = S_{ij-k} = S_{ijk} \tag{6}$$

(invariance under rotations and reflections about the x axis) and

$$S_{-ijk} = -S_{ijk} \tag{7}$$

(must be odd along the x axis). Since the derivative does not care which point we choose as the origin, it is then sufficient to solve e.g. for S_{100} at $x = y = z = 0$, where one easily finds

$$S_{100} = \frac{1 - 8h(S_{111} + S_{101})}{2h} \tag{8}$$

When this relation is satisfied, Eq. (5) holds everywhere.

Setting the off-axis weights S_{111} and S_{101} to zero reproduces the standard one-dimensional stencil, as it should, but we want to use them to improve the computation of some rotational invariant. A natural target is the gradient squared. It's enough to compute it for a plane wave with constant wave vector $\vec{k} = (k_x, k_y, k_x)$:

$$W(\vec{x}, \vec{k}) = e^{\imath \vec{k}\cdot\vec{x}} = e^{\imath(k_x x + k_y y + k_z z)} \tag{9}$$

$$(\nabla W(\vec{x}, \vec{k}))^2 = -\vec{k}^2 W^2(\vec{x}, \vec{k}) \tag{10}$$

Since $W(\vec{x}, \vec{k})$ is a Fourier basis, establishing invariance w.r.t. it establishes invariance for any (well behaved) field.

At the origin, where $(\nabla W(\vec{x}, \vec{k}))^2 = -\vec{k}^2$, applying our stencil yields

$$\begin{aligned}
&\left(\sum_{i,j,k=-1}^{1} S_{ijk} e^{\imath h(ik_x + jk_y + kk_z)}\right)^2 \\
+ &\left(\sum_{i,j,k=-1}^{1} S_{jik} e^{\imath h(ik_x + jk_y + kk_z)}\right)^2 \\
+ &\left(\sum_{i,j,k=-1}^{1} S_{kji} e^{\imath h(ik_x + jk_y + kk_z)}\right)^2 \\
= &\; -\vec{k}^2 \\
&+ \frac{h^2}{3}(k_x^4 + k_y^4 + k_z^4) \\
&+ 8h^3(S_{101} + 2S_{111})(k_x^2 k_y^2 + k_x^2 k_z^2 + k_y^2 k_z^2) \\
&+ \mathcal{O}(h^5)
\end{aligned} \tag{11}$$

(the stencil for ∂_y is obtained by swapping i and j in S_{ijk}, the stencil for ∂_z by swapping i and k).

At first sight, this is not encouraging. The leading error term is not proportional to some constant expression which could be made to vanish by an appropriate choice of stencil coefficients, and it is not rotationally invariant. But we can choose S_{111} and S_{101} so as to complete the squares: any

$$S_{101} + 2S_{111} = \frac{1}{12h} \tag{12}$$

will reduce the $\mathcal{O}(h^2)$ error term to $(h\vec{k}^2)^2/3$, which is manifestly isotropic. Since we knew from the outset that the error would be $\mathcal{O}(h^2)$, this is the best result we could have hoped for. It is now easily verified that the improved stencil also produces an isotropic leading error $h^2(k_A \cdot k_B)(k_A^2 + k_B^2)/6$ in the generalized case $\nabla W(\vec{x}, \vec{k_A}) \cdot \nabla W(\vec{x}, \vec{k_B})$, and the same leading error term as for gradient squared when applied twice to compute the Laplacian, $\nabla^2 W(\vec{x}, \vec{k})$.

Absent further targets for improvement, we can stop here and simply choose to minimize the number of multiplications and additions by setting e.g. the "corner" coefficient S_{111} to zero. The entire stencil is then given by

$$S_{0jk} = 0 \tag{13}$$

$$S_{1jk} = -S_{-1jk} = \frac{1}{12h}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{14}$$

Note that the sum of the weights in S_{1jk} equals the single weight in the one-dimensional stencil. The improved stencil essentially combines its one-dimensional equivalent with a low-pass filter along the orthogonal axes.

B. $\mathcal{O}(h^4)$ stencil

The construction of a stencil with $\mathcal{O}(h^4)$ isotropic error proceeds along the same lines. From the one-dimensional case, we know that at least $r = 2$ is required. Applying the symmetry conditions of Eq. (6) and (7) reduces the number of independent stencil weights from $5^3 = 125$ to 12. The test polynomial of Eq. (3) is now P_4, and we demand again that our stencil act on it like a derivative w.r.t. x. Applying this condition at the origin eliminates three more independent weights, which can be taken to be e.g.

$$\begin{aligned} S_{100} &= 4S_{111} + 8S_{201} + 12S_{102} + 16S_{211} \\ &\quad +32(S_{112} + S_{202} + S_{122}) + 64S_{222} \\ &\quad +80S_{212} + 2/(3h) \end{aligned} \tag{15}$$

$$\begin{aligned} S_{200} &= (4(S_{201} + S_{202} + S_{211} + S_{222}) \\ &\quad +8S_{212} + 1/h)/(-12) \end{aligned} \tag{16}$$

$$\begin{aligned} S_{101} &= -2(S_{111} + S_{201} + 2(S_{102} + S_{211})) \\ &\quad -8(S_{202} + S_{122}) - 10S_{112} - 16S_{222} \\ &\quad -20S_{212} \end{aligned} \tag{17}$$

When these relations are satisfied, the stencil acts on $P_4(x, y, z)$ like ∂_x everywhere.

As expected, setting the off-axis weights to zero reproduces the standard one-dimensional $\mathcal{O}(h^4)$ stencil ($S_{100} = 2/(3h)$, $S_{200} = -1/(12h)$) but again, we can use them to ensure that the gradient squared of an arbitrary plane wave is reproduced with an isotropic leading error term. At the origin, the error in $(\nabla W(\vec{x}, \vec{k}))^2$ introduced by our stencil is

$$\begin{aligned} & h^4(k_x^6 + k_y^6 + k_z^6)/15 \\ - \; & 4h^5(\\ & \quad 3k_x^2k_y^2k_z^2 \\ & \qquad (S_{111} + 2S_{211} + 8S_{112} + 16(S_{122} + S_{212}) \\ & \qquad\quad +32S_{222}) \\ & \quad -(k_x^2k_y^4 + k_x^4k_y^2 + k_x^2k_z^4 + k_x^4k_z^2 + k_y^2k_z^4 + k_y^4k_z^2) \\ & \qquad (S_{102} + S_{201} + 2(S_{112} + S_{211} + S_{122}) \\ & \qquad\quad +12S_{202} + 24S_{222} + 28S_{212}) \\ & \quad) \\ + \; & \mathcal{O}(h^6) \end{aligned} \tag{18}$$

Completing the squares, e.g. by substituting

$$\begin{aligned} S_{111} &= 2(2(S_{102}+S_{201})+3S_{211}-4S_{122} \\ &\quad +8S_{222}+12S_{202}+20S_{212}) \\ &+\frac{1}{6h} \qquad (19) \\ S_{112} &= -\frac{1}{2}(S_{102}+S_{201}+2(S_{211}+S_{122}) \\ &\quad +6S_{202}+12S_{222}+14S_{212}) \\ &-\frac{1}{40h} \qquad (20) \end{aligned}$$

this becomes $h^4(\vec{k}^2)^3/15+\mathcal{O}(h^6)$. It is again straightforward to verify that the improved stencil also produces the same leading error when applied twice to compute the Laplacian. But to get an isotropic leading error in the more general case $\nabla W(\vec{x},\vec{k_A})\cdot\nabla W(\vec{x},\vec{k_B})$, we need to repeat the exercise and complete the squares once more. With

$$S_{201} = -2(S_{211}+2S_{202}+4S_{222}+5S_{212}) - \frac{1}{30h} \qquad (21)$$

the error becomes $h^4(k_A\cdot k_B)((k_A^2)^2+(k_B^2)^2)/30+\mathcal{O}(h^6)$. Stopping here and setting the six remaining independent weights $S_{202}=S_{211}=S_{212}=S_{222}=S_{102}=S_{122}=0$, the stencil becomes

$$\begin{aligned} S_{0jk} &= 0 \qquad (22) \\ S_{1jk} &= \begin{bmatrix} 0 & S_{112} & 0 & S_{112} & 0 \\ S_{112} & S_{111} & S_{101} & S_{111} & S_{112} \\ 0 & S_{101} & S_{100} & S_{101} & 0 \\ S_{112} & S_{111} & S_{101} & S_{111} & S_{112} \\ 0 & S_{112} & 0 & S_{112} & 0 \end{bmatrix} \qquad (23) \\ S_{100} &= \frac{4}{15h} \qquad (24) \\ S_{101} &= \frac{1}{12h} \qquad (25) \\ S_{111} &= \frac{1}{30h} \qquad (26) \\ S_{112} &= \frac{-1}{120h} \qquad (27) \end{aligned}$$

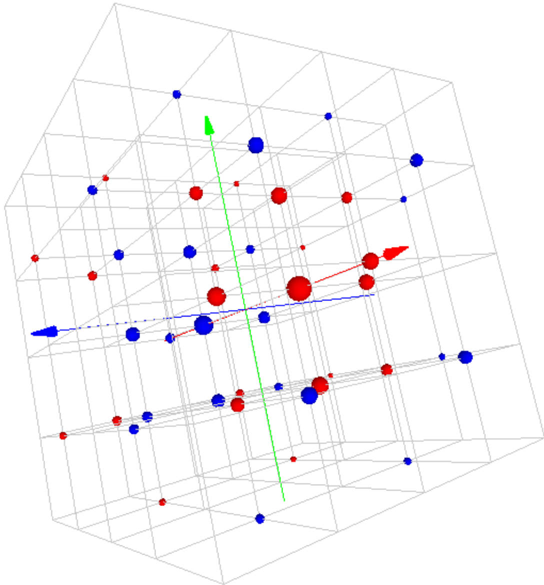

FIG. 1: The $\mathcal{O}(h^4)$ stencil (x axis in red). Red balls are positive weights, blue balls negative. Volume is proportional to weight.

$$S_{2jk} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -S_{111} & 0 & 0 \\ 0 & -S_{111} & S_{200} & -S_{111} & 0 \\ 0 & 0 & -S_{111} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (28)$$

$$S_{200} = \frac{1}{20h} \quad (29)$$

$$S_{-ijk} = -S_{ijk} \quad (30)$$

Again, the weights in S_{ijk} sum to the corresponding single weights in the one-dimensional stencil.

III. IMPROVED LOW-PASS FILTERS

A. $\mathcal{O}(h^4)$ filter

Besides differentiation, which is essentially a roughening operation, one often needs to perform the opposite task, smoothing. The same approach used for derivatives can be applied to construct improved smoothing operators: write down the most generic stencil with extension $2r+1$, subject to the total symmetry condition

$$S_{ikj} = S_{-ijk} = S_{ikj} = S_{i-jk} = S_{ij-k} = S_{ijk} \tag{31}$$

apply it to a plane wave and demand that the result be isotropic up to some power of h. In the simplest non-trivial case, $r=1$, symmetry allows only four independent weights, which we can take to be S_{000}, S_{001}, S_{011} and S_{111}. Applying the stencil to $W(\vec{x}, \vec{k_A})$ at the origin and Taylorizing in h yields

$$\begin{aligned}
& \sum_{i,j,k=-1}^{1} S_{ijk} e^{\imath h(ik_x + jk_y + kk_z)} \\
= \; & S_{000} + 6S_{001} + 12S_{011} + 8S_{111} \\
& -h^2\vec{k}^2(S_{001} + 4(S_{011} + S_{111})) \\
& +h^4(\\
& \qquad (k_x^4 + k_y^4 + k_z^4)S_{001} \\
& \qquad +4\,(k_x^4 + k_y^4 + k_z^4 + 3(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2))\,S_{011} \\
& \qquad +4\,(k_x^4 + k_y^4 + k_z^4 + 6(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2))\,S_{111} \\
& \quad)/12 \\
& +\mathcal{O}(h^6)
\end{aligned} \tag{32}$$

This is already isotropic up to $\mathcal{O}(h^2)$. We can complete the squares in the $\mathcal{O}(h^4)$ terms by imposing

$$S_{011} = (S_{001} - 8S_{111})/2 \tag{33}$$

It is possible to push on to higher order, but if the effect of the stencil is to depend on $|\vec{k}|$, we need the remaining independent weights.

Given (approximate) isotropy, we can analyze the frequency response along any convenient direction. On the x axis, applying the stencil to $W(\vec{x}, \vec{k_A})$ (at the origin, as usual) has the effect of multiplying the latter by the frequency response function

$$\begin{aligned}
H(\omega) \; = \; & S_{000} + 6S_{001} - 16S_{111} \\
& +6(S_{001} - 4S_{111})\cos(\omega)
\end{aligned} \tag{34}$$

where $\omega = k_x h$ is the circular frequency. For this to be as close to an ideal low-pass filter as possible, we want $H(0) = 1$ and $H(\pi) = 0$ ($\omega = \pi$ is the Nyquist frequency, beyond which signals are aliased to lower frequencies due to the finite resolution of the lattice). The first condition is satisfied by imposing

$$S_{111} = \frac{S_{000} + 12S_{001}}{40} - 1 \tag{35}$$

the second one by

$$S_{001} = 4S_{111} + 1/12 \tag{36}$$

With these choices,

$$H(\omega) = \frac{1 + \cos(\omega)}{2} \tag{37}$$

and the stencil reduces to

$$S_{0jk} = \begin{bmatrix} S_{011} & S_{012} & S_{011} \\ S_{012} & S_{000} & S_{012} \\ S_{011} & S_{012} & S_{011} \end{bmatrix} \tag{38}$$

$$S_{011} = \frac{1 + 6S_{000}}{24} \tag{39}$$

$$S_{012} = \frac{1 - 6S_{000}}{12} \tag{40}$$

$$S_{1jk} = S_{-1jk} = \begin{bmatrix} S_{111} & S_{011} & S_{111} \\ S_{011} & S_{012} & S_{011} \\ S_{111} & S_{011} & S_{111} \end{bmatrix} \tag{41}$$

$$S_{111} = -\frac{S_{000}}{8} \tag{42}$$

This can be viewed as an interpolator which seeks to determine the value of the central lattice site from those of its nearest neighbors and mixes the result with the original value, in proportion to the remaining independent weight S_{000}.

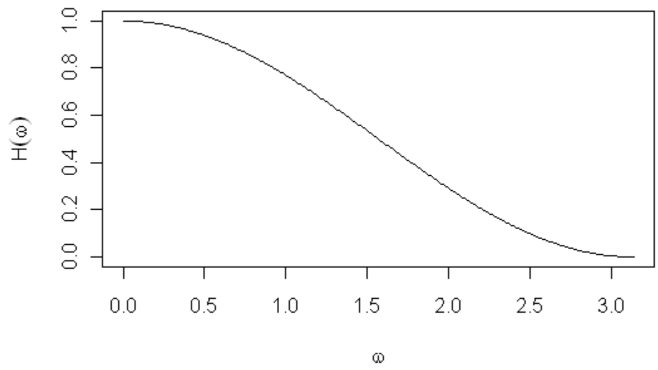

FIG. 2: Frequency response $H(\omega)$ of the improved low-pass filter for circular frequency ω.

B. $\mathcal{O}(h^6)$ filter

With $r = 2$, completing the squares leaves enough independent weights for a low-pass filter with $H(\pi) = 0$ up to $\mathcal{O}(h^6)$. To that order, isotropy holds when

$$\begin{aligned} S_{001} &= 16S_{112} + 8S_{111} - 20S_{012} \\ &\quad -100S_{122} - 128S_{022} \end{aligned} \tag{43}$$

$$\begin{aligned} S_{002} &= 40S_{222} + 31S_{122} + 5S_{112} + 2S_{022} \\ &\quad +(S_{111} - 5S_{012})/2 \end{aligned} \tag{44}$$

$$\begin{aligned} S_{011} &= 256S_{222} + 120S_{122} + 30S_{112} + 4S_{111} \\ &\quad -64S_{022} - 20S_{012} \end{aligned} \tag{45}$$

The twin requirements $H(0) = 1$ and $H(\pi) = 0$ can then be satisfied with

$$\begin{aligned} S_{122} &= (22080S_{112} - 136704S_{022} - 20352S_{012} \\ &\quad +8304S_{111} + 512S_{000} - 97)/99840 \end{aligned} \tag{46}$$

At this point, the frequency response still has a dependence on S_{000}, which can be removed by imposing

$$S_{112} = \frac{-2S_{000}}{135} \tag{47}$$

so that

$$\begin{aligned} H(\omega) &= \frac{1+\cos(\omega)}{832} \\ &\quad ((3888S_{111} - 27648S_{022} + 3456S_{012} - 37)\cos(\omega) \\ &\quad -3888S_{111} + 27648S_{022} - 3456S_{012} + 453) \end{aligned} \tag{48}$$

For a simple low-pass filter,

$$S_{111} = \frac{27648 S_{022} - 3456 S_{012} + 37}{3888} \tag{49}$$

reduces Eq. (48) to Eq. (37). Setting $S_{012} = S_{022} = 0$ then produces the final result

$$\begin{aligned}
S_{0jk} &= \begin{bmatrix} 0 & 0 & S_{002} & 0 & 0 \\ 0 & S_{011} & S_{001} & S_{011} & 0 \\ S_{002} & S_{001} & S_{000} & S_{001} & S_{002} \\ 0 & S_{011} & S_{001} & S_{011} & 0 \\ 0 & 0 & S_{002} & 0 & 0 \end{bmatrix} && (50) \\
S_{001} &= \frac{-1368 S_{000} + 305}{3240} && (51) \\
S_{002} &= \frac{63 S_{000} + 2}{1620} && (52) \\
S_{011} &= \frac{2(9 S_{000} + 2)}{135} && (53)
\end{aligned}$$

$$\begin{aligned}
S_{1jk} &= \begin{bmatrix} S_{122} & S_{112} & 0 & S_{112} & S_{122} \\ S_{112} & S_{111} & S_{011} & S_{111} & S_{112} \\ 0 & S_{011} & S_{001} & S_{011} & 0 \\ S_{112} & S_{111} & S_{011} & S_{111} & S_{112} \\ S_{122} & S_{112} & 0 & S_{112} & S_{122} \end{bmatrix} && (54) \\
S_{111} &= \frac{37}{3888} && (55) \\
S_{112} &= \frac{-2 S_{000}}{135} && (56) \\
S_{122} &= \frac{72 S_{000} - 7}{38880} && (57) \\
S_{-1jk} &= S_{1jk} && (58)
\end{aligned}$$

$$\begin{aligned}
S_{2jk} &= \begin{bmatrix} S_{222} & S_{122} & 0 & S_{122} & S_{222} \\ S_{122} & S_{112} & 0 & S_{112} & S_{122} \\ 0 & 0 & S_{002} & 0 & 0 \\ S_{122} & S_{112} & 0 & S_{112} & S_{122} \\ S_{222} & S_{122} & 0 & S_{122} & S_{222} \end{bmatrix} && (59) \\
S_{222} &= \frac{27 S_{000} + 1}{19440} && (60) \\
S_{-2jk} &= S_{2jk} && (61)
\end{aligned}$$

When the smoothing filter is used together with $\mathcal{O}(h^4)$ derivative stencils, there is little reason to go beyond this point.

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