Derivative Estimation from Marginally Sampled Vector Point Functions

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ABSTRACT

Several aspects of the problem of estimating derivatives from an irregular, discrete sample of vector observations are considered. It is shown that one must properly account for transformations from one vector representation to another, if one is to preserve the original properties of a vector point function during such a transformation (e.g., from u and v wind components to speed and direction). A simple technique for calculating the linear kinematic properties of a vector point function (translation, curl, divergence, and deformation) is derived for any noncolinear triad of points. This technique is equivalent to a calculation done using line integrals, but is much more efficient.

It is shown that estimating derivatives by mapping the vector components onto a grid and taking finite differences is not equivalent to estimating the derivatives and mapping those estimates onto a grid, whenever the original observations are taken on a discrete, irregular network. This problem is particularly important whenever the data network is sparse relative to the wavelength of the phenomena. It is shown that conventional mapping/differencing schemes fail to use all the information in the data, as well. Some suggestions for minimizing the errors in derivative estimation for general (nonlinear) vector point functions are discussed.

1. Introduction

Information about the derivatives of a function can be as important, if not more important, as that concerning the function itself. That is, the relative distribution may be of more interest than the particular values. Derivatives of the wind field, a vector point function, have important kinematic and dynamic significance; such derivatives permeate the diagnostic and prognostic equations of meteorology, so that obtaining good wind field derivative estimates becomes a matter of substantial concern.

However, it is not always easy to fulfill this need. Part of the problem in obtaining good wind representations for use in meteorological diagnosis/prognosis is the sparseness of meteorological data. This problem is compounded by the irregularity of the sample points' spatial distribution. Given a limited number of irregularly distributed wind observations, the goal is to extract the maximum amount of useful information from that sample.

The traditional approach to determining wind field derivatives begins with an "objective analysis" scheme (e.g., see Cressman, 1959), applied to the irregularly-distributed point values of the u and v wind components as if they were independent scalars. The objective analysis maps the wind components from the original sample points onto a regular grid. Once on the grid, the wind component derivatives are obtained via finite differencing. It is also relevant that analysis schemes which do not require the mapped fields to replicate exactly the observations at the sample points provide a simultaneous smoothing of the data (Stephens and Polan, 1971). Since meteorological data always contain some unknown amount of noise, this is a desirable property. That is, noise in the data tends to increase the amplitudes of short-wavelength spectral components, which are then magnified further by finite difference computations (Barnes, 1986).

In a previous paper (Schaefer and Doswell, 1979—hereafter referred to as SD79), two-dimensional wind field diagnosis was approached in a manner quite different from this traditional scheme. By calculating two-dimensional vorticity (ζ) and divergence (D) directly from the irregularly-distributed sample points via line integrals, SD79 demonstrated considerable improvement in the estimated derivative properties of the wind field by applying the technique to analytically specified vector functions.

This paper explores the origins of the improvements shown in SD79. We will show that derivative estimation for general vector point functions may involve treating them differently than pure scalar fields when the density of the sample data is not high enough to allow one to assume quasi-continuous data. However, it will be shown that one must account for the vector nature of the function only when the sampling density falls below a level to be defined. A computationally

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simple technique for estimating wind field derivatives is introduced which is equivalent to the line integral method, but gives additional information as well. Further, it will be demonstrated that the traditional approach fails to utilize all the information contained in the wind observations, whereas the line integral concept does, thus accounting for improved derivative estimates. Distortions introduced into the derivative estimates by the standard approach can be avoided or reduced by using the concepts developed here.

Although we have noted that wind field derivative estimates are an important part of initialization for numerical weather prediction models, it is not our intent to pursue the implications of this study with respect to prognostic models. Our primary concern is for diagnostic evaluation of wind field derivatives from observations, rather than the use of those diagnoses in the complex context of modern forecast models. The issues we explore, even within this restricted domain, are subtle and complex enough.

The main point of this paper is to develop a theoretical basis for improved wind field interpolation techniques. While much of this theory can be applied to scalar functions, we are concentrating on the unique nature of vector fields, so we shall not explore the ramifications of this theory with respect to scalar analysis. Application and empirical validation of the concepts developed here will be pursued in a subsequent publication.

2. The properties of vector point functions

A vector point function specifies a vector at every point within some domain. Given discrete sampling, nothing is known about the vector function between sample points, and yet it is this change in the vector function from one point in the domain to another that determines the derivatives of the function. With traditional approaches, the diagnosed wind component fields can match the observations at the sample points rather closely and yet not describe the derivative fields at all well, as we shall attempt to show.

An issue raised in SD79 concerns the question of what vector representation is appropriate for interpolating vectors linearly. For the hypothetical example given in SD79 involving only two observations of the wind along a line (see their Fig. 1), a rather troubling paradox arises. By linearly interpolating different representations of the wind field (u and v wind components versus wind speed, S, and direction,[1] θ) to the midpoint of the line connecting the two samples, SD79 pointed out that different answers for the interpolated wind speed at the midpoint are obtained. It was suggested that this difference is attributable to "the somewhat arbitrary nature of the vector norm" but the ambiguity was never resolved.

For the example given in SD79, a complex picture is revealed by considering other points along the connecting line in addition to the midpoint. In order to illustrate the difference in the two representations, we employ the (nonlinear) transformation between them:

$$u' = S\cos\theta, \quad S' = (u^2 + v^2)^{1/2},$$
$$v' = S\sin\theta, \quad \theta' = \tan^{-1}(v/u).$$

Thus, as shown in Fig. 1, if u and v are characterized by a linear variation between the end points, the resulting S' and θ' variations are nonlinear. Conversely, if S and θ vary linearly, the implied u' and v' distributions between the endpoints are nonlinear. A resolution of this issue can be found by considering the nature of a vector point function.

a. *Linear vector functions*

This section assumes that we are in two-dimensional orthogonal cartesian (OC) space, and the vector function (**V**) is linear. By definition then, following Saucier (1955, p. 318) and Doswell (1984), the components of **V** can be expressed by the linear terms in a Taylor's series expansion:

$$\left.\begin{aligned} u(x, y) &= u(x_0, y_0) + \frac{\partial u}{\partial x}\bigg]_0 (x - x_0) + \frac{\partial u}{\partial y}\bigg]_0 (y - y_0), \\ v(x, y) &= v(x_0, y_0) + \frac{\partial v}{\partial x}\bigg]_0 (x - x_0) + \frac{\partial v}{\partial y}\bigg]_0 (y - y_0), \end{aligned}\right\} \tag{1}$$

where (x_0, y_0) is some point at which the values of u and v and their derivatives are known,[2] while (x, y) is the point where the values of u and v are to be determined. If we define the following quantities:

$$\left.\begin{aligned} 2a &= \frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \equiv \mathrm{def_{str}}(\mathbf{V}), \\ 2b &= \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \equiv \mathrm{div}(\mathbf{V}) = D, \\ 2a' &= \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \equiv \mathrm{def_{shr}}(\mathbf{V}), \\ 2c &= \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \equiv \mathrm{rot}(\mathbf{V}) = \zeta. \end{aligned}\right\} \tag{2}$$

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[1] Note that in going from one representation to the other, a transformation is involved, but it is not a transformation of coordinates. Rather, it is a transformation of vector representations. Yet a third type of transformation may be involved, as when the underlying space is transformed; e.g., the case of going from points on the surface of a sphere to a flat plane. This latter transformation is not considered in this paper.

[2] As discussed in SD79, the line integral definition of the kinematic properties involves a limit as the area of the triangle goes to zero. Thus, the values computed properly apply at the centroid. For the case of a linear field, these values are constant, so they do not change as the area of the triangle shrinks.

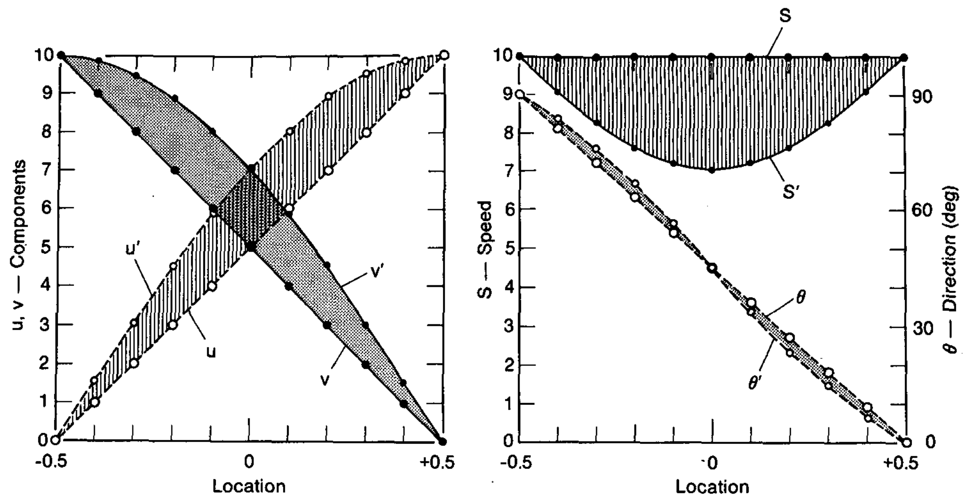

FIG. 1. Illustration of how a linear variation in u and v components implies a nonlinear variation of the speed and direction (a) and, conversely, how a linear variation of speed and direction forces a nonlinear variation of the u and v components (b). See text for the meaning of u', v', S' and θ'. Horizontal distance units are arbitrary, referring to arc length along a line connecting two wind observations, as in Schaefer and Doswell (1979).

then it is straightforward to show from (1) and (2) that a linear wind field satisfies

$$\left.\begin{aligned} u &= u_0 + a\delta x + a'\delta y + b\delta x - c\delta y, \\ v &= v_0 - a\delta y + a'\delta x + b\delta y + c\delta x, \end{aligned}\right\} \tag{3}$$

where u_0, v_0, a, a', b and c are constants. In (3), $u_0 = u(x_0, y_0)$, $v_0 = v(x_0, y_0)$, $\delta x = (x - x_0)$, and $\delta y = (y - y_0)$. As noted in Doswell (1984), the applicability of the linearity assumption depends on the length scale associated with the spatial variation of the wind components. This is discussed at some length below. For now, consider how to employ (3) in describing the linear behavior of a vector field from the wind observations.

There are six unknowns in (3): u_0, v_0, a, a', b and c. These quantities are referred to in this paper as the *kinematic* properties of the wind field. Specification of values for these provides a complete description of a linear wind field. It is reasonable to ask why one would not prefer to specify such a vector function by providing u_0, v_0, and the four derivatives $\partial u/\partial x$, $\partial u/\partial y$, $\partial v/\partial x$ and $\partial v/\partial y$. The answer is that vorticity (ζ), divergence (D), and the resultant deformation (described by the square root of the sum of squares of the two deformations and the resultant axis of dilatation) are properties of the vector field which should remain invariant during transformations of the sort considered in this paper. Thus, while the u and v components are not invariant, certain combinations of their OC coordinate derivatives are; this suggests that treating u and v as independent scalars can cause problems.

Since there are six quantities needed to specify a linear vector field completely, this means that three wind observations, which provide six pieces of information about the wind field, are sufficient to solve for the six kinematic quantities. If we define the row vectors: $\mathbf{D} = (u_0, v_0, a, a', b, c)$ and $\mathbf{U} = (u_1, v_1, u_2, v_2, u_3, v_3)$, the latter of which contains the wind component observations at the triad of points (x_1, y_1), (x_2, y_2), and (x_3, y_3), then the system of equations one derives from (3) is simply $\mathbf{DX} = \mathbf{U}$, where $\mathbf{X}$ is the six by six matrix:

$$\begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ \delta x_1 & -\delta y_1 & \delta x_2 & -\delta y_2 & \delta x_3 & -\delta y_3 \\ \delta y_1 & \delta x_1 & \delta y_2 & \delta x_2 & \delta y_3 & \delta x_3 \\ \delta x_1 & \delta y_1 & \delta x_2 & \delta y_2 & \delta x_3 & \delta y_3 \\ -\delta y_1 & \delta x_1 & -\delta y_2 & \delta x_2 & -\delta y_3 & \delta x_3 \end{bmatrix} = \mathbf{X}.$$

Note that δx_i and δy_i ($i = 1, 2, 3$) are distances from the centroid of the three observation points. This system can be solved easily for $\mathbf{D} = \mathbf{UX}^{-1}$. Provided the three samples are taken at noncolinear points, $\mathbf{X}^{-1}$ exists and there should be no conditioning problems unless the three sample points are very close to colinearity (in which case det[$\mathbf{X}$] approaches zero).

We have tested the ability of this scheme to determine the kinematic properties of linear flow fields (see Fig. 2 for some examples). Values were specified for the components of the vector $\mathbf{D}$ and used in (3) to form a regular grid of wind vectors, as in Fig. 2. Then various combinations of any three noncolinear points were chosen to specify the components of $\mathbf{U}$ and a simple Gauss-Jordan algorithm was used to find $\mathbf{X}^{-1}$. The resulting calculated components of $\mathbf{D}$ were the same, to five decimal places, as the input values, using single precision arithmetic on an IBM PC-XT. It is note-

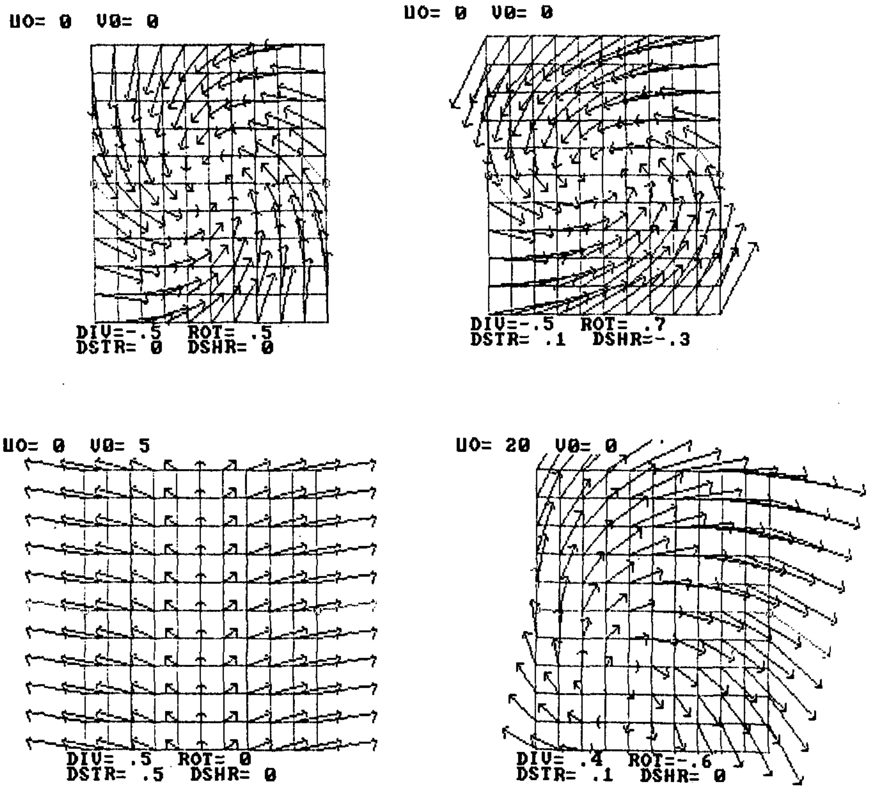

FIG. 2. Four examples of linear vector point functions. The six kinematic quantities are specified on each example, in arbitrary units.

worthy that this calculation gives values of vorticity and divergence that are equivalent to those found by SD79 in evaluating line integrals around triangles formed by three noncolinear data points. This can be shown by evaluating $\mathbf{X}^{-1}$ analytically. Further, this method also provides u_0 and v_0, the local translation components (see Saucier, 1955, p. 318). Zamora et al. (1987) provide an example of how this technique can be used to estimate the first derivatives of the wind field, for a situation in which $\mathbf{X}$ is fixed—once $\mathbf{X}^{-1}$ is determined in such a case, it need not be recalculated, making this approach quite efficient for derivative estimation.

Having established what we mean by a linear vector point function, let us return to the issue raised in SD79 about choosing a vector representation. When only two observations of the wind are given, this is insufficient to specify completely even a linear vector field. However, if the field is assumed to be linear, then along any arbitrary straight line the tips of the vectors whose tails are on that line also form a straight line. This can be seen by examining Fig. 2. In SD79, no explicit assumption about the character of the vector field was made. However, it was assumed that the *interpolation* was linear. Such an interpolation apportions any differences between observations linearly along the line. If this interpolation procedure is done for speed and direction, the tips of the interpolated vectors do not lie along a straight line, implying that the wind field is nonlinear. If the differences in u and v components are apportioned linearly, the resulting interpolated wind vector tips do, indeed, lie on a straight line. The choice between representations, when the wind field is assumed to be linear, is clearly that of u and v components. The resolution of the issue is achieved when the character of the vector field is specified. Of course, no true wind field can be completely linear, since the velocity components of linear fields increase in magnitude without limit as distances tend to infinity. Thus, we turn now to nonlinear vector point functions.

b. *Nonlinear vector functions*

When any of the kinematic quantities vary in space, the field is nonlinear. The Mean Value Theorem of the calculus implies that calculations of first derivatives [the relation between the kinematic quantities and the first derivatives is shown in (4) below] apply only locally, within a neighborhood of the point to which the quantities are assigned. The nonlinear nature of the flow must be accounted for by the point-to-point variation in kinematic properties. However, if the scale of the nonlinearity is on the order of the distance between sample points, then first derivative estimates can be seriously in error.

What is meant by "the scale of the nonlinearity"? If we suppose that the function is represented by a sinusoidal variation [e.g., $u(x) = A \sin(2\pi x/L)$, where L is a wavelength], then near the inflection points the function is well-approximated by a straight line over a length which is some fraction of L. However, near the extrema, curvature is so large that representation of that part of the function by a straight line is accurate only over a much smaller fraction of L than near the inflection points. One way to think of the scale of the nonlinearity is in terms of this length over which the variation of the function is well-approximated by a straight line. (In two dimensions, the analog to this is a region over which the gradient has nearly constant magnitude and direction.)

Another way to think of scaling the nonlinearity is to consider the Fourier spectrum of the function. When the spectrum has large amplitude only at wavelengths much larger than the sampling interval (say, Δ), the sample is capable of representing the field well. This means that for functions composed primarily of long wavelengths (relative to Δ), we can assume that nonlinearity in the flow field is well approximated as the point-to-point variation of the linear terms. Should there be significant amplitude present at scales on the order of Δ, the point-to-point variation of the first derivatives does not approximate the nonlinearity properly.

Three (noncolinear) observations of the vector function completely specify the linear variation but leave the nonlinear variations undetermined. If there are more than three observations, the local linear properties can be estimated for every suitable triad. Each such triad will, in general, have different values for the first derivative estimates, allowing estimation of the nonlinear terms (at least to second order) from spatial changes in the first derivatives. In the case of linear vector point functions, a, a', b and c were constants over the whole domain. For nonlinear functions, the kinematic quantities can be considered constant only over the triad of observations. That is, the obvious assumption to make is that the field is locally linear. By the Mean Value Theorem, there is some (unknown) point within that triad where the true derivative takes on that average value, and that point is considered to be the centroid (see footnote 2). Thus, although a, a', b and c are *locally* constant in a nonlinear situation, one has to account for spatial variation in those quantities—i.e., they have derivatives. Solving (3) for the OC coordinate derivatives, one has

$$\left.\begin{aligned} \frac{\partial u}{\partial x} &= a + b, \quad \frac{\partial u}{\partial y} = a' - c, \\ \frac{\partial v}{\partial x} &= a' + c, \quad \frac{\partial v}{\partial y} = b - a, \end{aligned}\right\} \tag{4}$$

so differentiating (4) gives the second derivatives of the field

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial b}{\partial x} + \frac{\partial a}{\partial x}, \quad \frac{\partial^2 v}{\partial x^2} = \frac{\partial a'}{\partial x} + \frac{\partial c}{\partial x},$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{\partial a'}{\partial y} - \frac{\partial c}{\partial y}, \quad \frac{\partial^2 v}{\partial y^2} = \frac{\partial b}{\partial y} - \frac{\partial a}{\partial y},$$

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial b}{\partial y} + \frac{\partial a}{\partial y} = \frac{\partial a'}{\partial x} - \frac{\partial c}{\partial x},$$

$$\frac{\partial^2 v}{\partial x \partial y} = \frac{\partial a'}{\partial y} + \frac{\partial c}{\partial y} = \frac{\partial b}{\partial x} - \frac{\partial a}{\partial x}.$$

Suppose the flow is nondivergent ($b = 0$) and the vorticity [$2c$, where $c = c(x, y)$] varies linearly. Then the spatial variation of c is specified by *constant* values of $\partial c/\partial x$ and $\partial c/\partial y$. Using the relationships above, these derivatives are simply

$$\frac{\partial c}{\partial x} = \frac{\partial a'}{\partial x} - \frac{\partial a}{\partial y}, \quad \frac{\partial c}{\partial y} = -\frac{\partial a}{\partial x} - \frac{\partial a'}{\partial y}. \tag{5}$$

In this situation, the fields a and a' (which together comprise the resultant deformation, an invariant) cannot both be constants, unless the vorticity vanishes altogether (a trivial case). In particular, both deformations cannot be zero. Hence, one cannot have a nondivergent flow with spatially varying vorticity, without also having deformation (which also must vary spatially), as stated without proof in Doswell (1984). A similar argument could be made for a vector field which is irrotational and has $b = b(x, y)$, an example of which might be the gradient of a scalar. A truly general vector point function has rotation (i.e., its curl), divergence, and deformation as general functions of space. (Note that giving the rotational and divergent parts of a flow is not equivalent to providing the irrotational and nondivergent parts, since deformation is both irrotational and nondivergent.)

We have already argued that in an OC space, treating u and v as independent scalars is capable of handling the linear variation of a vector field. For a nonlinear field the fact that we have written the series expansions for u and v independently suggests that they can always be treated independently. However, it turns out that for some situations, doing so creates some special problems. In order to explore these issues, we must turn our attention to the traditional mapping/differencing method.

3. Properties of the traditional approach

The starting point for derivative estimation via the traditional method from meteorological data is transforming data from sample points to a regular grid. Although this is done for the scalar components of the wind field, the mapping method can be used for any scalar. This process often takes the form of a weighted average[3]

$$u(x_g, y_g) = \sum_{i=1}^{N} \hat{u}(x_i, y_i)w(x_i - x_g, y_i - y_g), \quad (6)$$

where (x_g, y_g) is the point to which the data are to be mapped (usually but not necessarily a grid point, as shown by Caracena, 1987), while $\hat{u}(x_i, y_i)$ represents the sample data at points $i = 1, 2, \cdots, N$. Relationship (6) represents a type of discrete convolution of the sample with the weight function, w. By considering some idealized examples of the convolution process, we can see how the result of (6) influences the estimation of derivatives.

a. Continuous, unbounded data

Consider a situation where the data are continuous and unbounded. The analog to (6) in such a situation is

$$u(x, y) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \hat{u}(x', y') \times w(x' - x, y' - y)dx'dy' \equiv \hat{u}*w,$$

where the $*$ denotes a continuous convolution. Taking the first partial derivative of u with respect to x gives

$$\frac{\partial u}{\partial x} = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \hat{u}(x', y')\frac{\partial w}{\partial x}(x' - x, y' - y)dx'dy'. \quad (7)$$

Note that a second term involving $\partial\hat{u}/\partial x$ does not appear because $\hat{u}$ is not formally a function of x. By making a change of variable $\xi = x' - x$, it can be shown that $(\partial w/\partial x)dx' = (-\partial w/\partial x')dx'$. Then integrating (7) by parts gives

$$\frac{\partial u}{\partial x} = \int_{-\infty}^{+\infty}\left\{[\hat{u}w]_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} w\frac{\partial \hat{u}}{\partial x'}dx'\right\}dy' = \frac{\partial \hat{u}}{\partial x}*w. \quad (8)$$

The boundary terms vanish provided $w \rightarrow 0$ as $x' \rightarrow \pm\infty$, which is the case for most forms of the weight function. (Note that this argument is equally valid for nonhomogenous and/or anisotropic forms of the weight function, most of which also tend to zero with increasing distance.) If one goes through a similar argument for $v(x, y)$ and $\partial v/\partial y$, then it can be seen that the divergence (D) satisfies $D = \hat{D}*w$, and so forth for all the linear derivative properties of the field. This means that in the case of continuous, unbounded data, the derivative of the convolution of the data with the weight function is the same as the convolution of the weight function with the derivative. If the weight function has smoothing properties, as it usually does, then differentiating the smoothed data gives the same result as smoothing the derivatives. Therefore, for continuous, unbounded data, the invariant properties of the vector field are preserved if one treats u and v as independent scalars.

b. Continuous, bounded data

For continuous, but bounded data domains, one can make the same statement about the convolution as for unbounded data, but it is valid only for regions within the interior of the data domain. The critical part of the derivation of (8) is the vanishing of the boundary terms. For bounded data, the boundary terms can be neglected when far from the data boundaries. By "far from the boundaries", we mean that the weight function becomes negligible before the boundary is encountered. Away from boundaries, then, the derivative of the convolution of the data with the weight function is very nearly equal to the convolution of the weight function with the derivative. Near the boundaries, however, one obtains a different answer if one first smooths the u and v components and then calculates derivatives, than if the derivatives are estimated and then smoothed. This means that the invariant properties of the vector field are altered by the traditional approach, at least near the boundaries, even when the data are continuous.

c. Discrete data

One should consult Caracena (1987) for the details of what is involved in going from continuous to discrete mathematics in derivative estimation. It turns out that we can extend the results just obtained to the discrete convolution, under certain circumstances. That is, finite differencing of the data convolved with the weight function can be equivalent (or nearly so) to the convolution of the derivative with the weight function, but only when certain assumptions are met. In order to understand those circumstances which allow the extension to discrete data, we have to examine finite differentiation.

As a standard example,[4] define the finite difference operators on a general function, $f(x_g, y_g)$, defined on a grid (hence, the g-subscript) to be

[3] The process can take other forms, such as fitting polynomials, but virtually all such other forms can be re-cast in terms of weighted averages. This can be seen by noting that if one has a well-defined spectral response associated with the process, one can do an inverse Fourier transform of the spectral response to determine the effective weight function. Although we have confined our attention to homogeneous, isotropic forms of the weight function, w, more general forms of w can be used in our derivations, leading to complexities which are, for our purposes, of secondary importance.

[4] Although a second order centered difference operator is hardly the best differencing scheme available, it is used commonly in wind field diagnosis. Further, it serves to illustrate derivative estimation problems.

$$\nabla_x f(x_{gi}, y_{gj}) = (2\Delta x)^{-1}[f(x_{gi} + \Delta x, y_{gj}) - f(x_{gi} - \Delta x, y_{gj})], \quad (9)$$

$$\nabla_y f(x_g yi, y_{gj}) = (2\Delta y)^{-1}[f(x_{gi}, y_{gj} + \Delta y) - f(x_{gi}, y_{gj} - \Delta y)], \quad (10)$$

where Δx and Δy are the grid intervals in the x- and y-directions, respectively. First consider a situation wherein the data and grid points coincide and the domain is infinite. The discrete convolution of, say, $\hat{u}(x_i, y_j)$ with the weight function is

$$u(x_{gi}, y_{gj}) = \sum_{i=-\infty}^{+\infty} \sum_{j=-\infty}^{+\infty} \hat{u}(x_i, y_j) w(x_i - x_{gi}, y_j - y_{gj}). \quad (11)$$

When the ∇_x-operator in (9) is applied to (11) one obtains

$$\nabla_x u(x_{gi}, y_{gj}) = \sum_i \sum_j \hat{u}(x_i, y_j) \nabla_x w(x_i - x_{gi}, y_j - y_{gj}), \quad (12)$$

where, as in the continuous example, the data $\hat{u}(x_i, y_j)$ are not formally a function of (x_{gi}, y_{gj}), so a second term in (12) does not appear. Expanding $\nabla_x w$ in (12) using operator (9), we can take advantage of the symmetry in this situation in a manner analogous to that done by Sasaki (1969). Consider Figure 3, where the distances from grid points to data points along the x-direction are diagrammed. In Fig. 3 the data points and grid points have been displaced from each other to make the symmetry clear, but keep in mind that each grid point is also a data point, and vice-versa. Then the weight function gradient, $\nabla_x w$, can be written as (dropping the $[2\Delta x]^{-1}$ factor)

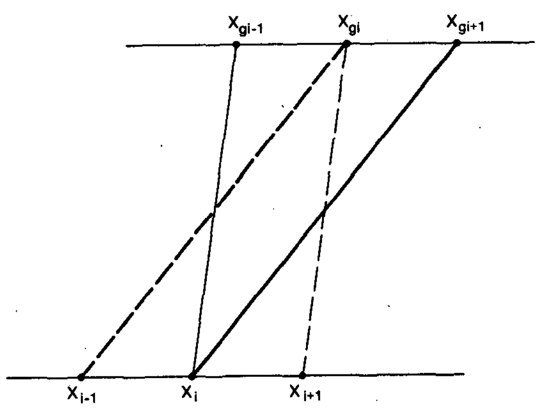

FIG. 3. Illustration of how x-distances from grid points (the three x-points with g-subscripts) to data points (the three x-points without g-subscripts) can be calculated equivalently from different point pairs. Although the line containing the grid points is displaced from the line with the data points, this is for illustration purposes only. Similarly, distances between the data and grid points are shown as slanting, but all are actually along the same x-direction line—this is done only to avoid overlapping lines.

$$w[x_i - (x_{gi} + \Delta x), y_j - y_{gj}] - w[x_i - (x_{gi} - \Delta x), y_j - y_{gj}] = w(x_i - x_{gi+1}, y_j - y_{gj}) - w(x_i - x_{gi-1}, y_j - y_{gj}),$$

which is identical to

$$w(x_{i-1} - x_{gi}, y_j - y_{gj}) - w(x_{i+1} - x_{gi}, y_j - y_{gj}) = -[w(x_{i+1} - x_{gi}, y_j - y_{gj}) - w(x_{i-1} - x_{gi}, y_j - y_{gj})],$$

because w depends only on distances between points and the symmetry permits the permutation of indices. For simplicity, we shall drop the y-dependence temporarily in what follows and consider some representative terms in the series (12)

$$\ldots + \hat{u}(x_i)[w(x_i - x_{gi+1}) - w(x_i - x_{gi-1})] + \hat{u}(x_{i+1})[w(x_{i+1} - x_{gi+2}) - w(x_{i+1} - x_{gi})] + \cdots,$$

which become, by what we have just seen,

$$\ldots - \hat{u}(x_i)[w(x_{i+1} - x_{gi}) - w(x_{i-1} - x_{gi})] - \hat{u}(x_{i+1})[w(x_{i+2} - x_{gi+1}) - w(x_i - x_{gi+1})] - \cdots.$$

It can be seen that by appropriately rearranging parts of consecutive terms, recalling that the series is infinite, (12) becomes

$$\nabla_x u = -\sum_j [\sum_i (-w\nabla_x \hat{u})] = \sum_i \sum_j w\nabla_x \hat{u} = \nabla_x \hat{u} * w. \quad (13)$$

In effect, we have accomplished a discrete integration by parts. Now (13) is a discrete analog to the continuous result, and it can be applied to the interior (far from the boundaries) of bounded, discrete domains as well, again provided the weight function becomes small as distances become large. Further reason for being far from the boundaries in this discrete case is that near the boundaries one does not have the appropriate terms in the series available for the rearrangement necessary in going from (12) to (13).

Therefore, as in the continuous case, we find that the invariant properties of the vector field are preserved. However, one serious limitation was introduced in order to make the rearrangement of terms in going from (12) to (13)—the data are assumed to be at the points of the computational grid. This situation is quite limited in terms of practical application; one hardly ever finds meteorological data on a uniform mesh of points.

A second case arises when the data are regular, but not colocated with grid points. This situation is rather uninteresting, because if this were the case, one certainly would wish to move the grid so as to bring the grid and the data into alignment. Hence, we have not performed an analysis of such a case.

The third, and most realistic, possibility is for irregularly-distributed, discrete data. If (9) is applied to (6), the form of the convolution applicable to irregularly-distributed data, the result analogous to (13) is (where the summation is now over the N data points)

$$\nabla_x u(x_{gi}, y_{gj}) = \sum_{n=1}^{N} [\hat{u}(x_n, y_n)\nabla_x w(x_n - x_{gi}, y_n - y_{gj})]. \quad (14)$$

The distinction between forms (14) and (13) is far more profound than mere notation. As with the previous forms, a second term in (14) does not appear, since the $\hat{u}$ are not defined on the grid, to which the operators like (9) and (10) are restricted. Derivatives of the data do not appear explicitly on the right-hand side of (14), while it appears that the derivative estimates depend as much on the spatial derivatives of the weight function as on the data values themselves! Furthermore, (14) cannot be manipulated as done to derive (13), since the irregularity of the data distribution prevents the rearranging of terms. In a regular grid of data, every point in the grid is identical to every other point in terms of the surrounding data distribution (at least far from the boundaries). This is not the case for irregular data meshes, thus making the manipulation used to show (13) impossible.

From a practical viewpoint, this is more than an interesting mathematical quirk of the way in which these problems are formulated. What is being said by (14) is that taking the finite difference form of the derivative after having used the convolution with the weight function to get the data to a grid is not the same as convolving the weight function with the derivative estimates. The conclusion one should draw is that *derivative estimation via the standard technique does not preserve the invariant properties of a vector point function.* Thus, it is preferable to estimate the derivatives first, since the invariants of the original vector field should be preserved in the transformation to a grid. This is the motivation for using the line integral technique, as in SD79; viz, it provides a way to obtain derivative estimates prior to transforming to a grid. Only in special situations—either continuous data (unbounded or in the interior of bounded domains), or discrete data on a regular grid (again, unbounded or interior to bounded domains)—can the traditional approach give an uncontaminated estimate of the derivatives.

If (14) characterizes the response of the standard techniques, two questions come to mind. First, it is clear that there have been many applications of the traditional approach (particularly in synoptic diagnosis) which do not seem to be seriously in error—are these applications essentially correct as they stand? Second, if this problem with derivative estimation via finite differencing of mapped (and smoothed) data is only serious under certain circumstances, what are those circumstances and how rarely (or often) do they arise? To help answer these questions, we must turn to sampling theory.

4. Sampling as it relates to derivative estimation

If we consider continuous data as a limiting case of discrete data, by oversampling the function heavily enough (say, 100 samples per wavelength), the errors made in treating the data as if they were continuous may become negligible. The problem is to know exactly (or even approximately) how much sampling is enough. In many fields other than meteorology, it is possible to obtain adequate sampling more or less at will. For example, in communication theory problems, one often can increase the temporal sampling rate to the desired level in order to meet perceived needs. In contrast, for much of operational meteorology, the sample points are fixed (and irregularly-distributed), so the question becomes one of deciding at what point information extraction becomes noise extraction. From the perspective of this paper, we need to know at what scales the data can usefully be approximated as "continuous", thus ensuring that the problem represented by (14) is not significant.

One can derive some rough guidelines by considering uniform, one-dimensional sampling. By ignoring the second spatial dimension, there is an error incurred—for purposes of establishing guidelines, the error is sufficiently minor that we have chosen to ignore it, although it may be important in some specialized situations (e.g., strongly anisotropic data distributions). In addition, irregular sampling can be thought of as increasing the *effective* sampling interval, provided the irregularity is not too extreme (Baer and Tribbia, 1976). That is, nonuniform data at some average interval Δ_1 is roughly equivalent to sampling uniformly at some larger interval Δ_2. Thus, the following should be understood to apply in situations where the data are reasonably uniformly (but not necessarily regularly) distributed.

In theory, the smallest detectable wavelength is the Nyquist interval ($2\Delta x$), which provides three samples per wave. As seen in Fig. 4, one's knowledge of such a wave depends on its phase relative to the sample points. As a worst case, when the sample points are at the inflection points, the wave is not detected at all (Fig. 4). Hence, sampling wavelengths at (or near) the Nyquist interval is not likely to generate reliable estimates of the function, much less its derivatives.

In fact, the fidelity with which the derivative information can be estimated is a good candidate for a quantitative measure of how "quasi-continuous" the sample data are. To see this, consider the standard centered difference estimate of the first derivative.[5] Barnes (1986) has shown that if $\delta f(x)$ is the finite difference form of the true derivative $f'(x)$, then

[5] As noted previously, one can find better differencing techniques. However there are trade-offs in doing so, and our intent here is to illustrate the effect of data density on finite differencing. Clearly, no matter how sophisticated one tries to be at differencing, this cannot make up for all the deficiencies in the sample data.

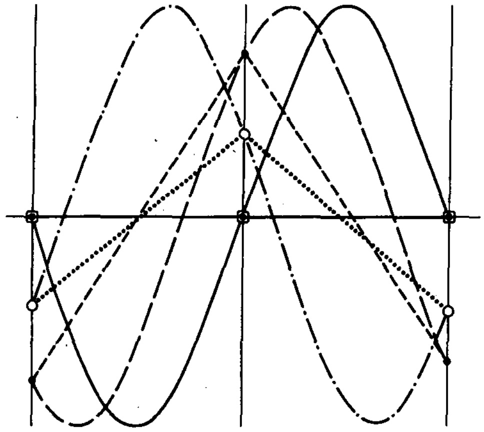

FIG. 4. Illustration of how a Nyquist interval wave gives virtually no derivative information. Three examples of such a wave are shown having different phase with respect to the grid (solid, dashed, and dash-dotted curves). The grid samples each example at different points (squares with filled circles, filled circles, and open circles, respectively). Straight lines connecting the sample points are shown for each example.

$$\delta f(x) = f'(x)\,\mathrm{diff}\left\{\frac{2\pi\Delta x}{L}\right\}, \tag{15}$$

where the function itself is given by

$$f(x) = A\sin\left\{\frac{2\pi x}{L}\right\},$$

Δx is the sampling interval, and $\mathrm{diff}(\tilde{x}) = \sin(\tilde{x})/\tilde{x}$ is the so-called diffraction function. Shown in Table 1 are the values of the diffraction function in (15) for various values of L as integer multiples of Δx. Long waves (i.e., in comparison to Δx) show very good response to the centered differencing, while wavelengths near the Nyquist show rather pronounced deterioration of the derivative estimates.

We can interpret $\mathrm{diff}(\tilde{x})$ in Table 1 as a quantitative measure of the quasi-continuity of the sampled function. Given some effective sampling interval, Δx, one can see that it is possible to make the continuum approximation with relatively negligible error (say, $\leqslant 5\%$) for long wavelengths (say, $L \geqslant 12\Delta x$). For purposes of this paper, sampling at wavelengths smaller than $6\Delta x$ is called *inadequate*. Similarly, we define *marginal* sampling to be in the range from $6\Delta x$ to $12\Delta x$. What this means to the previous discussion concerning derivative estimation (via the standard mapping/differencing technique) is that for wavelengths larger than $12\Delta x$, the data can be considered continuous for many practical purposes, and finite difference derivative estimates will be accurate to within five percent, at least within the interior of the grid.

Hence, one way to guarantee the fidelity of derivative estimation is to smooth out most of the amplitude at wavelengths below $12\Delta x$. This is not very satisfactory for many meteorological needs. For comparison purposes, a wave which is of length comparable to the entire east–west width of the United States is sampled roughly 9 to 12 times in the east–west direction by the operational sounding network. If we wish to retain signals in the marginally-sampled range (as we define the term), the traditional approach to derivative estimation is inevitably contaminated with noise of the form inherent in (14), because the continuous form of the convolution is no longer justifiable and the data are irregularly-distributed, which precludes using (13).

As if this were not enough of a problem, it is compounded by another difficulty. Recall from the above that a *regular* grid of samples can produce the proper form of derivative estimates, at least in the grid's interior. Such a sample obviously does not require remapping of the data to obtain a gridded dataset suitable for finite differencing, but there may be some smoothing desired for controlling the noise in the sample. Also, one might wish to map the data onto a finer mesh in order to limit truncation error during finite differencing. Thus, it may be desirable to apply the convolution with some weight function as a smoother, even when beginning with a regular, discrete dataset (see Bettge and Baumhefner, 1980, for an example). The theory above suggests that such a process introduces no contamination of the form suggested in (14), at least away from any boundaries, since the data distribution is regular.

However, even in this idealized situation, the difficulty is that finite differencing causes yet another problem. Consider Fig. 5, showing the centered finite difference stencil used in calculating the derivative estimates at the point (x_0, y_0). Four observation (grid) points, not including the center point, enter into the calculation of wind field derivatives (using the standard difference scheme), so there are eight pieces of information used to estimate the first derivative terms in (3). However, there are only four such quantities to be found, so that such a process is *overdetermined.* When estimating derivatives in this way, the actual information content of the data is not being used to its maximum extent.

TABLE 1. Values of the diffraction function for various wavelengths, L, as multiples of the grid interval, Δx.

$L = n\Delta x$ (n)	$2\pi\Delta x/L = \tilde{x}$	$\sin(\tilde{x})$	$\mathrm{diff}(\tilde{x})$
2	3.14159	0	0
3	2.094	.866	.413
4	1.571	1.0	.637
5	1.257	.951	.796
6	1.047	.866	.827
8	.785	.707	.9
10	.628	.588	.935
12	.524	.5	.955
15	.419	.406	.971
20	.314	.309	.984

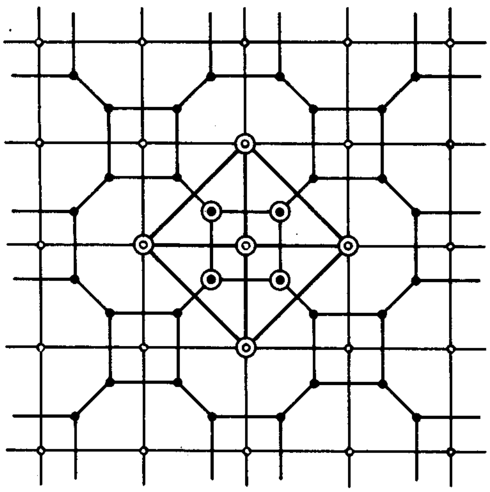

FIG. 5. The standard centered-difference stencil (double open circles) for first partial derivative estimates on a square grid (open circles and light lines) and the centroids (circled dots) of the four triangles (heavy lines) formed from the five points of that stencil. For the standard centered difference operator, only the four corner points of the stencil are used in the calculation. The lattice of triangle centroids (dots) derived from the original square grid is shown as the octagons and small squares.

When applying the line integral form of computation to a regular quadrilateral (instead of a triangle) like that of Fig. 5, precisely the same answer is obtained as that given by the standard centered difference approximation [see (3) and (4) in SD79]. Thus, a major part of the improvement demonstrated by SD79 in estimating the linear vector field properties does *not* arise through the line integral formulation, per se. Rather, it comes from two sources. First, using triangles means the wind data at the vertices are used to fullest possible extent. Second, by avoiding the problems inherent in (14), the derivative estimates are inherently more faithful to the data.

In order to circumvent the information loss inherent in the standard approach, the data grid can be used to construct a triangulation from which derivative information is extracted. Thus, one obtains a new mesh of points at which derivatives are available (i.e., the triangle centroids). For the special case of a square grid (Fig. 5), the centroids of the triangles formed from the squares create a lattice of octagons and squares having an average spacing about 11% greater than the original square grid. That is, within any $2\Delta x$ square area defined by nine points on the square grid, one finds eight triangle centroids. However, the square grid only uses half of the total information available for determining derivatives (as just pointed out above). An alternative interpretation is that since the triangle method incorporates information about derivatives directly, this can be thought of as a decrease in the effective sampling interval. (See Stephens, 1971, who concludes that the minimum definable scale is reduced by a factor of two when the analysis incorporates independent derivative estimates.) If we include the increase in average spacing (which, by the way, is a direct result of the irregularity of the centroid distribution), the net information gain associated with the triangle formulation can be modeled by using an effective data spacing somewhere between the original spacing and one-half of that. Although there is no rigorous way to defend the choice, we have approximated the net gain (probably conservatively) to be about equivalent to having a data spacing ¾ that of the original. Owing to the lack of rigor in specification of this reduction in the effective data interval, one should not interpret what follows too literally.

Repeating the calculations of Table 1 using a Δx which is ¾ that of the original yields the results shown in Fig. 6. The lower curve is a plot of the values in Table 1, while the upper curve reveals the possibilities inherent in using the data to their fullest. The improvement in the derivative estimate via this approach increases as the sampling rate decreases. Assuming that quasi-continuity begins at a diffraction function response of 95%, the triangulation form of derivative estimation achieves this at a sampling interval of about $8\Delta x$, instead of $12\Delta x$. Put another way, the quality of derivative estimates using triangulation for waves of $6\Delta x$ is equivalent to centered differencing at wavelengths of about $8\Delta x$. Yet another way of seeing how this influences derivative estimation is to note that within the marginal sampling range (from $6\Delta x$ to $12\Delta x$), triangular estimation of derivatives represents an improvement of from 10% to 3% (respectively) over the standard "rectangular" approach.

5. Discussion

In meteorology, it is safe to say that we rarely, if ever, have so much data that we can afford the luxury

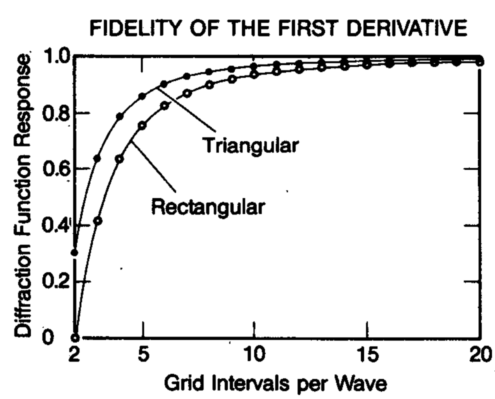

FIG. 6. Plot of the quality of derivative estimates using the traditional (rectangular) stencil and the equivalent graph for a triangular estimation of the derivative, having modeled the information gain associated with the triangular approach by means of an effective Δx which is ¾ that of the rectangular form (see text for discussion).

of not extracting the last possible measure of information. Given the great focus currently on "mesoscale" meteorology, it is desirable to push the data we have into revealing things on wavelengths which are marginally sampled. What this paper has tried to show is that the tools of analysis cannot be applied thoughtlessly when operating at the limits of the information contained within the data, especially when considering wind field derivative information.

Several complicating issues have not been treated within this discussion, such as measurement errors in the sample data, the effect of aliasing on the true information content, and so on. While these are nontrivial effects, they have been treated at length elsewhere (e.g., see Gandin, 1963; Jones, 1972; Bergman, 1978).

Instead, we have examined some basic characteristics of the traditional approach to derivative estimation, which involves a two-step process. It has been shown that remapping u and v to grid points produces a kind of contamination of the derivative estimates which becomes apparent only as one moves into the realm of marginally sampled phenomena. For marginal sampling, the traditional approach gives different estimates than those obtained from a direct evaluation of the derivatives. The fact that the answers differ becomes important because of the need to preserve the invariants of the vector wind field. Further, using the traditional scheme, the structure of the weight function becomes a potential source of contamination, depending on its properties.

For problems with real data, we have shown that many of the difficulties in derivative estimation are associated with nonuniform data distributions. Although not considered in detail, the data domain boundaries probably constitute the most important nonuniformity associated with real data distributions. One subsidiary issue tied to the data boundaries is described in the Appendix. We have shown that for bounded data domains, the only reliable analysis is far (as we have defined "far") from the contaminating effect of the boundary.

Another serious nonuniformity arises when significant gaps exist in the data. This creates a sort of *internal* boundary, which means that the second term of (A2) can become important in (14). If one examines the traditionally computed finite difference estimates of vorticity and divergence in SD79 (see their Figs. 5a and 6a), one sees immediately that many serious errors of traditional estimation arise within or near regions of inhomogeneity in the data distribution (data voids and/or boundaries). When the field itself is flat or when the data density is high (i.e., the field is locally linear), the conventional estimates can be reasonably good. However, the triangulation approach provides considerable improvement in precisely those areas where the conventional method breaks down (see SD79's Figs. 5b and 6b). Do not be deceived into thinking of this as a way of getting something for nothing. Some additional effort (computationally) is required and there is no known substitute for adequate data.

We can answer the two questions we posed at the end of section 3 with one generalization. The standard approach to derivative estimation always is characterized by distortions of the sort we have described. However, these distortions only begin to be significant whenever the sampling rate falls into the range we have defined as marginal. Clearly, the short wavelength components of a wind field will suffer the most degradation. While one may be willing to accept this sort of error in derivative estimation, we have shown that it is possible to improve the quantitative estimates of wind field derivatives through the approach we have advocated. We also have provided a scheme for more efficient calculation than the line integral method of SD79, but which gives identical answers.

It is worth pointing out that the quality of derivative estimates may well be of relatively little importance to a particular application of objective analysis to the wind field. Whenever the vector field itself, and not its derivatives, is of primary interest, a traditional u and v component mapping of the data to a grid may indeed be sufficient for one's needs. By examining the results shown by SD79 in detail, it is clear that the adjustments needed to improve the calculation of the field's derivative properties do not result in substantial changes to the u and v components. For instance, their Table 1 shows that the root-mean-square difference between the two techniques is generally less than one m s^{-1}, hardly worth all the extra effort. Indeed, it is probably true that the benefit is not worth the cost, provided that the object of the process happens not to require accurate *derivative* information on scales which are marginally sampled. The fact that it seems possible to increase the quality of the derivative estimates without degrading the function itself is an encouraging aspect of the results seen in SD79.

We have shown that in order to preserve the differential invariants of the vector field, one should calculate them directly from the data without a prior mapping of the components to a grid, in the traditional way. For a two-dimensional vector field, the first derivative invariants are *scalars* (vorticity, divergence, and resultant deformation), except for specification of the deformation's dilatation axis. Curiously, for a scalar field, the first derivative invariant is a *vector* (the gradient). Although we have concentrated on vector fields, one can apply this approach to scalar fields, as well.

Finally, consider the subject of how to incorporate the derivative information in producing a consistent wind field analysis. The approach advocated in SD79 involved formulating variational constraints, and solving the resulting elliptic-type equations to reconstruct the wind field. We believe that it is possible to blend the derivative estimates with the wind observations without having to solve elliptic partial differential equations. This topic is beyond the scope of the current report, but it will be covered in detail in a forthcoming paper.

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APPENDIX

Although it is not of primary concern within the body of this work, the weight functions we have been considering are normalized. That is, they are of the form

$$w(x_n - x_{gi}, y_n - y_{gj}) = \frac{W(x_n - x_{gi}, y_n - y_{gj})}{\sum_{k=1}^{N} W_k}, \quad \text{(A1)}$$

where the $W_k = W(x_k - x_{gi}, y_k - x_{gj})$ represent the *unnormalized* weights. Thus, the sum of the weights at each point is constrained to be unity. This normalization is done to prevent introducing bias into the resulting fields when convolution of the weight function with the data is done.

In the fortunate circumstance of uniformly distributed data, the normalizing factor $N_0 \equiv \sum W_k$ in the denominator of (A1) does not vary from point to point. Applying the gradient operator to (A1) gives

$$\nabla w = (\nabla W)/N_0 - \left\{\frac{W}{N_0^2}\right\}\nabla N_0, \quad \text{(A2)}$$

which reduces to $(\nabla W)/N_0$ for uniform data. Note that the data need not be regular for the second term in (A2) to be negligible—merely that the irregularity be sufficiently minor that the sum of weights is nearly constant from point to point within the domain.

One significant violation of uniformity occurs around the boundaries. As shown in Barnes (1964, his Fig. 4), there is a substantial drop-off in the number of stations influencing the analysis as one approaches the boundaries of a finite data domain. Boundary problems in general have been examined in detail by Caracena et al. (1984) and Achtemeier (1986).

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