

GENERALISED SPLINE SURFACES

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ABSTRACT

A variational approach to objective analysis using splines and cross validation for meteorological applications has been described by Wahba and Wendelberger (1980). The method can be considered as an extension of a variational approach to smoothing spline interpolation developed originally by Carl Reinsch in the late 1960s. The theoretical and conceptual basis of these methods is reviewed, and some analogies drawn between their spatial properties and properties of other deterministic and stochastic methods. Certain properties of generalised spline (GS) analysis are strikingly similar to those of the stochastic method known as universal kriging (UK), which can itself be considered as generic to what meteorologists refer to as Optimal Interpolation (OI) and the potential advantages and disadvantages of GS over UK and OI methods are considered.

Some examples of the GS method applied to the assimilation of conventional observations in 2-d and 3-d spatial domains are used to illustrate possible applications in finescale analysis.

1. THEORETICAL BACKGROUND

1.1 Smoothing Splines

Reinsch (1967) considered the following 'classical' estimation problem: given n discrete observations $x_j = x(t_j) + z_j$, $j = 1, 2, \dots, n$, where $x(t)$ is an unknown function of an independent variable t , and z_j a random normal error with zero mean and variance σ_j^2 , estimate $x(t)$ as a linear function of $\{x_j\}$, i.e. as

$$\hat{x}(t) = \sum_{j=1}^n w_j x_j \quad . \quad (1)$$

At that time two classical methods were commonly applied to the above problem. In deterministic methods, it is assumed that $x(t)$ may be approximated everywhere by a single expansion consisting of a weighted sum of

linearly independent functions of t , such as polynomials. Having specified such a parametric model for $x(t)$, the estimated model parameters (and hence $\hat{x}(t)$) are solved by linear regression, for which the object function to be minimized is the sum of squared residuals between x and \hat{x} on data locations. In stochastic methods, it is assumed that $x(t)$ is a random function with a stationary covariance function $v(\tau)$, where τ is a lag in t -space, which is known or can be approximated by some parametric model. At any point t , $\hat{x}(t)$ is obtained by finding w_j , $j = 1, 2 \dots n$ to minimize the estimation error variance - the optimal interpolation method, as it is known in meteorology (after Gandin, 1963).

Both deterministic and stochastic methods involve specifying a parametric model, either for $x(t)$ or $v(\tau)$, before (1) can be solved. In the case of deterministic models, it may be difficult to find a suitable space of functions or truncation point in the model expansion which interpolates $\hat{x}(t)$ smoothly while adequately approximating $\{x_j\}$. In stochastic methods, a suitable model for $v(\tau)$ may either not be available, or may be based on a dubious assumption, such as that $v(\tau)$ is well approximated by fitting a model to 'between-station' covariances estimated from independent sets of observations.

Reinsch avoided these problems by seeking a solution for $\hat{x}(t)$ which satisfies the requirements of smooth interpolation and approximation but which does not involve specifying a parametric model for either $x(t)$ or $v(\tau)$. Instead, his method involves finding a solution for $\hat{x}(t)$ which minimizes the functional $f[\hat{x}(t)]$ given by

$$f[x(t)] = \int_{\Gamma} \left[\frac{\partial^2 \hat{x}(t)}{\partial t^2} \right]^2 dt + \lambda \left[\frac{1}{n} \sum_j \left(\frac{\hat{x} - x}{\sigma} \right)_j^2 - S^2 + \gamma^2 \right] \quad , \quad (2)$$

A λB

where λ and γ are unknown positive constants, and S a prescribed approximation parameter. Term A expresses smoothness with reference to the integral of squared curvature over the domain Γ , while term B expresses approximation with reference to the requirement that the mean square residual of \hat{x}_j weighted by σ_j^{-1} should be less than or equal to S . Except in the special case where this variational problem can be satisfied by a straight line in x, t space, the solution for $\hat{x}(t)$ turns out to be a cubic spline in t , with n knots on data locations; and γ is then identically equal to zero. Reinsch showed that with $\gamma = 0$, λ could be obtained by finding the zero of a function of λ , the location of that zero being

determined by S , the values of the observations $\{x_j\}$, and by $\{\sigma_j\}$, (see also Reinsch, 1971). Given λ , the calculation of parameters weighting the individual terms in the cubic spline representation for $\hat{x}(t)$ is straightforward, and details can be found in Reinsch (1967). If $\sigma_1 = \sigma_2 = \dots = \sigma_n$ is a reasonable assumption, then the approximation requirement in (2) is equivalent to requiring that the mean square residual of $\hat{x}(t)$ is equal to some prescribed value. Reinsch's 'smoothing spline' approach is easily extended to estimation of $x(\underline{t})$, when \underline{t} measures location in a bivariate Euclidean space, using the 'thin-plate' spline solution obtained by Duchon (1976).

1.2 Generalized splines with cross validation

For geophysical applications, there are three difficulties with Reinsch's approach to smoothing spline analysis. Firstly, even if σ_j is known for all j , then it is nevertheless difficult to specify a value for S which should minimize estimation error variance (see Wahba, 1975). Secondly, even if S is correctly prescribed, then the method still requires that σ_j is known, even when $\sigma_1 = \sigma_2 = \dots = \sigma_j$ is a reasonable assumption. Thirdly, Reinsch's smoothness criterion based on second derivative properties of $\hat{x}(t)$ might not be appropriate for the estimation of geophysical fields, even though it might be appropriate for modelling the behaviour of some simple physical systems, such as bent beams and plates (see de Boor, 1978).

These difficulties are apparently overcome in the more generalized approach to the variational analysis problem presented by Wahba and Wendelberger (1980; hereafter WW). These authors again consider a variational approach to solving for $\hat{x}(t)$, though with t replaced by the point $\underline{t} = t_1, t_2, \dots, t_d$ in a d -dimensional Euclidean space.[†] However, WW define the variational problem rather differently than does Reinsch by seeking $\hat{x}(\underline{t})$ to minimize

$$g[\hat{x}(\underline{t})] = \int_{-\infty}^{\infty} \left[\frac{\partial^m \hat{x}(\underline{t})}{\partial \underline{t}^m} \right]^2 d\underline{t} + \frac{\lambda}{n} \sum_j \left(\frac{\hat{x} - x}{\sigma} \right)_j^2 \quad (3)$$

A λB

where λ is an unknown multiplier and m an unknown positive constant. Here, the 'smoothness term' A has been written in shorthand form: the term in parenthesis represents the sum of all m 'th order derivatives of $\hat{x}(\underline{t})$ with

[†] Solutions in a spherical curvilinear space are given in Wahba (1981).

respect to all combinations of the d location variables; and the integration is over the infinite volume of d -space. Apart from the fact that term A in (3) has a more general form than that in (2), we note that the approximation criterion now relates to the requirement that the mean weighted square residual of \hat{x}_j should be minimized. This formulation has the advantage that if $\sigma_1 = \sigma_2 = \dots = \sigma_n$ is a reasonable assumption, then it is not necessary to specify σ_j , since any arbitrary scaling can be absorbed by the multiplier λ .

WW state that for prescribed positive values of m and λ , this variational problem has a unique analytical solution given by

$$\hat{x}(\underline{t}) = \underline{\phi}'(\underline{t})\underline{\alpha} + \sum_{j=1}^n \beta_j \kappa(\tau_j) . \quad (4)$$

In (4), $\underline{\phi}(\underline{t})$ represents a vector of polynomials complete to order $(m - 1)$ in the d -location variables, and $\underline{\alpha}$ is an associated vector of parameters; β_j is one of n parameters associated with the function $\kappa(\tau_j)$ where τ_j is the distance in Euclidean d -space between \underline{t} and \underline{t}_j , with $\kappa(\tau)$ being given by

$$\begin{aligned} \kappa(\tau) &= \tau^{2m-d} \ln \tau, \quad d \text{ even}^* \\ &= \tau^{2m-d}, \quad d \text{ odd}^* . \end{aligned}$$

Solution (4) can be considered as a generalized spline (GS) surface in the sense that the piecewise-continuous property of $\hat{x}(\underline{t})$ is similar to that of simple univariate splines: $\hat{x}(\underline{t})$ is continuous and differentiable to order m , but its m 'th order derivative changes discretely at observing locations, and no higher order derivatives exist at a point. With $m = 2$ and $d = 1$, $\hat{x}(\underline{t})$ takes the form of a cubic spline, while with $m = 2$ and $d = 2$ $\hat{x}(\underline{t})$ takes the form of a 'thin-plate' spline.

Given values of m and λ , the parameters in (4) can be obtained by solving the linear system

$$\begin{pmatrix} (\underline{K} + n\lambda \underline{D}_{\sigma}) & \underline{\Phi} \\ \underline{\Phi}' & \underline{0} \end{pmatrix} \begin{pmatrix} \underline{\beta} \\ \underline{\alpha} \end{pmatrix} = \begin{pmatrix} \underline{x} \\ \underline{0} \end{pmatrix} . \quad (5)$$

Here \underline{K} is a symmetric $n \times n$ matrix of $\kappa(\tau)$ values corresponding to all pairs of observing stations, $\underline{\Phi}$ is a polynomial matrix with n rows, and \underline{x} the n -

* WW include a constant multiplier in these expressions; but that constant may be absorbed in β_j , and has been omitted here.

vector of observations. Strictly, \underline{D}_σ is a diagonal matrix containing σ_j^2 data. However, if $\sigma_1^2 = \sigma_2^2 = \dots = \sigma_n^2$ is a reasonable assumption, then \underline{D}_σ may be replaced by the $n \times n$ identity matrix.

System (5) can be solved using Reinsch's method provided that suitable values of m and mean square residual can be specified *a priori*. However, WW suggest a potentially more powerful approach based on a generalized cross-validation (GCV) method. Conceptually at least, the cross-validation method is based on finding m and λ such that the square of the estimation error $[\hat{x}(\underline{t}) - x(\underline{t})]$ is minimized when averaged over all d -space. In practice, the GCV approach uses a suitably weighted sum of squared residuals (on observing locations) to track the behaviour of estimation error variance averaged over the available observing locations. The location of the minimum of this GCV variable $G(\lambda, m)$ in G, λ, m space estimates the location of the minimum mean square estimation error. Full details of how the GCV method may be effected numerically, together with theoretical sources, are described in WW.

Sample analyses in WW demonstrate the ability of the GCV method to result in accurate interpolation of the signal function $x(\underline{t})$ when applied to discrete noisy data simulating synoptic observations of geopotential disturbance fields and it is not difficult to reproduce WW's results following the numerical procedures described in their paper. WW also suggest how the method may be extended to incorporate assimilation of multivariate observations.

2. ANALOGIES

2.1 Variable resolution

The GS solution (4) of the variational problem (3) may be written concisely as

$$\hat{x}(\underline{t}) = \underbrace{\hat{\mu}(\underline{t})}_M + \underbrace{\kappa'(\underline{t})\beta}_S \quad . \quad (6)$$

An important property of this solution is that as $\|\underline{t} - \underline{t}_j\|$ becomes large for all \underline{t}_j , term S tends to zero. Hence $\hat{x}(\underline{t})$ always relaxes onto an 'infinitely smooth' polynomial surface M both in observation-sparse regions of \underline{t} -space and outside the convex region enclosing observations. Whilst that property does not guarantee that $\hat{x}(\underline{t})$ has reasonable extrapolation properties ($\hat{\mu}(\underline{t})$ is not generally the same as a least squares estimated polynomial trend surface), it does at least mean that $\hat{x}(\underline{t})$ and its

derivatives tend to be reasonably smooth along boundaries enclosing the observation space. Furthermore, the above result implies that term S can be thought of as a 'short-range' component of $\hat{x}(\underline{t})$, which provides more information about the derivative structure of $x(\underline{t})$ in regions of enhanced observation density. (Notice that although the differentiability of $\hat{x}(\underline{t})$ is limited to $\leq m$ at a point, higher derivatives can be estimated via finite differencing provided that the differencing interval is greater than the local 'mean-station-separation'). Hence GS analysis provides a form of variable resolution analysis in regions where observations are not distributed homogeneously and is, in this sense, analogous to some successive approximation methods (following the approach introduced by Cressman, 1959); except that unlike successive approximation via a distance weighting formulation, GS analysis is optimally formulated with respect to a least-squares criterion.

2.2 Kriging and OI

A more specific analogy exists between the GS solution (6) and the solution provided by the statistical method known as universal kriging (UK) developed originally by Matheron (1970), who also later noted a similarity between UK and spline analysis (Matheron, 1981). In UK $x(\underline{t})$ is considered as a purely random function consisting of a stochastic trend or 'drift' $\mu(\underline{t})$ plus a spatially stationary stochastic component $x'(\underline{t})$ the correlation scale of which is smaller than the scale of the convex region enclosing observations. Subject to a suitable choice of parametric model for $\mu(\underline{t})$ and covariance model for $x'(\underline{t})$, the UK solution minimizing estimation error variance can be written as

$$\hat{x}(\underline{t}) = \hat{\mu}(\underline{t}) + \underline{v}'(\underline{t}) (\underline{v} + \underline{D})^{-1} (\underline{x} - \hat{\underline{\mu}}) \quad (7)$$

where $\hat{\mu}(\underline{t})$ is the estimated drift component, $\underline{v}(\underline{t})$ a vector of 'station'-to-gridpoint covariances, and $(\underline{v} + \underline{D})$ the observation covariance matrix wherein \underline{D} is a diagonal matrix of the observation error variances $\{\sigma_j^2\}$. The GS solution takes a similar form if (5) is used to substitute for $\underline{\beta}$ in (6), leading to

$$\hat{x}(\underline{t}) = \hat{\mu}(\underline{t}) + \underline{k}'(\underline{t}) (\underline{k} + \underline{D}(\lambda))^{-1} (\underline{x} - \hat{\underline{\mu}}) \quad (8)$$

where $\underline{D}(\lambda)$ is again a diagonal matrix, the elements of which depend on λ and the relative magnitudes of the observation error variances $\{\sigma_j^2\}$.

Comparing (7) and (8) suggests that the function $\kappa(\tau)$ in the GS solution models the short-range covariance function $\nu(\tau)$, though actually $\kappa(\tau)$ behaves more like the short-range variogram function $\eta(\tau)$ (or "structure function" as it became known following Gandin, 1963) which is related to $\nu(\tau)$ by

$$\eta(\tau) = [\nu(0) - \nu(\tau)] \quad .$$

The above analogy points to both the essential similarity and difference between the UK and GS methods: in UK, the success of the analysis in recovering $x(\underline{t})$ depends on correct specification of a parametric model for $\mu(\underline{t})$ and $\nu(\tau)$, though the former might not be critical in practice. In GS, via the GCV method, the success of the analysis depends on there being sufficient information in a single realization of the sampled spatial process to provide suitable values for m and λ .

Universal kriging can be considered as generic to meteorological optimal interpolation (OI) analysis of univariate field data in the sense that in OI $\mu(\underline{t})$ is assumed to be zero for all \underline{t} , or, equivalently, that $\hat{\mu}$ in (7) can be replaced by a forecast datum x^f and $\nu(\tau)$ by a covariance model for the increment variable $(x - x^f)$. If reliable values for $\nu(\tau)$ and σ^2 are available, then neither UK nor GS methods appear to offer any advantage over OI. However, it is worth noting the following potential weaknesses of OI which might be particularly relevant to the problem of finescale analysis:

- I. Even if a prescribed covariance model $\hat{\nu}(\tau)$ is a good approximation to $\nu(\tau)$, OI does not necessarily return a minimum variance estimate of $x(\underline{t})$ when the analysis 'box', i.e. the region containing the n observations defined by (1), has a spatial scale not much greater than the correlation scale of $\nu(\tau)$, the reason being that under these circumstances the observation covariance matrix tends to be ill-conditioned, and its inverse relatively sensitive to small errors in $\hat{\nu}(\tau)$.
- II. OI cannot be expected to interpolate highly anisotropic field structures faithfully if its formulation is based on averaging statistics from independent sets of observations. (The latter process inevitably tends to suppress the effect of anisotropy except in a climatological sense).
- III. The assumption that sufficient averaging of covariance data leads to reliable estimates of $\nu(\tau)$ may be highly dubious in the context of fine-scale analysis, where 'unusual' structures, such as frontal regions, are

unlikely to be represented in an unbiased way in the forecast field data.

With regard to point I, both UK and GS offer a solution: by incorporating a trend of 'drift' component in the explicit (for UK) or implicit (for GS) data model, the correlation scale of the residual field $\{x(t) - \mu(t)\}$ must be smaller than that of the total field $\{x(t)\}$. This means that the final analysis should be relatively insensitive to errors in the explicit (for UK) or implicit (for GS) model for the short-range component $x'(t)$, provided that the large scale trend model accounts for an appreciable component of the total observed variation in $\{x_j\}$.

With regard to point II, UK and GS represent only the short range component $x'(t)$ via an explicit or implicit isotropic structure function. The drift or trend component can represent any degree of larger-scale field anisotropy which is 'left over' by the estimated short range structure. WW have furthermore suggested that the GS method could be formulated to cope with field anisotropy on all scales by suitable rescaling of spatial coordinates, this scaling having been optimised via the GCV method.

With regard to point III, GS has a potential advantage over UK and OI in relying on only one realization of a spatial process in arriving at an optimal interpolation of the signal field $x(t)$. Whether or not that is a real advantage in practice will depend on the nature of the field being sampled, and on the density of sampling points. At present there appears to be no objective means of estimating which approach is likely to yield the best interpretation of an interpolated field structure for a given sampling situation; in diagnostic case studies, we may have to rely on subjective evaluation of the competing analyses.

3. PRACTICAL ASPECTS AND EXAMPLES

3.1 General

Although the GCV method provides in principle an estimate of the best GS model approximating the sampled data, practical experience suggests that there may be a tendency for the noise/signal variance parameter λ to be underestimated by this method if there is insufficient sampling of the observed field structure within the domain of interest. Fortunately, it is found that the GS analysis is relatively insensitive to the prescribed value of m in (3) (as noted by WW), so that the GCV estimate of m is probably not critical for many meteorological sampling situations.

Furthermore, the numerical procedure for solving a GS surface described in WW can easily be extended to incorporate the principle described in Reinsch (1967); algorithmically, the two methods differ only in the method by which λ is estimated. Consequently, it is easy to override a GCV estimate of λ in favour of one based on a prescribed value for rms residual with little extra computational effort. In practice, it might often be desirable to impose some 'extra smoothing' in order to suppress coherent but small-scale features from the analysis, and for this purpose Reinsch's method has the obvious advantage over GCV.

3.2 Scalar map

Figures 1 illustrate GS surface analyses applied to 1000 mb height data derived from 132 synoptic m.s.l. pressure reports from stations lying within 500 km of map centre. Points to note about the raw data are that they sample a highly anisotropic field structure and are distributed non-uniformly over the area of interest. The GCV method results in the analysis shown in Fig. 1a. The interpretation of the pressure field in the vicinity of the surface front (marked by the dashed line) is quite similar to that usually employed in a subjective analysis, in which fronts are often drawn as first order discontinuities in the pressure field. However, elsewhere the GS and GCV analysis results in rather less smoothing than that usually effected by subjective analysis. In this case one feels that GCV underestimates the optimal degree of smoothing, as evidenced by the somewhat unrealistic derived geostrophic vorticity field shown in Figure 1b. Figures 1b and 1c illustrate the effect of increasing the smoothing by prescribing the rms residual following Reinsch's method. Notice that despite the considerable degree of smoothing which results when rms = 5 gpm, the essential anisotropy of the height field in the vicinity of the frontal zone has not been lost.

3.3 Vector map

A GS analysis can also be applied to vector field data, either by assimilating components quite independently, or by using common λ, m values determined from the minimum of a GCV variable obtained as a function of the rms vector error before fitting GS surfaces to the component data. Both approaches assume implicitly that the vector observing error has an rms value independent of direction, but the latter method is computationally more efficient. Figure 2 shows the result of this method applied to surface (10 metre) wind reports. (Here it has been assumed that surface

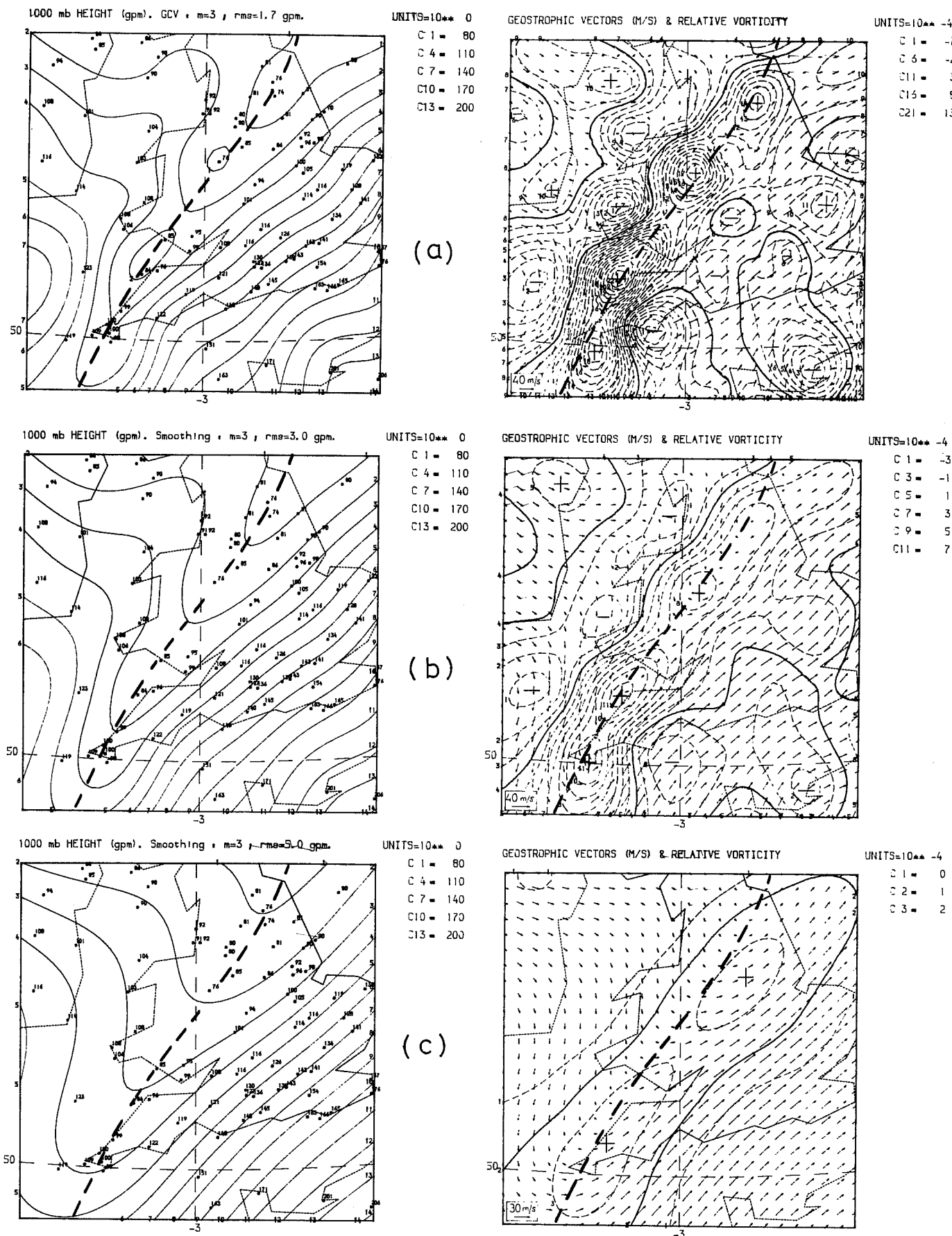


Figure 1. GS analysis of 1000 mb height field, with derived geostrophic vectors and relative vorticity (s^{-1}). (a) is via GCV; (b) and (c) are with prescribed r.m.s. residuals.

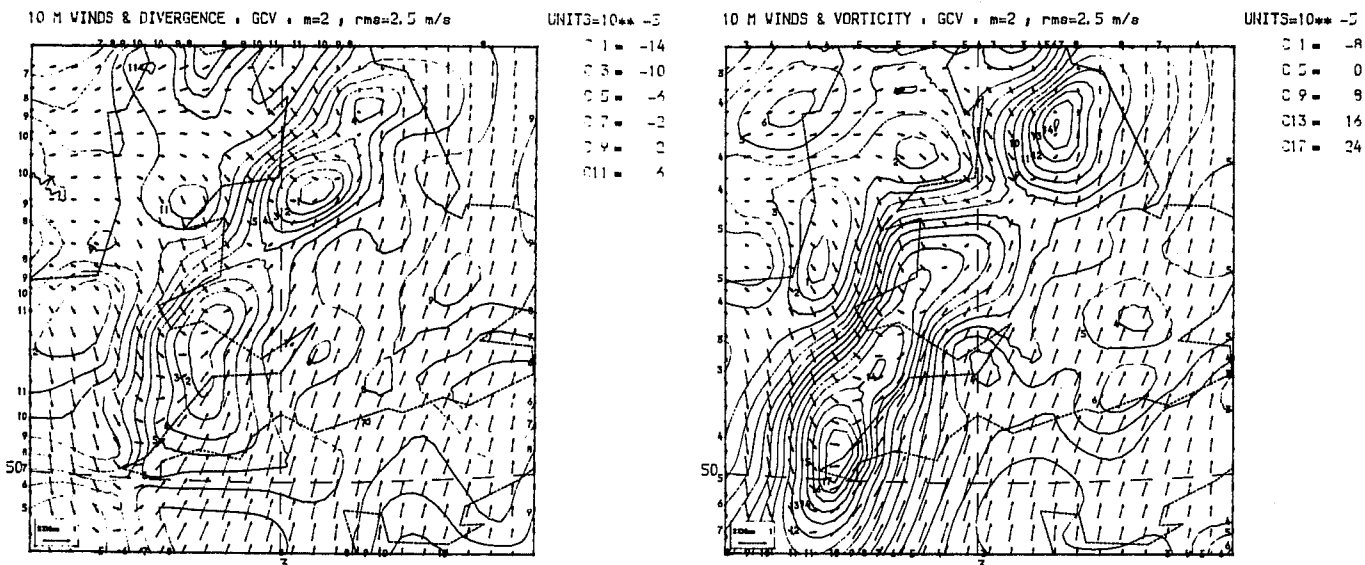


Figure 2. GS analysis of 10 metre wind field (same case as Fig. 1) with derived divergence and vorticity (s^{-1}).

wind error is proportional to reported wind speed, so that \underline{D}_0 in (5) has not in this case been replaced by an identity matrix.) Despite the relatively high noise level of surface wind observations (arising largely from local effects on scales smaller than the between-station separation scale), the resulting GS analysis provides a relatively smooth and convincing interpretation of the 10 metre kinematic structure associated with a surface front.

A method of GCV vector spline analysis on a sphere incorporating constraints on the relationship between velocity potential and stream-function variables has been developed by Wahba (1982). However, I have no experience of that method applied to real observations.

3.4 Scalar/Vector analysis in 3-space

The GS formulation is easily extended to the estimation of fields in a 3-dimensional Euclidean space. Figures 3 to 6 show some vertical sections derived by this method applied to all standard and significant point reports from 16 upper-air stations in and around the British Isles (involving up to 275 input data between 1000 and 250 mb). The GCV method was applied in the analysis of potential temperature and equivalent potential temperature fields resulting in rms residuals of just under 1 K. Wind component data were analysed to result in a root-mean-vector residual of 1 m s^{-1} , the GCV method having returned an unrealistically small value of the noise/signal variance ratio parameter λ . For this type of analysis it is necessary to carry out relative scaling of coordinate variables in order to ensure that the vertical component of short range variation has a similar scale to its horizontal component in the transformed location space. In these experiments the magnification of the vertical coordinate scale (ICAO height) was fixed at $\times 100$, though WW have suggested that an optimal scaling might be derived using the GCV approach.

Despite the relatively coarse sampling in the horizontal domain, these examples illustrate the ability of the GS analysis to resolve subtle variations in cross-sectional structure along a frontal zone (Figure 3). The cross-section fields of derived quasi-geostrophic variables in Figure 4 (ageostrophic forcing or 'Q-vectors' in the cross-frontal plane and the total geostrophic frontogenesis fields) reveal structure on a localised scale, consistent with a frontal-scale development. Figure 5 shows a vertical section of horizontal wind divergence derived directly from the

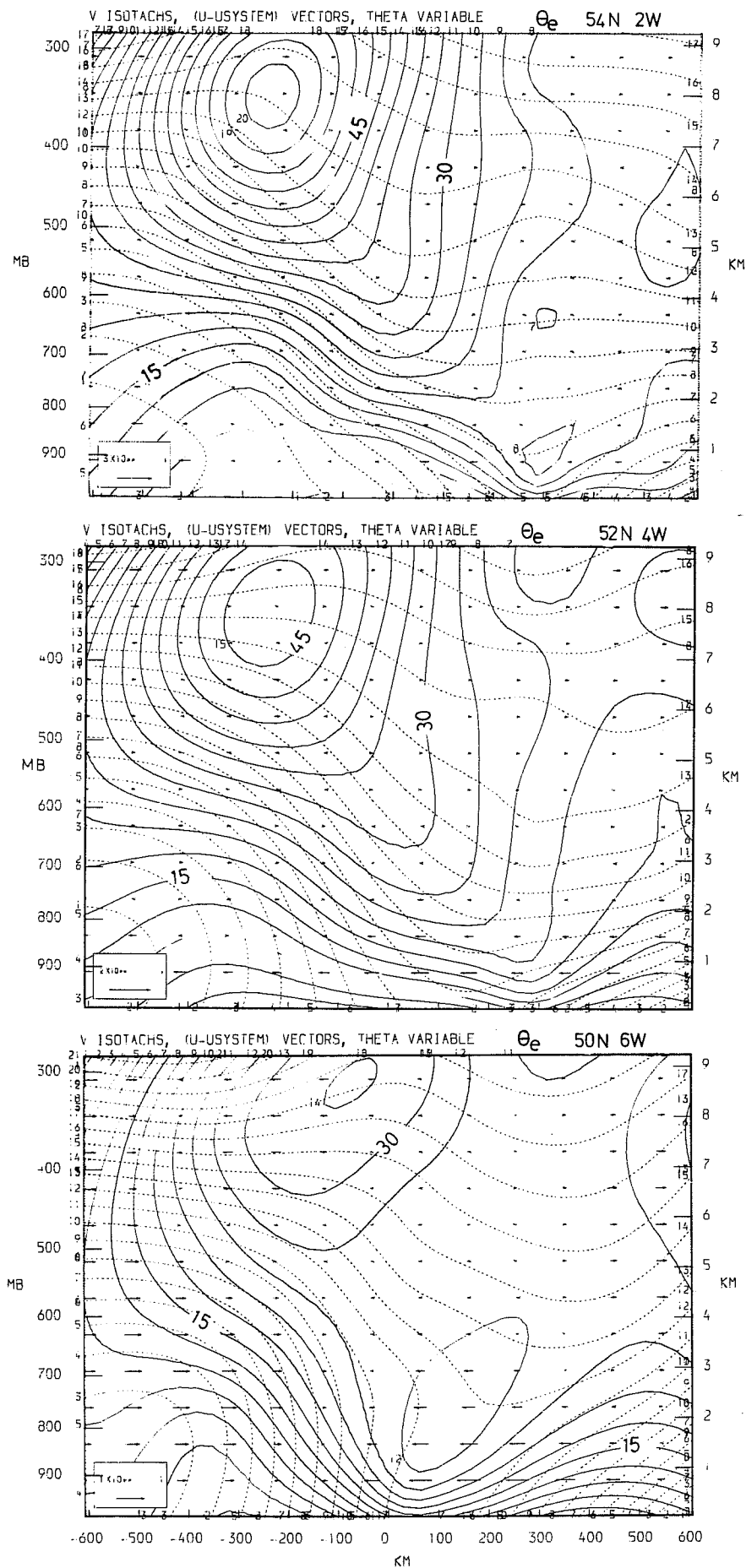


Figure 3. Cold front sections derived from GS analysis of synoptic UA data. Latitude, longitude values refer to centre of section orientated normal to surface front. θ_e (dashed) every 2K. u and v in $m s^{-1}$.

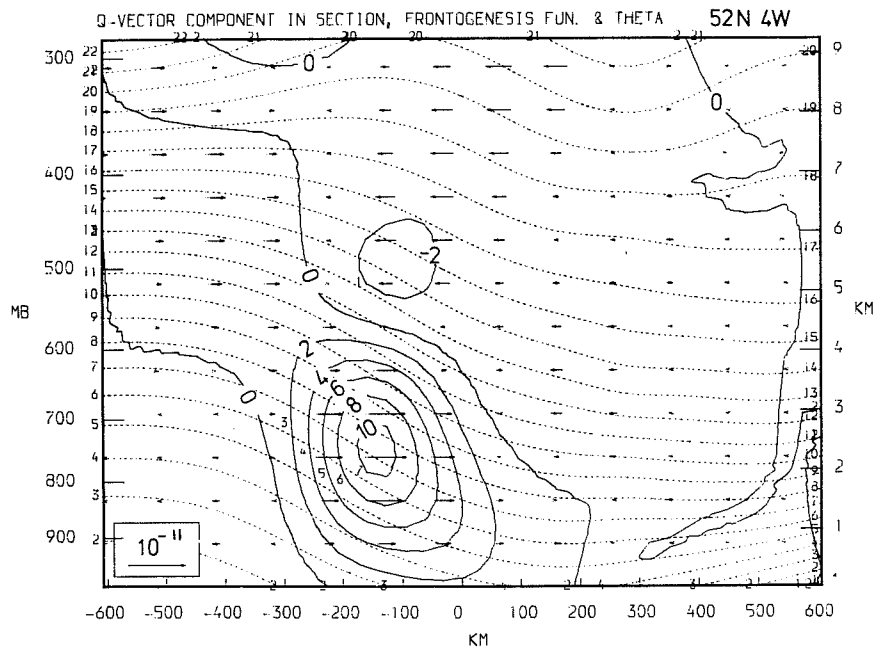


Figure 4. Q-vector components ($\text{m}^2 \text{s}^{-1} \text{kg}^{-1}$) in section and geostrophic frontogenesis function ($10^{-14} \text{K}^2 \text{m}^{-2} \text{s}^{-1}$) superimposed on θ (every 2K). Other details as in Fig. 3.

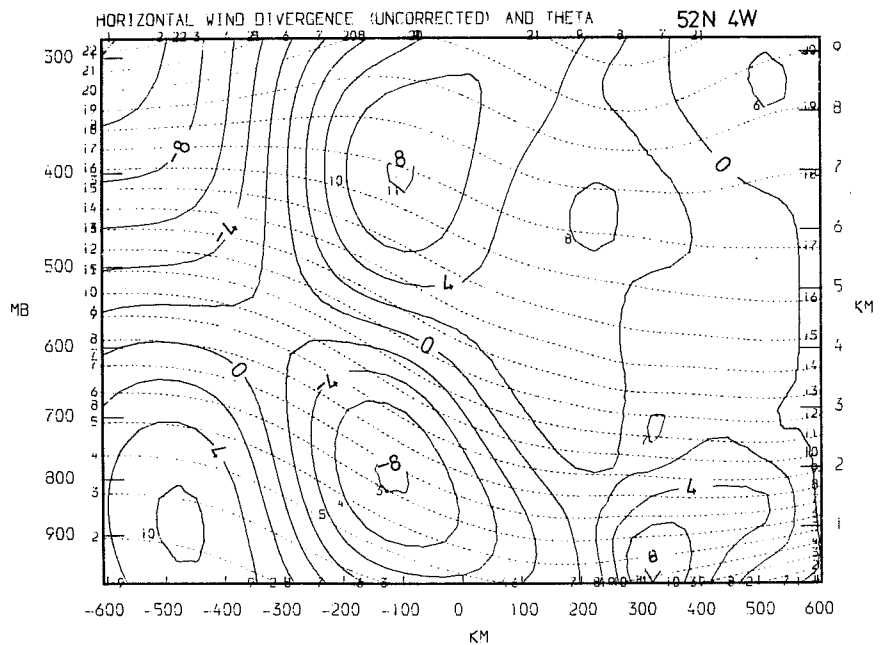


Figure 5. Horizontal wind divergence (10^{-5}s^{-1}) superimposed on θ (every 2K). Other details as in Fig. 3.

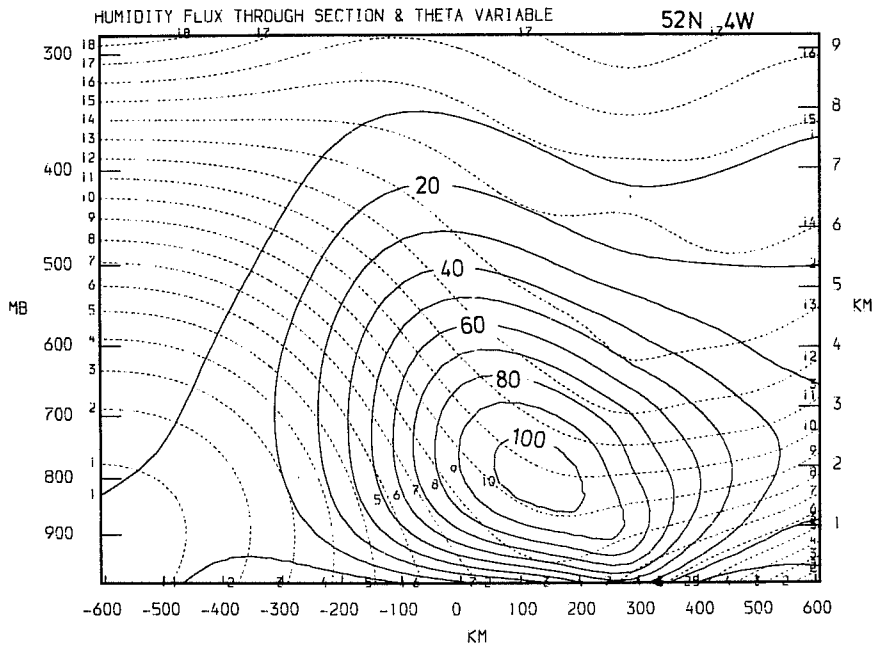


Figure 6. Humidity flux through cold front section ($\text{g m}^{-2} \text{s}^{-1}$) derived from GS analysis of log (specific humidity) and wind component data, superimposed on θ_e (every 2K). Other details as in Fig. 3.

vector wind field analysis: although the vertical distribution of divergence is not everywhere realistic, the divergence profile within the cold front zone is reasonably well balanced, and indicates a change from ascent (maximum $\omega \approx 15 \mu\text{b s}^{-1}$) to descent (maximum $\omega \approx 15 \mu\text{b s}^{-1}$) taking place over a horizontal distance of the order of 300 km, again consistent with a relatively high resolution analysis of the structure of a cold front zone. Figure 6 shows a vertical section of specific humidity flux into the plane of the section derived via the wind field analysis and a GS analysis of log specific humidity, the latter having been derived using Reinsch's approach with a prescribed rms residual equivalent to 10% of the observed specific humidity.

4. CONCLUDING COMMENTS

Surface or hypersurface spline analysis of spatial fields sampled by scattered noisy observations appears to be well suited for exploratory analysis where an optimal balance between smoothness and approximation is a primary analysis goal. In the absence of a prior covariance model for the sampled data, Wahba and Wendelberger's generalized cross validation approach to an optimal spline analysis could be superior to universal kriging or OI methods, though their method does appear to require a large number of independent observations of the sampled field if it is to result in realistic smoothing. However, there is no such limitation if Reinsch's smoothing spline method is used to estimate a suitable value for one of the two 'tuning parameters' required in Wahba and Wendelberger's formulation. Compared with other methods for interpolating meteorological fields, spline surface analysis with cross validation is numerically expensive and as yet untested for very large amounts of data ($n \geq 300$). However, it has obvious possibilities in diagnostic analysis of sub-synoptic scale events based on fine-scale observation nets, for which it might be difficult to prescribe suitable prior covariance models for the observed or forecast increment data.

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