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CROSS VALIDATED SPLINE METHODS FOR DIRECT AND INDIRECT SENSING EXPERIMENTS

by

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Cross Validated Spline Methods for Direct and Indirect Sensing Experiments

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Abstract

We first give an overview of cross-validated smoothing spline methods for the analysis of data from direct and indirect sensing experiments. Then we summarize some results involving two particular applications of the approach - (1) a deconvolution problem with nonnegativity constraints on the solution; (2) estimation of horizontal divergence and vorticity from discrete, scattered, global measurements of the upper air wind field.

1. Overview of Cross Validated Spline Methods for Direct and Indirect Sensing Experiments.

For several years, we have been developing data analysis techniques for a fairly general class of (direct and indirect) sensing experiments. The model may be described as follows: f is some unknown function of one or more variables, which is assumed to be in a (Hilbert) space H of "smooth" functions, and one observes $\{y_i\}$

$$y_i = L_i f + \varepsilon_i \qquad i = 1,2,\ldots,n, \tag{1.1}$$

where the data functionals $L_1,\ldots,L_n$ are n bounded linear functionals on H and the ε_i are independent, zero mean measurement errors, with variances $w_i\sigma^2$, $i = 1,2,\ldots,n$. The parameter σ^2 may be unknown. Examples of L_i are

(1) $L_i f = f(P_i)$

(2) $L_i f = \int_\Omega K(P_i,P)f(P)dP$

(3) $L_i f = \sum a_{\underset{\sim}{\alpha}}(P_i)\dfrac{\partial^{\alpha_1+\ldots\alpha_d}}{\partial x_1^{\alpha_1}\ldots\partial x_d^{\alpha_d}} f(x_1,\ldots,x_d).$

Example (1) corresponds to the "direct sensing" problem, example (2) to a Fredholm integral equation of the first kind given discrete, noisy data, and example (3) corresponds to a partial differential equation. Example (2) is pervasive in many problems in geophysics, meteorology and medicine. Usually one desires to estimate f(P), for all $P \varepsilon$ some set S. Sometimes only moments $\int w_i(P)f(P)dP$ are desired, in other applications derivatives of f may be desired. Side information may frequently be available, such as

$$\begin{array}{ll} 0 \le f(P) & \text{positivity} \\ a(P) \le f(P) \le b(P) & \text{boundedness} \\ 0 \le f'(P) & \text{monotonicity} \\ 0 \le f''(P) & \text{convexity} \end{array} \tag{1.2}$$

etc. More generally we have considered the case where $f \varepsilon C \subset H$, where C is any closed convex set in H which is the intersection of a "smoothly varying" family of hyperplanes. See [2]. H can be chosen so that there exists a C with the requisite properties for each of the examples in (1.2).

The general approach to the estimation of f we have developed and tested goes as follows: The estimate, call it f_λ, is the solution to the minimization problem: Find $f \varepsilon H$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}(y_i-L_i f)^2/w_i + \lambda J_{m,\delta}(f), \tag{1.3}$$

subject to $f \varepsilon C$. Here $J_{m,\delta}$ is a seminorm on H, or "penalty function" indexed by the parameters m and δ, (to be described in a monent), and λ is the bandwidth or smoothing parameter. Some examples of J are

(1) $J_m(f) = \int_0^1 (f^{(m)}(P))^2 dP$

(2) $J_{2,\delta}(f) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (f_{xx}{}^2 + 2\delta f_{xy}{}^2 + \delta^2 f_{yy}{}^2)\,dxdy$ or, in d dimensions

$$J_m(f) = \sum_{\alpha_1+\alpha_2+\ldots\alpha_d=m} \frac{m!}{\alpha_1!\alpha_2!,,,\alpha_d!} \int\cdot\cdot\int \left(\frac{\partial^m f}{\partial x_1^{\alpha_1}\ldots\partial x_d^{\alpha_d}}\right)^2 dx_1\ldots dx_d.$$

(3) $J_m(f) = \int_{\text{sphere}} (\Delta^m f)^2 dP$

where Δ is the Laplace-Beltrami operator on the sphere

$$\Delta f = \frac{1}{\cos^2\phi} f_{\lambda\lambda} + \frac{1}{\cos\phi}(\cos\phi f_\phi)_\phi,\ \lambda = \text{longitude},\ \phi = \text{latitude}.$$

Another example appears in Section 3 below, where the parameter δ plays a different role. The important bandwidth parameter λ, and sometimes m and δ, can be estimated by the method of generalized cross validation (GCV). The GCV method has recently been extended to cover problems where the constraints $f\varepsilon C$ are imposed [21,24]. In example (1), if the $L_i f$ are point evaluation functionals, that is, $L_i f = f(P_i)$, then f_λ is a polynomial smoothing spline, in example (2) f_λ will be a thin plate spline [11,13] and in example (3) f_λ will be a spline on the sphere [20].

f_λ can be shown to be a Bayes estimate, with a certain prior determined by H and J ([1,6]). On the other hand, it can be shown that f_λ is a natural generalization of the output of a low pass filter, see [7]. If the $L_i f$'s are derivatives, and the limit is taken as $\lambda\to 0$, then spline collocation methods for the solution to differential equations results [10].

Table 1 gives a list of some of the problems involved in estimating f by cross validated spline methods, and relevant references of the author, her collaborators, and students. In Table 1, $\hat{\lambda}$ is the GCV estimate of λ.

Table 1

Problems in the estimation of f, with references

(1) Explicit representation of the minimizer of (1.3) in various contexts [1,4,5,11,13,18,20,22].

(2) Generalized cross validation methods for choosing λ,m, and δ [4,7,8,21,24].

(3) Use of prior information to choose H and J [22,23].

(4) Smoothing of multidimensional scattered data [11,13].

(5) Smoothing splines on the sphere [20,22].

(6) Numerical methods for computing $f_{\hat{\lambda}}$ with large data sets [14,21,25].

(7) Quadrature methods tailored to specific integral equation problems [19,28].

(8) Optimal design (choice of $t_1,\ldots,t_n$)[10,17].

(9) Convergence properties of $f_{\hat{\lambda}}$ [3,4,7,12].

(10) Convergence properties when the constraints are discretized [2].

(11) Confidence intervals for $f_{\hat{\lambda}}$ [26].

(12) Relation of $f_{\hat{\lambda}}$ to Bayes estimates and Weiner filtering [1,6].

(13) Nonlinear data functionals [29].

Four expecially interesting areas of application are

(1) Smoothing of scattered, noisy data in two and higher dimensions with thin plate splines [11,13]. Transportable code is available from the Madison, WI Academic Computing Center.

(2) Approximate solution of Abel's Integral Equations, as they occur in stereology and computerized tomography [16,28]. These equations have a singular kernel.

(3) Equations of radiative transfer as they occur, for example in the estimation of vertical temperature profiles from satellite-observed radiances [29]. These equations are mildly nonlinear.

(4) As an alternative to logistic regression [27].

The integral equation methods have found use in a number of engineering applications, for example in the determination of adsorption energy distributions from an adsorption isotherm experiment [30] and in the recovery of aerosol size distributions from Marple impactor data [31].

For lack of space we have omitted explicit mention of recent related work by others, in particular by Cox; Chow, Geman and Wu; Rosenblatt; Lii; Silverman; Speckman, and Utreras.

In the remainder of this paper we briefly review recent numerical results in two interesting areas: Section 2: Deconvolution with positivity constraints and Section 3: Estimation of wind horizontal divergence and vorticity from scattered noisy wind vector measurements.

2. Deconvolution with Nonnegativity Constraints

We numerically studied the convolution equation

$$y_i = \int_0^1 k(\tfrac{i}{n}-s)f(s)ds + \varepsilon_i, \qquad i = 1,2,\ldots,n \tag{2.1}$$

$$f(s) \geq 0, \; 0 \leq s \leq 1$$

with $J(f) = \int_0^1 (f''(s))^2 ds$. The results appear in [24]. The cross validated spline method prescribes the estimate of the solution, call it f_λ, say, as the minimizer of

$$\frac{1}{n}\sum_{i=1}^{n} \int_0^1 k(\tfrac{i}{n}-s)f(s)ds + \lambda\int_0^1 (f''(s))^2 ds \tag{2.2}$$

in the nonnegative quadrant of a certain Sobolev space $W_2{}^2$, (which we will not discuss further).

For n of moderate size (say 32-256) a good, readily computable approximation to the minimizer f_λ of (2.2) may be found by approximating f_λ by a trignometric polynomial of the form

$$f_\lambda(x) = \alpha_0 + \sum_{\nu=1}^{n/2} \alpha_\nu \cos 2\pi\nu x + \sum_{\nu=1}^{n/2-1} \beta_\nu \sin 2\pi\nu x$$

and finding the α's and β's to minimize (2.2) subject to the discretized positivity constraints

$$f(\tfrac{i}{n}) \geq 0, \quad i = 1,2,\ldots,n.$$

For fixed λ, a quadratic programming problem with n unknowns and n linear inequality constraints results. GCV for constrained problems may be used to choose λ; for each trial value of λ a q.p. must be solved, a good starting guess can be obtained by applying GCV to the unconstrained problem. (Thus, the method is not "cheap", however it can be very cheap compared to the cost of some experiments.)

We give here a single numerical example, from [24]. Fig. 2.1 gives a plot of the convolution kernel k(t) (assumed periodic). Fig. 2.2 gives a plot of the (true) test solution f(x), $0 \leq x \leq 1$, "exact" data g(x),

$$g(x) = \int_0^1 k(x-s)f(s)ds \quad 0 \leq x \leq 1$$

and simulated measured data

$$y_i = g(\tfrac{i}{n}) + \varepsilon_i, \; i = 1,2,\ldots,n$$

for n = 64. The ε_i were independent normally distributed pseudorandom variables with common standard deviation $\sigma = .05$. The fact that there are two distinct peaks in the true f is not at all obvious from the measured data. Fig. 2.3 gives the true f (again) and it gives $f_{\hat{\lambda}}$, which is the crossvalidated spline estimate of f obtained <u>without</u> imposing positivity constraints. Fig. 2.3 also gives $f_{\hat{\lambda}_C}^C$, which is the estimate for f with the nonnegativity constraints imposed. $\hat{\lambda}_C$ is the GCV estimate of λ for constrained problems.

The unconstrained cross-validated spline estimate is not bad, however, spurious oscillations are clearly visible. The constrained solution not only eliminates the spurious oscillations, it enhances the resolution of the two peaks. This innocuous looking problem is illposed to a high degree.

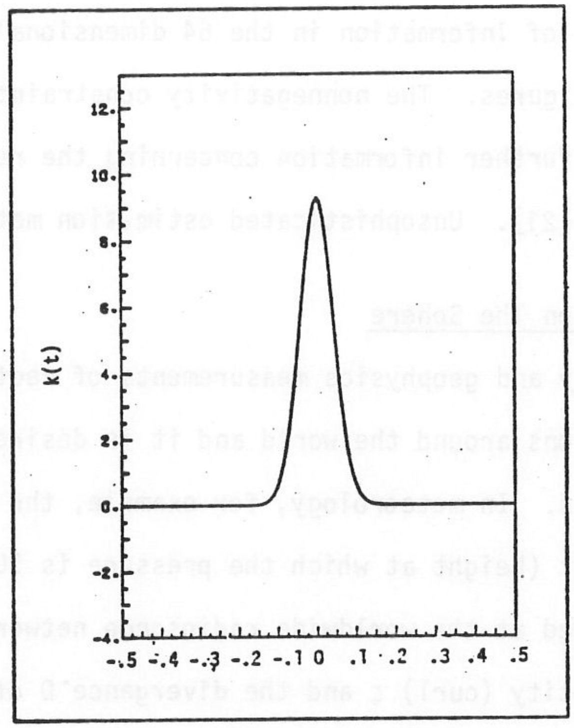

Figure 2.1. The convolution kernel k(t).

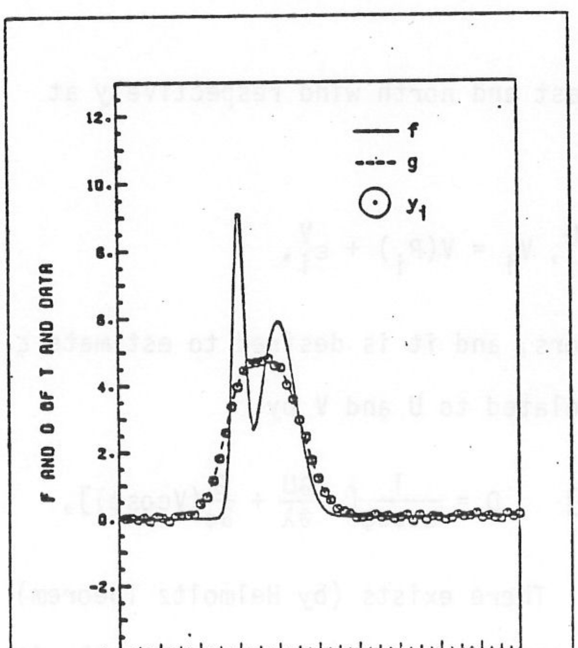

Figure 2.2

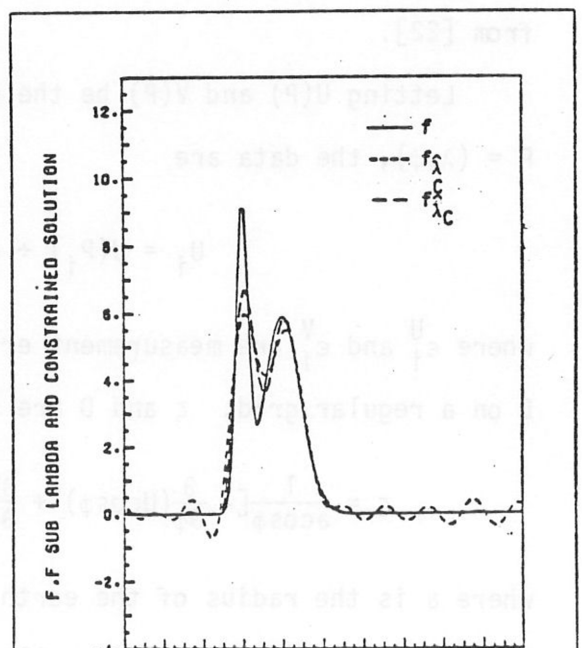

Figure 2.3

f, g, data, f_λ and $f^C_{\hat{\lambda}_C}$

If there were no measurement error, there would be only about 20 linearly independent pieces of information in the 64 dimensional data vector recorded to 8 significant figures. The nonnegativity constraints are adding important information. For further information concerning the relative degree of illposedness, see [21]. Unsophisticated estimation methods will give garbage.

3. Vector Fields on The Sphere

In meteorology and geophysics measurements of vector fields are made at discrete locations around the world and it is desired to estimate the global vector field. In meteorology, for example, the wind field at the 500 millibar height (height at which the pressure is 500 millibars) and other heights, is measured at the worldwide radiosonde network. It is desired to estimate the vorticity (curl) ζ and the divergence D of this wind field on a regular grid, to be used as initial conditions for the differential equations of numerical weather forecasting. The following is abstracted from [22].

Letting U(P) and V(P) be the east and north wind respectively at $P = (\lambda,\phi)$, the data are

$$U_i = U(P_i) + \varepsilon_i^U, \quad V_i = V(P_i) + \varepsilon_i^V, \tag{3.1}$$

where ε_i^U and ε_i^V are measurement errors, and it is desired to estimate ζ and D on a regular grid. ζ and D are related to U and V by

$$\zeta = \frac{1}{a\cos\phi}\left[-\frac{\partial}{\partial\phi}(U\cos\phi) + \frac{\partial V}{\partial\lambda}\right] \qquad D = \frac{1}{a\cos\phi}\left[\frac{\partial U}{\partial\lambda} + \frac{\partial}{\partial\phi}(V\cos\phi)\right], \tag{3.2}$$

where a is the radius of the earth. There exists (by Helmoltz Theorem) two functions $\Psi(P)$ and $\Phi(P)$, called the stream function and the velocity potential respectively, with the following properties:

$$U = \frac{1}{a}\left(-\frac{\partial\Psi}{\partial\phi} + \frac{1}{\cos\phi}\frac{\partial\Phi}{\partial\lambda}\right),\ V = \frac{1}{a}\left(\frac{1}{\cos\phi}\frac{\partial\Psi}{\partial\lambda} + \frac{\partial\Phi}{\partial\phi}\right); \tag{3.3}$$

$$\zeta = \Delta\Psi,\quad D = \Delta\Phi. \tag{3.4}$$

We estimate ζ and D from U_i and V_i by solving a minimization problem of the form: Find Ψ and Φ in an appropriate function space to minimize

$$\frac{1}{n}\sum_{i=1}^{n}\left(-\frac{1}{a}\frac{\partial\Psi}{\partial\phi}(P_i) + \frac{1}{a\cos\phi_i}\frac{\partial\Phi}{\partial\lambda}(P_i) - U_i\right)^2 + \frac{1}{n}\sum_{i=1}^{n}\left(\frac{1}{a\cos\phi_i}\frac{\partial\Psi}{\partial\lambda}(P_i) + \frac{1}{a}\frac{\partial\Phi}{\partial\phi}(P_i) - V_i\right)$$
$$+ \lambda[J^{(1)}(\Psi) + \frac{1}{\delta}J^{(2)}(\Phi)] \tag{3.5}$$

and then obtaining ζ and D analytically as $\Delta\Psi$ and $\Delta\Phi$. The parameter λ is the usual bandwidth parameter and the parameter δ controls the relative amount of energy in the divergent and nondivergent part of the wind. An approximation to the minimizer of (3.5) may be obtained by first approximating Ψ and Φ as a finite number of spherical harmonics

$$\Psi = \sum_{\ell=1}^{N}\sum_{s=-\ell}^{\ell}\alpha_{\ell s}Y_\ell^s,\ \Phi = \sum_{\ell=1}^{N}\sum_{s=-\ell}^{\ell}\beta_{\ell s}Y_\ell^s. \tag{3.6}$$

The spherical harmonics $\{Y_\ell^s\}$ are the eigenfunctions of the Laplace-Beltrami operator Δ,

$$\Delta Y_\ell^s = -\ell(\ell+1)Y_\ell^s,$$

and approximating Ψ and Φ this way is analogous to the approximation of f in Section 2 by a finite number of sines and cosines. It can be shown that if $J^{(1)}$ and $J^{(2)}$ are isotropic seminorms (isotropic = unchanged under arbitrary rotations of the coordinate system) then for Ψ and Φ of (3.6),

$$J^{(1)}(\Psi) = \sum_{\ell=1}^{N} \sum_{s=-\ell}^{\ell} \frac{\alpha_{\ell s}^{2}}{\lambda_{\ell s}^{(1)}}, \quad J^{(2)}(\Phi) = \sum_{\ell=1}^{N} \sum_{s=-\ell}^{\ell} \frac{\beta_{\ell s}^{2}}{\lambda_{\ell s}^{(2)}} \tag{3.7}$$

for some $\{\lambda_{\ell s}^{(1)}, \lambda_{\ell s}^{(2)}\}$. For more details, and in particular for a discussion concerning the choice of the $\{\lambda_{\ell s}\}$ from historical data, see [22].

By substituting (3.7) into (3.5), for fixed λ,δ, the minimization problem reduces to finding the $\{\alpha_{\ell s}, \beta_{\ell s}\}$ which minimize a quadratic form. The parameters λ and δ are estimated by GCV.

To see how well this method may be expected to do on real meteorological data, realistic "true" 500 millibar stream function-velocity potential pairs (Ψ,Φ) were generated and the "true" wind fields at 114 North American weather stations determined using (3.3). Realistic measurement errors (s.d. in each component of 2.5 meters/sec) were added. Fig. 3.1 gives the simulated wind data, and Fig. 3.2 gives the estimated wind field, which is obtained by using (3.3) in conjunction with the estimated (Ψ,Φ). Figs. 3.3 and 3.4 give the "true" and estimated vorticity and divergence respectively. The results appear to be excellent when compared to previous estimation methods. One of the results of this experiment was that the estimates were sensitive to changes in δ as well as λ and, the GCV method gives a good estimate of an optimal δ as well as λ. In a problem like this, it can be very important to parameterize J in a physically meaningful way, as well as in a mathematically well posed way. Methods for doing this are discussed in [22], see also [15].

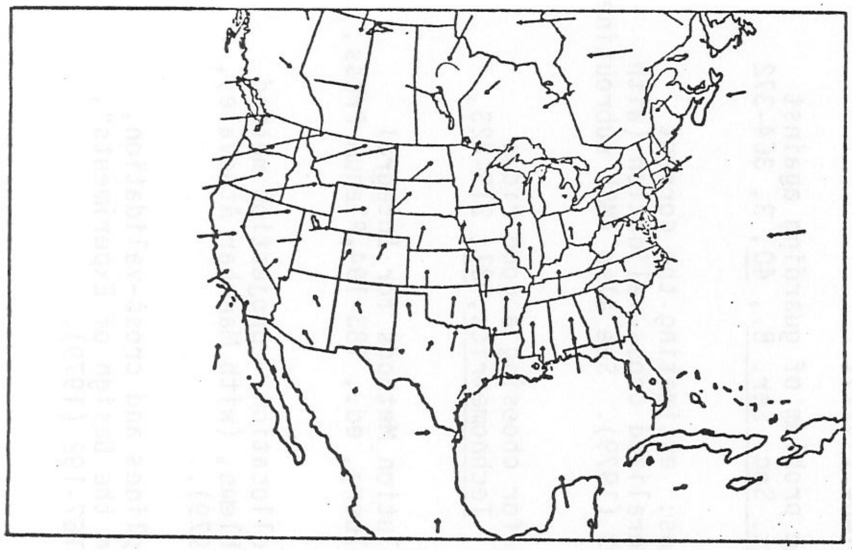

Figure 3.1 Simulated Wind Data

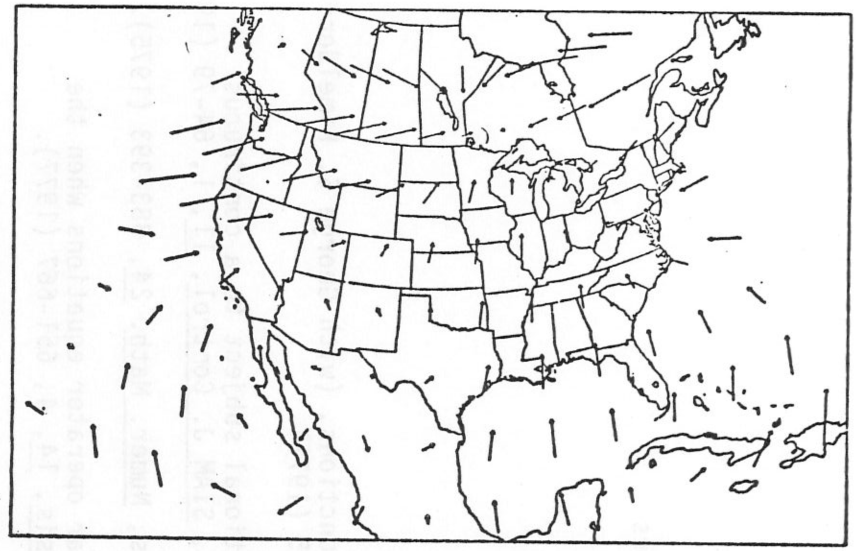

Figure 3.2 Estimated Wind Field

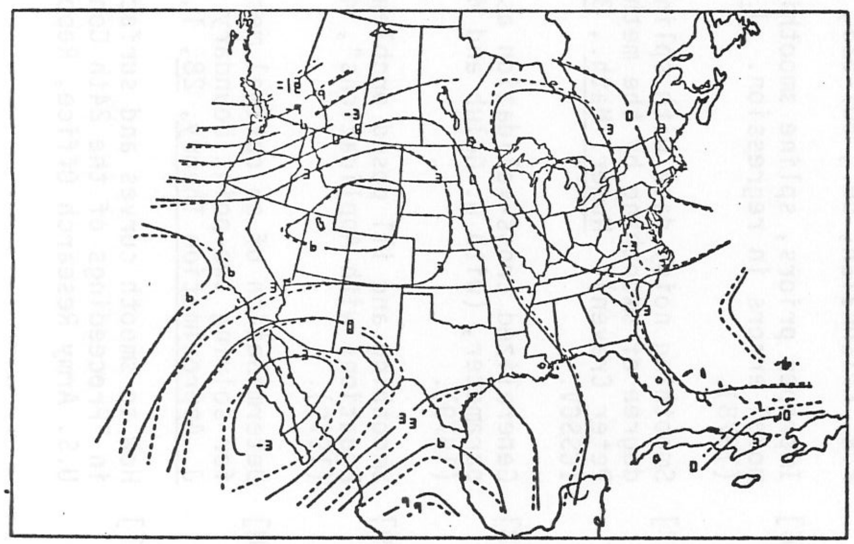

Figure 3.3 Model and Estimated Vorticity, X 10^{-5}/sec.

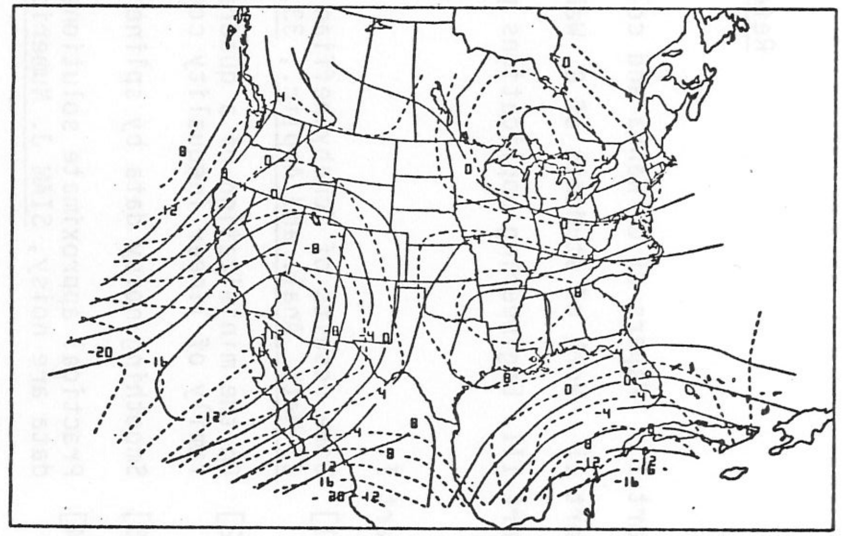

Figure 3.4 Model and Estimated Divergence, X 10^{-6}/sec.

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Part III Engineering applications papers

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

We first give an overview of cross validated smoothing spline methods for the analysis of data from direct and indirect sensing experiments. Then we summarize some results involving two particular applications of the approach - (1) a deconvolution problem with nonnegativity constraints on the solution; (2) estimation of horizontal divergence and vorticity from discrete, scattered, global measurements of the upper air wind field.

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