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PARTIAL SPLINE MODELS FOR THE INCLUSION OF TROPOPAUSE AND FRONTAL BOUNDARY INFORMATION IN OTHERWISE SMOOTH TWO AND THREE DIMENSIONAL OBJECTIVE ANALYSIS

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ABSTRACT

A new method, based on partial spline models, is developed for including specified discontinuities in otherwise smooth two and three dimensional objective analyses. The method is appropriate for including tropopause height information in two and three dimensional temperature analyses, using the O'Sullivan-Wahba physical variational method for analysis of satellite radiance data, and may in principle be used in a combined variational analysis of observed, forecast, and climate information. A numerical method for its implementation is described and a prototype two dimensional analysis based on simulated radiosonde and tropopause height data is shown. The method may also be appropriate for other geophysical problems, such as, modelling the ocean thermocline, fronts, discontinuities, etc.

1. Introduction

In this paper partial spline models are used to obtain otherwise smooth analyses of direct and indirectly sensed atmospheric data, which retain prescribed information concerning the location of certain types of discontinuities. The focus is on modelling a jump in the vertical first derivative of the two and three dimensional atmospheric temperature distribution which is characteristic of the tropopause and frontal boundaries. It is assumed that a (spline) analysis of tropopause height (or other inversion layer if used) is available separately. Such an analysis may be available from radiosonde data, total ozone content (Munteanu, Westwater and Grody (1984)), VHF radar, (Gage and Green, (1979)), a forecast, or other information. The objective of this paper is to show how partial spline models can be used to combine this information with direct (i.e. radiosonde) and/or indirect (i.e. satellite radiance) data to obtain a two or three dimensional analysis of atmospheric temperature. For radiance data a two or three dimensional version of the O'Sullivan-Wahba (1985) (O'S-W) physical variational method is incorporated into the partial spline model.

It is conjectured (but not explicitly demonstrated) that early combination of these different types of information will prove synergistic, since satellite radiance data has high resolution in the horizontal and low resolution in the vertical, particularly near the tropopause, while radiosonde data, when available, has the reverse.

Partial spline models involve functions of one or several variables, which are the sum of a smoothing spline or related function plus one or more parametric functions which carry other information. These models have found a variety of applications in the statistical literature and may even be used for probability forecasting (see Wahba (1985a), Shiau (1985) and references cited there).

Partial spline models using thin plate splines in several variables were proposed in Wahba (1984a,b, 1985a) (see Wahba and Wendelberger (1980) for a discussion of smoothing thin plate splines). A general theory of otherwise smooth functions of several variables with sharp edges along specified curves or boundary layers has been proposed by Shiau (1985). The basic mathematical theory for the characterization of partial spline models as solutions to variational problems may be found as special cases of the theory in Kimeldorf and Wahba (1971).

In Section 2 a one dimensional partial spline model for modelling an otherwise smooth curve with a jump in the first derivative at a specified point is presented. Such a model is appropriate to describe a vertical temperature profile including the first order discontinuity at the tropopause.

In Section 3 the method is extended to perform an otherwise smooth two dimensional thin plate spline analysis of temperature for a cross section through the atmosphere from a hypothetical array of radiosondes oriented on a latitude circle. The longitudinal dependence of the tropopause height as a discontinuity in the first derivative of temperature is prescribed within the plane of the cross section. The method immediately extends to a three dimensional analysis with the height of the discontinuity being specified as a two dimensional surface representing the tropopause. The methods given in this section are also appropriate for an analysis of frontal structures and the three dimensional ocean temperature where it is desired to build in information on the location of the thermocline; and it may be appropriate for certain other meteorological and geophysical problems.

In Section 4 a theoretical discussion of partial spline models is presented to show how these methods may be used in conjunction with general covariance functions to superimpose two and three dimensional break curves or surfaces on otherwise smooth fields.

In Section 5 partial spline models are used to merge tropopause height and frontal boundary information with satellite radiance data to obtain two and three dimensional temperature retrievals via the physical variational method proposed by O'Sullivan and Wahba (1985), and further studied by Wahba (1985b). Svensson (1985) has already implemented a one dimensional retrieval using this form of variational method, tropopause height information, and, moreover imposing a constraint on the dry adiabatic lapse rate.

Sections 2 through 5 end with a variational problem with a finite number of unknowns to be computed and one or more smoothing parameters to be chosen. In the appendix we show how these variational problems can be transformed so as to utilize recently developed transportable code (Bates, Lindstrom, Wahba and Yandell (1985)) which solves the variational problem and chooses the smoothing parameter(s) by generalized cross validation, for several hundred unknowns, using a super mini computer.

2. Theory of one dimensional smoothing splines with a jump in the first derivative at a specified location.

The development of the method begins by briefly reviewing some of the theory of one dimensional smoothing splines. Our discussion will be limited to certain aspects of univariate splines which generalize to partial thin plate and other spline models in many dimensions, and is not intended to describe the most efficient ways of operating with univariate polynomial splines. For a description of numerical methods which take advantage of the special structure of one dimensional polynomial splines, see Hutchinson and deHoog (1985), Shiau (1985) and references cited there.

The data model is

$$y_i = g(z(i)) + \varepsilon_i, \qquad i = 1,2,\ldots,n$$

where g is a smooth function of the variable z, and the ε_i are zero mean, approximately independent disturbances with about the same variance. One may obtain a smooth estimate g_λ of g by finding g in the (Sobolev) space W^m of all functions with m - 1 continuous derivatives and square integrable mth derivative which minimizes

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - g(z(i)))^2 + \lambda\int_{-\infty}^{\infty}(g^{(m)}(z))dz. \tag{2.1}$$

The limits on the integral may be replaced by any $a \leq z(1)$ and $b \geq z(n)$, if $z(1) < z(2) < \ldots < z(n)$, and the answer between a and b will be the same. Weights may also be included in the sum of squares term if appropriate, their discussion is omitted.

It is well known that, for fixed $\lambda>0$, with $n \geq m$, the minimizer g_λ is unique, and is in a certain n dimensional subspace which is characterized by the following properties:

(1) g_λ is a polynomial of degree m-1 for $z\varepsilon(-\infty, z(1)]$ and $z\varepsilon[z(n),\infty)$

(2) g_λ is a polynomial of degree 2m-1 in each interval $[z(j),z(j+1)]$, $j = 1,2,\ldots,n-1$

(3) The polynomial pieces are joined at each $z(1),\ldots,z(n)$ in such a way that g_λ has 2m-2 continuous derivatives.

See e.g. de Boor (1978).

This space is designated $\mathcal{S}_n^{m,1}(z(1),\ldots,z(n))$. It is assumed that $m \geq 2$, and hence g_λ will always have a continuous first derivative. In principle one may construct g_λ by constructing n linearly independent basis functions for $\mathcal{S}_n^{m,1}(z(1),\ldots,z(n))$. Substituting a representation for g in terms of the basis functions into (2.1) results in a quadratic form in the unknown coefficients which is then minimized to obtain g_λ. The smoothing parameter λ may be chosen by generalized cross validation (GCV) (see Craven and Wahba (1979), Wahba and Wendelberger (1980)). Define the influence matrix $A(\lambda)$ by

$$\begin{pmatrix} g_\lambda(z(1)) \\ \cdot \\ \cdot \\ \cdot \\ g_\lambda(z(n)) \end{pmatrix} = A(\lambda)y \quad , \tag{2.2}$$

where $y = (y_1,\ldots,y_n)'$. The GCV estimate of λ is the minimizer $\hat{\lambda}$ of $V(\lambda)$ defined by

$$V(\lambda) = \frac{1}{n}||(I-A(\lambda))y||^2/(\frac{1}{n}\mathrm{Trace}(I-A(\lambda)))^2. \tag{2.3}$$

Software for computing $\hat{\lambda}$ and $g_{\hat{\lambda}}$ is available in IMSL (1983) and a very fast code has recently been developed by Hutchinson (1985). m may also be chosen by minimizing V with respect to λ for several values of m of interest and then minimizing with respect to m.

By specializing the above variational problem to periodic functions on the circle and equally spaced data, one can establish that if $y_i = \cos 2\pi\omega\frac{i}{n}$ then $g_\lambda(\frac{i}{n}) \cong \Phi_{\lambda,m}(\omega)\cos 2\pi\omega\frac{i}{n}$, for $\omega = 1,2,\ldots,n/2$, where the filter function $\Phi_{\lambda,m}(\omega)$ is

$$\Phi_{\lambda,m}(\omega) = 1/(1+\lambda(2\pi\omega)^{2m}). \tag{2.4}$$

Methods for making this calculation may be found in Wahba (1982a). Thus the smoothing spline may be viewed as a generalization of a low pass filter to the non periodic, nonequally spaced data case, with frequency response $\Phi_{\lambda,m}(\omega)$. As a low pass filter, the output g_λ can be expected to smooth over sharp corners.

Now suppose that our data model is

$$y_i = f(z(i)) + \varepsilon_i, \qquad i = 1,2,\ldots,n$$

where a possible jump is allowed in the first derivative of f at $z = z^*$, where z^* is fixed value of z. In a partial spline f is modelled as

$$f(z) = g(z) + \theta\gamma(z) \ , \tag{2.5}$$

where $g(z)\varepsilon W^m$ for some $m\geq 2$ and $\gamma(z) = |z-z^*|$. Then

$$\left.\frac{\partial f}{\partial z}\right|_{z=z^*_+} - \left.\frac{\partial f}{\partial z}\right|_{z=z^*_-} = 2\theta. \tag{2.6}$$

A partial spline estimate of f is obtained by finding $f_\lambda = g_\lambda + \theta\gamma$ where $g\varepsilon W^m$ and θ are chosen to minimize

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - g(z(i))-\theta\gamma(z(i)))^2 + \lambda\int_{-\infty}^{\infty}(g^{(m)}(z))^2dz. \qquad (2.7)$$

It can be shown, using the theory in Kimeldorf and Wahba (1971), that if there exists a unique minimizing pair (g_λ,θ), then g_λ will be in $\mathcal{S}_n^{m,1}(z(1),\ldots,z(n))$, and there will be a unique minimizer provided that a certain $n\times(m+1)$ dimensional matrix defined below is of rank m+1. Let $\phi_1(z),\ldots,\phi_m(z)$ span the polynomials of degree less than m and let T be the $n\times m$ matrix with $i\nu$th entry $\phi_\nu(z(i))$. Let T_1 be the $n\times 1$ matrix with ith entry $\gamma(z(i))$. There will be a unique minimizer of (2.5) for each $\lambda>0$ if the matrix $(T:T_1)$ is of rank m + 1. λ and m may be chosen by GCV by defining $A(\lambda)$ now as

$$\begin{pmatrix} f_\lambda(z(1)) \\ \cdot \\ \cdot \\ \cdot \\ f_\lambda(z(n)) \end{pmatrix} = A(\lambda)y$$

and minimizing $V(\lambda)$ as before. The details can be inferred as special cases of the two and three dimensional partial spline models in the next Section, and in the Appendix.

The use of this method is illustrated in the hypothetical vertical temperature data of Figure 2.1. The solid line is a hypothetical vertical "true" temperature profile and the circles are (noisy) hypothetical measured temperature observations. The "true" temperature profile has a jump in the vertical first derivative at z*. The dashed line represents the estimate $\hat{f}_\lambda$ obtained by minimizing (2.7) for m = 2 with the true z* given and $\hat{\lambda}$ being the GCV estimate of λ.

3. Two and three dimensional thin plate partial splines with breaks and jumps

Thin plate smoothing splines appeared in the meteorological literature as a variational method for objective analysis in Wahba and Wendelberger (1980) based on mathematical foundations due to Duchon (1976) and Meinquet (1979). Since then a number of researchers have considered them in meteorological contexts, i.e. Hoffman (1984), Seaman and Hutchinson (1984), Testud and Chong (1983), Lee and Houghton (1984) and others. We will first review relevant portions of the thin plate spline theory and then give the partial spline model.

In the remainder of this paper let s and t be points in Euclidean d-space, $t = (x_1,\ldots,x_d)$, $t(i) = (x_1(i),\ldots,x_d(i))$ where $d = 1,2$, or 3 depending on whether a function of 1,2 or 3 variables is being modelled. If desired, time may be included as a fourth variable in a straightforward manner. Also, to distinguish between vertical and one or two horizontal coordinates let $t = (z,\ell)$ or (z,ℓ_1,ℓ_2) if there are, respectively, one or two horizontal (Euclidean) coordinates.

First, the model for the observations is assumed to be

$$y_i = g(t(i)) + \varepsilon_i, \qquad i = 1,2,\ldots,n \tag{3.1}$$

where g is a smooth function of $t = (x_1,\ldots,x_d)$ and ε_i are independent zero mean measurement errors or high frequency disturbances with about the same variance. $d = 2,3,4$ are the cases of most meteoroogical interest. g is assumed to be in $X^{m,d}$, a space of "smooth" functions of d variables whose derivatives of total order m are square integrable, see Meinguet (1979) for a rigorous definition. Given the data

$y = (y_1,\ldots,y_n)'$, one obtains an analysis as the minimizer in $X^{m,d}$ of

$$\frac{1}{n}\sum_{i=1}^{n}(y_i-g(t(i)))^2 + \lambda J(g), \tag{3.2}$$

where $J(g)$ is the thin plate penalty functional. For $d = 2$, $m = 2$,

$$J(g) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(g_{x_1x_1}{}^2 + 2g_{x_1x_2}{}^2 + g_{x_2x_2}{}^2)dx_1dx_2 \tag{3.3a}$$

and for general m,d

$$J(g) = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\sum_{\sum\alpha_i=m}\frac{m!}{\alpha_1!\ldots\alpha_d!}\left(\frac{\partial^m f}{\partial x_1^{\alpha_1}\ldots\partial x_d^{\alpha_d}}\right)^2 dx_1\ldots dx_d. \tag{3.3b}$$

In order that the minimizer g_λ be a well defined continuous function it is necessary that $2m-d>0$. The penalty functional is isotropic, but can be made elliptical by rescaling some of the independent variables $x_1,\ldots,x_d$ at the outset.

Let $\phi_1(t),\ldots,\phi_M(t)$ span the $M = \binom{m+d-1}{d}$ polynomials of total degree less than m in the d variables $x_1,\ldots,x_d$, and let T be the $n\times M$ matrix with $i\nu$th entry $\phi_\nu(t(i))$. If T is of rank M then (3.2) will have a unique minimizer; that is known to be in a certain n dimensional subspace to be called $\mathcal{S}_n^{m,d}(t(1),\ldots,t(n))$ which is now described.

For a description of this subspace, let

$$E_m(|t|) = \theta_{m,d}||t||^{2m-d}\log||t|| \qquad 2m-d \text{ an even integer}$$

$$= \theta_{m,d}||t||^{2m-d} \qquad 2m-d \text{ not an even integer} \tag{3.4}$$

where $||t|| = ||x_1{}^2+\ldots+x_d{}^2||^{1/2}$ and

$$\theta_{m,d} = \frac{(-1)^{(d/2)+1+m}}{2^{2m-1}\pi^{d/2}(m-1)!(m-d/2)!} \qquad d \text{ even,}$$

$$= \frac{\Gamma((d/2)-m)}{2^{2m}\pi^{d/2}(m-1)!} \qquad d \text{ odd.}$$

$\mathcal{S}_n^{m,d}(t(1),\ldots,t(n))$ consists of all functions g of the form

$$g(t) = \sum_{i=1}^{n} c_i E_m(|t-t(i)|) + \sum_{\nu=1}^{M} d_\nu \phi_\nu(t) \tag{3.5}$$

with $c = (c_1,\ldots,c_n)'$ satisfying the M conditions $T'c = 0$. If the $\{t(i)\}$ are distinct and T is of rank M, then $\mathcal{S}_n^{m,d}(t(1),\ldots,t(n))$ is of dimension n. It is known that if g is in $\mathcal{S}_n^{m,d}$ then

$$J(g) = c'Kc \tag{3.6}$$

where K is the n×n matrix with ijth entry $E_m(|t(i)-t(j)|)$. K is not a positive definite matrix but c'Kc will be nonnegative if T'c = 0. Using these facts, g of the form (3.5) can be substituted into (3.2) and it can be shown that the c and $d = (d_1,\ldots,d_M)'$ which minimize (3.2) satisfy

$$\begin{aligned} (K+n\lambda I)c + Td &= y \\ T'c &= 0. \end{aligned} \tag{3.7}$$

See Wahba and Wendelberger (1980). The minimizer g_λ will be continuous and have a continuous first partial derivative with respect to any one of the variables $x_1,\ldots,x_d$ if $2m-d \geq 2$.

By an argument similar to the one dimensional case, it can be shown that the smoothing thin plate spline in d dimensions is a generalization of a low pass filter with filter function

$$\Phi_{\lambda,m}(\omega_1,\ldots,\omega_d) = 1/(1+\lambda(2\pi|\omega|)^{2m}), \tag{3.8}$$

$$\text{where } \omega = (\omega_1^2+\omega_2^2+\ldots+\omega_d^2)^{1/2}.$$

Thus if the true g in the model has a sharp break, as might occur at the tropopause or a frontal boundary, it is likely that a smoothing thin plate spline analysis of the data will smooth it out.

Figure 3.1 gives 10 hypothetical temperature curves (solid lines) as might be observed from 10 hypothetical stations equally spaced along a latitude circle. The curves have been displaced a unit horizontal distance on the page so that the temperature scale goes with only one of the curves. The horizontal distance unit ℓ has been scaled so that the scale length in vertical and horizontal distance units is about the same. The given temperature scale actually goes with the leftmost curve. Figure 3.2 shows the tropopause height $z^*(\ell)$. $z^*(\ell)$ may be represented by a univariate spline function. Figure 3.3 shows a function $f(z,\ell)$ which specifies the sharp temperature minimum at the tropause and interpolates the 10 "true" vertical profiles of Figure 3.1. This hypothetical "true" function has been modeled with the aid of a thin plate spline $g(z,\ell)$ and a tropopause "break function" $\gamma(z,\ell)$ defined by

$$\gamma(z,\ell) = |z-z^*(\ell)| \tag{3.9}$$

where $z^*(\ell)$ is a univariate spline. If

$$f(z,\ell) = g(z,\ell) + \theta(\ell)\gamma(z,\ell) \tag{3.10}$$

and $\frac{\partial g}{\partial z}$ is continuous for each ℓ, then

$$\left.\frac{\partial f}{\partial z}\right|_{z=z^*(\ell)_+} - \left.\frac{\partial f}{\partial z}\right|_{z=z^*(\ell)_-} = 2\theta(\ell) \quad .$$

Thus the break function γ carries the location of the discontinuity in the vertical first derivative of f and the coefficient $\theta(\ell)$ carries the information concerning its size. Figure 3.4 gives the tropopause break function

corresponding to the tropopause height of Figure 3.2. If $\theta(\ell) = 0$ for some ℓ, then there is no break in the vertical first derivative of f. We shall see that if sufficient data is available and suitable assumptions are made on $\theta(\ell)$, then $\theta(\ell)$ can be treated as an unknown and estimated from the data.
Only the location $z^*(\ell)$ of the break is assumed known a priori.

The small circles in Figure 3.1 give the hypothetical data as might be observed by 10 (rather noisy) radiosondes at the stations of Figure 3.1. Figure 3.5 presents an analysis of the temperature given the location $z^*(\ell)$ of the tropopause of Figure 3.2 and the data of Figure 3.1. Temperature measurements at the tropopause are not assumed. For comparison the dashed lines in Figure 3.1 are cross sections of the two dimensional analysis of Figure 3.5. In the analysis it was assumed that tropopause height was known exactly.

Figure 3.6 presents a cross section of the "true" and estimated temperature as a function of z and ℓ while Figure 3.7 shows the true and estimated potential temperature. Results in practice will be degraded further to the extent that an erroneous tropopause height is prescribed.

We now describe the partial spline objective analysis which was used to obtain the temperature analysis of Figure 3.5. The data model is

$$y_i = f(z(i),\ell(i)) + \varepsilon_i$$

where

$$f(z,\ell) = g(z,\ell) + \theta(\ell)\gamma(z,\ell), \qquad (3.11)$$

and where $g \varepsilon X^{m,d}$ with m = 2, d = 2. The break function coefficient was modelled by $\theta(\ell) = \theta_1 + \theta_2\ell$, where θ_1 and θ_2 are to be estimated, see Shiau (1985). Then g_λ, θ_1 and θ_2 were obtained as the solution to the minimization problem:

Find $g \epsilon X^{2,2}$, θ_1 and θ_2 to minimize

$$\frac{1}{n} \sum_{i=1}^{n} (y_i - g(z(i),\ell(i)) - (\theta_1+\theta_2\ell(i))\gamma(z(i),\ell(i)))^2 + \lambda J(g), \qquad (3.12)$$

and λ was obtained by GCV. The $n = 150 = 10 \times 15$ data points $t(i) = (z(i),\ell(i))$ were the 15 data points associated with each of the 10 "true" curves of Figure 3.1.

Let $\gamma_1(t) = \gamma(t)$, $\gamma_2(t) = \ell\gamma(t)$ and T_1 be the $n \times 2$ matrix with iqth entry $\gamma_q(t(i))$. If the $n \times (M+2)$ matrix $(T:T_1)$ has rank $M + 2$ then it can again be shown, using the methods in Kimeldorf and Wahba (1971), that (3.12) has a unique minimizer $(g_\lambda, \theta_1, \theta_2)$ and that g_λ must be in $\mathcal{S}_n^{m,2}(t(1),\ldots,t(n))$. f_λ is then of the form

$$f_\lambda(t) = \sum_{i=1}^{n} c_i E_m(|t-t(i)|) + \sum_{\nu=1}^{M} d_\nu \phi_\nu(t) + \sum_{q=1}^{2} \theta_q \gamma_q(t)$$

where c, d and $\theta = (\theta_1, \theta_2)$ minimize

$$\frac{1}{n}||y - Kc - Td - T_1\theta||^2 + \lambda c'Kc \qquad (3.13)$$

subject to $T'c = 0$.

The three dimensional partial spline model is constructed the same way. Let ℓ_1 and ℓ_2 be horizontal distance coordinates and let the tropopause height be $z^*(\ell_1,\ell_2)$. The tropopause break function $\gamma(t)$, $t = (z_1,\ell_1,\ell_2)$, is

$$\gamma(t) = |z - z^*(\ell_1,\ell_2)| \; . \qquad (3.14)$$

In practice z^* would be obtained by a separate analysis of tropopause height data. The partial spline model is

$$f(t) = g(t) + \theta(\ell_1,\ell_2)\gamma(t).$$

$g \varepsilon X^{m,3}$ and $\theta(\ell_1,\ell_2)$ is modelled as

$$\theta(\ell_1,\ell_2) = \sum_{q=1}^{r} \theta_q \psi_q(\ell_1,\ell_2) \tag{3.15}$$

where the ψ_q are given. With $\gamma_q(t) = \psi_q(\ell_1,\ell_2)\gamma(t)$, and data assumed to be given from the model

$$y_i = f(t(i)) + \varepsilon_i, \quad i = 1,2,\ldots,n, \tag{3.16}$$

let $f_\lambda = g_\lambda + \sum \theta_q\gamma_q$ where g_λ in $X^{m,3}$ and $\theta = (\theta_1,\ldots,\theta_r)$ are the minimizers of

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - g(t(i)) - \sum_{q=1}^{r}\theta_q\gamma_q(t(i)))^2 + \lambda J(g).$$

If the $n\times(M+r)$ matrix $(T:T_1)$, where T_1 is the $n\times r$ matrix with iqth entry $\theta_q(t(i))$ is of rank $M + r$, then there will be a unique minimizer, g_λ which is in $\mathcal{S}_n^{m,3}(t(1),\ldots,t(n))$, so

$$g_\lambda(t) = \sum_{i=1}^{n} c_i E_m(|t-t(i)|) + \sum_{\nu=1}^{M} d_\nu\phi_\nu(t) + \sum_{q=1}^{r}\theta_q\gamma_q(t)$$

while c, d and θ are the minimizers of

$$\frac{1}{n}||y - Kc - Td - T_1\theta||^2 + \lambda c'Kc$$

with $T'c = 0$.

4. General partial spline models for modelling discontinuities of the vertical first derivative in 2 and 3 dimensions

4.1 General Theory

In this section a general theory of partial spline models which may be used with a wide class of penalty functionals is described. The choice of penalty functional can be related to a choice of prior covariance. Thin plate spline penalty functionals have proved to be good first approximations to describe atmospheric phenomena in rectangular coordinates, with an isotropic or elliptical covariance such that the energy decay with wavenumber depends on m. Splines on the sphere (Wahba (1981a)) have the same properties. However, partial spline models can be built around general covariances, and the theory may be described here in its natural context of general reproducing kernel Hilbert spaces (r.k.h.s.). Some mathematical background on r.k.h.s. may be found in Aronzajn (1950) and Kimeldorf and Wahba (1971).

Partial spline models can be used with general bounded linear functionals,

$$y_i = L_i f + \varepsilon_i, \qquad i = 1,2,\ldots,n \tag{4.1.1}$$

not just evaluation functionals,

$$y_i = f(t(i)) + \varepsilon_i. \tag{4.1.2}$$

The interesting bounded linear functionals are typically of the form $L_i f = \int K(t_i,s)f(s)ds$. The evaluation functionals are bounded in r.k.h.s.'s and thus these spaces play a key role when it is desired to combine direct data as in (4.1.2) with indirect data as in (4.1.1). In an r.k.h.s., (4.1.2) is just a special case of (4.1.1).

In the remainder of this paper P will stand for 1 or 2 horizontal coordinates, t = (z,P), in particular P may be (latitude, longitude).

The function f(t), $t\varepsilon\Omega$ to be estimated is modelled as

$$f(t) = g(t) + \theta(P)\gamma(t) \quad . \tag{4.1.3}$$

In this equation $\gamma(t) = |z-z^*(P)|$, and the break function coefficient $\theta(P)$ is parameterized as $\sum \theta_q\psi_q(P)$ where the ψ_q are given functions. Ω is some region containing the region of interest. A second break function e.g. $|z-z^{**}(P)|$, may be added if there is a second break, we omit the details. g is assumed to be in an r.k.h.s. of real valued functions defined for all $t\varepsilon\Omega$ which have all their first derivatives everywhere continuous. $\mathcal{H}$ is decomposed into two orthogonal subspaces, $\mathcal{H}_1$ and $\mathcal{H}_0$, where $\mathcal{H}_0$ is an M dimensional subspace such that the desired penalty functional J(g) is 0 if g is in $\mathcal{H}_0$. Formally $\mathcal{H}$, $\mathcal{H}_1$ and $\mathcal{H}_0$ are chosen so that $J(g) = ||P_1g||^2$, where P_1 is the orthongonal projection onto $\mathcal{H}_1$ in $\mathcal{H}$ and $||.||$ is the norm in $\mathcal{H}$. Letting $\{\phi_1,\ldots,\phi_M\}$ be a basis for $\mathcal{H}_0$, the model is expressed as

$$f(t) = g_1(t) + \sum_{\nu=1}^{M} d_\nu\phi_\nu(t) + \sum_{q=1}^{r} \theta_q\gamma_q(t), \tag{4.1.4}$$

where $g_1\varepsilon\mathcal{H}_1$ and $\gamma_q(t) = \psi_q(P)\gamma(t)$. It is assumed that γ_q is not in $\mathcal{H}$. Now consider data y_i of the form

$$y_i = L_if + \varepsilon_i, \qquad i = 1,2,\ldots,n, \tag{4.1.5}$$

where L_i is a bounded linear functional on $\mathcal{H}\oplus\{\gamma_q\}$. f is estimated by finding

g_1 in $\mathcal{H}_1$ and $d = (d_1,\ldots,d_M)'$ and $\theta = (\theta_1,\ldots,\theta_r)'$ to minimize

$$\frac{1}{n}\sum_{i=1}^{n}(y_i - L_i(g_1 + \sum_{\nu=1}^{M} d_\nu\phi_\nu + \sum_{q=1}^{r}\theta_q\gamma_q))^2 + \lambda J(g_1). \tag{4.1.6}$$

(A concrete example of $J(g_1)$ is found in Section 4.4.)

Let $Q(s,t)$, $s,t \in \Omega$ be the reproducing kernel for $\mathcal{H}_1$. (Q is also a prior covariance, see Section 4.2 below.)

Let $\xi_j(t) = L_{j(s)}Q(t,s)$ where $L_{j(s)}$ means that L_j is to be applied to what follows considered as a function of s. Then it can be shown that if there is a unique minimizer of (4.1.6), then g_1 must be of the form

$$g_1 = \sum_{j=1}^{n} c_j\xi_j. \tag{4.1.7}$$

(See, e.g. Kimeldorf and Wahba (1971)).

Let T be the $n\times M$ matrix with $i\nu$th entry $L_i\phi_\nu$, let T_1 be the $n\times r$ matrix with iqth entry $L_i\gamma_q$ and let Σ be the $n\times n$ matrix with ijth entry $L_{i(s)}L_{j(t)}Q(s,t) = L_i\xi_j \equiv \langle\xi_i,\xi_j\rangle$, where $\langle\cdot,\cdot\rangle$ is the inner product in $\mathcal{H}_1$. If $(T:T_1)$ has rank M+r and Σ has rank n, then (4.1.6) will have a unique minimizer and the minimization of (4.1.6) reduces to finding c, d, and θ to minimize

$$\frac{1}{n}||y - \Sigma c - Td - T_1\theta||^2 + \lambda c'\Sigma c. \tag{4.1.8}$$

4.2 Partial splines as Bayes (Gandin) estimates

Let f_λ be the estimate of f obtained by minimizing (4.1.6). It can be shown that f_λ is a Bayes (Gandin) estimate for f under the model

$$y_i = f(t_i) + \varepsilon_i, \qquad i = 1,2,\ldots,n$$

$$f(t) = g_1(t) + \sum_{\nu=1}^{M} d_\nu\phi_\nu(t) + \sum_{q=1}^{r}\theta_q\gamma_q(t)$$

where $g_1(t)$ is a zero mean normally distributed stochastic process with $Eg_1(s)g_1(t) = bQ(s,t)$, and the ε_i are independent normal random variables with variance σ^2, and $\lambda = \sigma^2/nb$ (see Kimeldorf and Wahba (1971), Wahba (1978)).

4.3 Use of basis functions for computational efficiency

If n is very large, instead of attempting to obtain the exact minimizer of (4.1.6) by minimizing (4.1.8), it may be adequate to minimize (4.1.6) by approximating g_1 by a linear combination of $N << n$ basis functions. Basis functions which have generally good approximation-theoretic properties in $\mathcal{H}_1$ are: the first n eigenfunctions of the r.k. Q (see, e.g. Micchelli and Wahba (1981)) and representers of evaluation $\{q_{s(\ell)}\ \ell=1,2,\ldots,N\}$ in $\mathcal{H}_1$, where $q_{s(\ell)}(t) = Q(t,s(\ell))$ (also known as "sections of the r.k." and as "structure functions") and $s(1),\ldots,s(N)$ are spread throughout the region of interest. It can be shown that the N dimensional space of thin plate basis functions $\mathcal{S}_n^{m,d}(s(1),\ldots,s(N))$ span the same N dimensional space as sections of r.k. for $X^{m,d}$, thus the thin plate basis functions make a good set. (See Wahba (1980), Hutchinson (1984)). A sufficiently large number N of basis functions should be used to avoid losing resolution that may be contained in the data. Let $B_1,\ldots,B_N$ be the basis functions. If $Q(s,t) = \sum \lambda_j B_j(s)B_j(t)$, that is, the B_j's are eigenfunctions of Q, then $J(\sum c_j B_j) = \sum c_j^2/\lambda_j$. If $B_j(t) = q_{s(j)}(t)$, that is, a section of the r.k., then $J(\sum_{j=1}^{N} c_j q_{s(j)}) = \sum_{j,k=1}^{N} c_j c_k Q(s(j),s(k))$.

If the thin plate penalty functional is used we let $g = g_1 + \sum d_\nu \phi_\nu$ and then we minimize for g in $\mathcal{S}_n^{m,d}(s(1),\ldots,s(N))$, thus $g(t) = \sum c_j E_m(|t-t(j)|) + \sum d_\nu \phi_\nu(t)$ with $S'\underset{\sim}{c} = 0$, S being the $N\times M$ matrix with $j\nu$th entry $\phi_\nu(s(j))$, and $J(g) = c'Kc$ where K is the $N\times N$ matrix with ijth entry $E_m(|s(i)-s(j)|)$. See Hutchinson (1984).

Letting T and T_1 be as before, and letting X be the n×N matrix with ijth entry L_iB_j, we obtain

$$f = \sum_{j=1}^{N} c_jB_j + \sum_{\nu=1}^{M} d_\nu\phi_\nu + \sum_{q=1}^{r} \theta_q\gamma_q \quad (4.3.1)$$

by finding c, d and θ to minimize

$$\frac{1}{n}||y-Xc-Td-T_1\theta||^2 + \lambda c'Jc \quad (4.3.2)$$

where now J is the N×N matrix such that $J(\sum_{j=1}^{N} c_jB_j) = c'Jc$. If thin plate basis functions are used, then $B_j(t) = E_m(|t-s(j)|)$ in (4.3.1) and c must satisfy the side condition $S'c = 0$. Numerical methods for obtaining c, d and θ in (4.3.2) along with the GCV estimate of λ are discussed in the Appendix.

4.4 Example: Global partial splines

$$\text{Let } Q(t,t') = \sum_{\ell=1}^{\infty} \sum_{s=-\ell}^{\ell} \sum_{j=1}^{q} \sum_{k=1}^{q} \lambda_{\ell s,j,k} h_j(z)h_k(z')Y_{\ell s}(P)Y_{\ell s}(P') \quad (4.4.1)$$

where $t = (z,P)$ and $s = (z',P')$ and the h_j are q linearly independent continuously differentiable vertical basis functions and the $Y_{\ell s}$ are (surface) spherical harmonics. The stochastic model associated with Q(s,t) is

$$g_1(t) = b^{1/2} \sum_{\ell s} \sum_{j} g_{\ell s,j} h_j(z) Y_{\ell s}(P) \quad (4.4.2)$$

where $Eg_{\ell s,j} = 0$, $Eg_{\ell s,j}g_{\ell 's',k} = 0$, $\ell s \neq \ell 's'$, $Eg_{\ell s,j}g_{\ell s,k} = \lambda_{\ell s,j,k}$ (i.e., $Eg_1(s)g_1(t) = bQ(s,t)$). The penalty functional is

$$J(g_1) = \sum_{\ell s} \sum_{j,k} g_{\ell s,j} \lambda_{\ell s}^{jk} g_{\ell s,k} \qquad (4.4.3)$$

where $\{\lambda_{\ell s}^{jk}\}$ are the entries of $\Lambda_{\ell s}$, the q×q matrix with jkth entry $\lambda_{\ell s,j,k}$. The r.k.h.s. $\mathcal{H}_1$ consists of functions possessing a representation of the form (4.4.2) with (4.4.3) finite. In this example $\mathcal{H}_0$ might be span $\{h_j(z)Y_{00}(P)\}$. There should be more vertical basis functions than the vertical resolution desired to avoid losing information at this stage. The eigenfunctions of Q are $\{\tilde{h}_j(z)Y_{\ell s}(P)\}$ where the $\{\tilde{h}_j\}$ are linear combinations of the h_j such that $\sum_j \tilde{h}_j^2(z)\delta_{\ell sj} = (h_1(z),\ldots,h_q(z))'\Lambda_{\ell s}(h_1(z),\ldots,h_q(z))$. Conditions on the rate of decay of the $\delta_{\ell sj}$ with horizontal wavenumber ℓs that are characteristic of the atmosphere should be assumed, see. e.g. Wahba (1982d).

5. Analysis of two and three dimensional atmospheric temperature distributions from satellite radiance data

An important potential application of partial spline theory is to the analysis of two and three dimensional atmospheric temperature fields via the physical variational method of O'Sullivan and Wahba (1985) (O'S-W).

The observed radiance y_i from a particular channel and look direction indexed by i is modelled as

$$y_i = N_i(f) + \varepsilon_i, \qquad i = 1,2,\ldots,n$$

where f is the two or three dimensional atmospheric temperature distribution, N_i is a nonlinear functional, involving the radiative transfer equation with an integral over f along the line of sight and the ε_i represent measurement noise or other high frequency phenomena it is desired to eliminate. Dependence on surface temperature and atmospheric water vapor is included but we omit explicit expression of this dependency. (See Smith, Woolf and Schreiner (1985) or Svensson (1985)).

Merging the O'S-W method with partial spline theory, in 2 or 3 dimensions, and assuming suitable basis functions, f is modelled as

$$f = \sum_{j=1}^{N} c_j B_j + \sum_{\nu=1}^{M} d_\nu \phi_\nu + \sum_{q=1}^{r} \theta_q \gamma_q . \tag{5.1}$$

Then, following O'S-W one finds f of the form (5.1) to minimize

$$\frac{1}{n} \sum_{i=1}^{n} (y_i - N_i(f))^2 + \lambda c' J c. \tag{5.2}$$

Goldberg et al (1985) have recently argued that choice of an appropriate J is important. O'S-W use a Gauss-Newton iteration to minimize expressions like (5.2) and an extended form of GCV to choose λ. The method goes as follows: Write $N_i(f) = N_i(c,d,\theta)$ and let $X_{n\times N}{}^k$, $T_{n\times M}{}^k$ and $T_{1,n\times r}{}^k$ be matrices whose dimensions are indicated by the subscripts a×b with entries

$$\left.\frac{\partial N_i}{\partial c_j}\right|_k , \quad \left.\frac{\partial N_i}{\partial d_\nu}\right|_k \quad \text{and} \quad \left.\frac{\partial N_i}{\partial \theta_q}\right|_k$$

respectively where the subscript k indicates that the partial derivative is to be evaluated at $(c:d:\theta) = (c^k:d^k:\theta^k)$. Expanding N_i to first order in a Taylor series expansion gives

$$N_i(c^{k+1}, d^{k+1}, \theta^{k+1}) \simeq N_i(c^k, d^k, \theta^k) + \sum_{j=1}^{N} \left.\frac{\partial N_i}{\partial c_j}\right|_k (c_j{}^{k+1} - c_j{}^k)$$
$$+ \sum_{\nu=1}^{M} \left.\frac{\partial N_i}{\partial d_\nu}\right|_k (d_\nu{}^{k+1} - d_\nu{}^k) + \sum_{q=1}^{r} \left.\frac{\partial N_i}{\partial \theta_q}\right|_k (\theta_q{}^{k+1} - \theta_q{}^k)$$

(5.3)

Letting $z_i^k = y_i - N_i(c^k, d^k, \theta^k) + \sum_{j=1}^{N} \frac{\partial N_i}{\partial c_j}\Big|_k c_j^k + \sum_{\nu=1}^{M} \frac{\partial N_i}{\partial d_\nu}\Big|_k d_\nu^k + \sum_{q=1}^{r} \frac{\partial N_i}{\partial \theta_q}\Big|_k \theta_q^k$,

and $z^k = (z_1^k, \ldots, z_n^k)'$, and substituing (5.3) into (5.2) gives:

$$\frac{1}{n}||z^k - X^k c^{k+1} - T^k d^{k+1} - T_1^k \theta^{k+1}||^2 + \lambda c^{k+1'} J c^{k+1}. \tag{5.4}$$

c^{k+1}, d^{k+1} and θ^{k+1} are obtained given c^k, d^k and θ^k by minimizing (5.4). For fixed λ, given c^0, d^0, θ^0, iterative minimization of (5.2) takes place by minimizing (5.4) for $k = 0,1,2,\ldots$, then the GCV function $V(\lambda)$ is evaluated for the quadratic minimization problem of (5.4) at convergence. The process is repeated with a different value of λ, until the λ which minimizes $V(\lambda)$ is found. If thin plate basis functions are used then at each stage c^{k+1} must satisfy $S'c^{k+1} = 0$ where S is as before. The methods in the appendix can be used for each step in the iteration (5.4). An additonal useful feature of the O'S-W method is its ability to accommodate side conditions. Svensson (1985) has implemented this approach in one dimension (a single column) and has imposed inequality constraints resulting from constraints on the dry adiabatic lapse rate. (For use of GCV when inequality constraints are present, see Villalobos and Wahba (1985), Wahba (1982a)). In a 2 or 3 dimensional analysis, occasional radiosonde data may provide a very important complement to the radiance data, particularly since the radiosonde data has high vertical resolution and poor horizontal resolution, whereas the radiance data has high horizontal resolution and poor vertical resolution. If some radiosonde data is available within the region and time of interest, this data can be analyzed simultaneously by including it in the sum of squares term in (5.2) with appropriate weights, that is, $\tilde{y}_1, \ldots, \tilde{y}_L$ are direct temperature observations at (z_ℓ, P_ℓ), $\ell = 1,2,\ldots,L$, this adds a term $\frac{1}{L}\sum_{\ell=1}^{L}(y_\ell - f(z_\ell, P_\ell))^2\omega$ to the left hand side of (5.2), where ω is an appropriate weight. It is also possible to include forecast information in the same variational problem, see Wahba (1982c, 1985b, Section 5).

It is not known a priori whether or not it is worthwhile to reestimate λ with each new data set, or whether the same λ may be used for similar data sets. Seaman and Hutchinson (1985) have recently suggested (in another context) that reestimation with each data set may provide some ability to compensate for a suboptimal covariance (Q).

APPENDIX

A numerical algorithm for medium sized data sets

Bates, Lindstrom, Wahba and Yandell (1985) (BLWY) have developed transportable code for certain core calculations that are common to the variational problems described here. The methods use matrix decompositions in LINPACK (Dongarra, et. al. (1979), and appear to be quite satisfactory for several hundred unknowns (i.e. state variables) on the U.W. Madison Statistics Department VAX 11/750 running UNIX. BLWY find δ_λ to minimize

$$||y - Y\delta||^2 + \lambda\delta'\Sigma\delta, \tag{A.1}$$

where $y_{n\times 1}$, $Y_{n\times p}$, $\delta_{p\times 1}$ and $\Sigma_{p\times p}$ have the given dimensions, and Σ is symmetric non-negative. p may be larger than n, and neither Y nor Σ is required to be of full rank although the program requires the intersection of the nullspace of Y and Σ to be empty. (If it is not, the minimizer δ is not unique. The minimal norm δ could be taken but this is not done.) The program computes the GCV estimate of λ (or uses a fixed value, if requested) and also returns certain singular values and other diagnostic information. The code uses the truncated singular value decompositon of Bates and Wahba (1983), to speed up the calculation and is based on the algorithm given there. The minimization problems of (3.13), (4.1.8), (4.3.2) and (5.4) can be reduced to this form. First consider the minimization of

$$\frac{1}{n}||z - Xc - Td - T_1\theta||^2 + \lambda c'Jc \tag{A.2}$$

with no side conditions on c. Then (A.2) is of the form (A.1) with

$$Y = (X:T:T_1)$$

$$\delta' = (c':d':\theta')$$

$$\sum = \begin{pmatrix} J:0:0 \\ \cdots\cdots \\ 0:0:0 \\ \cdots\cdots \\ 0:0:0 \end{pmatrix}.$$

If c must satisfy the side condition $T'c = 0$, then take a QR decompositon of $T_{n\times M}$ as

$$T = QR = (Q_1:Q_2)\begin{pmatrix} R_1 \\ \cdots \\ 0 \end{pmatrix},$$

where Q is orthogonal and R_1 is lower triangular $M\times M$. The $n-M$ columns of Q_2 are all perpendicular to the columns of T so we can set $c = Q_2\gamma$ where γ is $n-M$, this insures that $T'c = 0$. Substituting into (A.2) gives

$$\frac{1}{n}||z - XQ_2\gamma - Td - T_1\theta||^2 + \lambda\gamma'Q_2'JQ_2\gamma,$$

which is of the form of (A.1) with

$$Y = (XQ_2'T:T_1)$$

$$\sum = \begin{pmatrix} Q_2'JQ_2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\delta' = (\gamma':d':\theta').$$

Hoffman (1984), Testud and Chong (1983) and others have solved very large optimization problems with thin plate penalty functionals using conjugate gradient algorithms. Purser (1985) has proposed multigrid methods for solving similar problems. It remains to be seen whether conjugate gradient, multigrid or other methods suitable for very large state vectors can be applied to the inclusion of break functions and the GCV choice of λ in very large problems.

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Figure Captions

Figure 2.1. True (simulated) temperature, (simulated) data, and estimated temperature with a break in the first derivative at the tropopause.

Figure 3.1. True (simulated) temperature, simulated data, and estimated temperature curves, with a break in the first derivative, for 10 observing locations equally spaced along a fixed latitude.

Figure 3.2. The tropopause, $z^*(\ell)$.

Figure 3.3. True (simulated) temperature, as a function of z and ℓ.

Figure 3.4. The tropopause break function $\gamma(z,\ell)$.

Figure 3.5. Analysis of the temperature data of Figure 3.1, with the use of $z^*(\ell)$, the tropopause height.

Figure 3.6. True (a) and estimated (b) temperature contour plots corresponding to Figures 3.3 and 3.5.

Figure 3.7. True (a) and estimated (b) potential temperature.

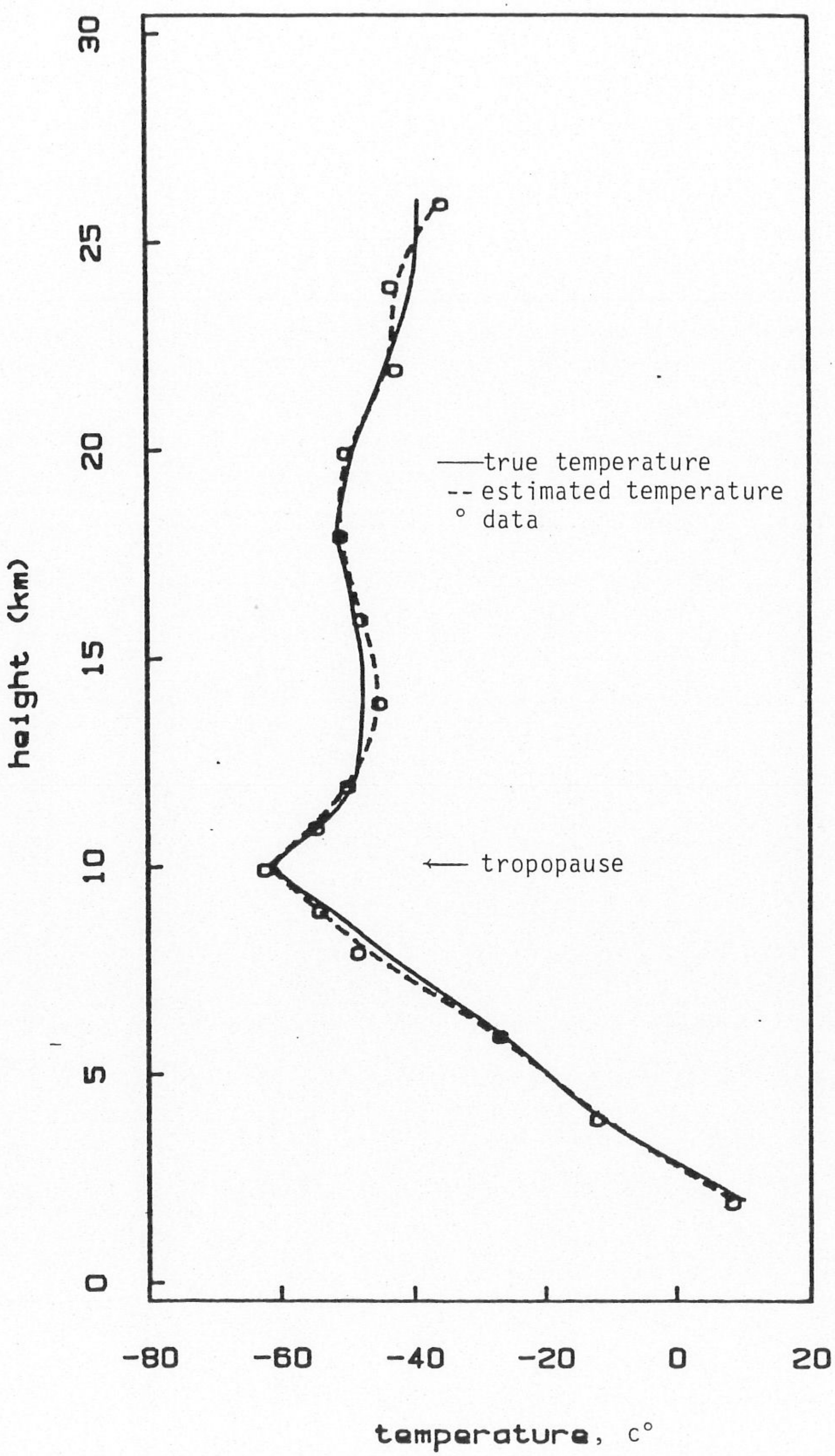

Figure 2.1 True (simulated) temperature, (simulated) data, and estimated temperature with a break in the first derivative at the tropopause.

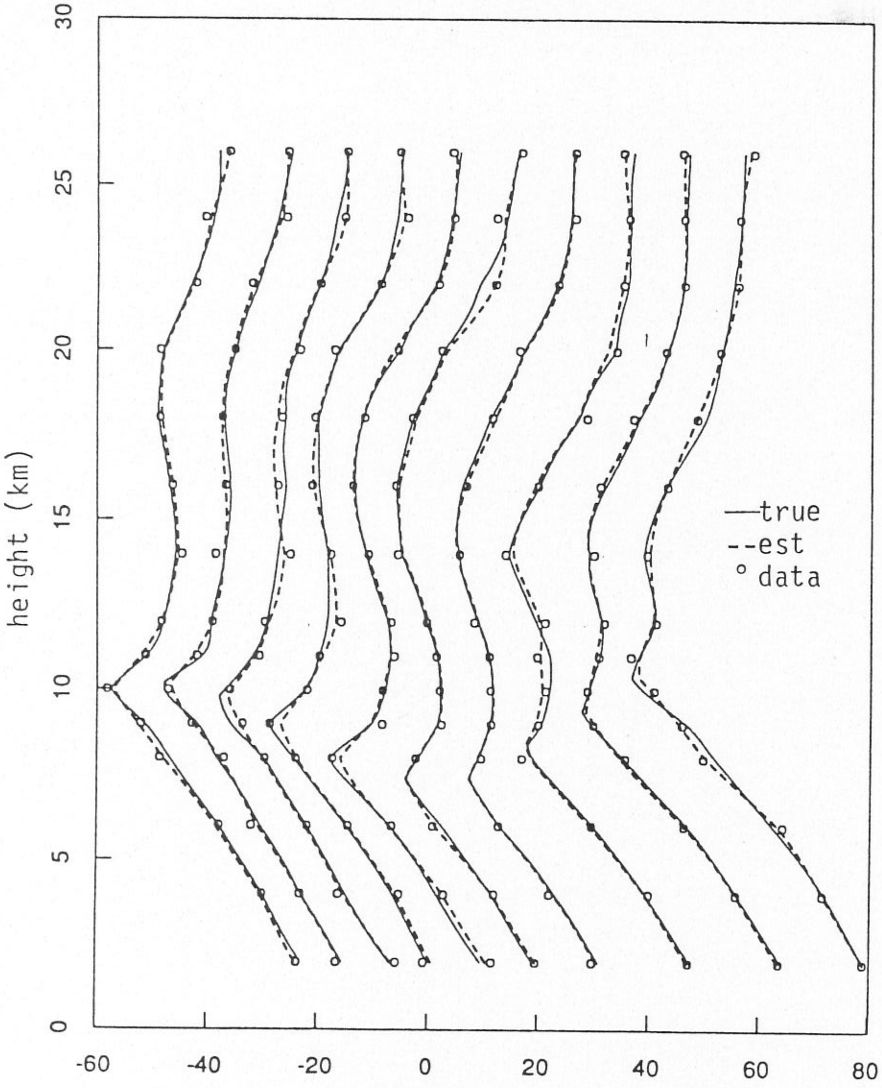

Figure 3.1 True (simulated) temperatures, simulated data, and estimated temperature curves, with a break in the first derivative, for 10 observing locations equally spaced along a fixed latitude.

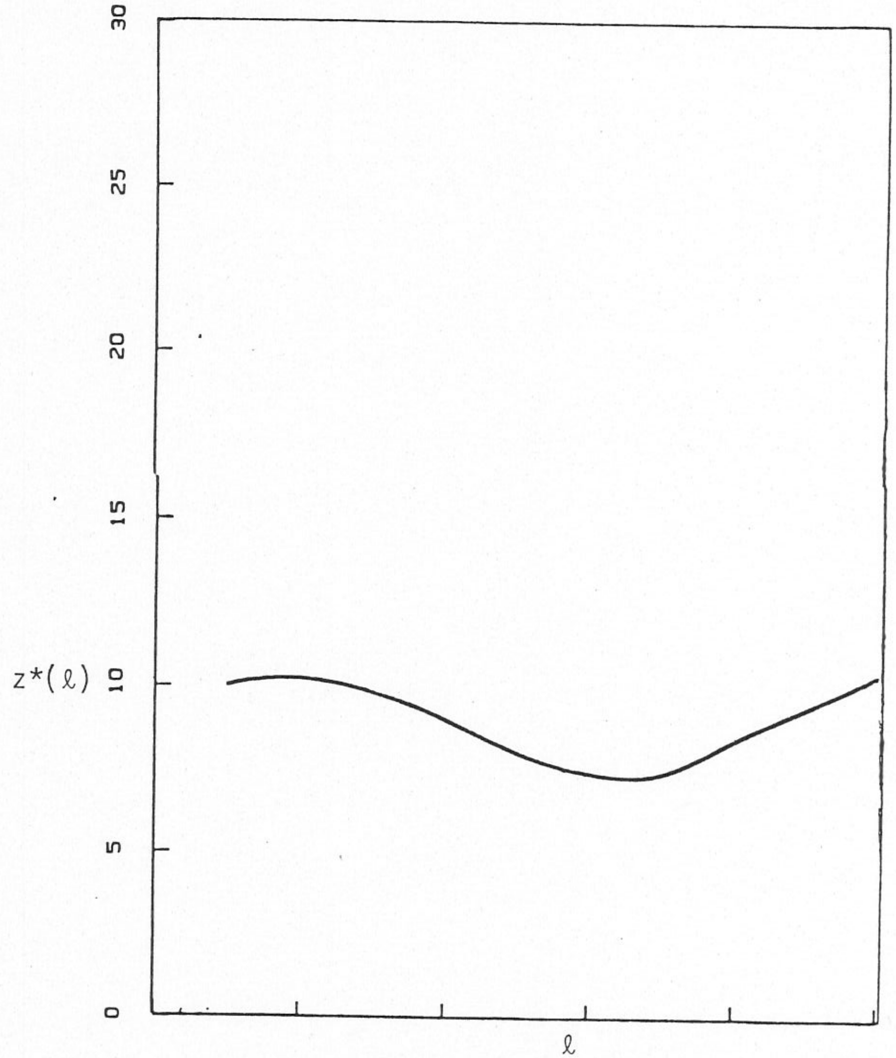

Figure 3.2 The tropopause, z*(ℓ)

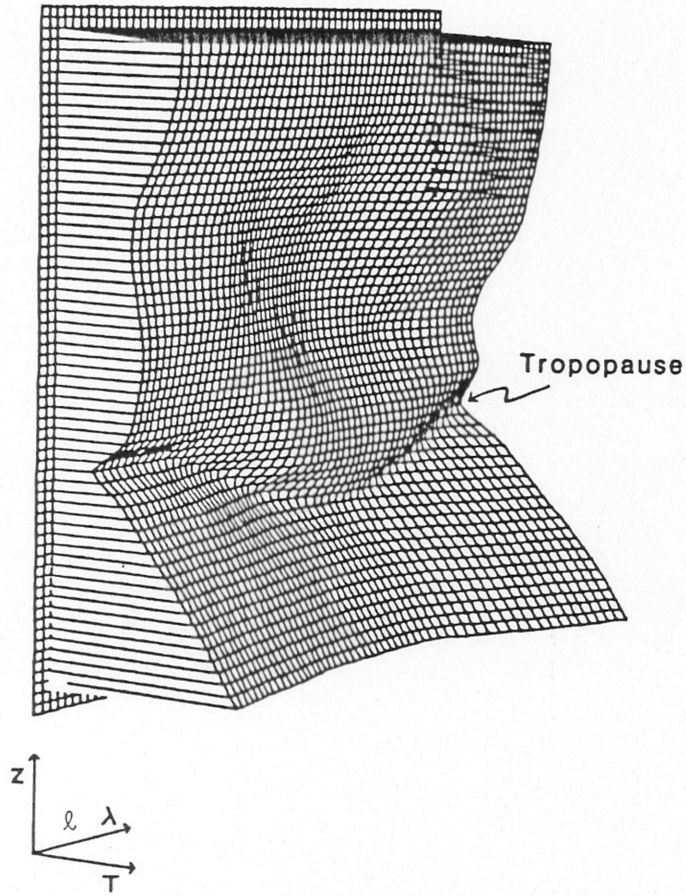

Figure 3.3 True (simulated) temperature, as a function of z and ℓ.

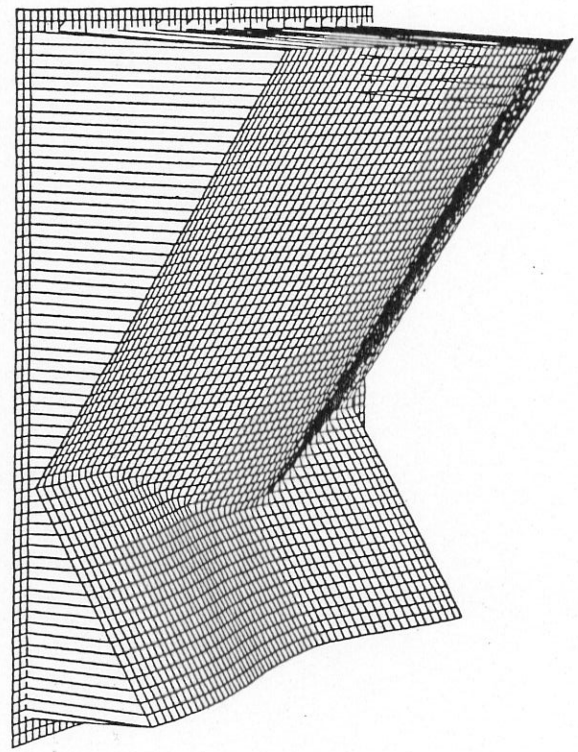

Figure 3.4 The tropopause break function $\gamma(z,\ell)$.

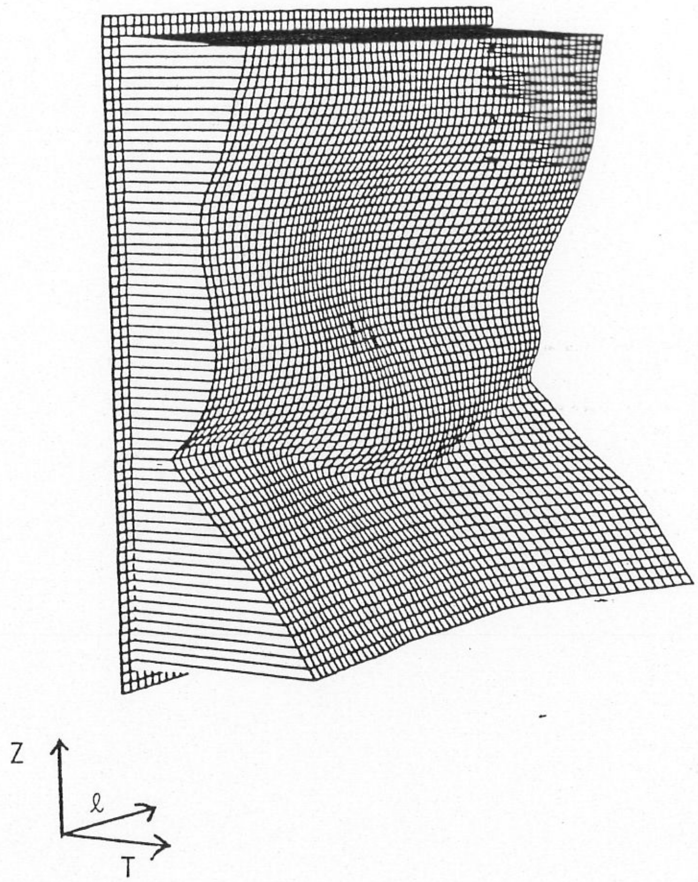

Figure 3.5 Analysis of the temperature data of Figure 3.1, with the use of $z^*(\ell)$, the tropopause height.

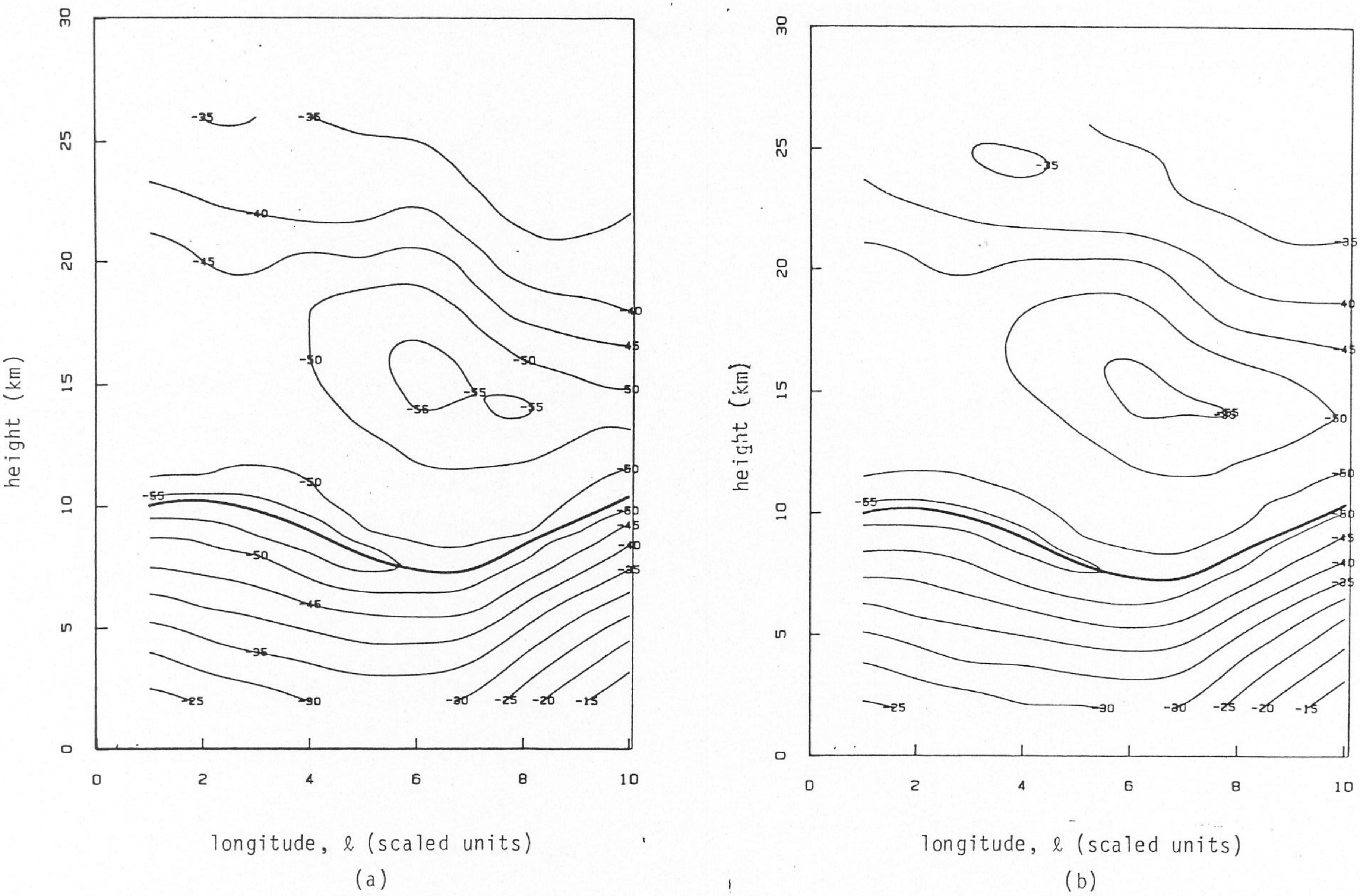

Figure 3.6. True (a) and estimated (b) temperature contour plots corresponding to Figures 3.3 and 3.5 .

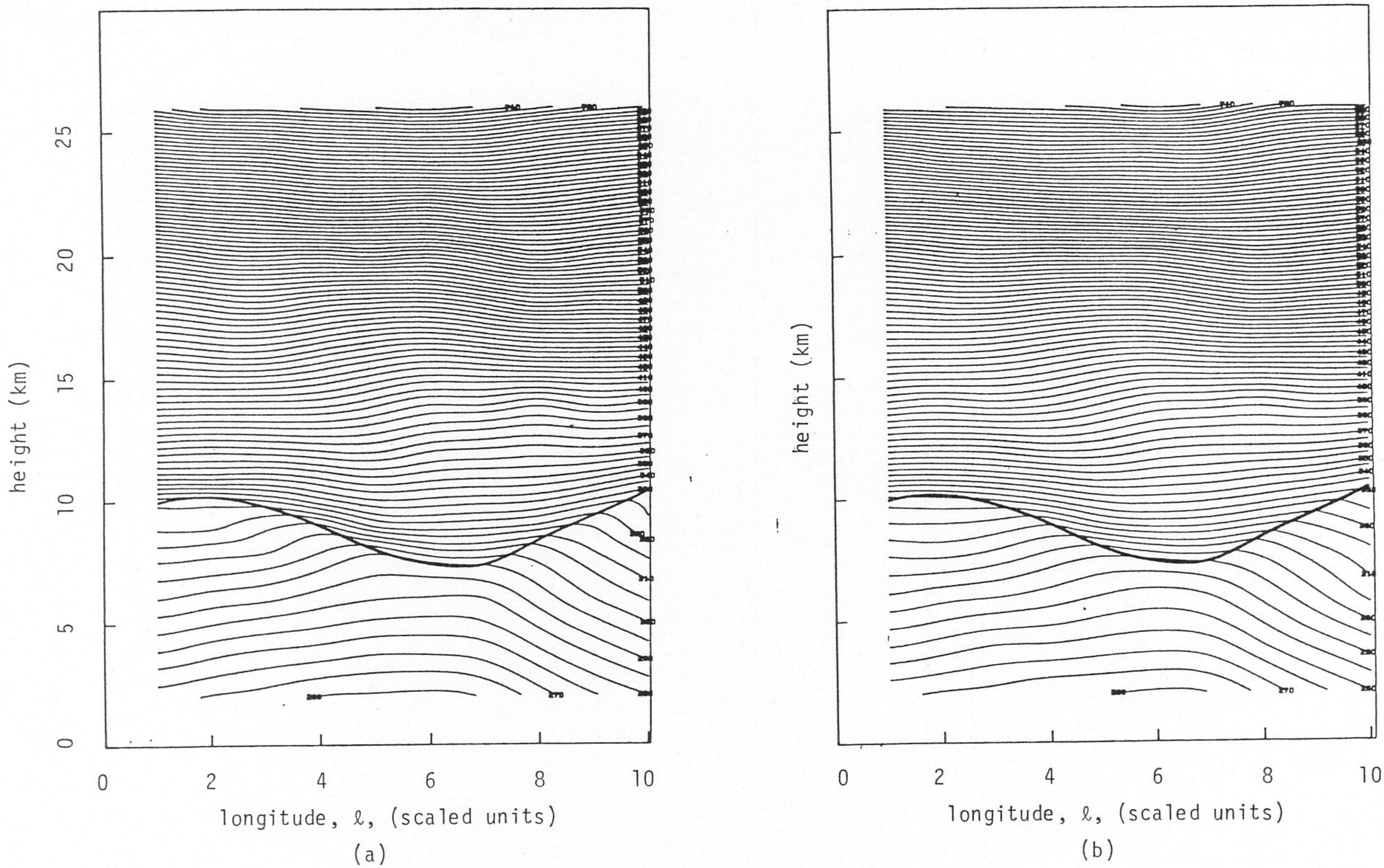

Figure 3.7. True (a) and estimated (b) potential temperature.