SOLVING OF THE INVERSE PROBLEM OF SENSING THE GASEOUS COMPOSITION OF THE ATMOSPHERE BASED ON DESCRIPTIVE SMOOTHING SPLINES

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Received October 1, 1990

A new approach to solving the problem on interpretation of the data of lidar sensing of the gaseous composition of the atmosphere has been considered. The approach is based on the use of the descriptive smoothing splines, which make it possible to take into account the a priori information on the function sought, assigned in the form of a system of inequalities for the values of the spline–approximated function or its derivatives. Results of both numerical modeling and processing of the real experimental data are given.

INTRODUCTION

Many approaches to the interpretation of the data of lidar sensing of the gaseous composition of the atmosphere are connected with smoothing and differentiation of the experimental data. By way of an example we can give the processing of the data that have been obtained either by the Raman scattering (RS) method or the fluorescence technique with the purpose of determining the profile of concentration of the gases over the slanted and horizontal paths. An extraction of the information about the profile of the gas concentration in the differential absorption method (DA) is performed by differentiation of the logarithm of the ratio of the signals that have been obtained inside and outside of the absorption line.[1,2]

One of the techniques of stable solution of the considered problems of interpretation is based on the use of the smoothing cubic splines.[3,4] However, in the case in which the data are strongly distorted by the measurement "noise" (for example, in processing of "weak" lidar returns which have been obtained from high altitudes and recorded in the photon counting mode) a suitable from the physical viewpoint solution of the problem cannot be always obtained (the negative values of the function sought have been arisen when it is to be nonnegative).

In this paper we propose a new approach to the solution of the interpretation problems which makes it possible to take into account the *a priori* information assigned in the form of a system of inequalities for the values of the approximated function or its derivatives.

DESCRIPTIVE SMOOTHING SPLINES

Let us assume that the investigated functional dependence $f(x)$ is represented by its values measured at the points n, namely,

$$\tilde{f}_1 = f(x_1) + \eta_1,\ 1 \le i \le n, \tag{1}$$

where η_1 is the measurement noise with zero mean and variance σ_2^1 and x_1 are the nodes of measurement in the order of increasing.

In order to provide stable calculation of $f(x)$ and its derivatives $f'(x)$ and $f''(x)$ from the-table $\{x_1, \tilde{f}_1\}$, the so–called smoothing splines are quite often used.[3,4] A polynomial of the third degree with a continuous second derivative on the interval (x_1, x_n) is such a cubic smoothing spline $S_{n,\alpha}(x)$ that on each interval $[x_1, x_{i+1}]$ admits the following representation:

$$S_{n,\alpha} = a_1 + b_1(x - x_1) + c_1(x - x_1)^2 + d_1(x - x_1)^3 . \tag{2}$$

In order to provide a uniqueness of the smoothing spline the corresponding boundary conditions,[3] which are determined by the values of $f(x)$ or its derivatives, are assigned at the points x_1 and x_n. If the variational approach is used, the spline $S_{n,\alpha}(x)$ is estimated from the condition of the minimum of the functional

$$F_\alpha(S,\tilde{f}) = \alpha \int_{x_1}^{x_n} (S''(x))^2\, dx + \sum p_1 \left(S(x_1) - \tilde{f}_1\right)^2 , \tag{3}$$

where α is the smoothing parameter, $p_1 > 0$ are the weighting factors, which finally leads to the certain algebraic relations from which the spline coefficients a_1, b_1, c_1, and d_1 are estimated.[3] By means of a selection of the optimal smoothing parameter we succeed in minimization of the rms error (RMSE) of smoothing[3]

$$\Delta^2(\alpha) = M\left[\sum_{i=1}^{n}\left(f(x_1) - S_{n,\alpha}(x)^2\right)\right].$$

where M[.] is the operator of mathematical expectation.

The so-called splines of the convex sets[5] are constructed based on the conditional minimization of the functional

$$F[S] = \int (S''(x))^2\, dx \tag{4}$$

subject to the limitations

$$\left|S(x_1) - \tilde{f}_1\right| \le \varepsilon_1,\ 1 \le i \le n, \qquad (5)$$

where ε_1 is the "half–width" of the confidence interval. The conditions of the uniqueness and existence of such splines have been analyzed in Ref. 5.

When interpreting the data of the remote sensing of the atmosphere, an "intermediate" situation arises, namely, it would be desirable to construct a spline adequately approximating the function $f(x)$ (in the sense of RMSE smoothing) and simultaneously satisfying the *a priori* limitations which originate from the physical concepts with regard to the problem. Such a spline is similar to the descriptive one and we shall consider its construction as a variational problem, namely, to minimize $F_\alpha[S, \tilde{f}\,]$ (see expression (3)) subject to the limitations

$$d_i^{\mathrm{L}} \le D^{l_i}\ S(x_i) \le d_i^{\mathrm{U}},\ i \in I_t$$

where D^{L_1} is the operator of differentiation of the l_ith order (l_i = 0, 1, 2); I_t is the set of indices $N_t \subseteq \{1, 2, \ldots, n\}$ (here N_t is the total number of limitations), d_i^L and d_i^U are the lower and upper limits of the value $D^{\mathrm{L}_1}\,S(x_1)$. We denote $S^*_{n,\alpha}(x)$ by the spline which is a solution of this problem.

The proposed definition of the descriptive spline differs from Eqs. (4) and (5) by two points. First, it permits one to take simultaneously into account the a priori information on the function $f(x)$ in different, forms (including its first and second derivatives as well as the limitations in the form of the equality $d_i^L = d_i^U$). Second, if the number of limitations is small or the limitations are of qualitative character (for example, $S'(x) \ge 0$), then such an *a priori* information happens to be insufficient for constructing an appropriate spline from the viewpoint of RMSE smoothing. When going over from Eq. (4) to the functional (3), we remove this difficulty with the appropriate choice of the smoothing parameter.

THE ALGORITHM FOR CONSTRUCTING THE DESCRIPTIVE SMOOTHING SPLINE

It is shown in the Appendix that functional (4) can be represented in the form of a quadratic form $S^{\mathrm{T}}Qs$. It then directly follows from Eq. (3) that:

$$F[\tilde{f}\,,\ S] = \alpha\ S^{\mathrm{T}}QS + (S - \tilde{f}\,)^{\mathrm{T}}\ P(S - \tilde{f}\,) \qquad (7)$$

where $P = \mathrm{diag}\{p_1, \ldots, p_n\}$ is the diagonal matrix, $s = |S_{n,\alpha}(x_1, \ldots, S_{n,\alpha}|^{\mathrm{T}}$ is the vector of spline values at the nodes x_1, and Q is the $n \times n$ matrix defined in the Appendix.

Let us consider first the unilateral limitations

$$D^{\mathrm{L}_1}\ S_{n,\alpha}(x_1) \le d_i,\ i \in I_t,$$

which, with account of Eq. A5, assumes the form

$$DS \le d,$$

where D is the $N_t \times n$ matrix. Taking into account Eq. (7), we arrive at the problem of quadratic programming

$$\min\left\{\frac{1}{2}\,S^{\mathrm{T}}U\alpha S + S^{\mathrm{T}}U + \mathrm{const}\right\} \qquad (8)$$

subject to the limitations

$$DS \le d^{\mathrm{U}} \qquad (9)$$

where D^{U} are the upper limitations.

Let us dwell on the existence and uniqueness of the solution S^*_α of problem (8) and (9). The existence of the solution is determined by the consistency of system of limitations (9), which is *a priori* assumed. Furthermore, for arbitrary $\alpha > 0$ the matrix U_α is positively defined, and the functional minimized is strictly convex. The valid non-empty set of vectors s, which satisfy Eq (9), is a convex set. Therefore, the formulated problem of conditional minimization has a unique solution S^*_α.[6]

In order to find S^*_α we use the technique proposed in Ref. 7. The problem, which is dual after Lagrange, consists in minimizing the functional

$$\psi(\mu) = \frac{1}{2}\mu^{\mathrm{T}} D U_\alpha^{-1} D^{\mathrm{T}}\mu + \mu^{\mathrm{T}}\left(D U_\alpha^{-1} U + d^{\mathrm{U}}\right)$$

subject to the limitation $\mu \ge 0$, where μ is the N_t – dimensional vector. After finding the solution μ of this problem, we calculate the vector S^*_α from the formula

$$S^*_\alpha = S_\alpha - U_\alpha^{-1}\ D^{\mathrm{T}}\mu^*, \qquad (10)$$

where S_α is the vector, which provides for an unconditional minimum of the functional (8). Thus, the algorithm for constructing the descriptive spline can be described by the following stages:

1. The smoothing parameter α is assigned and system of equations

$$\left(A + \alpha H P^{-1} H^{\mathrm{T}}\right) m_\alpha = H\,\tilde{f} \qquad (11)$$

is solved for the $(n - 2)$–dimensional vector m_α (the "natural" boundary conditions).

2. The vector

$$S_\alpha = \tilde{f} - \alpha P^{-1} H^{\mathrm{T}} m_\alpha \qquad (12)$$

is calculated.

It is shown in Appendix 2 that the spline S_α constructed according to formulas (11) and (12) coincides with the solution which provides unconditional minimum of Eq. (8). Scheme (11) and (12) is more efficient for the numerical estimate of the spline, since the matrix $HP^{-1}H^{\mathrm{T}}$ is incomplete (pentadiagonal), while the matrix U_α in Eq. (8) is entirely complete (see Appendix 1).

3. If limitations (9) are satisfied, it should be assumed that $S^*_\alpha = S_\alpha$ and the spline construction is finished.

4. If limitations (9) are not valid, the solution μ^* of the adjoint problem is constructed.

5. The vector S^*_α is calculated from Eq. (10).

6. The system $Am = HS^*_\alpha$ with (a tridiagonal matrix A is solved. The coefficients b_i, c_i, and d_i (Ref. 3) of the descriptive smoothing spline ($a_i = \{S_\alpha\}_i$) are estimated based on the determined vector m.

In the case of bilateral limitations (see the expression (A6)) the descriptive spline is constructed according to the same algorithm after we go over to the unilateral limitations

$\tilde{D}\,S \le \tilde{d}$,

where $\tilde{D} = |-D \vdots D|$ is the $2N_t \times n$ matrix and $\tilde{d} = |d^L \vdots d^U|^T$ is the $2N_t$ – dimensional vector.

Note that the value of the smoothing parameter α in the foregoing algorithm for construction of the descriptive spline has an appreciable effect on the approximation accuracy. It is possible to use several approaches in order to chose it.

Thus when choosing a the a priori information introduced can bo neglected, i.e., the vector S_α defined by Eqs. (11) and (12) can be used instead of S^*_α . At the same time, in order to find the optimal value α_{opt}, we use the algorithms constructed on the basis of the optimizing criterion and of the cross–significance technique.[3] It should be taken into account that an introduction of the *a priori* information has, as a rule, a "regularization" effect and, therefore, the determined value of α can be reduced by an order of magnitude. The numerical experiment performed has demonstrated the expedience of such a procedure, which makes it possible to improve the spline resolution. A choice of α based on the given accuracy characteristics of the spline is also possible.[8] We have used the optimal criterion in this paper. In an alternative approach to the determination of the smoothing parameter, α_{opt} is estimated by the same algorithms, into which, however, the vector S^*_α now enters, so that the steps 1–5 are repeated at each iteration of the selection algorithm for α, which essentially increases the expenditures of the computer time (by an order of magnitude and even more).

NUMERICAL EXPERIMENT

In order to investigate the algorithm for construction of the descriptive spline, which has been discussed above, extensive computational experiments were carried out. Let us represent the results of one experiment.

The function $f(x)$ in the interval [0, 6] was assigned by the expression

$$f(x) = \frac{1}{2}\exp\left\{-\frac{(x-20)^2}{500}\right\} + 5\exp\left\{-\frac{(x-4)^2}{0.5}\right\}. \qquad (13)$$

The plots of $f(x)$ and $f'(x)$ are given in Figs. 1 and 2. Note that such a function is "difficult" for the investigated smoothing problem, since it contains sections with essentially distinct values of the first derivative. The values of $f(x)$ were determined at the points $x_1 = 6(I - 1)/(n - 1)$, where $n = 40$, and subsequently distorted by an additive noise with variance $\sigma_i^2 = \text{const} = \delta[f(x_i)]_{max}/2$, where δ is the noise level, $[f(x_1)]_{max}$ is the maximum values of the function in the interval [0, 6]. The splines $S^*_\alpha(x)$ and $S_\alpha(x)$ were constructed based on the values of $\tilde{f}_i$, $1 \le I \le n$. The descriptive spline was subject to the limitations: $S(x) \ge 0$; $x \in [0, 6]$; $S'(x) \ge 0$; $x \in [0, 3.5]$; $S'(x = 3.50) \ge 5.7$; $S'(x = 4.5) \le -5.7$; $S''(x) \ge 0$; $x \in [0, 3.5]$; $x \in [4.5, 6]$. The splines were constructed using the following values of α:
$\alpha_1 = \alpha_{opt}$ and $\alpha_2 = 0.1\ \alpha_{opt}$.

The results of modeling of smoothing the function $f(x)$ are given in Fig. 1 and those of its derivative $f(x)$ are plotted in Fig. 2, the noise level being assigned equal to 10%. It can be seen from Figs. 1 and 2 that the spline S^*_α is more accurate in approximating $f(x)$ and its derivative $f'(x)$ for $\alpha = \alpha_2$ and, which is rather important, S^*_α satisfies the "physical concepts" on the function $f(x)$ approximated and its derivative $f'(x)$. It is pertinent to note that this large body of an a priori information about the function $f(x)$ and its derivatives is frequently inaccessible for an experimenter (especially the information abort the second derivative), so we give our results only in order to demonstrate the possibilities of the algorithm.

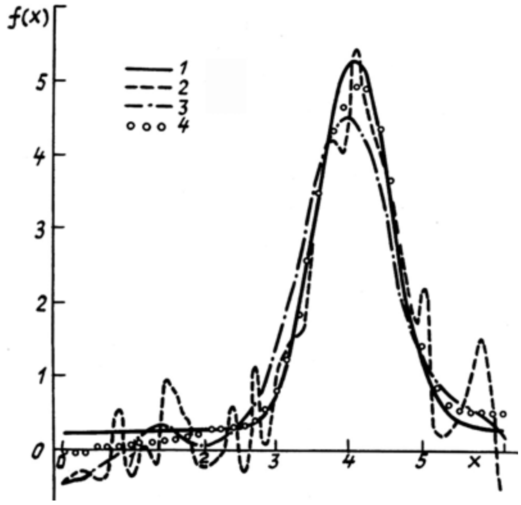

FIG. 1. Spline approximation of the function f(x): the exact curve f(x) (see Eq. (13)) (1), the "noisy" curve with the noise level δ = 10% (2), the spline S_α constructed for $\alpha_1 = \alpha_{opt}$ (3), and the descriptive spline S^*_α constructed for $\alpha_2 = 0.1\ \alpha_{opt}$ (4).

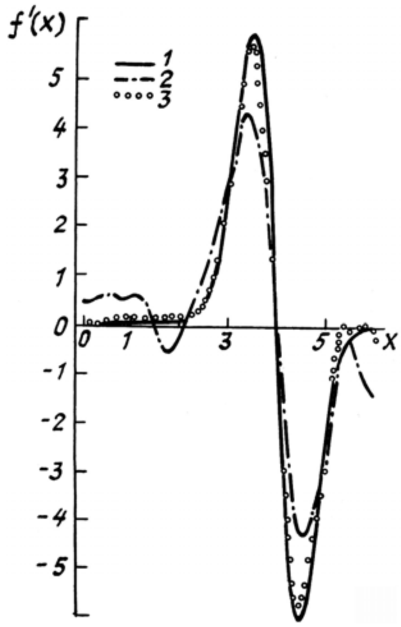

FIG. 2. Spline approximation of the first derivative $f'(x)$: the exact curve $f'(x)$ (see Eq. (13)) (1), the curve $S'_\alpha(x)$ for $\alpha_1 = \alpha_{opt}$ (2), and the curve $[S^*_\alpha(x)]'$ for $\alpha_2 = 0.1\ \alpha_{opt}$ (3).

PROCESSING OF THE DATA OF THE FIELD EXPERIMENT

By way of an example, we present the results of processing of the data of lidar sensing of ozone, which have been obtained at the Institute of Atmospheric Optics.[9] As a consequence of a considerable separation of the spectral channels (λ_1 = 398 nm and λ_2 = 532 nm), the primary processing of the signals was performed according to a procedure based on the spectral dependence of the aerosol extinction coefficient of the form $\alpha_a \sim \lambda^{-4}$ (see Ref. 10), where λ is the wavelength. The absorption coefficient of ozone will be then writ ten as follows:

$$\tilde{\alpha}_{O_3}(x) = -\frac{1}{2}\frac{d}{dx}\ln\left[\frac{(N(x)-N_{BG})x^2}{0.2\beta_m(x)(4+R(x)T^2(x)}\right], \quad (14)$$

where $N(x)$ is the lidar return at a wavelength of 308 nm, which has been obtained from the sensing range x, N_{BC} is the background signal, $R(x)$ is the scattering ratio measured at a wavelength of 532 nm, β_M is the molecular backscattering coefficient (it is taken from the model), and T^2(x) is the squared atmospheric transparency associated with the total extinction due to the molecular scattering and aerosol extinction of light:

$$T^2(x) = \exp\left\{-2\cdot 1.67\int_0^x \beta_M(x')(4R(x')+1)dx'\right\}. \quad (15)$$

The error of the starting data was calculated according to the following formula:

$$\sigma_\alpha^2(x) = \frac{1}{4}\left\{\frac{N(x)+N_{BG}}{(N(x)-N_{BG})^2} + \frac{\sigma_R^2(x)}{(4+R(x))^2}\right\}. \quad (16)$$

Here $\sigma_R^2 = \sigma_R^2 \cdot R^2(x)$ is the error variance in the scattering ratio. The value of δ_R, in accordance with the data of Ref. 11, was assigned equal to 7%.

The lidar returns, which were recorded at different dates (January–March, 1989), were used for the processing. The profiles of the molecular absorption coefficient of ozone α_{O_3} which have been obtained on January 4 and 6, February 22 and 28 (Fig. 3*a*), and March 3, 1989 (Fig. 3*b*) reconstructed from the lidar data are plotted in Fig. 3. It is easy to convert from α_{O_3} into the concentration of ozone, if the ozone absorption cross–section at a wavelength 308 nm is known. The profiles of α_{O_3} in Fig. 3*a* have been obtained with the help of the smoothing splines from the solution of unconditional problem (7) and those in Fig. 3*b* — using the descriptive splines. It can be seen, at least qualitatively, that the profiles of α_{O_3} do not contradict the physical concepts about the altitude distribution of ozone. In order to interprete quantitatively the lidar returns with any degree of confidence, it is necessary to make a comparison with the results of an independent experiment carried out synchronously with the lidar sensing (e.g., a comparison with the data of an ozone meter).

In conclusion, let us note that the algorithm for construction of the descriptive smoothing splines can be successfully used for processing of the data of lidar sensing of the atmosphere.

The authors are grateful to V.N. Marichev and A.V. Yel'nikov for kindly providing experimental data of lidar sensing of the ozone layer of the atmosphere.

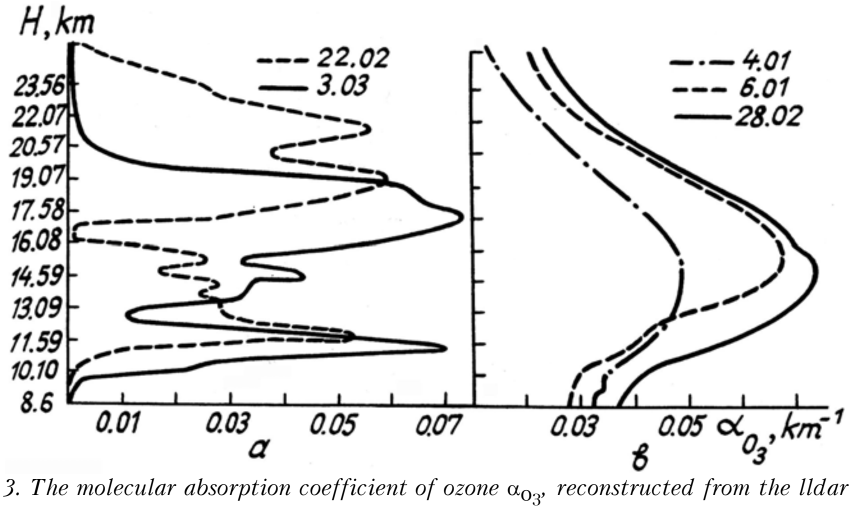

FIG. 3. The molecular absorption coefficient of ozone α_{O_3}, reconstructed from the lldar data.

APPENDIX 1

Let us introduce a vector of the second derivatives

$$m = |\ S''_{n,\alpha}(x_1),\ S''_{n,\alpha}(x_2),\ \ldots,\ S''_{n,\alpha}(x_n)|^T,$$

which is related to a vector of the spline values

$$S = |\ S_{n,\alpha}(x_1),\ S_{n,\alpha}(x_2),\ \ldots,\ S_{n,\alpha}(x_n),|^T,$$

by the matrix expression[3]

$$Am = Hs \quad (A1)$$

The elements of tridiagonal matrices A and H are determined by the accepted boundary conditions.[3] Here, we restrict ourselves by writing down the expressions for the elements of the matrices A and H with the "natural" boundary conditions

$$S''_{n,\alpha}(x_1) = S''_{n,\alpha}(x_n) = 0.$$

The vector m then has the form

$m = | S''_{n,\alpha}(x_2), \ldots, S''_{n,\alpha}(x_{n-1}), |^T$

and the elements of the $(n-2)\times(n-2)$ matrix A are determined as

$A_{i,i} = (h_i + h_{i+1})/3,\ 1 \le i \le n-2;$

$A_{i,i+1} = A_{i+1,I} = h_{i+1}/6,\ 1 \le i \le n-3;$

where

$h_i = x_{i+1} - x_i > 0,\ 1 \le i \le n-1.$

The $(n-2)\times n$ matrix H has the elements

$H_{i,i} = 1/h_i;\ H_{i,i+1} = -(1/h_1 + 1/h_{i+1});$

$H_{i,i+2} = 1/h_{i+1};\ 1 \le i \le n-2.$

If the boundary conditions are different, we shall have the $(n \times n)$ matrices A and H that differ by the first and last row. Using the vector m, the functional (4) assumes the form

$$F(S) = \int_{x_1}^{x_n} (S''(x))^2 dx = m^T Am. \quad \text{(A2)}$$

It then follows immediately from Eqs. (Al) and (A2) that

$$F(S) = S^T H^T A^{-1} Hs = s^T Qs, \quad \text{(A3)}$$

where Q is the $n \times n$ matrix,

$$Q = H^T A^{-1} H. \quad \text{(A4)}$$

Let us consider the relations between the spline coefficients a_i, b_i, c_i. and d_i of Eq. (2) and the vector s. It can be shown that the vectors a, b, and c composed from the coefficients a_i, b_i, and c_i are related to the following matrix expressions:

$a = D_0 s,\ b = D_1 s,\ c = D_2 s,$

where D_0 is the unitary matrix and D_1 and D_2 are the $n \times n$ and $(n-2)\times n$ matrices:

$$D_1 = L + TA^{-1}H,\ D_2 = \frac{1}{2}A^{-1}H.$$

Here L is the matrix of the size $(n \times n)$ with the elements

$L_{i,i} = -1/h_i;\ L_{i,i+1} = 1/h_i,\ 1 \le i \le n-1,$

$L_{n,n-1} = 1/h_{n-1},\ L_{n,n} = 1/h_{n-1},$

T is the $n \times (n-2)$ matrix with the elements

$T_{i,i} = -h_i/6,\ T_{i+1,i} = -h_{i+1}/3,\ 1 \le i \le n-2,$

$T_{n,n-2} = -h_{n-1}/6.$

With an account of the notations used, the l_1 th derivative of limitations (6) assumes the form

$$D^{l_i} S_{n,\alpha}(x_i) = \begin{cases} D^{0,1}s, & l_1 = 0 \\ D^{1,1}s, & l_1 = 1 \\ D^{2,1}s, & l_1 = 2 \end{cases} \quad \text{(A5)}$$

where $D^{l}{}_i$ denotes the ith row of the corresponding matrix D^l, $l = 0, 1, 2$. Taking into consideration Eq. (A4), system of limitations (6) can be represented in the form of the matrix inequality

$$d^L \le Ds \le d^U, \quad \text{(A6)}$$

in which the $N_t \times n$ matrix D is composed of the elements of the rows $D^{l}{}_i$, $1 \le i \le N_t$.

APPENDIX 2

The spline s_α, which has been obtained from Eqs. (11) and (12), can be represented, on the one hand, as

$$S_\alpha = \tilde{f} - \alpha P^{-1}H^T m_\alpha = \tilde{f} - \alpha P^{-1}H^T(A + \alpha HP^{-1}H^T)^{-1}H\tilde{f} = R\tilde{f},$$

where

$$R = I - \alpha P^{-1}H^T(A + \alpha HP^{-1}H^T)^{-1}H. \quad \text{(A7)}$$

On the other hand, the solution $\tilde{S}_\alpha$ which provides the unconditional minimum of Eq. (8), has the form

$$\tilde{S}_\alpha = (\alpha Q + P)^{-1} P\tilde{f}$$

or with an account of Eq. (A4)

$$\tilde{S}_\alpha = (\alpha H^T A^{-1} H + P)^{-1} P\tilde{f} = \tilde{R}\tilde{f}, \quad \text{(A8)}$$

where

$$\tilde{R} = (\alpha H^T A^{-1} H + P)^{-1} P$$

It can be shown that the matrices R and $\tilde{R}$ are identical and, consequently, the spline $S_\alpha = \tilde{S}_\alpha$.

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