Summary. In this paper we generalize the results of [4] and modify the algorithm presented there to obtain a better rate of convergence.

In the space of real valued functions with absolutely continuous \((m-1)\)-st derivative and square integrable \(m\)-th derivative define the two functionals

\[
J(f) = \int_{-\infty}^{\infty} (D^m f)^2 \, dx,
\]

\[
E(f) = \sum_{i=1}^{n} \left( \frac{y_i - f(x_i)}{\delta y_i} \right)^2
\]

with \(\delta y_i (i = 1, \ldots, n)\) given positive numbers. In 1964 Schoenberg [5] introduced the following two problems:

(A) minimize \(J(f) + \phi E(f)\), \(0 \leq \phi < \infty\) (given),

(B) minimize \(J(f)\) subject to the constraint \(E(f) \leq S\), \(0 \leq S < \infty\) (given).

\(\phi \to \infty\) or \(S = 0\) yields \(E(f) = 0\), i.e., the interpolation problem \(f(x_i) = y_i (i = 1, \ldots, n)\) with a natural spline function of degree \(2m-1\) as solution. For other values of \(\phi\) resp. \(S\), we may interpret the objectives as a compromise between the smoothing and the closeness of fit to the prescribed values, the parameter \(\phi\) or \(S\) allowing one to control the extent of smoothing. Here, too, the solutions to both problems are spline functions; in fact, for (A) Schoenberg states the following result.

Theorem 1. For \(m \leq n\) there exists a unique solution \(s_p(x)\) to (A). It is a natural spline of degree \(2m-1\) with knots \(x_1, \ldots, x_n\).

Anselone and Laurent [1] have generalized the problem (A) in the following way: Let \(X\) and \(Y\) be two real Hilbert spaces. Let \(T\) be a continuous linear operator on \(X\) into \(Y\), and let \(N\) denote the nullspace of \(T\), \(m\) its dimension. Let \(n\) bounded linear functionals in \(X\) be given which according to the Riesz Representation Theorem may be represented by innerproducts with \(n\) elements \(k_1, \ldots, k_n\) of \(X\); \(K^\perp\) denote the orthogonal complement of the span of \(\{k_1, \ldots, k_n\}\). The generalization of the two functionals (1), (2) for all \(f \in X\) is

\[
J(f) = (Tf, Tf)_Y,
\]

\[
E(f) = \sum_{i=1}^{n} \left( \frac{y_i - (k_i, f)X}{\delta y_i} \right)^2.
\]

Then, Anselone and Laurent prove the following two theorems.
Theorem 2. If \( N \cap K = \{ \theta \} \) and if the range of \( T \) is closed, then there exists a unique element \( s_p \in X \) minimizing \( J(f) + \rho E(f) \) among all \( f \in X \).

Theorem 3. Under the same assumptions there exist \( n - m \) linearly independent elements \( M_1, \ldots, M_{n-m} \) of \( Y \) such that for all \( f \in X \) \( (M_i, Tf)_Y \) can be expressed as a linear combination of the \( (k_j, f)_X \), say

\[
(M_i, Tf)_Y = \sum_{j=1}^{n} q_{i,j} (k_j, f)_X \quad (i = 1, \ldots, n - m).
\]

For any such set, \( T s_p \) has a representation

\[
T s_p = \sum_{i=1}^{n-m} c_i M_i,
\]

and the coefficients \( c_i \) together with the values of the functionals for \( s_p \),

\[
(a_j = (k_j, s_p)_X \quad (j = 1, \ldots, n),
\]

uniquely determine \( s_p \). They are obtained from the linear system with positive definite coefficient matrix

\[
\begin{align*}
(W + \frac{1}{\rho} Q^T D^2 Q) c &= Q^T y, \\
(a &= y - \frac{1}{\rho} D^2 Q c,
\end{align*}
\]

with \( w_{i,j} = (M_i, M_j)_Y \) and \( D = \text{diag}(\delta y_1, \ldots, \delta y_n) \).

In the special case considered by Schoenberg, \( T = D^m \) and \( (k_i, f)_X = f(x_i) \), the \( M_i \) are the minimum-support-splines [2, 6] of degree \( m - 1 \), and the \( q_{i,j} \) are the coefficients of the \( m \)-th order divided differences based on \( y_1, \ldots, y_{i+m} \). Then, \( W \) and \( Q^T D^2 Q \) are band matrices of width \( 2m - 1 \) and \( 2m + 1 \) respectively. For the most important case, \( m = 2 \), the algorithm was given in [4].

The numerical treatment of (5), (6) may cause trouble if

(i) the \( k_i \) are linearly dependent (meaningful!) or almost dependent,

(ii) some of the \( \delta y_i \) are very large compared with the remaining ones.

One has to concede that the Problem (A) has no immediate practical importance. The reason is that one usually wants to specify the amount of smoothing very carefully while one has here to prescribe a technical parameter, viz. \( \rho \), having no direct significance. In contrast to this, the parameter \( S \) of Problem (B) has that direct meaning. Schoenberg has pointed out that there is a strong relation between the two problems. Indeed, for the interesting functionals we have

\[
\begin{align*}
J(s_p) &= e^T W c = \rho^2 y^T Q (\rho W + Q^T D^2 Q)^{-1} W (\rho W + Q^T D^2 Q)^{-1} Q^T y, \\
E(s_p) &= (y - a)^T D^{-2} (y - a) = \| D Q (\rho W + Q^T D^2 Q)^{-1} Q^T y \|^2_2.
\end{align*}
\]

Obviously, both are rational functions of \( \rho \), the former increasing from zero to an asymptotic value, the latter strictly decreasing from \( E(s_0)^* \) to zero. Hence,

\[
* s_0 = \lim_{\rho \to 0} s_\rho \text{ is the element from } N \text{ minimizing } E(f).
\]
if $0 \leq S \leq E(s_0)$, there exists exactly one $\rho$ such that $E(s_\rho) = S$, or using (8)

$$F(\rho) = \|DQ(\rho W + Q^TD^2Q)^{-1}Q^T y\|^2 = S^2. \tag{9}$$

This equation defines $\rho = \rho(S)$ on $[0, E(s_0)]$.

In [5] Schoenberg states that the $s_\rho$ corresponding to $\rho(S)$ is also the solution to Problem (B). In fact, we have

**Theorem 4.** If the conditions of Theorem 2 are satisfied then there exists for all non-negative values of $S$ an element $s_\rho \in X$ minimizing $J(f)$ among all $f \in X$ under the constraint $E(f) \leq S$. Equality holds here if $0 \leq S \leq E(s_0)$. Then, $s_\rho$ is uniquely determined and agrees with $s_\rho$, the solution to Problem (A) with $\rho(S)$ defined by (9).

**Proof.** If $S > E(s_0)$, any element from $N$ is a solution to Problem (B). Otherwise, define $\tilde{\rho}$ by (9) with corresponding $s_\rho$ and assume $\tilde{s}_\rho = s_\rho$. This would require

$$J(\tilde{s}_\rho) \leq J(s_\rho) \quad \text{and} \quad E(\tilde{s}_\rho) \leq S = E(s_\rho),$$

hence

$$J(\tilde{s}_\rho) + \rho E(\tilde{s}_\rho) \leq J(s_\rho) + \rho E(s_\rho)$$

which is clearly a contradiction to the fact that $s_\rho$ is the unique solution to Problem (A). Q.E.D.

Hence, Problem (B) is reduced to the much simpler Problem (A) if there is a reasonable algorithm to determine $\rho$ such that (9) holds for given $S$. In [4] a Newton iteration was used to solve

$$F(\rho) = S^2$$

since the required derivative $dF/d\rho$ can be evaluated with very little extra costs. When starting with $\rho^{(0)} = 0$, this iteration produces a strictly increasing sequence $\rho^{(r)}$, $r = 1, 2, \ldots$, converging to the correct value of $\rho$, for $F(\rho)$ is convex and strictly decreasing. This can easily be seen from the fact that it has a representation

$$F(\rho)^2 = \sum_{i=1}^{n-m} \left(\frac{z_i}{\lambda_i + \rho}\right)^2 \tag{10}$$

where the $\lambda_i$ are the eigenvalues of $Q^TDQ = \lambda Wv$. They are positive so that each term in the right-hand member of (10) is convex and decreasing, and the same holds then for $F(\rho)$ since the Euclidean norm is monotonic.

Unfortunately, the method is too slow to be always applicable. $F(1/\rho)$ is frequently (but not necessarily) a concave function of $\rho$ in the interesting interval, and the Newton process with this function gave a reduced number of iterations for the examples which were tried. However, there is no guarantee of global convergence and the resulting smoothing may be larger than specified by the given quantity $S$.

Convergence in the large and a reduced number of iterations is achieved using $1/F(\rho)$ in a Newton iteration to solve

$$1/F(\rho) = S^{-\frac{1}{2}}.$$

Equivalently, the process may be described as a modified Newton iteration on $F(\rho)$ where the tangent line is replaced by the tangent hyperbola which obviously
approximates $F(p)$ much better. The corresponding correction of an approximate root $p$ is given by

$$
\Delta p = \frac{F(p)^{-1} - S^{-1}}{F'(p) F(p)^{-2}} = \frac{F(p) \cdot S^4 - F(p)}{S^4 F'(p)}
$$
or $F/S^4$ times larger than for the original method. In particular, the slow convergence of the latter for small values of $S$ is removed. It remains to show that \(1/F(p)\) is concave, i.e., that

$$
\frac{1}{F(q)} \leq \frac{1}{F(p)} - (q - p) \frac{F'(p)}{F(p)^2} \quad (p, q \geq 0),
$$
(the right-hand side is the tangent line of $1/F(q)$ at the point $p$). Inserting the representation (10) in the above inequality we obtain

$$
\left(\frac{\mu_0}{\mu_2}\right)^{1/4} \leq \mu_{-1}/\mu_0
$$

where

$$
\mu_k = \sum_{i=1}^{n-m} \left(\frac{z_i}{\lambda_i + p}\right)^2 \left(\frac{\lambda_i + p}{\lambda_i + q}\right)^k
$$

are the $k$-th order moments of the positive quantities $(\lambda_i + p)/(\lambda_i + q)$. Thus, our assertion reduces to the well known mean value inequality (see, e.g., Thm. 16 in [3]).

Note that there is only one modification in the algorithm as outlined in [4]: the Newton correction for $p$, $(e - (Se)^i)/(f - p g)$, in step (iii) is enlarged by a factor $(e/S)^i > 1$. The matrices $W$ and $Q$, of course, depend on the choice of the operator $T$ and the functionals $k_i$, and the same holds for the integration of (4) with the multi-point boundary conditions (4').

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References

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