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CUBIC SPLINES WITH MINIMAL NORM*

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Abstract. Natural cubic interpolatory splines are known to have a minimal L_2-norm of its second derivative on the C^2 (or W_2^2) class of interpolants. We consider cubic splines which minimize some other norms (or functionals) on the class of interpolatory cubic splines only. The cases of classical cubic splines with defect one (interpolation of function values) and of Hermite C^1 splines (interpolation of function values and first derivatives) with spline knots different from the points of interpolation are discussed.

Keywords: cubic interpolatory spline, minimal norm interpolation

MSC 2000: 41A15, 65D05, 65D07

1. Introduction

Let us be given an increasing spline knotset x_i, $i = 0(1)n+1$ on the real axis with prescribed values s_i, $i = 0(1)n+1$ at the knots x_i. The cubic splines $s(x) = s_{31}(x) \in C^2$ interpolating the prescribed function values have two free parameters which can be used for some boundary condition prescribed or to optimization purposes. The natural cubic interpolatory spline (with BC $s''(x_0) = s''(x_{n+1}) = 0$) is known to minimize the L_2-norm of the second derivative on the class of interpolants from $C^2(W_2^2)$ (see [2], [5]). We can search for cubic splines minimizing some other norms of the spline or of the vector of the corresponding derivative values at knots (or another functional which can give a measure of some geometric or physical properties of the process described by the data given). When at a knot x_i we are given the function value $s_i = s(x_i)$ and the value $m_i = s'(x_i)$ of the first derivative, then the Hermite local cubic interpolatory spline $s_{32}(s) \in C^1$ is determined uniquely. To obtain

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some free parameters, let us prescribe such data at some *points of interpolation* t_i, $i = 0(1)n$; $x_i < t_i < x_{i+1}$; $g_i = s_{31}(t_i)$, $p_i = s'_{31}(t_i)$. We obtain again some free parameters which can be used for minimization purposes. There is an open question of the optimal position of knots with respect to the data given.

We will consider the cases of minimized functionals (spline norms squared)

$$J_k(s) = \int_{x_0}^{x_{n+1}} [s^{(k)}(x)]^2 \, \mathrm{d}x, \quad k = 0, 1, 2, 3$$

or the corresponding discrete analogs

$$J_{kd}(s) = \sum_{i=0}^{n+1} w_i [s^{(k)}(x_i)]^2, \quad k = 0, 1, 2.$$

In the simplest cases (J_{kd} with $w_i = 1$) we can obtain the optimal parameters using the pseudoinverse solution of the system of continuity conditions (see [1]). The cases when the functional $J_{kd}(s)$ can be expressed as a scalar product with a symmetric positive definite (SPD) matrix can be treated with a special least-squares (LSQ) technique (see [6]). More generally, we can use the quadratic programming techniques (equality constrains are given by the spline continuity conditions)—see e.g. [4].

2. Classical cubic spline

2.1. Local representation with the second derivative.

With the prescribed knotset and function values given $[\{x_i, s_i\},\ i = 0(1)n+1]$ let us denote $h_i = x_{i+1} - x_i$, $u = (x - x_i)/h_i$, $M_i = s''_{31}(x_i)$. Then the local representation of the spline $s_{31}(x) = s(x)$ in the interval $[x_i, x_{i+1}]$ can be written as

$$\begin{aligned} s(x) = s(x_i + uh_i) = (1-u)s_i + us_{i+1} - \tfrac{1}{6}h_i^2 u(1-u) \\ \times [(2-u)M_i + (1+u)M_{i+1}]. \end{aligned} \tag{1}$$

The *spline continuity conditions* (CC) which guarantee C^2-smoothness can be written for this local representation as the recurrence (see e.g. [5])

$$\begin{aligned} h_{i-1}M_{i-1} + 2(h_{i-1} + h_i)M_i + h_i M_{i+1} = 6(h_{i-1} + h_i)[x_{i-1}, x_i, x_{i+1}]s, \\ i = 1(1)n. \end{aligned} \tag{2}$$

The $(n, n+2)$-matrix on the left-hand side of CC has the full row rank. The unknown local parameters M_i of the unique cubic spline which minimizes the functional

$J_{2d}(s) = \|\mathbf{M}\|_2^2 = \sum\limits_{i=0}^{n+1} M_i^2$ can be simply computed as the unique solution with minimal norm of the underdetermined system (2) using the pseudoinverse matrix (see [1]).

For the functionals $J_k(s)$ mentioned above we can obtain the expressions

$$
\begin{aligned}
(3) \qquad J_0(s) = {} & \frac{1}{7560} \sum_{i=0}^{n} h_i [2520(s_i^2 + s_i s_{i+1} + s_{i+1}^2) \\
& + h_i^4 (16M_i^2 + 31 M_i M_{i+1} + 16 M_{i+1}^2)] \\
& - \frac{1}{7560} \sum_{i=0}^{n} h_i^3 [336(s_i M_i + s_{i+1} M_{i+1}) + 294(s_i M_{i+1} + s_{i+1} M_i)],
\end{aligned}
$$

$$
(4) \qquad J_1(s) = \sum_{i=0}^{n} \frac{1}{h_i} \Big[(s_i - s_{i+1})^2 + \frac{h_i^4}{180} (4M_i^2 + 7 M_i M_{i+1} + 4 M_{i+1}^2) \Big],
$$

$$
(5) \qquad J_2(s) = \frac{1}{3} \sum_{i=0}^{n} h_i (M_i^2 + M_i M_{i+1} + M_{i+1}^2) = \frac{1}{6} \mathbf{M^T R_2 M},
$$

$$
(6) \qquad J_3(s) = \sum_{i=0}^{n} \frac{1}{h_i} (M_{i+1} - M_i)^2 = \mathbf{M^T R_3 M}.
$$

The existence of optimal solutions we search for follows from the nonnegativity of the functionals J_k, J_{kd}. The matrices of the quadratic forms $J_0(s)$, $J_1(s)$, $J_2(s)$ (with respect to the unknown parameters M_i) can be written as symmetric positive definite (SPD) matrices, the matrix $\mathbf{R_3}$ in $J_3(s)$ is singular. We can use the LSQ approach (see [6], [3]) to the CC as recurrences (difference equations) for computing the optimal values of parameters M_i. More generally we can use algorithms of quadratic programming with equality constrains. The positive definiteness of the matrix of the quadratic form causes then the uniqueness of the minimizer. We can see that in the "continuous" case of $J_3(s)$ the solution exists, but need not be unique (there is no discrete analog). In the case of an equidistant spline knotset we can prove the uniqueness of the minima of $J_3(s)$—when we denote by $\mathbf{Z}$ the matrix of the nullspace of the system of CC conditions (2), then the $(2,2)$-matrix $\mathbf{Z^T R_3 Z}$ is SPD (the result should be valid also for slightly nonequidistant knotsets).

To discuss the discrete variant with $J_{1d}(s)$, we have to use another local representation. The results obtained till now will be stated in a theorem in the next subsection.

2.2. Local representation with the first derivative.

We can use the unknown values of $s'(x_i) = m_i$ as local parameters in the cubic spline representation ($u = (x - x_i)/h_i$)

$$s(x) = (1-u)^2(1+2u)s_i + u^2(3-2u)s_{i+1} + h_i u(1-u)[(1-u)m_i - u m_{i+1}]. \tag{7}$$

The *continuity conditions* can be now written as recurrences (see [7], [5])

$$a_i m_{i-1} + 2m_i + c_i m_{i+1} = f_i, \quad i = 1(1)n \tag{8}$$

with coefficients

$$a_i = \frac{h_i}{h_{i-1} + h_i}; \quad c_i = 1 - a_i; \quad f_i = 3\Big[c_i \frac{s_{i+1} - s_i}{h_i} + a_i \frac{s_i - s_{i-1}}{h_{i-1}}\Big]. \tag{9}$$

The matrix of CC has the full rank and so we can compute the local parameters m_i of the unique spline with minimal l_2-norm of the vector $\mathbf{m}$ using the pseudoinverse approach to the system (8).

We can compute again the expressions for functionals $J_k(s)$ and obtaining

$$\begin{aligned} J_0(s) = \frac{1}{210} \sum_{i=0}^{n} h_i [&h_i^2(2m_i^2 - 3m_i m_{i+1} + 2m_{i+1}^2) \\ &+ h_i(22s_i + 13s_{i+1})m_i - h_i(13s_i + 22s_{i+1})m_{i+1} \\ &+ 78s_i^2 + 54s_i s_{i+1} + 78s_{i+1}^2], \end{aligned} \tag{10}$$

$$\begin{aligned} J_1(s) = \sum_{i=0}^{n} \Big[&\frac{h_i}{15}(2m_i^2 - m_i m_{i+1} + 2m_{i+1}^2) \\ &+ \frac{1}{5}(s_i - s_{i+1})(m_i + m_{i+1}) + \frac{6}{5h_i}(s_i - s_{i+1})^2\Big], \end{aligned} \tag{11}$$

$$\begin{aligned} J_2(s) = 4\Big[&\sum_{i=0}^{n} \frac{1}{h_i}(m_i^2 + m_i m_{i+1} + m_{i+1}^2) \\ &+ \sum_{i=0}^{n} \frac{3}{h_i^2}(m_i + m_{i+1})(s_i - s_{i+1}) + \sum_{i=0}^{n} \frac{3}{h_i^3}(s_i - s_{i+1})^2\Big], \end{aligned} \tag{12}$$

$$J_3(s) = 36 \sum_{i=0}^{n} \frac{1}{h_i^5}[2(s_i - s_{i+1}) + h_i(m_i + m_{i+1})]^2. \tag{13}$$

We can see again the positive definiteness of matrices of quadratic parts in the functionals $J_k(s)$, $k = 0, 1, 2$, which ensures the uniqueness of the minima. For the functional $J_3(s)$ we have again positiveness only—but on the equidistant knotset we can prove uniqueness similarly as in the foregoing case (positive definiteness of the projection of the matrix of the quadratic form to the nullspace of CC).

The optimal solutions to our problem can be computed using quadratic programming algorithms. On the equidistant knotset we can use the special LSQ technique for solutions of difference equations, described in [6]. The following theorem completes our results for the functionals $J_k(s)$ and $J_{kd}(s)$.

Theorem 1. *For given spline knots* $\mathbf{x}$ *and function values* $\mathbf{s}$ *at the knots there exists a unique cubic interpolatory spline with minimal value of* $J_{1d}(s)$ *or* $J_{2d}(s)$*. Its local parameters* $m_i = s'(x_i)$ *or* $M_i = s''(x_i)$ *can be computed as the pseudoinverse solution to the underdetermined system of CC* (8) *or* (2)*.*

There exist also unique cubic splines with minimal values of $J_k(s)$*,* $k = 0, 1, 2$*. Their local parameters* m_i *or* M_i *can be computed by quadratic programming algorithms or some special LSQ algorithms as minimizers of* $J_k(s)$ *under the corresponding continuity conditions.*

On the equidistant spline knotset there exists also unique cubic spline with minimal value of $J_3(s)$*.*

E x a m p l e 1. For the discrete data $\mathbf{x} = 0 : 1 : 20$,

```
s=[15 11 3 5 0 -2 -7 -1 6 10 12 16 19 17 13 12 8 6 4 1 0]
```

we have computed the cubic natural spline and the cubic splines with minimal norms of the vectors $\mathbf{m}, \mathbf{M}$. The very similar results are plotted in Fig. 1.

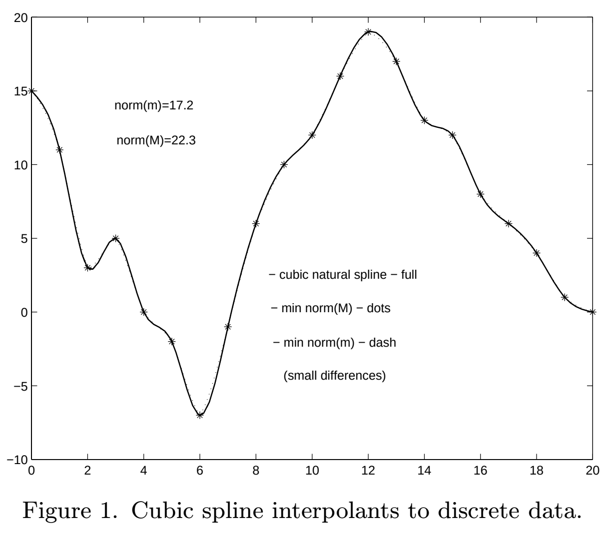

Figure 1. Cubic spline interpolants to discrete data.

3. Hermite cubic spline

When we are given the function value and the first derivative value at each knot x_i, then there exists a unique Hermite spline $s_{32}(x)$ interpolating these values—there are no free parameters for any optimization. But we can consider the same problem with the data t_i, $g_i = s(t_i)$, $p_i = s'(t_i)$; $i = 0(1)n$ with different spline knots x_i, $i = 0(1)n+1$ (the connection of neighbouring segments with possible jumps in the second derivative will be between the points of interpolation; we can then influence the curve shape by the choice of the knots). For the most frequently used case of $t_i = (x_i + x_{i+1})/2$ we can write the spline local representation with the local variable $u = (x - x_i)/h_i$ as

$$\begin{aligned} s_{32}(x) = {} & (2u-1)^2[(1-u)s_i + us_{i+1}] \\ & + 4u(1-u)g_i + 2h_i u(1-u)(2u-1)p_i. \end{aligned} \tag{14}$$

The condition of the first derivative continuity gives the *spline continuity conditions* as the recurrences ($i = 0(1)n-1$)

$$\begin{aligned} & -\frac{1}{h_i}s_i + 5\Big(\frac{1}{h_i} + \frac{1}{h_{i+1}}\Big)s_{i+1} - \frac{1}{h_{i+1}}s_{i+2} \\ & \qquad = 4\Big(\frac{1}{h_i}g_i + \frac{1}{h_{i+1}}g_{i+1}\Big) + 2(p_i - p_{i+1}). \end{aligned} \tag{15}$$

Similarly as with classical cubic splines we have now two free parameters, which we can use to fulfil some boundary conditions or for optimization purposes. We can see that the matrix of CC (15) has the full rank. When we want to have the interpolant from C^2 with the same knots, then we have not to prescribe the derivatives p_i, but to compute them so that the conditions for the second derivative continuity

$$\begin{aligned} & -\frac{1}{h_i^2}s_i + 2\left(\frac{1}{h_i^2} - \frac{1}{h_{i+1}^2}\right)s_{i+1} + \frac{1}{h_{i+1}^2}s_{i+2} \\ & \qquad = \left(\frac{1}{h_i^2}g_i - \frac{1}{h_{i+1}^2}g_{i+1}\right) + \frac{3}{2}\left(\frac{1}{h_i}p_i + \frac{1}{h_{i+1}}p_{i+1}\right) \end{aligned} \tag{16}$$

are also valid. Both systems (15), (16) of such CC form now a block system of equations for computing the local parameters s_i, p_i with three free parameters. Using the pseudoinverse approach we can compute the local parameters s_i, p_i of the spline with minimal norm of the vector $[\mathbf{s}, \mathbf{p}]$.

From the representation (14) we can compute the values of the functionals $J_k(s)$—we obtain

$$J_0(s) = \frac{1}{105}\sum_{i=0}^{n} h_i[(14g_i - 3h_ip_i)s_i + (14g_i + 3h_ip_i)s_{i+1} + 9s_i^2 + 3s_is_{i+1} + 9s_{i+1}^2 + 56g_i^2 + 2h_i^2p_i^2], \tag{17}$$

$$J_1(s) = \frac{1}{15}\sum_{i=0}^{n} \frac{1}{h_i}[-(80g_i - 24h_ip_i)s_i - (80g_i + 24h_ip_i)s_{i+1} + 47s_i^2 - 14s_is_{i+1} + 47s_{i+1}^2 + 80g_i^2 + 12h_i^2p_i^2], \tag{18}$$

$$J_2(s) = 16\sum_{i=0}^{n} \frac{1}{h_i^3}[-(4g_i - 6h_ip_i)s_i - (4g_i + 6h_ip_i)s_{i+1} + 4s_i^2 - 4s_is_{i+1} + 4s_{i+1}^2 + 4g_i^2 + 3h_i^2p_i^2], \tag{19}$$

$$J_3(s) = 576\sum_{i=0}^{n} \frac{1}{h_i^5}[s_{i+1} - s_i - h_ip_i]^2. \tag{20}$$

We can see here the positive definiteness of the matrices of the quadratic forms $J_k(s)$, $k = 0, 1, 2$ and together with the full rank of the matrices in CC (15) we can so prove the uniqueness of their minima. The matrix of the quadratic form $J_3(s)$ is singular. Contrary to the case of cubic splines $s_{31}(x)$ there is not a unique minimum. To the given input data $\{g_i, p_i\}$ we can find such a constant p that the Hermite spline with input data $\{g_i, p_i + p\}$ gives the same value to the functional $J_3(s)$. A simpler construction of such counterexample will be given in the next section. We summarize the results of this section in the following theorem.

Theorem 2. *On the spline knotset with points of interpolation at the midpoints of intervals there exist unique Hermite interpolatory splines which have minimal values of $J_k(s)$, $k = 0, 1, 2$ and $J_{0d}(s)$ for the data $[x_i, g_i, p_i]$ given.*

Remark. We can expect similar results in the case of slightly shifted knots x_i. When we denote $u = (x - x_i)/h_i$, $d_i = (t_i - x_i)/h_i$, we can obtain the spline local representation for such a general knotset as

$$\begin{aligned} s(x) = {} & \frac{1}{d_i^2}[d_i^2 + d_i(1 - d_i)u + (1 + 2d_i)u^2 - u^3]s_i \\ & + \frac{1}{(1 - d_i)^2}u(u + d)^2 s_{i+1} \\ & + \frac{u}{d_i^2(1 - d_i)^2}[d_i(2 - 3d_i) + (3d_i^2 - 1)u + (1 - 2d_i)u^2]g_i \\ & + \frac{h_iu}{d_i(d_i - 1)}[d_i - (1 + d_i)u + u^2]p_i. \end{aligned}$$

The first derivative CC can be written in such a general case as

$$\text{(21)}\quad \frac{1}{h_i}\Big(\frac{d_i-1}{d_i}\Big)^2 s_i + \Big[\frac{1}{h_i}\frac{d_i-3}{d_i-1} + \frac{1}{h_{i+1}}\frac{d_{i+1}+2}{d_{i+1}}\Big] s_{i+1} - \frac{1}{h_{i+1}}\Big(\frac{d_{i+1}}{d_{i+1}-1}\Big)^2 s_{i+2}$$
$$= \frac{1}{h_i}\frac{3d_i-1}{d_i^2(d_i-1)} g_i + \frac{1}{h_{i+1}}\frac{2-3d_{i+1}}{d_{i+1}(d_{i+1}-1)^2} g_{i+1}$$
$$+ \frac{1}{d_i} p_i + \frac{1}{d_{i+1}-1} p_{i+1}.$$

To write down the expressions for functionals considered and to discuss the uniqueness of the optimal solution is more involved now.

4. First derivative as the local parameter

With the given data $[t_i, g_i, p_i]$ from the foregoing section we can choose the values $[m_i, m_{i+1}]$, $m_j = s'(x_j)$ of the Birkhoff interpolation problem as completing local parameters. The corresponding local representation in the simpler case of $t_i = (x_i + x_{i+1})/2$ $(d_i = 1/2)$ is

$$\text{(22)}\quad s(x) = g_i + h_i\Big[\Big(\frac{2}{3}u^3 - \frac{3}{2}u^2 + u - \frac{5}{24}\Big) m_i$$
$$- \Big(\frac{4}{3}u^3 - 2u^2 + \frac{1}{3}\Big) p_i + \Big(\frac{2}{3}u^3 - \frac{1}{2}u^2 + \frac{1}{24}\Big) m_{i+1}\Big].$$

The spline continuity conditions for $s(x) \in C^1$ are now $(i = 0(1)n-1)$

$$\text{(23)}\quad -h_i m_i + 5(h_i + h_{i+1}) m_{i+1} - h_{i+1} m_{i+2}$$
$$= 24\Big[g_{i+1} - g_i - \frac{1}{3}(h_i p_i + h_{i+1} p_{i+1})\Big].$$

The matrix on the left-hand side of these CC has full rank. With help of the pseudoinverse we can compute from this system of n equations with $n+2$ unknown parameters m_i the solution with the minimal value of $J_{1d}(s)$. When we do not prescribe the values p_i, we can compute them so as to obtain $s(x) \in C^2$ which obeys the CC (23) and the following C^2 conditions:

$$\text{(24)}\quad \frac{1}{h_i} m_i + 3\Big(\frac{1}{h_i} + \frac{1}{h_{i+1}}\Big) m_{i+1} + \frac{1}{h_{i+1}} m_{i+2} = 4\Big(\frac{1}{h_i} p_i + \frac{1}{h_{i+1}} p_{i+1}\Big).$$

We have again three free parameters in a block system of equations. We can also use these relations in *the derivative interpolation problem*, where only the values p_i are given. We can now find the pseudoinverse solution $\mathbf{m}$ from (24), to choose the value g_0 and then compute recursively the remaining values g_i from the first part of CC (23).

We can compute the expressions for the functionals $J_k(s)$ in such a representation—we obtain

$$(25)\quad J_0(s) = \frac{1}{20160}\sum_{i=0}^{n}[h_i(256h_ip_i - 1680g_i) + h_i(256h_ip_i + 1680g_i)m_{i+1} + h_i^2(83m_i^2 - 86m_im_{i+1} + 83m_{i+1}^2) + 20160g_i^2 + 1088h_i^2p_i^2],$$

$$(26)\quad J_1(s) = \frac{1}{15}\sum_{i=0}^{n}[2p_i(m_i + m_{i+1}) + 2m_i^2 - m_im_{i+1} + 2m_{i+1}^2 + 8p_i^2],$$

$$(27)\quad J_2(s) = \frac{1}{3}\sum_{i=0}^{n}\frac{1}{h_i^3}[7m_i^2 + 2m_im_{i+1} + 7m_{i+1}^2 - 16p_i(m_i + m_{i+1}) + 16p_i^2],$$

$$(28)\quad J_3(s) = 16\sum_{i=0}^{n}\frac{1}{h_i^5}(m_i + m_{i+1} - 2p_i)^2.$$

We can establish again the positive definiteness of the matrices of the quadratic forms for $k = 0, 1, 2$, which—together with the full rank of the matrix in CC—ensures the uniqueness of the optimal spline, as stated above in Theorem 2. The matrix in $J_3(s)$ is again singular. Now it is easier to see that the two different splines determined by the data $[g_i, p_i]$ and $[g_i + g, p_i]$ with an arbitrary constant g correspond to splines with equal values m_i (see (23)) and an equal value of the functional. We can complete our results now as follows.

Theorem 3. *For a given spline knotset* $[x_i]$ *and data* $[t_i, g_i, p_i]$ *with* $t_i = \frac{1}{2}(x_i + x_{i+1})$ *there exists a unique Hermite interpolatory spline with a minimal value of* $J_{1d}(s)$. *We can compute its parameters* $\mathbf{m}$ *as the pseudoinverse solution to the system* (23).

There is no unique Hermite spline with a minimal value of $J_3(s)$.

Given the data $[x_i]$, $[p_i = s'(t_i)]$, $t_i = \frac{1}{2}(x_i + x_{i+1})$, $i = 0(1)n$ *only, then the spline* $s_{31}(x)$ *interpolating the derivative values* p_i *with a minimal value of* $J_{1d}(s)$ *is determined uniquely up to an additive constant (initial condition).*

Remark. For the general position of the points of interpolation t_i between the knots x_i, x_{i+1}—described by the parameters $d_i = (t_i - x_i)/h_i$—the local Hermite spline representation can be written as

$$s_{32}(u) = g_i + \frac{h_i}{6d_i}[d_i^2(d_i - 3) + 6d_i u - 3(1 + d_i) + 2u^3]m_i + \frac{h_i}{6(1 - d_i)}[d_i^3 - 3d_i u^2 + 2u^3]m_{i+1} - \frac{h_i}{6d_i(1 - d_i)}\left[d_i^2(3 - 2d_i) - 3u^2 + 2u^3\right]p_i. \tag{29}$$

The continuity conditions for the first derivatives are now

$$-\frac{h_i}{d_i}(1 - d_i)^3 m_i + [h_i(1 + d_i - d_i^2) + h_{i+1}d_{i+1}(3 - d_{i+1}]m_{i+1} - \frac{h_{i+1}}{1 - d_{i+1}}d_{i+1}^3 m_{i+2}$$
$$= 6(g_{i+1} - g_i) - \frac{h_i}{d_i}(1 - d_i)(2d_i + 1)p_i - \frac{h_{i+1}}{1 - d_{i+1}}d_{i+1}(3 - 2d_{i+1})p_{i+1}.$$

The expressions for the values of the functionals $J_k(s)$ are too lengthy to be written here.

Remark. It would be possible to consider also the problem of the mean value interpolation (histopolation) with cubic splines. In such a case we could not use the function value at the midpoint as the local parameter.

Example 2. For $\mathbf{x} = -1 : 2 : 11$; $\mathbf{t} = 0 : 2 : 10$ and the values of the function $f(u) = (5 - u)\cos(u)$ and its derivative we have computed the natural cubic spline with knots and values at the knots x_i, the cubic spline with a minimal norm of the vector $\mathbf{m}$ and Hermite interpolants with points of interpolation t_i and minimal norms of vectors $\mathbf{s}, \mathbf{m}$. The results obtained are plotted in Fig. 2.

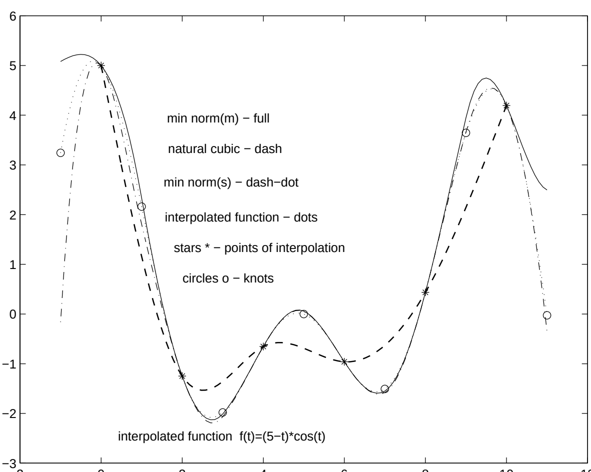

Figure 2. Hermite spline interpolants.

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