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Dedicated to Professor Ioan A. RUS on the occasion of his 70^{th} anniversary

Least squares data shape preserving

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ABSTRACT. Least squares data fitting is an important task in many fields of applied mathematics ([3, 4]). Essentially, in two dimensions it means to find an element from a a given class of functions which best approximates a given set of points in the real plane, by also preserving their shape. In this paper we use for such an approximation, classical and Bernstein polynomials. The (generally inconsistent) least squares problems so obtained are solved by both a Kaczmarz-like projection method, and an approximate orthogonalization technique (previously developed by the one of the authors in [1, 2]). Numerical experiments and comparisons are also provided.

1. INTRODUCTION

We shall present in this section the generalized interpolation (for short, **GI**) problem with respect to the linear subspace of real polynomial functions of degree less or equal than a given value $n \geq 1$, denoted by $\mathcal{P}_n$. We shall suppose that a basis $\{P_1,\ P_2, \ldots, P_{n+1}\}$ is known in $\mathcal{P}_n$. With these assumptions we can state the **GI** problem as follows: if $N_1(x_1, y_1)$,...,$N_m(x_m, y_m)$ are $m \geq 1$ given points (nodes) in the real plane $\mathbb{R}^2$, find a polynomial $f \in \mathcal{P}_n$, such that the "orthogonal" distances $d_i, i = 1, ..., m$ defined by (see (1.1) and Figure 1)

$$d_i = \mathrm{dist}\{N_i(x_i, y_i), (x_i, f(x_i)\} = |y_i - f(x_i)| \tag{1.1}$$

satisfy

$$\sum_{i=1}^{m} d_i^2 = \min!, \tag{1.2}$$

where the notations $\|Ax^* - b\| = \min!$ means that we want to find $x^* \in \mathbb{R}^n$ with the property $\|Ax^* - b\| = \inf\{\|Ax - b\|, x \in \mathbb{R}^n\}$.

Because $f \in \mathcal{P}_n$, we have

$$f(x) = a_1 P_1 + ... + a_{n+1} P_{n+1}, \tag{1.3}$$

which introduced in (1.1)-(1.2) gives

$$\sum_{i=1}^{m} \left[\sum_{j=1}^{n+1} a_j P_j(x_i) - y_i \right]^2 = \min!. \tag{1.4}$$

If we define the $m \times (n+1)$ matrix A, m-vector b and $(n+1)$-vector u by

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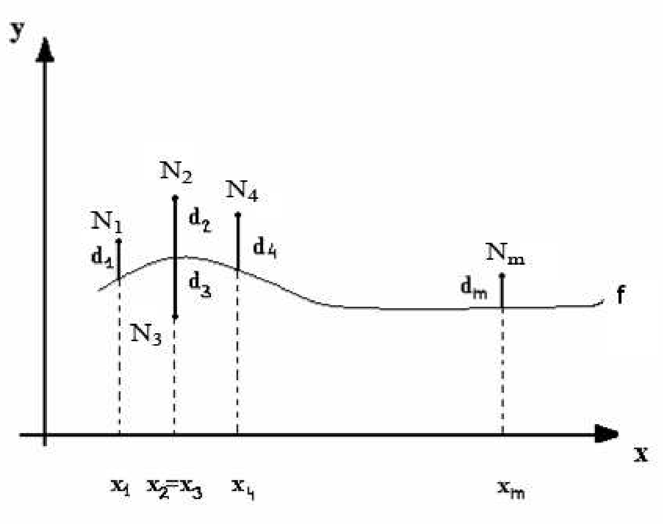


FIGURE 1. Generalized interpolation, $f \in \mathcal{P}_n$

$$A = \begin{bmatrix} P_1(x_1) & P_2(x_1) & P_3(x_1) & \cdot & P_{n+1}(x_1) \\ P_1(x_2) & P_2(x_2) & P_3(x_2) & \cdot & P_{n+1}(x_2) \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ P_1(x_m) & P_2(x_m) & P_3(x_m) & \cdot & P_{n+1}(x_m) \end{bmatrix}, \tag{1.5}$$

$$b = (y_1, y_2, \dots, y_m)^t, \ u = (a_1, a_2, \dots, a_{n+1})^t, \tag{1.6}$$

then, (1.2) (or (1.4)) can be written as a least squares problem: find $u \in \mathbb{R}^{n+1}$ such that

$$\|Au - b\|^2 = \min !. \tag{1.7}$$

We shall denote by $LSS(A; b)$ the set of all solutions for (1.7) and by u_{LS} the minimal norm one.

Remark 1.1. Usually the number m of the given data $N_1, \dots, N_m$ exceeds the number of fitting function parameters $(a_1, a_2, \dots, a_{n+1}$, in our case), i.e the problem (1.7) is overdetermined. Moreover, the abscissas $x_1, \dots, x_m$ of the given points $N_1, \dots, N_m$ have no special properties (i.e. may exist points N_i and $N_j,\ i \neq j$ with the same abscissas $x_i = x_j$). This means that the matrix A in (1.5) will have no more full row or column rank, thus (1.7) will also be rank-defficient.

2. STANDARD AND BERNSTEIN-LIKE POLYNOMIALS

In our procedure, we used the following two different basis $\{P_1, P_2, \dots, P_{n+1}\}$ in $\mathcal{P}_n$:

I. Standard polynomials

$$P_1(x) = 1, P_i(x) = x^{i-1}, i = 2, \ldots, n+1,\ x \in [0,1]\,; \tag{2.8}$$

II. Bernstein-like polynomials

$$P_i(x) = C_n^{i-1} x^{i-1}(1-x)^{n-i+1},\ i = 1, \ldots, n+1,\ x \in [0,1]\,. \tag{2.9}$$

Remark 2.2. In practical applications, the interval $[a, b]$ from (2.8) is defined such that

$$\min_{1 \le i \le m} x_i = a < b = \max_{1 \le i \le m} x_i \tag{2.10}$$

where $x_1, \ldots, x_m$ are the abscissas of the points $N_1, \ldots, N_m$ from (1.1).

Remark 2.3. The polynomials in (2.8) or (2.9) are restricted to the unit interval $[0, 1] \subset \mathbb{R}$. For an arbitrary interval $[a, b]$ (e.g. as in (2.10)) we consider the translation φ

$$\varphi : [a, b] \to [0, 1]\,,\ \varphi(x) = \frac{x-a}{b-a} \tag{2.11}$$

and define the basis $\{\hat{P}_1, \ldots, \hat{P}_{n+1}\}$ by

$$\hat{P}_i(x) = P_i(\varphi(x)),\ x \in [a, b]\,. \tag{2.12}$$

With the above notations and definitions, we have the following result.

Proposition 2.1. *Let $\mathcal{P}_n\left([0,1]\right)$ be the vector space of the restrictions $f|_{[0,1]}$ of the elements $f \in \mathcal{P}_n$. Then $\{P_1, \ldots, P_{n+1}\}$ with P_i from* (2.8) *or* (2.9) *is a basis in $\mathcal{P}_n\left([0,1]\right)$.*

Proof. The result is clear for P_i from (2.8). Let $P_i,\ i = 1, \ldots, n+1$ be given by (2.9) such that

$$\alpha_1 P_1(x) + \ldots + \alpha_{n+1} P_{n+1}(x) = 0,\ \forall x \in [0,1] \tag{2.13}$$

and suppose that it exists an index $i \in \{1, \ldots m\}\}$ such that $\alpha_i \neq 0$. Then from (2.13) we get

$$E_1(x) + \alpha_i + E_2(x) = 0,\ \forall x \in (0,1) \tag{2.14}$$

with

$$E_1(x) = \sum_{j=1}^{i-1} \alpha_j \frac{C_n^{j-1}}{C_n^{i-1}} \frac{(1-x)^{i-j}}{x^{i-j}},\ E_2(x) = \sum_{j=i+1}^{n+1} \alpha_j \frac{C_n^{j-1}}{C_n^{i-1}} \frac{x^{j-i}}{(1-x)^{j-i}} \tag{2.15}$$

$x \in (0, 1)$, thus

$$\lim_{x \to 0, x>0} E_1(x) = \lim_{x \to 1, x<1} E_2(x) = \pm\infty;\ \lim_{x \to 0, x>0} E_2(x) = \lim_{x \to 1 x<1} E_1(x) = 0, \tag{2.16}$$

from which we obtain that

$$\alpha_1 = \ldots = \alpha_{i-1} = \alpha_{i+1} = \ldots = \alpha_{n+1} = 0 \tag{2.17}$$

and together with (2.14) we get $\alpha_i = 0$. But, this contradicts our initial assumption about α_i. It rests that all the α_i 's from the linear combination (2.13) are zero and the proof is complete. □

Corollary 2.1. *$\{\hat{P}_1, \ldots, \hat{P}_{n+1}\}$ with $\hat{P}_i$ from* (2.12) *and P_i from* (2.8) *or* (2.9) *is a basis in the vector space $\mathcal{P}_n\left([a,b]\right)$ (defined as $\mathcal{P}_n\left([0,1]\right)$) w.r.t. $[a, b]$).*

Remark 2.4. The Bernstein-like polynomial (on $[0,1]$), $B_n(x) = \sum_{i=1}^{n+1} a_i P_i(x)$(with $P_i(x)$ from (2.9)) is a convex combination of the numbers a_i. For this we expect a "better shape preserving" by using them for the **GI** problem (see the next section of the paper).

3. Numerical experiments

We used as numerical (iterative) solvers for the problem (1.7) the *Kaczmarz Extended* **(KE)** and the *Right hand side Kovarik* **(rhs-Ko)** algorithms. In what follows, we shall briefly describe the above mentioned methods. For details, see [1, 2].

Kaczmarz Extended **(KE)**

Let $a_i,\ i = 1,\ldots,m,\ \alpha_j,\ j = 1,\ldots,n$ be the i-th row and the j-th column of A respectively, and b_i the i-th component of b; assume that $a_i \neq 0,\ \alpha_j \neq 0,\ (\forall)\ i = 1,\ldots,m,\ j = 1,\ldots,n$. We define the projections (see e.g. [1]) $f_i(b;\cdot),\ F(b;\cdot) : \mathbb{R}^n \to \mathbb{R}^n$ and $\varphi_j,\ \phi : \mathbb{R}^m \to \mathbb{R}^m$ by

$$\begin{aligned} &f_i(b;u) = u - \tfrac{<u,a_i>-b_i}{\|a_i\|^2} a_i,\ F(b;u) = (f_1 \circ \ldots \circ f_m)(b;u),\ u \in \mathbb{R}^n, \\ &\varphi_j(y) = y - \tfrac{<y,\alpha_j>}{\|\alpha_j\|^2}\alpha_j,\ j = 1,\ldots,n,\ \phi(y) = (\varphi_1 \circ \ldots \circ \varphi_n)(y),\ y \in \mathbb{R}^m. \end{aligned} \tag{3.18}$$

Let $y^0 = b,\ x^0 \in \mathbb{R}^n$ (arbitrary) and $u^k \in \mathbb{R}^n$ already computed. The next iteration, u^{k+1}, is obtained as follows

$$y^{k+1} = \phi(y^k),\ b^{k+1} = b - y^{k+1},\ u^{k+1} = F(b^{k+1};u^k),\ k \geq 0. \tag{3.19}$$

Theorem 3.1. ([1]) *Under the above assumptions, the sequence* $(u^0)_{k\geq 0}$ *generated by the algorithm* (3.19) *converges, and* $\lim_{k\to\infty} u^k = u^* \in LSS(A;b)$. *Moreover, for* $u^0 = 0$ *we get* $u^* = u_{LS}$.

Right hand side Kovarik **(rhs-KO)**

Let $A_0 = A,\ b_0 = b$; for $k = 0, 1, \ldots$ do

$$H_k = I - A_k A_k^t;\ \Gamma_k = I + \frac{1}{2} H_k,\ A_{k+1} = \Gamma_k A_k,\ b^{k+1} = \Gamma_k b^k. \tag{3.20}$$

Theorem 3.2. ([2]) *With the following scaling*

$$A = A \cdot \frac{1}{\sqrt{\|AA^t\|_\infty + 1}};\ b = b \cdot \frac{1}{\sqrt{\|AA^t\|_\infty + 1}},$$

the sequence $(A_k^t b^k)_{k\geq 0}$ *generated in the iterations in* (3.20), *converges and*

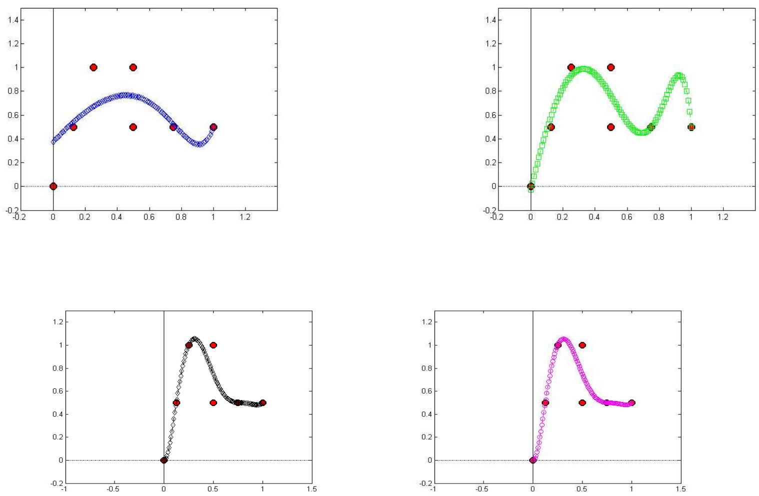
$$\lim_{k\to\infty} A_k^t b^k = u_{LS}.$$

We considered in our experiments the following set of points

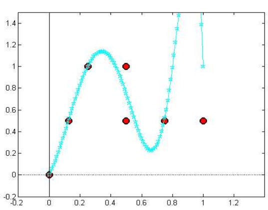
Problem 1. Input data							
x	0.0	0.125	0.25	0.5	0.5	0.75	1.0
y	0.0	0.5	1.0	1.0	0.5	0.5	0.5

Problem 2. Input data									
x	0.0	0.1	0.3	0.35	0.45	0.45	0.6	0.8	0.9
y	0.2	0.1	0.3	0.8	0.6	0.8	0.3	0.9	1.0

The tests were performed with $\dim(\mathcal{P}_n) = 11$ for Problem 1 and $\dim(\mathcal{P}_n) = 13$ for Problem 2. The results are shown in Figures 2-5. As it shall be noticed, the results obtained by MATLAB function are the worst in both cases, since it obtains graphs with very high "amplitudes". In comparison, the Bernstein polynomials give us a better "shape" of the graph, as it was expected. With respect to the solver, in this particular cases, the **rhs-KO** is better than the **KE**. As future work, we want to improve the implementation of **KE** and **rhs-KO** algorithms and find an appropriate hybrid **KE–rhs-KO** method, to solve the problem for closed contours, and to extend the above mentioned algorithms to surfaces.

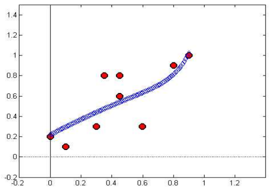


Interpolation using **KE** solver   Interpolation using **rhs-KO** solver

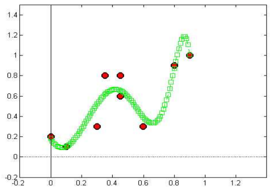


Interpolation using **MATLAB** function

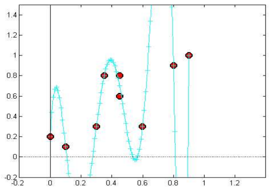
FIGURE 2. Problem 1-Bernstein polynomials



Interpolation using **KE** solver

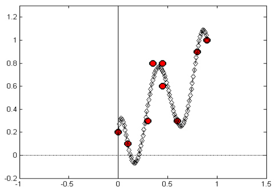


Interpolation using **rhs-KO** solver

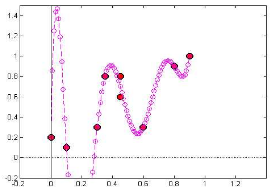


Interpolation using **MATLAB** function

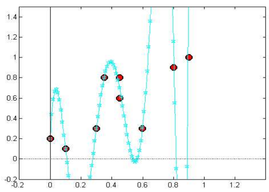
FIGURE 3. Problem 2-Standard polynomials



Interpolation using **KE** solver



Interpolation using **rhs-KO** solver



Interpolation using **MATLAB** function

FIGURE 4. Problem 2-Bernstein polynomials

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