

# Bernstein-Vandermonde matrices, and applications II

**José-Javier Martínez**

Departamento de Física y Matemáticas,  
Universidad de Alcalá.

Research partially supported by Spanish research grant  
MTM2012-31544 (Gobierno de España)

**3rd ALAMA Courses on Totally Positive and  
Totally Negative Matrices**, Castro Urdiales, 5 - III - 2015

## Outline of the talk

- Introduction
- Application: Polynomial least squares fitting
- Total positivity and Neville elimination
- Bidiagonal factorization
- Polynomial least squares fitting: an example
- Basic result and algorithms
- Numerical experiments
- Another application: Singular value computation
- References

## Some history...

NJH: A little later, in 1969, you have a paper *Matrix Decompositions and Statistical Calculation*. Was this motivated by your earlier statistical interests?

GHG: Yes, and the fact that I worked on all these orthogonal decompositions and so forth. So I tried to get the statisticians interested in doing numerical computations, A few people were interested in it, but I don't think it had a heavy influence in statistics. I doubt if today people really use decomposition methods rather than normal equations. Statisticians are fairly fixed in their ways.

[N. J. Higham. An Interview with Gene Golub. MIMS EPrint 2008.8. The University of Manchester, 2008]

# Important aspects

- The structure of the matrix.
- The choice of the basis for the polynomial space.

## References to our work

- A. Marco, J. J. Martínez. A fast and accurate algorithm for solving Bernstein-Vandermonde linear systems. *Linear Algebra Appl.* 422 (2007), 616–628.
- A. Marco, J. J. Martínez. Polynomial least squares fitting in the Bernstein basis. *Linear Algebra Appl.* 433 (2010), 1254–1264.

## References to our work, II

- A. Marco, J. J. Martínez. Accurate computations with totally positive Bernstein-Vandermonde matrices. *Electronic Journal of Linear Algebra*: Vol. 26, Article 24 (2013).
- A. Marco, J. J. Martínez. Ajuste polinómico por mínimos cuadrados usando la base de Bernstein. *La Gaceta de la RSME*, Vol. 18 (2015), núm. 1, 135–153.

## Why the Bernstein basis?

- In the Vandermonde case (corresponding to the usual choice of the monomial basis  $\{1, t, t^2, \dots, t^n\}$ ) we also have total positivity, so we must look for some advantage of the Bernstein polynomial basis.
- J. Delgado, J. M. Peña. Optimal conditioning of Bernstein collocation matrices. *SIAM J, Matrix Analysis Appl.* 31 (2009), 990–996.
- R. Farouki. The Bernstein polynomial basis: A centennial retrospective. *Computer Aided Geometric Design* 29 (6) (2012), 379-419.

## Statement of the problem

Given  $\{x_i\}_{1 \leq i \leq l+1}$  pairwise distinct real points and  $\{f_i\}_{1 \leq i \leq l+1} \in \mathbf{R}$ , let us consider a degree  $n$  polynomial

$$P(x) = c_0 + c_1x + \dots + c_nx^n$$

for some  $n < l$ . Such a polynomial is a *least squares fit* to the data if it minimizes the sum of the squares of the deviations from the data,

$$\sum_{i=1}^{l+1} |P(x_i) - f_i|^2.$$



Computing the coefficients  $c_j$  of that polynomial  $P(x)$  is equivalent to solve, in the least squares sense, the overdetermined linear system  $Ac = f$ , where  $A$  is the rectangular  $(l + 1) \times (n + 1)$  Vandermonde matrix corresponding to the nodes  $\{x_i\}_{1 \leq i \leq l+1}$ .

Taking into account that  $A$  has full rank  $n + 1$ , the problem has a unique solution given by the unique solution of the linear system

$$A^T A c = A^T f,$$

the normal equations.

Since  $A$  is usually an ill-conditioned matrix, it was early recognized that solving the normal equations was not an adequate method. Golub [Golub - 65], following previous ideas by Householder, suggested the use of the  $QR$  factorization of  $A$ , which involves the solution of a linear system with the triangular matrix  $R$ .

Let us observe that, if  $A = QR$  with  $Q$  being an orthogonal matrix, then using the condition number in the spectral norm we have

$$\kappa_2(R) = \kappa_2(A),$$

that is,  $R$  inherits the ill-conditioning of  $A$  while

$$\kappa_2(A^T A) = \kappa_2(A)^2.$$

In addition, as it was already observed by Golub in [Golub - 69] (see also Section 20.1 of [Higham - 2002]),

*although the use of the orthogonal transformation avoids some of the ill effects inherent in the use of normal equations, the value  $\kappa_2(A)^2$  is still relevant to some extent.*

Consequently a good idea is to use, instead of the monomial basis, a polynomial basis which leads to a matrix  $A$  with smaller condition number than the Vandermonde matrix.

A basis which leads to a matrix  $A$  better conditioned than the Vandermonde matrix is **the Bernstein basis** of polynomials, a widely used basis in Computer Aided Geometric Design due to the good properties that it possesses (see, for instance, [Carnicer-Peña - 93]).

J. Delgado, J. M. Peña. Optimal conditioning of Bernstein collocation matrices. SIAM J, Matrix Analysis Appl. 31 (2009), 990–996.

So we will solve the following problem:

Let  $\{x_i\}_{1 \leq i \leq l+1} \in (0, 1)$  a set of points such that  $0 < x_1 < \dots < x_{l+1} < 1$ . Our aim is to compute a polynomial

$$P(x) = \sum_{j=0}^n c_j b_j^{(n)}(x)$$

expressed in the Bernstein basis

$$\mathcal{B}_n = \left\{ b_j^{(n)}(x) = \binom{n}{j} (1-x)^{n-j} x^j, \quad j = 0, \dots, n \right\}$$

such that  $P(x_i) = f_i$  for  $i = 1, \dots, l+1$ , with  $l \geq n$ .

This problem is equivalent to solving the overdetermined linear system  $Ac = f$  in the least squares sense, where

$$A = \begin{pmatrix} \binom{n}{0}(1-x_1)^n & \binom{n}{1}x_1(1-x_1)^{n-1} & \cdots & \binom{n}{n}x_1^n \\ \binom{n}{0}(1-x_2)^n & \binom{n}{1}x_2(1-x_2)^{n-1} & \cdots & \binom{n}{n}x_2^n \\ \vdots & \vdots & \ddots & \vdots \\ \binom{n}{0}(1-x_{l+1})^n & \binom{n}{1}x_{l+1}(1-x_{l+1})^{n-1} & \cdots & \binom{n}{n}x_{l+1}^n \end{pmatrix} \quad (1,1)$$

is the  $(l+1) \times (n+1)$  *Bernstein-Vandermonde matrix* for the Bernstein basis  $\mathcal{B}_n$  and the nodes  $\{x_i\}_{1 \leq i \leq l+1}$ ,

# Totally nonnegative matrices

- Numerical computing with **structured totally nonnegative matrices** is a classical subject in numerical linear algebra which has recently received a renewed attention [Demmel et al, 08].
- A matrix is said to be **totally nonnegative** or **totally positive (strictly totally positive)** if all its minors are nonnegative (positive).
- A **nonsingular totally nonnegative** matrix can be decomposed as a product of **nonnegative bidiagonal factors** [Fallat, 01],[Gasca-Peña, 92; 94]. This fact was used by Koev [Koev, 05; 07] to develop several **accurate algorithms** for the general class of TN matrices.

## Previous work with totally positive matrices

Examples of totally nonnegative matrices whose **bidiagonal decompositions** can be **computed** in an **accurate** and **efficient** way are: **Vandermonde** [Björck-Pereyra, 70; Higham, 02], **and Cauchy** [Boros-Kailath-Olshevsky, 99].



## Neville elimination

The main theoretical tool for obtaining the results presented in this talk is **Neville elimination** [Gasca-Peña, 92; 94].

Neville elimination makes zeros in a matrix adding to a given row an **appropriate multiple of the previous one**:

Given  $A = (a_{i,j}) \in \mathbf{R}^{l \times n}$  with  $l \geq n$ , it consists on  $n - 1$  steps

$$A := A_1 \rightarrow A_2 \rightarrow \dots \rightarrow A_n$$

where  $A_t = (a_{i,j}^{(t)}) \in \mathbf{R}^{l \times n}$  has zeros below its main diagonal in the  $t - 1$  first columns.

# Neville elimination

- $p_{i,j} := a_{i,j}^{(j)}$  **pivot**  $(i, j)$   $(1 \leq j \leq n; j \leq i \leq l)$

- If all the pivots are nonzero:
  - No row exchanges are needed.
  - $p_{i,1} = a_{i,1} \forall i$

$$p_{i,j} = \frac{\det A[i-j+1, \dots, i | 1, \dots, j]}{\det A[i-j+1, \dots, i-1 | 1, \dots, j-1]}$$

$(1 < j \leq n, j \leq i \leq l)$  [Gasca-Peña, 92].

- $m_{i,j} = \frac{p_{i,j}}{p_{i-1,j}}$  **multiplier**  $(1 \leq j \leq n; j < i \leq l)$

## Neville elimination

- $U := A_n$  is upper triangular with the **diagonal pivots**  $p_{i,i}$  in its main diagonal.
- The **complete Neville elimination** of a  $A$  consists of performing the Neville elimination of  $A$  for obtaining  $U$  and then continue with the Neville elimination of  $U^T$ .
- When no row exchanges are needed in the Neville elimination of  $A$  and  $U^T$  the multipliers of the complete Neville elimination of  $A$  are:
  - The multipliers of the Neville elimination of  $A$  if  $i \geq j$
  - The multipliers of the Neville elimination of  $A^T$  if  $j > i$ .

# Total positivity

Neville elimination allows one to characterize strictly totally positive matrices [Gasca-Peña, 92]:

**THEOREM 1:** A matrix is strictly totally positive if and only if its complete Neville elimination can be performed without row and column exchanges, the multipliers of the Neville elimination of  $A$  and  $A^T$  are positive, and the diagonal pivots of the Neville elimination of  $A$  are positive.

## Bidiagonal factorization of $A$

For the case of **rectangular** Bernstein-Vandermonde matrices we have:

**THEOREM 2:** Let  $A \in \mathbf{R}^{(l+1) \times (n+1)}$  be a Bernstein-Vandermonde matrix whose nodes satisfy  $0 < x_1 < x_2 < \dots < x_l < x_{l+1} < 1$ . Then

$$A = F_l F_{l-1} \cdots F_1 D G_1 G_2 \cdots G_n,$$

where  $G_i$  are  $(n+1) \times (n+1)$  upper triangular bidiagonal matrices ( $i = 1, \dots, n$ ),  $F_i$  are  $(l+1) \times (l+1)$  lower triangular bidiagonal matrices ( $i = 1, \dots, l$ ), and  $D$  is a  $(l+1) \times (n+1)$  diagonal matrix.





# Bidiagonal factorization of $A$

$$D = \text{diag}\{p_{1,1}, p_{2,2}, \dots, p_{n+1,n+1}\} \in \mathbf{R}^{(l+1) \times (n+1)}$$

$p_{i,j}$  are the **diagonal pivots** of the Neville elimination of  $A$ .



# The matrix $BD(A)$

- [P. Koev, 2005], [P. Koev, 2007], [Demmel et al., 2008]
- Its bidiagonal decomposition is the (unique) representation of a TN matrix in order to perform accurate computations.
- Being able to compute all  $n^2$  initial minors of  $A$  accurately is a necessary and sufficient condition for computing the bidiagonal decomposition  $BD(A)$  accurately.

## The matrix $BD(A)$

- It is convenient to store the  $n^2$  nontrivial entries of  $BD(A)$  as a matrix  $B$ . In position  $(i, j)$  we store the multiplier  $m_{ij}$ , and on the diagonal we store  $D$ .
- Starting from an accurate bidiagonal decomposition of the original matrix, virtually all linear algebra with TN matrices can be performed accurately.

## Fast and accurate algorithms for $BD(A)$

- Fast algorithms for computing  $BD(A)$  can be found by using in an appropriate way **explicit expressions** for the involved minors (determinants).
- They have **high relative accuracy** because they satisfy the NIC (no inaccurate cancellation) condition [Demmel et al., 08].
- **NIC:** The algorithm only multiplies, divides, adds (resp., subtracts) real numbers with like (resp., differing) signs, and otherwise only adds or subtracts input data.

# Example

For the  $4 \times 2$  Bernstein-Vandermonde matrix

$$A = \begin{pmatrix} 4/5 & 1/5 \\ 3/5 & 2/5 \\ 2/5 & 3/5 \\ 1/5 & 4/5 \end{pmatrix}$$

its bidiagonal factorization is

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1/2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 2/3 & 1 & 0 \\ 0 & 0 & 3/2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 3/4 & 1 & 0 & 0 \\ 0 & 4/3 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 4/5 & 0 \\ 0 & 1/4 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1/4 \\ 0 & 1 \end{pmatrix}$$

The corresponding  $\mathcal{BD}(A)$  is

$$\mathcal{BD}(A) = \begin{pmatrix} 4/5 & 1/4 \\ 3/4 & 1/4 \\ 2/3 & 4/3 \\ 1/2 & 3/2 \end{pmatrix}.$$

## A small example

Let us consider the problem of fitting, by a polynomial of degree less or equal to 2, the following data:

$$f(-1) = 1, f(1) = 3, f(2) = 10, f(3) = 29.$$

So we have

$$x_1 = -1, x_2 = 1, x_3 = 2, x_4 = 3,$$

$$f = (1, 3, 10, 29)^T.$$

The (rectangular) Vandermonde matrix obtained when using the monomial basis  $1, x, x^2$  will be:

$$V = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{pmatrix}.$$



The solution  $c$  (in the least squares sense) of  $Vc = f$  is given by the solution of the normal equations:

$$c = (V^T V)^{-1} V^T f = (-20/11, 13/55, 36/11)^T,$$

i.e. the desired polynomial is

$$p_1(x) = (-20/11) + (13/55)x + (36/11)x^2.$$

The projection  $p$  of the vector  $f$  on the column space of  $V$  is

$$p = \hat{f} = Vc = V(V^T V)^{-1} V^T f = (67/55, 93/55, 646/55, 1559/55)^T.$$

Matrix  $H = V(V^T V)^{-1}V^T$  is the projection matrix on the column space of matrix  $V$ , and that matrix is

$$H = \begin{pmatrix} 109/110 & 3/55 & -4/55 & 3/110 \\ 3/55 & 37/55 & 24/55 & -9/55 \\ -4/55 & 24/55 & 23/55 & 12/55 \\ 3/110 & -9/55 & 12/55 & 101/110 \end{pmatrix}.$$

**Remark.** The projection matrix  $H$  in many statistics texts is called *the hat matrix*, since

$$\hat{f} = Hf.$$

A classic paper that studies the properties of matrix  $H$  and its application in regression problems is due to Hoaglin.  $H$ , of size  $(l + 1) \times (l + 1)$ , in addition to being symmetric and idempotent ( $H^2 = H$ ), has the eigenvalue 1 with multiplicity  $n + 1$  (the rank of  $V$ ) and the eigenvalues 0 with multiplicity  $l - n$ , so the sum of its diagonal entries (the trace of  $H$ ) is  $n + 1$ .

The projection matrix on the orthogonal complement (in  $\mathbb{R}^{l+1}$ ) of the column space of  $V$  is  $P = I - H$ , where  $I$  is the identity matrix. The vector

$$r = f - \hat{f} = f - Hf = Pf$$

is the *residual vector*, which in our example is

$$r = (-12/55, 72/55, -96/55, 36/55)^T.$$

For changing to the interval  $(0, 1)$  (by means of a change of variable of the form  $t = g(x) = a_0 + a_1x$ ) there is not a unique way. It is important, from a numerical point of view (and for having the Bernstein-Vandermonde matrix strictly totally positive), to avoid the boundary points 0 and 1. If, for instance, we choose to have  $g(-1) = 1/6$  and  $g(3) = 5/6$  then  $g(x)$  is determined as

$$g(x) = (x + 2)/6,$$

so that the corresponding points in  $(0, 1)$  will be  $t_1 = 1/6, t_2 = 1/2, t_3 = 2/3, t_4 = 5/6$ .

The corresponding Vandermonde matrix will now be

$$V_0 = \begin{pmatrix} 1 & 1/6 & 1/36 \\ 1 & 1/2 & 1/4 \\ 1 & 2/3 & 4/9 \\ 1 & 5/6 & 25/36 \end{pmatrix}.$$

Now it is important to observe that *the data vector remains the same* for the problem shifted to  $(0, 1)$ :

$$f = (1, 3, 10, 29)^T.$$

The relationship between both Vandermonde matrices  $V$  and  $V_0$  is the following one:

$$V_0 = VS,$$

where  $S$  is the matrix

$$S = \begin{pmatrix} 1 & 1/3 & 1/9 \\ 0 & 1/6 & 1/9 \\ 0 & 0 & 1/36 \end{pmatrix}$$

which depends on the change of variable  $t = (x + 2)/6$ .

With that change we have

$$t = (x + 2)/6 = (1/3) + (1/6)x$$

y

$$t^2 = (1/9) + (1/9)x + (1/36)x^2,$$

which gives the second and third columns of  $S$ , an upper triangular and invertible matrix. It is clear this fact would be true in general for a change of the form  $t = g(x) = a_0 + a_1x$  with  $a_1$  different from zero: the diagonal entries of  $S$  are the powers of  $a_1$ .



This relationship between  $V$  and  $V_0$  implies that for both matrices the projection matrix  $H$  on the column space is the same (i.e.  $V_0$  and  $V$  have the same column space). So in both cases  $\hat{f} = Hf$  is the same vector.

On the contrary, the vector  $c$  will be different. For the problem in  $(0, 1)$  the solution will be

$$c = (54/5, -4242/55, 1296/11)^T,$$

i.e the fitting polynomial is

$$p_2(t) = (54/5) + (-4242/55)t + (1296/11)t^2.$$

This polynomial allows us to evaluate at the points of the original interval, taking into account that  $t = (x + 2)/6.$ , For example,

$$p_1(0) = p_2(1/3) = -20/11.$$

Finally, we will use in  $(0, 1)$  the Bernstein basis (of degree  $\leq 2$  in our example):

$$b_0^{(2)}(t) = (1 - t)^2 = 1 - 2t + t^2,$$

$$b_1^{(2)}(t) = 2(1 - t)t = 2t - 2t^2,$$

$$b_2^{(2)}(t) = t^2.$$

The Bernstein-Vandermonde matrix corresponding to the nodes  $t_1 = 1/6$ ,  $t_2 = 1/2$ ,  $t_3 = 2/3$ ,  $t_4 = 5/6$  will be:

$$A = \begin{pmatrix} 25/36 & 5/18 & 1/36 \\ 1/4 & 1/2 & 1/4 \\ 1/9 & 4/9 & 4/9 \\ 1/36 & 5/18 & 25/36 \end{pmatrix}.$$

Now, the relationship between the Vandermonde matrix  $V_0$  and the Bernstein-Vandermonde matrix  $A$  is the following one:

$$A = V_0 C.$$

The lower triangular and invertible matrix  $C$  is now the matrix given by the change of basis from the monomial basis to the Bernstein basis:

$$C = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 2 & 0 \\ 1 & -2 & 1 \end{pmatrix}.$$

Consequently, also in the case of general  $n$  we have this kind of relationship ( $A = V_0 C$  with  $C$  invertible), which implies that the projection matrix  $H$  on the column space of  $A$  will be the same as the projection matrix on the column space of  $V_0$ , which in turn is the same as the projection matrix on the column space of the original matrix  $V$ . **Therefore we can solve the original problem by using the Bernstein basis on  $(0, 1)$ .**

The solution  $c$  is now

$$c = (54/5, -1527/55, 2832/55)^T,$$

i.e. the fitting polynomial (which is the same as  $p_2$ ) expressed in the Bernstein basis is

$$p_3(t) = (54/5)b_0^{(2)}(t) + (-1527/55)b_1^{(2)}(t) + (2832/55)b_2^{(2)}(t).$$

This polynomial  $p_3$  can be used to obtain values of  $p_1$  at points of the original interval. For instance,

$$p_1(-1) = p_3(1/6) = 67/55.$$

It is important to remark that for evaluating the polynomial expressed in the Bernstein basis it is convenient to use the *de Casteljau algorithm*. This algorithm evaluates the polynomial by computing only convex combinations of data obtained in previous stages, which makes the algorithm numerically stable.



## Basic result for the least squares problem

**THEOREM 3:** [Björck, 96] Let  $A \in \mathbf{R}^{(l+1) \times (n+1)}$  with  $\text{rank}(A) = n + 1$ ,  $l \geq n$ ,  $x \in \mathbf{R}^{n+1}$  and  $b \in \mathbf{R}^{l+1}$ . Let the QR decomposition of  $A$ :

$$A = Q \begin{pmatrix} R \\ 0 \end{pmatrix},$$

where  $Q \in \mathbf{R}^{(l+1) \times (l+1)}$  is an orthogonal matrix and  $R \in \mathbf{R}^{(n+1) \times (n+1)}$  is an upper triangular matrix with positive diagonal entries. Then **the solution of the least squares problem**  $\min_x \|b - Ax\|_2$  is obtained from

$$\begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = Q^T b, \quad Rx = d_1, \quad r = Q \begin{pmatrix} 0 \\ d_2 \end{pmatrix},$$

where  $d_1 \in \mathbf{R}^{n+1}$ ,  $d_2 \in \mathbf{R}^{l-n}$  and  $r = b - Ax$ .

# Algorithm for the least squares problem

**INPUT:** The nodes  $t_i$  ( $i = 1, \dots, l + 1$ ), the degree  $n$  and the vector  $b$ .

**OUTPUT:** The vector  $x$  minimizing  $\|Ax - b\|_2$ .

**Step 1:** Computation of the bidiagonal decomposition of  $A$  by using our algorithms.

**Step 2:** Given the result of Step 1, computation of the QR decomposition of  $A$  by using TNQR ([Koev, 07]; package TNTTool).

**Step 3:** Computation of  $d = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} = Q^T b$  (MATLAB).

**Step 4:** Solution of  $Rx = d_1$  by using TNSolve (package TNTTool).

# The projection matrix and least squares

## Definition

- $p = Ac = A(A^T A)^{-1} A^T f$  is the **projection** of  $f$  onto the column space of  $A$ .
- $P = A(A^T A)^{-1} A^T$  is the **projection matrix**.

## Proposition

Let  $Ac = f$  be the least squares problem whose projection matrix  $P$  we are interested in computing. Let

$$A = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$$

be the  $QR$  factorization of  $A$ , where  $Q$  is an  $(m+1) \times (m+1)$  orthogonal matrix and  $R$  is an  $(n+1) \times (n+1)$  upper triangular matrix with positive diagonal entries, and let  $Q_1$  be the  $(m+1) \times (n+1)$  matrix with the first  $n+1$  columns of  $Q$ . Then

$$P = Q_1 Q_1^T.$$

# Algorithms in MATLAB

TNTool package (Accurate Computations with Totally Nonnegative Matrices):

- P. Koev. <http://www.math.sjsu.edu/~koev>

## Numerical experiments - Initial example

We will consider in the first place (with a slight adaptation) an example which appears in Lecture 19 of the book of Trefethen and Bau, a chapter devoted to the stability of the algorithms for least squares problems. We must slightly adapt the problem because we must avoid the points 0 and 1 to have the Bernstein-Vandermonde matrix strictly totally positive.

Also, taking into account the perturbation theory presented in Marco-Martínez (2013, ELA), it is important to have the greatest node not very close to 1.

Choosing  $m = 101$  and  $n = 15$  (the degree of the fitting polynomial will be 14) we have 100 nodes in  $(0, 1)$   $(1/101, \dots, 100/101)$  which we can introduce in MATLAB by means of the instruction

```
t = (1:m-1)'/m;
```

The corresponding Vandermonde matrix of size  $100 \times 15$  has condition number  $\kappa_2(A) = 2,99e + 10$ . We consider the fitting of the function  $f(t) = e^{\sin(4t)}$ , introducing the data vector  $f$  by means of the instruction (after the definition of the nodes  $t_i$ )

```
f = exp(sin(4*t));
```

We will compare the numerical results with the corresponding “exact” solutions obtained by using *Maple* with extended precision arithmetic (in this case we do not use exact rational arithmetic because the data vector is obtained evaluating the function  $f(t)$ ). By using the command  $c = A \backslash f$  of *MATLAB* we obtain the solution vector, and comparing with the exact solution  $c_e$  we obtain a relative error

$$\frac{\|c - c_e\|_2}{\|c_e\|_2} = 1,87e - 07,$$

a quantity close to that indicated in the example of Trefethen-Bau.



The authors comment this is a consequence of the fact that the condition number of  $A$  is of the order of  $10^{10}$  (very close to ours, in spite of the modification of the nodes) and that therefore the loss of accuracy in the solution is not due to the instability of the algorithm, but to the high condition number of  $A$ , which in the book is associated to the fact that the monomial basis  $1, t, \dots, t^{14}$  is an *ill-conditioned basis*.

If for the same problem we use the Bernstein basis the results are much better. We use our algorithm for computing the bidiagonal factorization of the corresponding Bernstein-Vandermonde matrix  $BV$ :

$$B = \text{TNBDBVR}(cf, 15);,$$

where the row vector  $cf$  is obtained by transposing the node vector:  $cf = t'$ .

From this matrix  $B$  we compute the  $QR$  factorization of the Bernstein-Vandermonde matrix  $BV$  (let us observe that  $BV$  is not constructed) by means of the algorithm  $\text{TNQR}$  of P. Koev.

The Bernstein-Vandermonde matrix for this problem has condition number  $\kappa_2(BV) = 1,07e + 04$ . The relative error in the computation of the coefficients of the fitting polynomial (now expressed in the Bernstein basis, given in the vector  $cb$ ) is

$$\frac{\|cb - cb_e\|_2}{\|cb_e\|_2} = 7,9e - 13,$$

which clearly shows the advantage of using a better conditioned basis.

## Numerical experiments

We compute the solution vector  $\bar{x}$  by means of:

- 1 Our approach.
- 2  $A \setminus b$  MATLAB command: Least squares based on QR.

We compute the relative errors by using the exact solution obtained in *Maple*.

## Numerical experiments - Example 1

We consider:

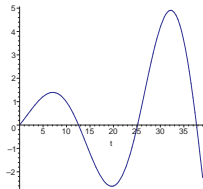
- The Bernstein–Vandermonde matrix  $A$  corresponding to the nodes

$$\begin{array}{l} \frac{1}{25} < \frac{9}{200} < \frac{1}{20} < \frac{53}{1000} < \frac{11}{200} < \frac{59}{1000} < \frac{31}{500} < \frac{67}{1000} < \frac{71}{1000} < \frac{77}{1000} < \\ \frac{83}{1000} < \frac{23}{250} < \frac{1}{10} < \frac{11}{100} < \frac{3}{25} < \frac{3}{20} < \frac{17}{100} < \frac{21}{100} < \frac{1}{4} < \frac{29}{100} < \frac{9}{25} < \\ \frac{11}{25} < \frac{1}{2} < \frac{11}{20} < \frac{279}{500} < \frac{281}{500} < \frac{283}{500} < \frac{143}{250} < \frac{577}{1000} < \frac{73}{125} < \frac{59}{100} < \frac{3}{5} < \\ \frac{61}{100} < \frac{63}{100} < \frac{16}{25} < \frac{67}{100} < \frac{7}{10} < \frac{73}{100} < \frac{37}{50} < \frac{149}{200} \end{array}$$

- The Vandermonde matrix  $V$  corresponding to the same nodes.
- The same vector  $b$  for both matrices (see Figure). Note that the desired polynomial is the same, expressed in the Bernstein basis or in the monomial basis.

The condition numbers are:  $\kappa_2(A) = 5,4e + 06$ ,  $\kappa_2(V) = 1,1e + 12$

Function for Example 1:  $f(x) = \sin(x/4) * \exp(x/20)$



## The original problem

- The data (vector  $b$ ) are computed by evaluating the function at the corresponding nodes in  $(0, 39)$ .
- For the problem in  $(0, 39)$  the corresponding Vandermonde matrix has the condition number

$$\kappa_2(V) = 2,06e + 23$$

## Relative errors in Example 1

| $\kappa_2(V)$ | $ex_1$  | $ex_2$  |
|---------------|---------|---------|
| 1.1e+12       | 7.5e-11 | 6.8e-08 |

**Vandermonde case**

| $\kappa_2(A)$ | $ex_1$  | $ex_2$  |
|---------------|---------|---------|
| 5.4e+06       | 1.7e-11 | 9.6e-11 |

**Bernstein-Vandermonde case**



## Triangular systems $Rx = d$

- (For triangular systems) the behaviour of the forward error, however, is intriguing, because the forward error is often surprisingly small -much smaller than we would predict from the normwise condition number  $\kappa$ .

(N. J. HIGHAM, Accuracy and Stability of Numerical Algorithms, second ed. SIAM, Philadelphia, 2002)

- The solution of triangular systems are usually computed to high accuracy. This fact... cannot be proved in general, for counter examples exist.

(G. W. STEWART, Introduction to Matrix Computations, 1973)

## Triangular systems $Rx = d$

In the factorization  $A = QR$ ,  $R$  inherits the spectral condition number of  $A$ , i.e.

$$\kappa_2(R) = \kappa_2(A).$$

Also, the accuracy of the solution of a totally positive triangular system  $Rx = d$  depends on  $d$ .

## Computation of $p = A\bar{x}$

- Having computed the solution vector  $\bar{x}$ , the projection vector  $p = A\bar{x}$  can be computed by using the *de Casteljau algorithm*, which evaluates a polynomial given by its coefficients in the Bernstein basis.
- Note that  $A$  is never constructed.

## Example 2: Projection matrix

We consider:

- The 40 nodes:

$$\begin{array}{cc}
 \frac{1}{25} < \frac{9}{200} < \frac{1}{20} < \frac{53}{1000} < \frac{11}{200} < \frac{59}{1000} < \frac{31}{500} < \frac{67}{1000} < \frac{71}{1000} < \frac{77}{1000} < \\
 \frac{83}{1000} < \frac{23}{250} < \frac{1}{10} < \frac{11}{100} < \frac{3}{25} < \frac{3}{20} < \frac{17}{100} < \frac{21}{100} < \frac{1}{4} < \frac{29}{100} < \frac{9}{25} < \\
 \frac{11}{25} < \frac{1}{2} < \frac{11}{20} < \frac{279}{500} < \frac{281}{500} < \frac{283}{500} < \frac{143}{250} < \frac{577}{1000} < \frac{73}{125} < \frac{59}{100} < \frac{3}{5} < \\
 \frac{61}{100} < \frac{63}{100} < \frac{16}{25} < \frac{67}{100} < \frac{7}{10} < \frac{73}{100} < \frac{37}{50} < \frac{149}{200}
 \end{array}$$

- The monomial basis of  $\Pi_{15}(x)$  ( $\Rightarrow A$  is Vandermonde).
- The Bernstein basis of  $\Pi_{15}(x)$  ( $\Rightarrow A$  is Bernstein-Vandermonde).

We compute the **relative error** of each computed projection matrix by using the exact projection matrix computed in *Maple*.

## Relative errors in Example 2

We compute the projection matrix by means of:

- Our algorithm.
- By using the  $QR$  factorization of **MATLAB**.

### Vandermonde case

| $\kappa_2(A)$ | Our alg. | MATLAB  |
|---------------|----------|---------|
| 1.1e+12       | 2.6e-15  | 1.1e-06 |

### Bernstein-Vandermonde case

| $\kappa_2(A)$ | Our alg. | MATLAB  |
|---------------|----------|---------|
| 5.5e+06       | 2.7e-15  | 1.5e-10 |

## QR factorization and our algorithm

- If  $A = QR$  with  $Q$  orthogonal, then  $\kappa_2(A) = \kappa_2(R)$ .  
 $R$  inherits the ill-conditioning of  $A$ .
- We compute the projection matrix by means of  $P = Q_1 Q_1^T$ .  
 **$R$  is not involved.**
- $Q_1$  is computed in an **efficient and accurate way**. The structure of  $A$  is taken into account.
- **$P$  is computed in an efficient and accurate way.**
- In Example 2 the relative errors are:
  - $A$  is a Vandermonde matrix:  $2.6e-15$
  - $A$  is a Bernstein-Vandermonde matrix:  $2.7e-15$

# Singular value computation.

**AIM:** To compute the singular values of a Bernstein-Vandermonde matrix  $A \in \mathbf{R}^{(l+1) \times (n+1)}$ ,  $l > n$ .

**INPUT:** The nodes  $x_i$  ( $i = 1, \dots, l + 1$ ) and the degree  $n$ .

**OUTPUT:** A vector  $x$  containing the singular values of  $A$ .

*Step 1:* Computation of the bidiagonal decomposition of  $A$  by using TNBDBV.

*Step 2:* Given the result of Step 1, computation of the singular values by using TNSingularValues ([Koev, 05]; package TNTTool).

## Example (singular values)

We consider:

- The Bernstein basis  $\mathcal{B}_{15}$ .
- The Bernstein-Vandermonde matrix  $A \in \mathbf{R}^{21 \times 16}$  generated by
$$\frac{1}{22} < \frac{1}{20} < \frac{1}{18} < \frac{1}{16} < \frac{1}{14} < \frac{1}{12} < \frac{1}{10} < \frac{1}{8} < \frac{1}{6} < \frac{1}{4} < \frac{1}{2} < \frac{23}{42} < \frac{21}{38} < \frac{19}{34} < \frac{17}{30} < \frac{15}{26} < \frac{13}{22} < \frac{11}{18} < \frac{9}{14} < \frac{7}{10} < \frac{5}{6}.$$

•



## Example

Its condition number is:  $\kappa_2(A) = 5,3e + 08$ .

We compute the **relative error** of each computed singular value by using the singular values calculated in *Maple 10* with 50-digit arithmetic.

## Example

We present **the two greatest relative errors** obtained when computing the singular values of  $A$  by means of:

- **Our algorithm:**
  - $1,8e - 15$  (15th singular value).
  - $1,1e - 15$  (10th singular value).
- **svd** from MATLAB:
  - $3,9e - 10$  (15th singular value).
  - $2,5e - 10$  (16th singular value).

**OBS:** We consider the singular values sorted from the largest to the smallest one.

## References

- A. Björck. Numerical Methods for Least Squares Problems. SIAM, Philadelphia, 1996.
- A. Björck, V. Pereyra. Solution of Vandermonde Systems of equations. *Mathematics of Computation* 24 (1970), 893–903.
- T. Boros, T. Kailath, V. Olshevsky. A fast parallel Björck-Pereyra-type algorithm for solving Cauchy linear equations. *Linear Algebra Appl.* 302/303 (1999), 265–293.
- J. M. Carnicer, J.M. Peña, Shape preserving representations and optimality of the Bernstein basis, *Advances in Computational Mathematics* 1 (1993), 173–196.
- J. Demmel, I. Dumitriu, O. Holtz, P. Koev. *Accurate and efficient expression evaluation and linear algebra*. *Acta Numerica*, 17 (2008), 1–59.

## References

- S. M. Fallat. Bidiagonal factorizations of totally nonnegative matrices. *American Mathematical Monthly* 108 (2001), 697–712.
- R. Farouki. The Bernstein polynomial basis: A centennial retrospective. *Computer Aided Geometric Design* 29 (6) (2012), 379-419.
- M. Gasca, J. M. Peña. Total positivity and Neville elimination. *Linear Algebra Appl.* 165 (1992), 25–44.
- M. Gasca, J. M. Peña. A matricial description of Neville elimination with applications to total positivity. *Linear Algebra Appl.* 202 (1994), 33–45.

## References

- N. J. Higham. Accuracy and Stability of Numerical Algorithms, second ed. SIAM, Philadelphia, 2002.
- N. J. Higham. An Interview with Gene Golub. MIMS EPrint 2008.8. The University of Manchester, 2008.
- P. Koev. <http://www.math.sjsu.edu/~koev>
- P. Koev. Accurate eigenvalues and SVDs of totally nonnegative matrices. SIAM J. Matrix Anal. Appl. 21 (2005), 1–23.
- P. Koev. Accurate computations with totally nonnegative matrices. SIAM J. Matrix Anal. Appl. 29 (2007), 731–751.

## References

- A. Marco, J. J. Martínez. *A fast and accurate algorithm for solving Bernstein-Vandermonde linear systems*. *Linear Algebra Appl.*, 422 (2007), 616–628.
- A. Marco, J. J. Martínez. Polynomial least squares fitting in the Bernstein basis. *Linear Algebra Appl.* 433 (2010), 1254–1264.
- A. Marco, J. J. Martínez. Accurate computations with totally positive Bernstein-Vandermonde matrices. *Electronic Journal of Linear Algebra: Vol. 26 Article 24* (2013).
- A. Marco, J. J. Martínez. Ajuste polinómico por mínimos cuadrados usando la base de Bernstein. *La Gaceta de la RSME*, Vol. 18 (2015), núm. 1, 135–153.

## References

- J. J. Martínez, J. M. Peña. Factorizations of Cauchy-Vandermonde matrices with one multiple pole, in: O. Pordavi (Eds.), *Recent Research on Pure and Applied Algebra*, Nova Sci. Publ., Hauppauge, NY, 2003, pp. 85–95.
- G. Mühlbach, M. Gasca. A test for strict total positivity via Neville elimination. In: *Current Trends in Matrix Theory* (F. Uhlig and R. Grone, eds.), North-Holland, 1987, pp. 225-232.
- J. M. Peña. Tests for the recognition of total positivity. *SeMA Journal* 62 (2013), 61–73.