Fast and Tight Bound Functions for Multivariate Polynomials with Applications to the Reliable Analysis of Structural Frames

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Outline

- The Bernstein expansion for polynomials and its properties
- Monomial analysis and an implicit representation
- Examples
- Earlier and recent applications
- Application to the solution of parametric linear systems

Bernstein Polynomials

$B_i(x) = \binom{l}{i} x^i (1-x)^{l-i}, \qquad 0 \le i \le l$

given: $p(x) = \sum_{i=0}^{l} a_i x^i$

wanted: $p(I) = \{p(x) \mid x \in I\}$ w.l.o.g. $I = [0,1]$

power form $\longrightarrow$ Bernstein form

$p(x) = \sum_{i=0}^{l} b_i B_i(x)$, where

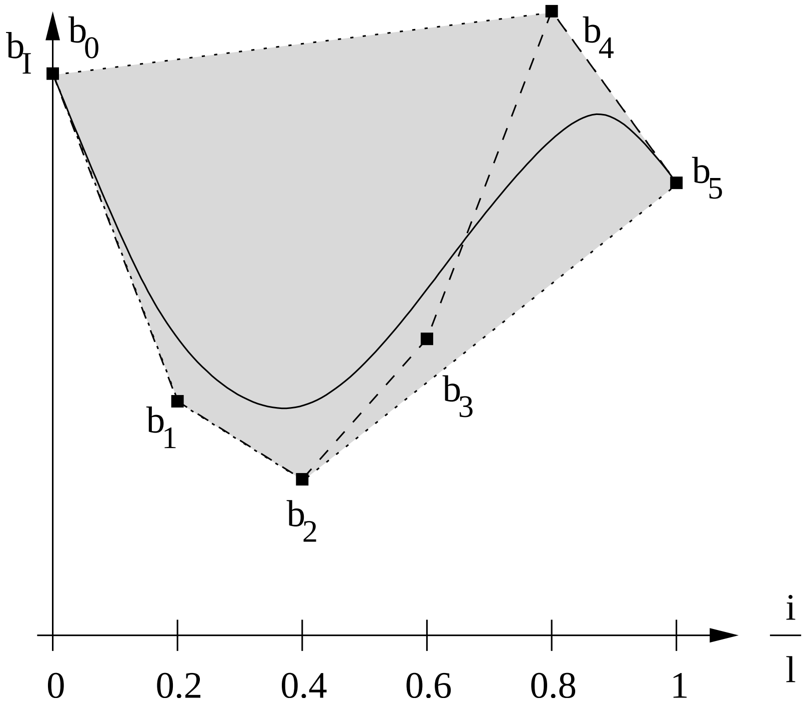
$$b_i = \sum_{j=0}^{i} \frac{\binom{i}{j}}{\binom{l}{j}} a_j, \quad 0 \le i \le l \qquad \textit{Bernstein coefficients}$$

in particular, $b_0 = a_0 = p(0), \qquad b_l = \sum_{i=0}^{l} a_i = p(1)$

can be calculated economically by difference table method (similarly to the de Casteljau algorithm).

Convex Hull Property

$$\left\{\binom{x}{p(x)} \;:\; x \in I\right\} \quad \subseteq \quad conv\left\{\binom{i/l}{b_i} \;:\; 0 \le i \le l\right\}.$$



Interval Enclosing Property

Theorem 1 *For all* $x \in I$

$$\min_{0 \le i \le l} b_i \le p(x) \le \max_{0 \le i \le l} b_i.$$

Notations

Multiindices $i = (i_1, \ldots, i_n)^T$ are vectors, where the components are nonnegative integers. (The vector 0 denotes the multiindex with all components equal to 0.)
Comparisons and arithmetic operators on multiindices are defined componentwise such that $i \odot l := (i_1 \odot l_1, \ldots, i_n \odot l_n)^T$, for $\odot = +, -, \times$, and / (with $l > 0$).
For $x \in \mathbf{R}^n$ its multipowers are $x^i := \prod_{\mu=1}^{n} x_\mu^{i_\mu}$.
We use the notations $\sum_{i=0}^{l} := \sum_{i_1=0}^{l_1} \ldots \sum_{i_n=0}^{l_n}$ and $\binom{l}{i} := \prod_{\mu=1}^{n} \binom{l_\mu}{i_\mu}$.

Interval Enclosing Property

Theorem 1 *For all* $x \in I$

$$\min_{0 \le i \le l} b_i \le p(x) \le \max_{0 \le i \le l} b_i.$$

Monomial Analysis

Now suppose that we have a polynomial

$$p(x) = \sum_{i=0}^{l} a_i x^i, \quad x = (x_1, \ldots, x_n),$$

in n variables, $x_1, \ldots, x_n$, of degree $l = (l_1, \ldots, l_n)$, and a box

$$X := [\underline{x}_1, \overline{x}_1] \times \ldots \times [\underline{x}_n, \overline{x}_n].$$

The generalised Bernstein coefficients b_i over X are given by

$$b_i = \sum_{j=0}^{i} \frac{\binom{i}{j}}{\binom{l}{j}} (\overline{x} - \underline{x})^j \sum_{k=j}^{l} \binom{k}{j} \underline{x}^{k-j} a_k, \quad 0 \le i \le l.$$

Bernstein coefficients of monomials

Theorem 2 *The multivariate Bernstein coefficients of a monomial are the products of the univariate Bernstein coefficients of its monomial components.*

Theorem 3 *Let $p(x) = a_k x^k$, $x = (x_1, \ldots, x_n)$, for some $0 \leq k \leq l$ and let X be a box which is restricted to a single orthant of $\mathbf{R}^n$. Then the Bernstein coefficients of p (of degree l) over X are monotone wrt each variable x_j, $j = 1, \ldots, n$.*

In this case, it is not necessary to explicitly compute the whole set of Bernstein coefficients. For boxes which intersect two or more orthants of $\mathbf{R}^n$, the box can be bisected, and the Bernstein coefficients of each single-orthant sub-box can be computed separately.

An implicit Bernstein form for polynomials

If the polynomial p consists of t terms, i.e.

$$p(x) = \sum_{j=1}^{t} a_{i_j} x^{i_j}, \quad 0 \leq i_j \leq l, \quad x = (x_1, \ldots, x_n),$$

then (due to the linearity of the Bernstein form) each Bernstein coefficient is equal to the sum of the corresponding Bernstein coefficients of each term:

$$b_i = \sum_{j=1}^{t} b_i^{(j)}, 0 \leq i \leq l,$$

where $b_i^{(j)}$ are the Bernstein coefficients of the jth term of p.

Instead of computing and storing the whole set of Bernstein coefficients, we can instead, for each term, compute the Bernstein coefficients of each component univariate monomial.

The space complexity is $\mathrm{O}(nt(\hat{l}+1))$, as opposed to $\mathrm{O}((\hat{l}+1)^n)$ for the explicit form, where $\hat{l} := \max\{l_j \,|\, j = 1, \ldots, n\}$.

Each Bernstein coefficient can be computed as required from the implicit form as a sum of t products, requiring $(n+1)t$ arithmetic operations.

Example

Let $n := 2$, $p(x) := x_1^3 x_2^2 - 30x_1x_2$, $l := (3,2)$, and the box $X := [1,2] \times [2,4]$. The sum of the corresponding Bernstein coefficients of each term gives the Bernstein coefficients of p:

$$\{b_i\} = \begin{pmatrix} 4 & 8 & 16 \\ 8 & 16 & 32 \\ 16 & 32 & 64 \\ 32 & 64 & 128 \end{pmatrix} + \begin{pmatrix} -60 & -90 & -120 \\ -80 & -120 & -160 \\ -100 & -150 & -200 \\ -120 & -180 & -240 \end{pmatrix}$$

$$= \begin{pmatrix} -56 & -82 & -104 \\ -72 & -104 & -128 \\ -84 & -118 & -136 \\ -88 & -116 & -112 \end{pmatrix}.$$

The implicit form of these coefficients can be depicted as

$$\begin{matrix} \mathbf{1} & \begin{pmatrix} 4 & 8 & 16 \end{pmatrix} \\ \begin{pmatrix} 1 \\ 2 \\ 4 \\ 8 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \end{matrix} + \begin{matrix} \mathbf{-30} & \begin{pmatrix} 2 & 3 & 4 \end{pmatrix} \\ \begin{pmatrix} 1 \\ \frac{4}{3} \\ \frac{5}{3} \\ 2 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \end{matrix}.$$

Determination of the minimum (or maximum) Bernstein coefficient

We wish to determine the value of the multiindex $i_{\min}$, $0 \le i_{\min} \le l$, of the minimum Bernstein coefficient in each direction. In order to reduce the search space (among the $(\hat{l}+1)^n$ Bernstein coefficients) we can exploit Theorem 3 and employ the following tests:

- **Uniqueness**: If a variable x_j appears only once, then the Bernstein coefficients of the term in which it appears determines $i_{\min_j}$.
- **Monotonicity**: If all terms containing x_j are likewise monotone wrt x_j, then $i_{\min_j} = 0$ or l_j.
- **Dominance**: Otherwise, all the terms containing x_j can be split into two sets, depending on whether they are increasing or decreasing wrt x_j. If the width of the Bernstein enclosure of one set is less than the minimum difference between Bernstein coefficients among the terms of the other set, then the first set can make no contribution to the determination of $i_{\min_j}$, and the monotonicity clause applies.

Example

$$p(x) = 3x_1x_2^5 + 2x_1^4x_2 - 8x_1^2x_3^6x_4^2 - x_1x_4^8 + 3x_2^3x_5 - 10x_4^5x_5^5x_6^5 + 0.01x_5^2x_6^2 + 4x_5^3x_7^4$$

$$X = [1, 2]^7.$$

The degree, l, is $(4, 5, 6, 8, 5, 5, 4)$ and the number of Bernstein coefficients is 340200 $(5 \times 6 \times 7 \times 9 \times 6 \times 6 \times 5)$.

$$p(x) = 3x_1x_2^5 + 2x_1^4x_2 - 8x_1^2x_3^6x_4^2 - x_1x_4^8 + 3x_2^3x_5 - 10x_4^5x_5^5x_6^5 + 0.01x_5^2x_6^2 + 4x_5^3x_7^4$$

- Uniqueness: x_3 appears only in term 3, which is decreasing wrt it. Therefore $i_{\mathsf{min}3} = 6$.

- Uniqueness: x_7 appears only in term 8, which is increasing wrt it. Therefore $i_{\mathsf{min}7} = 0$.

- Monotonicity: x_2 appears in terms 1 and 2, both of which are increasing wrt it. Therefore $i_{\mathsf{min}2} = 0$.

- Monotonicity: x_4 appears in terms 3, 4, and 6, all of which are decreasing wrt it. Therefore $i_{\mathsf{min}4} = 8$.

- Dominance: x_6 appears in terms 6 and 7, one of which is decreasing and one of which is increasing wrt it. However term 6 dominates term 7 to such an extent that term 7 plays no role in determining $i_{\mathsf{min}6}$. Therefore $i_{\mathsf{min}6} = 5$, since term 6 is decreasing wrt x_6.

$$p(x) = 3x_1x_2^5+2x_1^4x_2-8x_1^2x_3^6x_4^2-x_1x_4^8+3x_2^3x_5-10x_4^5x_5^5x_6^5+0.01x_5^2x_6^2+4x_5^3x_7^4$$

$$i_{\mathsf{min}} = (?, 0, 6, 8, ?, 5, 0)$$

The dimensionality of the search space has thus been reduced from 7 to 2. The number of Bernstein coefficients to compute is consequently reduced from 340200 to 30 (5×6), plus those needed for the implicit Bernstein form, 78 ($8 + 7 + 13 + 11 + 6 + 18 + 6 + 9$), 108 total.

Numerical Results

- Simulation of a branch and bound approach:
  - A bisection in each direction in turn is performed.
  - One of the two resulting subboxes is retained and the other is discarded.
  - After each bisection, the Bernstein enclosure is recomputed over the new box.
  - This process is iterated 100 times.
- Verified computation: the Bernstein coefficients are stored as intervals, and interval arithmetic is used.

The first test problem (test1) is

$$p(x) = 3x_1^2x_2^3x_3^4 + 1x_1^3x_2x_3^4 - 5x_1x_2x_4^5 + 1x_3x_4x_5^3$$

over the box

$$X = [1,2] \times [2,3] \times [4,6] \times [-5,-2] \times [2,10].$$

The second (test2) is the example previously presented. The remaining test problems are drawn from GLOBALLib; where unspecified, a suitable single-orthant starting box of unit width was chosen.

A. P. Smith *"Fast construction of constant bound functions for sparse polynomials"*, J. Global Optimization **43** (2-3), pp. 445–458 (2009)

J. Garloff, A. P. Smith *"Rigorous affine lower bound functions for multivariate polynomials and their use in global optimisation"*, Lect. Notes Management Sci. **1**, pp. 199–211 (2008)

				Bernstein Form			Implicit Bernstein Form		
Name	n	t	l	Iters.	# BCs	time (s)	Iters.	# BCs	time (s)
test1	5	4	$(3,3,4,5,3)$	1-100	1920	0.01	1-3 4-5 6-100	60 12 2	0.0001
test2	7	8	$(4,5,6,8,$ $5,5,4)$	1-100	340200	6.05	1-9 10-100	60 12	0.0004
mhw4d	5	17	$(2,3,4,4,4)$	1-100	1500	0.04	1-3 4-100	1000 200	0.0068
meanvar	7	49	$(2,2,2,2,$ $2,2,2)$	1-100	2187	0.24	1-100	2	0.0008
ex2_1_5	10	16	$(2,2,2,2,2,$ $2,2,1,1,1)$	1-100	17496	0.83	1-100	2	0.0003
harker	20	40	$(3,3,3,3,3,$ $3,3,3,3,3,$ $3,3,3,3,2,$ $2,2,2,2,2)$	1-100	1.96 $\times 10^{11}$	$> 10^5$	1-100	2	0.0019

Earlier Applications

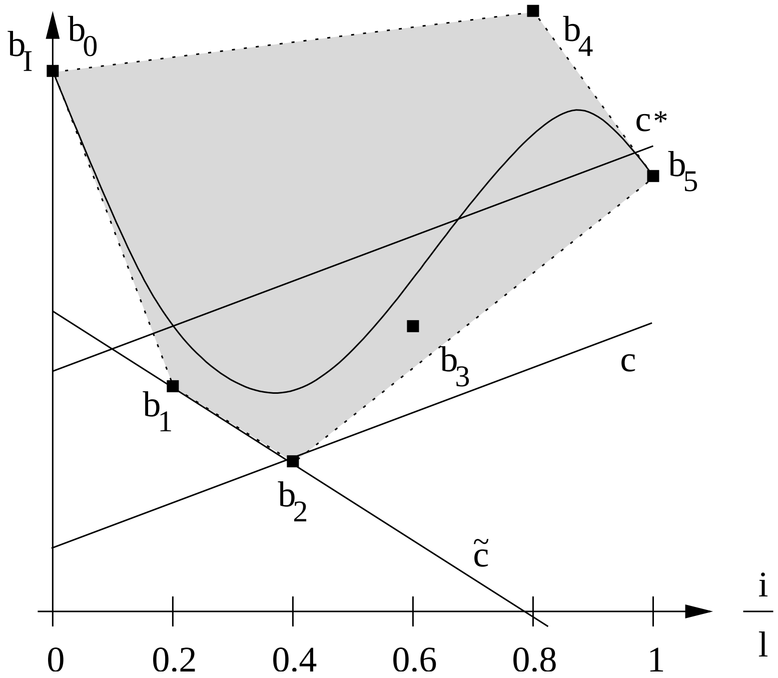
- Robust control problems, e.g., checking stability of a polynomial with coefficients depending polynomially on parameters varying in given intervals

- Enclosure of the solution set of systems of polynomial equations and inequalities

Recent Applications to Global Optimization

- We have a constrained global optimization problem, where one or more of the objective or constraint functions are multivariate polynomials.

- In a branch and bound framework, relaxations may be used. For each subbox, the objective function and some of the constraints may be replaced by bounding functions (convex, affine, constant) which are easier to handle.



b_I
b_0
b_4
c*
b_5
b_3
c
b_1
b_2
c̃
i
l
0
0.2
0.4
0.6
0.8
1

Rigorous Bound Functions

Due to rounding errors, inaccuracies may be introduced into the calculation of the Bernstein coefficients and the corresponding bound functions. As a result, the computed affine function may not stay below the given polynomial over the box of interest. We also wish to consider the case of uncertain polynomial coefficients, assuming that for each coefficient a lower and an upper bound are known. In either case, it is often desirable to compute the affine lower bound functions in such a way that it can be *guaranteed* to stay below the given polynomial.

Verified version for interval data

1. Compute the Bernstein coefficients as before, using interval arithmetic. Since each polynomial coefficient contributes only once to each Bernstein coefficient, this can be done without overestimation.

2. Compute the linear least squares approximation as before, using the midpoints of the control points / Bernstein coefficients.

3. Compute the discrepancy and perform downward shift according to lower bounds of the control points / Bernstein coefficients.

Only the first and last steps need to be performed rigorously, so that little extra computational effort is required.

Application to Parametric Linear Systems

Given: $A(p) \cdot x = b(p)$,

where $A(p) \in \mathbf{R}^{n \times n}$, $b(p) \in \mathbf{R}^n$ are depending on $p \in [p] = ([p_1], \ldots, [p_k])^T$.

Parametric solution set

$$\mathbf{\Sigma}_p = \mathbf{\Sigma}(A(p), b(p), [p]) := \{x \in \mathbf{R}^n \,|\, A(p) \cdot x = b(p) \text{ for some } p \in [p]\}$$

wanted: $\square\Sigma_p = [\inf \Sigma_p, \sup \Sigma_p]$ or a tight enclosure for it.

Parametric Residual Iteration (Popova '05, Rump '90)

Define $\breve{p} := \mathrm{mid}([p])$, $\breve{A} := A(\breve{p})$, $\breve{b} := b(\breve{p})$.
Let $R \approx \breve{A}^{-1}$, $\tilde{x} \approx R\breve{b}$ and define $[z],[y] \in \mathbf{IR}^n$, $[C] \in \mathbf{IR}^{n\times n}$ by

$$\begin{aligned}
[z] &:= \Box\left\{R(b(p) - A(p)\tilde{x}) \mid p \in [p]\right\},\\
[y] &:= [z] + [-\varepsilon,\varepsilon]\cdot \mathrm{rad}([z]),\\
[C] &:= \Box\left\{I - R\cdot A(p) \mid p \in [p]\right\}.
\end{aligned}$$

Define $[v] \in \mathbf{IR}^n$ by means of the following Einzelschrittverfahren

$$1 \le i \le n \quad : \quad [v_i] := \left\{[z] + [C]\cdot([v_1],\dots,[v_{i-1}],[y_i],\dots,[y_n])^T\right\}_i .$$

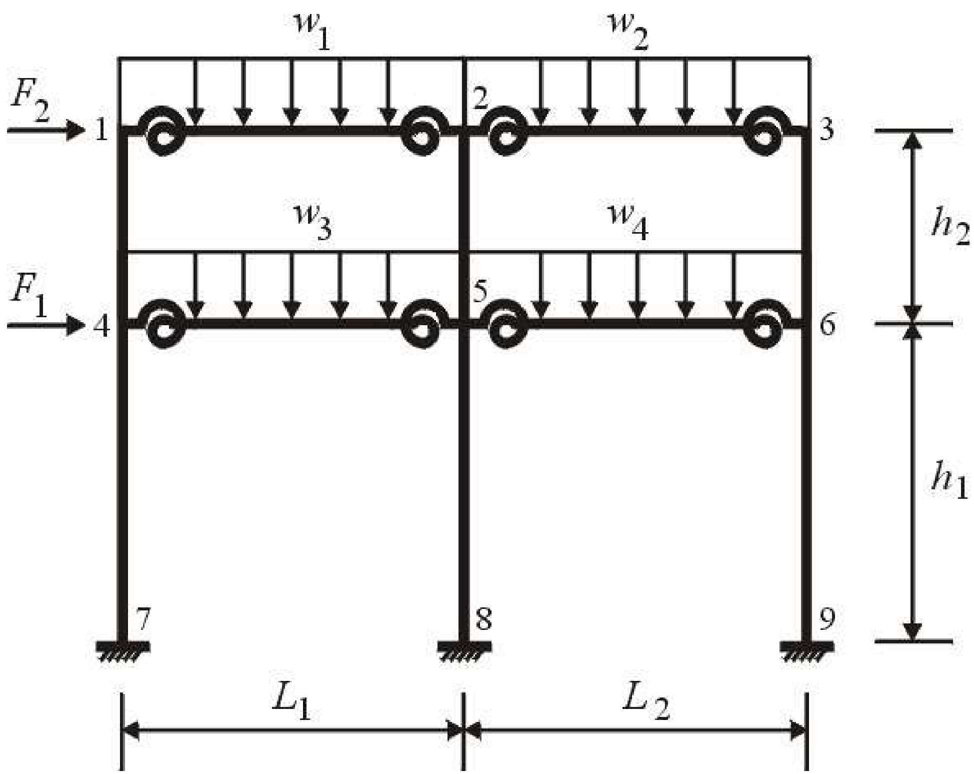
If $[v] \overset{\subset}{\neq} [y]$, then R and every matrix $A(p)$ with $p \in [p]$ are regular, and for every $p \in [p]$ the unique solution $\hat{x} = A^{-1}(p)b(p)$ satisfies $\hat{x} \in \tilde{x} + [v]$.

Software tools for the rigorous enclosure of the solution set of a parametric linear system involving rational dependencies provided by E. Popova in a *Mathematica* environment:

`Parametic_Solve`: Based on the arithmetic of proper and improper intervals.

`polyRational_Solve`: Uses software for the Bernstein enclosure provided by A. P. Smith (based on the `C++` interval library `filib++`).

Example: Two-Bay Two-Story Frame



1st problem: Parametric linear system of order 18 with 13 uncertain parameters

	Columns (HE 280 B)	Beams (IPE 400)
Cross-sectional area	$A_c = 0.01314\,\mathrm{m}^2$,	$A_b = 0.008446\,\mathrm{m}^2$
Moment of inertia	$I_c = 19270 * 10^{-8}\,\mathrm{m}^4$,	$I_b = 23130 * 10^{-8}\,\mathrm{m}^4$
Modulus of elasticity	$E_c = 2.1 * 10^8\,\mathrm{kN/m}^2$,	$E_b = 2.1 * 10^8\,\mathrm{kN/m}^2$
Rotational spring stiffness	$c = 10^8\,\mathrm{kN}$	
Uniform vertical load	$w_1 = \ldots = w_4 = 30\,\mathrm{kN/m}$	
Concentrated lateral forces	$f_1 = f_2 = 100\,\mathrm{kN}$	

tolerances: material properties 1%, spring stiffness and all applied loadings 10%

`Parametic_Solve`	ca. 14 s
`polyRational_Solve`	ca. 1.3 s

2nd problem: Same structure as before, but assuming that each structural element has properties varying independently (within 1% tolerance) results in a system with 37 parameters.

`Parametic_Solve`	ca. 13 min
`polyRational_Solve`	ca. 4 min

Present Work

- More complex models of the FEM, e.g., problems with uncertain node locations.

Future Work

- Construction of affine bound functions for polynomials, based upon the implicit Bernstein form. Affine bound functions provide shape information and bound the graph of the polynomial more tightly, but (currently) require many explicit Bernstein coefficients.
- Further deployment and testing of the constant and affine bound functions in the branch and bound framework in existing software packages for the solution of global optimization problems, e.g., at the University of Vienna (COCONUT) and at the Indian Institute of Technology Bombay.