Multivariate Polynomials (with MacaulayLab) for Beginners

Flanders Al Research Day

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Why multivariate polynomials?



Outline

1 | Introduction

- 2 | Definitions, Examples, and Applications
- 3 | Different Solution Approaches
 - a | Normal Form Methods
 - b | Homotopy Continuation Methods
- 4 | Very Short MacaulayLab Demo
- 5 | Multiparameter Eigenvalue Problems
- 6 | Conclusion

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Multivariate polynomials

A multivariate polynomial p(x), or $p(x_1, \ldots, x_n)$, in n variables is a finite linear combination of monomials x^{α} from K^n with coefficients c_{α} from K:

$$p(\boldsymbol{x}) = \sum_{\mathcal{A}} c_{\boldsymbol{lpha}} \boldsymbol{x}^{\boldsymbol{lpha}}$$

where the summation runs over all the exponents in the set \mathcal{A} .

- K can be any field: complex numbers \mathbb{C} , real numbers \mathbb{R} , or finite numbers \mathbb{F}_q
- $\boldsymbol{\alpha}=(\alpha_1,\ldots,\alpha_n)$ indexes the monomials $\boldsymbol{\alpha}^{\boldsymbol{lpha}}$ and coefficients $c_{\boldsymbol{lpha}}$
- set of monomials, \mathcal{C}_d^n , consists out of $\binom{d+n}{n}$ elements
- example: $p(\boldsymbol{x}) = 3 + \sqrt{5}x_1 + (1+i)x_2 + \frac{3}{2}x_1^2x_2^8$

Multivariate polynomials

• Typically, multivariate polynomials appear in systems of multivariate polynomial equations:

$$egin{cases} p_1(oldsymbol{x}) &= \sum_{\mathcal{A}} c^{(1)}_{oldsymbol{lpha}} oldsymbol{x}^{oldsymbol{lpha}} = 0, \ dots \ p_s(oldsymbol{x}) &= \sum_{\mathcal{A}} c^{(s)}_{oldsymbol{lpha}} oldsymbol{x}^{oldsymbol{lpha}} = 0, \end{split}$$

where we look for the solutions of s multivariate polynomials in n variables.

• Every polynomial has a total degree: $d_i = \max(|\boldsymbol{\alpha}|)$.

Combinatorial explosion



Combinatorial explosion of the number of monomials in the set C_d^n with respect to the maximum total degree d and number of variables n. The cardinality of C_d^n is given for n = 1 (--), n = 2 (--), n = 3 (--), n = 4 (--), and n = 5 (--).

Two limit cases

univariate polynomial (n = 1)

linear systems $(d_i = 1)$

$$\left\{egin{aligned} p_1(oldsymbol{x}) &= b_1 + \sum_{j=1}^n a_{1j} x_j \ dots \ p_s(oldsymbol{x}) &= b_s + \sum_{j=1}^n a_{sj} x_j \ \psi \ oldsymbol{A} oldsymbol{x} &= oldsymbol{b} \end{aligned}
ight.$$

These are well-known problems from linear algebra

Different polynomial basis

$$p(\boldsymbol{x}) = \sum_{\mathcal{W}} \tilde{c}_{\boldsymbol{\omega}} t_{\boldsymbol{\omega}(\boldsymbol{x})}$$

A multivariate Chebyshev polynomial of degree $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$:

$$t_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \prod_{i=1}^{n} t_{\alpha_i}^*(x_i) = \prod_{i=1}^{n} \cos\left(\alpha_i \cos^{-1}(x_i)\right),$$

where $t^*_{\alpha_i}(x_i)$ corresponds to the univariate Chebyshev polynomial of degree α_i .

Examples:

$$t_2(x) = 2x^2 - 1$$

$$t_{13}(x_1, x_2) = x_1 (4x_2^3 - 3x_2)$$

$$t_{162}(x_1, x_2, x_3) = x_1 (32x_2^6 - 48x_2^4 + 18x_2^2 - 1) (2x_3^2 - 1)$$

polynomial optimization problems

$$\min_{oldsymbol{x}\in K^n}g(oldsymbol{x})$$
 subject to $h_1(oldsymbol{x})=\cdots=h_l(oldsymbol{x})=0$ \downarrow

This can be solved via the Lagrangian $\mathcal{L}(\boldsymbol{x},\lambda_1,\ldots,\lambda_l)$:

$$\mathcal{L}(\boldsymbol{x},\lambda_1,\ldots,\lambda_l)=g(\boldsymbol{x})-\lambda_1h_1(\boldsymbol{x})-\cdots-\lambda_lh_l(\boldsymbol{x})$$

The first-order necessary conditions are given by the partial derivatives:

$$\frac{\partial \mathcal{L}}{\partial x_1} = \cdots = \frac{\partial \mathcal{L}}{\partial x_n} = h_1(\boldsymbol{x}) = \cdots = h_l(\boldsymbol{x}) = 0$$



robotics and kinematics



computational chemistry

The (bio)chemical reaction network of the T-cell signal transduction model:





computer graphics

Estimating internal calibration parameters of a camera from point correspondences in a sequence of (noisy) images:



system identification and time series



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Find all the values for $x \in \bar{K}^n$ such that $p_1(x) = \cdots = p_s(x) = 0$, i.e., the variety of the polynomial system

$$\mathcal{V}(p_1,\ldots,p_s) = \left\{ \boldsymbol{a} \in \bar{K}^n : p_i(\boldsymbol{a}) = 0, \forall i = 1,\ldots s \right\}$$

- Typically, we consider polynomial systems which are well-determined! This can be for both square and rectangular systems.
- Some solution approaches can deal with over-determined polynomial systems.
- Under-determined polynomial systems could be solved in a certain sense, but what does it mean?



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Everything depends on the ground field that you consider!



This polynomial system has 9 solutions in $\mathbb{C}^2,\,1$ solution in $\mathbb{R}^2,$ and 0 solutions in \mathbb{Q}^2

Some examples:

- C: homotopy continuation, particle physics
- R: optimization, chemical reaction networks, robotics
- Q: discriminants/resultants, Grassmannians, number theory
- \mathbb{F}_q : cryptography
- $\mathbb{C}\{\{t\}\}, \mathbb{Q}_p$: tropical geometry

Number of solutions?

- For univariate polynomials (i.e., n = 1), the fundamental theorem of algebra states that a degree d polynomial has d roots.
- The theorem of Bézout is the multivariate extension of that theorem.

For any square system (i.e., s = n) of multivariate polynomial equations $p_1(\boldsymbol{x}), \ldots, p_n(\boldsymbol{x})$, the number of isolated solutions in the projective space \mathbb{P}^n when the solution set is zero-dimensional, i.e., the number of isolated points in the zero-dimensional variety $\mathcal{V}(p_1(\boldsymbol{x}), \ldots, p_n(\boldsymbol{x})) \subset \mathbb{P}^n$, is exactly equal to

$$m_b = d_1 \cdots d_n = \prod_{i=1}^n d_i,$$

where d_i is the total degree of the polynomial $p_i(x)$.

Number of solutions?

 The theorem of Bézout counts the number of isolated solutions in the projective space:

$$m_b = m_a + m_\infty$$

- For generic systems, $m_b = m_a$, but in practice this is not the case
- There exist more refined bounds on the number of affine solutions (e.g., Kushnirenko, BKK, etc.)



Different solution approaches

When we consider an algebraically closed field, there are two main methods to solve systems of multivariate polynomial equations:

normal form methods

- reduce problem to a univariate problem
- (numerical) linear algebra
- any field K^n
- rectangular systems: $s \ge n$
- $m_b < \pm 10\,000$ solutions

homotopy continuation methods

- continuously deform a system with known solutions
- ordinary differential equations
- field of complex numbers \mathbb{C}^n
- square systems: s = n
- $m_b < \pm 1\,000\,000$ solutions

Implementations

normal form methods

- Macaulay2
- Singular
- Magma
- msolve
- Mathematica
- Oscar.jl
- Maple
- MacaulayLab

• ...

homotopy continuation methods

- HomotopyContinuation.jl
- Bertini
- NAG4M2
- Hom4PS-3
- PHCpack
- . . .

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Normal form methods and the Macaulay matrix

 $\begin{cases} p_1(\boldsymbol{x}) = \boldsymbol{a}_{00} + \boldsymbol{a}_{10}x_1 + \boldsymbol{a}_{01}x_2 + \boldsymbol{a}_{20}x_1^2 + \boldsymbol{a}_{11}x_1x_2 + \boldsymbol{a}_{02}x_2^2 = 0\\ p_2(\boldsymbol{x}) = \boldsymbol{b}_{00} + \boldsymbol{b}_{10}x_1 + \boldsymbol{b}_{01}x_2 + \boldsymbol{b}_{20}x_1^2 + \boldsymbol{b}_{11}x_1x_2 + \boldsymbol{b}_{02}x_2^2 = 0 \end{cases}$ ∜ x_{1}^{2} x_1 x_2 a_{10} a_{20} $p_1(x) = a_{00}$ a_{01} 0 0 $x_1 p_1(x)$ a_{00} a_{10} $\begin{array}{c} x_1 x_2 \\ x_2^2 \\ x_1^3 \\ x_1^2 x_2 \\ x_1 x_2^2 \end{array}$ 0 0 0 0 $x_2 p_1(\boldsymbol{x})$ a_{00} a_{10} a_{01} a_{20} a_{11} a_{02} = 0 b_{10} b_{20} b_{11} $b_{02} = 0 = 0$ 0 b_{01} 0 $p_2(\boldsymbol{x})$ b_{00} 0 b_{10} b_{01} 0 b_{20} b_{11} b_{02} 0 0 b_{00} $x_1 p_2(\boldsymbol{x})$ b_{10} b_{01} 0 b_{20} b_{02} 0 0 b_{00} 0 b_{11} $x_2 p_2(\boldsymbol{x})$ Macaulay matrix

Structured right null space

Basis matrix of the right null space can be written in terms of the solutions $(d \ge d_*)$

- solutions can be described by the dual vector space of the quotient space
- from the rank-nullity theorem

$$n_d = q_d - r_d$$

= dim $\mathcal{P}_d^n / \left\langle p_1^h(\tilde{\boldsymbol{x}}), \dots, p_s^h(\tilde{\boldsymbol{x}}) \right\rangle_d$

• requires dual vector space $C_d^{n'}$ of C_d^n and differential functionals

$$\left. \partial_{\boldsymbol{i}}(\cdot) \right|_{(j)} \triangleq \left. \frac{1}{i_1! \dots i_n!} \frac{\partial^{|\boldsymbol{i}|}(\cdot)}{\partial x_1^{i_1} \dots \partial x_n^{i_n}} \right|_{(j)}$$

confluent multivariate Vandermonde basis matrix (projective setting) $x_0^2|_{(1)}$ $x_0 x_1|_{(1)}$ $x_0 x_1$ $x_0 x_2|_{(1)}$ $|x_0x_2|_{(2)}$ x_{1}^{2} $x_1 x_2$ x_{2}^{2} $\left.\partial_{00}(oldsymbol{v})
ight|_{(1)}$ $\partial_{10}(\boldsymbol{v})|_{(1)}$ $\partial_{00}(\boldsymbol{v})|_{(2)}$

one projective solution





one projective solution



Note that we consider differential functionals in $\mathcal{C}_2^{2'}$ in this exposition.



multiple simple projective solutions



multiple projective solutions with multiplicity greater than one



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Note that we consider differential functionals in $\mathcal{C}_2^{2'}$ in this exposition.

multiple affine solutions with multiplicity greater than one



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select the linearly independent rows of V_d

Note that we consider differential functionals in $\mathcal{C}_2^{2'}$ in this exposition.

multiple affine solutions with multiplicity greater than one



eigenvalue problem!

 $\boldsymbol{S}_1 \boldsymbol{V}_d \boldsymbol{D}_{x_1} = \boldsymbol{S}_{x_1} \boldsymbol{V}_d$

Three difficulties

$$\boldsymbol{S}_1 \boldsymbol{V}_d \boldsymbol{D}_{x_1} = \boldsymbol{S}_{x_1} \boldsymbol{V}_d$$

• Solutions/confluent Vandermonde basis vectors are not known in advanced:

numerical basis matrix Z_d of the right null space $(V_d = Z_d T)$ $\downarrow \downarrow$ $(S_1 Z_d) T D_{x_1} = (S_{x_1} Z_d) T$ $T D_{x_1} T^{-1} = (S_1 Z_d)^{-1} (S_{x_1} Z_d)$

• Not possible to numerically stable compute Jordan normal form:

numerically stable Schur decomposition

$$\downarrow$$

 $\boldsymbol{Q} \boldsymbol{U}_{x_1} \boldsymbol{Q}^{-1} = (\boldsymbol{S}_1 \boldsymbol{Z}_d)^{-1} (\boldsymbol{S}_{x_1} \boldsymbol{Z}_d)$

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• Solutions at infinity need to be deflated via a column compression

(Dreesen, 2013; Corless et al., 1997; Vermeersch and De Moor, 2021)

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Homotopy continuation methods





Homotopy continuation methods

$$Q(\boldsymbol{x}) = (q_1(\boldsymbol{x}), \dots, q_n(\boldsymbol{x})) \rightarrow P(\boldsymbol{x}) = (p_1(\boldsymbol{x}), \dots, p_n(\boldsymbol{x}))$$

$$H(\boldsymbol{x},t) = (1-t)Q(\boldsymbol{x}) + tP(\boldsymbol{x}), \quad t = 0 \to 1$$





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MacaulayLab toolbox

www.macaulaylab.net



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Multiparameter eigenvalue problem

The multiparameter eigenvalue problem (MEP) $\mathcal{M}(\lambda)z = 0$ consists in finding all *n*-tuples $\lambda = (\lambda_1, \ldots, \lambda_n) \in \mathbb{C}^n$ and corresponding vectors $z \in \mathbb{C}^{l \times 1} \setminus \{0\}$, so that

$$\mathcal{M}(oldsymbol{\lambda})oldsymbol{z} = \left(\sum_{\{oldsymbol{\omega}\}}oldsymbol{A}_{oldsymbol{\omega}}oldsymbol{\lambda}^{oldsymbol{\omega}}
ight)oldsymbol{z} = oldsymbol{0},$$

with $\| \boldsymbol{z} \|_2 = 1$.

- $oldsymbol{\omega}=(\omega_1,\ldots,\omega_n)$ indexes the monomials $oldsymbol{\lambda}^{oldsymbol{\omega}}$ and coefficient matrices $oldsymbol{A}_{oldsymbol{\omega}}$
- rectangular[†] coefficient matrices $A_{\omega} = A_{(\omega_1,...,\omega_n)} \in \mathbb{R}^{k \times l}$ with $k \ge l + n 1$
- example: $(A_{000} + A_{200}\lambda_1^2 + A_{013}\lambda_2\lambda_3^3)z = 0$

[†]We consider only rectangular problems in this presentation, so we no longer mention the term "rectangular" explicitly.

Unifying framework for (multiparameter) eigenvalue problems

Different types of (multiparameter) eigenvalue problems in a two-dimensional grid[†].

Spectral parameter(s)	Linear	Polynomial
Eigenvalues $(n = 1)$	Type I	Type II
	$\{1,\lambda\}$	λ^ω
	$oldsymbol{A}-oldsymbol{B}\lambda$	$oldsymbol{A}_0+oldsymbol{A}_1\lambda+\dots+oldsymbol{A}_d\lambda^d$
	SEP/GEP	PEP
Eigentuples $(n > 1)$ $(i = 1, \dots, n)$	Type III	Type IV
	λ_i	$oldsymbol{\lambda}^{oldsymbol{\omega}} = \prod_{i=1}^n \lambda_i^{\omega_i}$
	$oldsymbol{A}_{00}+oldsymbol{A}_{10}\lambda_1+oldsymbol{A}_{01}\lambda_2$	$oldsymbol{A}_{00}+oldsymbol{A}_{11}\lambda_1\lambda_2+oldsymbol{A}_{03}\lambda_2^3$
	linear MEP	polynomial MEP

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[†] SEP = standard eigenvalue problem, GEP = generalized eigenvalue problem, and PEP = polynomial eigenvalue problem

Examples and applications



- Identification of misfit-versus-latency models
- Model order reduction in the \mathcal{H}_2 -norm

Extension to the block Macaulay matrix



Two solution approaches





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- Multivariate polynomials are omnipresent in science and engineering
- There exist many different solution approaches
- Depending on the application, there could be a lot of structure available



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