# Hypatia Graduate School 2024
# Basics on methods from computational algebra

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**Our goal for this class:**

Present basic computational tools to deal with polynomials.

# Our setting

- (Bio)chemical reaction networks define systems of ordinary differential equations with (in general, unknown) parameters
- We will assume: Mass Action Kinetics (MAK). Then, the associated system of differential equations in an autonomous polynomial dynamical system $\dot{x} = f(x)$ in many variables.
- We will present a super quick introduction to Gr´obner bases and elimination of variables.
- We will also recall Descartes rule of signs and Sturm theorem about real roots of univariate polynomial with real coefficients.

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# Dealing with polynomials in several variables

A good reference is the book Ideals, varieties and algorithms, by Cox, Little and O'Shea.

Definition: A term order $\prec$ is a total order on the monomials $x^\alpha = x_1^{\alpha_1} \dots x_n^{\alpha_n}$ (or on their exponents $\alpha \in \mathbb{Z}^n_{\geq 0}$) such that if $x^\alpha \prec x^\beta$, for any $\gamma$ we have that $x^{\alpha+\gamma} \prec x^{\beta+\gamma}$ and $1 \prec x^\alpha$, for any $\alpha$.
For instance, we can consider a lexicographic order (associated with an order of the variables), a degree-lexicographic order, the reverse degree-lexicographic order, orders given by weights, etc.

The polynomial ideal $I_f$ generated by a finite number of polynomials $f_1, \dots, f_s \in k[x_1, \dots, x_n]$ is given by all the linear combinations $\sum_{i=1}^{s} g_i f_i$ with $g_1, \dots, g_s$ polynomials in $k[x_1, \dots, x_s]$. All polynomial ideals are of this form. A Gröbner basis (GB) of $I_f$ associated with a given term order $\prec$ is a system of generators of $I_f$ with good properties.

## An example

- We compute a GB of the ideal generated by $f_1 = x^2, f_2 = x - y^2$ w.r. to the lexicographic order with $y \prec x$.
- $f_3 = S(f_1, f_2) = f_1 - xf_2 = x^2 - x^2 + xy^2 = xy^2$.
- $S(f_1, f_3) = 0$ (monomials).
- $f_4 = S(f_2, f_3) = y^2 f_2 - f_3 = y^2 x - y^4 - xy^2 = -y^4$.
- All further $S$-polynomials are 0. A GB is given by $\{f_1, f_2, f_3, f_4\}$, but in fact as the respective leading terms are $x^2, x, xy^2, y^4$, also $\{f_2, f_4\} = \{x - y^2, y^4\}$ is a (reduced) GB of $I_f$.
- As the zero set of $f_1$ and $f_2$ (and of all the polynomials in $I_f$) is the origin $(0, 0)$ then, as $y$ vanishes there, Hilbert Nullstellensatz asserts that there is a power of $y$ that lies in the ideal, and we found such a power (the minimal one).
- If we take the lexicographic order with $x \prec y$, the leading terms are $f_1 = x^2, f_2 = x - y^2$, which are coprime, and thus they are already a GB of $I_f$ for this other term order.

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# Some comments

- For a linear system, lexicographic Gröbner basis = Gauss elimination.
- We can use GB computations to find all linear relations (with constant coefficients, not polynomial coefficients). Problem: How?.
- In the previous example $y^4 = -(x+y^2)(x-y^2) + 1\, x^2$ but it cannot be obtained only with constant coefficients, we need polynomial coefficients. How can we know this?
- GB's are implemented in all CAS = Computer algebra systems (e.g. Macaulay2, Singular, Sage, etc. (free) or Maple, Mathematica, etc. (commercial)) and perform elimination of variables (in general, not computing a lexicographic GB because the computational complexity is high). There are many improvements in the original algorithm (now they even use AI to decide what reductions to make).

# Elimination of variables

Elimination of variables is not as simple over the polynomial ring as the triangulation of linear systems

Take $f_1 = x^2+y+z-1, f_2 = y^2+x+z-1, f_3 = z^2+x+y-1$ in $k[x,y,z]$. We would like to *triangulate* the system. But this is the answer we can get (a GB for the lex order $z \prec y \prec x$:

$$p = z^6 - 4\,z^4 + 4\,z^3 - z^2, z^4 + 2\,yz^2 - z^2,$$

$$y^2 - z^2 - y + z, z^2 + x + y - 1.$$

This ideal has a finite number of zeros in $\mathbb{C}^n$. Do you see why?

However, the ideal is not radical: there are polynomials vanishing on the common zeros but not in the ideal.

# Shape lemma

Assume $I_f \subset k[x_1, \ldots, x_n]$ ($k$ any field contained in $\mathbb{C}$) has a finite number of complex solutions $V(I_f)$ and it is radical. Assume also that $x_1$ separates points of $V(I_f)$, that is, the first coordinates of all the points in $V(I_f)$ are all different. Then, a reduced lexicographic GB of $I_f$ where $x_1$ is the smallest variable has the form:

$$G = \{g_1(x_1), x_2 - g_2(x_1), \ldots, x_n - g_n(x_n),$$

with $\deg(g_1) \leq \#V(I_f)$, and for $i > 1$ $\deg(g_i) \leq \#V(I_f) - 1$.

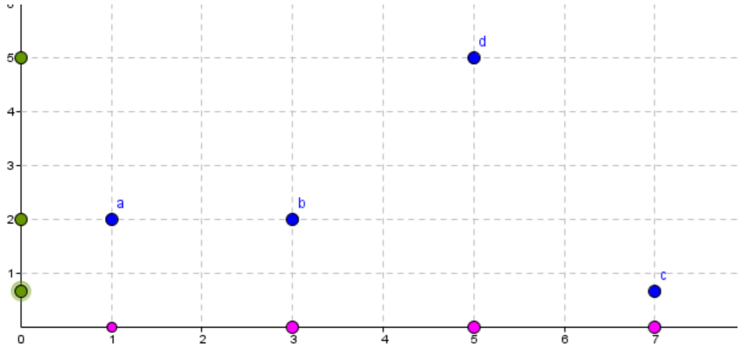


Figure: $V(I_f) = \{a, b, c, d\}$ the blue dots

$g_1 = \prod_{a \in V(I_f)}(x_1 - a_1)$, $g_2, \dots, g_n$ are interpolators.

# Ideals vs. $\mathbb{R}$-subspaces

## Shinar and Feinberg network, Science '10

This chemical reaction system exhibits Absolute Concentration Robustness (ACR) in $Y_p$.

$$\begin{gathered}
XD \underset{\kappa_{21}}{\overset{\kappa_{12}}{\rightleftarrows}} X \underset{\kappa_{32}}{\overset{\kappa_{23}}{\rightleftarrows}} XT \overset{\kappa_{34}}{\to} X_p \\
X_p + Y \underset{\kappa_{65}}{\overset{\kappa_{56}}{\rightleftarrows}} X_pY \overset{\kappa_{67}}{\to} X + Y_p \\
XT + Y_p \underset{\kappa_{98}}{\overset{\kappa_{89}}{\rightleftarrows}} XTY_p \overset{\kappa_{9,10}}{\to} XT + Y \\
XD + Y_p \underset{\kappa_{12,11}}{\overset{\kappa_{11,12}}{\rightleftarrows}} XDY_p \overset{\kappa_{12,13}}{\to} XD + Y
\end{gathered} \tag{1}$$

Denote by $x_1, \ldots, x_{Y_p} = x_7, x_8, x_9$ the species concentrations.

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# Ideals vs. $\mathbb{R}$-subspaces

## Toric steady states and ACR

The reduced Gröbner basis with respect to the lexicographical order $x_1 > x_2 > x_4 > x_5 > x_6 > x_8 > x_9 > x_3 > x_7$ of the ideal $f_1, \ldots, f_9$ consists of the following binomials:

$$
\begin{aligned}
g_1 &= [\kappa_{89}\kappa_{12}\kappa_{23}\kappa_{9,10}(\kappa_{12,11}+\kappa_{12,13}) + \kappa_{11,12}\kappa_{21}\kappa_{12,13}(\kappa_{98}+\kappa_{9,10})(\kappa_{32}+\kappa_{34})]x_3x_7 + \\
&\quad + [-\kappa_{23}\kappa_{34}\kappa_{12}(\kappa_{12,11}+\kappa_{12,13})(\kappa_{98}+\kappa_{9,10})]x_3 \\
g_2 &= [-\kappa_{11,12}\kappa_{21}\kappa_{34}(\kappa_{98}+\kappa_{9,10})(\kappa_{32}+\kappa_{34})]x_3 + \\
&\quad + [\kappa_{11,12}\kappa_{21}\kappa_{12,13}(\kappa_{98}+\kappa_{9,10})(\kappa_{32}+\kappa_{34}) + \kappa_{12}\kappa_{23}\kappa_{89}\kappa_{9,10}(\kappa_{12,11}+\kappa_{12,13})]x_9 \\
g_3 &= [-\kappa_{23}\kappa_{34}\kappa_{89}\kappa_{12}(\kappa_{12,11}+\kappa_{12,13})]x_3 + \\
&\quad + [\kappa_{23}\kappa_{9,10}\kappa_{89}\kappa_{12}(\kappa_{12,11}+\kappa_{12,13}) + \kappa_{11,12}\kappa_{21}\kappa_{12,13}(\kappa_{98}+\kappa_{9,10})(\kappa_{32}+\kappa_{34})]x_8 \\
g_4 &= \kappa_{67}x_6 - \kappa_{34}x_3 \\
g_5 &= \kappa_{56}\kappa_{67}x_4x_5 + \kappa_{34}(-\kappa_{65}-\kappa_{67})x_3 \\
g_6 &= \kappa_{23}x_2 + (-\kappa_{32}-\kappa_{34})x_3 \\
g_7 &= -\kappa_{21}(\kappa_{32}+\kappa_{34})x_3 + \kappa_{12}\kappa_{23}x_1
\end{aligned}
$$

Therefore, the network has toric steady states (for any *generic* choice of positive reaction rate constants) because the steady state ideal can be generated by $g_1, g_2, \ldots, g_7$ (and shows ACR in $Y_p$).

However, we can prove that linear combinations only with real coefficients cannot reveal these properties.

# Parameters

The reduced lexicographic GB of $\{ax + by, cx + dy\}$ with respect to the lexicographic order with $y \prec x$ equals $\{y, x\}$. Is this true for any value of $a, b, c, d$?

This computation is made in $\mathbb{Q}(a, b, c, d)[x, y]$. The coefficients lie in the field of rational functions of the variables $a, b, c, d$, so we are allowed to divide by polynomials in the parameters $a, b, c, d$.

# Parameters

The reduced lexicographic GB of $\{ax+by, cx+dy\}$ with respect to the lexicographic order with $d \prec c \prec b \prec a \prec y \prec x$ equals $\{ady - bcy, cx+dy, ax+by\}$

This computation is made in $\mathbb{Q}[a,b,c,d,x,y]$, so we are not allowed to divide by polynomials in the parameters $a,b,c,d$

So, if $ad - bc \neq 0$ we get that $y = 0$ from the first polynomial, and then either $a$ or $c$ are nonzero and we get that $x = 0$ using the other two polynomials.

The computation with $a,b,c,d$ as parameters and only 2 variables is much faster!

# Descartes' rule of signs

- Descartes' rule of signs was proposed by René Descartes in 1637 in "La Géometrie", an appendix to his "Discours de la Méthode".
- Given a univariate real polynomial $f(x) = c_0 + \sum_{j=1}^{r} c_j x^j$, the number of positive real roots $n_f$ of $f$ (counted with multiplicity) is bounded by the number of sign variations in the ordered sequence of coefficient signs $\sigma(c_0), \ldots, \sigma(c_r)$ (where we discard the 0's in this sequence and we add a 1 each time two consecutive signs are different) and both quantities have the same parity.
- For instance, if $f = c_0 + 3x - 90x^6 + 2x^8 + x^{111}$, the sequence of coefficient signs (discarding 0's) is: $\sigma(c_0), +, -, +, +$. So, $n_f$ equals 2 if $c_0 \geq 0$ and 3 if $c_0 < 0$. Then, $f$ has at most 2 or 3 positive real roots.
- If the number of sign variations $s$ is odd, then there is at least 1 positive root (or $3, 5, \ldots, s$).

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- Note that one consequence is that we can bound the number of real roots in terms of the number of nonzero terms of $f$, independently of its degree.

- The rule is sharp in the sense that given a sequence of signs, there exist polynomials with coefficients of these signs with $n_f$ equal to the number of sign variations. We'll see how to get these polynomials in the forthcoming lecture on Thursday.

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# Sturm's theorem

- Sturm sequence: Given a univariate polynomial $p \in \mathbb{R}[x]$, the associated Sturm sequence equals: $p_0 = p,\ p_1 = p'$, and $p_{i+1} = -\text{rem}(p_{i-1}, p_i)$, for $i \geq 1$. The sequence stops when $p_{i+1} = 0$. The $p_i$'s can be replaced by any positive multiple.
- For $c \in \mathbb{R}$, let $var(c)$ denote the number of sign changes in the sequence $p_0(c), \ldots, p_m(c)$.
- Sturm's theorem (1829): Let $a < b$ and assume that neither $a$ nor $b$ are multiple roots of $p(x)$. Then, the number of distinct roots of $p$ in $(a, b]$ equals the difference $var(a) - var(b)$.

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- $p = x^3 - x^2 + x - 1 = (x-1)(x^2+1)$. Its Sturm sequence equals $x^3 - x^2 + x - 1, x^2 - 2/3x + 1/3, -x + 2, -1$.

Then, the number of distinct roots of $p$ in $(0, r]$ for $r$ big, equals the difference between $var(0)$ = the sign variation of $-1, 1/3, 2, -1 = 2$ and $var(r)$ = sign variation of the leading coefficients $1, 1, -1, -1 = 1$, that is $p$ has a single root in $(0, r]$. Note that this is the number of positive roots of $p$ in $(0, +\infty) = \mathbb{R}_{>0}$.