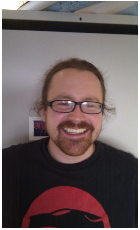
# Back to the Roots

## at the occasion of Anders Lindquist 75 !

**Philippe Dreesen**

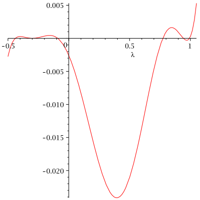
**Kim Batselier**

**Bart De Moor**

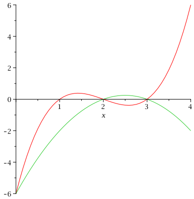
**KU Leuven**
Department of Electrical Engineering
ESAT-STADIUS

# Outline

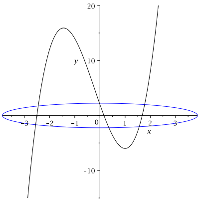
$$p(\lambda) = \det(A - \lambda I) = 0$$



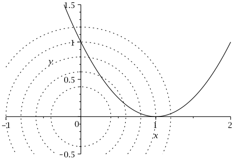

$$\begin{aligned} (x-1)(x-3)(x-2) &= 0 \\ -(x-2)(x-3) &= 0 \end{aligned}$$



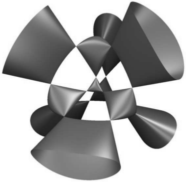

$$\begin{aligned} x^2 + 3y^2 - 15 &= 0 \\ y - 3x^3 - 2x^2 + 13x - 2 &= 0 \end{aligned}$$

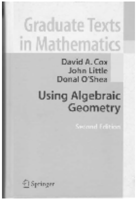



$$\begin{aligned} \min_{x,y} \quad & x^2 + y^2 \\ \text{s.t.} \quad & y - x^2 + 2x - 1 = 0 \end{aligned}$$



- Algebraic Geometry: 'Queen of mathematics' (literature = huge !)
- Computer algebra: symbolic manipulations
- Computational tools: Gröbner Bases, Buchberger algorithm





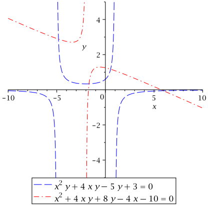

**Wolfgang Gröbner**
(1899-1980)

**Bruno Buchberger**

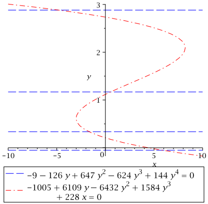
# Example: Gröbner basis

**Input system:**

$$
\begin{aligned}
x^2y + 4xy - 5y + 3 &= 0 \\
x^2 + 4xy + 8y - 4x - 10 &= 0
\end{aligned}
$$




- Generates simpler but equivalent system (same roots)
- Symbolic eliminations and reductions
- Exponential complexity
- Numerical issues
  - NO floating point but integer arithmetic
  - Coefficients become very large




**Gröbner Basis:**

$$
\begin{aligned}
-9 - 126y + 647y^2 - 624y^3 + 144y^4 &= 0 \\
-1005 + 6109y - 6432y^2 + 1584y^3 + 228x &= 0
\end{aligned}
$$

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# Outline

- **Characteristic Polynomial**
  The eigenvalues of $A$ are the roots of

$$p(\lambda) = \det(A - \lambda I) = 0$$

- **Companion Matrix**
  Solving

$$q(x) = 7x^3 - 2x^2 - 5x + 1 = 0$$

leads to

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1/7 & 5/7 & 2/7 \end{bmatrix} \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix} = x \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}$$

Consider the univariate equation

$$x^3 + a_1 x^2 + a_2 x + a_3 = 0,$$

having three distinct roots $x_1$, $x_2$ and $x_3$

$$\begin{bmatrix} a_3 & a_2 & a_1 & 1 & 0 & 0 \\ 0 & a_3 & a_2 & a_1 & 1 & 0 \\ 0 & 0 & a_3 & a_2 & a_1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ x_1^2 & x_2^2 & x_3^2 \\ x_1^3 & x_2^3 & x_3^3 \\ x_1^4 & x_2^4 & x_3^4 \\ x_1^5 & x_2^5 & x_3^5 \end{bmatrix} = 0$$

- Banded Toeplitz; linear homogeneous equations
- Null space: (Confluent) Vandermonde structure
- Corank (nullity) = number of solutions
- Realization theory in null space: eigenvalue problem

Consider

$$\begin{aligned} x^3 + a_1 x^2 + a_2 x + a_3 &= 0 \\ x^2 + b_1 x + b_2 &= 0 \end{aligned}$$

Build the Sylvester Matrix:

$$\left[\begin{array}{ccccc} 1 & a_1 & a_2 & a_3 & 0 \\ 0 & 1 & a_1 & a_2 & a_3 \\ \hline 1 & b_1 & b_2 & 0 & 0 \\ 0 & 1 & b_1 & b_2 & 0 \\ 0 & 0 & 1 & b_1 & b_2 \end{array}\right] \left[\begin{array}{c} 1 \\ x \\ x^2 \\ x^3 \\ x^4 \end{array}\right] = 0$$

| Row Space | Null Space |
|---|---|
| **Ideal**<br>=union of ideals<br>=multiply rows with powers of $x$ | **Variety**<br>=intersection of null spaces |

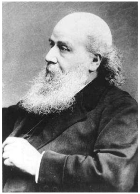
- Corank of Sylvester matrix = number of common zeros
- null space = intersection of null spaces of two Sylvester matrices
- common roots follow from realization theory in null space
- notice ‘double’ Toeplitz-structure of Sylvester matrix

- **Sylvester Resultant**
  Consider two polynomials $f(x)$ and $g(x)$:

$$f(x) = x^3 - 6x^2 + 11x - 6 = (x-1)(x-2)(x-3)$$
$$g(x) = -x^2 + 5x - 6 = -(x-2)(x-3)$$

Common roots iff $S(f,g) = 0$

$$S(f,g) = \det \left[\begin{array}{ccccc} -6 & 11 & -6 & 1 & 0 \\ 0 & -6 & 11 & -6 & 1 \\ \hline -6 & 5 & -1 & 0 & 0 \\ 0 & -6 & 5 & -1 & 0 \\ 0 & 0 & -6 & 5 & -1 \end{array}\right]$$


**James Joseph Sylvester**

The corank of the Sylvester matrix is 2!

Sylvester's result can be understood from

$$\begin{array}{l} f(x)=0 \\ x\cdot f(x)=0 \\ g(x)=0 \\ x\cdot g(x)=0 \\ x^2\cdot g(x)=0 \end{array} \qquad \begin{array}{c} \begin{array}{ccccc} 1 & x & x^2 & x^3 & x^4 \end{array} \\ \begin{bmatrix} -6 & 11 & -6 & 1 & 0 \\ & -6 & 11 & -6 & 1 \\ -6 & 5 & -1 & & \\ & -6 & 5 & -1 & \\ & & -6 & 5 & -1 \end{bmatrix} \end{array} \begin{bmatrix} 1 & 1 \\ x_1 & x_2 \\ x_1^2 & x_2^2 \\ x_1^3 & x_2^3 \\ x_1^4 & x_2^4 \end{bmatrix} = 0$$

where $x_1 = 2$ and $x_2 = 3$ are the common roots of $f$ and $g$

The vectors in the Vandermonde kernel $K$ obey a ‘shift structure’:

$$\begin{bmatrix} 1 & 1 \\ x_1 & x_2 \\ x_1^2 & x_2^2 \\ x_1^3 & x_2^3 \end{bmatrix} \begin{bmatrix} x_1 & 0 \\ 0 & x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \\ x_1^2 & x_2^2 \\ x_1^3 & x_2^3 \\ x_1^4 & x_2^4 \end{bmatrix}$$

or

$$\underline{K}.D = S_1 K D = \overline{K} = S_2 K$$

The Vandermonde kernel $K$ is not available directly, instead we compute $Z$, for which $ZV = K$. We now have

$$\begin{aligned} S_1 K D &= S_2 K \\ S_1 Z V D &= S_2 Z V \end{aligned}$$

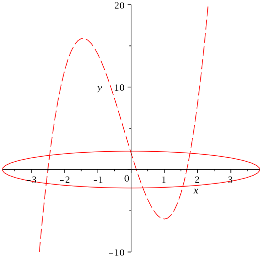
leading to the generalized eigenvalue problem

$$(S_2 Z) V = (S_1 Z) V D$$

# Outline

- Consider

$$\begin{cases} p(x,y) &= x^2 + 3y^2 - 15 = 0 \\ q(x,y) &= y - 3x^3 - 2x^2 + 13x - 2 = 0 \end{cases}$$




- Fix a monomial order, e.g., $1 < x < y < x^2 < xy < y^2 < x^3 < x^2y < \ldots$

- Construct $M$: write the system in matrix-vector notation:

| | $1$ | $x$ | $y$ | $x^2$ | $xy$ | $y^2$ | $x^3$ | $x^2y$ | $xy^2$ | $y^3$ |
|---|---|---|---|---|---|---|---|---|---|---|
| $p(x,y)$ | $-15$ | | | $1$ | | $3$ | | | | |
| $q(x,y)$ | $-2$ | $13$ | $1$ | $-2$ | | | $-3$ | | | |
| $x \cdot p(x,y)$ | | $-15$ | | | | | $1$ | | $3$ | |
| $y \cdot p(x,y)$ | | | $-15$ | | | | | $1$ | | $3$ |

$$\begin{cases} p(x,y) &= x^2 + 3y^2 - 15 = 0 \\ q(x,y) &= y - 3x^3 - 2x^2 + 13x - 2 = 0 \end{cases}$$

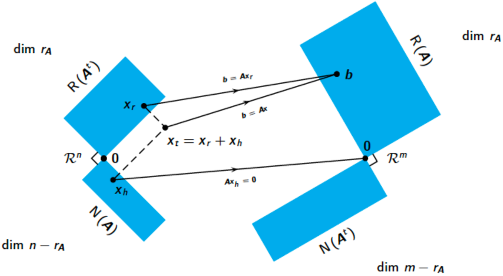
Continue to enlarge $M$:

| it # | form | $1$ | $x$ | $y$ | $x^2$ | $xy$ | $y^2$ | $x^3$ | $x^2y$ | $xy^2$ | $y^3$ | $x^4$ | $x^3y$ | $x^2y^2$ | $xy^3$ | $y^4$ | $x^5$ | $x^4y$ | $x^3y^2$ | $x^2y^3$ | $xy^4$ | $y^5$ | → |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $d=3$ | $p$ | −15 | | | 1 | | 3 | | | | | | | | | | | | | | | | |
| | $xp$ | | −15 | | | | | 1 | | 3 | | | | | | | | | | | | | |
| | $yp$ | | | −15 | | | | | 1 | | 3 | | | | | | | | | | | | |
| | $q$ | −2 | 13 | 1 | −2 | | | −3 | | | | | | | | | | | | | | | |
| $d=4$ | $x^2p$ | | | | −15 | | | | | | | 1 | | 3 | | | | | | | | | |
| | $xyp$ | | | | | −15 | | | | | | | 1 | | 3 | | | | | | | | |
| | $y^2p$ | | | | | | −15 | | | | | | | 1 | | 3 | | | | | | | |
| | $xq$ | | −2 | | 13 | 1 | | −2 | | | | −3 | | | | | | | | | | | |
| | $yq$ | | | −2 | | 13 | 1 | | −2 | | | | −3 | | | | | | | | | | |
| $d=5$ | $x^3p$ | | | | | | | −15 | | | | | | | | | 1 | | 3 | | | | |
| | $x^2yp$ | | | | | | | | −15 | | | | | | | | | 1 | | 3 | | | |
| | $xy^2p$ | | | | | | | | | −15 | | | | | | | | | 1 | | 3 | | |
| | $y^3p$ | | | | | | | | | | −15 | | | | | | | | | 1 | | 3 | |
| | $x^2q$ | | | | −2 | | | 13 | 1 | | | −2 | | | | | −3 | | | | | | |
| | $xyq$ | | | | | −2 | | | 13 | 1 | | | −2 | | | | | −3 | | | | | |
| | $y^2q$ | | | | | | −2 | | | 13 | 1 | | | −2 | | | | | −3 | | | | |
| | ↓ | | | | | | | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ | ⋱ |

- $\#$ rows grows faster than $\#$ cols $\Rightarrow$ overdetermined system
- If solution exists: rank deficient by construction!

- **Row space**:
  - ideal; Hilbert Basis Theorem
  - *Subspace based elimination theory*
- **Left null space**:
  - syzygies, Hilbert Syzygy Theorem
  - *Syzygy: numerical linear algebra paper bdm/kb*
- **Right null space**:
  - Variety; Hilbert Nullstellensatz (existence of solutions); Hilbert polynomial (number of solutions = nullity)
  - *Modelling the Macaulay null space with nD singular autonomous systems*
- **Column space**: *Rank tests: Affine roots, roots at* $\infty$

**David Hilbert**

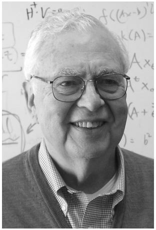


$$A = USV^t = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} S_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^t \\ V_2^t \end{pmatrix}$$

with

$$U_1^t U_1 = I_{r_A} \qquad V_1^t V_1 = I_{r_A}$$
$$U_2^t U_2 = I_{m-r_A} \qquad V_2^t V_2 = I_{n-r_A}$$
$$U_1^t U_2 = 0 \qquad V_1^t V_2 = 0$$

| Geometry | Basis |
|---|---|
| $\mathrm{R}(A)$ | $U_1$ |
| $\mathrm{N}(A^t)$ | $U_2$ |
| $\mathrm{R}(A^t)$ | $V_1$ |
| $\mathrm{N}(A)$ | $V_2$ |



**Gene Howard Golub**

**(Dr. SVD)**

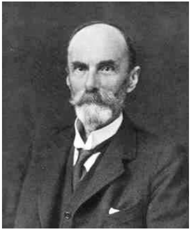
- Macaulay matrix $M$:

$$M = \begin{bmatrix} \times & \times & \times & \times & 0 & 0 & 0 \\ 0 & \times & \times & \times & \times & 0 & 0 \\ 0 & 0 & \times & \times & \times & \times & 0 \\ 0 & 0 & 0 & \times & \times & \times & \times \end{bmatrix}$$

- Solutions generate vectors in kernel of $M$:

$$MK = 0$$

- Number of solutions $s$ follows from corank



**Francis Sowerby Macaulay**

Vandermonde nullspace $K$ built from $s$ solutions $(x_i, y_i)$:

$$\left[\begin{array}{c|c|c|c} 1 & 1 & \ldots & 1 \\ \hline x_1 & x_2 & \ldots & x_s \\ y_1 & y_2 & \ldots & y_s \\ \hline x_1^2 & x_2^2 & \ldots & x_s^2 \\ x_1y_1 & x_2y_2 & \ldots & x_sy_s \\ y_1^2 & y_2^2 & \ldots & y_s^2 \\ \hline x_1^3 & x_2^3 & \ldots & x_s^3 \\ x_1^2y_1 & x_2^2y_2 & \ldots & x_s^2y_s \\ x_1y_1^2 & x_2y_2^2 & \ldots & x_sy_s^2 \\ y_1^3 & y_2^3 & \ldots & y_s^3 \\ \hline x_1^4 & x_2^4 & \ldots & x_4^4 \\ x_1^3y_1 & x_2^3y_2 & \ldots & x_s^3y_s \\ x_1^2y_1^2 & x_2^2y_2^2 & \ldots & x_s^2y_s^2 \\ x_1y_1^3 & x_2y_2^3 & \ldots & x_sy_s^3 \\ y_1^4 & y_2^4 & \ldots & y_s^4 \\ \hline \vdots & \vdots & \vdots & \vdots \end{array}\right]$$

- Choose $s$ linear independent rows in $K$

$$S_1 K$$

- This corresponds to finding linear dependent columns in $M$

$$\begin{bmatrix} 1 & 1 & \ldots & 1 \\ \hline x_1 & x_2 & \ldots & x_s \\ y_1 & y_2 & \ldots & y_s \\ \hline x_1^2 & x_2^2 & \ldots & x_s^2 \\ x_1 y_1 & x_2 y_2 & \ldots & x_s y_s \\ y_1^2 & y_2^2 & \ldots & y_s^2 \\ \hline x_1^3 & x_2^3 & \ldots & x_s^3 \\ x_1^2 y_1 & x_2^2 y_2 & \ldots & x_s^2 y_s \\ x_1 y_1^2 & x_2 y_2^2 & \ldots & x_s y_s^2 \\ y_1^3 & y_2^3 & \ldots & y_s^3 \\ \hline x_1^4 & x_2^4 & \ldots & x_4^4 \\ x_1^3 y_1 & x_2^3 y_2 & \ldots & x_s^3 y_s \\ x_1^2 y_1^2 & x_2^2 y_2^2 & \ldots & x_s^2 y_s^2 \\ x_1 y_1^3 & x_2 y_2^3 & \ldots & x_s y_s^3 \\ y_1^4 & y_2^4 & \ldots & y_s^4 \\ \hline \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

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# Shifting the selected rows gives (shown for 3 columns)

$$\left[\begin{array}{c|c|c} 1 & 1 & 1 \\ \hline x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ \hline x_1^2 & x_2^2 & x_3^2 \\ x_1 y_1 & x_2 y_2 & x_3 y_3 \\ y_1^2 & y_2^2 & y_3^2 \\ \hline x_1^3 & x_2^3 & x_3^3 \\ x_1^2 y_1 & x_2^2 y_2 & x_3^2 y_3 \\ x_1 y_1^2 & x_2 y_2^2 & x_3 y_3^2 \\ y_1^3 & y_2^3 & y_3^3 \\ \hline x_1^4 & x_2^4 & x_4^4 \\ x_1^3 y_1 & x_2^3 y_2 & x_3^3 y_3 \\ x_1^2 y_1^2 & x_2^2 y_2^2 & x_3^2 y_3^2 \\ x_1 y_1^3 & x_2 y_2^3 & x_3 y_3^3 \\ y_1^4 & y_2^4 & y_3^4 \\ \hline \vdots & \vdots & \vdots \end{array}\right] \longrightarrow \text{“shift with } x\text{”} \longrightarrow \left[\begin{array}{c|c|c} 1 & 1 & 1 \\ \hline x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ \hline x_1^2 & x_2^2 & x_3^2 \\ x_1 y_1 & x_2 y_2 & x_3 y_3 \\ y_1^2 & y_2^2 & y_3^2 \\ \hline x_1^3 & x_2^3 & x_3^3 \\ x_1^2 y_1 & x_2^2 y_2 & x_3^2 y_3 \\ x_1 y_1^2 & x_2 y_2^2 & x_3 y_3^2 \\ y_1^3 & y_2^3 & y_3^3 \\ \hline x_1^4 & x_2^4 & x_4^4 \\ x_1^3 y_1 & x_2^3 y_2 & x_3^3 y_3 \\ x_1^2 y_1^2 & x_2^2 y_2^2 & x_3^2 y_3^2 \\ x_1 y_1^3 & x_2 y_2^3 & x_3 y_3^3 \\ y_1^4 & y_2^4 & y_3^4 \\ \hline \vdots & \vdots & \vdots \end{array}\right]$$

simplified:

$$\left[\begin{array}{c|c|c} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ x_1 y_1 & x_2 y_2 & x_3 y_3 \\ x_1^3 & x_2^3 & x_3^3 \\ x_1^2 y_1 & x_2^2 y_2 & x_3^2 y_3 \end{array}\right] \left[\begin{array}{ccc} x_1 & & \\ & x_2 & \\ & & x_3 \end{array}\right] = \left[\begin{array}{c|c|c} x_1 & x_2 & x_3 \\ x_1^2 & x_2^2 & x_3^2 \\ x_1 y_1 & x_2 y_2 & x_3 y_3 \\ x_1^2 y_1 & x_2^2 y_2 & x_3^2 y_3 \\ x_1^4 & x_2^4 & x_4^4 \\ x_1^3 y_1 & x_2^3 y_2 & x_3^3 y_3 \end{array}\right]$$

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- Finding the $x$-roots: let $D_x = \mathrm{diag}(x_1, x_2, \ldots, x_s)$, then

$$S_1 K D_x = S_x K,$$

where $S_1$ and $S_x$ select rows from $K$ w.r.t. shift property

- **Realization Theory** for the unknown $x$

We have

$$S_1 K D_x = S_x K$$

Generalized Vandermonde $K$ is not known as such, instead a null space basis $Z$ is calculated, which is a linear transformation of $K$:

$$ZV = K$$

which leads to

$$(S_x Z)V = (S_1 Z)V D_x$$

Here, $V$ is the matrix with eigenvectors, $D_x$ contains the roots $x$ as eigenvalues.

It is possible to shift with $y$ as well...

We find

$$S_1 K D_y = S_y K$$

with $D_y$ diagonal matrix of $y$-components of roots, leading to

$$(S_y Z)V = (S_1 Z)V D_y$$

Some interesting results:

- same eigenvectors $V$!
- $(S_x Z)^{-1}(S_1 Z)$ and $(S_y Z)^{-1}(S_1 Z)$ commute
  $\Longrightarrow$ 'commutative algebra'

## Basic Algorithm outline

Find a basis for the nullspace of $M$ using an SVD:

$$M = \begin{bmatrix} \times & \times & \times & \times & 0 & 0 & 0 \\ 0 & \times & \times & \times & \times & 0 & 0 \\ 0 & 0 & \times & \times & \times & \times & 0 \\ 0 & 0 & 0 & \times & \times & \times & \times \end{bmatrix} = \begin{bmatrix} X & Y \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} W^T \\ Z^T \end{bmatrix}$$

Hence,

$$MZ = 0$$

We have

$$S_1 K D = S_{\text{shift}} K$$

with $K$ generalized Vandermonde, not known as such. Instead a basis $Z$ is computed as

$$ZV = K$$

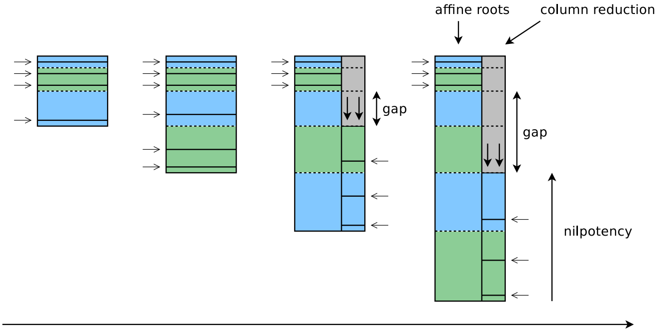
which leads to

$$(S_{\text{shift}} Z)V = (S_1 Z)VD$$

$S_1$ selects linear independent rows; $S_{\text{shift}}$ selects rows 'hit' by the shift.

# *'Mind the Gap' and 'A Bout de Souffle'*

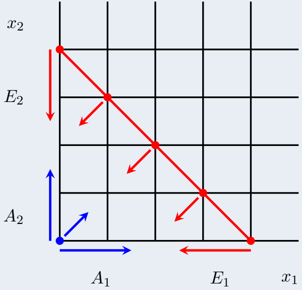
- Dynamics in the null space of $M(d)$ for increasing degree $d$: The index of some of the linear independent rows stabilizes (=affine zeros); The index of other ones keeps increasing (=zeros at $\infty$).
- 'Mind-the-gap': As a function of $d$, certain degree blocks become and stay linear dependent on all preceeding rows: allows to count and seperate affine zeros from zeros at $\infty$
- 'A bout de souffle': Effect of zeros at $\infty$ 'dies' out (nilpotency).



- Weierstrass Canonical Form decoupling affine and infinity roots

$$\left(\frac{v(k+1)}{w(k-1)}\right) = \left(\begin{array}{c|c} A & 0 \\ \hline 0 & E \end{array}\right) \left(\frac{v(k)}{w(k)}\right),$$

- Action of $A_i$ and $E_i$ represented in grid of monomials



# Roots at Infinity: $n$D Descriptor Systems

Weierstrass Canonical Form decouples affine/infinity

$$\left[\begin{array}{c} v(k+1) \\ \hline w(k-1) \end{array}\right] = \left[\begin{array}{c|c} A & 0 \\ \hline 0 & E \end{array}\right] \left[\begin{array}{c} v(k) \\ \hline w(k) \end{array}\right]$$

Singular $n$D Attasi model (for $n = 2$)

$$\begin{array}{rcl} v(k+1,l) & = & A_x v(k,l) \\ v(k,l+1) & = & A_y v(k,l) \\ \\ w(k-1,l) & = & E_x w(k,l) \\ w(k,l-1) & = & E_y w(k,l) \end{array}$$

with $E_x$ and $E_y$ nilpotent matrices.

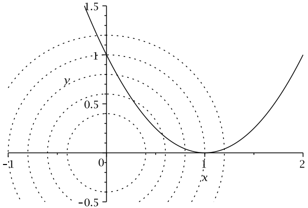
# Summary

- Rooting multivariate polynomials
  - = (numerical) linear algebra
  - = (fund. thm. of algebra) $\bigcap$ (fund. thm. of linear algebra)
  - = nD realization theory in null space of Macaulay matrix
- Decisions based upon (numerical) rank
  - Dimension of variety = degree of Hilbert polynomial: follows from corank (nullity);
  - For 0-dimensional varieties ('isolated' roots): corank stabilizes = # roots (nullity)
  - 'Mind-the-gap' splits affine zeros from zeros at $\infty$
  - # affine roots (dimension column compression)
- not discussed
  - Multiplicity of roots ('confluent' generalized Vandermonde matrices)
  - Macaulay matrix columnspace based methods ('data driven')

# Outline

# Polynomial Optimization Problems EVP

$$\begin{aligned} \min_{x,y} \quad & x^2 + y^2 \\ \text{s. t.} \quad & y - x^2 + 2x - 1 = 0 \end{aligned}$$




**Lagrange multipliers**: necessary conditions for optimality:

$$L(x, y, z) = x^2 + y^2 + z(y - x^2 + 2x - 1)$$

$$\begin{aligned} \partial L/\partial x = 0 \quad & \rightarrow \quad 2x - 2xz + 2z = 0 \\ \partial L/\partial y = 0 \quad & \rightarrow \quad 2y + z = 0 \\ \partial L/\partial z = 0 \quad & \rightarrow \quad y - x^2 + 2x - 1 = 0 \end{aligned}$$

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Observations:

- all equations remain polynomial
- all 'stationary' points (local minima/maxima, saddle points) are roots of a system of polynomial equations
- shift with objective function to find minimum: only minimizing roots are needed !

Let

$$A_x V = V D_x$$

and

$$A_y V = V D_y$$

then find minimum eigenvalue of

$$(A_x^2 + A_y^2)V = V(D_x^2 + D_y^2)$$

# Outline



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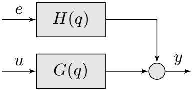
- PEM System identification
- Measured data $\{u_k, y_k\}_{k=1}^N$
- Model structure

$$y_k = G(q)u_k + H(q)e_k$$




- Output prediction

$$\hat{y}_k = H^{-1}(q)G(q)u_k + (1 - H^{-1})y_k$$

- Model classes: ARX, ARMAX, OE, BJ

$$A(q)y_k = B(q)/F(q)u_k + C(q)/D(q)e_k$$

| Class | Polynomials |
|---|---|
| ARX | $A(q), B(q)$ |
| ARMAX | $A(q)$, $B(q)$, $C(q)$ |
| OE | $B(q)$, $F(q)$ |
| BJ | $B(q)$, $C(q)$, $D(q)$, $F(q)$ |

- Minimize the prediction errors $y - \hat{y}$, where

$$\hat{y}_k = H^{-1}(q)G(q)u_k + (1 - H^{-1})y_k,$$

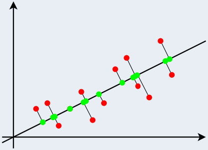
subject to the model equations

- Example

ARMAX identification: $G(q) = B(q)/A(q)$ and $H(q) = C(q)/A(q)$, where $A(q) = 1 + aq^{-1}$, $B(q) = bq^{-1}$, $C(q) = 1 + cq^{-1}$, $N = 5$

$$\begin{aligned}
\min_{\hat{y},a,b,c} \quad & (y_1 - \hat{y}_1)^2 + \ldots + (y_5 - \hat{y}_5)^2 \\
\text{s. t.} \quad & \hat{y}_5 - c\hat{y}_4 - bu_4 - (c-a)y_4 = 0, \\
& \hat{y}_4 - c\hat{y}_3 - bu_3 - (c-a)y_3 = 0, \\
& \hat{y}_3 - c\hat{y}_2 - bu_2 - (c-a)y_2 = 0, \\
& \hat{y}_2 - c\hat{y}_1 - bu_1 - (c-a)y_1 = 0,
\end{aligned}$$

## Static Linear Modeling



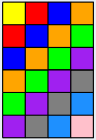
- Rank deficiency
- minimization problem:

$$\begin{array}{ll} \min & \|[\,\Delta A \quad \Delta b\,]\|_F^2\,, \\ \text{s. t.} & (A+\Delta A)v = b+\Delta b, \\ & v^T v = 1 \end{array}$$

- Singular Value Decomposition:
  find $(u, \sigma, v)$ which minimizes $\sigma^2$
  Let $M = [\,A \quad b\,]$

$$\left\{\begin{array}{rcl} Mv &=& u\sigma \\ M^T u &=& v\sigma \\ v^T v &=& 1 \\ u^T u &=& 1 \end{array}\right.$$

## Dynamical Linear Modeling



- Rank deficiency
- minimization problem:

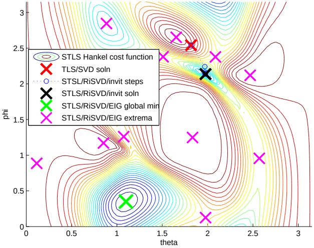
$$\begin{array}{ll} \min & \|[\Delta A \quad \Delta b]\|_F^2\,, \\ \text{s. t.} & (A+\Delta A)v = b+\Delta b, \\ & v^T v = 1 \\ & [\Delta A \quad \Delta b] \text{ structured} \end{array}$$

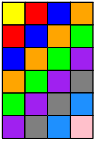
- Riemannian SVD:
  find $(u, \tau, v)$ which minimizes $\tau^2$

$$\left\{\begin{array}{rcl} Mv &=& D_v u\tau \\ M^T u &=& D_u v\tau \\ v^T v &=& 1 \\ u^T D_v u &=& 1\ (= v^T D_u v) \end{array}\right.$$

## Structured Total Least Squares

$$\begin{aligned} \min_{v} \quad & \tau^2 = v^T M^T D_v^{-1} M v \\ \text{s.t.} \quad & v^T v = 1. \end{aligned}$$



| method | TLS/SVD | STLS inv. it. | STLS eig |
|---|---|---|---|
| $v_1$ | .8003 | .4922 | **.8372** |
| $v_2$ | -.5479 | -.7757 | **.3053** |
| $v_3$ | .2434 | .3948 | **.4535** |
| $\tau^2$ | 4.8438 | 3.0518 | **2.3822** |
| global solution? | no | no | **yes** |

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## CpG Islands

- genomic regions that contain a high frequency of sites where a cytosine (C) base is followed by a guanine (G)
- rare because of methylation of the C base
- hence CpG islands indicate functionality

## Given observed sequence of DNA:

CTCACGTGATGAGAGCATTCTCAGA
CCGTGACGCGTGTAGCAGCGGCTCA

## Problem

Decide whether the observed sequence came from a CpG island

## The model

- 4-dimensional state space $[m] = \{\mathrm{A}, \mathrm{C}, \mathrm{G}, \mathrm{T}\}$
- Mixture model of 3 distributions on $[m]$
  1. : CG rich DNA
  2. : CG poor DNA
  3. : CG neutral DNA
- Each distribution is characterised by probabilities of observing base A,C,G or T

Table: Probabilities for each of the distributions (Durbin; Pachter & Sturmfels)

| DNA Type | A | C | G | T |
|---|---|---|---|---|
| CG rich | 0.15 | 0.33 | 0.36 | 0.16 |
| CG poor | 0.27 | 0.24 | 0.23 | 0.26 |
| CG neutral | 0.25 | 0.25 | 0.25 | 0.25 |

- The probabilities of observing each of the bases $A$ to $T$ are given by

$$\begin{aligned} p(A) &= -0.10\,\theta_1 + 0.02\,\theta_2 + 0.25 \\ p(C) &= +0.08\,\theta_1 - 0.01\,\theta_2 + 0.25 \\ p(G) &= +0.11\,\theta_1 - 0.02\,\theta_2 + 0.25 \\ p(T) &= -0.09\,\theta_1 + 0.01\,\theta_2 + 0.25 \end{aligned}$$

- $\theta_i$ is probability to sample from distribution $i$ $(\theta_1 + \theta_2 + \theta_3 = 1)$
- Maximum Likelihood Estimate:

$$(\hat{\theta_1}, \hat{\theta_2}, \hat{\theta_3}) = \arg\max_{\theta} \; l(\theta)$$

where the log-likelihood $l(\theta)$ is given by

$$l(\theta) = 11\,\log p(A) + 14\,\log p(C) + 15\,\log p(G) + 10\,\log p(T)$$

- Need to solve the following polynomial system

$$\begin{cases} \frac{\partial l(\theta)}{\partial \theta_1} = \sum_{i=1}^{4} \frac{u_i}{p(i)} \frac{\partial p(i)}{\partial \theta_1} = 0 \\ \frac{\partial l(\theta)}{\partial \theta_2} = \sum_{i=1}^{4} \frac{u_i}{p(i)} \frac{\partial p(i)}{\partial \theta_2} = 0 \end{cases}$$

## Solving the Polynomial System

- corank$(M)$ = 9
- Reconstructed Kernel

$$K = \begin{bmatrix} 1 & 1 & 1 & 1 & \dots \\ 0.52 & 3.12 & -5.00 & 10.72 & \dots \\ 0.22 & 3.12 & -15.01 & 71.51 & \dots \\ 0.27 & 9.76 & 25.02 & 115.03 & \dots \\ 0.11 & 9.76 & 75.08 & 766.98 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \begin{matrix} 1 \\ \theta_1 \\ \theta_2 \\ \theta_1^2 \\ \theta_1\theta_2 \\ \vdots \end{matrix} .$$

- $\theta_i$'s are probabilities: $0 \leq \theta_i \leq 1$
- Could have introduced slack variables to impose this constraint!
- Only solution that satisfies this constraint is $\hat{\theta} = (0.52, 0.22, 0.26)$

Applications are found in

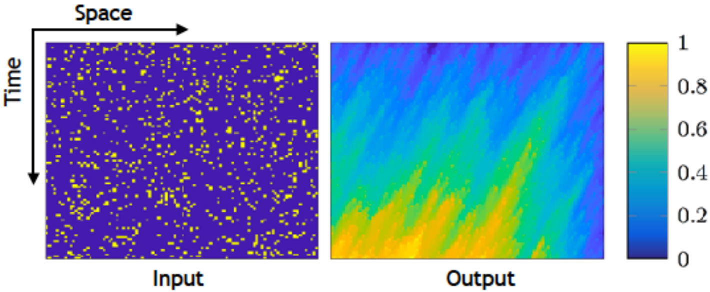
- Polynomial Optimization Problems
- Structured Total Least Squares
- $H_2$ Model order reduction
- Analyzing identifiability of nonlinear model structures (differential algebra)
- Robotics: kinematic problems
- Computational Biology: conformation of molecules
- Algebraic Statistics
- Signal Processing
- nD dynamical systems; Partial difference equations
- ...

# Outline

- Finding roots: linear algebra and realization theory!
- Polynomial optimization: extremal eigenvalue problems
- (Numerical) linear algebra/systems theory translation of algebraic geometry/symbolic algebra
- Many problems are in fact eigenvalue problems !
    - Algebraic geometry
    - System identification (PEM)
    - Numerical linear algebra (STLS, affine EVP $Ax = x\lambda + a$, etc.)
    - Multilinear algebra (tensor least squares approximation)
    - Algebraic statistics (HMM, Bayesian networks, discrete probabilities)
    - Differential algebra (Glad/Ljung)
- Projecting up to higher dimensional space (difficult in low number of dimensions; ‘easy’ (=large EVP) in high number of dimensions)

Current work:

- Subspace identification for spatially-temporarilly correlated signals (partial difference equations)
- Modelling in the era of IoT (Internet-of-Things) with its tsunami of data: in space and time (e.g. trajectories over time); or e.g. in MSI (mass spectrometry imaging): spectrum (1D) per space-voxel (3D) over time (1D) = 5D-tensor. How to model ?
- Example: Advection - diffusion equation space-time with input-output data:



## Conceptual/Geometric Level

- Polynomial system solving is an eigenvalue problem!
- Row and Column Spaces: Ideal/Variety $\leftrightarrow$ Row space/Kernel of $M$, ranks and dimensions, nullspaces and orthogonality
- Geometrical: intersection of subspaces, angles between subspaces, Grassmann's theorem,...

## Numerical Linear Algebra Level

- Eigenvalue decompositions, SVDs,...
- Solving systems of equations (consistency, nb sols)
- QR decomposition and Gram-Schmidt algorithm

## Numerical Algorithms Level

- Modified Gram-Schmidt (numerical stability), GS 'from back to front'
- Exploiting sparsity and Toeplitz structure (computational complexity $O(n^2)$ vs $O(n^3)$), FFT-like computations and convolutions,...
- Power method to find smallest eigenvalue ($=$ minimizer of polynomial optimization problem)

"At the end of the day,
the only thing we really understand,
is linear algebra".

Sculpture by Joos Vandewalle

A variety in algebraic geometry

Anders 'free will' Lindquist

Ad multos annos !!