Robots, Reactions, Surfaces, and Sudoku

Social Event with a Scientific Twist

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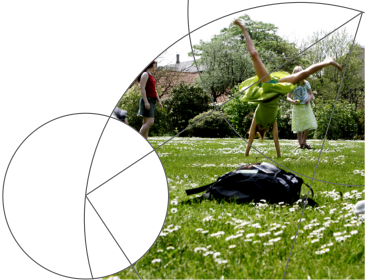


Mathematics & Computer Science

Mogens

Professor

Henrik

Thomas

Morten

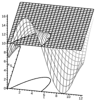
Associate Professors

Henrik

Assistant Professor

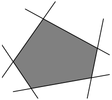
(Aug. 2007 – Feb. 2012)

My Teaching



Matematik og Databehandling (block 1, class teacher)

– Mathematical modelling
– Differential equations
– Functions of two variables



Matematik og Planlægning (block 3, lecturer)

– Linear programming
– Convex optimization
– Dynamic programming

My Research

- Dimension theory,

$$\mathrm{id}_{\mathbb{Z}}(\mathbb{Q}) = 1 \quad , \quad \mathrm{depth}(\mathbb{Z}/4\mathbb{Z}) = 0.$$

- Hyperhomological algebra,

$$\mathcal{A}_D(R) \underset{\mathbf{R}\mathrm{Hom}_R(D,-)}{\overset{D\otimes^{\mathbf{L}}_R -}{\rightleftarrows}} \mathcal{B}_D(R) \quad \text{is an equivalence.}$$

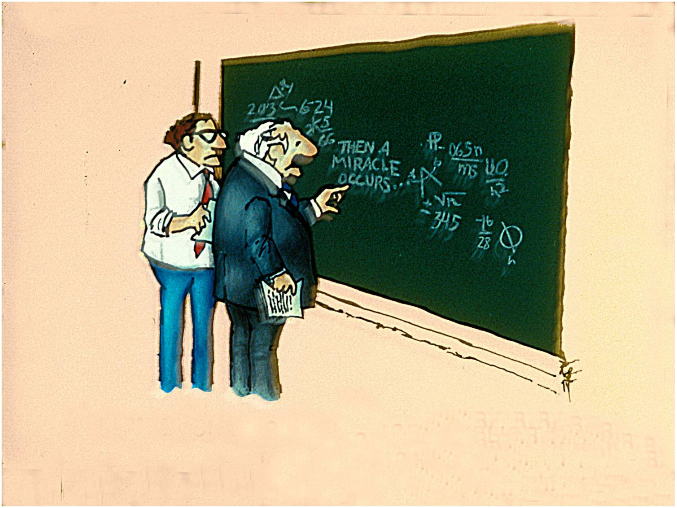
- Relative homological algebra,

$$\mathrm{Prod}\left\{ \mathrm{Hom}_{\mathbb{Z}}(M, \mathbb{Q}/\mathbb{Z}) \,\middle|\, M \in \mathcal{M} \right\} \quad \text{is enveloping.}$$

- Triangulated categories,

$$K\left(\mathrm{Inj}\, \frac{\mathbb{R}[x,y,z]}{(xy, z^2+y)} \right) \quad \text{is compactly generated.}$$

A Mathematical Miracle



"I think you should have been more explicit here in step two."

Buchberger's Algorithm

Input

List of equations:

$$f_1(x, y, z, \ldots) = a_1$$

$$\vdots$$

$$f_r(x, y, z, \ldots) = a_r$$

Monomial order:

$$<_{\text{lex}},\ <_{\text{grlex}},\ <_{\text{grevlex}},\ \cdots$$

$$\xrightarrow[\text{“Then a miracle occurs...”}]{\text{Buchberger's algorithm}}$$

Output

Gröbner equations:

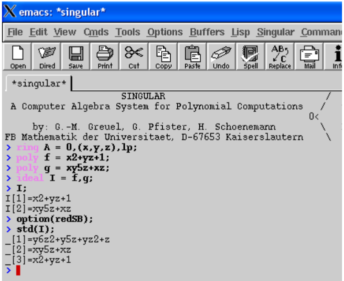
$$g_1(x, y, z, \ldots) = b_1$$

$$\vdots$$

$$g_s(x, y, z, \ldots) = b_s$$

SINGULAR

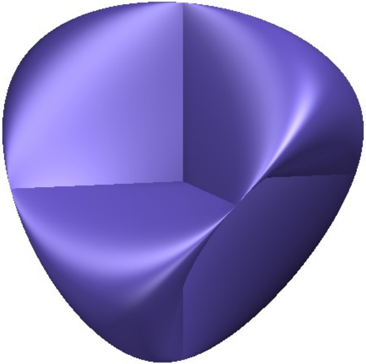
Buchberger's algorithm =



Gröbner equations for mathematicians

Surfaces 1 / 7

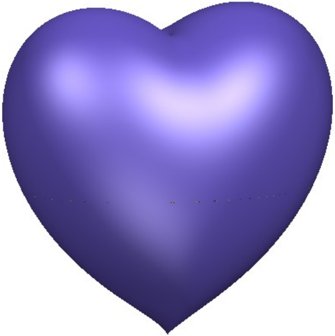
Example 1: *Steiner surface*



$$x^2y^2 + x^2z^2 + y^2z^2 - xyz = 0$$

Surfaces 2 / 7

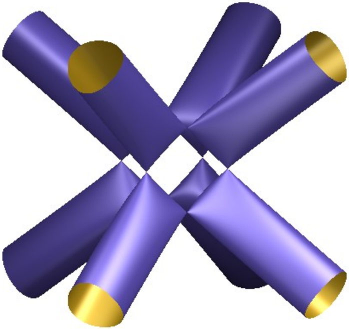
Example 2: *Heart*



$$(2x^2 + y^2 + z^2 - 1)^3 - \frac{1}{10}x^2z^3 - y^2z^3 = 0$$

Surfaces 3 / 7

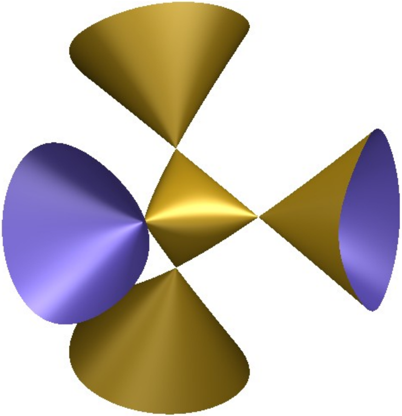
Example 3: *Kummer surface*



$$x^4 + y^4 + z^4 - x^2y^2 - x^2z^2 - y^2z^2 - x^2 - y^2 - z^2 = -1$$

Surfaces 4 / 7

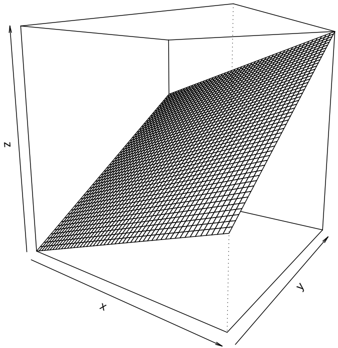
Example 4: *Cayley's cubic*



$$x^2 + y^2 + z^2 - x^2 z + y^2 z - 1 = 0$$

Surfaces 5 / 7

There are two ways to describe a hyperplane in 3D-space:



Parametric equation:

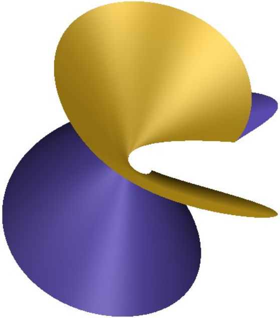
$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = t \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + u \begin{pmatrix} 3 \\ 0 \\ 1 \end{pmatrix}$$

Cartesian equation:

$$x + 2y - 3z = 0$$

Surfaces 6 / 7

Can we find the Cartesian equation from the parametric one?



Parametric equation:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} t+u \\ t^2+2tu \\ t^3+3t^2u \end{pmatrix}$$

Cartesian equation:

$$z^2 - 6xyz + \cdots = 0$$

Surfaces 7 / 7

We are given the parametric equations:

$$x = t + u$$
$$y = t^2 + 2tu$$
$$z = t^3 + 3t^2u$$

Surfaces 7 / 7

We are given the parametric equations:

$$
\begin{aligned}
x &= t + u \\
y &= t^2 + 2tu \\
z &= t^3 + 3t^2u
\end{aligned}
$$

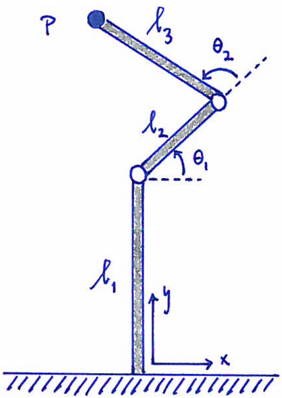
We compute the Gröbner equations:

$$
\begin{aligned}
z^2 - 6xyz + 4x^3z + 4y^3 - 3x^2y^2 &= 0 \\
2ty - 2tx^2 - z + xy &= 0 \\
2tz - 2tx^3 - 5xz + 4y^2 + x^2y &= 0 \\
t^2 - 2tx + y &= 0 \\
u + t - x &= 0
\end{aligned}
$$

We seek out the equation not depending on t and u.
This is the desired Cartesian equation.

Gröbner equations for other scientists

Robotics 1 / 6

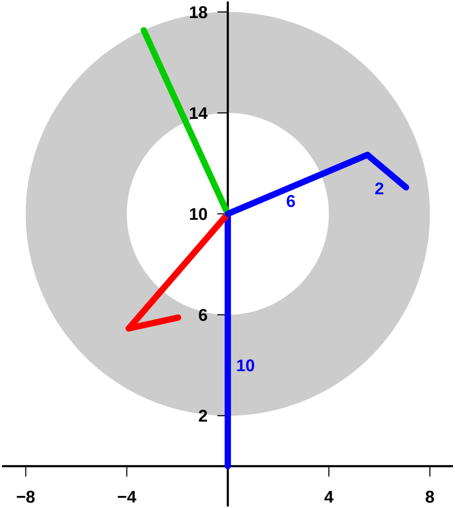


The position of the robot hand is:

$$P = P(\ell_1, \ell_2, \ell_3, \theta_1, \theta_2) = \begin{pmatrix} \ell_2 \cos\theta_1 + \ell_3 \cos(\theta_1 + \theta_2) \\ \ell_1 + \ell_2 \sin\theta_1 + \ell_3 \sin(\theta_1 + \theta_2) \end{pmatrix}$$

Robotics 2 / 6

The possible positions of the robot hand are:



Robotics 3 / 6

The inverse kinematic problem: Given $(a, b) \in \mathbb{R}^2$, solve:

$$P = \begin{pmatrix} \ell_2 \cos\theta_1 + \ell_3 \cos(\theta_1 + \theta_2) \\ \ell_1 + \ell_2 \sin\theta_1 + \ell_3 \sin(\theta_1 + \theta_2) \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

for θ_1, θ_2 (the lengths ℓ_1, ℓ_2, ℓ_3 are assumed to be fixed).

Robotics 3 / 6

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for θ_1, θ_2 (the lengths ℓ_1, ℓ_2, ℓ_3 are assumed to be fixed).

Solution: Gröbner equations don't work with cos and sin.

$$\begin{aligned} c_i &:= \cos\theta_i \\ s_i &:= \sin\theta_i \\ c_i^2 + s_i^2 &= 1 \\ \cos(\theta_1 + \theta_2) &= \cos\theta_1 \cos\theta_2 - \sin\theta_1 \sin\theta_2 = c_1 c_2 - s_1 s_2 \\ \sin(\theta_1 + \theta_2) &= \sin\theta_1 \cos\theta_2 + \sin\theta_2 \cos\theta_1 = s_1 c_2 + s_2 c_1 \end{aligned}$$

Robotics 4 / 6

Hence the inverse kinematic problem becomes:

$$\begin{cases} \ell_2 c_1 + \ell_3(c_1 c_2 - s_1 s_2) = a \\ \ell_1 + \ell_2 s_1 + \ell_3(s_1 c_2 + s_2 c_1) = b \\ c_1^2 + s_1^2 = 1 \\ c_2^2 + s_2^2 = 1 \end{cases}$$

with c_1, s_1, c_2, s_2 as unknowns.

Robotics 4 / 6

Hence the inverse kinematic problem becomes:

$$\begin{cases} \ell_2 c_1 + \ell_3(c_1 c_2 - s_1 s_2) = a \\ \ell_1 + \ell_2 s_1 + \ell_3(s_1 c_2 + s_2 c_1) = b \\ c_1^2 + s_1^2 = 1 \\ c_2^2 + s_2^2 = 1 \end{cases}$$

with c_1, s_1, c_2, s_2 as unknowns. The Gröbner equations are:

$$\begin{cases} c_2 - \dfrac{a^2+(b-\ell_1)^2-\ell_2^2-\ell_3^2}{2\ell_2\ell_3} = 0 \\ s_2 + \dfrac{a^2+(b-\ell_1)^2}{a\ell_3} s_1 - (b-\ell_1)\dfrac{a^2+(b-\ell_1)^2+\ell_2^2-\ell_3^2}{2a\ell_2\ell_3} = 0 \\ c_1 + \dfrac{b-\ell_1}{a} s_1 - \dfrac{a^2+(b-\ell_1)^2+\ell_2^2-\ell_3^2}{2a\ell_2} = 0 \\ s_1^2 + (b-\ell_1)\dfrac{a^2+(b-\ell_1)^2+\ell_2^2-\ell_3^2}{\ell_2(a^2+(b-\ell_1)^2)} s_1 + \dfrac{(a^2+(b-\ell_1)^2+\ell_2^2-\ell_3^2)^2-4a^2\ell_2^2}{4\ell_2^2(a^2+(b-\ell_1)^2)} = 0 \end{cases}$$

...which are easily solved for c_1, s_1, c_2, s_2.

Robotics 5 / 6

E.g. for $\ell_1 = 10$, $\ell_2 = 6$, $\ell_3 = 2$, and $(a, b) = (4, 15)$ one gets:

$$\begin{cases} c_2 - \frac{1}{24} & = 0 \\ s_2 + \frac{41}{8} s_1 - \frac{365}{96} & = 0 \\ c_1 + \frac{5}{4} s_1 - \frac{73}{48} & = 0 \\ s_1^2 - \frac{365}{246} s_1 + \frac{3025}{5904} & = 0 \end{cases}$$

These equations have two solutions:

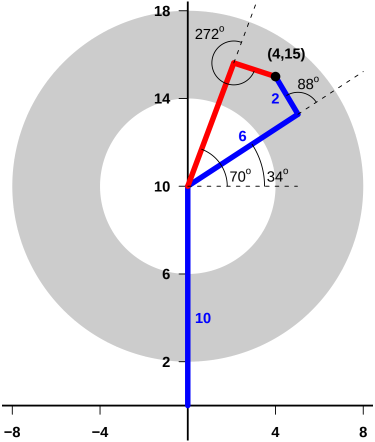
$$\begin{aligned} s_1 &= \sin\theta_1 = 0.55 \\ c_1 &= \cos\theta_1 = 0.84 \\ s_2 &= \sin\theta_2 = 1.00 \\ c_2 &= \cos\theta_2 = 0.04 \end{aligned} \qquad \text{or} \qquad \begin{aligned} s_1 &= \sin\theta_1 = 0.94 \\ c_1 &= \cos\theta_1 = 0.35 \\ s_2 &= \sin\theta_2 = -1.00 \\ c_2 &= \cos\theta_2 = 0.04 \end{aligned}$$

It follows that the desired angles are:

$$\begin{aligned} \theta_1 &= 34^\circ \\ \theta_2 &= 88^\circ \end{aligned} \qquad \text{or} \qquad \begin{aligned} \theta_1 &= 70^\circ \\ \theta_2 &= 272^\circ \end{aligned}$$

Robotics 6 / 6

Lengths	*Point*	*Angles*	*Angles*
$\ell_1 = 10$			
$\ell_2 = 6$	$(4, 15)$	$\theta_1 = 34^\circ$	$\theta_1 = 70^\circ$
$\ell_3 = 2$		$\theta_2 = 88^\circ$	$\theta_2 = 272^\circ$



Enzyme Reactions 1 / 4

$$E + A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} EA$$

$$EA + B \underset{k_4}{\overset{k_3}{\rightleftharpoons}} EAB$$

$$EAB \underset{k_6}{\overset{k_5}{\rightleftharpoons}} EPQ$$

$$EPQ \underset{k_8}{\overset{k_7}{\rightleftharpoons}} EQ + P$$

$$EQ \underset{k_9}{\overset{k_{10}}{\rightleftharpoons}} E + Q$$

E	enzyme
A, B	substrates
P, Q	products
EA, EQ, EAB, EPQ	complexes
$k_1, \dots, k_{10}$	rate constants

Enzyme Reactions 2 / 4

Rate equations:

$$\frac{\partial(EA)}{\partial t} = k_1 EA + k_4(EAB) - k_2(EA) - k_3(EA)B$$
$$\frac{\partial(EQ)}{\partial t} = k_7(EPQ) + k_9 EQ - k_{10}(EQ) - k_8(EQ)P$$
$$\frac{\partial(EAB)}{\partial t} = k_3(EA)B + k_6(EPQ) - k_4(EAB) - k_5(EAB)$$
$$\frac{\partial(EPQ)}{\partial t} = k_5(EAB) + k_8(EQ)P - k_6(EPQ) - k_7(EPQ)$$
$$\frac{\partial Q}{\partial t} = k_{10}(EQ) - k_9 EQ$$

Steady-state assumption:

$$\frac{\partial(EA)}{\partial t} = \frac{\partial(EQ)}{\partial t} = \frac{\partial(EAB)}{\partial t} = \frac{\partial(EPQ)}{\partial t} = 0.$$

Constant enzyme concentration:

$$E_0 = E + (EA) + (EQ) + (EAB) + (EPQ).$$

Enzyme Reactions 3 / 4

Thus, our assumptions are:

$$\begin{cases} 0 &= k_1 EA + k_4(EAB) - k_2(EA) - k_3(EA)B \\ 0 &= k_7(EPQ) + k_9 EQ - k_{10}(EQ) - k_8(EQ)P \\ 0 &= k_3(EA)B + k_6(EPQ) - k_4(EAB) - k_5(EAB) \\ 0 &= k_5(EAB) + k_8(EQ)P - k_6(EPQ) - k_7(EPQ) \\ E_0 &= E + (EA) + (EQ) + (EAB) + (EPQ) \end{cases}$$

Under these assumptions, we wish to express

$$\frac{\partial Q}{\partial t} = k_{10}(EQ) - k_9 EQ$$

as a function of only E_0, A, B, P, and Q. That is, we want to eliminate the variables E, (EA), (EQ), (EAB), (EPQ).

Enzyme Reactions 4 / 4

We get 25 Gröbner equations:

$$g_1(E, (EA), (EQ), (EAB), (EPQ), E_0, A, B, P, Q, \frac{\partial Q}{\partial t}) = 0$$

$$\vdots$$

$$g_{25}(E, (EA), (EQ), (EAB), (EPQ), E_0, A, B, P, Q, \frac{\partial Q}{\partial t}) = 0$$

Surprisingly, g_1 does not(!) involve the red variables. We get:

Enzyme Reactions 4 / 4

We get 25 Gröbner equations:

$$g_1(E, (EA), (EQ), (EAB), (EPQ), E_0, A, B, P, Q, \tfrac{\partial Q}{\partial t}) = 0$$

$$\vdots$$

$$g_{25}(E, (EA), (EQ), (EAB), (EPQ), E_0, A, B, P, Q, \tfrac{\partial Q}{\partial t}) = 0$$

Surprisingly, g_1 does not(!) involve the red variables. We get:

$$\frac{\partial Q}{\partial t} = \frac{(k_1k_3k_5k_7k_{10}AB - k_2k_4k_6k_8k_9PQ)E_0}{\begin{array}{l} k_1k_3k_5k_7AB + k_1k_3k_5k_8ABP + k_1k_3k_5k_{10}AB + \\ k_1k_3k_6k_8ABP + k_1k_3k_6k_{10}AB + k_1k_3k_7k_{10}AB + \\ k_1k_4k_6k_8AP + k_1k_4k_6k_{10}A + k_1k_4k_7k_{10}A + \\ k_1k_5k_7k_{10}A + k_2k_4k_6k_8P + k_2k_4k_6k_9Q + k_2k_4k_6k_{10} + \\ k_2k_4k_7k_9Q + k_2k_4k_7k_{10} + k_2k_4k_8k_9PQ + k_2k_5k_7k_9Q + \\ k_2k_5k_7k_{10} + k_2k_5k_8k_9PQ + k_2k_6k_8k_9PQ + \\ k_3k_5k_7k_9BQ + k_3k_5k_7k_{10}B + k_3k_5k_8k_9BPQ + \\ k_3k_6k_8k_9BPQ + k_4k_6k_8k_9PQ \end{array}}$$

Gröbner equations
for
everybody

Sudoku 1 / 6

Problem: Complete the 4×4 sudoku:

			4
4		2	
	3		1

Sudoku 1 / 6

Problem: Complete the 4×4 sudoku:

			4
4		2	
	3		1

Solution:

3	2	1	4
4	1	2	3
2	3	4	1
1	4	3	2

Sudoku 2 / 6

x_1	x_2	x_3	x_4
x_5	x_6	x_7	x_8
x_9	x_{10}	x_{11}	x_{12}
x_{13}	x_{14}	x_{15}	x_{16}

There are 40 sudoku equations in the variables $x_1, \dots, x_{16}$:

- Each variable has one of the values 1, 2, 3, or 4:

$$\begin{cases} (x_1-1)(x_1-2)(x_1-3)(x_1-4) = 0 \\ \vdots \\ (x_{16}-1)(x_{16}-2)(x_{16}-3)(x_{16}-4) = 0 \end{cases}$$

- There are no repetitions in the 1st column:

$$\begin{cases} x_1+x_5+x_9+x_{13} = 10 \\ x_1x_5x_9x_{13} = 24 \end{cases}$$

- ...

Sudoku 3 / 6

To complete the sudoku

			4
4		2	
	3		1

we consider the 45 equations in the variables $x_1, \ldots, x_{16}$:

$$\left\{ \begin{array}{l} \text{The 40 sudoku equations} \\ \quad x_4 = 4 \\ \quad x_5 = 4 \\ \quad x_7 = 2 \\ \quad x_{10} = 3 \\ \quad x_{12} = 1 \end{array} \right.$$

Sudoku 4 / 6

The Gröbner equations turn out to be:

$$\begin{cases} x_1 = 3 & x_2 = 2 & x_3 = 1 & x_4 = 4 \\ x_5 = 4 & x_6 = 1 & x_7 = 2 & x_8 = 3 \\ x_9 = 2 & x_{10} = 3 & x_{11} = 4 & x_{12} = 1 \\ x_{13} = 1 & x_{14} = 4 & x_{15} = 3 & x_{16} = 2 \end{cases}$$

Hence we have found the unique solution:

3	2	1	4
4	1	2	3
2	3	4	1
1	4	3	2

Sudoku 5 / 6

What about the following sudoku ($x_{12} = 1$ is removed)?

			4
4		2	
	3		

This time the Gröbner equations are:

$$
\begin{array}{rclrclrclrcl}
x_1 &=& 3 & x_2 &=& 2 & x_3 &=& 1 & x_4 &=& 4 \\
x_5 &=& 4 & x_6 &=& 1 & x_7 &=& 2 & x_8 &=& 3 \\
x_9 &=& x_{16} & x_{10} &=& 3 & x_{11} &=& 4 & x_{12} &=& 3 - x_{16} \\
x_{13} &=& 3 - x_{16} & x_{14} &=& 4 & x_{15} &=& 3 & (x_{16} - 1)(x_{16} - 2) &=& 0
\end{array}
$$

Sudoku 6 / 6

Consequently, the sudoku:

			4
4		2	
	3		

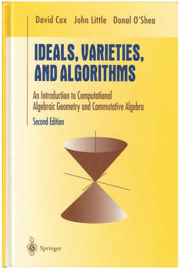
has exactly two solutions:

3	2	1	4
4	1	2	3
1	3	4	2
2	4	3	1

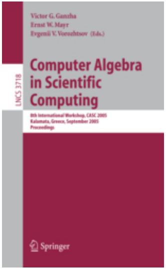
and

3	2	1	4
4	1	2	3
2	3	4	1
1	4	3	2

References



(Chapters 2, 3, 6)



(Pages 155–165)

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Application of Gröbner Bases theory to derive rate equations for enzyme catalysed reactions with two or more substrates or products

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