Convex Hulls of Trajectories

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joint with Daniel Ciripoi, Andreas Löhne, and Bernd Sturmfels

Brown University

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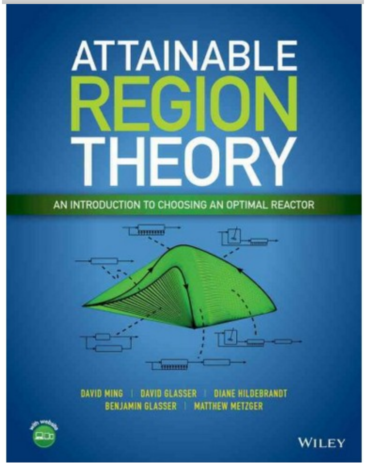
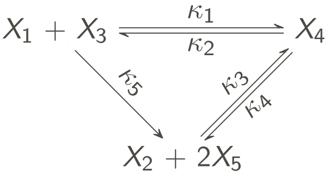

ATTAINABLE
REGION
THEORY
AN INTRODUCTION TO CHOOSING AN OPTIMAL REACTOR
DAVID MING | DAVID GLASSER | DIANE HILDEBRANDT
BENJAMIN GLASSER | MATTHEW METZGER
WILEY

Attainable Region Theory

Attainable Region (AR) theory is a branch of chemical reaction engineering that incorporates elements of geometry and mathematical optimization to understand how chemical reactor networks—termed *reactor structures*—can be designed and improved.

AR theory is unique in that it is **geometric** in nature, and is particularly useful for understanding complex reactions (involving many competing reactions and species).

Chemical Reaction Networks (CRN)



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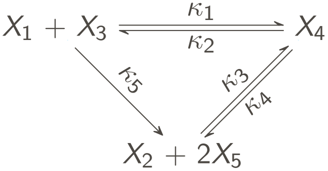

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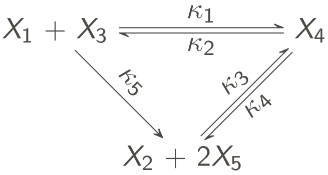

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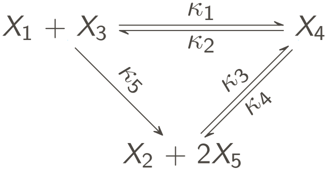

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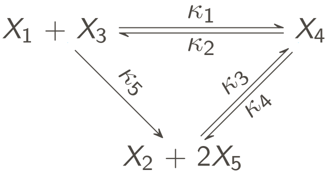

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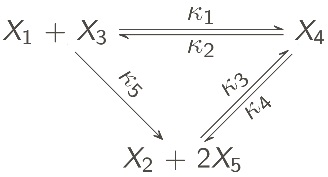
Definition (Chemical Reaction Networks)

A chemical reaction network (CRN) is a graph whose vertices are chemical complexes and edges are the chemical reactions weighted by their reaction rates.

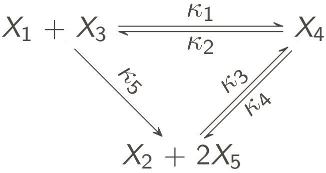


$$\dot{x} = \frac{dx}{dt} = \Psi(x) \cdot A_\kappa \cdot Y$$

$$\Psi(x) = \begin{bmatrix} x_1 x_3 & x_4 & x_2 x_5^2 \end{bmatrix}$$

$$A_\kappa = \begin{bmatrix} -\kappa_1 - \kappa_5 & \kappa_1 & \kappa_5 \\ \kappa_2 & -\kappa_2 - \kappa_4 & \kappa_4 \\ 0 & \kappa_3 & -\kappa_3 \end{bmatrix}$$

$$Y = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 2 \end{bmatrix}$$



$$\dot{x} = \frac{dx}{dt} = \Psi(x) \cdot A_\kappa \cdot Y$$

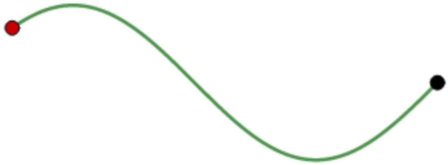
$$\dot{x}_1 = \frac{dx_1}{dt} = -\kappa_1 x_1 x_3 - \kappa_5 x_1 x_3 + \kappa_2 x_4$$

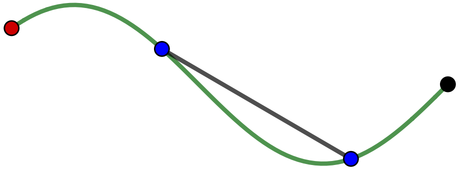
$$\dot{x}_2 = \frac{dx_2}{dt} = \kappa_5 x_1 x_3 + \kappa_4 x_4 - \kappa_3 x_2 x_5^2$$

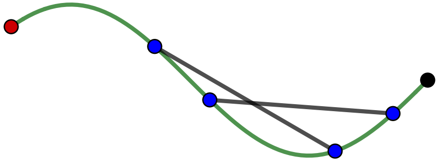
$$\dot{x}_3 = \frac{dx_3}{dt} = (-\kappa_1 - \kappa_5) x_1 x_3 + \kappa_2 x_4$$

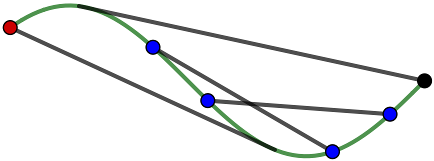
$$\dot{x}_4 = \frac{dx_4}{dt} = \kappa_1 x_1 x_3 + (-\kappa_2 - \kappa_4) x_4 + \kappa_3 x_2 x_5^2$$

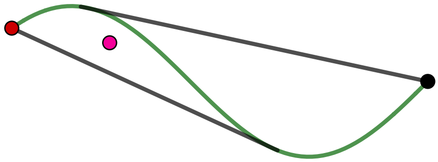
$$\dot{x}_5 = \frac{dx_5}{dt} = 2(\kappa_5 x_1 x_3 + \kappa_4 x_4 - \kappa_3 x_2 x_5^2).$$

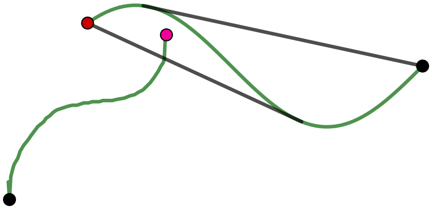


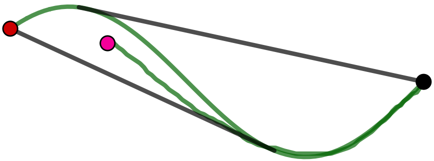












Attainable Region

Definition (Forward Closed)

A subset $S \subset \mathbb{R}^n$ is *forward closed* if the initial condition $x_0 \in S$ holds for the dynamical system then $x(t) \in S$ for all $t > 0$.

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Definition (Attainable Region)

For a given reaction network and starting point x_0 in $\mathbb{R}^n$, the *attainable region*, $\mathcal{A}(x_0)$, is the smallest subset of $\mathbb{R}^n$ that contains x_0 and is both convex and forward closed.

Definition (Spectrahedral Shadow)

$$S = \{(x_1, x_2, \ldots, x_m) \in \mathbb{R}^m | \ \exists \ (y_1, y_2, \ldots, y_p) \in \mathbb{R}^p : A_0 + \sum_i x_i A_i + \sum_j y_j B_j \succcurlyeq 0\}$$

where A_0, A_i and B_j are real symmetric matrices. We use the symbol $A \succcurlyeq 0$ to denote that the matrix A is positive semidefinite.

Linear Chemical Reaction Networks

A chemical reaction network is linear if all the complexes are single unit species.

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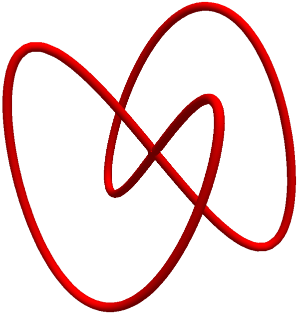
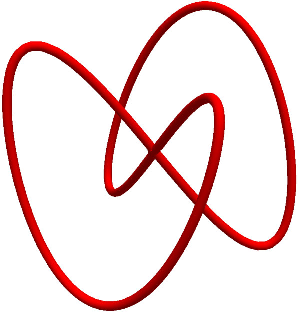
Proposition (K.)

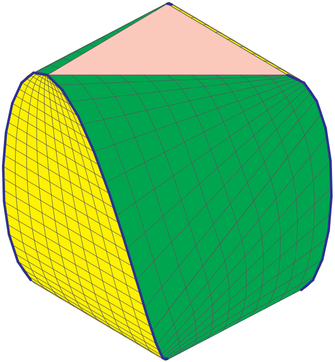
The convex hull of the trajectory of a linear chemical reaction network whose Laplacian has eigenvalues in rational ratio is a spectrahedral shadow.

Theorem (K.)

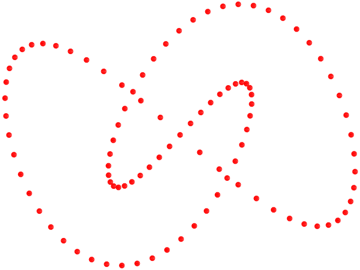
The attainable region of linear chemical reaction networks whose Laplacian has eigenvalues in rational ratio is spectrahedral shadow.

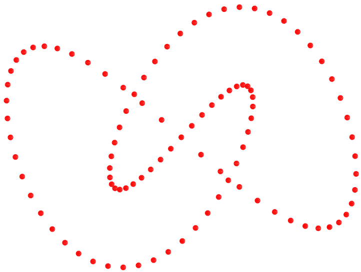


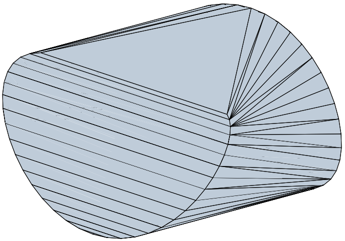




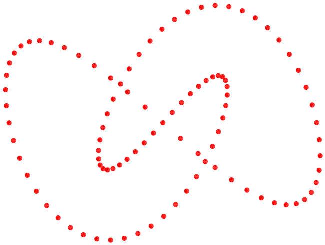
$$\dot{x} = \frac{dx}{dt} = f(x)$$

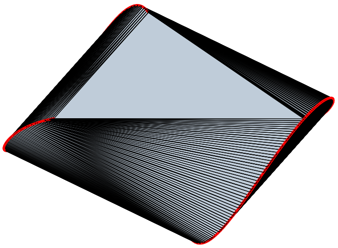






Using Bensolve





Using Bensolve

Computing Convex Hulls

The main idea involves computing the polytope given the points on the trajectories. More the points, the closer it is to actual convex hull.

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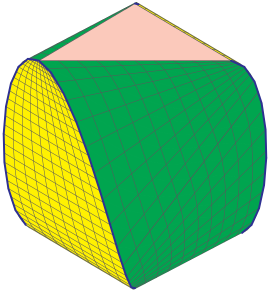

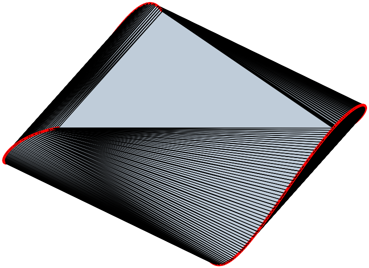

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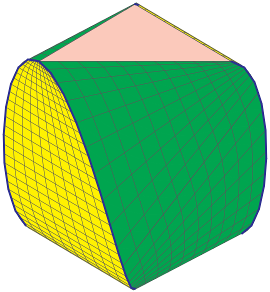

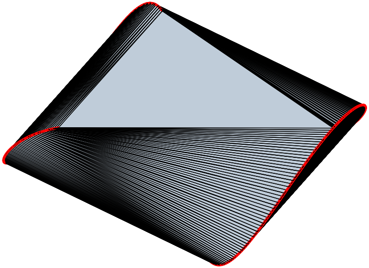

We use this to develop a theory on limiting faces of the polyhedral approximations.

Definition (ε-Approximation)

An ε-approximation of a given curve $\mathcal{C}$ is a finite subset $\mathcal{A}_\varepsilon \subset \mathcal{C}$ such that

$$\forall y \in \mathcal{C} \; \exists x \in \mathcal{A}_\varepsilon : \|y - x\| \leq \varepsilon.$$

Let $A_\varepsilon = \operatorname{conv}(\mathcal{A}_\varepsilon)$.

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Definition (Hausdorff Distance)

The *Hausdorff distance* of two compact sets B_1 and B_2 in $\mathbb{R}^n$ is defined as

$$d(B_1, B_2) = \max\left\{ \max_{x \in B_1} \min_{y \in B_2} \|x - y\|, \max_{y \in B_2} \min_{x \in B_1} \|x - y\| \right\}.$$

Limiting Faces

Theorem (Ciripoi, K., Löhne, Sturmfels)

With some genericity assumptions, let $\{F_\varepsilon\}_{\varepsilon \searrow 0}$ *be a Hausdorff convergent sequence of proper faces* F_ε *of* A_ε*. Then its limit* F *is a proper face of* $\mathrm{conv}(\mathcal{C})$*.*

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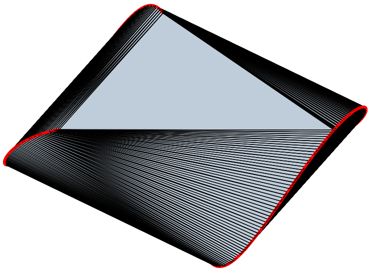
Theorem (Ciripoi, K., Löhne, Sturmfels)

Let every point on the curve $\mathcal{C}$ *that is in the boundary of* $\mathrm{conv}(\mathcal{C})$ *is an extremal point of* $\mathrm{conv}(\mathcal{C})$*. If* F *is a simplex which is a uniquely exposed face of* $\mathrm{conv}(\mathcal{C})$*, then* F *is the Hausdorff limit of a sequence* $\{F_\varepsilon\}_{\varepsilon \searrow 0}$ *of facets of* A_ε*.*

Patches



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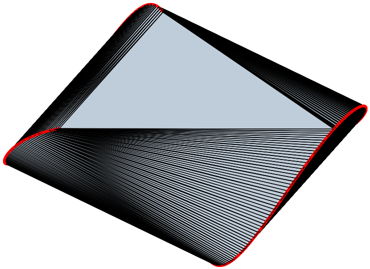

- The figure has four regions of 1-dimensional family of 1-dimensional faces.

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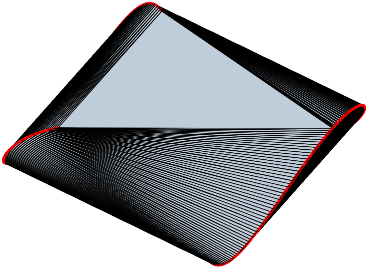

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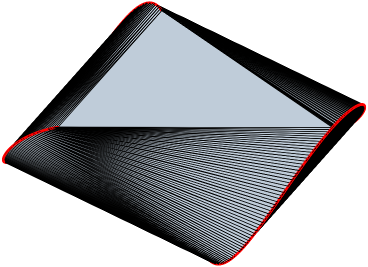

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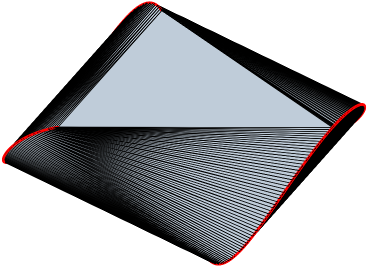

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We call these family of faces as patches. How do we define them?

Patches

Let C be a convex set and $C^\vee$ be its dual. Let $\mathcal{E} \subseteq \partial C^\vee$ be the set of exposed points of $C^\vee$. We define *Normal Cycle* as follows.

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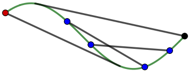
- ψ is maximal with these properties.

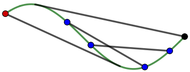


Algorithm

(Detection of edges and arcs for $n = 2$)

input : *A list $\mathcal{A}$ of points on a curve $\mathcal{C}$ in $\mathbb{R}^2$; a threshold value $\delta > 0$*

Boundary of Planar Convex Hulls



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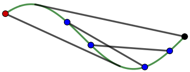

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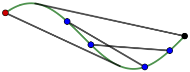
2 *Build a graph G with node set $\mathcal{H}$ such that two distinct edges H_1, H_2 of A form an edge of G if $H_1 \cap H_2 \neq \emptyset$ and both H_1 and H_2 have length $\leq \delta$.*



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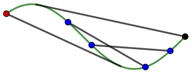
Boundary of Planar Convex Hulls



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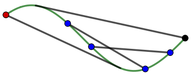
Output the number $\#_1$ of isolated nodes of G and the number $\#_0$ of remaining connected components G_i.

foreach *nonsingleton connected component G_i* **do**

  Output a list of curve points that are endpoints of those edges of A, that belong to G_i. This represents the ith arc of ∂C.

end



Algorithm

(Detection of edges and arcs for $n = 2$)

input : *A list* $\mathcal{A}$ *of points on a curve* $\mathcal{C}$ *in* $\mathbb{R}^2$*; a threshold value* $\delta > 0$

Compute the vertices $\mathcal{V}$ *and edges* $\mathcal{H}$ *of* $A = \text{conv}(\mathcal{A})$

Build a graph G *with node set* $\mathcal{H}$ *such that two distinct edges* H_1, H_2 *of* A *form an edge of* G *if* $H_1 \cap H_2 \neq \emptyset$ *and both* H_1 *and* H_2 *have length* $\leq \delta$.

Output the number $\#_1$ *of isolated nodes of* G *and the number* $\#_0$ *of remaining connected components* G_i.

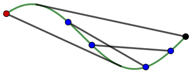
foreach *nonsingleton connected component* G_i **do**

    Output a list of curve points that are endpoints of those edges of A*, that belong to* G_i*. This represents the* i*th arc of* ∂C.

end

The edges H_j *of* A *that correspond to isolated nodes of* G *represent edges of* C.

Boundary of Planar Convex Hulls



Algorithm

(Detection of edges and arcs for $n = 2$)

input : *A list $\mathcal{A}$ of points on a curve $\mathcal{C}$ in $\mathbb{R}^2$; a threshold value $\delta > 0$*

Compute the vertices $\mathcal{V}$ and edges $\mathcal{H}$ of $A = \text{conv}(\mathcal{A})$

Build a graph G with node set $\mathcal{H}$ such that two distinct edges H_1, H_2 of A form an edge of G if $H_1 \cap H_2 \neq \emptyset$ and both H_1 and H_2 have length $\leq \delta$.

Output the number $\#_1$ of isolated nodes of G and the number $\#_0$ of remaining connected components G_i.

foreach *nonsingleton connected component G_i* **do**

   Output a list of curve points that are endpoints of those edges of A, that belong to G_i. This represents the ith arc of ∂C.

end

The edges H_j of A that correspond to isolated nodes of G represent edges of C.

output: *The numbers $\#_0$ and $\#_1$ of arcs and edges of $C = \text{conv}(\mathcal{C})$*
For each i: list of curve points that represent the ith arc of ∂C.
List of line segments that represent the edges of C.

degree 2d	6	8	10	12	14	16	18	20	22	24	26
max $\#_2$	6	9	13	16	20	21	24	26	28	30	30
tritangents	8	80	280	672	1320	2288	3640	5440	7752	10640	14168
max $\#_1$	10	14	20	25	30	32	35	37	41	42	43
edge surface	30	70	126	198	286	390	510	646	798	966	1150

Table: Census of random trigonometric curves in 3-space

Theorem (Ranestad, Sturmfels)

Let $\mathcal{C}$ be a general smooth compact curve of degree d and genus g in $\mathbb{R}^3$. The algebraic boundary ∂C of its convex hull C is the union of the edge surface and the tritangent planes. The edge surface is irreducible of degree $2(d-3)(d+g-1)$, and the number of complex tritangent planes equals
$8\binom{d+g-1}{3} - 8(d+g-4)(d+2g-2) + 8g - 8.$

degree 2d	6	8	10	12	14	16	18	20	22	24	26
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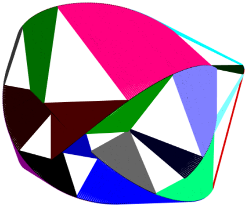
Table: Census of random trigonometric curves in 3-space



All implementations are available at
http://tools.bensolve.org/trajectories.

Thank You.