Challenge Problem 5: Polynomial Zonotopes in Julia

Niklas Kochdumper

Stony Brook University

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Curriculum vitae:

- **2018-2021:** PhD candidate in the research group of Prof. Althoff at the Chair of Robotics, Artificial Intelligence, and Embedded Systems (Technical University of Munich)
- **2021-now:** Postdoctoral researcher in the research group of Prof. Bak (Stony Brook University)

Research interests: Reachability analysis, set-based computing, neural network verification, control theory

Motivation

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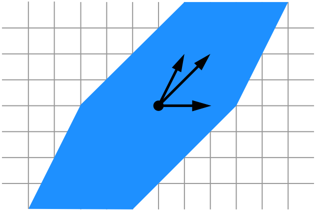
Exact reachable set of the Van-der-Pol oscillator at time $t = 3.15$s.

Polynomial zonotopes[1] are a novel non-convex set representation:

Zonotope:

$$\mathcal{Z} = \left\{ \begin{bmatrix} 2 \\ 0 \end{bmatrix} \alpha_1 + \begin{bmatrix} 1 \\ 2 \end{bmatrix} \alpha_2 + \begin{bmatrix} 2 \\ 2 \end{bmatrix} \alpha_3 \ \middle| \ \alpha_1, \alpha_2, \alpha_3 \in [-1, 1] \right\}$$



[1] N. Kochdumper and M. Althoff. *Sparse Polynomial Zonotopes: A Novel Set Representation for Reachability Analysis*, Transactions on Automatic Control, 2021

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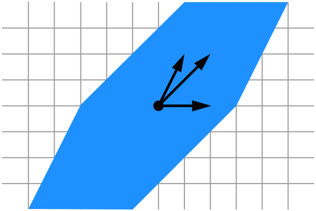

Polynomial Zonotope:

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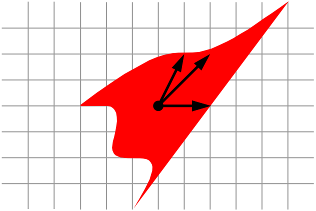

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Sparse Representation of Polynomial Zonotopes

Sparse Polynomial Zonotope

Given a constant offset $c \in \mathbb{R}^n$, a generator matrix $G \in \mathbb{R}^{n \times h}$, and an exponent matrix $\mathbb{N}_{\geq 0}^{p \times h}$, a sparse polynomial zonotope $\mathcal{PZ} \subset \mathbb{R}^n$ is

$$\mathcal{PZ} = \left\{ c + \sum_{i=1}^{h} \left(\prod_{k=1}^{p} \alpha_k^{E_{(k,i)}} \right) G_{(\cdot,i)} \;\middle|\; \alpha_k \in [-1,1] \right\}.$$

For a concise notation we use the shorthand $\mathcal{PZ} = \langle c, G, E \rangle_{PZ}$.

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Sparse representation of the polynomial zonotope on the previous slide:

$$\begin{aligned} \mathcal{PZ} &= \left\{ \begin{bmatrix} 2 \\ 0 \end{bmatrix} \alpha_1 + \begin{bmatrix} 1 \\ 2 \end{bmatrix} \alpha_2 + \begin{bmatrix} 2 \\ 2 \end{bmatrix} \alpha_1^3 \alpha_2 \;\middle|\; \alpha_1, \alpha_2 \in [-1,1] \right\} \\ &= \left\langle \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 & 1 & 2 \\ 0 & 2 & 2 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 3 \\ 0 & 1 & 1 \end{bmatrix} \right\rangle_{PZ} \end{aligned}$$

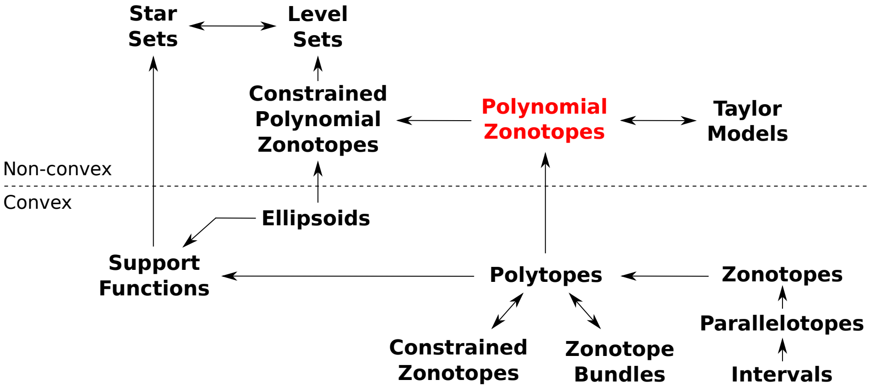
Set Operations

✓ closed under operation, — closed, but no formula, ✗ not closed

Set Representation	Lin. Map	Mink. Sum	Cart. Prod.	Conv. Hull	Quad. Map	Inter- section	Union
Interval	✗	✓	✓	✗	✗	✓	✗
Zonotopes	✓	✓	✓	✗	✗	✗	✗
Polytopes	✓	✓	✓	✓	✗	✓	✗
Ellipsoids	✓	✗	✗	✗	✗	✗	✗
Support Functions	✓	✓	✓	✓	✗	—	✗
Taylor Models	✓	✓	✓	✓	✓	✗	✗
Level Sets	✓	—	✓	—	—	✓	✓
Star Sets	✓	✓	✓	—	—	✓	—
Polynomial Zonotopes	✓	✓	✓	✓	✓	✗	✗
Con. Poly. Zonotopes	✓	✓	✓	✓	✓	✓	✓

Family Tree for Set Representations

Visualization of the relations between the different set representations, where A $\rightarrow$ B denotes that B is a generalization of A.



Set Operations on Polynomial Zonotopes

Given two polynomial zonotopes $\mathcal{PZ}_1 = \langle c_1, G_1 \rangle_{PZ} \subset \mathbb{R}^n$, $\mathcal{PZ}_2 = \langle c_2, G_2 \rangle_{PZ} \subset \mathbb{R}^n$ and a matrix $M \in \mathbb{R}^{n \times n}$, basic set operations on polynomials are trivial to compute:

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- **Linear map:**

$$M\,\mathcal{PZ}_1 = \langle M\,c, M\,G, E \rangle_{PZ}$$

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- **Minkowski addition:**

$$\mathcal{PZ}_1 \oplus \mathcal{PZ}_2 = \left\langle c_1 + c_2, \begin{bmatrix} G_1 & G_2 \end{bmatrix}, \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix} \right\rangle_{PZ}$$

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- **Cartesian product:**

$$\mathcal{PZ}_1 \times \mathcal{PZ}_2 = \left\langle \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}, \begin{bmatrix} G_1 & 0 \\ 0 & G_2 \end{bmatrix}, \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix} \right\rangle_{PZ}$$

Quadratic Map

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Given a discrete set of quadratic matrices $\mathcal{Q} = \{Q_1, \dots, Q_m\}$, $Q_i \in \mathbb{R}^{n \times n}$ and a set $\mathcal{S} \subset \mathbb{R}^n$, the quadratic map is defined as

$$\mathtt{sq}(\mathcal{S}, \mathcal{Q}) = \left\{ x \in \mathbb{R}^m \;\middle|\; x_{(i)} = s^T Q_i \, s, \;\; s \in \mathcal{S}, \;\; i = 1, \dots, m \right\}.$$

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For a polynomial zonotope $\mathcal{PZ} = \langle c, G, E \rangle_{PZ} \subset \mathbb{R}^n$ the quadratic map is

$$\operatorname{sq}(\mathcal{PZ}, \mathcal{Q}) = \left\langle \overline{c}, \begin{bmatrix} \overline{G} & \widehat{G}_1 & \dots & \widehat{G}_h \end{bmatrix}, \begin{bmatrix} E & \widehat{E}_1 & \dots & \widehat{E}_h \end{bmatrix} \right\rangle_{PZ},$$

with

$$\overline{c} = \begin{bmatrix} c^T Q_1 c \\ \vdots \\ c^T Q_m c \end{bmatrix}, \quad \overline{G} = \begin{bmatrix} c^T (Q_1 + Q_1^T) G \\ \vdots \\ c^T (Q_m + Q_m^T) G \end{bmatrix}, \quad \widehat{G}_i = \begin{bmatrix} G_{(\cdot,i)}^T Q_1 G \\ \vdots \\ G_{(\cdot,i)}^T Q_m G \end{bmatrix}$$

$$\widehat{E}_i = E + \begin{bmatrix} E_{(\cdot,i)} & \dots & E_{(\cdot,i)} \end{bmatrix}, \quad i = 1, \dots, h$$

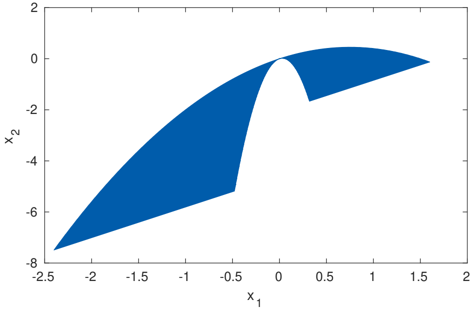
Example Quadratic Map

Given $\mathcal{PZ}$ and $\mathcal{Q} = \{Q_1, Q_2\}$ defined as

$$\mathcal{PZ} = \left\langle \begin{bmatrix} 0.2 \\ -0.6 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 0.4 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\rangle_{PZ}, \; Q_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \; Q_2 = \begin{bmatrix} -3.2 & 1.2 \\ 1.2 & 0 \end{bmatrix},$$

the quadratic map is

$$\mathrm{sq}(\mathcal{PZ}, \mathcal{Q}) = \left\langle \begin{bmatrix} -0.24 \\ -0.416 \end{bmatrix}, \begin{bmatrix} -1.2 & 0.16 & 0.8 & 0 \\ -2.72 & 0.192 & 0.96 & -3.2 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 1 & 2 \\ 0 & 1 & 1 & 0 \end{bmatrix} \right\rangle_{PZ}.$$



Linear Combination

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Given two set $\mathcal{S}_1 \subset \mathbb{R}^n$ and $\mathcal{S}_2 \subset \mathbb{R}^n$, their linear combination is

$$\mathtt{comb}(\mathcal{S}_1, \mathcal{S}_2) = \left\{ \frac{1}{2}(1+\lambda)s_1 + \frac{1}{2}(1-\lambda)s_2 \;\middle|\; s_1 \in \mathcal{S}_1,\ s_2 \in \mathcal{S}_2,\ \lambda \in [-1,1] \right\}.$$

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For polynomial zonotopes $\mathcal{PZ}_1 = \langle c_1, G_1, E_1 \rangle_{PZ} \subset \mathbb{R}^n$ and $\mathcal{PZ}_2 = \langle c_2, G_2, E_2 \rangle_{PZ} \subset \mathbb{R}^n$ the linear combination is

$$\texttt{comb}(\mathcal{PZ}_1, \mathcal{PZ}_2) = \Bigg\langle \frac{1}{2}(c_1 + c_2), \frac{1}{2}\begin{bmatrix}(c_1 - c_2) & G_1 & G_1 & G_2 & -G_2\end{bmatrix}, \begin{bmatrix} 0 & E_1 & E_1 & 0 & 0 \\ 0 & 0 & 0 & E_2 & E_2 \\ 1 & 0 & 1 & 0 & 1 \end{bmatrix} \Bigg\rangle_{PZ}$$

Linear Combination and Convex Hull

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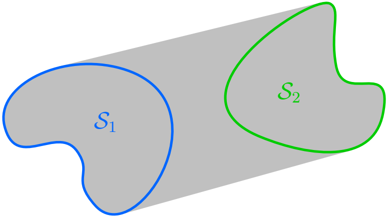
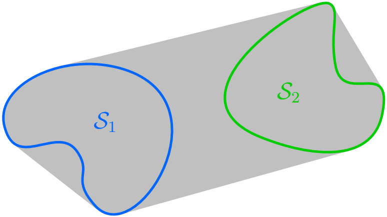


Convex Hull:



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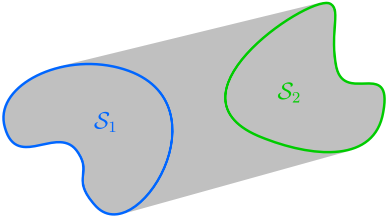

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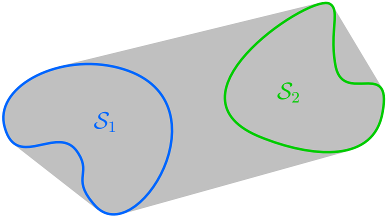


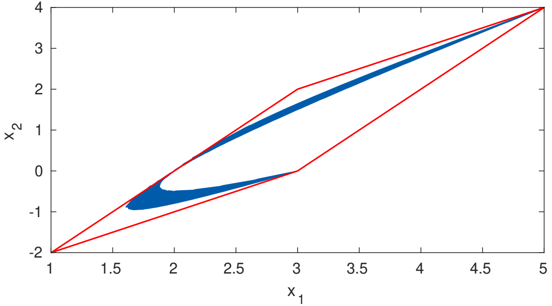
The convex hull $\texttt{conv}(\mathcal{S}_1, \mathcal{S}_2)$ can be computed using the linear combination:

$$\texttt{conv}(\mathcal{S}_1, \mathcal{S}_2) = \texttt{comb}\big(\texttt{comb}(\mathcal{S}_1, \mathcal{S}_1), \texttt{comb}(\mathcal{S}_2, \mathcal{S}_2)\big)$$

For the computation of zonotope enclosures, terms with **all-even exponents** can be enclosed more tightly:

$$\mathcal{PZ} = \left\{ \begin{bmatrix}2\\0\end{bmatrix} + \begin{bmatrix}1\\2\end{bmatrix} \underbrace{\alpha_1\alpha_2}_{\in[-1,1]} + \begin{bmatrix}2\\2\end{bmatrix} \underbrace{\alpha_1^4\alpha_2^2}_{\in[0,1]} \,\middle|\, \alpha_1,\alpha_2 \in [-1,1] \right\}$$

$$\subseteq \left\{ \begin{bmatrix}2\\0\end{bmatrix} + 0.5 \begin{bmatrix}2\\2\end{bmatrix} + \begin{bmatrix}1\\2\end{bmatrix} \alpha_3 + 0.5 \begin{bmatrix}2\\2\end{bmatrix} \alpha_4 \,\middle|\, \alpha_3,\alpha_4 \in [-1,1] \right\}$$



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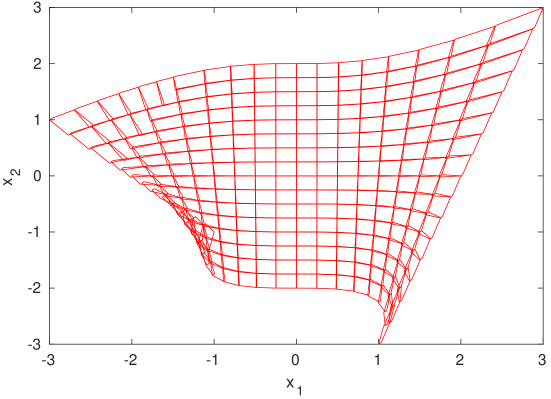
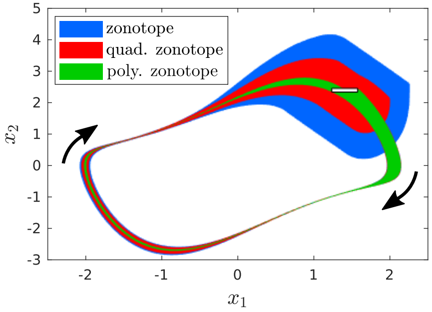
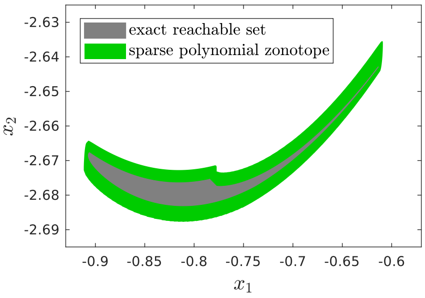


Van-der-Pol oscillator:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} x_2 \\ (1 - x_1^2)x_2 - x_1 \end{bmatrix}$$





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- ✓ With sparse polynomial zonotopes one can calculate very tight outer-approximations for reachable sets of nonlinear systems

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Good luck with the challenge problem!