Generalized Exponent Relaxation of Polynomial Zonotopes for Formally Verifying Neural Networks

Technical University of Munich

Department of Informatics

Chair of Robotics, Artificial Intelligence and Real-time Systems

Supervisor:
Prof. Dr.-Ing. Matthias Althoff

Advisor:
Tobias Ladner, M.Sc.

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For more information please contact us:

Phone: +49 (89) 289 - 18140

E-Mail: tobias.ladner@tum.de

Website: ce.cit.tum.de/cps/

Background

Formal neural network verification [3] aims to rigorously prove properties such as robustness to input perturbations, bounded outputs, or absence of unsafe behaviors under all admissible inputs.

One of the leading approaches to this problem is reachability analysis — computing a conservative outer approximation of all possible outputs the network can produce for a given set of inputs. To perform reachability analysis on neural networks, especially those with nonlinear activation functions or in feedback loops [7], we need expressive mathematical structures that can capture complex dependencies among variables.

Zonotopes and their extensions have become popular in this context [6]. Classical zonotopes [4] are an efficient set representation for linear reachability analysis, while polynomial zonotopes [5] extend this by including nonlinear monomials, allowing tighter approximations of nonlinear dynamics or activation functions. However, polynomial zonotopes can grow rapidly in complexity, making them computationally expensive to propagate through multiple layers or iterations.

To mitigate this, an exponent relaxation technique has been introduced by Ladner and Althoff [2] which simplifies polynomial zonotopes by reducing the degree of their monomials while preserving sound outer approximations. Still, existing approaches treat each monomial independently. This leads to unnecessary outer approximation and reduced scalability.

Description

This thesis aims to improve the scalability and tightness of exponent relaxation by developing a group-based relaxation method for polynomial zonotopes. The central idea is to identify sets of monomials that share structural or geometric characteristics and to relax their exponents collectively. The goal is to preserve underlying exponential dependencies while achieving a tighter and more efficient outer approximation.

Two primary grouping strategies will be evaluated alongside one exploratory topic:

1. Directional similarity: monomials whose associated generators point in the same (or similar) directions in space may be relaxed together, as they contribute coherently to the zonotope shape.
2. Parity-based exponent Structure: monomials with even-even or odd-odd exponent pairs tend to have consistent signs, allowing for tighter bounding of the error introduced by collective relaxation.
3. Use of Bernstein polynomial form (Exploratory): With recent developments in efficient conversion of multivariate polynomials to Bernstein form [8], this thesis will explore how the Bernstein representation can be exploited to improve polynomial zonotope computations. In particular, the focus will be on leveraging the bounding and convexity properties of Bernstein coefficients to more effectively estimate relaxation errors or simplify internal operations within the zonotope framework.

The thesis will also develop methods to quantify the relaxation error incurred when these grouped monomials are jointly relaxed. This involves theoretical analysis and/or symbolic estimation of the maximum deviation from the original zonotope.

Tasks

1. Background research: deepen understanding of polynomial zonotopes, exponent relaxation, and relevant algebraic properties of monomials.

2. Group identification criteria:
   - develop heuristics or algorithms to detect monomial groups based on directional similarity.
   - formulate rules based on exponent parity patterns.
3. Error estimation:
   - derive bounding techniques for the approximation error introduced by group relaxation.
   - analyze how dependency-preserving relaxation affects the overall zonotope conservativeness.
4. Implementation: integrate the grouping and relaxation algorithms into a prototype within CORA.
5. Experimental evaluation: Benchmark the group-based method against individual exponent relaxation in terms of runtime, tightness, and scalability on neural network verification problems.

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