Star Set based Reachability Analysis of Neural Networks with differing Layers and Activation Functions

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LuFG Theory of Hybrid Systems

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RWTH AACHEN UNIVERSITY

Outline

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Feedforward Neural Network

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- FFN transmits information forward through:

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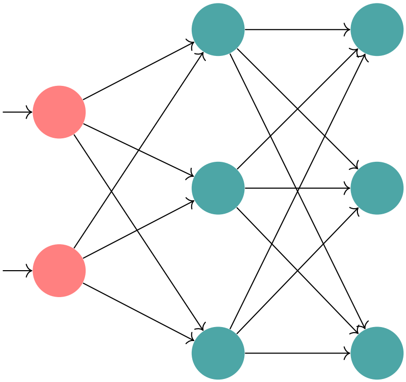

Feedforward Neural Network

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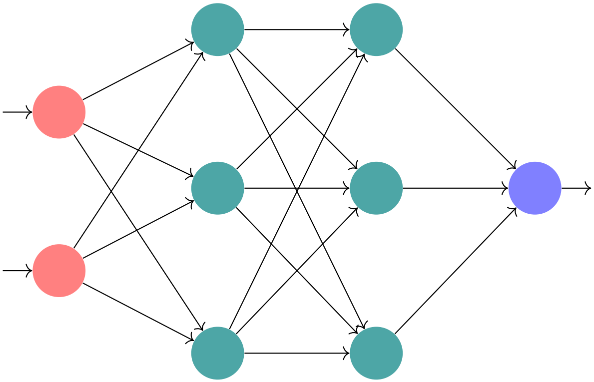

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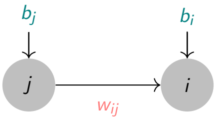

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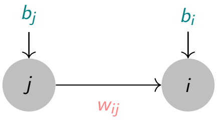

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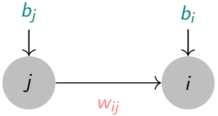

  - The activation function f
  - Overall y_i give the output of a neuron i by:

$$y_i = f(b_i + \sum_{j=1}^{n} w_{ij} x_j)$$

Star Set Representation

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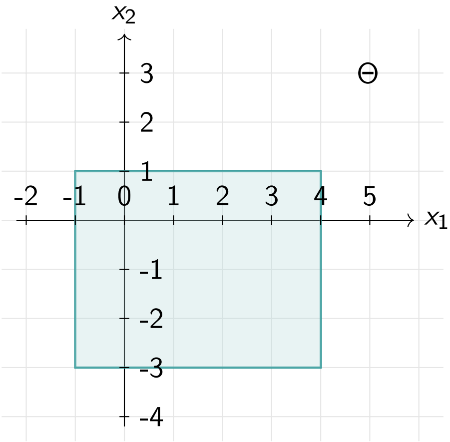
- The set of states:

$$[\![\Theta]\!] = \{x \mid x = c + \sum_{i=1}^{m}(\alpha_i v_i) \text{ such that } P(\alpha) = \top)\}$$

Affine Mapping of a Star



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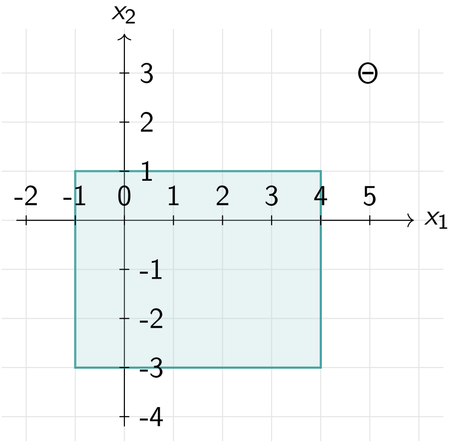

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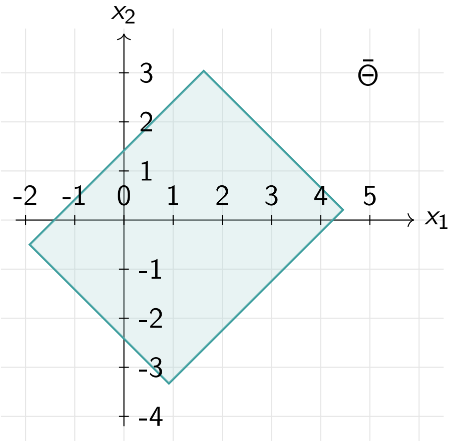
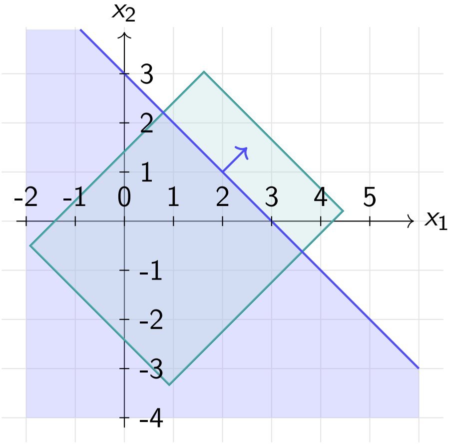


$\langle \bar{c}, \bar{V}, \bar{P} \rangle$

$$\bar{c} = Wc + b, \ \ \bar{V} = \{Wv_1, \dots, Wv_m\}, \ \ \bar{P} \equiv P$$

Star and Half-space Intersection



$\Theta = \langle c, V, P \rangle$ and $\mathscr{H} \triangleq \{x \mid Hx \leq g\}$

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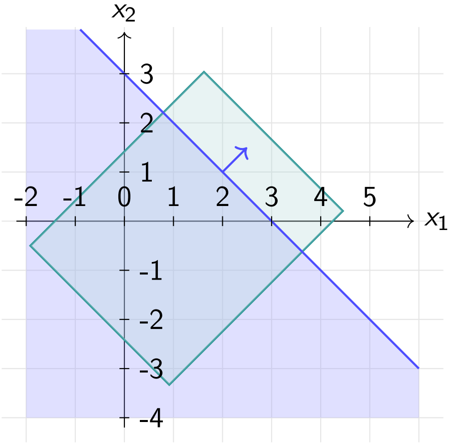

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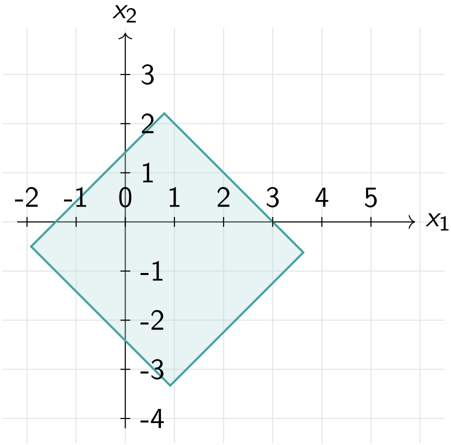
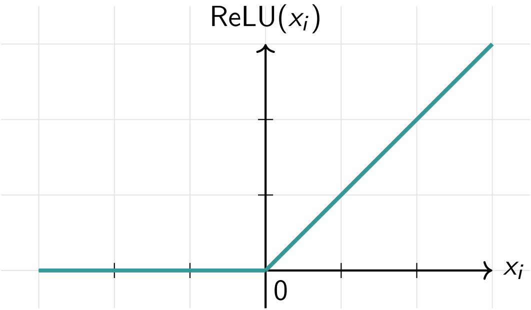


$\bar{\Theta} = \Theta \cap \mathscr{H} = \langle c, V, \bar{P} \rangle$ with $\bar{P} = P \wedge P'$, where
$P'(\alpha) \triangleq (H \times V)\alpha \leq g - H \times c, \;\; V = [v_1, \ldots, v_m]$

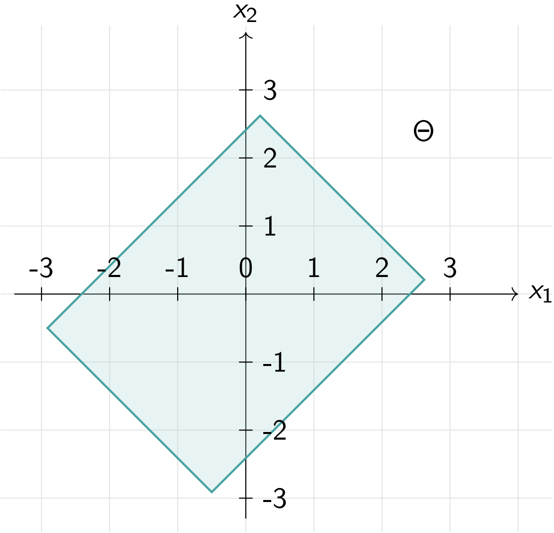
Reachability Analysis of FNNs with ReLU

- Given the input x,

$$ReLU(x) = \begin{cases} x, & x \geq 0 \\ 0, & x < 0 \end{cases} = max(0, x)$$



Exact Analysis



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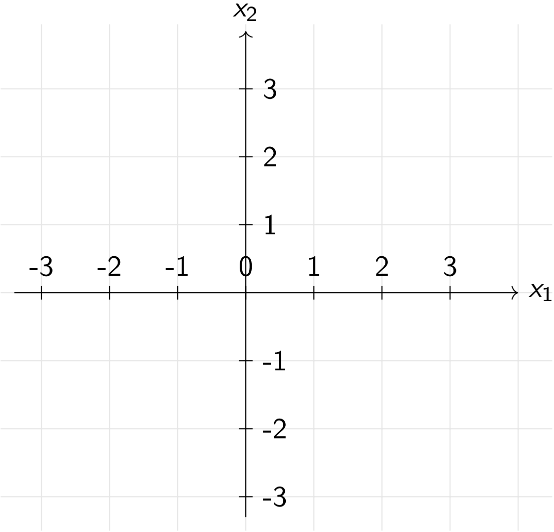

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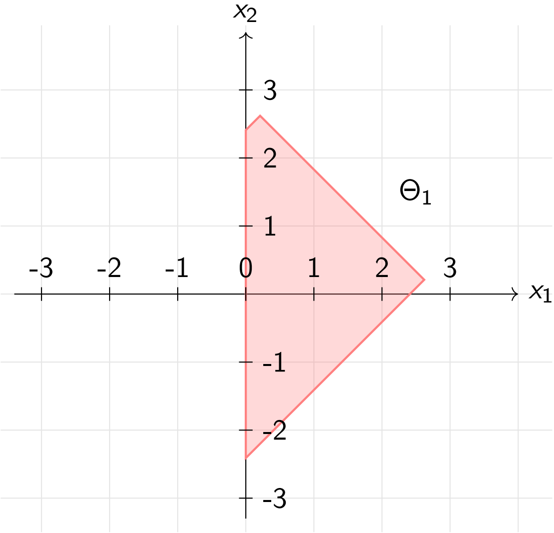

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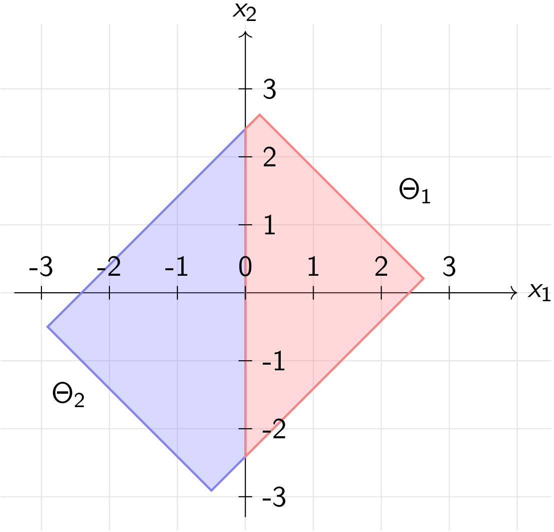

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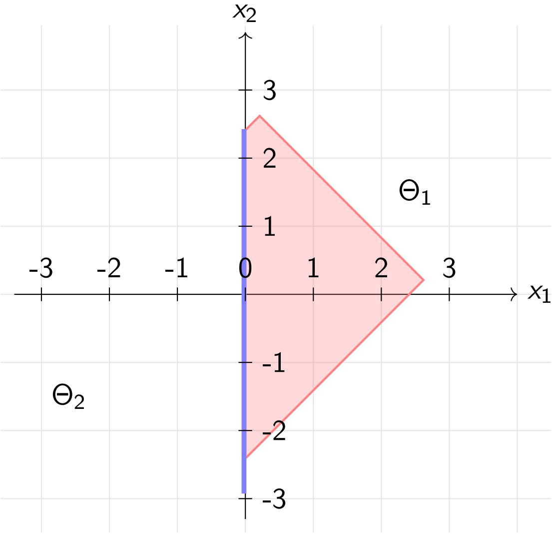

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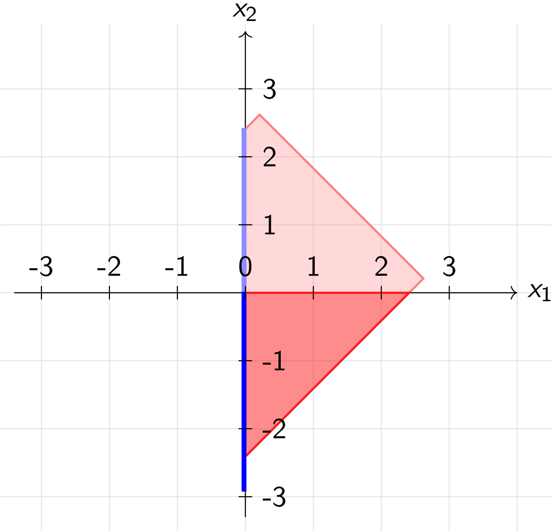

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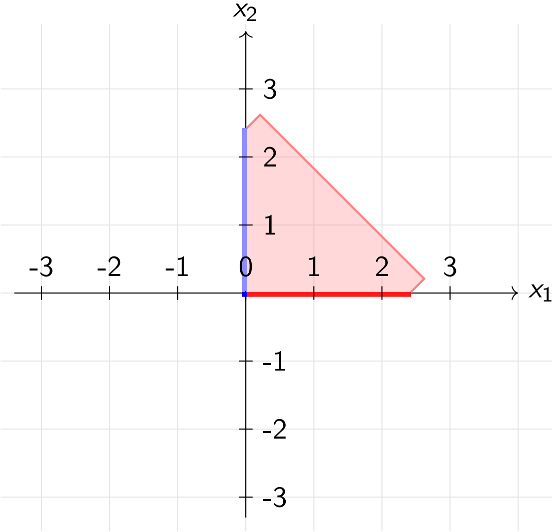
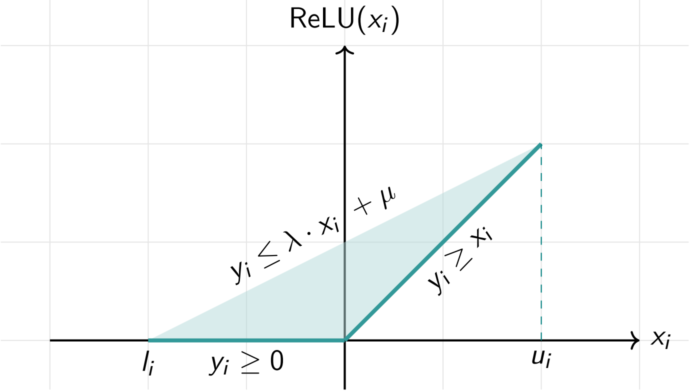


Over-approximate Analysis Convex Relaxation



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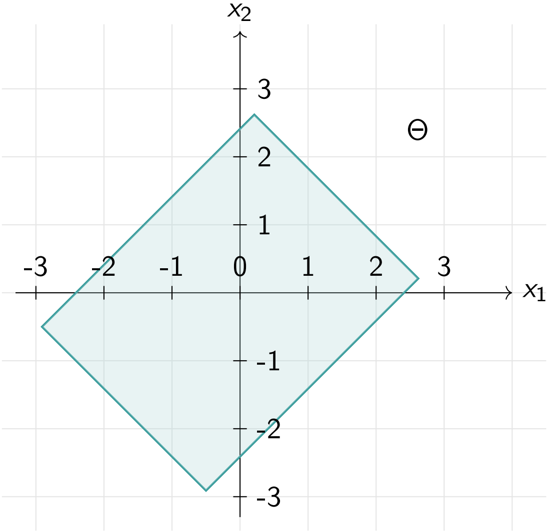

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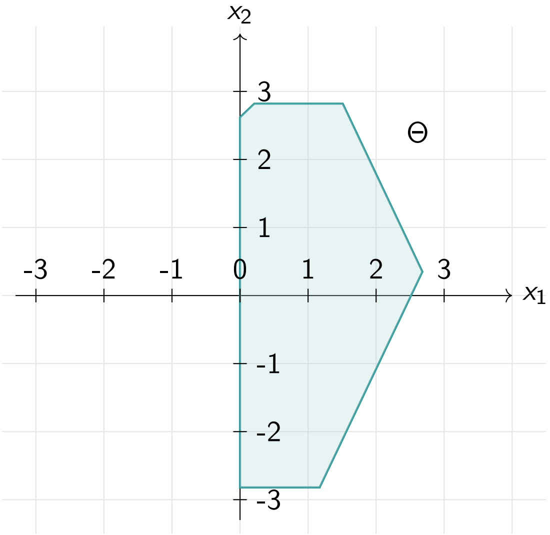

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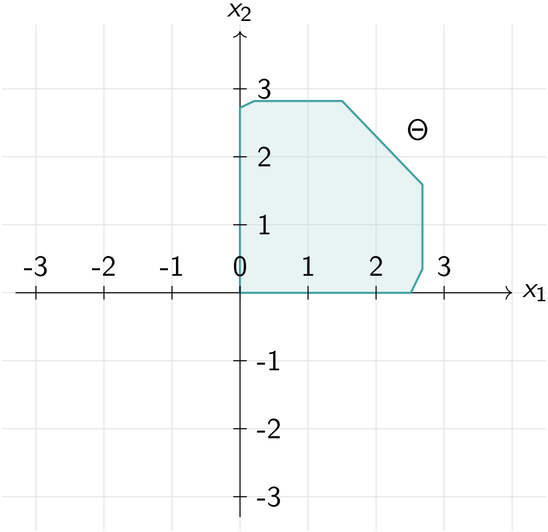

Outline

Motivation

Neural networks process and learn from complex, non-linear datasets

$\Rightarrow$ Non-linear activation functions to prevent linearity

$\Rightarrow$ Verifying neural networks to ensure their reliability, robustness, and safety

Methodology and Implementation

We investigate star set based reachability analysis of . . .

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- Leaky ReLU Layer

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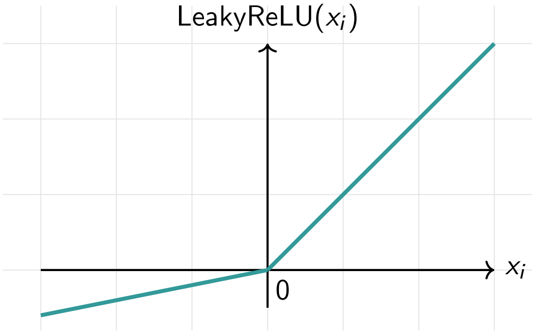
for exact and over-approximation on bounded/unbounded sets.

Leaky ReLU Function

- Given the input x,

$$LeakyReLU(x) = \begin{cases} x, & x > 0 \\ \gamma \cdot x, & x \leq 0 \end{cases} = max(\gamma \cdot x, x)$$

where $\gamma \in (0, 1)$



Exact Analysis

Case 1 | Case 2 | Case 3

Exact Analysis

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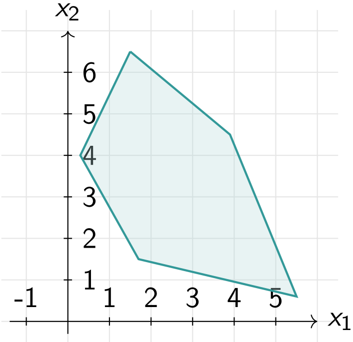

Case 2

Case 3

Exact Analysis

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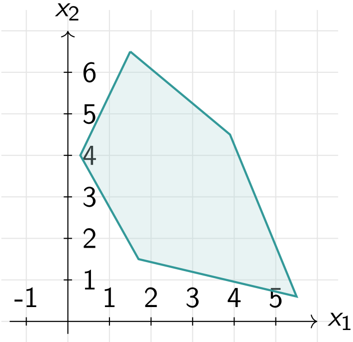

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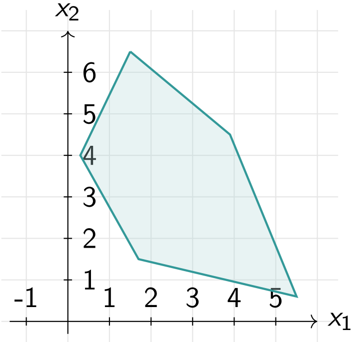

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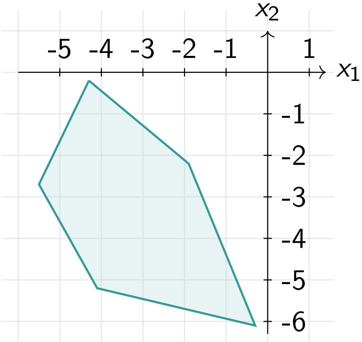

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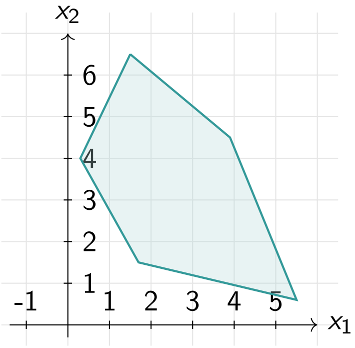

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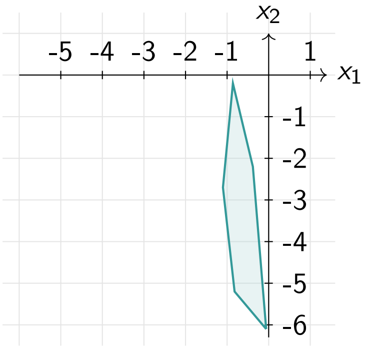

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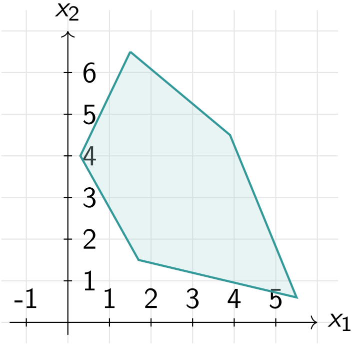

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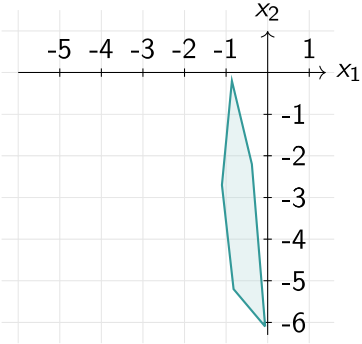

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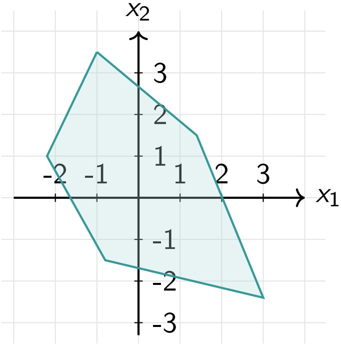

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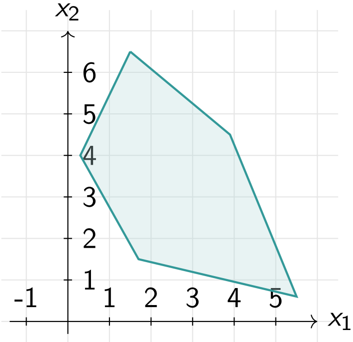

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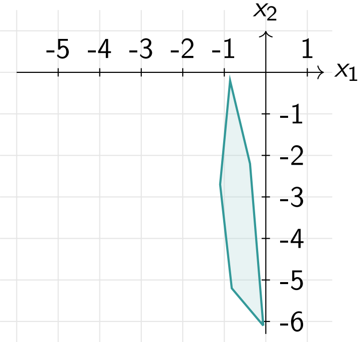

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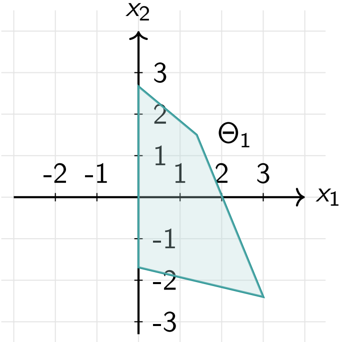

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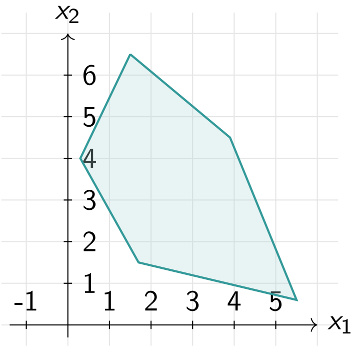

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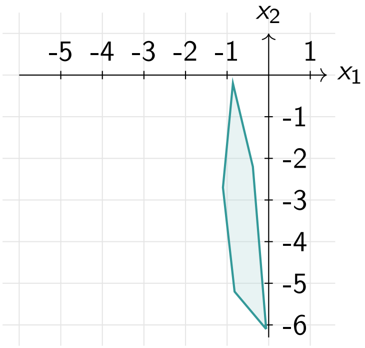

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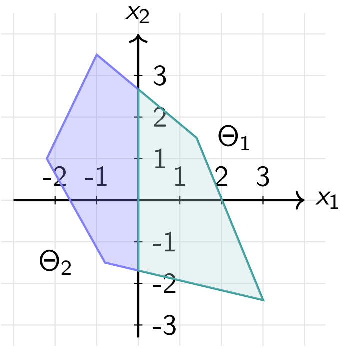

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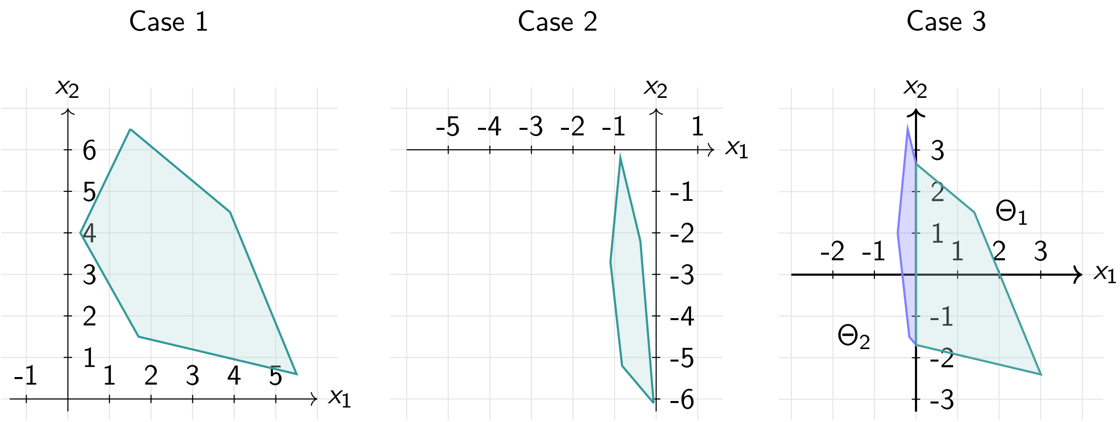

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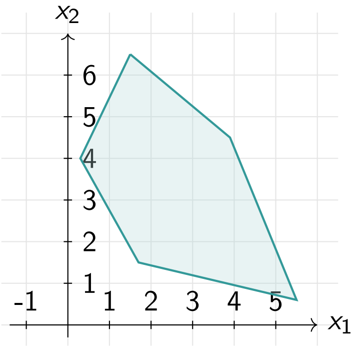

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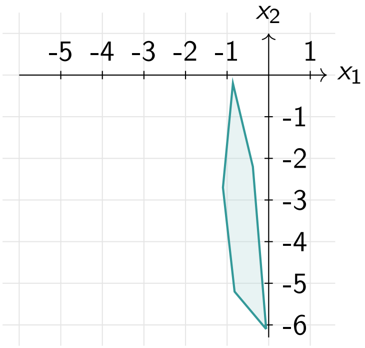

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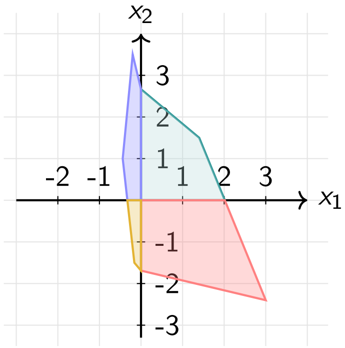

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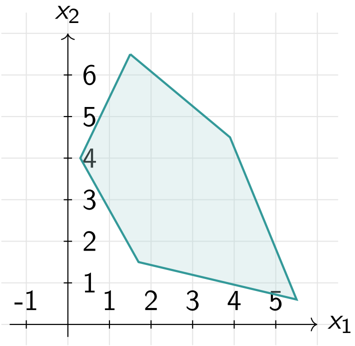

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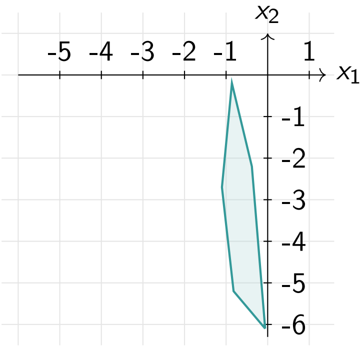

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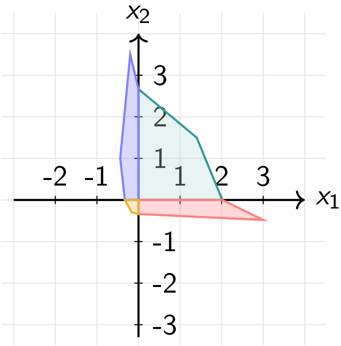
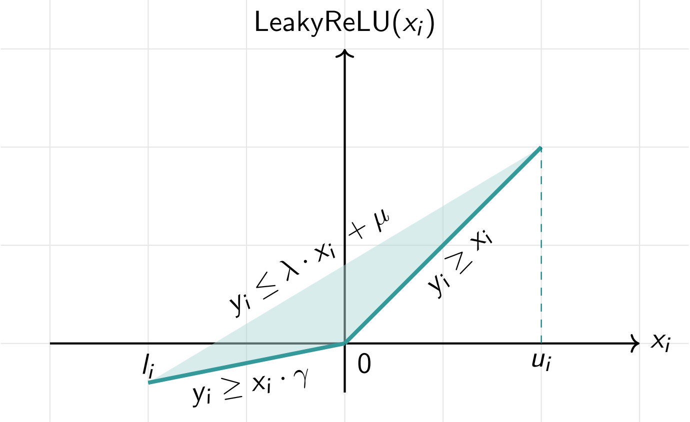


Over-approximate Analysis Convex Relaxation



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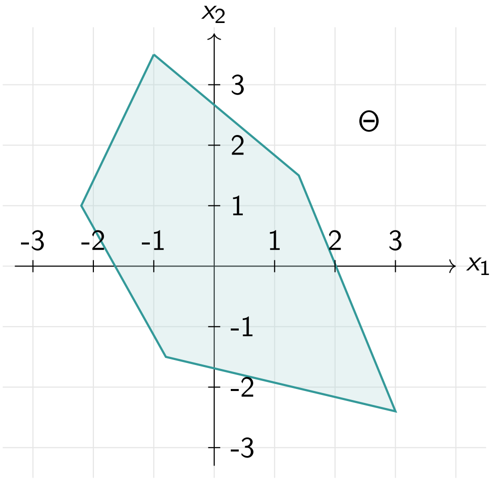

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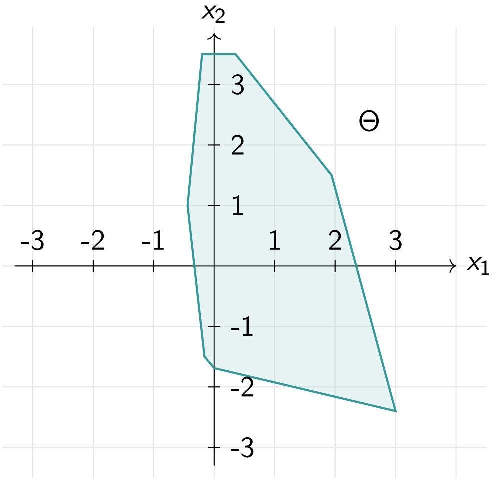

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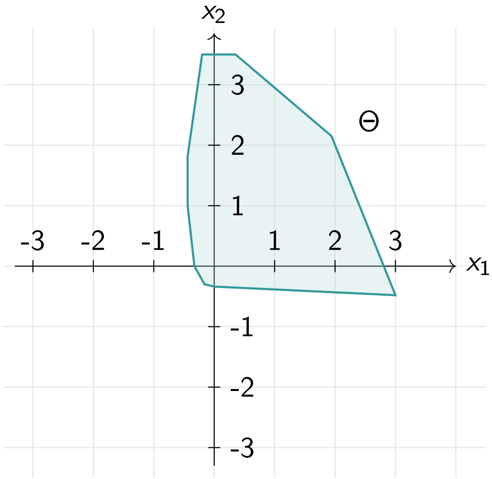
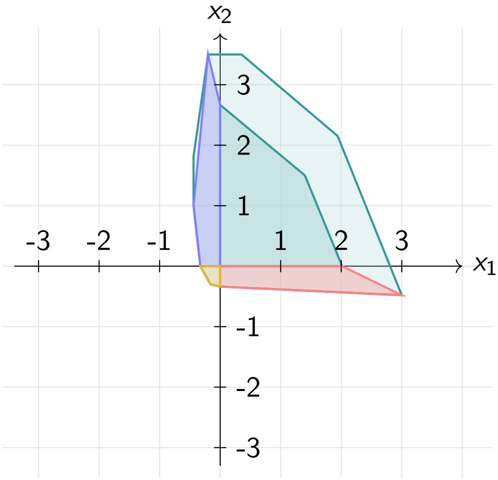


Comparison

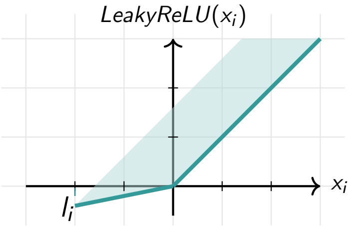


Unbounded Analysis

Case 1 | Case 2 | Case 3

Unbounded Analysis

No upper bound

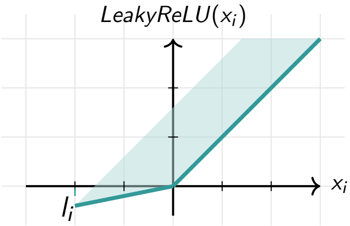


Case 2

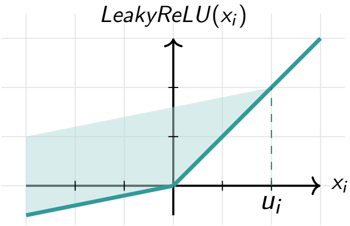
Case 3

Unbounded Analysis

No upper bound



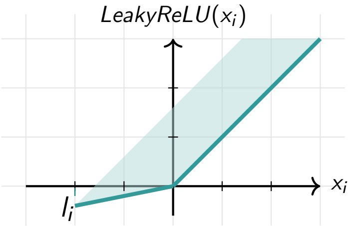
No lower bound



Case 3

Unbounded Analysis

No upper bound



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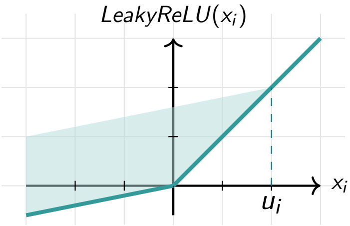
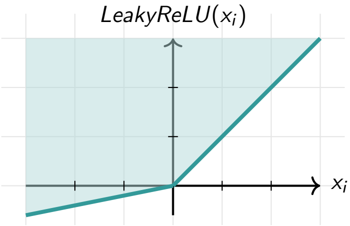


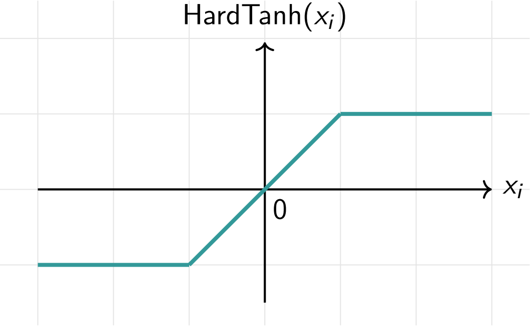
No bounds



Hard Tanh Function

- For the input x,

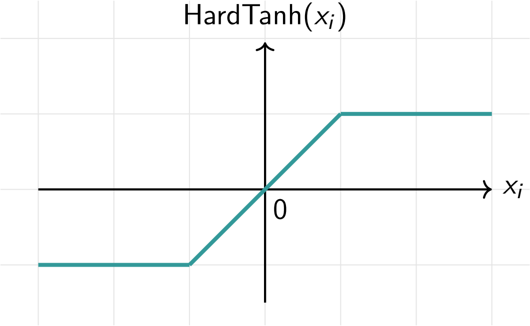
$$HardTanh(x) = \begin{cases} -1 & x < -1 \\ 1 & x > 1 \\ x & -1 \leq x \leq 1 \end{cases}$$



Hard Tanh Function

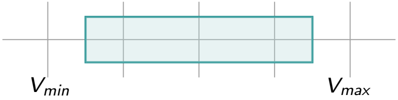
- For the input x,

$$HardTanh(x) = \begin{cases} V_{min}, & x < V_{min} \\ V_{max}, & x > V_{max} \\ x, & V_{min} \leq x \leq V_{max} \end{cases}$$



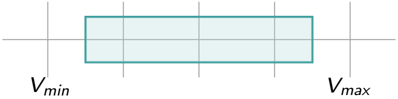
Exact Analysis

Exact Analysis

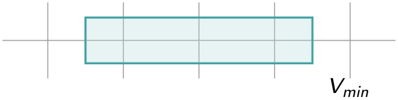


$\Rightarrow$ Remain the same

Exact Analysis

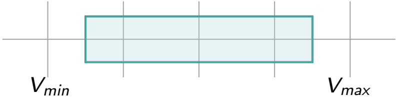


$\Rightarrow$ Remain the same

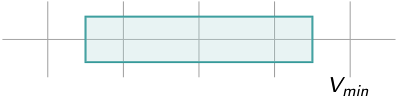


$\Rightarrow$ Project onto V_{min}

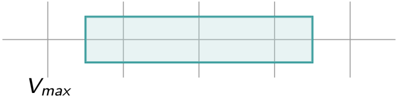
Exact Analysis



$\Rightarrow$ Remain the same

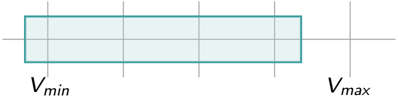


$\Rightarrow$ Project onto V_{min}



$\Rightarrow$ Project onto V_{max}

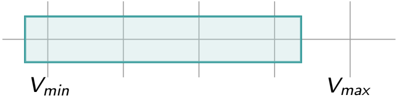
Exact Analysis



$\Rightarrow$ Decompose into two subsets

$$\Theta_1 = \Theta \wedge (V_{min} \leq x_i \leq V_{max})$$
$$\Theta_2 = \Theta \wedge (x_i < V_{min})$$

Exact Analysis



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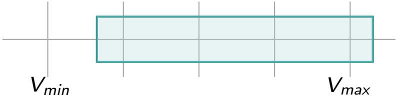
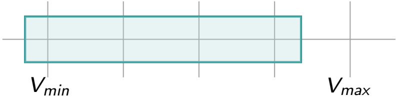


$\Rightarrow$ Decompose into two subsets

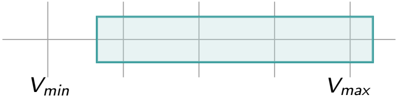
$$\Theta_1 = \Theta \wedge (V_{min} \leq x_i \leq V_{max})$$
$$\Theta_2 = \Theta \wedge (x_i > V_{max})$$

Exact Analysis



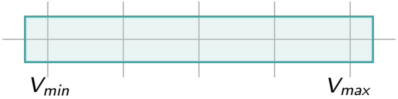
$\Rightarrow$ Decompose into two subsets

$$\Theta_1 = \Theta \wedge (V_{min} \leq x_i \leq V_{max})$$
$$\Theta_2 = \Theta \wedge (x_i < V_{min})$$



$\Rightarrow$ Decompose into two subsets

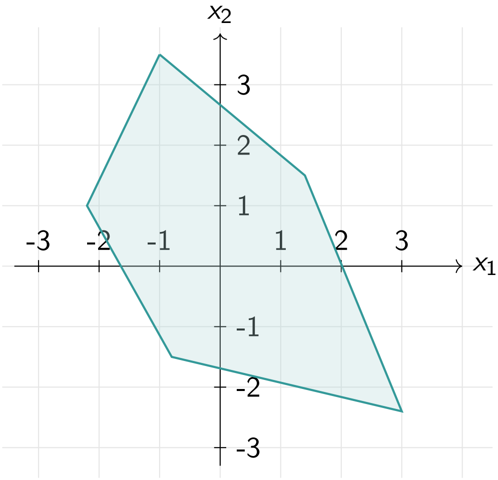
$$\Theta_1 = \Theta \wedge (V_{min} \leq x_i \leq V_{max})$$
$$\Theta_2 = \Theta \wedge (x_i > V_{max})$$



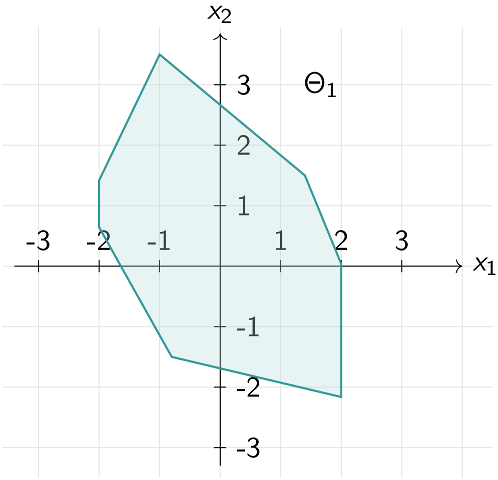
$\Rightarrow$ Decompose into three subsets

$$\Theta_1 = \Theta \wedge (V_{min} \leq x_i \leq V_{max})$$
$$\Theta_2 = \Theta \wedge (x_i < V_{min})$$
$$\Theta_3 = \Theta \wedge (x_i > V_{max})$$

Exact Analysis



Exact Analysis



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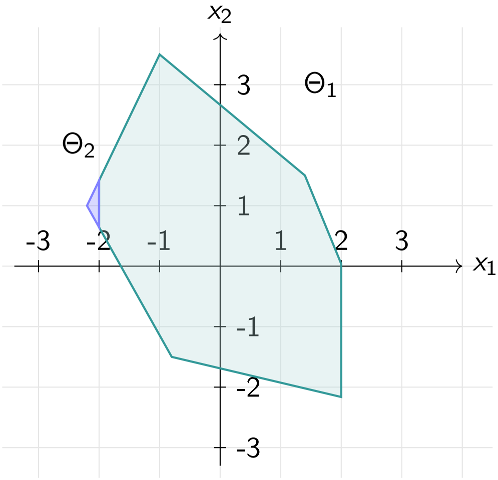

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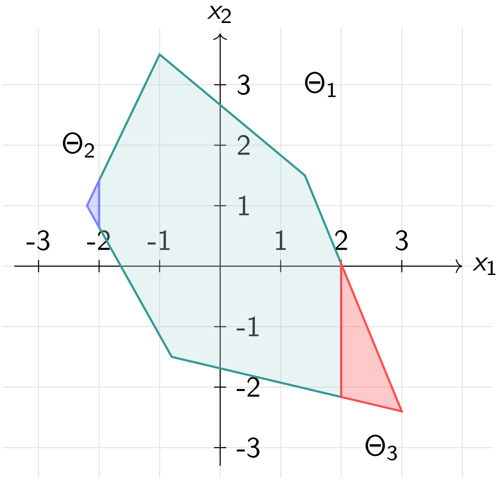

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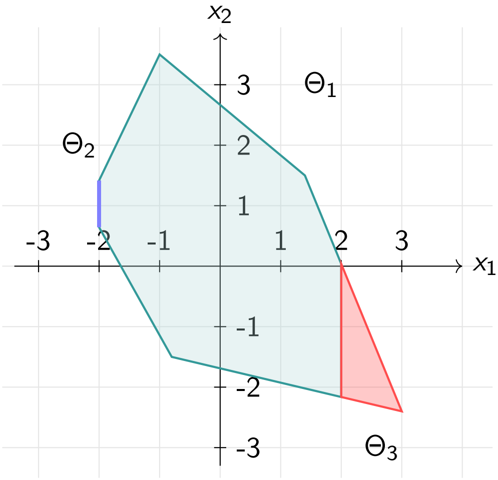

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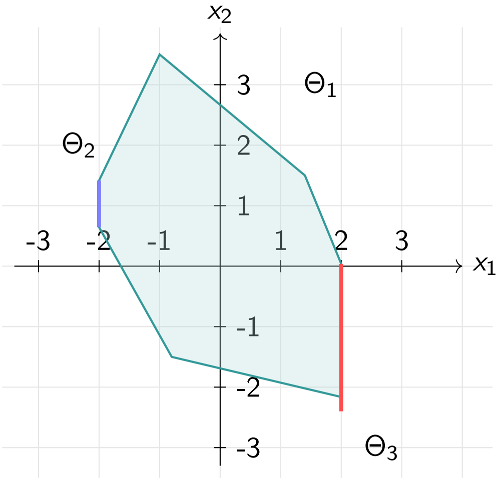
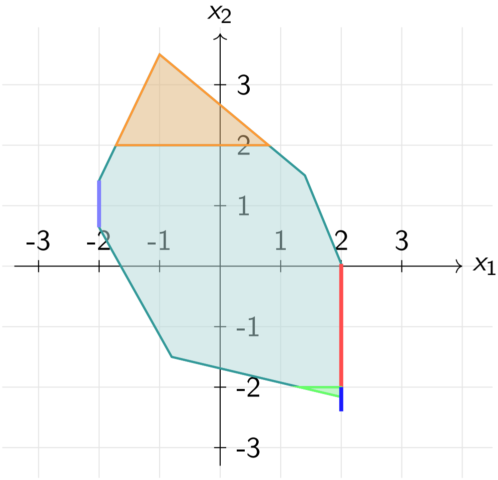
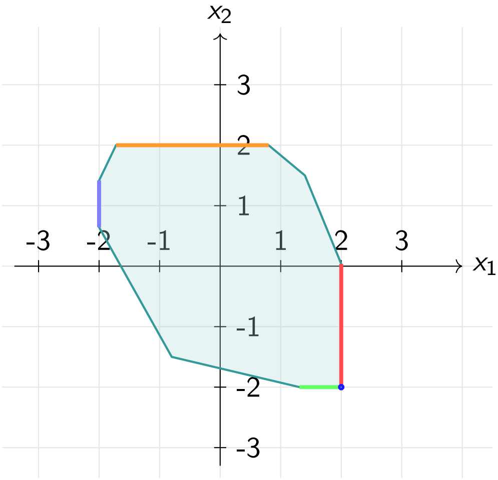


Exact Analysis



Exact Analysis



Over-approximate Analysis Convex Relaxation

Case 1, 2, and 3 equivalent to exact analysis

Over-approximate Analysis Convex Relaxation

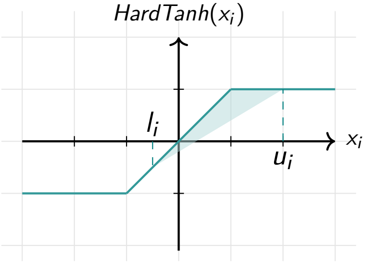
Case 4

Case 5

Case 6

Over-approximate Analysis Convex Relaxation

Case 4

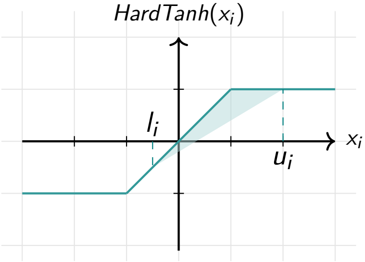


Case 5

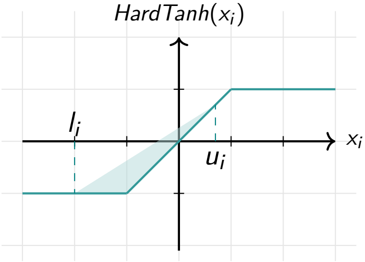
Case 6

Over-approximate Analysis Convex Relaxation

Case 4



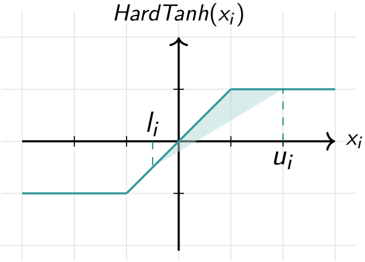
Case 5



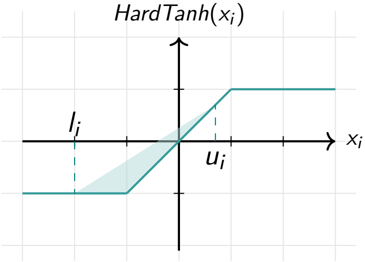
Case 6

Over-approximate Analysis Convex Relaxation

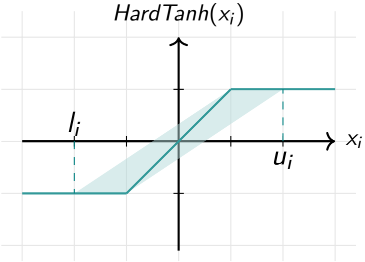
Case 4



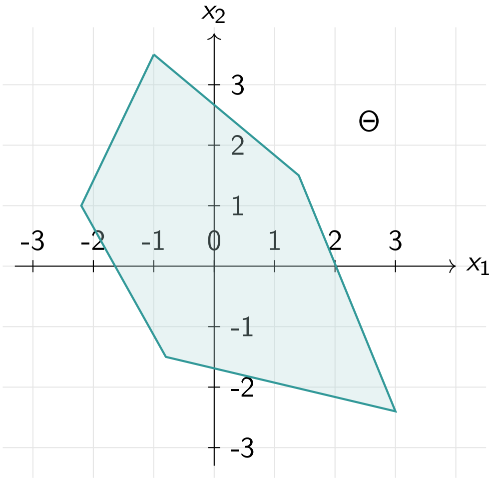
Case 5



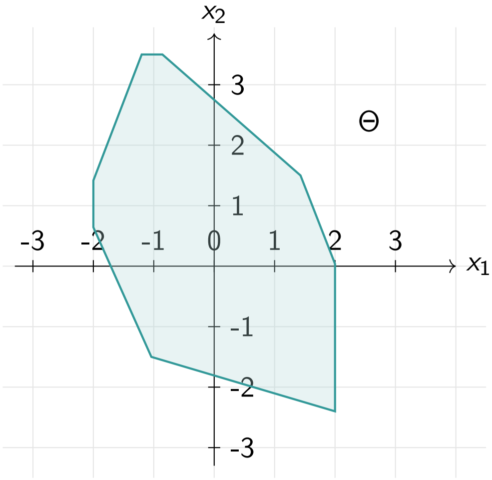
Case 6



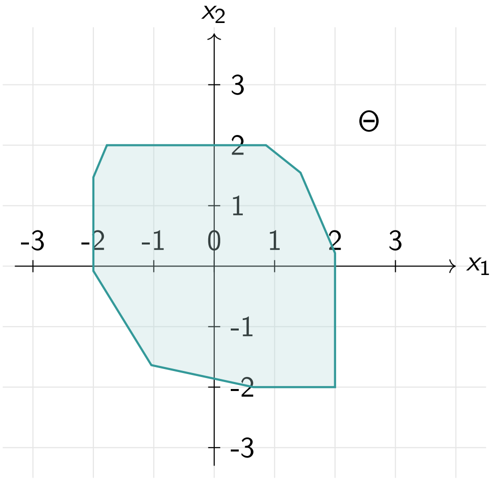
Over-approximate Analysis



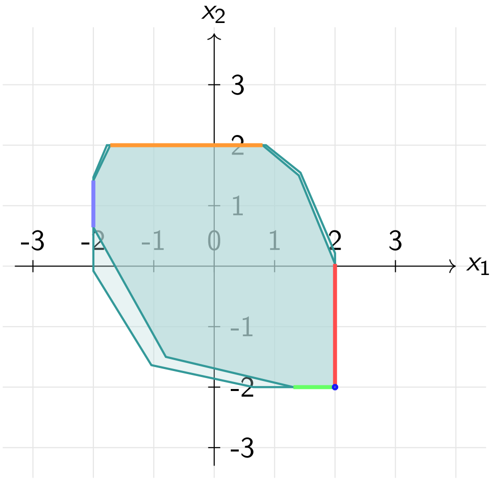
Over-approximate Analysis



Over-approximate Analysis



Comparison



Unbounded Analysis

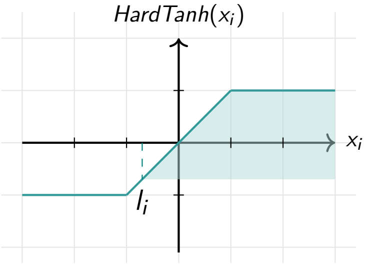
Case 1

Case 2

Case 3

Unbounded Analysis

No upper bound

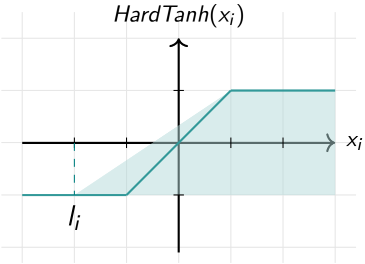


Case 2

Case 3

Unbounded Analysis

No upper bound

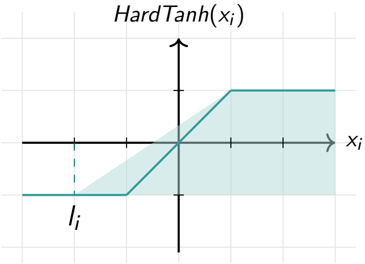


Case 2

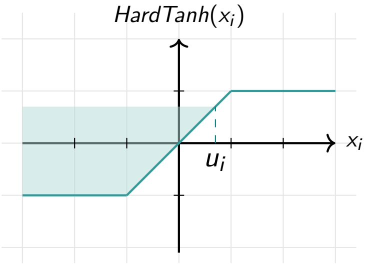
Case 3

Unbounded Analysis

No upper bound



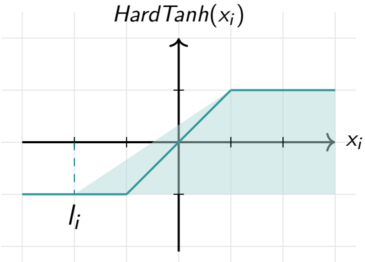
No lower bound



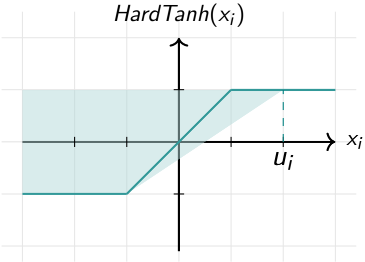
Case 3

Unbounded Analysis

No upper bound



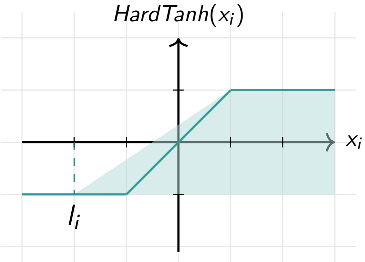
No lower bound



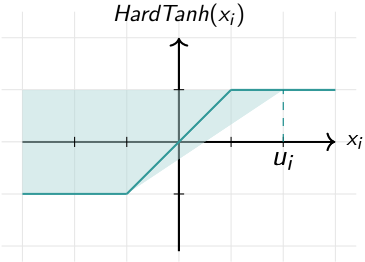
Case 3

Unbounded Analysis

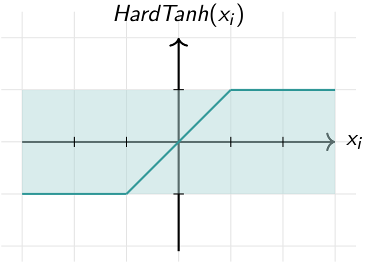
No upper bound



No lower bound



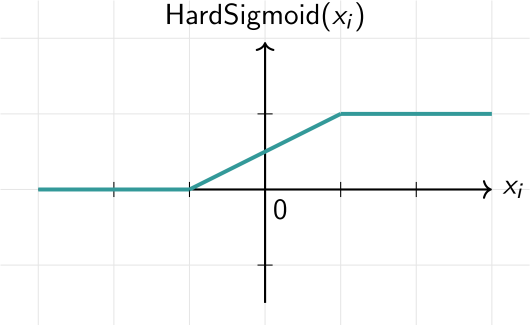
No bounds



Hard Sigmoid Function

- For the input x,

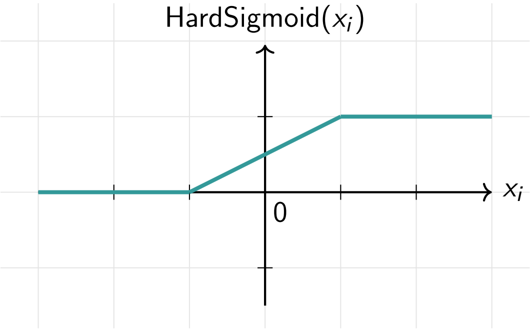
$$HardSigmoid(x) = \begin{cases} 0 & x \leq -1 \\ 1 & x \geq 1 \\ \frac{1}{2} \cdot x + \frac{1}{2} & -1 < x < 1 \end{cases} = max(0, min(\frac{1}{2} \cdot x + \frac{1}{2}))$$



Hard Sigmoid Function

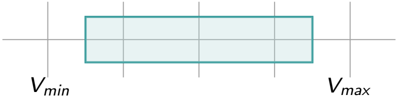
- For the input x,

$$HardSigmoid(x) = \begin{cases} 0 & x \leq V_{min} \\ 1 & x \geq V_{max} \\ \frac{1}{V_{max} - V_{min}} \cdot x + \frac{V_{min}}{V_{min} - V_{max}} & V_{min} < x < V_{max} \end{cases}$$



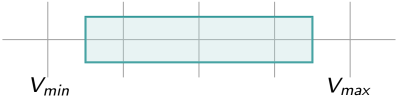
Exact Analysis

Exact Analysis

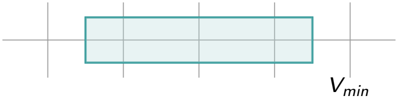


$\Rightarrow$ Correspond to the function

Exact Analysis

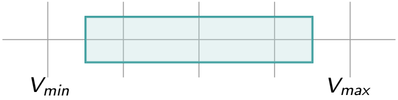


$\Rightarrow$ Correspond to the function

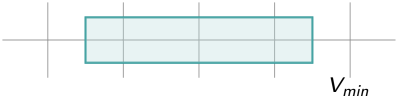


$\Rightarrow$ Project onto 0

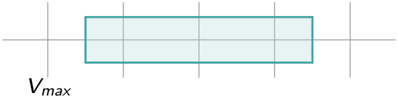
Exact Analysis



$\Rightarrow$ Correspond to the function

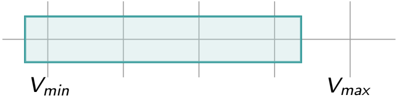


$\Rightarrow$ Project onto 0



$\Rightarrow$ Project onto 1

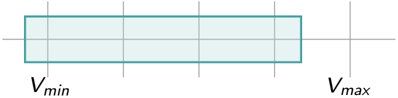
Exact Analysis



$\Rightarrow$ Decompose into two subsets

$$\Theta_1 = \Theta \wedge (V_{min} < x_i < V_{max})$$
$$\Theta_2 = \Theta \wedge (x_i \leq V_{min})$$

Exact Analysis



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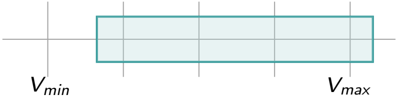
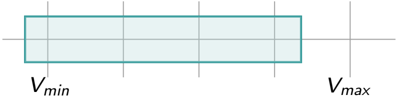


$\Rightarrow$ Decompose into two subsets

$$\Theta_1 = \Theta \wedge (V_{min} < x_i < V_{max})$$
$$\Theta_2 = \Theta \wedge (x_i \geq V_{max})$$

Exact Analysis



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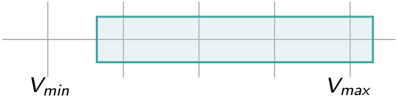

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$$\Theta_1 = \Theta \wedge (V_{min} < x_i < V_{max})$$
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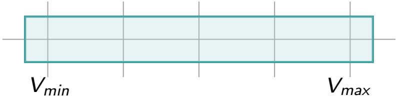

$\Rightarrow$ Decompose into three subsets

$$\Theta_1 = \Theta \wedge (V_{min} < x_i < V_{max})$$
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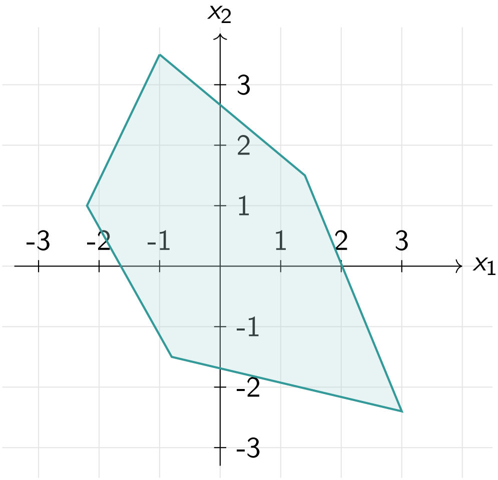
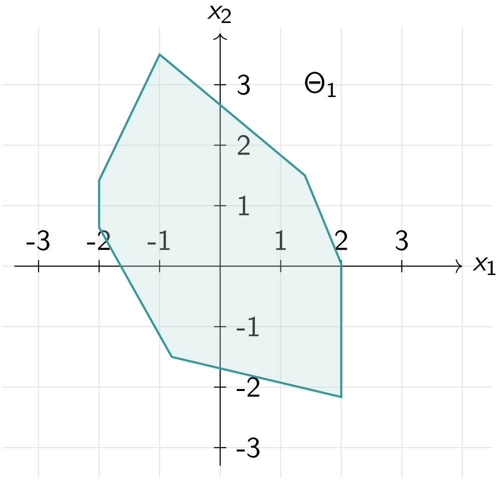
$$\Theta_3 = \Theta \wedge (x_i \geq V_{max})$$

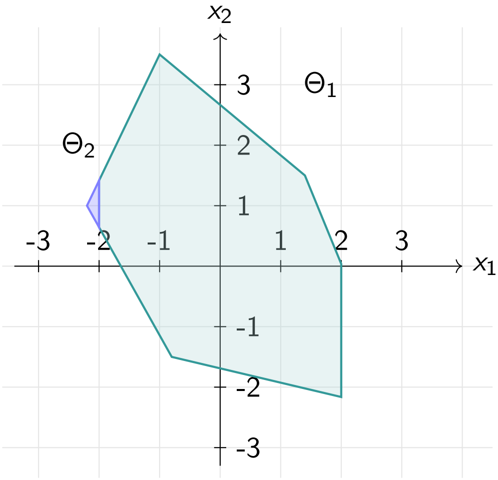
Exact Analysis



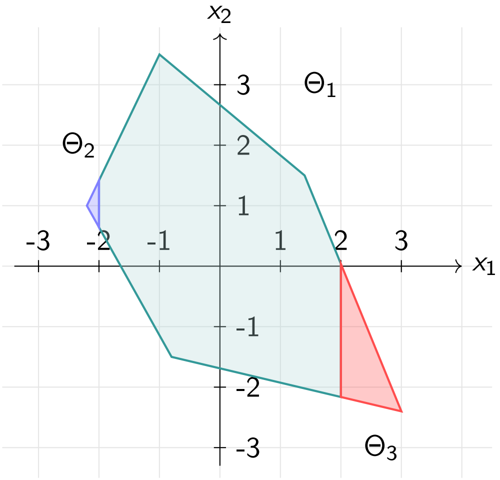
Exact Analysis



Exact Analysis



Exact Analysis



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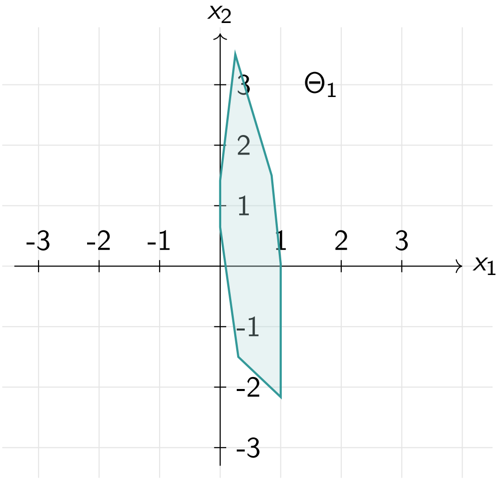

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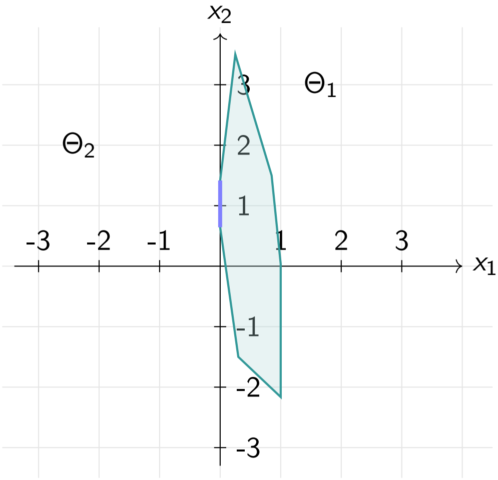
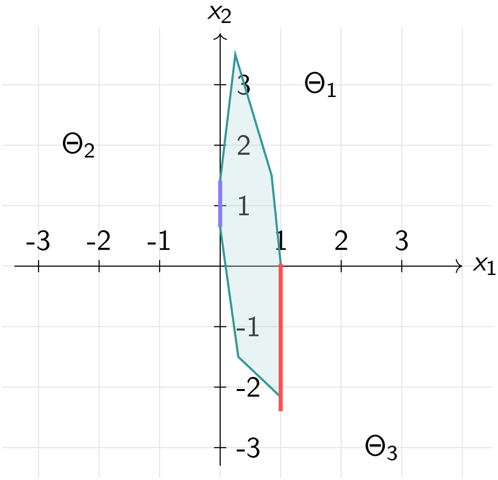
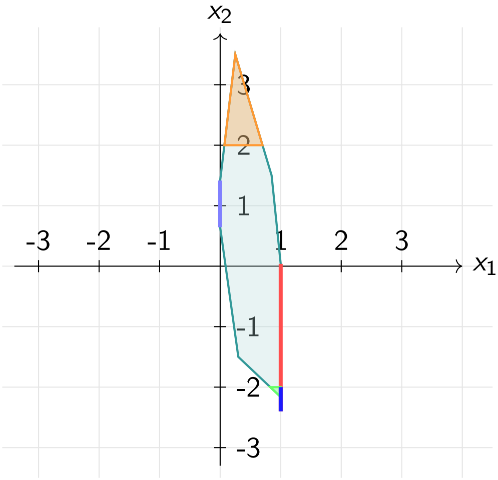


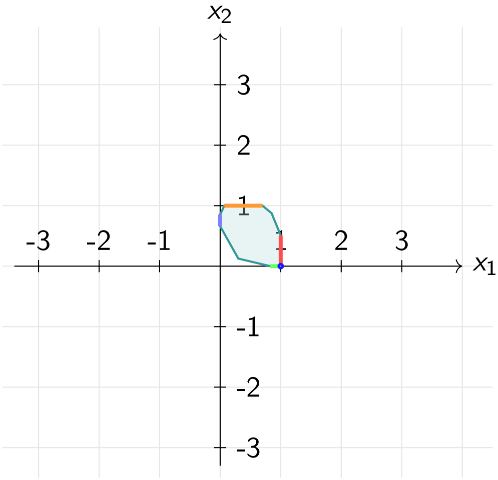
Exact Analysis



Exact Analysis



Exact Analysis

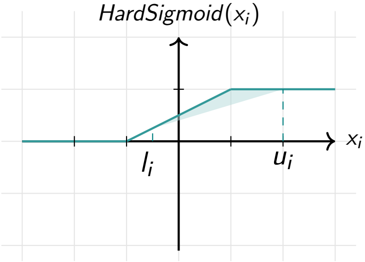


Over-approximate Analysis Convex Relaxation

Case 1 Case 2 Case 3

Over-approximate Analysis Convex Relaxation

Case 1

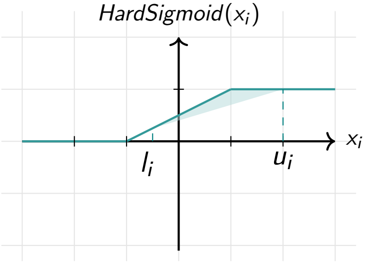


Case 2

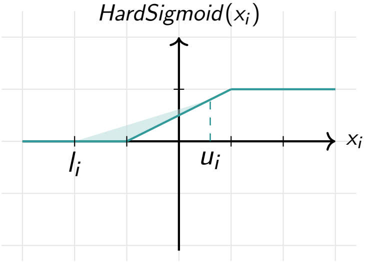
Case 3

Over-approximate Analysis Convex Relaxation

Case 1



Case 2



Case 3

Over-approximate Analysis Convex Relaxation

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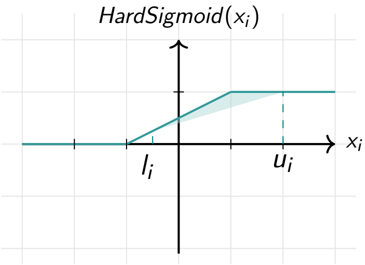
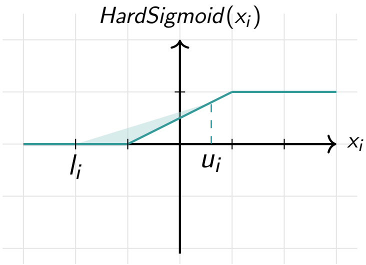
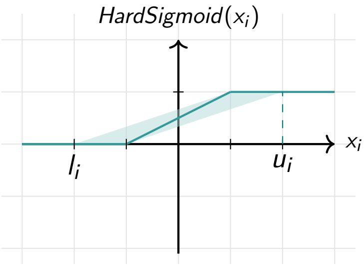


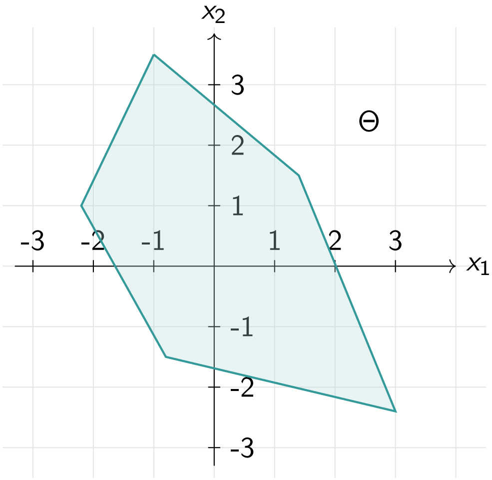
Case 2



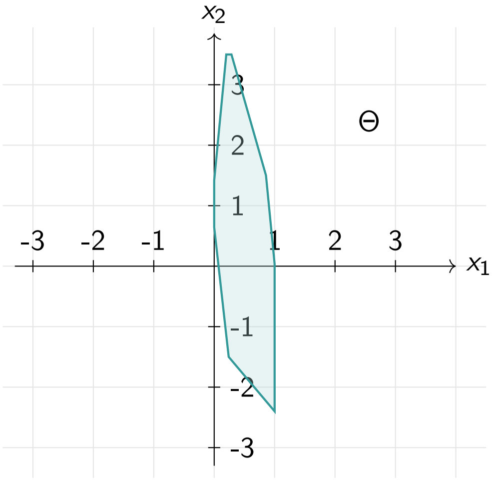
Case 3



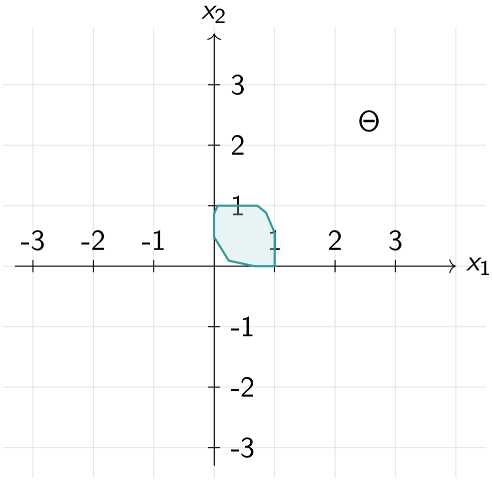
Over-approximate Analysis



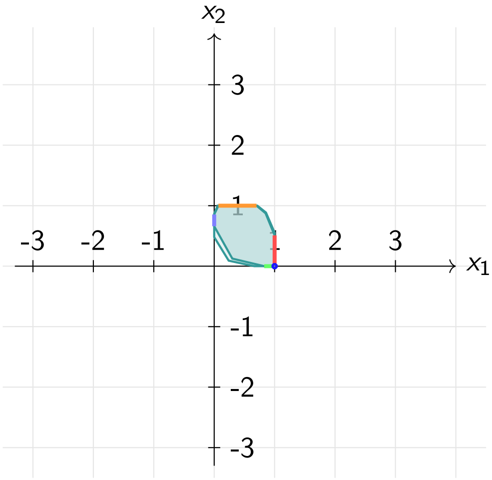
Over-approximate Analysis



Over-approximate Analysis



Comparison



Unbounded Analysis

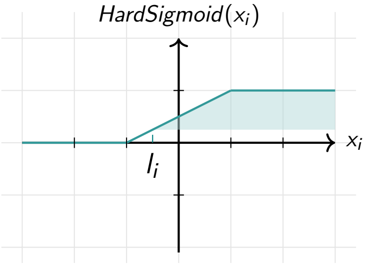
Case 1

Case 2

Case 3

Unbounded Analysis

No upper bound

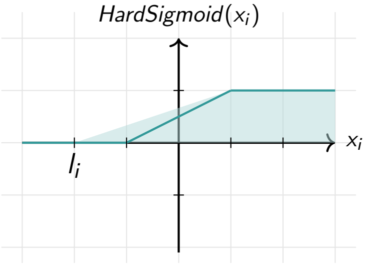


Case 2

Case 3

Unbounded Analysis

No upper bound

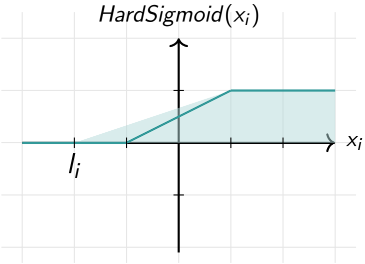


Case 2

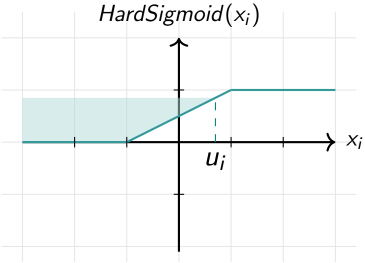
Case 3

Unbounded Analysis

No upper bound



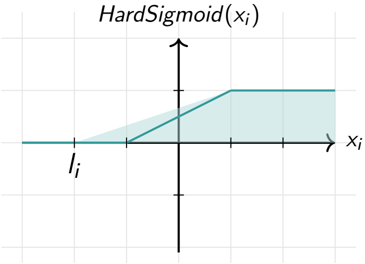
No lower bound



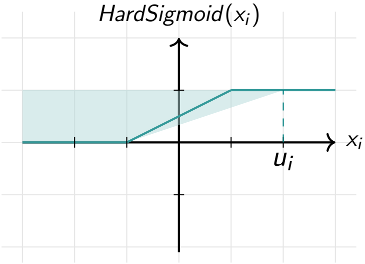
Case 3

Unbounded Analysis

No upper bound

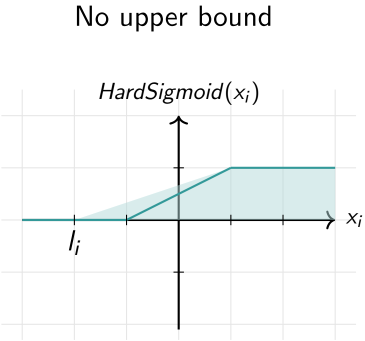


No lower bound



Case 3

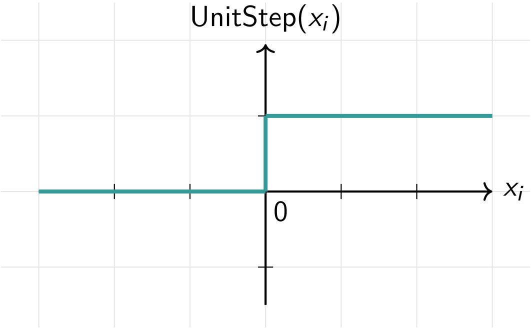
Unbounded Analysis



Unit step Function

- For the input x,

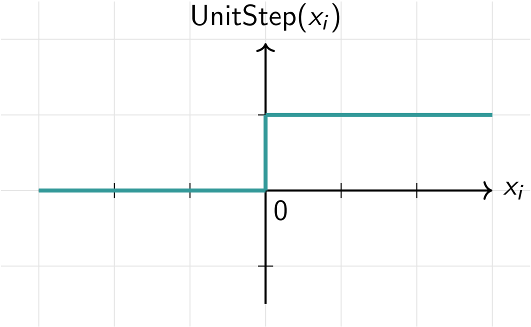
$$UnitStep(x) = \begin{cases} 0 & x \leq 0 \\ 1 & x > 0 \end{cases}$$



Unit step Function

- For the input x,

$$unitStep(x) = \begin{cases} V_{min} & x < V \\ V_{max} & x \geq V \end{cases}$$



Exact Analysis

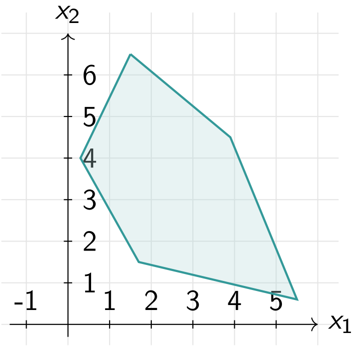
Case 1

Case 2

Case 3

Exact Analysis

Case 1

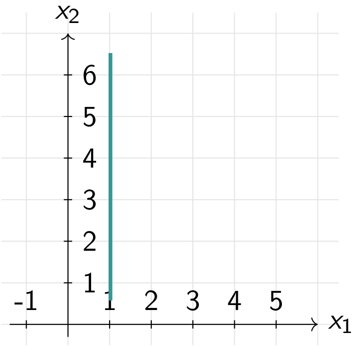


Case 2

Case 3

Exact Analysis

Case 1

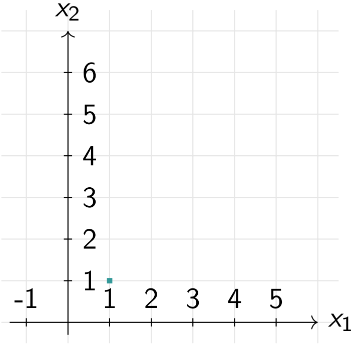


Case 2

Case 3

Exact Analysis

Case 1

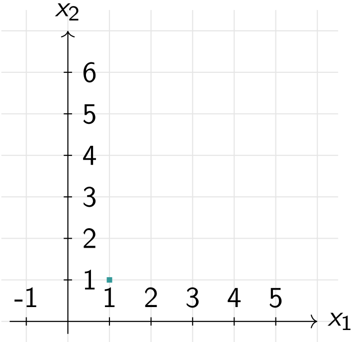


Case 2

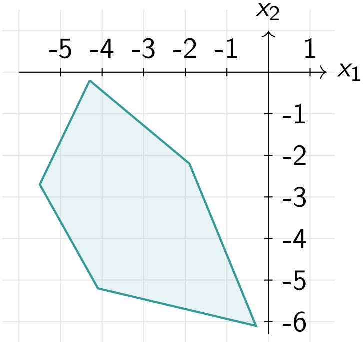
Case 3

Exact Analysis

Case 1



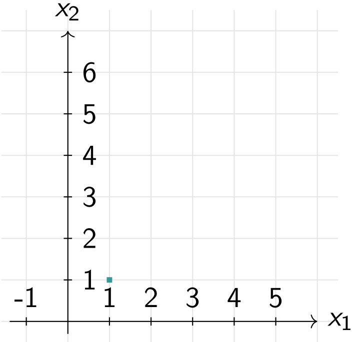
Case 2



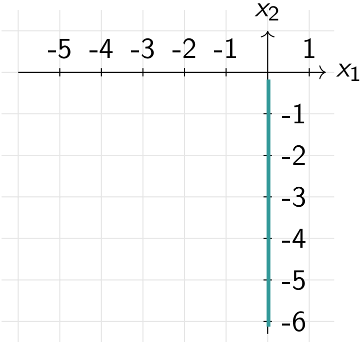
Case 3

Exact Analysis

Case 1



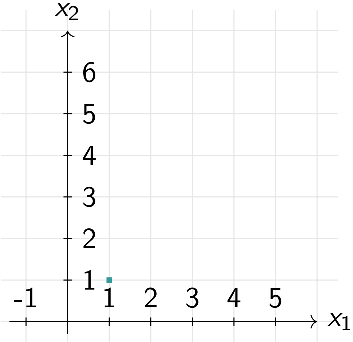
Case 2



Case 3

Exact Analysis

Case 1



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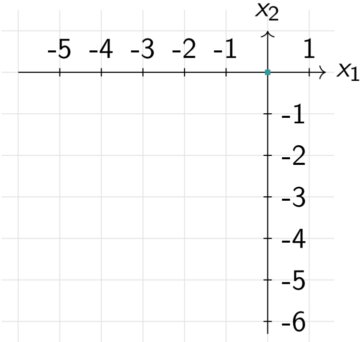
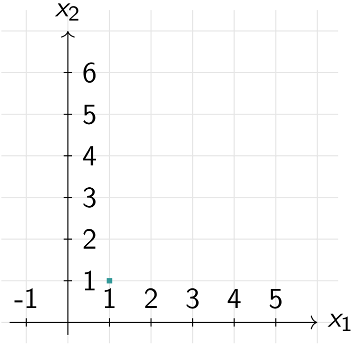


Case 3

Exact Analysis

Case 1



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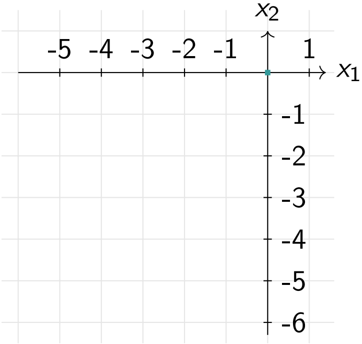
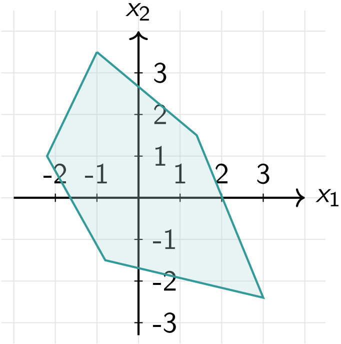
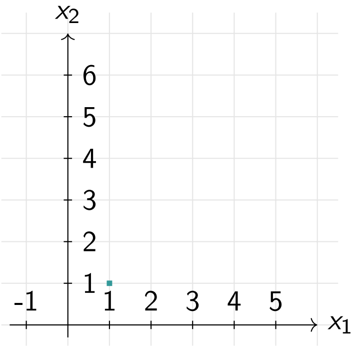


Case 3



Exact Analysis

Case 1



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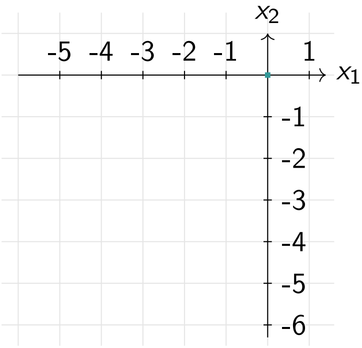
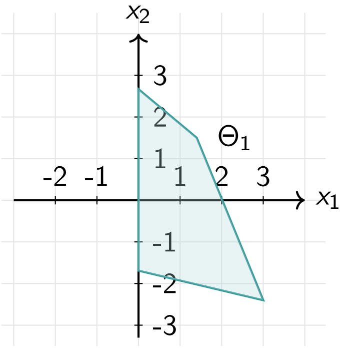
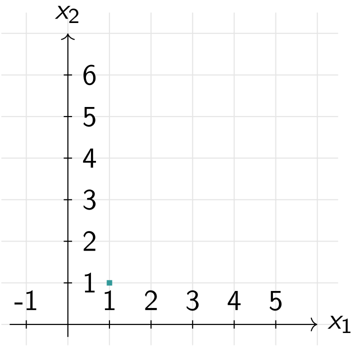


Case 3



Exact Analysis

Case 1



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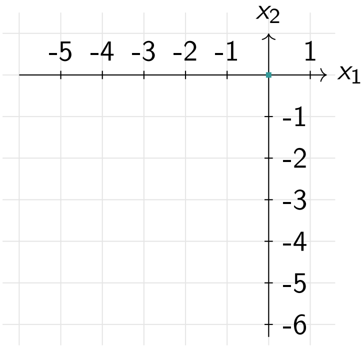

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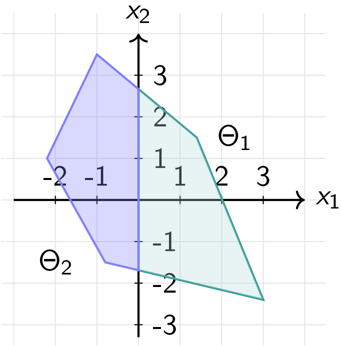
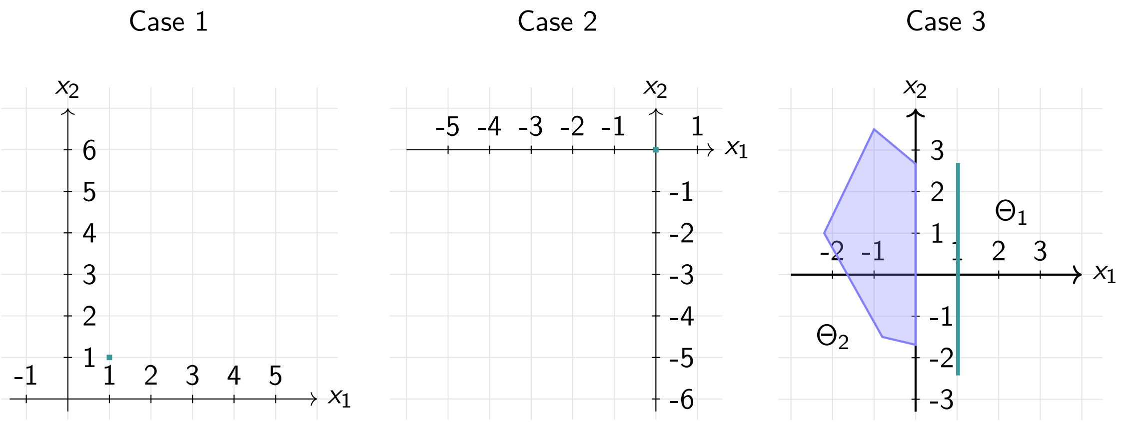
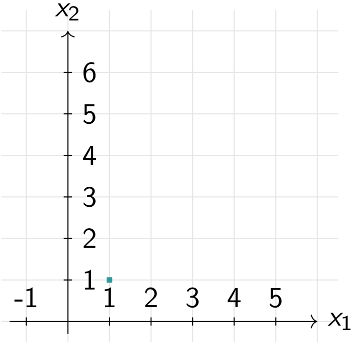


Exact Analysis

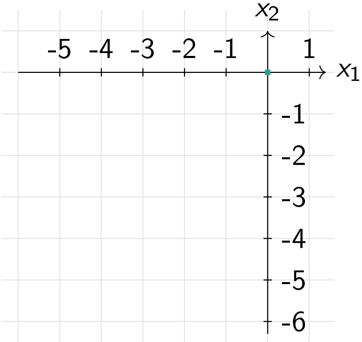


Exact Analysis

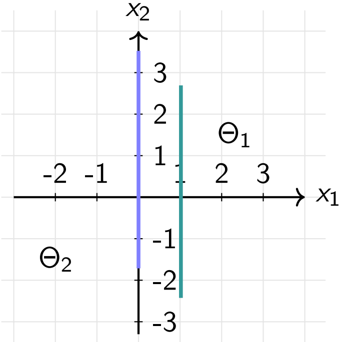
Case 1



Case 2

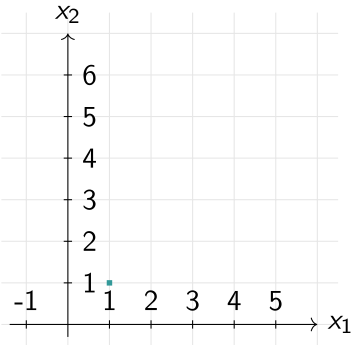


Case 3

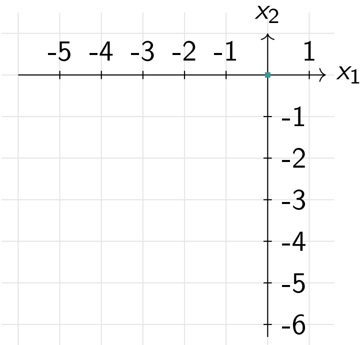


Exact Analysis

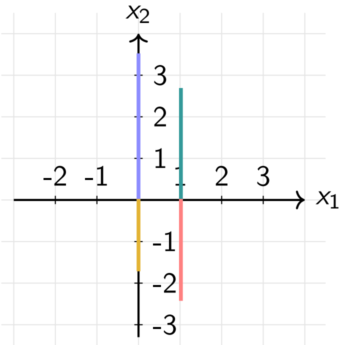
Case 1



Case 2

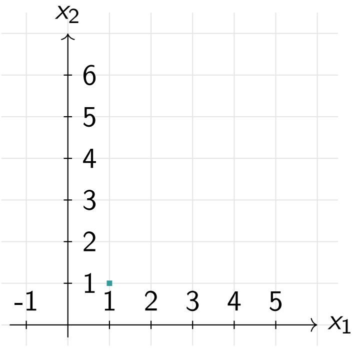


Case 3



Exact Analysis

Case 1



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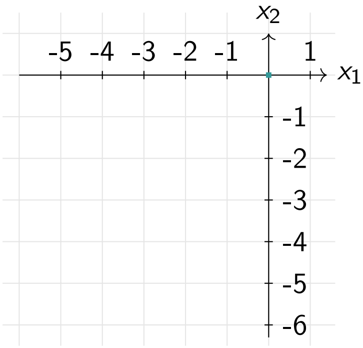
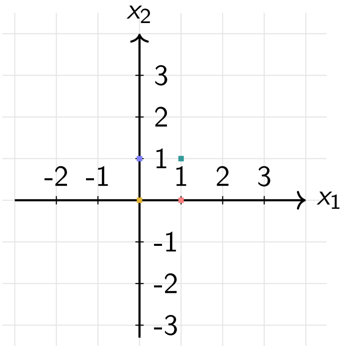
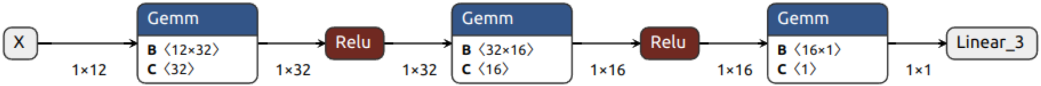


Case 3



ONNX Parser

- Open Neural Network Exchange (ONNX)
- Standard for representing deep learning models



Outline

ACAS Xu

- Airborne Collision Avoidance System Xu (ACAS Xu)
- A set of 45 feedforward neural networks, each with
  - 5 inputs,
  - 5 outputs,
  - 7 fully connected layers,
  - 300 neurons
- 10 properties to test the networks

ACAS Xu

For the evaluation, we

- compute the reachable set
- check the safety verification
- check the computation (RT) and the safety verification time (VT)

ACAS Xu

From the results,

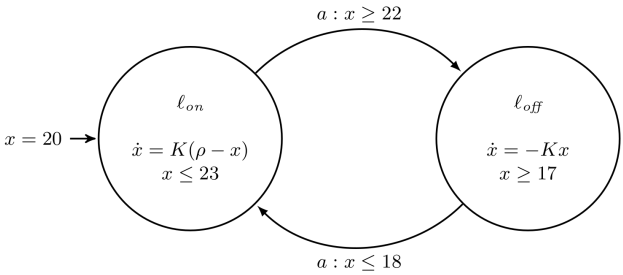
- the star set approach is, on average, faster than the Reluplex

properties	Exact	Overapproximation
	AVG RT(s)	AVG RT(s)
ϕ_1	29402.5067	2049.4807
ϕ_2	44631.003	1775.056
ϕ_3	254.60	10.38
ϕ_4	140.7655	9.4855
Sum	74428.8752	3844.4022

Average computation results for properties $\phi_1, \phi_2, \phi_3, \phi_4$

Thermostat

- Maintains room temperature between $17^\circ C$ and $23^\circ C$
- Neural network, with
  - 2 input neurons,
  - 2 hidden layers,
  - 1 output



The hybrid automaton model of the thermostat

Drones

- Drone takeoff and hover at chosen altitude
- A set of 8 feedforward neural networks

Architecture	Network ID	Neurons
Two layers	AC1	32, 16
	AC2	64, 32
	AC3	128, 64
	AC4	256, 128
Three layers	AC5	32, 16, 8
	AC6	64, 32, 16
	AC7	128, 64, 32
	AC8	256, 128, 64

Drones

For the evaluation, we check

- the computation time (RT)
- the safety verification time (VT)

Exact		Overapproximation	
RT(s)	VT(s)	RT(s)	VT(s)
232.37	8.86	4.94	1.37

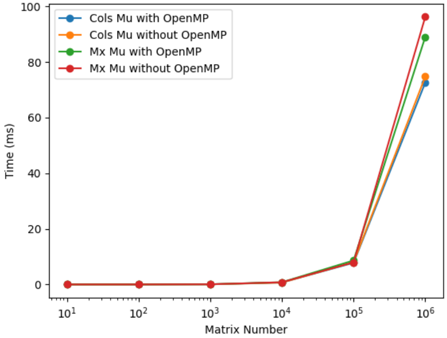
Average computation and verification time results

Sonar Binary Classifier

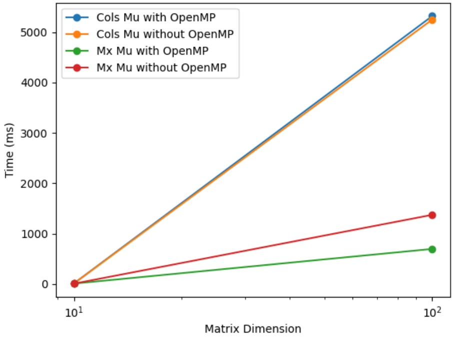
- Binary classification, distinguishing rocks from metal cylinders
- Neural network, with
  - 60 inputs,
  - 1 output,
  - 2 layers
- We check the local robustness of the neural network

Experimental Results

- Experiments to improve the running time of our algorithms, with
  - matrix multiplications vs. column multiplications



Run time with increasing matrix numbers



Run time with increasing matrix dimensions

Outline

Conclusion

- Reachability analysis
  - provides valuable insights into complex network behavior
  - ensures network safety and reliability
- Developed various activation functions, includes
  - exact analysis
  - over-approximate analysis

  for bounded and unbounded cases.
- ONNX parser for easier integration in Hypro

Questions?

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Appendix A

Lemma

The worst-case complexity of the number of stars in the reachable set of an N-neurons FNN is $\mathcal{O}(2^N)$.

Lemma

The worst-case complexity of the number of constraints of a star in the reachable set of an N-neurons FNN is $\mathcal{O}(N)$.

Lemma

The worst-case complexity of the number of variables and constraints in the reachable set of an N-neurons FNN is $N + m_0$ *and* $3N + n_0$, *respectively, where* m_0 *is the number of variables and* n_0 *the number of linear constraints of the predicate of the input set.*

Appendix B

Lemma

The worst-case complexity of the number of stars in the reachable set of an N-neurons FNN is $\mathcal{O}(3^N)$.

Lemma

The worst-case complexity of the number of constraints of a star in the reachable set of an N-neurons FNN is $\mathcal{O}(2N)$.

Lemma

The worst-case complexity of the number of variables and constraints in the reachable set of an N-neuron FNN is $N + m_0$ *and* $4N + n_0$, *where respectively* m_0 *is the number of variables and* n_0 *the number of linear constraints of the predicate of the input set.*

Appendix C

Lemma

The worst-case complexity of the number of stars in the reachable set of an N-neurons FNN is $\mathcal{O}(3^N)$.

Lemma

The worst-case complexity of the number of constraints of a star in the reachable set of an N-neurons FNN is $\mathcal{O}(2N)$.

Lemma

The worst-case complexity of the number of variables and constraints in the reachable set of an N-neurons FNN is $N + m_0$ *and* $4N + n_0$, *where respectively* m_0 *is the number of variables and* n_0 *the number of linear constraints of the predicate of the input set.*

Appendix D

Lemma

The worst-case complexity of the number of stars in the reachable set of an N-neurons FNN is $\mathcal{O}(2^N)$.

Lemma

The worst-case complexity of the number of constraints of a star in the reachable set of an N-neurons FNN is $\mathcal{O}(N)$.