Neural Network Approximation based on Hausdorff distance of Tropical Zonotopes

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International Conference on Learning Representations (ICLR) 2022

Our work: Neural Networks and Tropical Geometry

Contributions

- ✓ **Novel** bound on neural network approximation.
- ✓ 2 **new** algorithms for neural network compression.

Tropical Algebra

Tropical Geometry

Tropical Algebra

✓ **Tropical Semiring** $\mathbb{R}_{\max} = \mathbb{R} \cup \{-\infty\}$

$$a \vee b = \max(a, b)$$

$$a + b = a + b$$

- Replaces classical operations of addition and multiplication with max and $+$, respectively.

Tropical Geometry

Tropical Algebra

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✓ **Tropical Polynomials**

$$f(\boldsymbol{x}) = \max_{i \in [n]} \{\boldsymbol{a}_i^T \boldsymbol{x} + b_i\}$$

- Expressive for ReLU networks.

Tropical Geometry

Preface: Tropical Mathematics

Tropical Algebra

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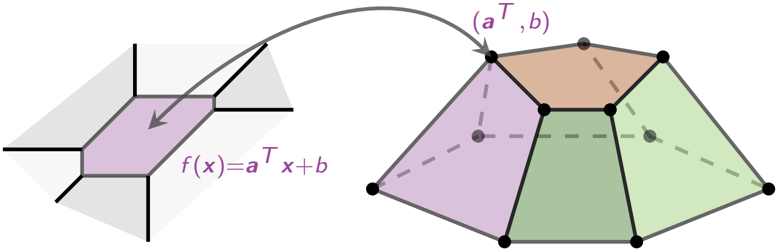
Tropical Geometry

✓ **Newton Polytopes**

$$\text{Newt}(f) = \text{conv}\{\boldsymbol{a}_i : i \in [n]\}$$
$$\text{ENewt}(f) = \text{conv}\{(\boldsymbol{a}_i, b_i) : i \in [n]\}$$

- They provide geometric interpretation for tropical polynomials.

Linear Regions and the Newton Polytope



- ✓ $1-1$ mapping: between linear regions and vertices. [1]
- ✓ The upper envelope determines the tropical polynomial and vice versa

$$f, g \in \mathbb{R}_{\max}[\boldsymbol{x}] : \quad f = g \Leftrightarrow UF(\text{ENewt}(f)) = UF(\text{ENewt}(g))$$

[1] Charisopoulos, V., Maragos, P. A tropical approach to neural networks with piecewise linear activations. *arXiv preprint arXiv:1805.08749*, 2018

Idea: What if we relax the previous equality?

Question: Would $\text{ENewt}(f) \approx \text{ENewt}(g)$ imply $f \approx g$?

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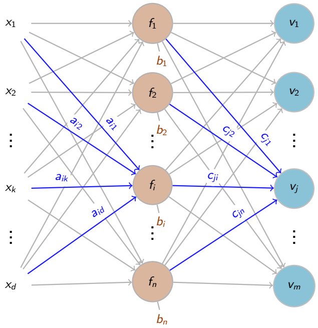
Proposition

Let $p, \tilde{p} \in \mathbb{R}_{max}[\boldsymbol{x}]$ be two tropical polynomials and let $P = ENewt\,(p)\,, \tilde{P} = ENewt\,(\tilde{p})$. Then,

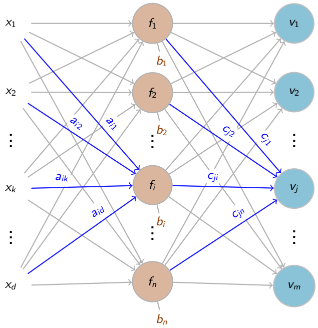
$$\max_{x \in \mathcal{B}} |p(\boldsymbol{x}) - \tilde{p}(\boldsymbol{x})| \leq \rho \cdot \mathcal{H}\left(P, \tilde{P}\right)$$

where $\mathcal{B} = \{\boldsymbol{x} \in \mathbb{R}^d : \|\boldsymbol{x}\| \leq r\}$ is the hypersphere of radius r, and $\rho = \sqrt{r^2 + 1}$.



ReLU neural network with 1 hidden layer

[2] L. Zhang, G. Naitzat, L.-H. Lim. "Tropical Geometry of Deep Neural Networks." in *International Conference on Machine Learning*, pages 5824–5832. 2018.
[3] P. Maragos, V. Charisopoulos and E. Theodosis, "Tropical Geometry and Machine Learning," in *Proceedings of the IEEE*, vol. 109, no. 5, pp. 728-755, May 2021, doi: 10.1109/JPROC.2021.3065238.



ReLU neural network with 1 hidden layer

✓ i−th hidden layer node.

$$f_i(\boldsymbol{x}) = \max\left(\boldsymbol{a}_i^T \boldsymbol{x} + b_i, 0\right)$$

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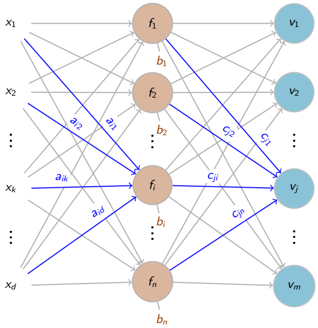

ReLU neural network with 1 hidden layer

- ✓ $i-$th hidden layer node.

$$f_i(\boldsymbol{x}) = \max\left(\boldsymbol{a}_i^T \boldsymbol{x} + b_i, 0\right)$$

- ✓ $j-$th output node.

$$v_j(\boldsymbol{x}) = p_j(\boldsymbol{x}) - q_j(\boldsymbol{x})$$

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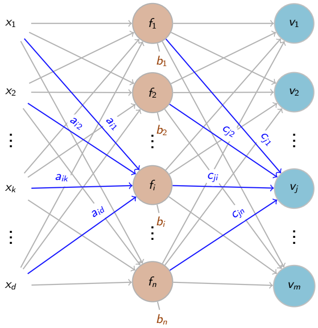

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Tropical Geometry

✓ ENewt (f_i) is linear segment with endpoints $\mathbf{0}$ and $(\boldsymbol{a}_i^T, b_i)$.

✓ $P_j =$ ENewt (p_j), $Q_j =$ ENewt (q_j) are Minkowski sums of segments ⇔ **zonotopes** [2,3].

✓ $(\boldsymbol{a}_i^T, b_i)$ are called **generators**.

[2] L. Zhang, G. Naitzat, L.-H. Lim. "Tropical Geometry of Deep Neural Networks." in *International Conference on Machine Learning*, pages 5824–5832. 2018.
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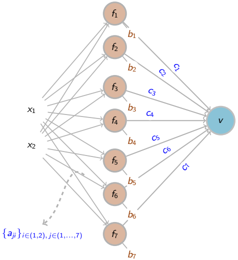
Neural Network Approximation

Theorem

Let $v, \tilde{v} \in \mathbb{R}_{max}[\mathbf{x}]$ be two neural networks with 1 hidden layer and $\tilde{P}_j, \tilde{Q}_j$ denote the positive and negative zonotopes of $\tilde{v}$. The following bound applies.

$$\max_{x \in \mathcal{B}} \|v(\mathbf{x}) - \tilde{v}(\mathbf{x})\|_1 \leq \rho \cdot \left(\sum_{j=1}^{m} \mathcal{H}\left(P_j, \tilde{P}_j\right) + \mathcal{H}\left(Q_j, \tilde{Q}_j\right) \right)$$

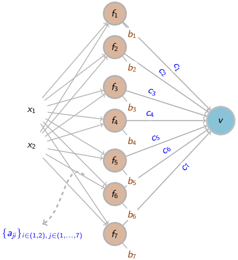
- ✓ Geometrical approximation problem.
- ✓ **Goal:** approximate the zonotopes.



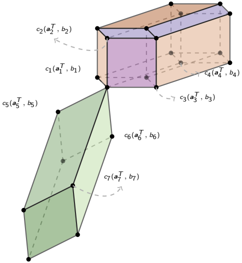
(a) Original network

✓ Applies only to networks with one output neuron.

Zonotope K-means



(a) Original network

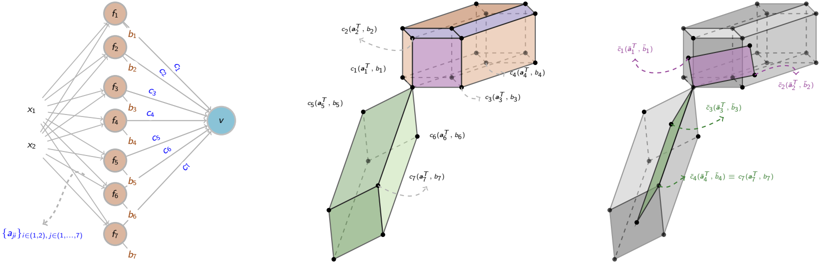


(b) Original zonotopes

✓ Applies only to networks with one output neuron.

Zonotope K-means

1. Split zonotope generators into positive and negative.

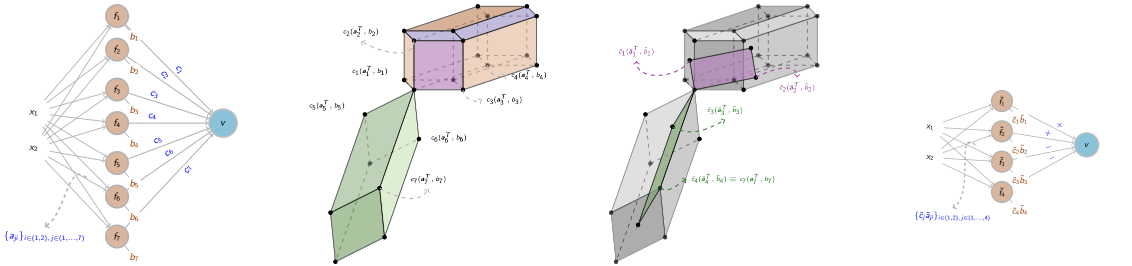


(a) Original network (b) Original zonotopes (c) Resulting zonotopes.

✓ Applies only to networks with one output neuron.

Zonotope K-means

1. Split zonotope generators into positive and negative.
2. Apply K-means to each generating set.



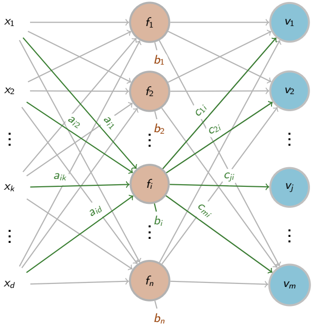
(a) Original network (b) Original zonotopes (c) Resulting zonotopes. (d) Compressed network.

✓ Applies only to networks with one output neuron.

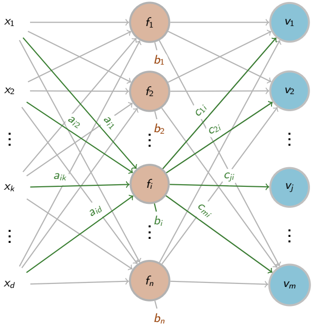
Zonotope K-means

1. Split zonotope generators into positive and negative.
2. Apply K-means to each generating set.
3. Construct final network.

Compression Algorithms II. Neural Path K-means



- Zonotope K-means doesn't generalize directly to multiple output nodes.



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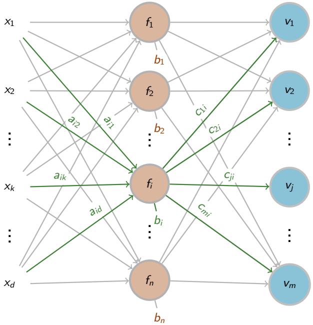
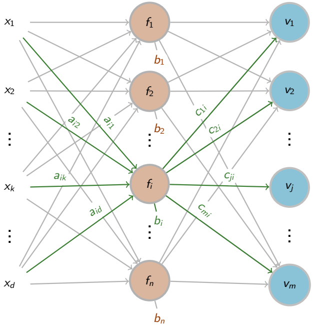
Neural Path K-means



- Zonotope K-means doesn't generalize directly to multiple output nodes.

Neural Path K-means

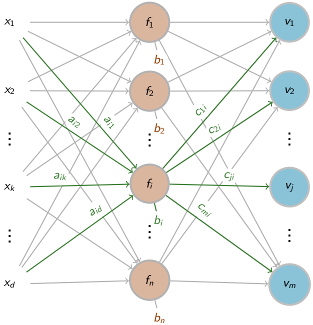
1. For each node form the vector of weights of incident edges.



- Zonotope K-means doesn't generalize directly to multiple output nodes.

Neural Path K-means

1. For each node form the vector of weights of incident edges.
2. Execute K-means to these vectors.



- Zonotope K-means doesn't generalize directly to multiple output nodes.

Neural Path K-means

1. For each node form the vector of weights of incident edges.
2. Execute K-means to these vectors.
3. Construct reduced network.

Theoretical Evaluation

Zonotope K-means Bound

$$\frac{1}{\rho} \cdot \max_{\boldsymbol{x} \in \mathcal{B}} |v(\boldsymbol{x}) - \tilde{v}(\boldsymbol{x})| \leq K \cdot \delta_{\max} + \left(1 - \frac{1}{N_{\max}}\right) \sum_{i=1}^{n} |c_i| \| \left(\boldsymbol{a}_i^T,\, b_i\right) \|$$

Neural Path K-means Bound

$$\frac{1}{\rho} \cdot \max_{\boldsymbol{x} \in \mathcal{B}} \|v(\boldsymbol{x}) - \tilde{v}(\boldsymbol{x})\|_1 \leq \sqrt{m} K \delta_{\max}^2 + \sqrt{m} \left(1 - \frac{1}{N_{\max}}\right) \sum_{i=1}^{n} \|C_{:,i}\| \left\| \left(\boldsymbol{a}_i^T,\, b_i\right) \right\| + \frac{\sqrt{m}\delta_{\max}}{N_{\min}} \sum_{i=1}^{n} \left(\left\| \left(\boldsymbol{a}_i^T,\, b_i\right) \right\| + \|C_{:,i}\| \right) + \sum_{j=1}^{m} \sum_{i \in \mathcal{N}_j} |c_{ji}| \left\| \left(\boldsymbol{a}_i^T,\, b_i\right) \right\|$$

- ✓ Bounds represent distances of zonotope vertices from K-means centers.
- ✓ Approximation is better when $K \approx n$. Both bounds become 0 when $K = n$.

Experimental Evaluation I: Comparison with tropical techniques.

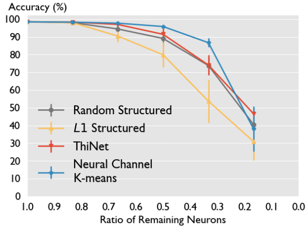
✓ Binary classification tasks.

Percentage of Remaining Neurons	MNIST 3/5			MNIST 4/9		
	Smyrnis et al., 2020	Zonotope K-means	Neural Path K-means	Smyrnis et al., 2020	Zonotope K-means	Neural Path K-means
100% (Original)	99.18 $\pm$ 0.27	99.38 $\pm$ 0.09	99.38 $\pm$ 0.09	99.53 $\pm$ 0.09	99.53 $\pm$ 0.09	99.53 $\pm$ 0.09
1%	99.11 $\pm$ 0.36	99.39 $\pm$ 0.05	99.32 $\pm$ 0.03	99.01 $\pm$ 0.09	99.46 $\pm$ 0.05	99.35 $\pm$ 0.17
0.3%	99.18 $\pm$ 0.36	99.25 $\pm$ 0.37	99.19 $\pm$ 0.41	98.81 $\pm$ 0.09	98.22 $\pm$ 1.38	98.22 $\pm$ 1.33

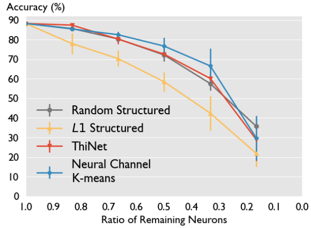
✓ Multiclass classification tasks.

Percentage of Remaining Neurons	MNIST		Fashion-MNIST	
	Smyrnis and Maragos, 2020	Neural Path K-means	Smyrnis and Maragos, 2020	Neural Path K-means
100% (Original)	98.60 $\pm$ 0.03	98.61 $\pm$ 0.11	88.66 $\pm$ 0.54	89.52 $\pm$ 0.19
10%	93.48 $\pm$ 2.57	96.89 $\pm$ 0.55	80.43 $\pm$ 3.27	86.04 $\pm$ 0.94
5%	92.93 $\pm$ 2.59	96.31 $\pm$ 1.29	–	83.68 $\pm$ 1.06

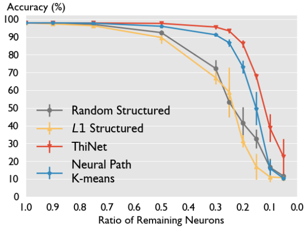
Experimental Evaluation II: Comparison with Thinet and baselines.



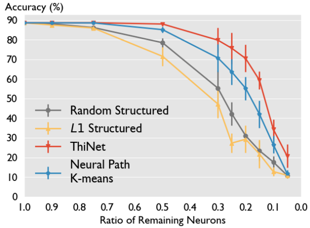
(a) LeNet5, MNIST



(b) LeNet5, F-MNIST



(c) deepNN, MNIST



(d) deepNN, F-MNIST

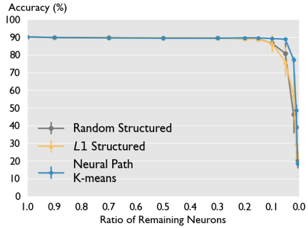
LeNet5

- ✓ 1 hidden layer with 84 neurons.

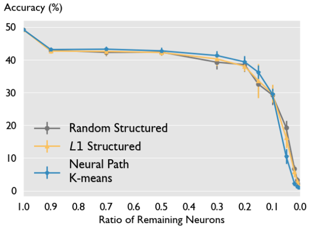
Custom deep network

- ✓ 3 hidden layers.

Experimental Evaluation III: Larger datasets



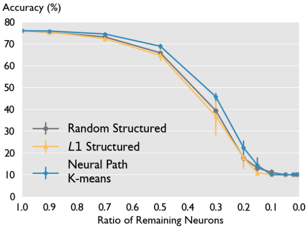
(a) CIFAR-VGG, CIFAR10



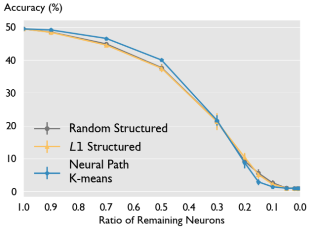
(b) CIFAR-VGG, CIFAR100

CIFAR-VGG

✓ 1 hidden layer of size 512.



(c) AlexNet, CIFAR10



(d) AlexNet, CIFAR100

AlexNet

✓ 2 hidden layers of size 512.

Thank you!

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