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Introduction to Tropical Geometry and its Applications to Machine Learning

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1

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What does TROPICAL mean?

- The adjective "tropical" was coined by French mathematicians Dominique Perrin and Jean-Eric Pin, to honor their Brazilian colleague Imre Simon, a pioneer of min-plus algebra as applied to finite automata in computer science.
- Tropical (Τροπικός in Greek) comes from the greek word «Τροπή» which means "turning" or "changing the way/direction".



Outline (and some introductory references)

1. Elements of Tropical Geometry

"a marriage between algebraic geometry and polyhedral geometry" [Maclagan & Sturmfels 2015]

- **Tropical semirings:** Max-plus & Min-plus Arithmetic
- Tropical Polynomials
- **Geometrical objects:** tropical curves/surfaces, halfspaces, Newton polytopes
- Max-plus Matrix Algebra: "linear algebra of DP & Combinatorics" [O.R., Graphs: Cuninghame-Green 1979], [DES, Nonlinear Control: Baccelli et al. 2001, Butkovic 2010], Optimization [Gaubert et al, Max-plus group], Mathematical Morphology & Image Analysis, Idempotent Mathematics [Maslov, Litvinov, et al]

2. Applications to Neural Networks:

- Tropical Geometry of NNs with PieceWise-Linear (PWL) Activations
- Advances in Morphological Networks: Training and Pruning
- **NN Minimization via Tropical Polynomial Division and Zonotopes**
- **3. Optimization and Tropical Regression:**
 - Optimal solutions of max-plus matrix equations
 - Tropical Regression: fitting tropical polynomials to data

Tropical Semirings

Scalar Arithmetic Rings

Integer/Real Addition-Multiplication Ring: $(\mathbb{R}, +, \times), (\mathbb{Z}, +, \times)$

Tropical Semirings

$$\mathbb{R}_{\max} = \mathbb{R} \cup \{-\infty\}, \ \mathbb{R}_{\min} = \mathbb{R} \cup \{+\infty\}$$

 $\vee = \max, \land = \min$

Max-plus semiring: $(\mathbb{R}_{max}, \lor, +)$

Min-plus semiring: $(\mathbb{R}_{\min}, \wedge, +)$

Correspondences between linear and (max, +) arithmeticLinear arithmetic(max, +) arithmetic+max×+0 $-\infty$ 10 $x^{-1} = 1/x$ $x^{-1} = -x$

Maslov Dequantization \rightarrow Log - Sum - Exp approximation

Log-Sum-Exp (LSE) approximation

(Maslov "Dequantization" in idempotent mathematics [Maslov 1987, Litvinov 2007])

$$\lim_{T \downarrow 0} T \cdot \log(e^{a/T} + e^{b/T}) = \max(a, b)$$
$$\lim_{T \downarrow 0} (-T) \log(e^{-a/T} + e^{-b/T}) = \min(a, b)$$



Graphs of Max-plus Tropical 1D Polynomials

 $y_{\text{t-line}} = \max(a+x,b), \quad y_{\text{t-parab}} = \max(a+2x,b+x,c)$



6

Max-plus and Min-Plus Tropical 1D Polynomials



Tropical Curve of Max/Min-Polynomials

Tropical curve of p(x,y) =

"Zero locus" of a max/min polynomial is the set of points where the max/min is attained by more than one of the "monomial" terms of the polynomial.



Tropical curve of the max-polynomial

$$p(x,y) = \max(2x,y,c)$$



Tropical curve of the min-polynomial

 $p'(x, y) = \min(2x, y, c)$

Tropical Curve vs Newton Polytope

Max polynomial

$$p(\mathbf{x}) = \max_{i \in 1, 2, \dots, k} \{ c_{i1}x_1 + c_{i2}x_2 + \dots + c_{in}x_n \} = \bigvee_{i=1}^{k} \mathbf{c}_i^T \mathbf{x}$$

"Zero locus" of a max polynomial is the set of points where the max is attained by more than two polynomial terms.



Newton polytope *N*(*p*) of max polynomial *p* is the convex hull of its coefficients' vectors.

$$\mathcal{N}(p) = \operatorname{conv}\left\{v_1, v_2, v_3\right\}$$

7



Duality between Newton polytope N(p) and tropical curve V(p)

Graph and Trop Curve of a tropical "Conic" polynomial

Tropical Polynomial of degree 2 in two variables

classical: " $ax^2 + bxy + cy^2 + dy + e + fx$ " tropical: $p(x, y) = \min(a + 2x, b + x + y, c + 2y, d + y, e, f + x)$ e**Graph** of p(x,y)x + fand y + dits **Tropical Curve** = set of (x, y) points where the min is attained by more than one terms. 2x + ax + y + b2y+c

Obtain Tropical Polynomials via Dequantization

Classic polynomial:
$$f(\mathbf{u}) = \sum_{k=1}^{K} c_k u_1^{a_{k1}} u_2^{a_{k2}} \cdots u_n^{a_{kn}}, \quad \mathbf{u} = (u_1, u_2, \dots, u_n)$$

Posynomial if $c_k > 0$, $\mathbf{a}_k = (a_{k1}, \dots, a_{kn}) \in \mathbb{R}^n$, $\mathbf{u} > 0$;

Log-Sum-Exp (Viro's "logarithmic paper" [Viro 2001]): $\mathbf{x} = \log(\mathbf{u}), \quad b_k = \log(c_k)$ $\lim_{T \downarrow 0} T \cdot \log f(e^{\mathbf{x}/T}) = \lim_{T \downarrow 0} T \cdot \sum_{k=1}^{K} \exp(\langle \mathbf{a}_k, \mathbf{x} / T \rangle + b_k / T) \rightarrow$ Tropical (max-plus) Polynomial = Piecewise-Linear Function

$$p(\mathbf{x}) = \bigwedge_{k=1}^{K} \left\{ \langle \mathbf{a}_{k}, \mathbf{x} \rangle + b_{k} \right\} = \bigwedge_{k=1}^{K} \left\{ a_{k1} x_{1} + \dots + a_{kn} x_{n} + b_{k} \right\}$$

11

Tropical Half-spaces and Polytopes in 2D

Tropical (affine) Half-space of \mathbb{R}^n_{\max} [Gaubert & Katz 2011]

$$\mathscr{T}(\mathbf{a},\mathbf{b}) \triangleq \{\mathbf{x} \in \mathbb{R}_{\max}^n : \max(a_{n+1},\bigvee_{i=1}^n a_i + x_i) \le \max(b_{n+1},\bigvee_{i=1}^n b_i + x_i)\}$$



The region separating boundaries are tropical lines (or hyper-planes).

Tropical **Polyhedra** are formed from finite intersections of tropical half-spaces. **Polytopes** are compact polyhedra.

Tropical Halfspaces and Polyhedra in 3D



(Extended) Newton Polytope

Let
$$p(x) = \max_{i=1,...,k} (a_i^T x + b_i)$$
 be a max-polynomial.
Definition ((Extended) Newton Polytope): We define as the
(Extended) Newton Polytope of p the following:
Newt $(p) = \operatorname{conv}\{a_i, i = 1, ..., k\}$
ENewt $(p) = \operatorname{conv}\{(a_i, b_i), i = 1, ..., k\}$

where conv signifies the convex hull of the given set.

<u>Theorem [Charisopoulos & Maragos, 2018; Zhang et al., 2018]</u>: Maxpolynomials with the same vertices in the upper hull of their Extended Newton Polytope correspond to the same function.

Examples of (Ext) Newton Polytopes



 $\max(3x, 2x + 1.5, x + 1, 0).$

Figure: Polytopes of $\max(2x, x + y + 1, x + 1, y + 1, 1).$

ENewt

Newt

1.0

0.8

0.6

0.4

0.2

0.0

Coefficient

Newton Polytope and Maxpolynomial Function

- "Upper" vertices of ENewt(p)
 define p(x) as a function.
- Geometrically: max(3x + 1, 2x + 1.25, x + 2, 0)= max(3x + 1, x + 2, 0)

(extra point is not on the upper hull).



ENewt(p), $p(x) = \max(3x + 1, x + 2, 0)$

Tropical Algebra of Max-plus Polynomials ←→ Tropical Geometry of their Newton Polytopes

Newt
$$(p_1 \lor p_2) = \operatorname{conv} (\operatorname{Newt} (p_1) \cup \operatorname{Newt} (p_2))$$

Newt $(p_1 + p_2) = \operatorname{Newt} (p_1) \oplus \operatorname{Newt} (p_2)$



Newton polytopes of (a) two max-polynomials

 $p_1(x,y) = max(x+y, 3x+y, x+2y)$ and $p_2(x,y) = max(0, -x, y, y-x)$, (b) their $max(p_1, p_2)$, and (c) their sum $p_1 + p_2$

Tropical Geometry of Neural Nets with Piecewise-Linear Activations

References:

- 1. Charisopoulos, V., & Maragos, P. (2017, May). *Morphological perceptrons: geometry and training algorithms*, ISMM '17.
- Charisopoulos, V., & Maragos, P. (2018). A Tropical Approach to Neural Networks with Piecewise Linear Activations. arXiv:1805.08749.
- 3. Zhang, Liwen and Naitzat, Gregory and Lim, Lek-Heng. *Tropical geometry of deep neural networks*, Proc. ICML(35) 2018.

Piecewise-linear functions used as *activation* functions σ :

- **1.** ReLU: $\max(0, v)$ or $\max(\alpha v, v)$, $\alpha \ll 1$ with $v := \boldsymbol{w}^\top \boldsymbol{x} + b$
- 2. Maxout: $\max_{k \in [K]} v_k$ with $v_k := W_k^\top x + b_k$



Linear regions: maximally connected regions of input space on which the NN's output is linear [Montufar et al., 2014].



Figure: Input space is subdivided into convex polytopes, each of which is a "linear region" for the NN. Reproduced from [Raghu et al., 2016]

Claim: more linear regions \equiv more expressive power

Convex + PWL: ideal to study under lens of tropical geometry

Formally: tropical semiring $(\mathbb{R} \cup \{-\infty\}, \lor, +)$

- binary "addition" $x \lor y := \max(x, y)$, "multiplication" x + y
- operations on vectors $oldsymbol{x}, oldsymbol{y}$:

$$\boldsymbol{x} \lor \boldsymbol{y} := \begin{pmatrix} \max(x_1, y_1) \\ \vdots \\ \max(x_n, y_n) \end{pmatrix}, \quad \boldsymbol{x}^\top \boxplus \boldsymbol{y} := \bigvee_{i=1}^n x_i + y_i$$

Key object: tropical {poly, posy, sig}nomials

An application of the fundamental theorem of LP yields:

Proposition [Charisopoulos & Maragos, 2017]

The number of linear regions for a single maxout unit $p(x) = \max_{j \in [k]} w_j^\top x + b_i$ are equal to the number of vertices on the upper hull of $\mathcal{N}(p)$

• subsumes **relu**

• all terms corresponding to interior vertices can be *removed* without affecting p(x) as a function.



Figure: Upper Hull example for $p(x) = \max(1 + 2x_1, 2 + x_1, 2, 2 + x_2, 2 + x_1 + x_2)$ For a collection of tropical polynomials, suffices to work with Minkowski sums:

Proposition [Charisopoulos & Maragos, 2018] [Zhang et al., 2018]

The number of linear regions of a layer with n inputs and m neurons is upper bounded by the number of vertices in the upper convex hull of

 $\mathcal{N}(p_1) \oplus \cdots \oplus \mathcal{N}(p_m),$

where \oplus denotes Minkowski sum.

Immediate application of a bound from [Gritzmann and Sturmfels, 1993] on faces of Minkowski sums gives

Proposition [Charisopoulos & Maragos, 2018]

The number of linear regions of n input, m output layer consisting of convex PWL activations of rank k is bounded above by

$$\min\left\{k^m, 2\sum_{j=0}^n \binom{m\frac{k(k-1)}{2}}{j}\right\}.$$

In case of ReLU, use symmetry of zonotopes to refine to

$$\min\left\{2^m, \sum_{j=0}^n \binom{m}{j}\right\}$$

Goal: given a network, count # of linear regions (exactly or approximately)

Exact counting using insight from Newton polytopes:

- ▷ vertex enumeration algorithm for Mink. sums [Fukuda, 2004] \Rightarrow requires solving $\Omega(|vert(P)|)$ LPs.
- impractical unless problem is small

MIP representability of NNs [Serra et al., 2018]:

- > Assumes bounded range of input space
- Requires enumerating solutions of MILPs

Geometric Algorithm: Randomized method for Sampling the Extreme Points of the Upper Hull of a Polytope [Charisopoulos & Maragos 2019, arXiv:1805.08749v2], [Maragos, Charisopoulos & Theodosis, Proc. IEEE 2021]

Geometry & Algebra of NNs with PWL Activations

<u>Theorem (Wang 2004)</u>: A continuous piecewise linear function is equal to the difference of two max-polynomials.

<u>Theorem (Charisopoulos & Maragos 2018)</u>: The essential terms of a tropical polynomial are in bijection 1 - 1 with the vertices on the upper convex hull of its extended Newton polytope.

<u>Theorem (Zhang et al. 2018)</u>: A neural network with ReLUtype activations can be represented as the difference of two max-polynomials, i.e. with a tropical rational function. [Calafiore et al., 2019] use the Maslov dequantization to design universal approximators for convex (+loglog-convex) data

$$f \text{ convex} \Rightarrow f \simeq f_{PWL} \Leftrightarrow f \simeq f_T,$$

where $f_{PWL} \leq f_T \leq T \log K + f_{PWL}$ and are given by

$$\begin{cases} f_{\text{PWL}} := \max_{k \in [K]} \langle \boldsymbol{a}_k, \boldsymbol{x} \rangle + b_k, \\ f_T := T \log \left(\sum_{k=1}^K \exp \left\{ b_k + \langle \boldsymbol{a}_k, \boldsymbol{x} \rangle \right\}^{1/T} \right) \end{cases}$$

In particular, fixing $\varepsilon > 0$ and compact C, a small enough T will satisfy

$$\sup_{\boldsymbol{x}\in\mathcal{C}}|f_T(\boldsymbol{x})-f(\boldsymbol{x})|\leq\varepsilon.$$

Morphological Networks: Geometry, Training, and Pruning

References:

•

V. Charisopoulos and P. Maragos, "Morphological Perceptrons: Geometry and Training Algorithms", Proc. ISMM 2017, LNCS 10225, Springer.

N. Dimitriadis and P. Maragos, "Advances in Morphological Neural Networks: Training, Pruning and Enforcing Shape Constraints", Proc. ICASSP, 2021.

Motivation

- Explosion of ML research in the last decade (now models with nearhuman or even human performance)
- Recent advances indicate shift towards nonlinearity, but...
- ...the "multiply-accumulate" (= linear) activations of the perceptron are still ubiquitous

Our Questions:

- Are dot products and convolutions the only biologically plausible models of neuronal computation?
- Can we use results and tools from "nonlinear" mathematics to reason about complexity and dimension of learning models in current literature?

Rosenblatt's perceptron

Introduced in 1943, still prevalent neural model

Activation:
$$\phi(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b$$

Nonlinearity at the output (e.g logistic sigmoid, ReLU):

$$y(\boldsymbol{x}) = \sigma(\phi(\boldsymbol{x}))$$

■ Multiply-accumulate architecture → archetypal building block of all architectures (e.g. fully-connected, convolutional etc.)



Maxplus Matrix Algebra

• vector/matrix **'addition'** = pointwise max

$$\mathbf{x} \lor \mathbf{y} = [x_1 \lor y_1, \dots, x_n \lor y_n]^T \mathbf{A} \lor \mathbf{B} = [a_{ij} \lor b_{ij}]$$

• vector/matrix 'dual addition' = pointwise min

$$\mathbf{x} \wedge \mathbf{y} = [x_1 \wedge y_1, \dots, x_n \wedge y_n]^T \mathbf{A} \wedge \mathbf{B} = [a_{ij} \wedge b_{ij}]$$

• vector/matrix 'multiplication by scalar'

$$c + \mathbf{x} = [c + x_1, \dots, c + x_n]^T$$

$$c + \mathbf{A} = [c + a_{ij}]$$

• (max, +) 'matrix multiplication'

$$[\mathbf{A} \boxplus \mathbf{B}]_{ij} = \bigvee_{k=1}^{n} a_{ik} + b_{kj}$$

• (min, +) 'matrix dual multiplication'

$$[\mathbf{A} \boxplus' \mathbf{B}]_{ij} = \bigwedge_{k=1}^{n} a_{ik} + b_{kj}$$

Morphological Operators on Lattices

(\leq = partial ordering, V = supremum, Λ = infimum)

- ψ is increasing iff $f \leq g \Rightarrow \psi(f) \leq \psi(g)$.
- δ is **dilation** iff $\delta(\vee_i f_i) = \vee_i \delta(f_i)$.
- ε is erosion iff $\varepsilon(\wedge_i f_i) = \wedge_i \varepsilon(f_i)$.

Then: ε is erosion, δ is dilation,

- α is **opening** iff increasing and antiextensive $(\alpha(f) \le f)$, and idempotent $(\alpha = \alpha^2)$.
- β is closing iff increasing and extensive (β(f) ≥ f),
 and idempotent (β = β²).
- (ε, δ) is adjunction iff $\delta(g) \le f \Leftrightarrow g \le \varepsilon(f)$.

(Galois connection) Residuation pair ("Tropical Adjoints")

 $\delta\varepsilon$ is opening (projection), $\varepsilon\delta$ is closing (projection).

[Serra 1988; Heijmans & Ronse 1990]

Solve Max-plus Equations

- Problems:
 - (1) Exact problem: Solve $\delta_A(\mathbf{x}) = \mathbf{A} \boxplus \mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \overline{\mathbb{R}}^{m \times n}, \ \mathbf{b} \in \overline{\mathbb{R}}^m$
 - (2) Approximate Constrained: Min $\|\mathbf{A} \boxplus \mathbf{x} \mathbf{b}\|_{p=1...\infty}$ s.t. $\mathbf{A} \boxplus \mathbf{x} \leq \mathbf{b}$
- **Theorem**: (a) The **greatest** (sub)solution of (1) and unique solution of (2) is

$$\hat{\mathbf{x}} = \varepsilon_A(\mathbf{b}) = \mathbf{A}^* \boxplus' \mathbf{b} = [\bigwedge_i b_i - a_{ij}], \quad \mathbf{A}^* \triangleq -\mathbf{A}^T$$

and yields the Greatest Lower Estimate (GLE) of data b:

$$\delta_A(\varepsilon_A(\mathbf{b})) = \mathbf{A} \boxplus (\mathbf{A}^* \boxplus' \mathbf{b}) \le \mathbf{b}$$

(b) Min Max Absolute Error (MMAE) unconstrained unique solution:

$$\tilde{\mathbf{x}} = \hat{\mathbf{x}} + \mu, \quad \mu = \|\mathbf{A} \boxplus \hat{\mathbf{x}} - \mathbf{b}\|_{\infty}/2$$

• Geometry: Operators δ, ε are vector dilation and erosion, and the GLE $\mathbf{b} \mapsto \delta \varepsilon(\mathbf{b})$ is an opening (lattice projection).

• **Complexity**: O(mn)

Morphological Perceptron

Introduced in the 1990's. Instead of multiply-accumulate, computes a dilation (max-of-sums):

$$\tau(\boldsymbol{x}) = \boldsymbol{w}^T \boxplus \boldsymbol{x} \triangleq \bigvee_{i=1}^n w_i + x_i$$

or an erosion:

$$\tau'(\boldsymbol{x}) = \boldsymbol{w}^T \boxplus' \boldsymbol{x} \triangleq \bigwedge_{i=1}^n w_i + x_i$$

Ritter & Urcid (2003): argued about biological plausibility and proved that every compact region in n-dim Euclidean space can be approximated by morphological perceptrons to arbitrary accuracy.

Related to a Maxout unit.

Feasible Regions & Separability Condition for Max-plus Percepton

Let $X \in \mathbb{R}_{\max}^{k \times n}$ be a matrix containing the patterns to be classified as its rows, let $x^{(k)}$ denote the k-th pattern (row) and let $\mathcal{C}_1, \mathcal{C}_0$ be the two classes

Max-plus perceptron
$$\tau(\boldsymbol{x}) = \boldsymbol{w}^T \boxplus \boldsymbol{x}$$

 $\tau(\boldsymbol{x}) = w_0 \lor (w_1 + x_1) \lor \cdots \lor (w_n + x_n) = w_0 \lor \left(\bigvee_{i=1}^n w_i + x_i\right)$

Feasible Region = Tropical Polyhedron

$$\mathcal{T}(\boldsymbol{X}_{\text{pos}}, \boldsymbol{X}_{\text{neg}}) = \{ \boldsymbol{w} \in \mathbb{R}^n_{\text{max}} : \boldsymbol{X}_{\text{pos}} \boxplus \boldsymbol{w} \ge 0, \ \boldsymbol{X}_{\text{neg}} \boxplus \boldsymbol{w} \le 0 \}$$

Separability Condition, equivalent to Nonempty Trop. Polyhedron

$$\mathbf{X}_{\mathrm{pos}}\boxplus(\mathbf{X}^*_{\mathrm{neg}}\boxplus'\mathbf{0})\geq\mathbf{0}$$

[Charisopoulos & Maragos, 2017]


Morphological Neural Nets (MNNs) and Training Approaches

• Constructive Algorithms

Dendrite Learning [Ritter & Urcid, 2003], Iterative Partitioning / Competitive Learning [Sussner & Esmi, 2011]: combine (max, +) and (min, +) classifiers, build "bounding boxes" around patterns

- "perfect" fit to data, no concept of outlier

Morphological Associative Memories

Introduce a Hopfield-type network, computing (noniteratively) a morphological/fuzzy response (e.g. Sussner & Valle, 2006):

Gradient Descent Variants

Min-max classifiers [Yang & Maragos, 1995], MRL nodes [Pessoa & Maragos, 2000], Dilation-Erosion Linear Perceptron [Araujo et al. 2012].

Recent Approaches:

Convex-Concave Programming (CCP) for Max-plus Perceptron and DEP (Binary Classification) [Charisopoulos & Maragos 2017]

Reduced Dilation-Erosion Perceptron (r-DEP) trained via CCP for Binary Classification [Valle 2020]

Dense Morphological Networks [Mondal et al. 2019]

Deep Morphological Networks [Franchi et al. 2020]

r-DEP for Multiclass Classification via CCP, L1 Pruning on Dense MNNs [Dimitriadis & Maragos 2021]

Our Approach for Training MP on Non-separable Data

Training a (max, +) perceptron can be stated as a difference-of-convex (DC) optimization problem. Solved iteratively (but global optimum not guaranteed) by the Convex-Concave Procedure (CCP) [Yuille & Rangarajan, 2003], implemented via DCCP [Shen et al. 2016]

Given a sequence of training data $\{x^{\kappa}\}_{k=1}^{n}$

$$\{x^k\}_{k=1}^K$$
 :

$$\begin{aligned} \text{Minimize } J(\boldsymbol{X}, \boldsymbol{w}, \boldsymbol{\nu}) &= \sum_{k=1}^{K} \nu_k \cdot \max(\xi_k, 0) \\ \text{s. t.} & \left\{ \begin{array}{l} \bigvee_{i=1}^{n} w_i + x_i^{(k)} \leq \xi_k & \text{ if } \boldsymbol{x}^{(k)} \in \mathcal{C}_0 \\ \bigvee_{i=1}^{n} w_i + x_i^{(k)} \geq -\xi_k & \text{ if } \boldsymbol{x}^{(k)} \in \mathcal{C}_1 \end{array} \right. \end{aligned}$$
 Negative

- Some measure of "being outlier" u_k
- ξ_k Positive only if misclassification occurs at k-th pattern

Gradient Descent vs. CCP for Training (max,+) Perceptron

Two Binary Classification Experiments.

Gradient descent with fixed N = 100 epochs vs. CCP using the DCCP toolkit for CvxPy (default parameters).

m	Riple	ys	WDBO	2	
η	SGD	WDCCP	SGD	WDCCP	
0.01	0.838 ± 0.011		0.726 ± 0.002		
0.02	0.739 ± 0.012		0.763 ± 0.006		
0.03	0.827 ± 0.008		0.726 ± 0.004		
0.04	0.834 ± 0.008		0.751 ± 0.007		
0.05	0.800 ± 0.009	0.902	0.783 ± 0.012	0.908	
0.06	0.785 ± 0.008	± 0.001	0.768 ± 0.01	± 0.001	
0.07	0.776 ± 0.009		0.729 ± 0.009		
0.08	0.769 ± 0.01		0.732 ± 0.01		
0.09	0.799 ± 0.009		0.730 ± 0.015		
0.1	0.749 ± 0.011		0.729 ± 0.009		
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	.P: more robu	JST results			

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Dilation-Erosion Perceptron Training

$$y = f(\mathbf{x}) = \lambda \delta_w(\mathbf{x}) + (1 - \lambda)\epsilon_m(\mathbf{x}) = \lambda \delta_w(\mathbf{x}) - (1 - \lambda)[-\epsilon_m(\mathbf{x})]$$

= convex - (-concave)
= convex - convex

Training as Difference-of-Convex Optimization via Convex-Concave Programming

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^{N} v_i \max\{0, \xi_i\} \\ \text{subject to} & \lambda \delta_{\mathsf{w}}(\mathbf{x}_i) + (1 - \lambda) \varepsilon_{\mathsf{m}}(\mathbf{x}_i) \geq -\xi_i \quad \forall \mathbf{x}_i \in \mathcal{P}, \\ & \lambda \delta_{\mathsf{w}}(\mathbf{x}_i) + (1 - \lambda) \varepsilon_{\mathsf{m}}(\mathbf{x}_i) \leq +\xi_i \quad \forall \mathbf{x}_i \in \mathcal{N} \end{array}$$

Effect of $\mathcal{N} \leftrightarrows \mathcal{P}$ and Ordering Vector Data

Double Moons example



Reduced ordering [Valle 2020] for better ordering feature patterns:

Let *V* be a nonempty set, \mathcal{L} be a complete lattice and $\rho: V \to \mathcal{L}$ be a surjective mapping. A reduced ordering is defined as: $x \leq_{\rho} y \Leftrightarrow \rho(x) \leq \rho(y) \forall x, y \in V$.

Can be obtained via a supervised training on a set of positive and negative examples.

Experiments: Multiclass r-DEP, CCP training

	MNIST	FashionMNIST
<i>n</i> = 5	$\textbf{97.72} \pm \textbf{0.01}$	88.21 ± 0.01
n = 10	97.72 ± 0.01	88.07 ± 0.01
<i>n</i> = 15	97.67 ± 0.01	88.11 ± 0.01
<i>n</i> = 20	97.64 ± 0.01	88.12 ± 0.01

Table: Results of Bagging *multiclass* r-DEP with *n* RBF kernels.

- Performance similar to MLP-ReLU architectures trained via SGD
- CCP training is more robust

Dense Morphological Networks



Dense Morphological Network with 2 hidden layers [similar to Mondal et al. 2019]

Focus on Sparsity [Dimitriadis & Maragos 2021] \rightarrow Apply ℓ_1 Pruning

Experiments: Pruning Dense MNN vs MLP-ReLU

		Adaptive Momentum Estimation		Stochastic Gradient Descent					
	p	δ	ε	(δ, ε)	FF-ReLU	 δ	ε	(δ, ε)	FF-ReLU
	100%	97.62	96.17	97.95	98.13	94.86	93.36	96.07	98.16
	75%	97.62	96.18	97.93	98.15	94.86	93.36	96.07	98.12
	50%	97.62	96.22	97.90	98.17	94.86	93.37	96.07	98.08
T	25%	97.62	96.09	97.87	97.51	94.86	93.40	96.06	98.01
SIN	10%	97.62	95.78	97.74	93.38	94.86	93.38	96.09	96.67
Μ	7.5%	97.62	95.42	97.76	90.17	94.86	93.38	96.10	95.56
	5%	97.62	94.51	97.66	83.39	94.86	93.40	96.10	92.96
	2.5%	97.62	93.43	97.37	68.93	94.86	93.39	96.09	80.48
	1%	97.62	91.17	97.08	44.22	94.86	93.38	96.08	58.07
	100%	86.31	86.82	88.32	88.82	82.06	85.23	86.21	87.79
	75%	86.30	86.81	88.30	88.88	82.00	85.23	86.21	87.75
ISI	50%	86.22	86.80	88.33	88.18	82.05	85.25	86.20	87.19
MN	25%	85.95	86.85	88.31	82.15	81.90	85.26	86.28	84.35
on	10%	85.58	86.27	88.05	65.89	81.67	85.27	86.23	73.22
shi	7.5%	85.47	86.15	87.99	57.93	81.63	85.27	86.21	63.95
Га	5%	85.37	85.81	87.76	49.12	81.52	85.24	86.22	47.73
	2.5%	84.91	85.47	87.56	42.48	81.14	85.26	86.22	38.84
	1%	81.14	84.86	86.85	28.13	80.68	85.27	86.18	35.46

Table: Accuracy of pruned networks on the MNIST and FashionMNIST datasets.

Models: $\delta \rightarrow$ only dilation neurons, $\varepsilon \rightarrow$ only erosion, $(\delta, \varepsilon) \rightarrow$ split equally, FF-ReLU \rightarrow FeedForward NN with ReLU.

shades of red showcase the degree of (severe) deterioration in accuracy green indicates the absence of performance loss

Qualitative Perspectives on Sparsity



Examples of hidden layer activations for various NN models (MNIST dataset) 46

Minimization of Neural Nets via Tropical Division and Newton Polytope Approximation

References:

- G. Smyrnis, P. Maragos and G. Retsinas, "*MaxPolynomial Division With Application to Neural Network Simplification*", Proc. ICASSP, 2020.
- G. Smyrnis and P. Maragos, "*Multiclass Neural Network Minimization Via Tropical Newton Polytope Approximation*", Proc. ICML 2020.
- P. Misiakos, G. Smyrnis, G. Retsinas and P. Maragos, "Neural Network Approximation based on Hausdorff distance of Tropical Zonotopes", Proc. ICLR 2022.

Tropical Polynomials

Tropical Semiring $(\mathbb{R}_{\max}, \lor, +)$

$$\mathbb{R}_{\max} = \mathbb{R} \cup \{-\infty\}$$
$$a \lor b = \max(a, b)$$
$$a + b = a + b$$

Tropical Polynomials

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

Newton Polytopes

Newton Polytopes

Newt
$$(f) = \operatorname{conv} \{ \boldsymbol{a}_i : i \in [n] \}$$

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

Polytope computation

ENewt $(f \lor g) = \operatorname{conv} \{ \operatorname{ENewt} (f) \cup \operatorname{ENewt} (g) \}$ ENewt $(f + g) = \operatorname{ENewt} (f) \oplus \operatorname{ENewt} (g)$

Example: Polytope Computation

$$f(x, y) = \max(2x + y + 1, 0)$$
$$g(x.y) = \max(x, y, 1)$$



$$f \lor g = \max(2x + y + 1, 0, x, y, 1)$$
$$f + g = \max(x, y, 1, 3x + y + 1, 2x + 2y + 1, 2x + y + 2)$$

General idea for Geometric NN Minimization



Original Network Polytope

Approximate Network Polytope

Maxpolynomial Division

Problem: Assume we have two maxpolynomials p(x), d(x) (dividend and divisor). We want to find two maxpolynomials q(x), r(x) (quotient and remainder) such that:

$$p(\mathbf{x}) = \max(q(\mathbf{x}) + d(\mathbf{x}), r(\mathbf{x}))$$

However! The above is not always feasible (non-trivially).

Approximate Division: We relax the requirements, so that the polynomials we want to find satisfy:

 $p(\mathbf{x}) \ge \max(q(\mathbf{x}) + d(\mathbf{x}), r(\mathbf{x}))$

We also require that q(x), r(x) satisfy the above maximally.

Algorithm for Approximate Maxpolynomial Division

- Let *C* be the set of possible vectors *c* by which we can h-shift Newt(*d*) (each of which corresponds to a linear term in *q*).
- 2. We raise the shifted version of ENewt(d) as high as possible so that it still lies below ENewt(p), and we mark the vertical shift as q_c .
- 3. We set the quotient equal to:

 $q(\boldsymbol{x}) = \max_{\boldsymbol{c} \in C} (q_{\boldsymbol{c}} + \boldsymbol{c}^T \boldsymbol{x})$

and add all terms not covered by a h-shift c to the remainder r(x).



Figure: Division Method Division of $p(x) = \max(3x, 2x + 1.5, x + 1, 0)$ by $d(x) = \max(x, 0)$.

Division Example (1)



Figure: Division of $p(x) = \max(3x, 2x + 1.5, x + 1, 0)$ by $d(x) = \max(x, 0)$.

Note: The Newton Polytope of the divisor is raised as much as possible, but it cannot match the polytope of the dividend exactly. Thus, only 3 out of the 4 vertices are perfectly matched.

Division Example (2)



Figure: Division of $p(x) = \max(3x, 2x + 1.5, x + 1, 0)$ by $d(x) = \max(x + 1, 0)$.

Note: In this case, the polytope of the divisor can match that of the dividend perfectly, so all vertices are covered.

Application to Neural Network Minimization

General idea: Our algorithm seeks to minimize the network by matching the most important vertices of the Newton Polytopes of its maxpolynomials.

2-layer 1-output NN:

The NNs considered are the difference of two maxpolynomials. For each of the two (+,-) maxpolynomials p(x) of the network, we first find a divisor d(x). This is done by: Finding the most important vertices of ENewt(p), via the weights of the network (based on which combination of neurons is activated).

Method for Single Output Neuron



- Final polytope (right) is precisely under the original (left).
- The process is a "smoothing" of the original polytope.
 (From the 8 vertices of the original-yellow polytope we keep only the 4 blue which comprise the vertices of the final-red polytope.)

Properties of Trop. Div. Approximation Method



Original Network Polytope

Approximate Network Polytope

- 1. Approximate polytope contains only vertices of the original.
- 2. The input samples activating the chosen vertices have the same output in the two networks.

3. At least
$$\frac{N}{\sum_{j=0}^{d} {n \choose j}} O(\log n')$$
 samples retain their output

(*N* is # of samples, n and n' the # of neurons in hidden layer before and after the approximation). Note: this is not a tight bound.

Extension with Multiple Output Neurons



Upper hull of polytope, Neuron 1

Upper hull of polytope, Neuron 2

- <u>What we have:</u> Multiple polytopes (one pair for each output neuron), interconnected (Minkowski sums of same hidden neurons but with different scaling weights).
- <u>What we want:</u> Simultaneous approximation of all polytopes.

One-Vs-All Framework



Experiments: Trop. Division NN Minimization

Neurons Kept	TropDiv Method, Avg. Accuracy	TropDiv Method, St. Deviation	MNIST
Original	98.604	0.027	Dataset
75%	96.560	1.245	
50%	96.392	1.177	
25%	95.154	2.356	
10%	93.748	2.572	
5%	92.928	2.589	

Neurons Kept	TropDiv Method, Avg. Accuracy	TropDiv Method, St. Deviation	Fashion-
Original	88.658	0.538	MNIST
75%	83.556	2.885	Dataset
50%	83.300	2.799	DataSCI
25%	82.224	2.845	
10%	80.430	3.267	

[G. Smyrnis & P. Maragos, "Multiclass Neural Net Minimization, Tropical Newton Polytope Approximation", ICML 2020]

Neural Network Tropical Geometry



1 hidden layer with ReLU activations

i- th hidden layer neuron

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

Tropical polynomial

j- th output layer neuron

$$\begin{aligned} \psi_j(\boldsymbol{x}) &= \sum_{i=1}^n c_{ji} f_i(\boldsymbol{x}) \\ &= \sum_{c_{ji}>0} |c_{ji}| f_i(\boldsymbol{x}) - \sum_{c_{ji}<0} |c_{ji}| f_i(\boldsymbol{x}) \\ &= p_j(\boldsymbol{x}) - q_j(\boldsymbol{x}) \end{aligned}$$

Tropical rational function

Neural Network Tropical Geometry



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

ENewt (f_i) is a linear segment

$$v_j(\boldsymbol{x}) = \sum_{c_{ji}>0} |c_{ji}| f_i(\boldsymbol{x}) - \sum_{c_{ji}<0} |c_{ji}| f_i(\boldsymbol{x})$$
$$= p_j(\boldsymbol{x}) - q_j(\boldsymbol{x})$$

 $P_{j} = \text{ENewt}(p_{j}) \qquad \begin{array}{l} \text{Positive} \\ Z_{j} = \text{ENewt}(q_{j}) \\ \hline for \ deep \end{array}$

Positive and Negative zonotopes – or polytopes for deeper NNs

 $c_{ji}\left(\boldsymbol{a}_{i}^{T}, b_{i}\right)$ Generators of the zonotopes

Approximate Extended Newton Polytopes



Approximate extended Newton polytopes

Approximate tropical polynomials

Proposition Let $p, \tilde{p} \in \mathbb{R}_{\max}[\boldsymbol{x}]$ and consider the polytopes $P = \text{ENewt}(p), \tilde{P} = \text{ENewt}(\tilde{p})$. Then,

Neural Network Approximation Theorem

Theorem: Consider two neural networks v, \tilde{v} with output size m and $P_j, Q_j, \tilde{P}_j, \tilde{Q}_j$ be the positive and negative extended Newton polytopes of v, \tilde{v} respectively. Then,

$$\max_{x \in \mathcal{B}} \|v(\boldsymbol{x}) - \tilde{v}(\boldsymbol{x})\|_{1} \le \rho \cdot \left(\sum_{j=1}^{m} \mathcal{H}\left(P_{j}, \tilde{P}_{j}\right) + \mathcal{H}\left(Q_{j}, \tilde{Q}_{j}\right)\right)$$

Approximately equal zonotopes

Approximately equivalent networks

Zonotope K-Means

K-means on the positive and negative *zonotope generators*



Single-output network

Original zonotopes

Approximated Zonotopes

Reduced network

Neural Path K-means



Generalization for multi-output networks

K-means on the vectors associated with the *neural paths*

Performance Results

Binary Classification Experiments

Percentage of		MNIST $3/5$		MNIST 4/9		
Remaining Neurons	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 ± 0.27	99.38 ± 0.09	99.38 ± 0.09	99.53 ± 0.09	99.53 ± 0.09	99.53 ± 0.09
5%	99.12 ± 0.37	99.42 ± 0.07	99.25 ± 0.04	98.99 ± 0.09	$99.52\ \pm 0.09$	99.48 ± 0.15
1%	99.11 ± 0.36	99.39 ± 0.05	99.32 ± 0.03	99.01 ± 0.09	99.46 ± 0.05	99.35 ± 0.17
0.5%	99.18 ± 0.36	99.41 ± 0.05	99.22 ± 0.11	98.81 ± 0.09	99.35 ± 0.24	98.84 ± 1.18
0.3%	99.18 ± 0.36	99.25 ± 0.37	99.19 ± 0.41	98.81 ± 0.09	98.22 ± 1.38	98.22 ± 1.33

Multiclass Classification Experiments

Percentage of	MNIST		Fashion-MNIST		
Remaining Neurons	Smyrnis and Maragos, 2020	Neural Path K-means	Smyrnis and Maragos, 2020	Neural Path K-means	
100% (Original)	98.60 ± 0.03	98.61 ± 0.11	88.66 ± 0.54	89.52 ± 0.19	
50%	96.39 ± 1.18	98.13 ± 0.28	83.30 ± 2.80	88.22 ± 0.32	
25%	95.15 ± 2.36	98.42 ± 0.42	82.22 ± 2.85	86.67 ± 1.12	
10%	93.48 ± 2.57	96.89 ± 0.55	80.43 ± 3.27	86.04 ± 0.94	
5%	92.93 ± 2.59	96.31 ± 1.29	_	83.68 ± 1.06	

[P. Misiakos, G. Smyrnis, G. Retsinas and P. Maragos, "Neural Network Approximation based on Hausdorff distance of Tropical Zonotopes", Proc. ICLR 2022]

Comparison with ThiNet and Baselines









Comparison with baselines

CIFAR10



AlexNet











Tropical Regression and Piecewise-Linear Surface Fitting

References:

- P. Maragos and E. Theodosis, "Multivariate Tropical Regression and Piecewise-Linear Surface Fitting", *Proc. ICASSP*, 2020.
- P. Maragos, V. Charisopoulos and E. Theodosis, "Tropical Geometry and Machine Learning", *Proceedings of the IEEE*, 2021.
Optimal Regression for Fitting Euclidean vs Tropical Lines

Problem: Fit a curve to data (x_i, y_i) , i = 1, ..., m**Euclidean**:

Fit a straight line y = ax + b by minimizing ℓ_2 -norm of error:

$$a = \frac{\sum x_i y_i - (\sum x_i) (\sum y_i) / m}{\sum (x_i)^2 - (\sum x_i)^2 / m} , \ b = \frac{1}{m} \sum_i y_i - ax_i$$

Tropical:

Fit a tropical line $y = \max(a + x, b)$ by minimizing some ℓ_p -norm of error:

Greatest Subsolution: $a = MIN y_i - x_i$, $b = MIN y_i$



Solve Max-plus Equations

• Problems:

(1) Exact problem: Solve $\delta_A(\mathbf{x}) = \mathbf{A} \boxplus \mathbf{x} = \mathbf{b}, \quad \mathbf{A} \in \overline{\mathbb{R}}^{m \times n}, \ \mathbf{b} \in \overline{\mathbb{R}}^m$

(2) Approximate Constrained: Min $\|\mathbf{A} \boxplus \mathbf{x} - \mathbf{b}\|_{p=1...\infty}$ s.t. $\mathbf{A} \boxplus \mathbf{x} \leq \mathbf{b}$

• **Theorem**: (a) The **greatest (sub)solution** of (1) and unique solution of (2) is

$$\hat{\mathbf{x}} = \varepsilon_A(\mathbf{b}) = \mathbf{A}^* \boxplus' \mathbf{b} = [\bigwedge_i b_i - a_{ij}], \quad \mathbf{A}^* \triangleq -\mathbf{A}^T$$

and yields the **Greatest Lower Estimate (GLE)** of data **b**:

$$\delta_A(\varepsilon_A(\mathbf{b})) = \mathbf{A} \boxplus (\mathbf{A}^* \boxplus' \mathbf{b}) \le \mathbf{b}$$

(b) Min Max Absolute Error (MMAE) unconstrained unique solution:

$$\tilde{\mathbf{x}} = \hat{\mathbf{x}} + \mu, \quad \mu = \|\mathbf{A} \boxplus \hat{\mathbf{x}} - \mathbf{b}\|_{\infty}/2$$

• Geometry: Operators δ, ε are vector dilation and erosion, and the GLE $\mathbf{b} \mapsto \delta \varepsilon(\mathbf{b})$ is an opening (lattice projection).

• **Complexity**: O(mn)

Sparse solutions: [Tsiamis & Maragos 2019], [Tsilivis et al. 2021]

Optimally Fitting Tropical Lines to Data

Problem: Fit a tropical line $y = \max(a + x, b)$ to noisy data (x_i, f_i) , i = 1, ..., m, where $f_i = y_i$ +error by minimizing $\ell_{1,...,\infty}$ norm of error: Greatest Subsolution (GLE): $\hat{w} = (\hat{a}, \hat{b})$, $\hat{a} = \min_i f_i - x_i$, $\hat{b} = \min_i f_i$ Min Max Abs. Error (MMAE) Solution: $\tilde{w} = \hat{w} + \mu$, $\mu = ||$ GLE error $||_{\infty} /2$



Numerical Examples of Optimally Fitting Tropical Lines to Data

Problem: Fit a tropical line $y = \max(a + x, b)$ to noisy data (x_i, f_i) , i = 1, ..., m = 200, where $f_i = y_i$ +error by minimizing $\ell_{1,...,\infty}$ of error: Greatest Subsolution (GLE): $\hat{w} = (\hat{a}, \hat{b})$, $\hat{a} = \min_i f_i - x_i$, $\hat{b} = \min_i f_i$ Min Max Abs. Error (MMAE) Solution: $\tilde{w} = \hat{w} + \mu$, $\mu = ||$ GLE error $||_{\infty} / 2$



(a) T-line with Gaussian Noise

(b) T-line with Uniform Noise

Optimal Fitting Max-Plus Tropical Planes to Data

Problem: Fit a tropical plane $z = \max(a + x, b + y, c)$ to noisy data (x_i, y_i, f_i) , where $f_i = z_i$ +error, i = 1, ..., m = 100, by minimizing $\ell_{1,...,\infty}$ norm of error: **Greatest Subsolution (GLE)**: $\hat{w} = (\hat{a}, \hat{b}, \hat{c})$

Min Max Abs. Error (MMAE) Solution: $\tilde{w} = \hat{w} + \mu$, $\mu = || \text{GLE error } ||_{\infty} / 2$



-5

0

x

5

-5

0

x

5

10

y

10

Optimal Fitting 2D Higher-degree Tropical Polynomials to Data

Data (noisy paraboloid): 3D tuples $(x_i, y_i, f_i) \in \mathbb{R}^3$ $f_i = x_i^2 + y_i^2 + \varepsilon_i$, $(x_i, y_i) \sim \text{Unif}[-1,1]$ $\varepsilon_i \sim \mathcal{N}(0, 0.25^2)$

Model:

Fit K-rank 2D trop. polynomial

 $p(x, y) = \underset{k=1}{\overset{K}{\operatorname{AX}}} \left\{ a_k x + b_k y + c_k \right\}$

by minimizing error
$$\|f_i - p(x_i, y_i)\|_{\alpha}$$

Estimation algorithm:

K – means on data gradients $\rightarrow a_k, b_k$ solve max-plus eqns $\rightarrow c_k$

Complexity: \approx Linear *O*(#data, #dimensions)

Conclusions

- Tropical Geometry, and its underlying max-plus algebra, provide many effective and insightful tools for the analysis of NNs with PWL activations and other ML systems.
- Morphological NNs (with max-plus & min-plus nodes): show similar performance and superior compression ability compared to their linear counterparts. (Trained via CCP or SGD/Adam.)
- Tropical Regression: Tropical Polynomials for multidimensional data fitting using PWL functions. Low-complexity algorithm based on optimal solutions of systems of max-plus equations.
- Approximation of NNs: Tropical geometry offers effective and insightful tools for compression of NNs.
- Future work: extensions to deeper networks and to more general functions using max-* algebra on weighted lattices.