Sparsity in Max-plus Algebra And Applications in Multivariate Convex Regression

Nikos Tsilivis ¹, Anastasios Tsiamis ², Petros Maragos ¹

¹School of ECE, National Technical University of Athens, Greece
²ESE Department, SEAS, University of Pennsylvania, USA

June 6-11, 2021





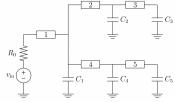
Overview

- Introduction
- Theory Sparsity in Max-plus algebra
- 3 Application to Multivariate Convex Regression
- 4 Conclusion

Convex regression - why?

<u>Problem: Learn a convex function from data.</u> Optimization





Machine Learning, Signal Processing & Finance



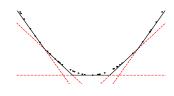


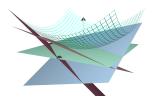
Data (\mathbf{x}_i, y_i) , where $y_i = f(\mathbf{x}_i)$, f an **unknown** convex function. How to estimate f?



Data (\mathbf{x}_i, y_i) , where $y_i = f(\mathbf{x}_i)$, f an **unknown** convex function. How to estimate f?

 $\label{eq:local_local_local} \begin{tabular}{l} Idea from Convex Analysis [Rockafellar 1970, Maragos 1994]: Any convex function \approx maximum of hyperplanes $a_i^Tx+b_j$. \end{tabular}$





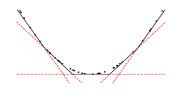
Data (\mathbf{x}_i, y_i) , where $y_i = f(\mathbf{x}_i)$, f an **unknown** convex function. How to estimate f?

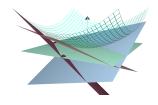
 $\label{eq:local_local_local} \begin{tabular}{ll} Idea from Convex Analysis [Rockafellar 1970, Maragos 1994]: Any convex function \approx maximum of hyperplanes $a_t^\intercal x + b_j$. \end{tabular}$

$$\max(\mathbf{a}_1^\mathsf{T}\mathbf{x}_1 + b_1, \dots, \mathbf{a}_K^\mathsf{T}\mathbf{x}_1 + b_K) = y_1$$

$$\max(\mathbf{a}_1^\mathsf{T}\mathbf{x}_2 + b_1, \dots, \mathbf{a}_K^\mathsf{T}\mathbf{x}_2 + b_K) = y_2$$

$$\dots$$





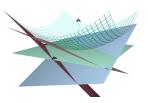
Data (\mathbf{x}_i, y_i) , where $y_i = f(\mathbf{x}_i)$, f an **unknown** convex function. How to estimate f?

 $\label{eq:local_local_local} \begin{array}{l} \mbox{Idea from Convex Analysis [Rockafellar 1970,} \\ \mbox{Maragos 1994]: Any convex function } \approx \\ \mbox{maximum of hyperplanes } \boldsymbol{a}_{,}^{T}\boldsymbol{x} + \boldsymbol{b}_{,}. \end{array}$

$$\max(\mathbf{a}_1^\mathsf{T}\mathbf{x}_1 + b_1, \dots, \mathbf{a}_K^\mathsf{T}\mathbf{x}_1 + b_K) = y_1$$

$$\max(\mathbf{a}_1^\mathsf{T}\mathbf{x}_2 + b_1, \dots, \mathbf{a}_K^\mathsf{T}\mathbf{x}_2 + b_K) = y_2$$





Question 1: How to *optimally* estimate $(\mathbf{a}_j, b_j)_{j=1}^K$ from these equations?

Question 2: How to keep # of hyperplanes as small as possible?

This is not a linear problem!

This is not a linear problem!

• But in a suitable algebra, it can be written in a linear like form.

This is not a linear problem!

- But in a suitable algebra, it can be written in a linear like form.
- Max-Plus Algebra: "Linear Algebra, but + becomes max, and \times becomes +".

This is not a linear problem!

- But in a suitable algebra, it can be written in a linear like form.
- Max-Plus Algebra: "Linear Algebra, but + becomes max, and \times becomes +".

$$\underbrace{\begin{pmatrix} \mathbf{a}_1^\mathsf{T} \mathbf{x}_1 & \mathbf{a}_2^\mathsf{T} \mathbf{x}_1 & \dots & \mathbf{a}_K^\mathsf{T} \mathbf{x}_1 \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_1^\mathsf{T} \mathbf{x}_m & \mathbf{a}_2^\mathsf{T} \mathbf{x}_m & \dots & \mathbf{a}_K^\mathsf{T} \mathbf{x}_m \end{pmatrix}}_{\mathsf{A}} \boxplus \underbrace{\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_K \end{pmatrix}}_{\mathsf{b}} = \underbrace{\begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}}_{\mathsf{y}},$$

where $[\mathbf{C} \boxplus \mathbf{D}]_{ij} = \max_{k=1}^{n} (c_{ik} + d_{kj}).$

This is not a linear problem!

- But in a suitable algebra, it can be written in a linear like form.
- Max-Plus Algebra: "Linear Algebra, but + becomes max, and \times becomes +".

$$\underbrace{\begin{pmatrix} \mathbf{a}_{1}^{\mathsf{T}} \mathbf{x}_{1} & \mathbf{a}_{2}^{\mathsf{T}} \mathbf{x}_{1} & \dots & \mathbf{a}_{K}^{\mathsf{T}} \mathbf{x}_{1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_{1}^{\mathsf{T}} \mathbf{x}_{m} & \mathbf{a}_{2}^{\mathsf{T}} \mathbf{x}_{m} & \dots & \mathbf{a}_{K}^{\mathsf{T}} \mathbf{x}_{m} \end{pmatrix}}_{\mathsf{A}} \boxplus \underbrace{\begin{pmatrix} b_{1} \\ b_{2} \\ \vdots \\ b_{K} \end{pmatrix}}_{\mathsf{b}} = \underbrace{\begin{pmatrix} y_{1} \\ \vdots \\ y_{m} \end{pmatrix}}_{\mathsf{y}},$$

where $[\mathbf{C} \boxplus \mathbf{D}]_{ij} = \max_{k=1}^{n} (c_{ik} + d_{kj}).$

• If we assume known slopes, problem reduces to solving a "linear" max-plus matrix equation $\mathbf{A} \boxplus \mathbf{b} = \mathbf{y}$.

This is not a linear problem!

- But in a suitable algebra, it can be written in a linear like form.
- Max-Plus Algebra: "Linear Algebra, but + becomes max, and \times becomes +".

$$\underbrace{\begin{pmatrix} \mathbf{a}_{1}^{\mathsf{T}}\mathbf{x}_{1} & \mathbf{a}_{2}^{\mathsf{T}}\mathbf{x}_{1} & \dots & \mathbf{a}_{K}^{\mathsf{T}}\mathbf{x}_{1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}_{1}^{\mathsf{T}}\mathbf{x}_{m} & \mathbf{a}_{2}^{\mathsf{T}}\mathbf{x}_{m} & \dots & \mathbf{a}_{K}^{\mathsf{T}}\mathbf{x}_{m} \end{pmatrix}}_{\mathsf{A}} \boxplus \underbrace{\begin{pmatrix} b_{1} \\ b_{2} \\ \vdots \\ b_{K} \end{pmatrix}}_{\mathsf{b}} = \underbrace{\begin{pmatrix} y_{1} \\ \vdots \\ y_{m} \end{pmatrix}}_{\mathsf{y}},$$

where $[\mathbf{C} \boxplus \mathbf{D}]_{ij} = \max_{k=1}^{n} (c_{ik} + d_{kj}).$

• If we assume known slopes, problem reduces to solving a "linear" max-plus matrix equation ${\bf A} \boxplus {\bf b} = {\bf y}.$

Question 1: How to optimally estimate $(\mathbf{a}_j, b_j)_{j=1}^K$ from these equations? \checkmark

Observation

If $b_j = -\infty$, then the maximum will never attain its value on the hyperplane $\mathbf{a}_j^\mathsf{T} \mathbf{x} + b_j \Rightarrow$ The whole region can be discarded.

Observation

If $b_j = -\infty$, then the maximum will never attain its value on the hyperplane $\mathbf{a}_j^\mathsf{T} \mathbf{x} + b_j \Rightarrow$ The whole region can be discarded.

e.g.
$$\max(5x + 3, 20x - \infty, x) = \max(5x + 3, x), \forall x$$

Observation

If $b_j = -\infty$, then the maximum will never attain its value on the hyperplane $\mathbf{a}_j^\mathsf{T} \mathbf{x} + b_j \Rightarrow$ The whole region can be discarded.

e.g.
$$\max(5x + 3, 20x - \infty, x) = \max(5x + 3, x), \forall x$$

Simpler & more robust approximation!

Observation

If $b_j = -\infty$, then the maximum will never attain its value on the hyperplane $\mathbf{a}_j^\mathsf{T} \mathbf{x} + b_j \Rightarrow$ The whole region can be discarded.

e.g.
$$\max(5x + 3, 20x - \infty, x) = \max(5x + 3, x), \forall x$$

Simpler & more robust approximation!

Idea

Force as many b_j as possible to be $-\infty$!

Observation

If $b_j = -\infty$, then the maximum will never attain its value on the hyperplane $\mathbf{a}_j^\mathsf{T} \mathbf{x} + b_j \Rightarrow$ The whole region can be discarded.

e.g.
$$\max(5x + 3, 20x - \infty, x) = \max(5x + 3, x), \forall x$$

Simpler & more robust approximation!

Idea

Force as many b_i as possible to be $-\infty$!

Question 2: How to keep # of hyperplanes as *small* as possible? \checkmark

Convex Regression as an Optimization Problem

Step 1. Enforce **sparsity** constraints - Optimization problem:

$$\arg\min_{b} |\operatorname{supp}(\mathbf{b})|$$

s.t.
$$\mathbf{A} \boxplus \mathbf{b} = \mathbf{y}$$
, where supp $(\mathbf{b}) \triangleq \{j \mid b_j \neq -\infty\}$.

Convex Regression as an Optimization Problem

Step 1. Enforce **sparsity** constraints - Optimization problem:

 $\arg\min_{\mathbf{b}}|\sup(\mathbf{b})|$

s.t. $\mathbf{A} \boxplus \mathbf{b} = \mathbf{y}$, where $supp(\mathbf{b}) \triangleq \{j \mid b_j \neq -\infty\}$.

Step 2. Account for **noise** - Optimization problem:

 $\underset{b}{\operatorname{arg min}} |\operatorname{supp}(\mathbf{b})|$

s.t. dist($\mathbf{A} \boxplus \mathbf{b}, \mathbf{y}$) $\leq \epsilon$.

• Prior work:

• Contributions:

- Prior work:
 - [Tsiamis & Maragos 2019] introduced sparsity in Max-plus algebra.

• Contributions:

- Prior work:
 - [Tsiamis & Maragos 2019] introduced sparsity in Max-plus algebra.
 - [Magnani & Boyd 2009, Kim et. al. 2010, Hannah & Dunson 2011] solve convex regression by alternating between partitioning the input and locally fitting affine functions.

Contributions:

- Prior work:
 - [Tsiamis & Maragos 2019] introduced sparsity in Max-plus algebra.
 - [Magnani & Boyd 2009, Kim et. al. 2010, Hannah & Dunson 2011] solve convex regression by alternating between partitioning the input and locally fitting affine functions.
 - [Maragos & Theodosis 2020] initiated the study of the problem through the lens of Max-plus algebra ⇒ complexity benefits.
- Contributions:

Prior work:

- [Tsiamis & Maragos 2019] introduced sparsity in Max-plus algebra.
- [Magnani & Boyd 2009, Kim et. al. 2010, Hannah & Dunson 2011] solve convex regression by alternating between partitioning the input and locally fitting affine functions.
- [Maragos & Theodosis 2020] initiated the study of the problem through the lens of Max-plus algebra ⇒ complexity benefits.

Contributions:

• Algorithms for sparse approximate solutions to max-plus matrix equations for any ℓ_p norm - Submodularity properties of the optimization problems.

Prior work:

- [Tsiamis & Maragos 2019] introduced sparsity in Max-plus algebra.
- [Magnani & Boyd 2009, Kim et. al. 2010, Hannah & Dunson 2011] solve convex regression by alternating between partitioning the input and locally fitting affine functions.
- [Maragos & Theodosis 2020] initiated the study of the problem through the lens of Max-plus algebra ⇒ complexity benefits.

Contributions:

- Algorithms for sparse approximate solutions to max-plus matrix equations for any ℓ_p norm Submodularity properties of the optimization problems.
- Application into the context of convex regression robust approximations with an approximately *minimum* number of affine regions.

Sparsity in Max-plus algebra

Definition (Sparsity)

We call a vector **x** sparse if it contains many $-\infty$ elements.

Sparsity in Max-plus algebra

Definition (Sparsity)

We call a vector **x** sparse if it contains many $-\infty$ elements.

Definition (Support set)

The *support set* of a vector is the set of indices of its values that are not equal to $-\infty$, that is: $\operatorname{supp}(\mathbf{x}) = \{j \mid x_j \neq -\infty\}$.

e.g.
$$|\text{supp}(1, 4, -\infty, -2, 0, 0)| = 5$$

Sparsity in Max-plus algebra

Definition (Sparsity)

We call a vector **x** sparse if it contains many $-\infty$ elements.

Definition (Support set)

The *support set* of a vector is the set of indices of its values that are not equal to $-\infty$, that is: $\operatorname{supp}(\mathbf{x}) = \{j \mid x_j \neq -\infty\}$.

e.g.
$$|\text{supp}(1, 4, -\infty, -2, 0, 0)| = 5$$

Theorem (Tsiamis & Maragos 2019)

Computing the sparsest solution of $\mathbf{A} \boxplus \mathbf{b} = \mathbf{y}$ is an NP-complete problem.

Sparse Approximate Solutions (1/3)

Problem formulation

$$\begin{split} \arg \min_{\mathbf{b}} &| \mathrm{supp}(\mathbf{b}) | \\ \mathrm{s.t.} & &\| \mathbf{y} - \mathbf{A} \boxplus \mathbf{b} \|_p^p \leq \epsilon, \\ &\mathbf{A} \boxplus \mathbf{b} \leq \mathbf{y}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{y} \in \mathbb{R}^m. \end{split}$$

Sparse Approximate Solutions (1/3)

Problem formulation

$$\begin{split} \arg \min_{\mathbf{b}} &| \mathrm{supp}(\mathbf{b}) | \\ \mathrm{s.t.} & &\| \mathbf{y} - \mathbf{A} \boxplus \mathbf{b} \|_p^p \leq \epsilon, \\ & \mathbf{A} \boxplus \mathbf{b} \leq \mathbf{y}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{y} \in \mathbb{R}^m. \end{split}$$

Notes

- We restrict the ℓ_p , $p < \infty$, error to be small
- We add an extra constraint $\mathbf{A} \boxplus \mathbf{b} \leq \mathbf{y}$: Technical reasons & enforce approximation from below!

Sparse Approximate Solutions (2/3)

Problem formulation

$$\begin{aligned} &\arg\min_{\mathbf{b}}|\mathrm{supp}(\mathbf{b})|\\ &\mathrm{s.t.}\ \|\mathbf{y}-\mathbf{A}\boxplus\mathbf{b}\|_{p}^{p}\leq\epsilon,\\ &\mathbf{A}\boxplus\mathbf{b}<\mathbf{y},\mathbf{A}\in\mathbb{R}^{m\times n},\mathbf{y}\in\mathbb{R}^{m}.\end{aligned} \tag{1}$$

Sparse Approximate Solutions (2/3)

Problem formulation

$$\arg \min_{\mathbf{b}} |\operatorname{supp}(\mathbf{b})|
s.t. \|\mathbf{y} - \mathbf{A} \boxplus \mathbf{b}\|_{p}^{p} \le \epsilon,
\mathbf{A} \boxplus \mathbf{b} \le \mathbf{y}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{y} \in \mathbb{R}^{m}.$$
(1)

Theorem

Problem (1) can be approximately solved in $\mathcal{O}(nm+n^2)$ time with a greedy algorithm.

Sparse Approximate Solutions (2/3)

Problem formulation

$$\arg \min_{\mathbf{b}} |\operatorname{supp}(\mathbf{b})|
s.t. \|\mathbf{y} - \mathbf{A} \boxplus \mathbf{b}\|_{p}^{p} \le \epsilon,
\mathbf{A} \boxplus \mathbf{b} \le \mathbf{y}, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{y} \in \mathbb{R}^{m}.$$
(1)

Theorem

Problem (1) can be approximately solved in $\mathcal{O}(nm + n^2)$ time with a greedy algorithm.

Technical details

Tools from Submodular Optimization \Rightarrow approximation ratio guarantees.

Sparse Approximate Solutions (3/3)

Approximating noise corrupted data from below might be problematic! Is it possible to remove the $\mathbf{A} \boxplus \mathbf{b} < \mathbf{y}$ contraint?

Sparse Approximate Solutions (3/3)

Approximating noise corrupted data from below might be problematic! Is it possible to remove the $\mathbf{A} \boxplus \mathbf{b} < \mathbf{y}$ contraint?

$$\underset{\mathbf{b}}{\arg\min}|\operatorname{supp}(\mathbf{b})|$$
s.t. $\|\mathbf{y} - \mathbf{A} \boxplus \mathbf{b}\|_{\infty} \le \epsilon, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{y} \in \mathbb{R}^{m}.$ (2)

Sparse Approximate Solutions (3/3)

Approximating noise corrupted data from below might be problematic! Is it possible to remove the $A \boxplus b \le y$ contraint?

$$\underset{\mathbf{b}}{\arg\min}|\operatorname{supp}(\mathbf{b})|$$
s.t. $\|\mathbf{y} - \mathbf{A} \boxplus \mathbf{b}\|_{\infty} < \epsilon, \mathbf{A} \in \mathbb{R}^{m \times n}, \mathbf{y} \in \mathbb{R}^{m}.$ (2)

Proposition

We can find a locally optimal solution of Problem (2) by solving Problem (1).

Input: Data $(\mathbf{x}_i, y_i) \in \mathbb{R}^{n+1}$, i = 1, 2, ..., m.

Input: Data $(\mathbf{x}_i, y_i) \in \mathbb{R}^{n+1}$, i = 1, 2, ..., m. Model: $\max(\mathbf{a}_1^\mathsf{T} \mathbf{x}_i + b_1, ..., \mathbf{a}_K^\mathsf{T} \mathbf{x}_i + b_K) = y_i, i = 1, 2, ..., m$.

Input: Data
$$(\mathbf{x}_i, y_i) \in \mathbb{R}^{n+1}$$
, $i = 1, 2, ..., m$.
Model: $\max(\mathbf{a}_1^\mathsf{T} \mathbf{x}_i + b_1, ..., \mathbf{a}_K^\mathsf{T} \mathbf{x}_i + b_K) = y_i, i = 1, 2, ..., m$.

Step 1: Estimate K slopes \mathbf{a}_k :

- Fixed values from an *n*-dimensional interval, or
- Numerical gradients of data.

Input: Data
$$(\mathbf{x}_i, y_i) \in \mathbb{R}^{n+1}$$
, $i = 1, 2, ..., m$.
Model: $\max(\mathbf{a}_1^\mathsf{T} \mathbf{x}_i + b_1, ..., \mathbf{a}_K^\mathsf{T} \mathbf{x}_i + b_K) = y_i, i = 1, 2, ..., m$.

Step 1: Estimate K slopes \mathbf{a}_k :

- Fixed values from an *n*-dimensional interval, or
- Numerical gradients of data.

Step 2: Solve Problem (1) (method called *Sparse Greatest Lower Estimate - SGLE*) or Problem (2) (called *Sparse Minimum Max Absolute Error - SMMAE*), and calculate intercepts b_k .

Input: Data
$$(\mathbf{x}_i, y_i) \in \mathbb{R}^{n+1}$$
, $i = 1, 2, ..., m$.
Model: $\max(\mathbf{a}_1^\mathsf{T} \mathbf{x}_i + b_1, ..., \mathbf{a}_K^\mathsf{T} \mathbf{x}_i + b_K) = y_i, i = 1, 2, ..., m$.

Step 1: Estimate K slopes \mathbf{a}_k :

- Fixed values from an *n*-dimensional interval, or
- Numerical gradients of data.

Step 2: Solve Problem (1) (method called *Sparse Greatest Lower Estimate - SGLE*) or Problem (2) (called *Sparse Minimum Max Absolute Error - SMMAE*), and calculate intercepts b_k .

Complexity: $\mathcal{O}(K^2 + K(n+1)m)$ or $\mathcal{O}(K^2 + K(n+2)m)$, respectively.

Input: Data
$$(\mathbf{x}_i, y_i) \in \mathbb{R}^{n+1}$$
, $i = 1, 2, ..., m$.
Model: $\max(\mathbf{a}_1^\mathsf{T} \mathbf{x}_i + b_1, ..., \mathbf{a}_K^\mathsf{T} \mathbf{x}_i + b_K) = y_i, i = 1, 2, ..., m$.

Step 1: Estimate K slopes \mathbf{a}_k :

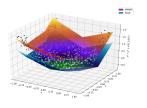
- Fixed values from an *n*-dimensional interval, or
- Numerical gradients of data.

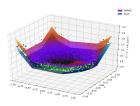
Step 2: Solve Problem (1) (method called *Sparse Greatest Lower Estimate - SGLE*) or Problem (2) (called *Sparse Minimum Max Absolute Error - SMMAE*), and calculate intercepts b_k .

Complexity: $\mathcal{O}(K^2 + K(n+1)m)$ or $\mathcal{O}(K^2 + K(n+2)m)$, respectively.

Output: A PWL convex approximation of the data with the approximately *minimum* number of affine regions needed for achieving the desired level of data fidelity.

Data from noisy paraboloid $z = x^2 + y^2 + \mathcal{N}(0, 1)$.





- (a) Approximation with 5 affine regions.
- (b) Approximation with 16 affine regions.

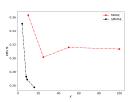


Figure: Comparison of SMMAE method (black line) with [Maragos & Theodosis 2020] (red line).

• Fundamental problem of convex regression through the lens of Max-plus algebra.

- Fundamental problem of convex regression through the lens of Max-plus algebra.
- Theoretical progress in algorithms for sparsity in this nonlinear space.

- Fundamental problem of convex regression through the lens of Max-plus algebra.
- Theoretical progress in algorithms for sparsity in this nonlinear space.
- Application into the problem of convex regression yields more robust estimators.

- Fundamental problem of convex regression through the lens of Max-plus algebra.
- Theoretical progress in algorithms for sparsity in this nonlinear space.
- Application into the problem of convex regression yields more robust estimators.

Future work: Statistical properties of the estimators & Sparsity in more abstract nonlinear spaces with an underlying lattice structure.

- Fundamental problem of convex regression through the lens of Max-plus algebra.
- Theoretical progress in algorithms for sparsity in this nonlinear space.
- Application into the problem of convex regression yields more robust estimators.

Future work: Statistical properties of the estimators & Sparsity in more abstract nonlinear spaces with an underlying lattice structure.

Thank you for your attention!

References



L. A. Hannah and D. B. Dunson. "Multivariate convex regression with adaptive partitioning". In: (2011). arXiv: 1105.1924.



J. Kim, L. Vandenberghe, and C.K.K. Yang. "Convex Piecewise-Linear Modeling Method for Circuit Optimization via Geometric Programming". In: *IEEE Trans. Computer-Aided Design of Integr. Circuits Syst.* 29.11 (Nov. 2010), pp. 1823–1827.



A. Magnani and S. P. Boyd. "Convex piecewise-linear fitting". In: *Optim. Eng.* 10 (2009), pp. 1–17.



P. Maragos. "Morphological Systems: Slope Transforms and Max-Min Difference and Differential Equations". In: *Signal Processing* 38.1 (July 1994), pp. 57–77.



P. Maragos and E. Theodosis. "Multivariate Tropical Regression and Piecewise-Linear Surface Fitting". In: *Proc. IEEE Int'l Conf. on Acoustics, Speech and Signal Processing (ICASSP)*. 2020, pp. 3822–3826.



R. T. Rockafellar. Convex Analysis. Princeton Univ. Press, 1970.



A. Tsiamis and P. Maragos. "Sparsity in Max-plus Algebra". In: *Discrete Events Dynamic Systems* 29 (2019), pp. 163–189.