Machine Learning with Tensors for Structured Data

Guillaume Rabusseau

IVADO - McGill University - Reasoning and Learning Lab





RL LAB

June 11, 2018 RIKEN AIP

Supervised Learning:

Supervised Learning:

- Classical learning algorithms assume $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}^p$.
- How to handle input/output structured data?

Supervised Learning:

- Classical learning algorithms assume $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}^p$.
- How to handle input/output structured data?
 - ► Tensor structured data: Images, videos, spatio-temporal data, ...



$$\in \mathbb{R}^{32 \times 32 \times 3} \simeq \mathbb{R}^{3072}$$

Supervised Learning:

Learn $f : \mathcal{X} \to \mathcal{Y}$ from a sample $\{(x_1, y_1), \cdots, (x_N, y_N)\} \subset \mathcal{X} \times \mathcal{Y}$.

- Classical learning algorithms assume $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}^p$.
- How to handle input/output structured data?
 - ► Tensor structured data: Images, videos, spatio-temporal data, ...
 - Discrete structured data: strings, trees, graphs, ...



Guillaume Rabusseau

Supervised Learning:

- Classical learning algorithms assume $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{Y} = \mathbb{R}^p$.
- How to handle input/output structured data?
 - ▶ Tensor structured data: Images, videos, spatio-temporal data, ...
 - Discrete structured data: strings, trees, graphs, ...
- In both cases, one can leverage linear and tensor algebra to design learning algorithms.

Tensors



$$\begin{split} \mathbf{M} \in \mathbb{R}^{d_1 \times d_2} & \mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3} \\ \mathbf{M}_{ij} \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2] & (\mathcal{T}_{ijk}) \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2], k \in [d_3] \end{split}$$

Tensors and Machine Learning

(i) Data has a tensor structure: color image, video, multivariate time series...





(ii) Tensors as parameters of a model: polynomial regression, higher-order RNNs, weighted automata on trees and graphs...



(iii) Tensors as tools: tensor method of moments [Anandkumar et al., 2014], layer compression in neural networks [Novikov et al., 2015], deep learning theoretical analysis [Cohen et al., 2015]...

Contributions

• Low rank regression for tensor data [NIPS'16, arXiv'17]



• Weighted automata for learning with discrete structured data [NIPS'17-a, AISTATS'18, JCSS'18, FoSSaCS'18]



• Tensor Method of Moments [NIPS'17-b, CAP'14]

Outline

- 1 Preliminaries: Tensors and Multilinear Algebra
- 2 Low-Rank Regression with Tensor Responses
- 3 Weighted Automata for Learning with Structured Data
- 4 Conclusion and Future Lines of Research

Tensors



$$\begin{split} \mathbf{M} \in \mathbb{R}^{d_1 \times d_2} & \mathcal{T} \in \mathbb{R}^{d_1 \times d_2 \times d_3} \\ \mathbf{M}_{ij} \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2] & (\mathcal{T}_{ijk}) \in \mathbb{R} \text{ for } i \in [d_1], j \in [d_2], k \in [d_3] \end{split}$$











Matrix product:

$$(\mathsf{AB})_{i_1,i_2} = \sum_k \mathsf{A}_{i_1k} \mathsf{B}_{ki_2}$$









Multilinear Maps

• Liner map $f : \mathbb{R}^d \to \mathbb{R}^p$ maps **x** to $\mathbf{W}\mathbf{x} = \mathbf{W} \times_2 \mathbf{x}$ for some $\mathbf{W} \in \mathbb{R}^{p \times d}$:



Multilinear Maps

• Liner map $f : \mathbb{R}^d \to \mathbb{R}^p$ maps **x** to $\mathbf{W}\mathbf{x} = \mathbf{W} \times_2 \mathbf{x}$ for some $\mathbf{W} \in \mathbb{R}^{p \times d}$:



Multilinear map g: ℝ^d₁ × ℝ^d₂ → ℝ^p maps (u, v) to W ×₂ u ×₃ v for some W ∈ ℝ^{p×d₁×d₂}:



Example: Multilinear Maps in Higher-Order RNNs

• Recurrent Neural Network (RNN):

$$(\mathsf{x}_1,\mathsf{x}_2,\mathsf{x}_3,\cdots)\mapsto (\mathsf{y}_1,\mathsf{y}_2,\mathsf{y}_3,\cdots)$$

• Simple RNN:

$$\mathbf{h}_t = g(\mathbf{U}\mathbf{x}_t + \mathbf{V}\mathbf{h}_{t-1}), \quad \mathbf{y}_t = g(\mathbf{M}\mathbf{h}_t)$$

Example: Multilinear Maps in Higher-Order RNNs

• Recurrent Neural Network (RNN):

$$(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \cdots) \mapsto (\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, \cdots)$$

• Simple RNN:

$$\mathbf{h}_t = g(\mathbf{U}\mathbf{x}_t + \mathbf{V}\mathbf{h}_{t-1}), \quad \mathbf{y}_t = g(\mathbf{M}\mathbf{h}_t)$$

• Second-order RNN [Giles et al., NIPS'90]:

$$\mathbf{h}_t = g(\boldsymbol{\mathcal{W}} \times_2 \mathbf{x}_t \times_3 \mathbf{h}_{t-1})$$

 \rightarrow order 2 multiplicative interactions: $[\mathbf{h}_t]_i = g\left(\sum_{j,k} \mathcal{W}_{ijk}[\mathbf{x}_t]_j[\mathbf{h}_{t-1}]_k\right)$.

Tensor Decomposition Techniques

• Matrix Decomposition:



 $\Rightarrow \operatorname{\mathsf{Rank}} \text{ of } \mathbf{M}: \text{ smallest } R \text{ such that } \mathbf{M} = \mathbf{UV}$ (with $\mathbf{U} \in \mathbb{R}^{m \times R}, \ \mathbf{V} \in \mathbb{R}^{R \times n}$).

Tensor Decomposition Techniques

• Tucker decomposition [Tucker, 1966 / Hitchcock, 1927]:



 $\Rightarrow \text{ Multilinear rank of } \mathcal{T}: \text{ smallest } (R_1, R_2, R_3) \text{ such that}$ $\mathcal{T} = \mathcal{G} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \mathbf{U}_3$

Tensor Decomposition Techniques

• Tucker decomposition [Tucker, 1966 / Hitchcock, 1927]:



 $\Rightarrow \text{ Multilinear rank of } \mathcal{T}: \text{ smallest } (R_1, R_2, R_3) \text{ such that}$ $\mathcal{T} = \mathcal{G} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \mathbf{U}_3$

Outline

Preliminaries: Tensors and Multilinear Algebra

- 2 Low-Rank Regression with Tensor Responses
 - Problem Setting
 - Higher-Order Low-Rank Regression
 - Theoretical Guarantees
 - Experiments
 - Discussion
 - 3 Weighted Automata for Learning with Structured Data
 - Conclusion and Future Lines of Research

Tensor Structured Data

• Data with tensor structure: EEG, hyperspectral images, videos, ...



Problem

Learn $f : \mathbb{R}^{d_0} \to \mathbb{R}^{d_1 \times \cdots \times d_p}$ from $\{(\mathbf{x}^{(n)}, \mathcal{Y}^{(n)})\}_{n=1}^N$ where $\mathcal{Y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.

Problem

Learn $f : \mathbb{R}^{d_0} \to \mathbb{R}^{d_1 \times \cdots \times d_p}$ from $\{(\mathbf{x}^{(n)}, \mathcal{Y}^{(n)})\}_{n=1}^N$ where $\mathcal{Y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.

• Multilinear Multitask Learning [Romera-Paredes et al., 2013]

 $f(\mathbf{x}) \in \mathbb{R}^{(\mathsf{Restaurant Critics}) imes (\mathsf{Evaluation Criteria})}$

Rest. 1	Critic 1	Critic 2	Critic 3
food quality	5	3	6
service quality	7	8	6.5
overall rating	5	6.5	4
	I		
Rest. 2	Critic 1	Critic 2	Critic 3
food quality	7	8	6
service quality	8.5	9	9
overall rating	0	0 5	7

. . .

Learn $f : \mathbb{R}^d \to \mathbb{R}^p$ from samples $\{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$ where $\mathbf{y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.



• Linear model: $f(\mathbf{x}) = \mathbf{W}^{\top}\mathbf{x}$ $(\mathbf{W} \in \mathbb{R}^{d \times p})$

Learn $f : \mathbb{R}^d \to \mathbb{R}^p$ from samples $\{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$ where $\mathbf{y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.



• Linear model:
$$f(\mathbf{x}) = \mathbf{W}^{ op} \mathbf{x}$$

$$\hat{\mathbf{W}} = \operatorname*{arg\,min}_{\mathbf{W} \in \mathbb{R}^{d \times p}} \|\mathbf{X}\mathbf{W} - \mathbf{Y}\|_{F}^{2} \qquad (\mathbf{X} \in \mathbb{R}^{N \times d}, \mathbf{Y} \in \mathbb{R}^{N \times p})$$

 $(\mathbf{W} \in \mathbb{R}^{d \times p})$

Learn $f : \mathbb{R}^d \to \mathbb{R}^p$ from samples $\{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$ where $\mathbf{y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.



• Linear model:
$$f(\mathbf{x}) = \mathbf{W}^{ op} \mathbf{x}$$
 $(\mathbf{W} \in \mathbb{R}^{d imes p})$

• Ordinary Least Squares

$$\hat{\mathbf{W}} = \operatorname*{arg\,min}_{\mathbf{W} \in \mathbb{R}^{d \times p}} \|\mathbf{X}\mathbf{W} - \mathbf{Y}\|_{F}^{2} \qquad (\mathbf{X} \in \mathbb{R}^{N \times d}, \mathbf{Y} \in \mathbb{R}^{N \times p})$$

 \Rightarrow Equivalent to perform *p* independent linear regressions! How can we capture linear dependencies in the output?

Learn $f : \mathbb{R}^d \to \mathbb{R}^p$ from samples $\{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^N$ where $\mathbf{y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.



• Linear model:
$$f(\mathbf{x}) = \mathbf{W}^{ op} \mathbf{x}$$
 $(\mathbf{W} \in \mathbb{R}^{d imes p})$

• Ordinary Least Squares

$$\hat{\mathbf{W}} = \operatorname*{arg\,min}_{\mathbf{W} \in \mathbb{R}^{d \times p}} \|\mathbf{X}\mathbf{W} - \mathbf{Y}\|_{F}^{2} \qquad (\mathbf{X} \in \mathbb{R}^{N \times d}, \mathbf{Y} \in \mathbb{R}^{N \times p})$$

• Reduced Rank Regression (Izenman, 1975)

$$\hat{\mathbf{W}} = \underset{\mathbf{W} \in \mathbb{R}^{d \times p}}{\arg \min} \|\mathbf{X}\mathbf{W} - \mathbf{Y}\|_{F}^{2} \quad \text{s.t. } \operatorname{rank}(\mathbf{W}) \leq R$$

Tensor-valued Regression

Learn $f : \mathbb{R}^{d_0} \to \mathbb{R}^{d_1 \times d_2}$ from $\{(\mathbf{x}^{(n)}, \mathcal{Y}^{(n)})\}_{n=1}^N$ where $\mathcal{Y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.



Tensor-valued Regression

Learn $f : \mathbb{R}^{d_0} \to \mathbb{R}^{d_1 \times d_2}$ from $\{(\mathbf{x}^{(n)}, \mathcal{Y}^{(n)})\}_{n=1}^N$ where $\mathcal{Y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.



• Vectorize outputs and use reduced rank regression?

 \rightarrow Need to capture higher order dependencies: multilinear rank constraint.

Tensor-valued Regression [GR, H. Kadri, NIPS'16]

Learn $f : \mathbb{R}^{d_0} \to \mathbb{R}^{d_1 \times d_2}$ from $\{(\mathbf{x}^{(n)}, \mathcal{Y}^{(n)})\}_{n=1}^N$ where $\mathcal{Y}^{(n)} \simeq f(\mathbf{x}^{(n)})$. $(iii) \quad (iii) \quad (ii$

• Linear model: $f(\mathbf{x}) = \mathcal{W} imes_1 \mathbf{x}$ $(\mathcal{W} \in \mathbb{R}^{d_0 imes d_1 imes d_2})$

Tensor-valued Regression [GR, H. Kadri, NIPS'16]

Learn $f : \mathbb{R}^{d_0} \to \mathbb{R}^{d_1 \times d_2}$ from $\{(\mathbf{x}^{(n)}, \mathcal{Y}^{(n)})\}_{n=1}^N$ where $\mathcal{Y}^{(n)} \simeq f(\mathbf{x}^{(n)})$.



- Linear model: $f(\mathbf{x}) = \mathbf{\mathcal{W}} \times_1 \mathbf{x}$ $(\mathbf{\mathcal{W}} \in \mathbb{R}^{d_0 \times d_1 \times d_2})$
- Low-Rank Regression for Tensor Structured Response

 $\underset{\mathcal{W} \in \mathbb{R}^{d_0 \times d_1 \times d_2}}{\operatorname{arg\,min}} \| \mathcal{W} \times_1 \mathbf{X} - \mathcal{Y} \|_F^2 \quad \text{ s.t. } \operatorname{rank}_{\mathit{ml}}(\mathcal{W}) \leq (\mathit{R}_0, \mathit{R}_1, \mathit{R}_2)$

Solving the Minimization Problem [GR, H. Kadri, NIPS'16]

Problem

$$rgmin_{\mathcal{W}\in\mathbb{R}^{d_0 imes d_1 imes d_2}} \|\mathcal{W} imes_1\mathbf{X}-\mathcal{Y}\|_F^2$$

s.t. $\operatorname{rank}_{ml}(\mathcal{W}) \leq (R_0, R_1, R_2)$

Solving the Minimization Problem [GR, H. Kadri, NIPS'16]

Problem

$$\underset{\mathcal{W} \in \mathbb{R}^{d_0 \times d_1 \times d_2}}{\operatorname{arg\,min}} \| \mathcal{W} \times_1 \mathbf{X} - \mathcal{Y} \|_F^2 \qquad s.t. \operatorname{rank}_{ml}(\mathcal{W}) \leq (R_0, R_1, R_2)$$

is equivalent to:

Problem

 $\underset{\mathsf{U}_0,\mathsf{U}_1,\mathsf{U}_2}{\arg\min \|\boldsymbol{\mathcal{Y}}\times_1\boldsymbol{\Pi}_0\times_2\boldsymbol{\Pi}_1\times_3\boldsymbol{\Pi}_2-\boldsymbol{\mathcal{Y}}\|_F^2} \qquad w.r.t. \ \mathbf{U}_i\in\mathbb{R}^{d_i\times R_i}$

s.t. $\mathbf{U}_i^{\top} \mathbf{U}_i = \mathbf{I}$ for $0 \le i \le 2$, $\mathbf{\Pi}_0 = \mathbf{X} \mathbf{U}_0 \left(\mathbf{U}_0^{\top} \mathbf{X}^{\top} \mathbf{X} \mathbf{U}_0 \right)^{-1} \mathbf{U}_0^{\top} \mathbf{X}^{\top}$, $\mathbf{\Pi}_i = \mathbf{U}_i \mathbf{U}_i^{\top}$ for i = 1, 2

- Find 3 low-dimensional subspaces U_0, U_1, U_2 such that projecting \mathcal{Y} along the corresponding modes is close to \mathcal{Y} .
- NP-hard... Solve $\arg \min_{U_i} \| \boldsymbol{\mathcal{Y}} \times_{i+1} \boldsymbol{\Pi}_i \boldsymbol{\mathcal{Y}} \|_F^2$ instead.
Theoretical Guarantees [GR, H. Kadri, NIPS'16]

Problem

$$(*) \underset{\mathcal{W} \in \mathbb{R}^{d_0 \times d_1 \times d_2}}{\operatorname{arg\,min}} \| \mathcal{W} \times_1 \mathbf{X} - \mathcal{Y} \|_F^2 \qquad s.t. \operatorname{rank}_{m/}(\mathcal{W}) \leq (R_0, R_1, R_2)$$

HOLRR is an order 3 approximation algorithm:

Theorem

Let \mathcal{W}^* be a solution of (*) and let $\hat{\mathcal{W}}$ be the regression tensor returned by HOLRR. Then,

$$\|\hat{\boldsymbol{\mathcal{W}}} imes_1 \boldsymbol{\mathsf{X}}-\boldsymbol{\mathcal{Y}}\|_F^2 \leq 3\|\boldsymbol{\mathcal{W}}^* imes_1 \boldsymbol{\mathsf{X}}-\boldsymbol{\mathcal{Y}}\|_F^2.$$

Theoretical Guarantees (cont'd) [GR, H. Kadri, NIPS'16]

Problem

$$(*) \underset{\boldsymbol{\mathcal{W}} \in \mathbb{R}^{d_0 \times d_1 \times d_2}}{\operatorname{arg\,min}} \| \boldsymbol{\mathcal{W}} \times_1 \boldsymbol{\mathsf{X}} - \boldsymbol{\mathcal{Y}} \|_F^2 \qquad s.t. \operatorname{rank}_{ml}(\boldsymbol{\mathcal{W}}) \leq (R_0, R_1, R_2)$$

• HOLRR is statistically consistent

Theoretical Guarantees (cont'd) [GR, H. Kadri, NIPS'16]

Problem

$$(*) \underset{\boldsymbol{\mathcal{W}} \in \mathbb{R}^{d_0 \times d_1 \times d_2}}{\operatorname{arg\,min}} \| \boldsymbol{\mathcal{W}} \times_1 \boldsymbol{\mathsf{X}} - \boldsymbol{\mathcal{Y}} \|_F^2 \qquad \textit{s.t.} \ \operatorname{rank}_{\textit{ml}}(\boldsymbol{\mathcal{W}}) \leq (R_0, R_1, R_2)$$

- HOLRR is statistically consistent
- Generalization bound for the class of functions

$$\mathcal{F}_{ml} = \left\{ \mathbf{x} \mapsto \mathcal{W} \times_1 \mathbf{x} : \operatorname{rank}_{ml}(\mathcal{W}) = (R_0, R_1, R_2) \right\}.$$

 $\rightarrow \text{ VC-dimension of } \mathcal{F}_{ml} \text{ is in } \mathcal{O}\left(\sqrt{R_0R_1R_2\log(d_1d_2d_3)}\right) \text{ instead of } \mathcal{O}\left(\sqrt{d_1d_2d_3}\right).$

Image Reconstruction from Noisy Measurements

- $\boldsymbol{\mathcal{W}} \in \mathbb{R}^{3 \times 50 \times 50}$ is an RGB image.
- Data is generated by $\mathbf{Y} = \mathcal{W} \times_1 \mathbf{x} + \boldsymbol{\xi}$ where $\mathbf{x} \sim \mathcal{N}(0, \mathbf{I})$ and $\boldsymbol{\xi}_{ij} \sim \mathcal{N}(0, 1)$.
- Training set of size 200.



Experiments on Real Data



Figure: Task: predict meteorological variables in different locations from their values in the preceding 3 time steps (average over 10 runs). Output is of size 17×125 for CCDS and $5 \times 16 \times 5$ for METEO-UK.

Discussion

- Multilinear extension of low/reduced-rank regression.
- Approximation algorithm rather than convex relaxation.
- Kernel extension \rightarrow nonlinear setting.
- Fast, efficient, theoretical guarantees.

Discussion

- Multilinear extension of low/reduced-rank regression.
- Approximation algorithm rather than convex relaxation.
- Kernel extension \rightarrow nonlinear setting.
- Fast, efficient, theoretical guarantees.

```
Leverage the tensor structure \Rightarrow \begin{cases} faster algorithms \\ better sample efficiency \end{cases}
```

Outline

Preliminaries: Tensors and Multilinear Algebra

- 2 Low-Rank Regression with Tensor Responses
- 3 Weighted Automata for Learning with Structured Data
 - Weighted Automata (WA) and Spectral Learning
 - Connections betweens WAs and RNNs
 - Beyond Strings and Trees: Graph Weighted Models

4 Conclusion and Future Lines of Research

Problem Statement

• How can one learn with structured objects such as strings and trees?



• Intersection of Theoretical Computer Science and Machine Learning...

Problem Statement

• How can one learn with structured objects such as strings and trees?



Intersection of Theoretical Computer Science and Machine Learning...

→ Weighted Automata: robust model to represent functions defined over structured objects (for example probability distributions).

Problem Statement

• How can one learn with structured objects such as strings and trees?



Intersection of Theoretical Computer Science and Machine Learning...

- → Weighted Automata: robust model to represent functions defined over structured objects (for example probability distributions).
 - String Weighted Automata (WA): generalize *Hidden Markov Models*, *Predictive State Representations* and closely related to *RNNs*.

String Weighted Automata (WA)

- Σ a finite alphabet (e.g. $\{a, b\}$), Σ^* strings on Σ (e.g. *abba*)
- A WA computes a function $f: \Sigma^* \to \mathbb{R}$

String Weighted Automata (WA)

- Σ a finite alphabet (e.g. $\{a, b\}$), Σ^* strings on Σ (e.g. *abba*)
- A WA computes a function $f: \Sigma^* \to \mathbb{R}$
- Weighted Automaton: $A = (oldsymbol{lpha}, \{oldsymbol{A}^\sigma\}_{\sigma\in\Sigma}, oldsymbol{\omega})$ where

$$\begin{split} & \boldsymbol{\alpha} \in \mathbb{R}^n \text{ initial weights vector} \\ & \boldsymbol{\omega} \in \mathbb{R}^n \text{ final weights vector} \\ & \mathbf{A}^{\sigma} \in \mathbb{R}^{n \times n} \text{ transition weights matrix for each } \sigma \in \boldsymbol{\Sigma} \end{split}$$

String Weighted Automata (WA)

- Σ a finite alphabet (e.g. $\{a, b\}$), Σ^* strings on Σ (e.g. *abba*)
- A WA computes a function $f: \Sigma^* \to \mathbb{R}$
- Weighted Automaton: $A = (\alpha, \{\mathbf{A}^\sigma\}_{\sigma \in \Sigma}, \omega)$ where

$$\begin{split} & \boldsymbol{\alpha} \in \mathbb{R}^n \text{ initial weights vector} \\ & \boldsymbol{\omega} \in \mathbb{R}^n \text{ final weights vector} \\ & \mathbf{A}^{\sigma} \in \mathbb{R}^{n \times n} \text{ transition weights matrix for each } \boldsymbol{\sigma} \in \boldsymbol{\Sigma} \end{split}$$

• A computes a function $f_A : \Sigma^* \to \mathbb{R}$ defined by

$$f_{\mathcal{A}}(\sigma_1\sigma_2\cdots\sigma_k)=\alpha^{\top}\mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_k}\boldsymbol{\omega}$$



Weighted Automata and Representation Learning



• A WA induces a mapping $\phi: \Sigma^* \to \mathbb{R}^n \ (\sim \text{ word embedding})$

Weighted Automata and Representation Learning



- A WA induces a mapping $\phi: \Sigma^* \to \mathbb{R}^n \ (\sim \text{ word embedding})$
- The mapping ϕ is compositional:

$$\phi(\lambda) = \boldsymbol{\alpha}^{\top}, \ \phi(\sigma_1) = \boldsymbol{\alpha}^{\top} \mathbf{A}^{\sigma_1}, \ \phi(\sigma_1 \sigma_2) = \boldsymbol{\alpha}^{\top} \mathbf{A}^{\sigma_1} \mathbf{A}^{\sigma_2} = \phi(\sigma_1) \mathbf{A}^{\sigma_2}, \ \dots$$

Weighted Automata and Representation Learning



- A WA induces a mapping $\phi: \Sigma^* \to \mathbb{R}^n \ (\sim \text{ word embedding})$
- The mapping ϕ is compositional:

$$\phi(\lambda) = \boldsymbol{\alpha}^{\top}, \ \phi(\sigma_1) = \boldsymbol{\alpha}^{\top} \mathbf{A}^{\sigma_1}, \ \phi(\sigma_1 \sigma_2) = \boldsymbol{\alpha}^{\top} \mathbf{A}^{\sigma_1} \mathbf{A}^{\sigma_2} = \phi(\sigma_1) \mathbf{A}^{\sigma_2}, \ \dots$$

• The output $f_A(x) = \langle \phi(x), \omega \rangle$ is linear in $\phi(x)$.

• $\mathbf{H}_f \in \mathbb{R}^{\Sigma^* \times \Sigma^*}$: Hankel matrix of $f : \Sigma^* \to \mathbb{R}$

Definition: prefix p, suffix $s \Rightarrow (\mathbf{H}_f)_{p,s} = f(ps)$

• $\mathbf{H}_f \in \mathbb{R}^{\Sigma^* \times \Sigma^*}$: Hankel matrix of $f : \Sigma^* \to \mathbb{R}$

Definition: prefix p, suffix $s \Rightarrow (\mathbf{H}_f)_{p,s} = f(ps)$

• Fundamental theorem [Carlyle and Paz, 1971; Fliess 1974]:

 $\operatorname{rank}(\mathbf{H}_f) < \infty \iff f$ can be computed by a WA

• $\mathbf{H}_f \in \mathbb{R}^{\Sigma^* \times \Sigma^*}$: Hankel matrix of $f : \Sigma^* \to \mathbb{R}$

Definition: prefix p, suffix $s \Rightarrow (\mathbf{H}_f)_{p,s} = f(ps)$

• Fundamental theorem [Carlyle and Paz, 1971; Fliess 1974]:

 $\operatorname{rank}(\mathbf{H}_f) < \infty \iff f$ can be computed by a WA

- Proof is constructive ⇒ Spectral Learning of WA:
 - 1. Estimate a sub-block of \mathbf{H}_f from training data
 - 2. Low rank decomposition **H** \simeq **PS**
 - 3. Build WA \hat{A} using **H**, **P** and **S**.
- \rightarrow Efficient and consistent learning algorithms for weighted automata [Hsu et al., 2009; Bailly et al. 2009; Balle et al., 2014, ...].

Connections betweens WAs and RNNs

Weighted Automata and Recurrent Neural Networks

• Recall that the hidden state of a second-order RNN (2-RNN) is computed by

$$\mathbf{h}_t = g(\boldsymbol{\mathcal{W}} \times_2 \mathbf{x}_t \times_3 \mathbf{h}_{t-1})$$

Weighted Automata and Recurrent Neural Networks

• Recall that the hidden state of a second-order RNN (2-RNN) is computed by

$$\mathbf{h}_t = g(\boldsymbol{\mathcal{W}} \times_2 \mathbf{x}_t \times_3 \mathbf{h}_{t-1})$$

• Similarly, the feature map of a WA $(lpha,\{{f A}^\sigma\}_{\sigma\in\Sigma},\omega)$ can be written as

$$\phi(x\sigma) = \mathcal{A} \times_2 \mathbf{e}_{\sigma} \times_3 \phi(x)$$

where

- $\boldsymbol{\mathcal{A}} \in \mathbb{R}^{n imes \Sigma imes n}$ is defined by $\boldsymbol{\mathcal{A}}_{:,\sigma,:} = (\boldsymbol{\mathsf{A}}^{\sigma})^{\top}$,
- \mathbf{e}_{σ} is the one-hot encoding of σ .

• For sequences of discrete symbols, WAs and second-order RNNs with linear activation functions are equivalent!

- For sequences of discrete symbols, WAs and second-order RNNs with linear activation functions are equivalent!
- \Rightarrow For the discrete case, the spectral learning algorithm is a consistent learning algorithm for linear second-order RNNs.

- For sequences of discrete symbols, WAs and second-order RNNs with linear activation functions are equivalent!
- ⇒ For the discrete case, the spectral learning algorithm is a consistent learning algorithm for linear second-order RNNs.
 - What about sequences of continuous vectors?
 - $\rightarrow\,$ Can we extend the spectral learning algorithm to linear 2-RNNs defined over continuous vectors?

- For sequences of discrete symbols, WAs and second-order RNNs with linear activation functions are equivalent!
- \Rightarrow For the discrete case, the spectral learning algorithm is a consistent learning algorithm for linear second-order RNNs.
 - What about sequences of continuous vectors?
 - $\rightarrow\,$ Can we extend the spectral learning algorithm to linear 2-RNNs defined over continuous vectors?
 - YES! By leveraging multilinear properties of linear RNNs and tensor sensing techniques.

WA A = (α, {A^σ}_{σ∈Σ}, ω): linear transition maps and linear termination function...

- WA A = (α, {A^σ}_{σ∈Σ}, ω): linear transition maps and linear termination function...
- Non-linear Weighted Automaton: $(\alpha, \{G_{\sigma}\}_{\sigma \in \Sigma}, F)$
 - α is the initial latent state
 - $G_{\sigma}: \mathbb{R}^n \to \mathbb{R}^n$ are non-linear transition maps
 - $F : \mathbb{R}^n \to \mathbb{R}$ is a non-linear termination function

$$f(\sigma_1\sigma_2\cdots\sigma_k)=F(G_{\sigma_k}(\cdots G_{\sigma_2}(G_{\sigma_1}(\alpha))\cdots)$$

(\simeq RNNs with one-hot encoding of the inputs)

- WA A = (α, {A^σ}_{σ∈Σ}, ω): linear transition maps and linear termination function...
- Non-linear Weighted Automaton: $(\alpha, \{G_{\sigma}\}_{\sigma \in \Sigma}, F)$
 - α is the initial latent state
 - $G_{\sigma}: \mathbb{R}^n \to \mathbb{R}^n$ are non-linear transition maps
 - $F : \mathbb{R}^n \to \mathbb{R}$ is a non-linear termination function

$$f(\sigma_1\sigma_2\cdots\sigma_k)=F(G_{\sigma_k}(\cdots G_{\sigma_2}(G_{\sigma_1}(\alpha))\cdots)$$

(\simeq RNNs with one-hot encoding of the inputs)

Two-stage learning algorithm:

- ► Learning $\phi: \Sigma^* \to \mathbb{R}^n$ using an encoder-decoder network to non-linearly decompose the Hankel matrix \mathbf{H}_f .
- Learning G_{σ} : feed-forward neural networks.

- Experiments on Penn Tree Bank data: 5,987 sentences over an alphabet of 33 symbols.
- Two evaluation metrics:

Table: Pautomac Score (\sim	perplexity)	on test data.
--------------------------------	-------------	---------------

Sample Size	SP	EM	RNN	NL-WA
1000	9.098	4.252	4.765	2.937
2000	4.995	3.723	4.6053	2.923
3000	4.532	3.570	4.398	2.894
4000	4.235	3.542	4.244	2.880
ALL	4.234	3.496	4.191	2.748

Table: Word error rate (one-step ahead prediction) on test data.

S	Sample Size	SP	EM	RNN	NL-WA
	1000	0.8432	0.808	0.806	0.7630
	2000	0.8342	0.793	0.788	0.7332
	3000	0.8195	0.781	0.736	0.7134
	4000	0.8141	0.776	0.692	0.6935
	ALL	0.8033	0.753	0.669	0.6831

Beyond Strings and Trees

A Look Back on String Weighted Automata

A Weighted Automaton $A = (\alpha, \{\mathbf{A}^{\sigma}\}_{\sigma \in \Sigma}, \omega)$ computes a function $f_A : \Sigma^* \to \mathbb{R}$ defined by

$$f_{A}(\sigma_{1}\sigma_{2}\cdots\sigma_{k})= \boldsymbol{\alpha}^{ op}\mathbf{A}^{\sigma_{1}}\mathbf{A}^{\sigma_{2}}\cdots\mathbf{A}^{\sigma_{k}}\boldsymbol{\omega}$$



Beyond Strings: Weighted Tree Automata

• A weighted tree automaton (WTA) is a tuple $A = \langle \alpha, \mathcal{T}, \{\omega_{\sigma}\}_{\sigma \in \Sigma} \rangle$

 $\alpha \in \mathbb{R}^n$: vector of initial weights $\mathcal{T} \in \mathbb{R}^{n \times n \times n}$: tensor of transition weights $\omega_{\sigma} \in \mathbb{R}^n$: vector of final weights associated with $\sigma \in \Sigma$

• A WTA computes a function $f_A : \mathfrak{T}_{\Sigma} \to \mathbb{R}$.



ML, Tensors & Structured Data

Graph Weighted Models [R. Bailly*, GR*, F. Denis, LATA'15/JCSS'18]

•
$$\mathcal{F} = \{a(\cdot), h(\cdot, \cdot), g(\cdot, \cdot, \cdot)\}$$

 v_1
 h^{1}
 v_2
 v_3
 v_4
 v_4

Figure: A graph on the ranked alphabet $\mathcal{F} = \{a(\cdot), h(\cdot, \cdot), g(\cdot, \cdot, \cdot)\}$.

n
•
$$\mathcal{F} = \{a(\cdot), h(\cdot, \cdot), g(\cdot, \cdot, \cdot)\}$$

 v_1
 h^1
 v_2
 v_3
 v_4

Figure: A graph on the ranked alphabet $\mathcal{F} = \{a(\cdot), h(\cdot, \cdot), g(\cdot, \cdot, \cdot)\}.$

• GWM: vector $\mathcal{M}^a \in \mathbb{R}^n$, matrix $\mathcal{M}^h \in \mathbb{R}^{n \times n}$, tensor $\mathcal{M}^g \in \mathbb{R}^{n \times n \times n}$

•
$$\mathcal{F} = \{a(\cdot), h(\cdot, \cdot), g(\cdot, \cdot, \cdot)\}$$

• GWM: vector $\mathcal{M}^a \in \mathbb{R}^n$, matrix $\mathcal{M}^h \in \mathbb{R}^{n \times n}$, tensor $\mathcal{M}^g \in \mathbb{R}^{n \times n \times n}$



•
$$\mathcal{F} = \{\alpha(\cdot), a(\cdot, \cdot), b(\cdot, \cdot), \omega(\cdot)\}$$

• GWM: $\mathcal{M}^{lpha}, \mathcal{M}^{\omega} \in \mathbb{R}^n$, $\mathcal{M}^a, \mathcal{M}^b \in \mathbb{R}^{n imes n}$



- $\mathcal{F} = \{a(\cdot, \cdot), b(\cdot, \cdot)\}$
- GWM: $\mathbf{M}^{a}, \mathbf{M}^{b} \in \mathbb{R}^{n \times n}$



Learning Graph Weighted Models

- Long term objective: extend the spectral learning algorithm to functions defined over graphs.
 - $\rightarrow\,$ learning general GWMs is very challenging.
- First step: study the problem of learning GWMs defined over simple families of graphs (circular strings, 2D grids).
- Minimization of GWMs over circular strings [GR, FoSSaCS'18]:
 - Minimizing WA \leftrightarrow linear algebra
 - Minimizing GWMs \leftrightarrow theory of finite dimensional algebras

Outline

- 1 Preliminaries: Tensors and Multilinear Algebra
- 2 Low-Rank Regression with Tensor Responses
- 3 Weighted Automata for Learning with Structured Data
- 4 Conclusion and Future Lines of Research

Conclusion

- Spectral methods for tensor and discrete structured data.
- \Rightarrow Leverage fundamental algebraic properties for learning:
 - Take tensor structure into account for better generalization.
 - Learning for structured data with weighted automata.
 - ► Spectral learning: efficient and consistent learning algorithms.

Multilinear algebra \leftrightarrow powerful models for learning with structured data.

Future Research Directions

- Learning with graphs.
 - Develop efficient learning algorithms for graph structured data.
 - Spectral learning of GWM \Rightarrow consistent learning algorithm.
 - Explore connections with graph neural networks (TCS insight).

Future Research Directions

• Learning with graphs.

- Develop efficient learning algorithms for graph structured data.
- Spectral learning of GWM \Rightarrow consistent learning algorithm.
- Explore connections with graph neural networks (TCS insight).
- Fast and scalable learning algorithms.
 - Tensor networks have been successfully used in numerical analysis and quantum physics to perform very large scale linear algebra.
 - Wide range of potential applications in ML.

Future Research Directions

• Learning with graphs.

- Develop efficient learning algorithms for graph structured data.
- Spectral learning of GWM \Rightarrow consistent learning algorithm.
- Explore connections with graph neural networks (TCS insight).

• Fast and scalable learning algorithms.

- Tensor networks have been successfully used in numerical analysis and quantum physics to perform very large scale linear algebra.
- Wide range of potential applications in ML.

• Nonlinear tensor learning.

- Combine the power of tensor algebra and deep learning.
- Revisit higher-order RNN through the lens of multilinear algebra.
- Both directions, e.g. non-linear extensions of tensor decomposition techniques / multilinear regularization in deep networks.

Thank you for your attention.

Image Reconstruction from Noisy Measurements

- $\boldsymbol{\mathcal{W}} \in \mathbb{R}^{3 \times 50 \times 50}$ is an RGB image.
- Data is generated by $\mathbf{Y} = \mathbf{W} \times_1 \mathbf{x} + \boldsymbol{\xi}$ where $\mathbf{x} \sim \mathcal{N}(0, \mathbf{I})$ and $\boldsymbol{\xi}_{ij} \sim \mathcal{N}(0, 1)$.
- Training set of size 200.



Image Reconstruction from Noisy Measurements

• $\boldsymbol{\mathcal{W}} \in \mathbb{R}^{3 \times 70 \times 70}$ is an RGB image.



Izenman, A. J. (1975). Reduced-rank regression for the multivariate linear model. *Journal of Multivariate Analysis*, 5(2):248–264.