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Training convolutional neural networks for biomedical data analysis: a tensor based approach

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Outline

PhD Purpose

Tensor-based training

Conclusion & Perspectives



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PhD

Multimodal analysis of Biomedical Data

- Funding: IDEX UCA^{JEDI}
- Project: Intégration et Analyse de Données Biomédicales (IADB)
- Mission: Extract biomarkers within workflow \rightarrow
- Multimodality:





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From Multimodality to Deep Learning for Biomedical Data analysis

- Deep learning (DL) widely used in computer vision and biomedical data analysis
- Convolutional Neural Networks (CNN) success: ad hoc, empirical design
 - Deep Convolutional Neural Networks and Learning ECG Features for Screening Paroxysmal Atrial Fibrillation Patients¹

	hand-crafted	end-to-end CNN	conv+KNN	conv+SVM
CCR^2 (%)	82	85	91	87



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Classical training of NN

Ad hoc success of NNs: problems of training/convergence of numerical optimization algorithms \rightarrow estimation $\theta = ?$



- \exists Challenges in Neural Network Optimization Optimization ³:
 - ill conditioning, local minima, long term dependencies ...



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Tensor based training of NNs

Estimate optimal neural network (NN) parameters: Tensor Decomposition (TD).





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Equivalence between Convolutional Arithmetic Circuits (ConvAC) architecture and tensor factorization

Estimate ConvAC parameters through tensor decomposition.

∃ Equivalence between network architecture and tensor factorization: Shallow networks (SN) ⇔ CP (rank-1) decomposition Deep network (DN) ⇔ Hierarchical Tucker decomposition (HT)

Theoretical formulation of expressive power: efficiency & <u>inductive bias</u> [Cohen, 2015-2017]



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ConvAC



• task: classifying an instance $X = (x_1, \dots, x_N)$ into categories $\mathcal{Y} := \{1, \dots, Y\}$

 x_1, \ldots, x_N patches around pixels, $x_i \in \mathbb{R}^s$

- score function: $\{h_y\}_{y \in \mathcal{Y}}$
- representation functions: $f_{\theta_1} \dots f_{\theta_M}$: $\mathbb{R}^s \to \mathbb{R}$

ConvAC Vs. SimNet

$$\underset{i=1,\dots,n}{MEX_{\xi}\{c_i\}} := \frac{1}{\xi} \log \left(\frac{1}{n} \sum_{i=1}^{n} \exp\{\xi \cdot c_i\}\right)$$



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Shallow ConvAC



⁴ joint decomposition: same vectors $a^{z,i}$ shared across $\forall classes_{v} \land \equiv v \land \equiv v$

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Shallow ConvAC as a tensor

$$h_{y}(x_{1},...,x_{N}) = \sum_{z=1}^{Z} a_{z}^{y} \prod_{i=1}^{N} \left(\sum_{d=1}^{M} a_{d}^{z,i} f_{\theta_{d}}(x_{i}) \right)$$
$$= \sum_{z=1}^{Z} a_{z}^{y} \left(\sum_{d_{1}=1}^{M} a_{d_{1}}^{z,1} f_{\theta_{d_{1}}}(x_{1}) \right)_{1} \dots \left(\sum_{d_{N}=1}^{M} a_{d_{N}}^{z,N} f_{\theta_{d_{N}}}(x_{N}) \right)_{N}$$
$$= \sum_{d_{1},d_{2}...,d_{N}}^{M} \mathcal{A}_{d_{1},...,d_{N}}^{y} \prod_{i=1}^{N} f_{\theta_{d_{i}}}(x_{i})$$



where
$$\mathcal{A}_{d_1,\ldots,d_N}^{y} = \sum_{z=1}^{Z} a_z^{y} a_{d_1}^{z,1} \ldots a_{d_N}^{z,N}$$
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Shallow ConvAC as CPD (1/2)

Canonical polyadic decomposition (CPD):

Tensor A sum of rank-1 tenors \mathcal{A} of dimensions $I_1 \times I_2 \times \cdots \times I_N$ A^n be matrices of size $I_n \times Z$ $a^{z,n}$ the z_{th} column of A^n

$$\mathcal{A} = \sum_{z=1}^{Z} \alpha_z a^{z,1} \otimes \cdots \otimes a^{z,N}, \quad a^{z,i} \in \mathbb{R}^{M_i}$$

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Shallow ConvAC as CPD (2/2)

Canonical polyadic decomposition (CPD):

Tensor ${\mathcal A}$ sum of rank-1 tenors 5

$$\mathcal{A} = \sum_{z=1}^{Z} a_{z} a^{z,1} \otimes \cdots \otimes a^{z,N}, \quad a^{z,i} \in \mathbb{R}^{M_{i}}$$
(3)

$$\mathcal{A}_{d_1,\ldots,d_N} = \sum_{z=1}^{Z} a_z a_{d_1}^{z,1} \ldots a_{d_N}^{z,N}$$
(4)



$$h_{y}(x_{1},...,x_{N}) = \sum_{(d_{1},...,d_{N})}^{M} \mathcal{A}^{y}_{d_{1},...,d_{N}} \prod_{i=1}^{N} f_{\theta_{d_{i}}}(x_{i}), \quad a_{z} := a_{z}^{y} \underbrace{(1, \sum_{\substack{(i \in D \land z \cup R) \\ COTE D \land z \cup R}}}_{\mathbb{C} O T E D \land z \cup R} \underbrace{0}_{\mathbb{C} O T E D \land Z} \underbrace{0}_{\mathbb{C} O T \boxtimes Z} \underbrace{0}_{\mathbb{C$$

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Parameter estimation





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Problem

- 1. Solve a system $h_y(X) = <\mathcal{A}^y, \mathcal{F}_ heta>$ for $y=1,\ldots,Y$ (*)
- 2. Solve (*) for a \bigcirc of input signals

Approach

• $\mathcal{A}^{y} = \sum_{z=1}^{Z} \frac{a_{z}^{y}}{a_{z}^{z}} a^{z,1} \otimes \cdots \otimes a^{z,N} \rightarrow \text{estimate } a^{z,i}$

Estimation

- vectorize (*) and solve
 - vec(A^y) = (vec(F_θ)vec(F_θ)')⁻¹vec(F)h_y, through normal equation
 - vec(A^y) through multilinear regression
- coupled CPD(\hat{A}^{y}) for a system y = 1, ..., Y of shared factors $a^{z,i}$'s
- standard convolution: $\forall i = 1 : N, a^{z,i} = a^z$ for z = 1 : Z



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Implementation in progress

- **ConvAC**: Keras is a high-level neural networks API. We introduce product pooling layer & add softmax (decision layer in ConvAC)
- **CPD**: Tensorlab is a Matlab toolbox that provides various tools for tensor computations/decomposition.
- **SimNet** on GitHub (*Caffe, TensorFlow*) Problems if incompatibilities



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Experimental results

- Synthetic data: 2 x random distributions of images 28x28 with μ_1 , σ_1 & μ_2 , σ_2 resp.
- vary $\mu 2$ to assess overlapping
- Divergence "related" to pooling layer





⁶product instability: [Appendix E, Cohen 2016]

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Recap: ConvAC as a tensor

ConvAC: ConvNet, choice of non-linearities:

• classify $X = (x_1, \dots, x_N)$ into categories $\mathcal{Y} := \{1, \dots, Y\}$

$$h_{y}(x_{1},...,x_{N}) = \sum_{(d_{1},...,d_{N})}^{M} \mathcal{A}_{d_{1},...,d_{N}}^{y} \prod_{i=1}^{N} f_{\theta_{d_{i}}}(x_{i})$$
(6)

• \mathcal{A}^{y} CPD of convolution filters.

Set Estimate CNN parameters from tensor characteristics: optimal CPD rank = # conv filters)

 \triangle Computational challenge: exponential number of entries M^N



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Perspectives 1



- 1. Validation: synthetic data & MNIST dataset
- 2. **Application**: biomedical data mainly electrocardiogram (ECG) for arrhythmia characterization, prediction of non recovery after ablation
- Biomarkers within IADB workflow.
 - ? Which biomedical topic, image?
 - ⑦ How to adapt NN design to the application, in practice?



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Perspectives 2

Deep network \Leftrightarrow HT decomposition of \mathcal{A}^{y}

Deep network with size-2 pooling:



corresponds to Hierarchical Tucker (HT) decomposition:

$$\begin{split} \phi^{1,j,\gamma} &= \sum_{\alpha=1}^{n_0} a_{\alpha}^{1,j,\gamma} \cdot \mathbf{a}^{0,2j-1,\alpha} \otimes \mathbf{a}^{0,2j,\alpha} \\ & \cdots \\ \phi^{l,j,\gamma} &= \sum_{\alpha=1}^{n_{-1}} a_{\alpha}^{l,j,\gamma} \cdot \phi^{l-1,2j-1,\alpha} \otimes \phi^{l-1,2j,\alpha} \\ & \cdots \\ \mathcal{A}^{y} &= \sum_{\alpha=1}^{n_{-1}} a_{\alpha}^{L,1,y} \cdot \phi^{l-1,1,\alpha} \otimes \phi^{l-1,2,\alpha} \end{split}$$

⁷The network, dubbed HT model, is universal: $\forall \{A^y\}_y$ represented by **CP** modely active in the represented by **HT** model with only a polynomial penalty in terms of resourcesuce 8 [N.Cohen, 2017]

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Eurasip Summer School

Tensor-Based Signal Processing. August 27 - 31, 2018, Leuven, Belgium





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Shallow ConvAC as a tensor

$$h_{y}(x_{1},...,x_{N}) = \sum_{(d_{1},...,d_{N})} \mathcal{A}_{d_{1},...,d_{N}}^{y} \prod_{i=1}^{N} f_{\theta_{d_{i}}}(x_{i})$$
(7)

 f_{θ} Gaussian / neurons (sigmoid or ReLU)

$$h_{y}(x_{1},...,x_{N}) = \sum_{(d_{1},...,d_{N})}^{M \text{ order of } 100} \mathcal{A}_{d_{1},...,d_{N}}^{y} \prod_{i=1}^{N} f_{\theta_{d_{i}}}(x_{i})$$
(8)

 $\exists \mathcal{A}^{y} \text{ tensor: multi-dimensional array} \\ N: \text{ order of } \mathcal{A}^{y} \\ M: \text{ dimension, } \# \text{ of values and index can take in particular model } i \\ M.N \times \mathcal{A}^{y}_{d_{1}d_{2}...d_{N}} \in \mathbb{R} \text{ entries of } \mathcal{A}^{y}, \text{ for } i \in [N] \text{ and } d \in [M_{i}] \\ \textcircled{0} \quad \underbrace{\mathsf{UNVERSITE}}_{(C) \in \mathcal{O} \times \mathbb{C}^{2}} \\ & \underbrace{\mathsf{UNVERSITE}}_{(C) \in \mathbb$

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Shallow ConvAC as CPD

Canonical polyadic decomposition (CPD): Tensor ${\cal A}$ sum of rank-1 ${\rm tenors}^9$

$$\mathcal{A} = \sum_{z=1}^{Z} a_{z} a^{z,1} \otimes \cdots \otimes a^{z,N}, \quad a^{z,i} \in \mathbb{R}^{M_{i}}$$
(9)

$$\mathcal{A}_{d_1,...,d_N} = \sum_{z=1}^{Z} a_z a_{d_1}^{z,1} \dots a_{d_N}^{z,N}$$
(10)





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Recap: ConvAC as a tensor

ConvAC: convNet, choice of non-linearities:

• classify $X = (x_1, \ldots, x_N)$ into categories $\mathcal{Y} := \{1, \ldots, Y\}$

EXAMPLE X an image, x_1, \ldots, x_N patches around pixels

- score function: $\{h_y\}_{y \in \mathcal{Y}}$
- representation functions $f_{\theta_1} \, \ldots \, f_{\theta_1} \colon \, \mathbb{R}^s \to \mathbb{R}$

$$h_{y}(x_{1},...,x_{N}) = \sum_{(d_{1},...,d_{N})}^{M} \mathcal{A}_{d_{1},...,d_{N}}^{y} \prod_{i=1}^{N} f_{\theta_{d_{i}}}(x_{i})$$
(12)

 A^y CPD of convolution operators / parameters.

 →

 Estimate NN parameters from tensor characteristics(rank, order,

 Image: Strain and Strain an

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SimNet & ConvAC

 In "Appendix E. Computation in Log-Space with SimNets" in paperhttps://arxiv.org/pdf/1509.05009.pdf: Authors suggest not to implementthe ConvAC in a standard way (the way we plan to do it) because of instability derived by product pooling. Instead, they suggest to use their" famous" simnet implementation

