Expressiveness of Convolutional Networks via Hierarchical Tensor Decompositions

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Sources

Deep SimNets
N. Cohen, O. Sharir and A. Shashua
Computer Vision and Pattern Recognition (CVPR) 2016

On the Expressive Power of Deep Learning: A Tensor Analysis
N. Cohen, O. Sharir and A. Shashua
Conference on Learning Theory (COLT) 2016

Convolutional Rectifier Networks as Generalized Tensor Decompositions
N. Cohen and A. Shashua
International Conference on Machine Learning (ICML) 2016

Inductive Bias of Deep Convolutional Networks through Pooling Geometry
N. Cohen and A. Shashua
International Conference on Learning Representations (ICLR) 2017

Tensorial Mixture Models
O. Sharir. R. Tamari, **N. Cohen** and A. Shashua
arXiv preprint 2017

Boosting Dilated Convolutional Networks with Mixed Tensor Decompositions
N. Cohen, R. Tamari and A. Shashua
arXiv preprint 2017

Deep Learning and Quantum Entanglement:
Fundamental Connections with Implications to Network Design
Y. Levine, D. Yakira, **N. Cohen** and A. Shashua
arXiv preprint 2017

Collaborators

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Outline

Statistical Learning Setup

$\mathcal{X}$ – instance space (e.g. $\mathbb{R}^{100\times100}$ for 100-by-100 grayscale images)

$\mathcal{Y}$ – label space (e.g. $\mathbb{R}$ for regression or $[k] := \{1, \ldots, k\}$ for classification)

$\mathcal{D}$ – distribution over $\mathcal{X} \times \mathcal{Y}$ (unknown)

$\ell : \mathcal{Y}\times\mathcal{Y} \rightarrow \mathbb{R}_{\geq 0}$ – loss func (e.g. $\ell(y, \hat{y}) = (y - \hat{y})^2$ for $\mathcal{Y} = \mathbb{R}$)

Task

Given training sample $S = \{(X_1, y_1), \ldots, (X_m, y_m)\}$ drawn i.i.d. from $\mathcal{D}$, return hypothesis (predictor) $h : \mathcal{X} \rightarrow \mathcal{Y}$ that minimizes population loss:

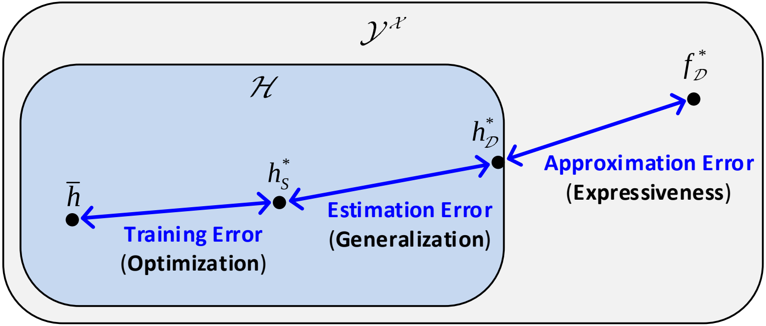
$$L_{\mathcal{D}}(h) := \mathbb{E}_{(X,y)\sim\mathcal{D}}[\ell(y, h(X))]$$

Approach

Predetermine hypotheses space $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$, and return hypothesis $h \in \mathcal{H}$ that minimizes empirical loss:

$$L_S(h) := \mathbb{E}_{(X,y)\sim S}[\ell(y, h(X))] = \frac{1}{m}\sum_{i=1}^{m} \ell(y_i, h(X_i))$$

Three Pillars of Statistical Learning Theory: Expressiveness, Generalization and Optimization



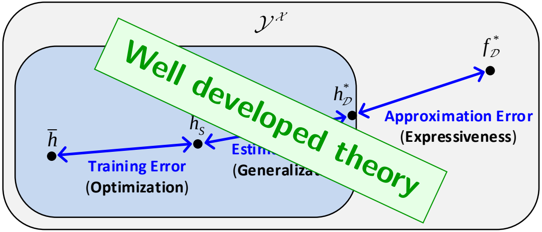
$f^*_{\mathcal{D}}$ – ground truth ($\text{argmin}_{f \in \mathcal{Y}^{\mathcal{X}}} L_{\mathcal{D}}(f)$)

$h^*_{\mathcal{D}}$ – optimal hypothesis ($\text{argmin}_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$)

h^*_S – empirically optimal hypothesis ($\text{argmin}_{h \in \mathcal{H}} L_S(h)$)

$\bar{h}$ – returned hypothesis

Classical Machine Learning



Optimization

Empirical loss minimization is a convex program:

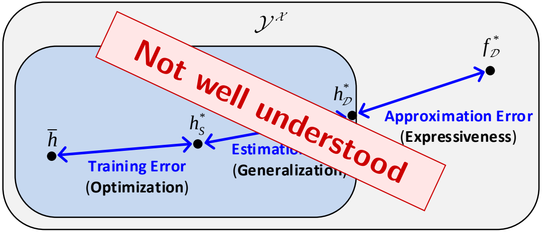
$$\bar{h} \approx h_S^* \quad (\text{ training err} \approx 0 \text{ })$$

Expressiveness & Generalization

Bias-variance trade-off:

$\mathcal{H}$	approximation err	estimation err
expands	$\searrow$	$\nearrow$
shrinks	$\nearrow$	$\searrow$

Deep Learning



Optimization

Empirical loss minimization is a non-convex program:

- h^*_S is not unique – many hypotheses have low training err
- Stochastic Gradient Descent somehow reaches one of these

Expressiveness & Generalization

Vast difference from classical ML:

- Some low training err hypotheses generalize well, others don't
- W/typical data, solution returned by SGD often generalizes well
- Expanding $\mathcal{H}$ reduces approximation err, but also estimation err!

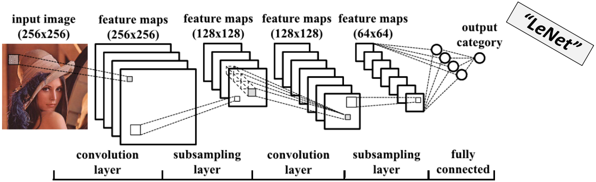
Outline

1. Reflection: The Mathematics of Deep Learning
2. Convolutional Networks as Hierarchical Tensor Decompositions
3. Expressiveness of Convolutional Networks
   - Efficiency of Depth *(C|Sharir|Shashua@COLT'16, C|Shashua@ICML'16)*
   - Modeling Interactions *(Levine|Yakira|C|Shashua@arXiv'17, C|Shashua@ICLR'17)*
   - Efficiency of Interconnectivity *(C|Tamari|Shashua@arXiv'17)*
4. Conclusion

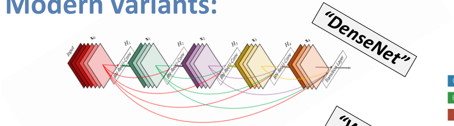
Convolutional Networks

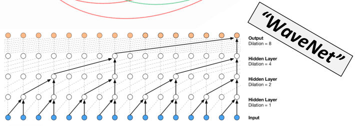
Most successful deep learning arch to date!

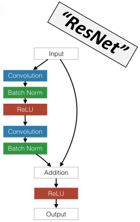
Classic structure:

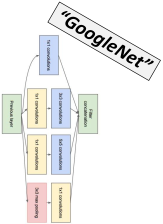


Modern variants:









Traditionally used for images/video, nowadays for audio and text as well

Tensor Product of L^2 Spaces

ConvNets realize func over many local elements (e.g. pixels, audio samples)

Let $\mathbb{R}^s$ be the space of such elements (e.g. $\mathbb{R}^3$ for RGB pixels)

Consider:

- $L^2(\mathbb{R}^s)$ – space of func over single element
- $L^2((\mathbb{R}^s)^N)$ – space of func over N elements

Fact

$L^2((\mathbb{R}^s)^N)$ is equal to the tensor product of $L^2(\mathbb{R}^s)$ with itself N times:

$$L^2((\mathbb{R}^s)^N) = \underbrace{L^2(\mathbb{R}^s) \otimes \cdots \otimes L^2(\mathbb{R}^s)}_{N \text{ times}}$$

Implication

If $\{f_d(\mathbf{x})\}_{d=1}^{\infty}$ is a basis[1] for $L^2(\mathbb{R}^s)$, the following is a basis for $L^2((\mathbb{R}^s)^N)$:

$$\left\{(\mathbf{x}_1, \ldots, \mathbf{x}_N) \mapsto \prod\nolimits_{i=1}^{N} f_{d_i}(\mathbf{x}_i)\right\}_{d_1 \ldots d_N = 1}^{\infty}$$

[1] Set of linearly independent func w/dense span

Coefficient Tensor

For practical purposes, restrict $L^2(\mathbb{R}^s)$ basis to a finite set: $f_1(\mathbf{x})\ldots f_M(\mathbf{x})$

We call $f_1(\mathbf{x})\ldots f_M(\mathbf{x})$ **descriptors**

General func over N elements can now be written as:

$$h(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\sum\nolimits_{d_1\ldots d_N=1}^{M}\mathcal{A}_{d_1\ldots d_N}\prod\nolimits_{i=1}^{N}f_{d_i}(\mathbf{x}_i)$$

w/func fully determined by the **coefficient tensor**:

$$\mathcal{A}\in\mathbb{R}^{\overbrace{M\times\cdots\times M}^{N\text{ times}}}$$

Example

- 100-by-100 images ($N=10^4$)
- pixels represented by 256 descriptors ($M=256$)

Then, func over images correspond to coeff tensors of:

- order 10^4
- dim 256 in each mode

Decomposing Coefficient Tensor $\longrightarrow$ Convolutional Arithmetic Circuit

$$h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum\nolimits_{d_1 \ldots d_N = 1}^{M} \mathcal{A}_{d_1 \ldots d_N} \prod\nolimits_{i=1}^{N} f_{d_i}(\mathbf{x}_i)$$

Coeff tensor $\mathcal{A}$ is exponential (in # of elements N)

$\implies$ directly computing a general func is intractable

Observation

Applying hierarchical decomposition to coeff tensor gives ConvNet w/linear activation and product pooling (**Convolutional Arithmetic Circuit**)!

decomposition type (mode tree, internal ranks etc)	$\longleftrightarrow$	network structure (depth, width, pooling etc)
decomposition parameters	$\longleftrightarrow$	network weights

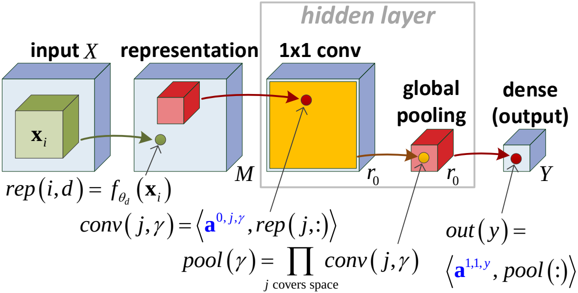
Example 1: CP Decomposition $\longrightarrow$ Shallow Network

$$h(\mathbf{x}_1,\ldots,\mathbf{x}_N)=\sum_{d_1\ldots d_N=1}^{M}\mathcal{A}_{d_1\ldots d_N}\prod_{i=1}^{N}f_{d_i}(\mathbf{x}_i)$$

W/CP decomposition applied to coeff tensor:

$$\mathcal{A}=\sum_{\gamma=1}^{r_0}a_\gamma^{1,1,y}\cdot\mathbf{a}^{0,1,\gamma}\otimes\mathbf{a}^{0,2,\gamma}\otimes\cdots\otimes\mathbf{a}^{0,N,\gamma}$$

func is computed by shallow network (single hidden layer, global pooling):



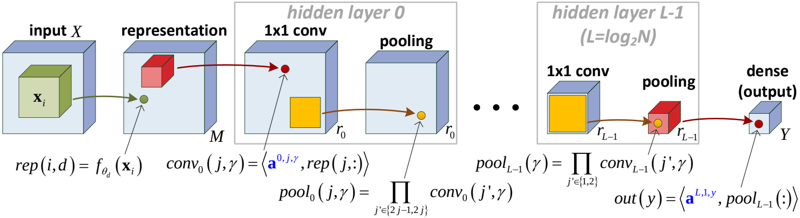
Example 2: HT Decomposition $\longrightarrow$ Deep Network

$$h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{d_1 \ldots d_N = 1}^{M} \mathcal{A}_{d_1 \ldots d_N} \prod_{i=1}^{N} f_{d_i}(\mathbf{x}_i)$$

W/Hierarchical Tucker (HT) decomposition applied to coeff tensor:

$$\begin{aligned}
\phi^{1,j,\gamma} &= \sum_{\alpha=1}^{r_0} a_\alpha^{1,j,\gamma} \cdot \mathbf{a}^{0,2j-1,\alpha} \otimes \mathbf{a}^{0,2j,\alpha} \\
&\cdots \\
\phi^{l,j,\gamma} &= \sum_{\alpha=1}^{r_{l-1}} a_\alpha^{l,j,\gamma} \cdot \phi^{l-1,2j-1,\alpha} \otimes \phi^{l-1,2j,\alpha} \\
&\cdots \\
\mathcal{A} &= \sum_{\alpha=1}^{r_{L-1}} a_\alpha^{L,1,y} \cdot \phi^{L-1,1,\alpha} \otimes \phi^{L-1,2,\alpha}
\end{aligned}$$

func is computed by deep network w/size-2 pooling windows:



Generalization to Other Types of Convolutional Networks

We established equivalence:

hierarchical tensor decompositions $\longleftrightarrow$ conv arith circuits (ConvACs)

ConvACs deliver promising empirical results,[1] but other types of ConvNets (e.g. w/ReLU activation and max/ave pooling) are much more common

The equivalence extends to other types of ConvNets if we generalize the notion of tensor product:[2]

Tensor product:

$$(\mathcal{A} \otimes \mathcal{B})_{d_1 \ldots d_{P+Q}} = \mathcal{A}_{d_1 \ldots d_P} \cdot \mathcal{B}_{d_{P+1} \ldots d_{P+Q}}$$

Generalized tensor product:

$$(\mathcal{A} \otimes_g \mathcal{B})_{d_1 \ldots d_{P+Q}} := g(\mathcal{A}_{d_1 \ldots d_P}, \mathcal{B}_{d_{P+1} \ldots d_{P+Q}})$$

(same as $\otimes$ but w/general $g : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ instead of mult)

[1] *Deep SimNets, CVPR'16* ; *Tensorial Mixture Models, arXiv'17*

[2] *Convolutional Rectifier Networks as Generalized Tensor Decompositions, ICML'16*

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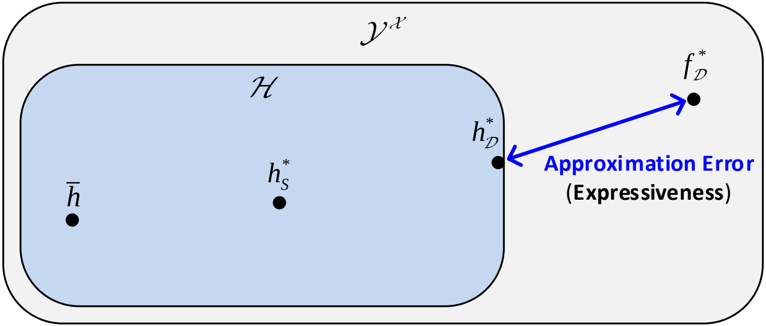
4. Conclusion

Expressiveness



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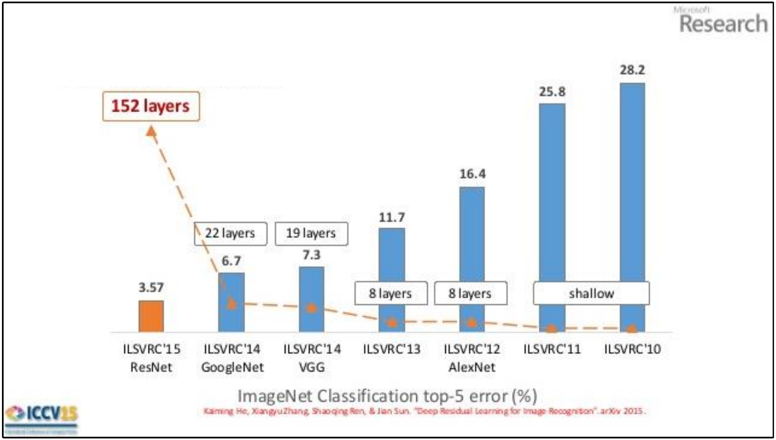
Outline

Efficiency of Depth



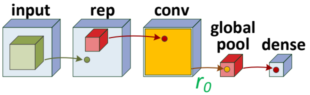
Longstanding conjecture

Efficiency of depth: deep ConvNets realize func that require shallow ConvNets to have exponential size (width)

Tensor Decomposition Viewpoint

$$h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum\nolimits_{d_1 \ldots d_N = 1}^{M} \mathcal{A}_{d_1 \ldots d_N} \prod\nolimits_{i=1}^{N} f_{d_i}(\mathbf{x}_i)$$

Shallow Network

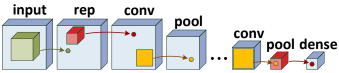


$\longleftrightarrow$

CP Decomposition

$$\mathcal{A} = \sum\nolimits_{\gamma=1}^{r_0} a_\gamma^{1,1,y} \cdot \mathbf{a}^{0,1,\gamma} \otimes \cdots \otimes \mathbf{a}^{0,N,\gamma}$$

Deep Network



$\longleftrightarrow$

HT Decomposition

$$\phi^{1,j,\gamma} = \sum\nolimits_{\alpha=1}^{r_0} a_\alpha^{1,j,\gamma} \cdot \mathbf{a}^{0,2j-1,\alpha} \otimes \mathbf{a}^{0,2j,\alpha}$$

$$\cdots$$

$$\phi^{l,j,\gamma} = \sum\nolimits_{\alpha=1}^{r_{l-1}} a_\alpha^{l,j,\gamma} \cdot \phi^{l-1,2j-1,\alpha} \otimes \phi^{l-1,2j,\alpha}$$

$$\cdots$$

$$\mathcal{A} = \sum\nolimits_{\alpha=1}^{r_{L-1}} a_\alpha^{L,1,y} \cdot \phi^{L-1,1,\alpha} \otimes \phi^{L-1,2,\alpha}$$

Efficiency of depth

HT decomposition realizes tensors that require CP decomposition to have exponential rank (r_0 exponential in N)

HT vs. CP Analysis

Theorem

Besides a negligible (zero measure) set, all parameter settings for HT decomposition lead to tensors w/CP-rank exponential in N

HT Decomposition

$$\phi^{1,j,\gamma} = \sum_{\alpha=1}^{r_0} a_\alpha^{1,j,\gamma} \cdot \mathbf{a}^{0,2j-1,\alpha} \otimes \mathbf{a}^{0,2j,\alpha}$$

$$\cdots$$

$$\phi^{l,j,\gamma} = \sum_{\alpha=1}^{r_{l-1}} a_\alpha^{l,j,\gamma} \cdot \phi^{l-1,2j-1,\alpha} \otimes \phi^{l-1,2j,\alpha}$$

$$\cdots$$

$$\mathcal{A} = \sum_{\alpha=1}^{r_{L-1}} a_\alpha^{L,1,y} \cdot \phi^{L-1,1,\alpha} \otimes \phi^{L-1,2,\alpha}$$

CP Decomposition

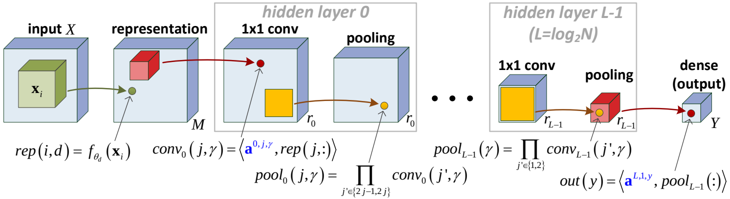
$$\mathcal{A} = \sum_{\gamma=1}^{\mathbf{r_0}} a_\gamma^{1,1,y} \cdot \mathbf{a}^{0,1,\gamma} \otimes \cdots \otimes \mathbf{a}^{0,N,\gamma}$$

HT vs. CP Analysis (cont'd)

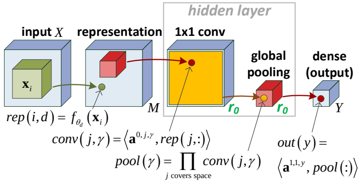
Corollary

Randomizing weights of deep ConvAC by a cont distribution leads, w.p. 1, to func that require shallow ConvAC to have exponential # of channels

Deep Network



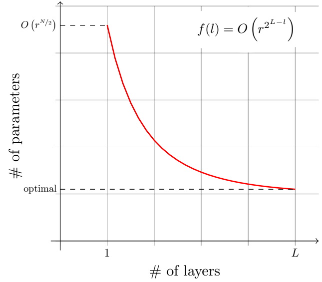
Shallow Network



HT vs. CP Analysis – Generalizations

HT vs. CP analysis may be generalized in various ways, e.g.:

- **Comparison between arbitrary depths**
  Penalty in resources is double-exponential w.r.t. # of layers cut-off



- **Adaptation to other types of ConvNets**
  W/ReLU activation and max pooling, deep nets realize func requiring shallow nets to be exponentially large, but not almost always

Efficiency of depth proven!

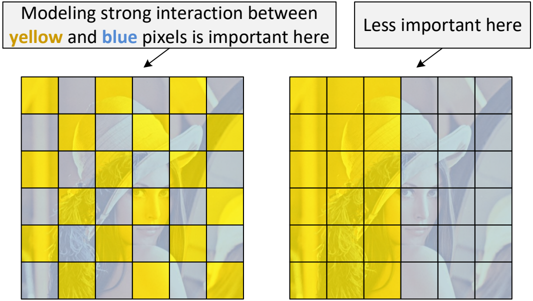
Outline

Modeling Interactions

ConvNets realize func over many local elements (e.g. pixels, audio samples)

Key property of such func:

interactions modeled between different sets of elements

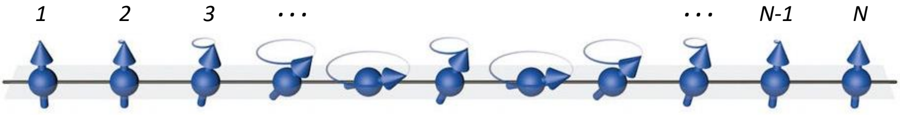


Partition A *Partition B*

Questions

- What kind of interactions do ConvNets model?
- How do these depend on network structure?

Quantum Entanglement



In quantum physics, state of particle is represented as vec in Hilbert space:

$$|\text{particle state}\rangle = \sum_{d=1}^{M} \underbrace{a_d}_{\text{coeff}} \cdot \underbrace{|\psi_d\rangle}_{\text{basis}} \in \mathbf{H}$$

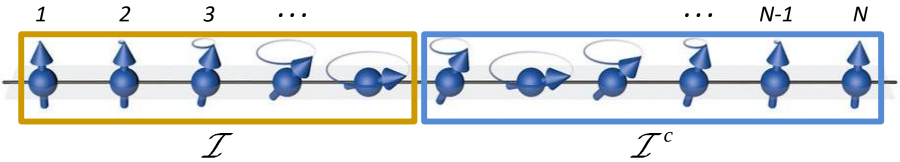
System of N particles is represented as vec in tensor product space:

$$|\text{system state}\rangle = \sum_{d_1 \ldots d_N=1}^{M} \underbrace{\mathcal{A}_{d_1 \ldots d_N}}_{\text{coeff tensor}} \cdot |\psi_{d_1}\rangle \otimes \cdots \otimes |\psi_{d_N}\rangle \in \underbrace{\mathbf{H} \otimes \cdots \otimes \mathbf{H}}_{N \text{ times}}$$

Quantum entanglement measures quantify interactions that a system state models between sets of particles

Quantum Entanglement (cont'd)

$$|\text{system state}\rangle = \sum_{d_1 \ldots d_N = 1}^{M} \mathcal{A}_{d_1 \ldots d_N} \cdot |\psi_{d_1}\rangle \otimes \cdots \otimes |\psi_{d_N}\rangle$$

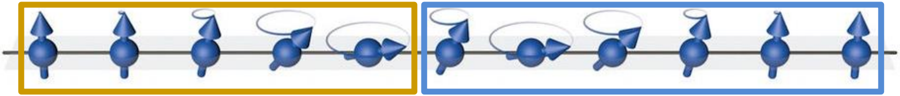


Consider partition of the N particles into sets $\mathcal{I}$ and $\mathcal{I}^c$

$[\![\mathcal{A}]\!]_{\mathcal{I}}$ – matricization of coeff tensor $\mathcal{A}$ w.r.t. $\mathcal{I}$:

- arrangement of $\mathcal{A}$ as matrix
- rows/cols correspond to modes indexed by $\mathcal{I}/\mathcal{I}^c$

Quantum Entanglement (cont'd)



$$|\text{system state}\rangle = \sum_{d_1 \ldots d_N = 1}^{M} \mathcal{A}_{d_1 \ldots d_N} \cdot |\psi_{d_1}\rangle \otimes \cdots \otimes |\psi_{d_N}\rangle$$

$[\![\mathcal{A}]\!]_{\mathcal{I}}$ – matricization of $\mathcal{A}$ w.r.t. $\mathcal{I}$

Let $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_R)$ be the singular vals of $[\![\mathcal{A}]\!]_{\mathcal{I}}$

Entanglement measures between particles of $\mathcal{I}$ and of $\mathcal{I}^c$ are based on $\boldsymbol{\sigma}$:

- Entanglement Entropy: entropy of $(\sigma_1^2, \ldots, \sigma_R^2) / \|\boldsymbol{\sigma}\|_2^2$
- Geometric Measure: $1 - \sigma_1^2 / \|\boldsymbol{\sigma}\|_2^2$
- **Schmidt Number**: $\|\boldsymbol{\sigma}\|_0 = \textit{rank}[\![\mathcal{A}]\!]_{\mathcal{I}}$

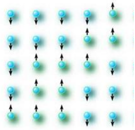
Entanglement with Convolutional Arithmetic Circuits

Structural equivalence:

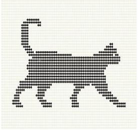
quantum system (many-body) state

$$|\text{system state}\rangle = \sum_{d_1 \ldots d_N = 1}^{M} \underbrace{\mathcal{A}_{d_1 \ldots d_N}}_{\text{coeff tensor}} \cdot |\psi_{d_1}\rangle \otimes \cdots \otimes |\psi_{d_N}\rangle$$

state of many particles



func over many pixels



func realized by ConvAC

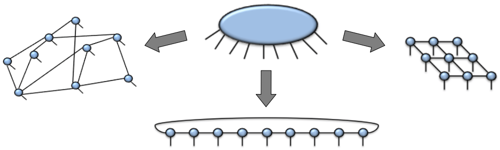
$$h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{d_1 \ldots d_N = 1}^{M} \underbrace{\mathcal{A}_{d_1 \ldots d_N}}_{\text{coeff tensor}} \cdot f_{d_1}(\mathbf{x}_1) \cdots f_{d_N}(\mathbf{x}_N)$$

We may quantify interactions ConvAC models between input sets by applying entanglement measures to its coeff tensor!

Quantum Tensor Networks

Coeff tensors of quantum many-body states are simulated via:

Tensor Networks



Tensor Networks (TNs):

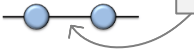
- Graphs in which: vertices ⟷ tensors edges ⟷ modes

scalar ***vector*** ***matrix*** ***order-3 tensor***

- Edge (mode) connecting two vertices (tensors) represents contraction

inner-product between vectors

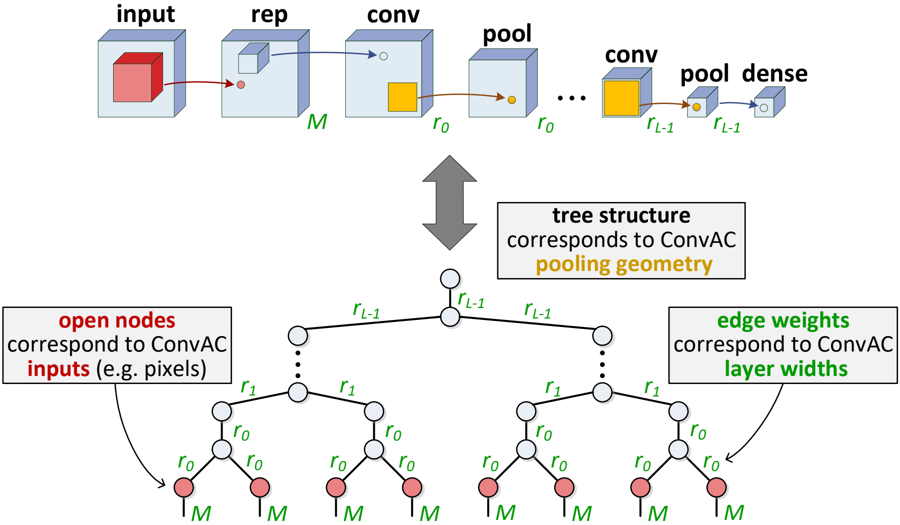
matrix multiplication



edges weighted by mode dimensions

Convolutional Arithmetic Circuits as Tensor Networks

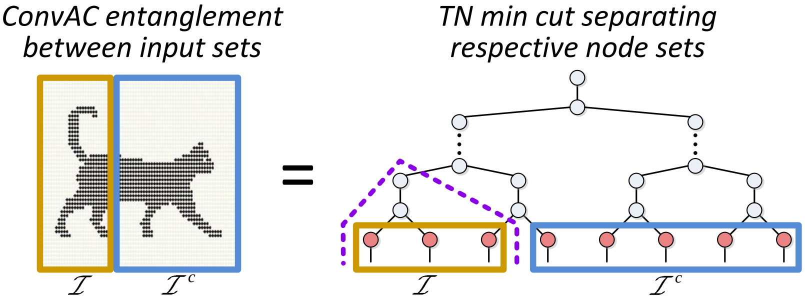
Coeff tensor of ConvAC may be represented via TN:



Entanglement via Minimal Cuts

Theorem

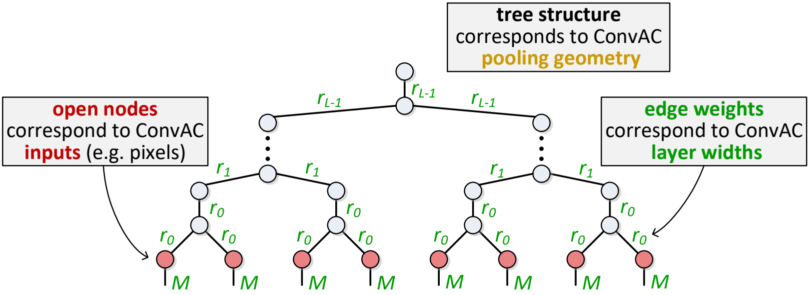
Maximal Schmidt entanglement ConvAC models between input sets $\mathcal{I}/\mathcal{I}^c$ is equal to min cut in respective TN separating nodes of $\mathcal{I}/\mathcal{I}^c$



Controlling Entanglement (Interactions)

Corollary

Controlling entanglement (interactions) modeled by ConvAC is equivalent to controlling min cuts in respective TN



Two sources of control: layer widths, pooling geometry

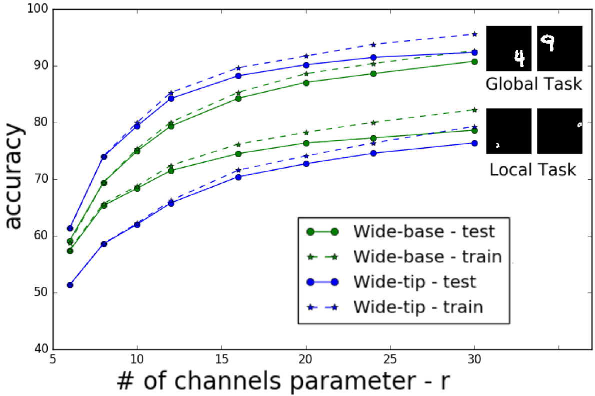
We may analyze the effect of ConvAC arch on the interactions (entanglement) it can model!

Controlling Interactions – Layer Widths

Claim

Deep (early) layer widths are important for long (short)-range interactions

Experiment



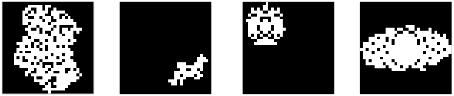
Controlling Interactions – Pooling Geometry

Claim

Input elements pooled together early have stronger interaction

Experiment

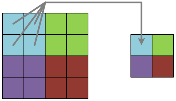
data



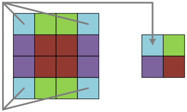
closedness: low	closedness: high	closedness: low	closedness: high
symmetry: low	symmetry: low	symmetry: high	symmetry: high

archs

square pooling
(local interactions)

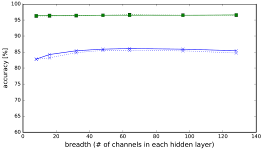


mirror pooling
(interactions between reflections)

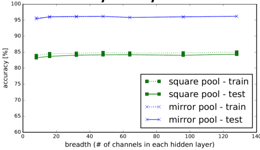


results

closedness task



symmetry task



Outline

1. Reflection: The Mathematics of Deep Learning

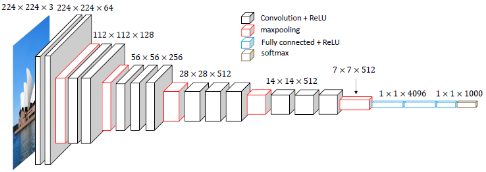
2. Convolutional Networks as Hierarchical Tensor Decompositions

3. Expressiveness of Convolutional Networks
   - Efficiency of Depth *(C|Sharir|Shashua@COLT'16, C|Shashua@ICML'16)*
   - Modeling Interactions *(Levine|Yakira|C|Shashua@arXiv'17, C|Shashua@ICLR'17)*
   - Efficiency of Interconnectivity *(C|Tamari|Shashua@arXiv'17)*

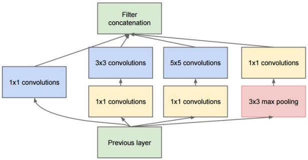
4. Conclusion

Efficiency of Interconnectivity

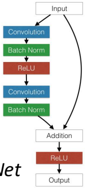
Classic ConvNets have feed-forward (chain) structure:



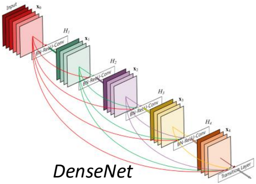
Modern ConvNets employ elaborate connectivity schemes:



Inception (GoogLeNet)



ResNet



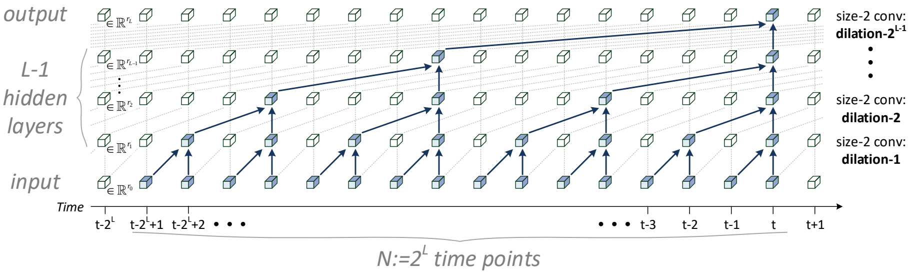
DenseNet

Question

Can such connectivities lead to more efficient representation of func?

Dilated Convolutional Networks

We focus on dilated ConvNets (D-ConvNets) for sequence data:

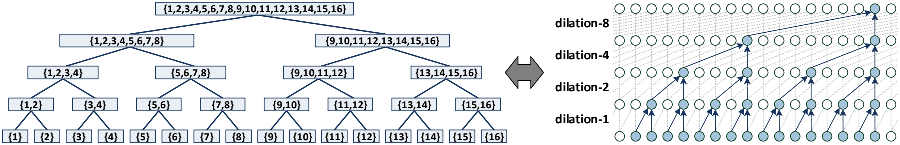


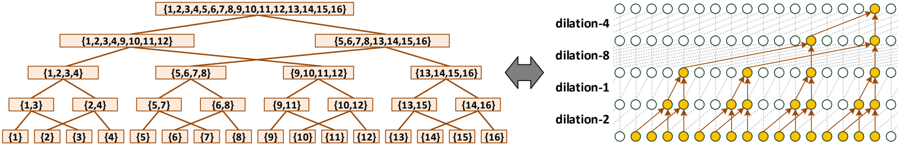
- 1D ConvNets
- No pooling
- Dilated (gapped) conv windows

Underlie Google's WaveNet & ByteNet – state of the art for audio & text!

Dilations and Mode Trees

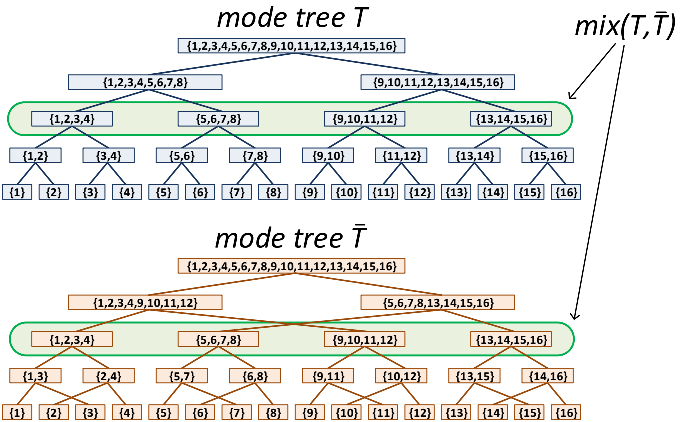
W/D-ConvNet, mode tree underlying corresponding tensor decomposition determines dilation scheme





Mixed Tensor Decompositions

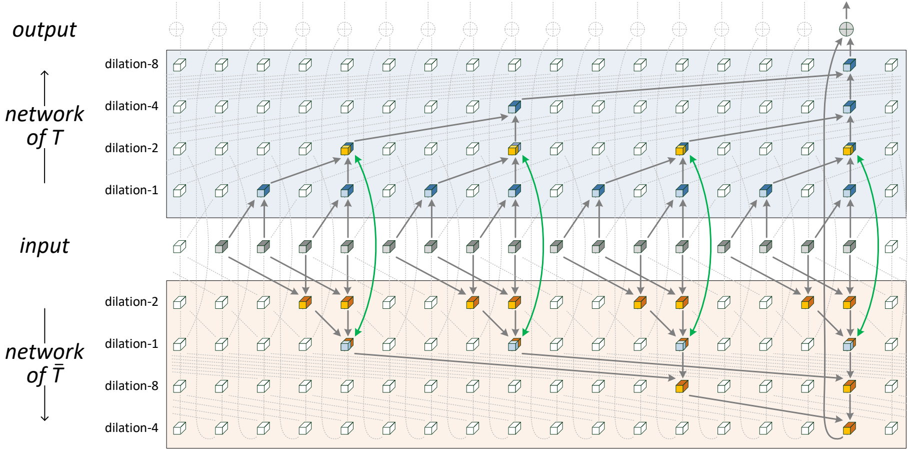
Let: T, $\bar{T}$ – mode trees ; $mix(T, \bar{T})$ – set of nodes present in both trees



A **mixed tensor decomposition** blends together T and $\bar{T}$ by running their decompositions in parallel, exchanging tensors in each node of $mix(T, \bar{T})$

Mixed Dilated Convolutional Networks

Mixed tensor decomposition corresponds to **mixed D-ConvNet**, formed by interconnecting the networks of T and $\bar{T}$:



Mixture $\longrightarrow$ Expressive Efficiency

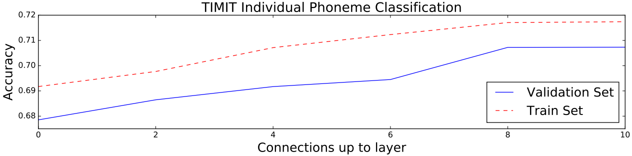
Theorem

Mixed tensor decomposition of T and $\bar{T}$ can generate tensors that require individual decompositions to grow quadratically (in terms of their ranks)

Corollary

Mixed D-ConvNet can realize func that require individual networks to grow quadratically (in terms of layer widths)

Experiment



Interconnectivity can lead to more efficient representation!

Outline

Conclusion

- Three pillars of statistical learning theory:

  Expressiveness Generalization Optimization

  - Well developed theory for classical ML
  - Limited understanding for Deep Learning

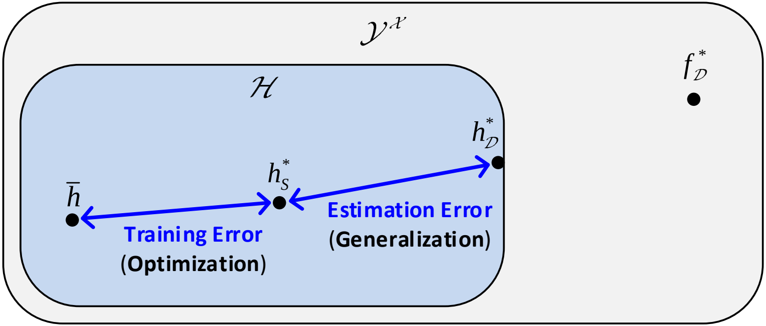
- We derive equivalence:

  ConvNets $\longleftrightarrow$ hierarchical tensor decompositions

- We use equivalence to **analyze expressiveness of ConvNets**:
  - Representational efficiency of depth
  - Input interaction (entanglement) modeling
  - Efficiency of interconnectivity schemes

- Results not only explanatory – provide **new tools for network design**

Future Work



$f^*_{\mathcal{D}}$ – ground truth ($\text{argmin}_{f \in \mathcal{Y}^{\mathcal{X}}} L_{\mathcal{D}}(f)$)

$h^*_{\mathcal{D}}$ – optimal hypothesis ($\text{argmin}_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$)

h^*_S – empirically optimal hypothesis ($\text{argmin}_{h \in \mathcal{H}} L_S(h)$)

$\bar{h}$ – returned hypothesis

Outline

Thank You