Expressive Efficiency and Inductive Bias of Convolutional Networks:

Analysis & Design via Hierarchical Tensor Decompositions

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The Hebrew University of Jerusalem

AAAI Spring Symposium Series 2017

Science of Intelligence: Computational Principles of Natural and Artificial Intelligence

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

Tractable Generative Convolutional Arithmetic Circuits
O. Sharir. R. Tamari, N. Cohen and A. Shashua
arXiv preprint 2017

On the Expressive Power of Overlapping Operations of Deep Networks
O. Sharir and A. Shashua
arXiv preprint 2017

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

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Yoav Levine

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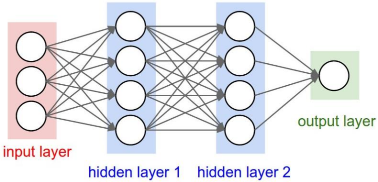
Classic vs. State of the Art Deep Learning

Classic



Multilayer Perceptron (MLP)

Architectural choices:

- depth
- layer widths
- activation types

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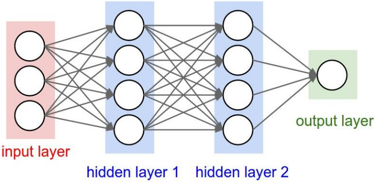

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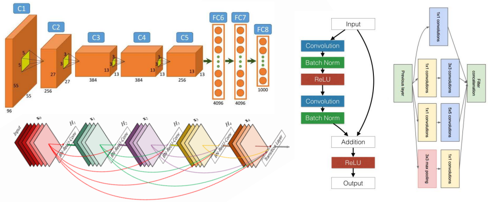

Convolutional Networks (ConvNets)

Architectural choices:

- depth
- layer widths
- activation types
- pooling types
- convolution/pooling windows
- convolution/pooling strides
- dilation factors
- connectivity
- and more...

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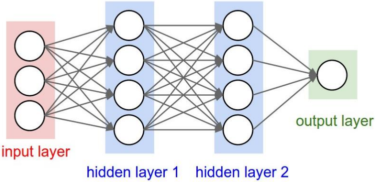

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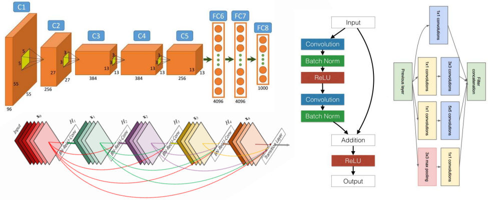

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Can the architectural choices of state of the art ConvNets be theoretically analyzed?

Outline

Expressiveness

Expressiveness:

- Ability to compactly represent rich and effective classes of func
- The driving force behind deep networks

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Fundamental theoretical questions:

- What kind of func can different network arch represent?
- Why are these func suitable for real-world tasks?
- What is the representational benefit of depth?
- Can other arch features deliver representational benefits?

Efficiency

Expressive efficiency compares network arch in terms of their ability to compactly represent func

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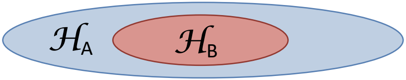
A is **efficient** w.r.t. B if $\mathcal{H}_B$ is a strict subset of $\mathcal{H}_A$



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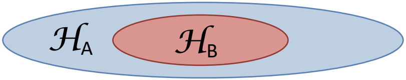
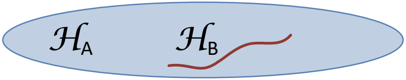


A is **completely efficient** w.r.t. B if $\mathcal{H}_B$ has zero "volume" inside $\mathcal{H}_A$



Efficiency – Formal Definition

Network arch A is **efficient** w.r.t. network arch B if:

(1) $\forall$func realized by B w/size r_B can be realized by A w/size $r_A \in \mathcal{O}(r_B)$

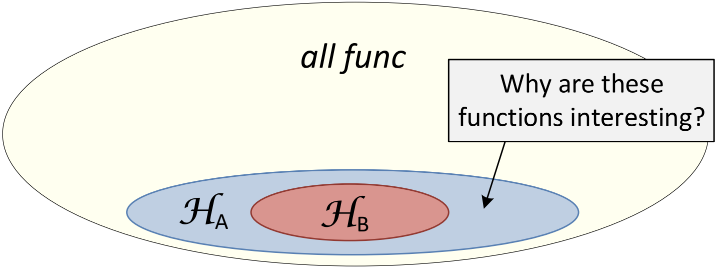
(2) $\exists$func realized by A w/size r_A requiring B to have size $r_B \in \Omega(f(r_A))$, where $f(\cdot)$ is super-linear

A is **completely efficient** w.r.t. B if (2) holds for all of its func but a set of Lebesgue measure zero (in weight space)

Inductive Bias

Networks of reasonable size can only realize a fraction of all possible func

Efficiency does not explain why this fraction is effective



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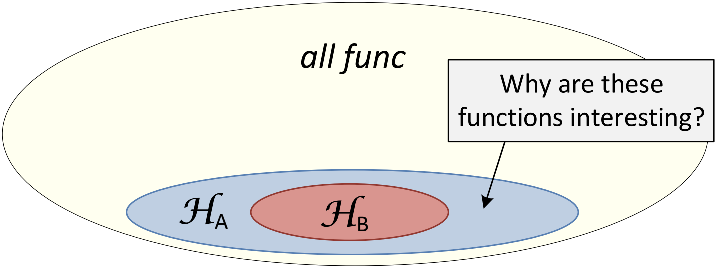


To explain the effectiveness, one must consider the **inductive bias**:

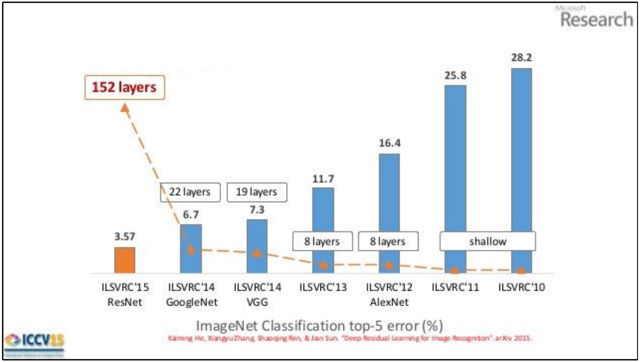
- Not all func are equally useful for a given task
- Network only needs to represent useful func

Outline

Efficiency of Depth

Longstanding conjecture, proven for MLP:

deep networks are efficient w.r.t. shallow ones



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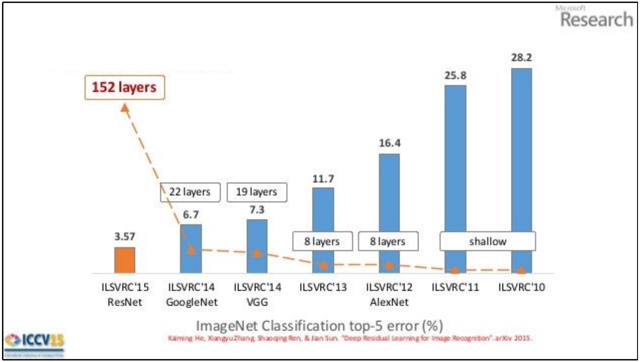

Q: *Can this be proven for ConvNets?*

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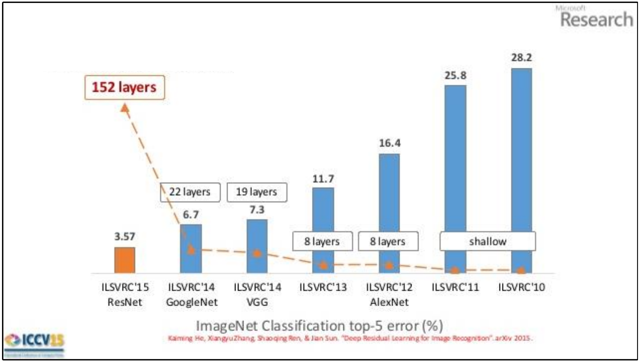
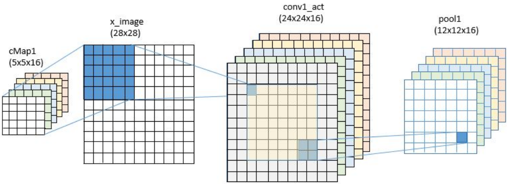


Q: *Can this be proven for ConvNets?*

Q: *Is their efficiency of depth complete?*

Inductive Bias of Convolution/Pooling Geometry

ConvNets typically employ square conv/pool windows



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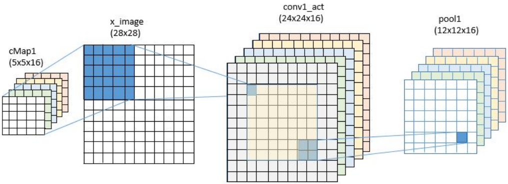
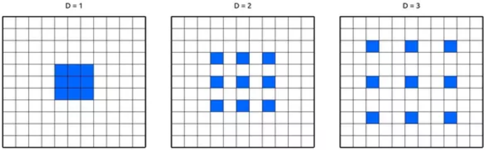


Recently, dilated windows have also become popular



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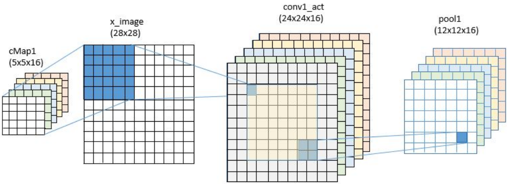

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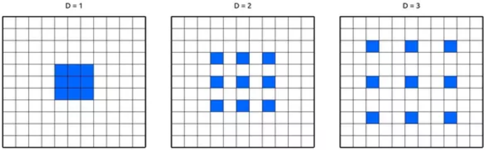

Q: *What is the inductive bias of conv/pool window geometry?*

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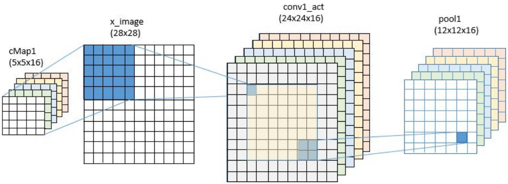

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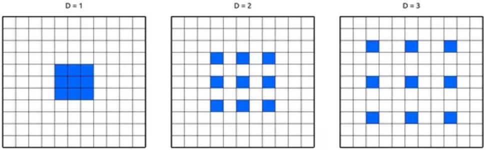
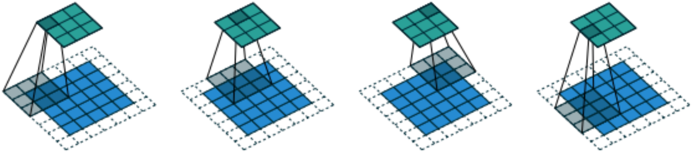


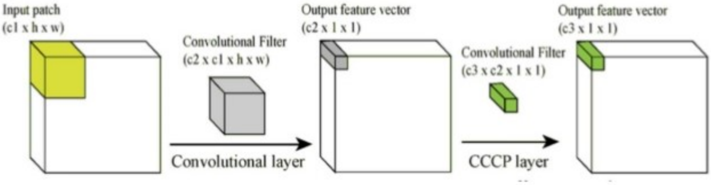
Q: *What is the inductive bias of conv/pool window geometry?*

Q: *Can the geometries be tailored for a given task?*

Efficiency of Overlapping Operations

Modern ConvNets employ both overlapping and non-overlapping conv/pool operations





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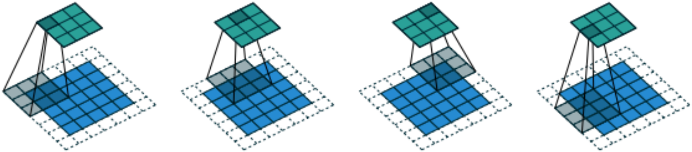
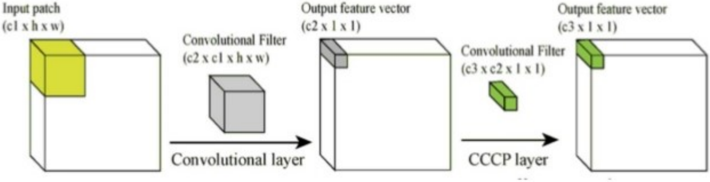
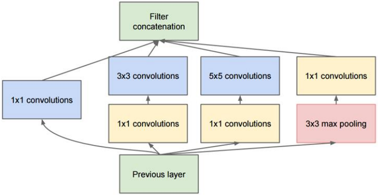




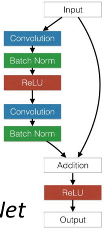
Q: *Do overlapping operations introduce efficiency?*

Efficiency of Connectivity Schemes

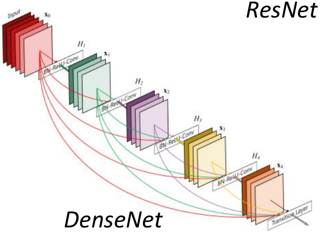
Nearly all state of the art ConvNets employ elaborate connectivity schemes



Inception (GoogLeNet)



ResNet



DenseNet

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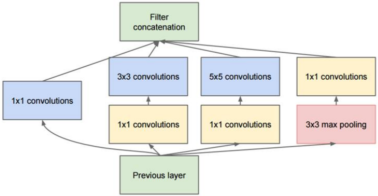

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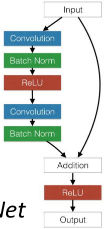

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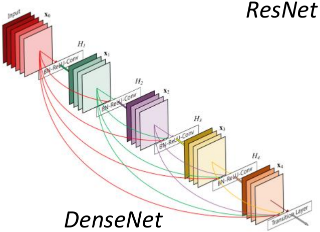

DenseNet

Q: *Can this be justified in terms of efficiency?*

Outline

Convolutional Arithmetic Circuits

To address raised questions, we consider a surrogate (special case) of ConvNets – **Convolutional Arithmetic Circuits (ConvACs)**

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ConvACs are equivalent to **hierarchical tensor decompositions**, allowing theoretical analysis w/mathematical tools from various fields, e.g.:

- Functional Analysis
- Measure Theory
- Matrix Algebra
- Graph Theory

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ConvACs are superior to ReLU ConvNets in terms of expressiveness[1]; deliver promising results in practice:

- Excel in computationally constrained settings[2]
- Classify optimally under missing data[3]

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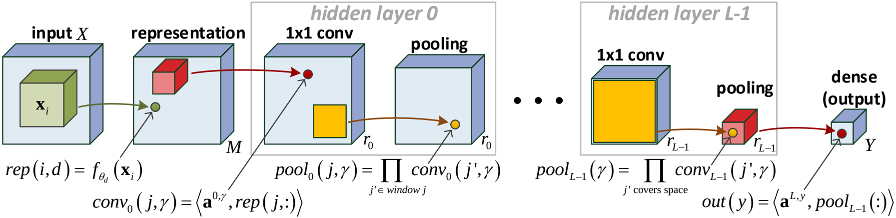
[1] *Convolutional Rectifier Networks as Generalized Tensor Decompositions, ICML'16*

[2] *Deep SimNets, CVPR'16*

[3] *Tractable Generative Convolutional Arithmetic Circuits, arXiv'17*

Baseline Architecture



Baseline ConvAC architecture:

- 2D ConvNet
- *Linear activation* ($\sigma(z) = z$), *product pooling* ($P\{c_j\} = \prod_j c_j$)
- 1×1 convolution windows
- Non-overlapping pooling windows

Grid Tensors

ConvNets realize func over many local structures:

$$f(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$\mathbf{x}_i$ – image patches (2D network) / sequence samples (1D network)

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$f(\cdot)$ may be studied by *discretizing* each $\mathbf{x}_i$ into one of $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(M)}\}$:

$$\mathcal{A}_{d_1 \ldots d_N} = f(\mathbf{v}^{(d_1)} \ldots \mathbf{v}^{(d_N)}) \quad , d_1 \ldots d_N \in \{1, \ldots, M\}$$

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The lookup table $\mathcal{A}$ is:

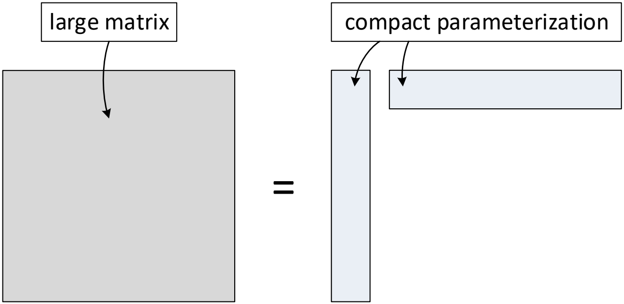
- an N-dim array (tensor) w/length M in each axis
- referred to as the **grid tensor** of $f(\cdot)$

Tensor Decompositions – Compact Parameterizations

High-dim tensors (arrays) are exponentially large – cannot be used directly

May be represented and manipulated via **tensor decompositions**:

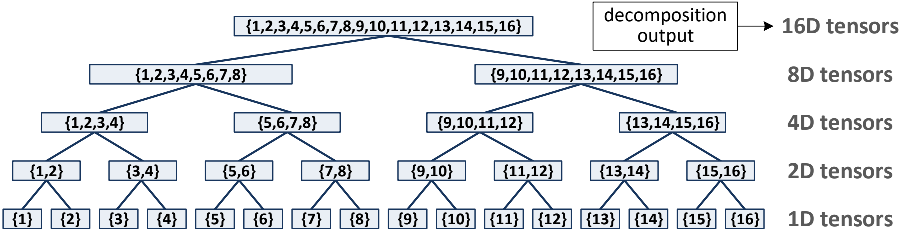
- Compact algebraic parameterizations
- Generalization of low-rank matrix decompositions



Hierarchical Tensor Decompositions

Hierarchical tensor decompositions represent high-dim tensors by incrementally generating intermediate tensors of increasing dim

Generation process can be described by a tree over tensor modes (axes)



Convolutional Arithmetic Circuits $\longleftrightarrow$ Hierarchical Tensor Decompositions

Observation

Grid tensors of func realized by ConvACs are given by hierarchical tensor decompositions:

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

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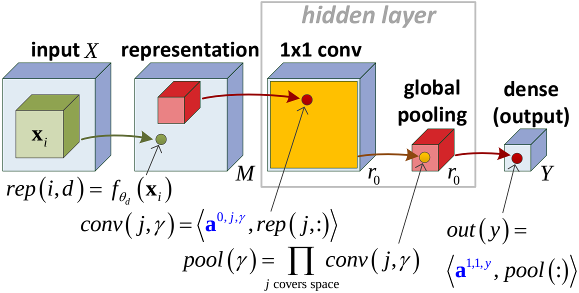
We can study networks through corresponding decompositions!

Example 1: Shallow Network $\longleftrightarrow$ CP Decomposition

Shallow network (single hidden layer, global pooling):



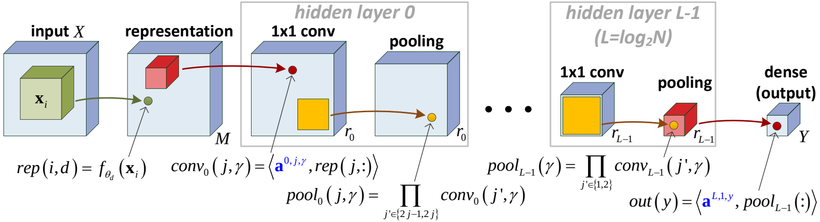
corresponds to classic **CP decomposition**:

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

($\otimes$ – outer product)

Example 2: Deep Network $\longleftrightarrow$ HT Decomposition

Deep network with size-2 pooling:



corresponds to **Hierarchical Tucker (HT) decomposition**:

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

$$\cdots$$

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

$$\cdots$$

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

Outline

Tensor Matricization

Let $\mathcal{A}$ be a tensor of order (dim) N

Let (I, J) be a partition of $[N]$, i.e. $I \dot{\cup} J = [N] := \{1, \ldots, N\}$

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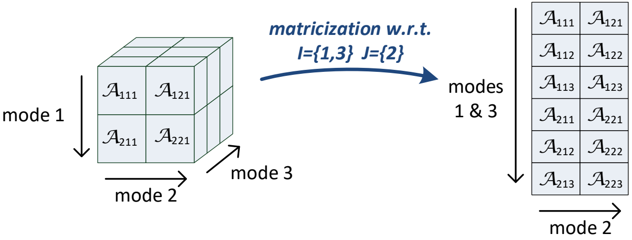
$[\![\mathcal{A}]\!]_{I,J}$ – **matricization of $\mathcal{A}$ w.r.t.** (I, J):

- Arrangement of $\mathcal{A}$ as matrix
- Rows correspond to modes (axes) indexed by I
- Cols -"- J



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Theorem

Consider the partition $I_{odd} = \{1, 3, \ldots, N-1\}$, $J_{even} = \{2, 4, \ldots, N\}$. Besides a set of measure zero, all param settings of HT decomposition give tensors that when matricized w.r.t. (I_{odd}, J_{even}), have exponential ranks.

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Since # of terms in CP decomposition corresponds to # of hidden channels in shallow ConvAC:

Corollary

Almost all func realizable by deep ConvAC cannot be replicated by shallow ConvAC with less than exponentially many hidden channels

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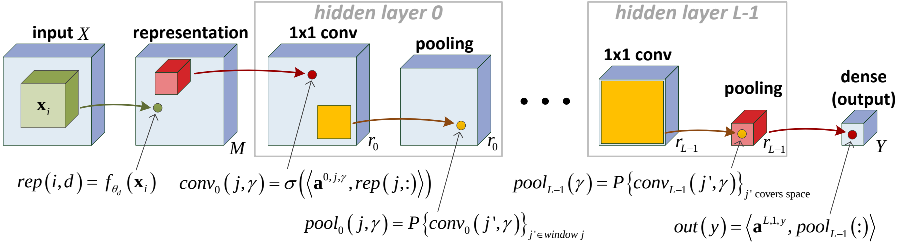
W/ConvACs efficiency of depth is exponential and complete!

From Convolutional Arithmetic Circuits to Convolutional Rectifier Networks



Transform ConvACs into **convolutional rectifier networks** (R-ConvNets):

linear activation $\longrightarrow$ ReLU activation: $\sigma(z) = \max\{z, 0\}$

product pooling $\longrightarrow$ max/average pooling: $P\{c_j\} = max\{c_j\}/mean\{c_j\}$

Most successful deep learning architecture to date!

Generalized Tensor Decompositions

ConvACs correspond to tensor decompositions based on tensor product $\otimes$:

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Generalized tensor decompositions are obtained by replacing $\otimes$ with $\otimes_g$

Convolutional Rectifier Networks $\longleftrightarrow$ Generalized Tensor Decompositions

Define the **activation-pooling operator**:

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Grid tensors of func realized by R-ConvNets are given by generalized tensor decompositions w/ $g(\cdot) \equiv \rho_{\sigma/P}(\cdot)$:

Shallow R-ConvNet	$\longleftrightarrow$	Generalized CP decomposition w/ $g(\cdot) \equiv \rho_{\sigma/P}(\cdot)$
Deep R-ConvNet	$\longleftrightarrow$	Generalized HT decomposition w/ $g(\cdot) \equiv \rho_{\sigma/P}(\cdot)$

Exponential But Incomplete Efficiency of Depth

By analyzing matricization ranks of tensors realized by generalized CP and HT decompositions w/$g(\cdot) \equiv \rho_{\sigma/P}(\cdot)$, we show:

Claim

There exist func realizable by deep R-ConvNet requiring shallow R-ConvNet to be exponentially large

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Developing optimization methods for ConvACs may give rise to an arch that is provably superior but has so far been overlooked

Outline

Separation Rank – A Measure of Input Correlations

ConvNets realize func over many local structures:

$$f(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)$$

$\mathbf{x}_i$ – image patches (2D network) / sequence samples (1D network)

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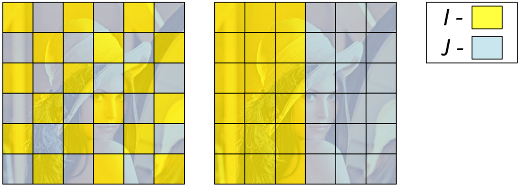
Separation rank:
Formal measure of these correlations



Partition A *Partition B*

Sep rank of $f(\cdot)$ w.r.t. input partition (I, J) measures dist from separability
(sep rank $\nearrow \implies$ more correlation between $(\mathbf{x}_i)_{i \in I}$ and $(\mathbf{x}_j)_{j \in J}$)

Deep Networks Favor Some Correlations Over Others

Claim

W/ConvAC sep rank w.r.t (I, J) *is equal to rank of* $[\![\mathcal{A}^y]\!]_{I,J}$ *– grid tensor matricized w.r.t.* (I, J)

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Maximal rank of tensor generated by HT decomposition, when matricized w.r.t. (I, J), is:

- *Exponential for "interleaved" partitions*
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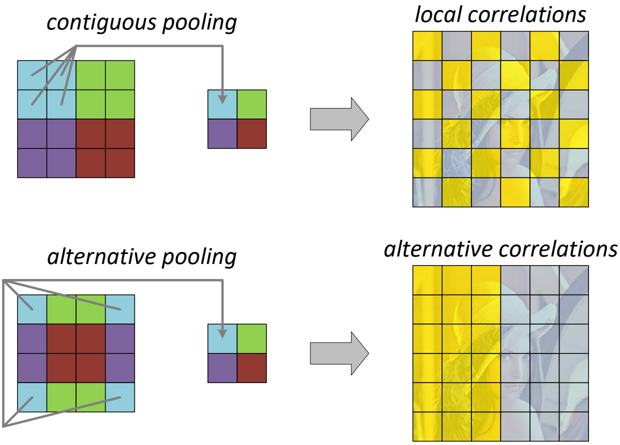
Corollary

Deep ConvAC can realize exponential sep ranks (correlations) for favored partitions, polynomial for others

Pooling Geometry Controls the Preference

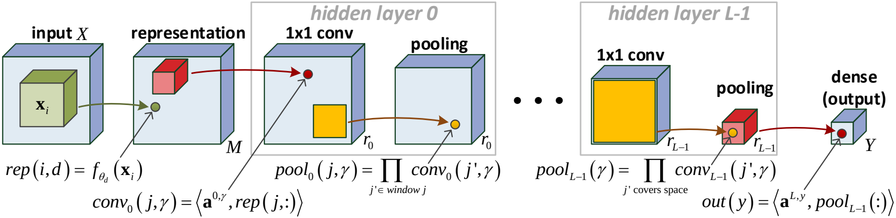


Pooling geometry of deep ConvAC determines which partitions are favored – controls the correlation profile (inductive bias)!

Outline

Overlapping Operations

Baseline ConvAC arch has non-overlapping conv and pool windows:



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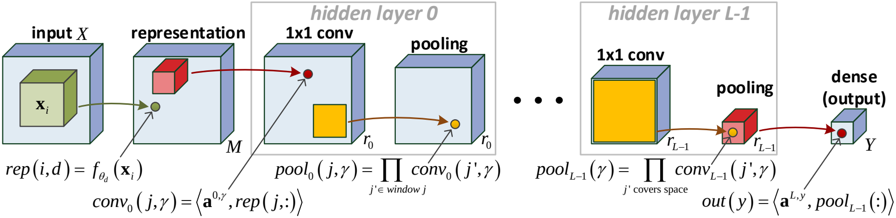
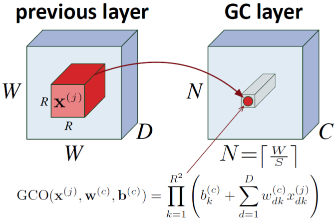


Replace those by (possibly) overlapping **generalized convolution**:



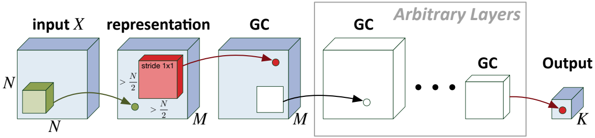
Exponential Efficiency

Theorem

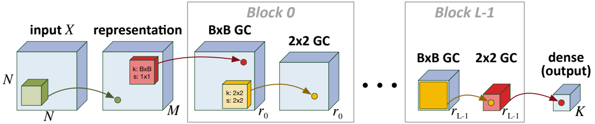
Various ConvACs w/overlapping GC layers realize func requiring ConvAC w/no overlaps to be exponentially large

Examples

- Network starts with large receptive field:



- Typical scheme of alternating $B \times B$ "conv" and 2×2 "pool":



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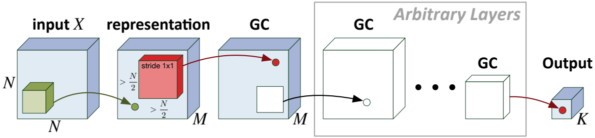

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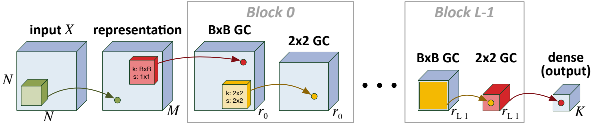


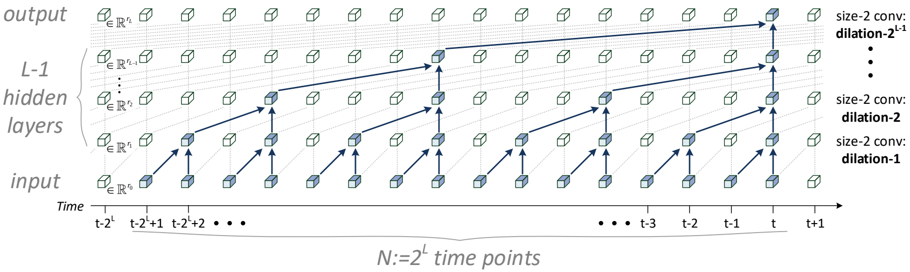
W/ConvACs overlaps lead to exponential efficiency!

Outline

1. Expressiveness
2. Expressiveness of Convolutional Networks – Questions
3. Convolutional Arithmetic Circuits
4. Efficiency of Depth *(Cohen+Sharir+Shashua@COLT'16, Cohen+Shashua@ICML'16)*
5. Inductive Bias of Pooling Geometry *(Cohen+Shashua@ICLR'17)*
6. Efficiency of Overlapping Operations *(Sharir+Shashua@arXiv'17)*
7. **Efficiency of Interconnectivity** *(Cohen+Tamari+Shashua@arXiv'17)*

Dilated Convolutional Networks

Study efficiency of interconnectivity w/**dilated convolutional networks**:

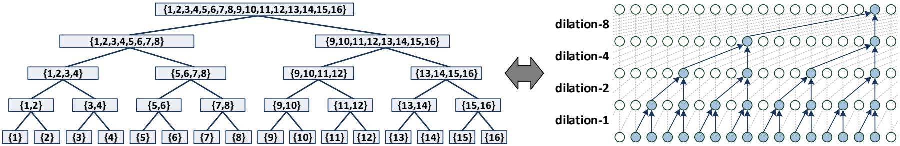


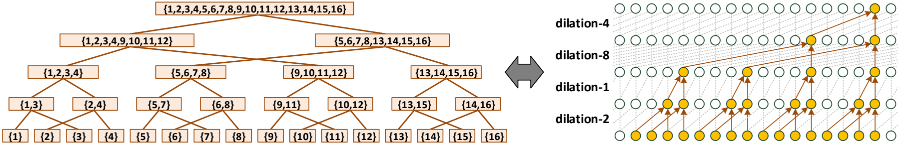
- 1D ConvNets (sequence data)
- Dilated (gapped) conv windows
- No pooling

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

Mixing Tensor Decompositions ⟶ Interconnectivity

With dilated ConvNets, mode (axes) tree underlying corresponding tensor decomposition determines dilation scheme





Mixed tensor decomposition blending different mode (axes) trees corresponds to interconnected networks with different dilations

Efficiency of Interconnectivity

Theorem

Mixed tensor decomposition generates tensors that can only be realized by individual decompositions if these grow quadratically

Corollary

Interconnected dilated ConvNets realize func that cannot be realized by individual networks unless these are quadratically larger

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W/dilated ConvNets interconnectivity brings efficiency!

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- We analyzed efficiency and inductive bias of ConvNet arch features:
  - depth
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  - overlapping operations
  - interconnectivity
- Fundamental tool underlying all of our analyses:

ConvNets $\longleftrightarrow$ **hierarchical tensor decompositions**

Thank You