Title: Expressiveness in Deep Learning via Tensor Networks and Quantum Entanglement - Nadev Cohen

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Abstract: <p>Three fundamental factors determine the quality of a statistical learning algorithm: expressiveness, generalization<wbr /> and optimization. The classic strategy for handling these factors is relatively well understood. In contrast, the radically different approach of deep learning, which in the last few years has revolutionized the world of artificial intelligence, is shrouded by mystery. This talk will describe a series of works aimed at unraveling some of the mysteries revolving expressiveness, arguably the most prominent factor behind the success of deep learning. I will begin by showing that state of the art deep learning architectures, such as convolutional networks, can be represented as tensor networks -- a computational model commonly employed in quantum physics. This connection will inspire the use of quantum entanglement for defining measures of data correlations modeled by deep networks. Next, I will turn to a quantum max-flow / min-cut theorem characterizing the entanglement captured by tensor networks. This theorem will give rise to new results that shed light on expressiveness in deep learning, and in addition, provide new tools for deep network design.</p>

<p> </p>

<p>Works covered in the talk were in collaboration with Yoav Levine, Or Sharir, David Yakira and Amnon Shashua.</p>

Expressiveness in Deep Learning via Tensor Networks and Quantum Entanglement

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Perimeter Institute for Theoretical Physics

7 August 2018

Sources

Deep SimNets
C + Sharir + Shashua
Computer Vision and Pattern Recognition (CVPR) 2016

On the Expressive Power of Deep Learning: A Tensor Analysis
C + Sharir + Shashua
Conference on Learning Theory (COLT) 2016

Convolutional Rectifier Networks as Generalized Tensor Decompositions
C + Shashua
International Conference on Machine Learning (ICML) 2016

Inductive Bias of Deep Convolutional Networks through Pooling Geometry
C + Shashua
International Conference on Learning Representations (ICLR) 2017

Boosting Dilated Convolutional Networks with Mixed Tensor Decompositions
C + Tamari + Shashua
International Conference on Learning Representations (ICLR) 2018

Deep Learning and Quantum Entanglement:
Fundamental Connections with Implications to Network Design
Levine + Yakira + *C* + Shashua
International Conference on Learning Representations (ICLR) 2018

Bridging Many-Body Quantum Physics and Deep Learning via Tensor Networks
Levine + Sharir + *C* + Shashua
arXiv preprint 2018

Collaborators

Yoav Levine

Or Sharir

Amnon Shashua

Ronen Tamari

David Yakira

Source

NVIDIA (`www.slideshare.net/openomics/the-revolution-of-deep-learning`)

Outline

1. Deep Learning Theory: Expressiveness, Generalization and Optimization
2. Convolutional Networks as Tensor Networks
3. Expressiveness of Convolutional Networks
    - Dependencies as Quantum Entanglement
    - Analysis of Supported Entanglement
4. Extensions
5. Conclusion

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)

$\ell : \mathcal{Y}\times\mathcal{Y} \to \mathbb{R}_{\geq 0}$ – 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) $h : \mathcal{X}\to\mathcal{Y}$ that minimizes population loss:

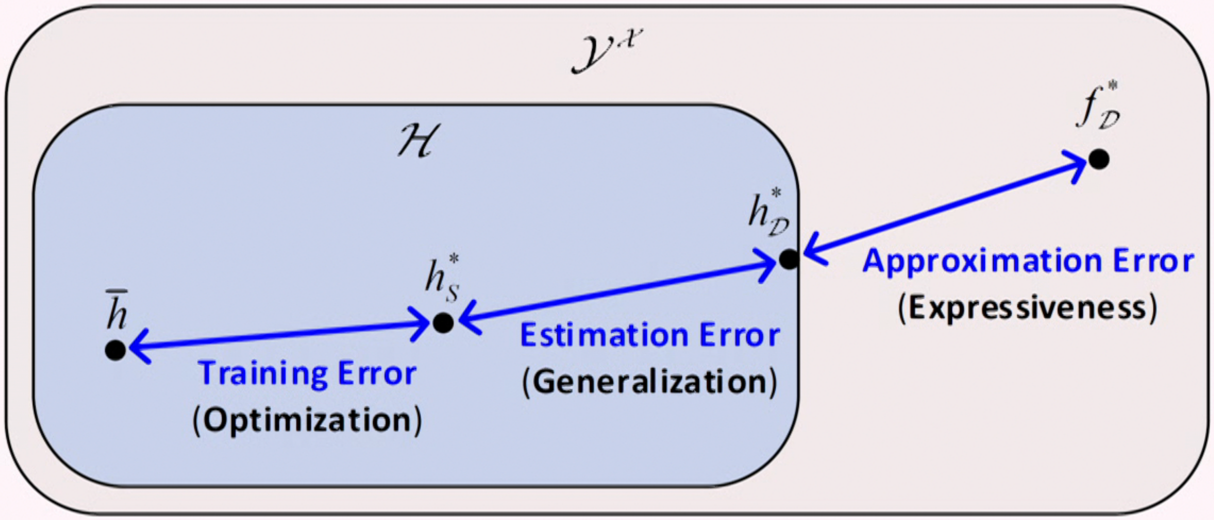
$$L_{\mathcal{D}}(h) := \mathbb{E}_{(X,y)\sim\mathcal{D}}[\ell(y,h(X))]$$

Approach

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

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

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



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

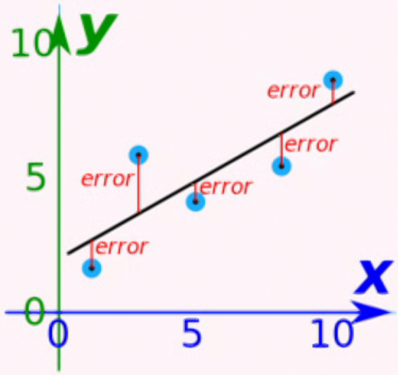
$h^*_{\mathcal{D}}$ – optimal hypothesis ($\text{argmin}_{h \in \mathcal{H}} L_{\mathcal{D}}(h)$)

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

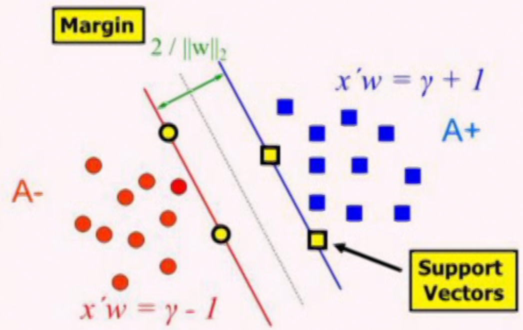
$\bar{h}$ – returned hypothesis

Classical Machine Learning

- Euclidean instance/label spaces: $\mathcal{X} = \mathbb{R}^d$, $\mathcal{Y} = \mathbb{R}^k$
- Linear hypotheses space: $\mathcal{H} = \{\mathbf{x} \mapsto W\mathbf{x} : W \in \mathbb{R}^{k,d}\}$

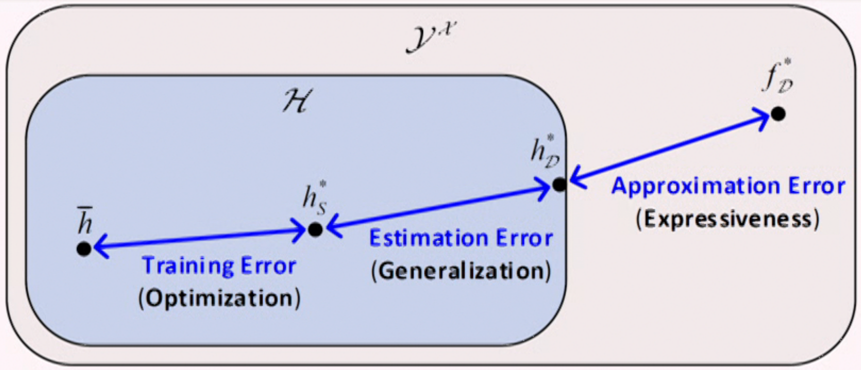


Least Squares Regression



Support Vector Machine

Classical Machine Learning – Three Pillars



Optimization

Empirical loss minimization is a convex program:

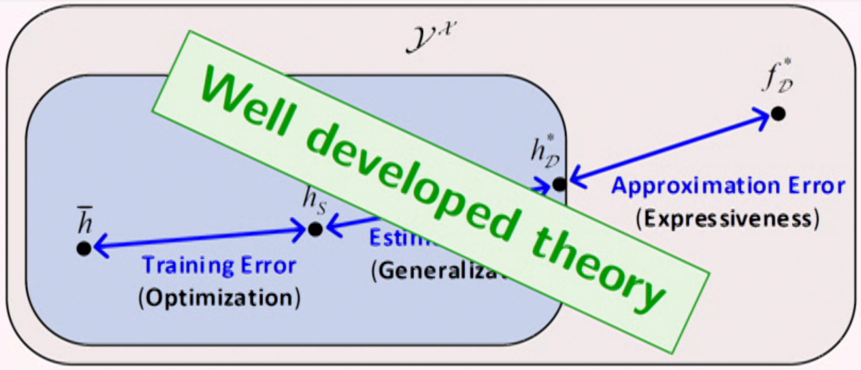
$$\bar{h} \approx h^*_S \quad (\text{ training err} \approx 0 \text{ })$$

Expressiveness & Generalization

Bias-variance trade-off:

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

Classical Machine Learning – Three Pillars



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Expressiveness & Generalization

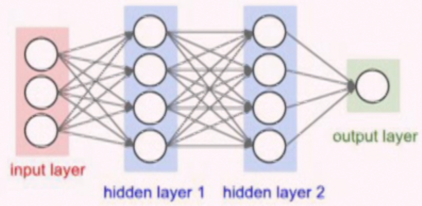
Bias-variance trade-off:

$\mathcal{H}$	approximation err	estimation err
expands	↘	↗
shrinks	↗	↘

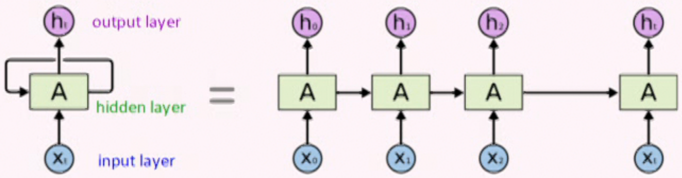
Deep Learning

- Euclidean instance/label spaces
- Composite (non-linear) hypotheses space

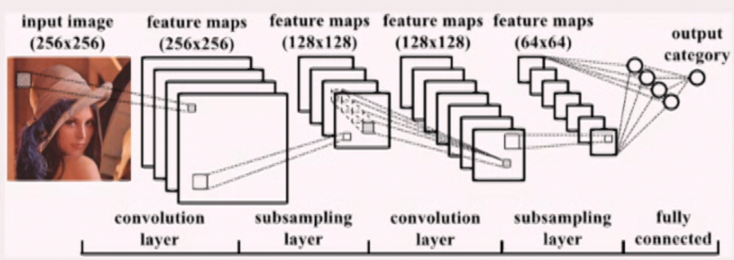
Fully-Connected Networks



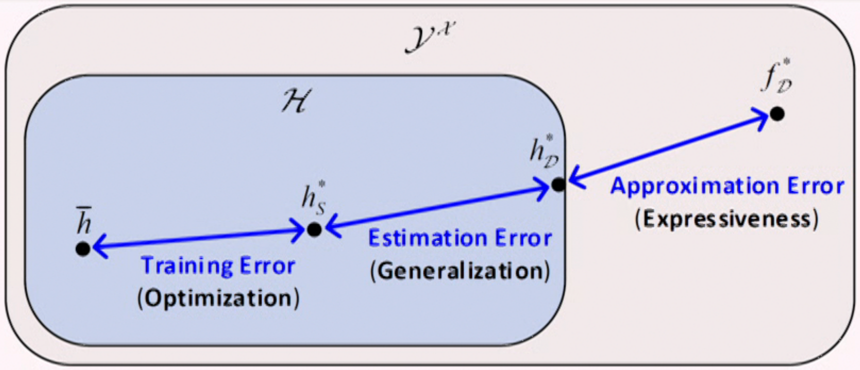
Recurrent Networks



Convolutional Networks



Deep Learning – Three Pillars



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

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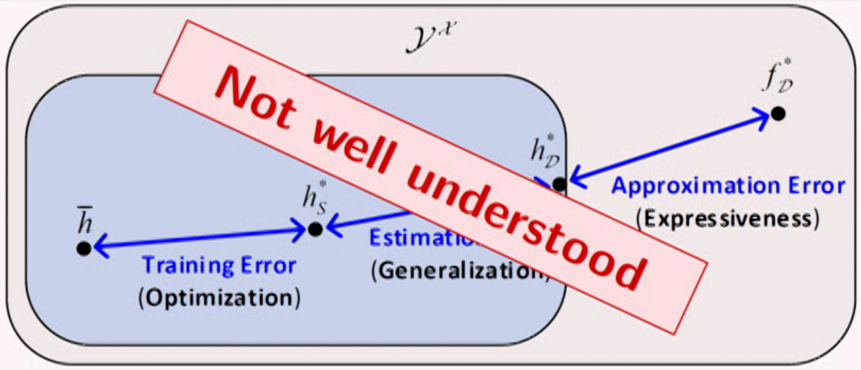
Deep Learning – Three Pillars



Optimization

Empirical loss minimization is a non-convex program:

- h^*_S is not unique – many hypotheses have low training err
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Expressiveness & Generalization

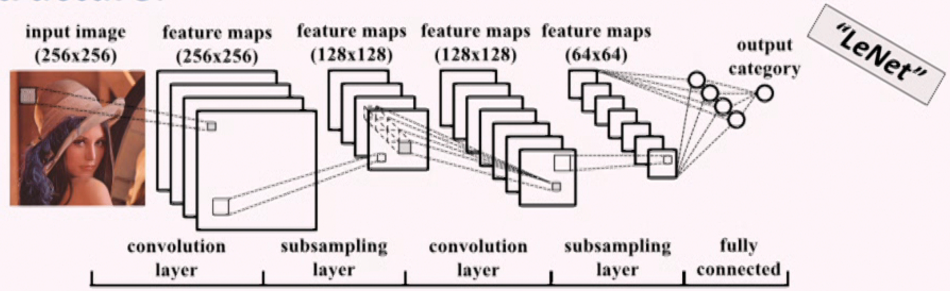
Vast difference from classical ML:

- 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!

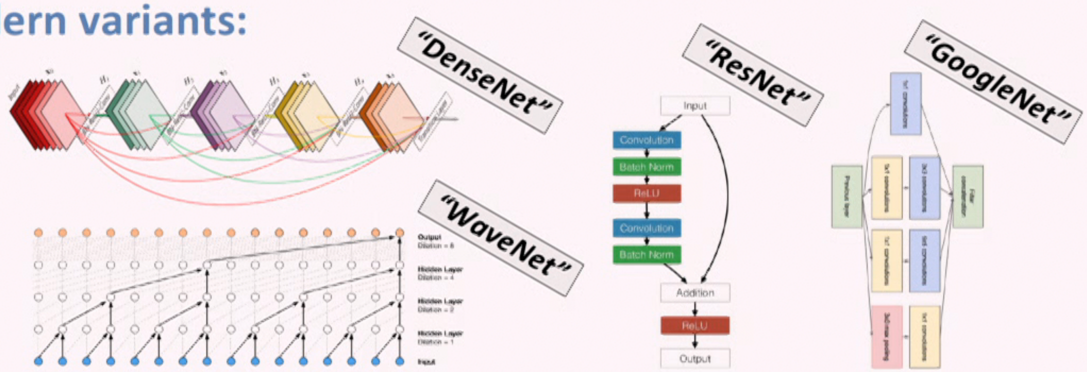
Convolutional Networks

Most successful deep learning arch to date!

Classic structure:



Modern variants:



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

Coefficient Tensor

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

Let $\mathbf{H} = span\{f_i(\mathbf{x})\}_{i=1}^{M}$ be Hilbert space of func over single element

Tensor product $\mathbf{H}^{\otimes N}$ is then Hilbert space of func over N elements

Any $h(\cdot) \in \mathbf{H}^{\otimes N}$ can be written as:

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

where:

- $\mathcal{F}(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ – product (rank-1) tensor, depends only on input

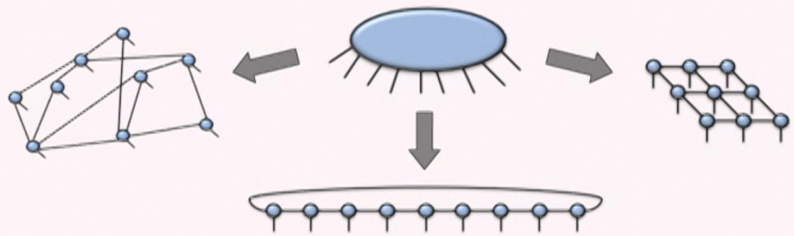
  $\left(\mathcal{F}(\mathbf{x}_1, \ldots, \mathbf{x}_N) := \mathbf{f}(\mathbf{x}_1) \otimes \cdots \otimes \mathbf{f}(\mathbf{x}_N) \; , \; \mathbf{f}(\mathbf{x}_i) := [f_1(\mathbf{x}_i), \ldots, f_M(\mathbf{x}_i)]^\top \right)$

- $\mathcal{A}$ – **coefficient tensor**, fully determines func $h(\cdot)$

Tensor Networks

In quantum physics, high-order tensors are simulated via:

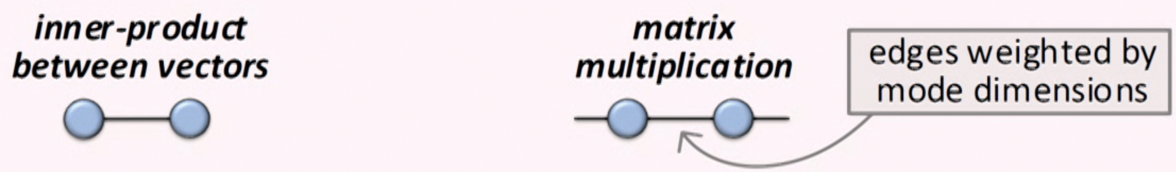
Tensor Networks



Tensor Networks (TN):

- Graphs in which: vertices $\longleftrightarrow$ tensors edges $\longleftrightarrow$ modes

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



Tree Tensor Network $\longrightarrow$ Convolutional Arithmetic Circuit

$$h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \Big\langle \underbrace{\mathcal{A}}_{\text{coeff tensor}} \Big| \underbrace{\mathcal{F}(\mathbf{x}_1, \ldots, \mathbf{x}_N)}_{\text{input product tensor}} \Big\rangle$$

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

$\Longrightarrow$ directly computing general func is intractable

Observation

Decomposing coeff tensor w/**tree TN** gives ConvNet w/linear activation and product pooling – **Convolutional Arithmetic Circuit** (ConvAC)!

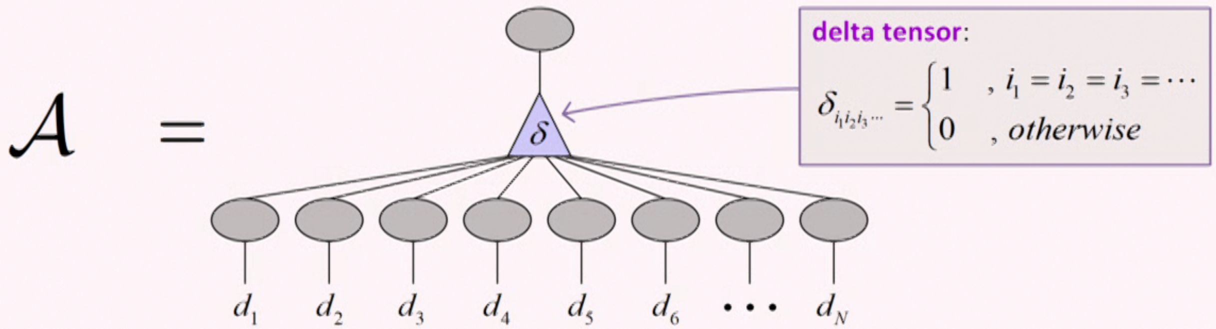
TN topology $\longleftrightarrow$ ConvAC arch

TN tensors $\longleftrightarrow$ ConvAC weights

Example 1: Shallow Model

$$h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \Big\langle \underbrace{\mathcal{A}}_{\text{coeff tensor}} \Big| \underbrace{\mathcal{F}(\mathbf{x}_1, \ldots, \mathbf{x}_N)}_{\text{input product tensor}} \Big\rangle$$

W/star TN applied to coeff tensor:

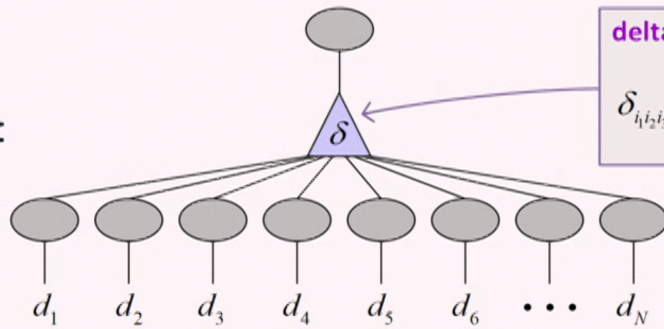


Example 1: Shallow Model

$$h(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \Big\langle \underbrace{\mathcal{A}}_{\text{coeff tensor}} \Big| \underbrace{\mathcal{F}(\mathbf{x}_1,\ldots,\mathbf{x}_N)}_{\text{input product tensor}} \Big\rangle$$

W/star TN applied to coeff tensor:

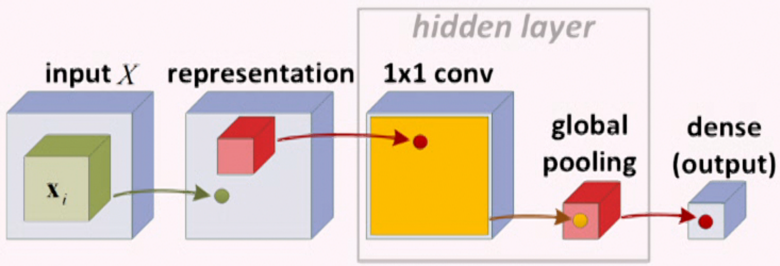
$\mathcal{A} =$



delta tensor:

$$\delta_{i_1 i_2 i_3 \cdots} = \begin{cases} 1 & , i_1 = i_2 = i_3 = \cdots \\ 0 & , \textit{otherwise} \end{cases}$$

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

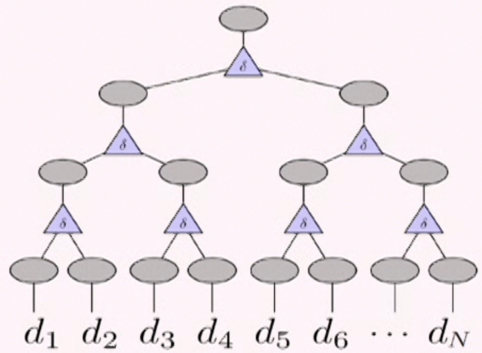


Example 2: Deep Model

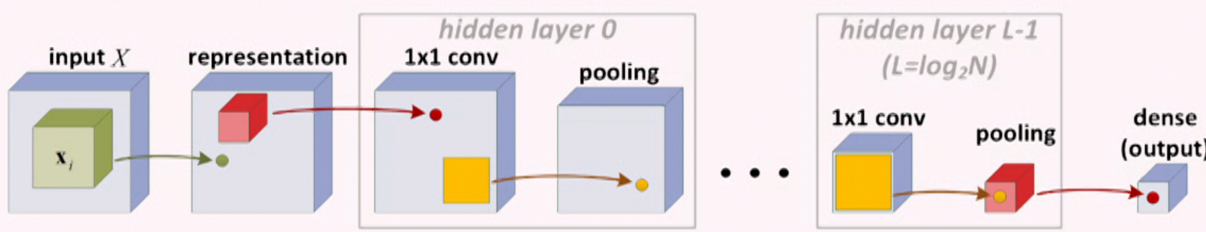
$$h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \Big\langle \underbrace{\mathcal{A}}_{\text{coeff tensor}} \Big| \underbrace{\mathcal{F}(\mathbf{x}_1, \ldots, \mathbf{x}_N)}_{\text{input product tensor}} \Big\rangle$$

W/binary tree TN applied to coeff tensor:

$\mathcal{A} =$



func is computed by deep ConvAC (size-2 pooling windows):

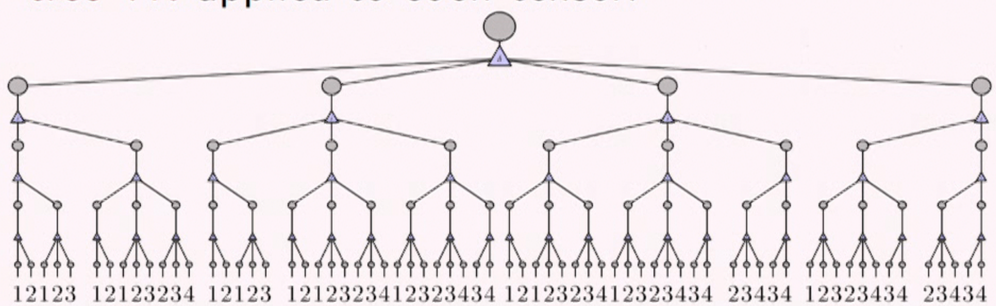


Example 3: Deep Model with Overlaps

$$h(\mathbf{x}_1,\ldots,\mathbf{x}_N) = \Big\langle \underbrace{\mathcal{A}}_{\text{coeff tensor}} \Big| \underbrace{\mathcal{F}(\mathbf{x}_1,\ldots,\mathbf{x}_N)}_{\text{input product tensor}} \Big\rangle$$

W/"duplicated" tree TN applied to coeff tensor:

$\mathcal{A}$ =



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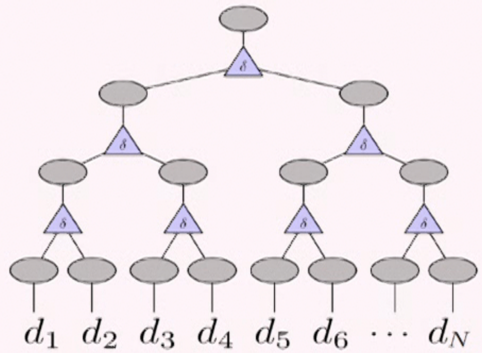
W/binary tree TN applied to coeff tensor:

$\mathcal{A} =$



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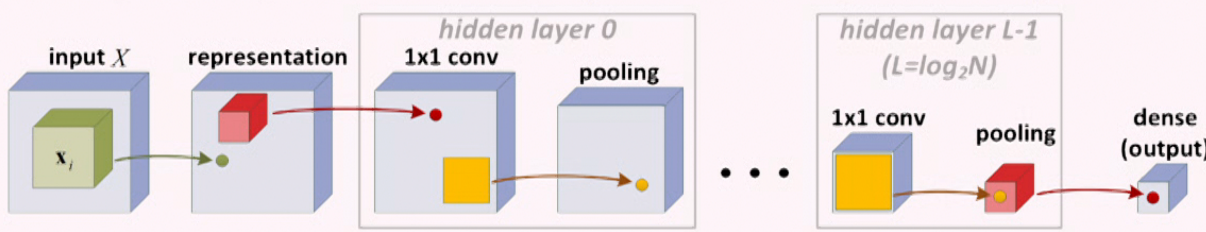
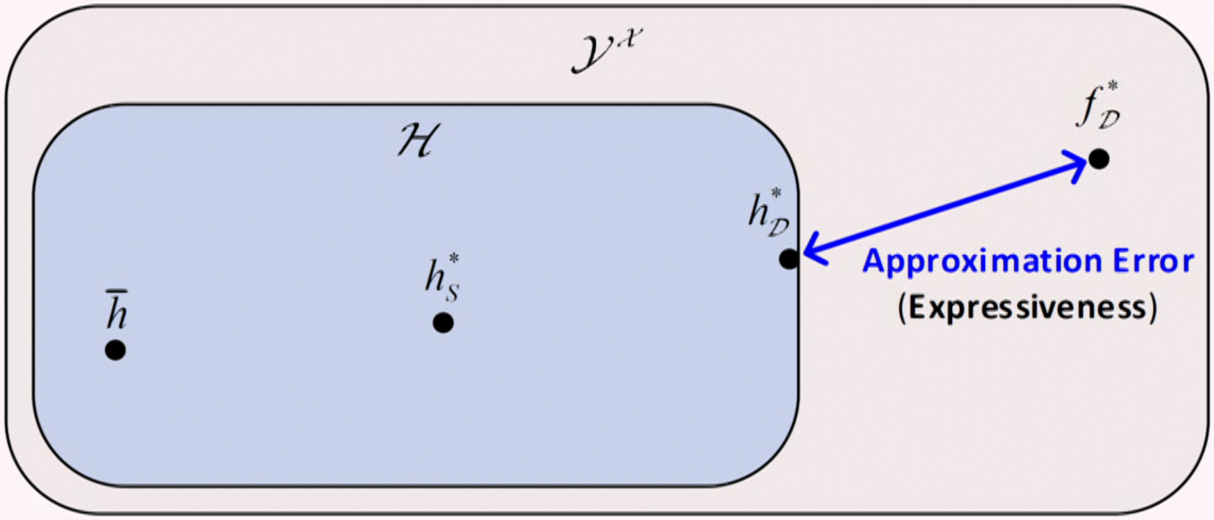


Expressiveness

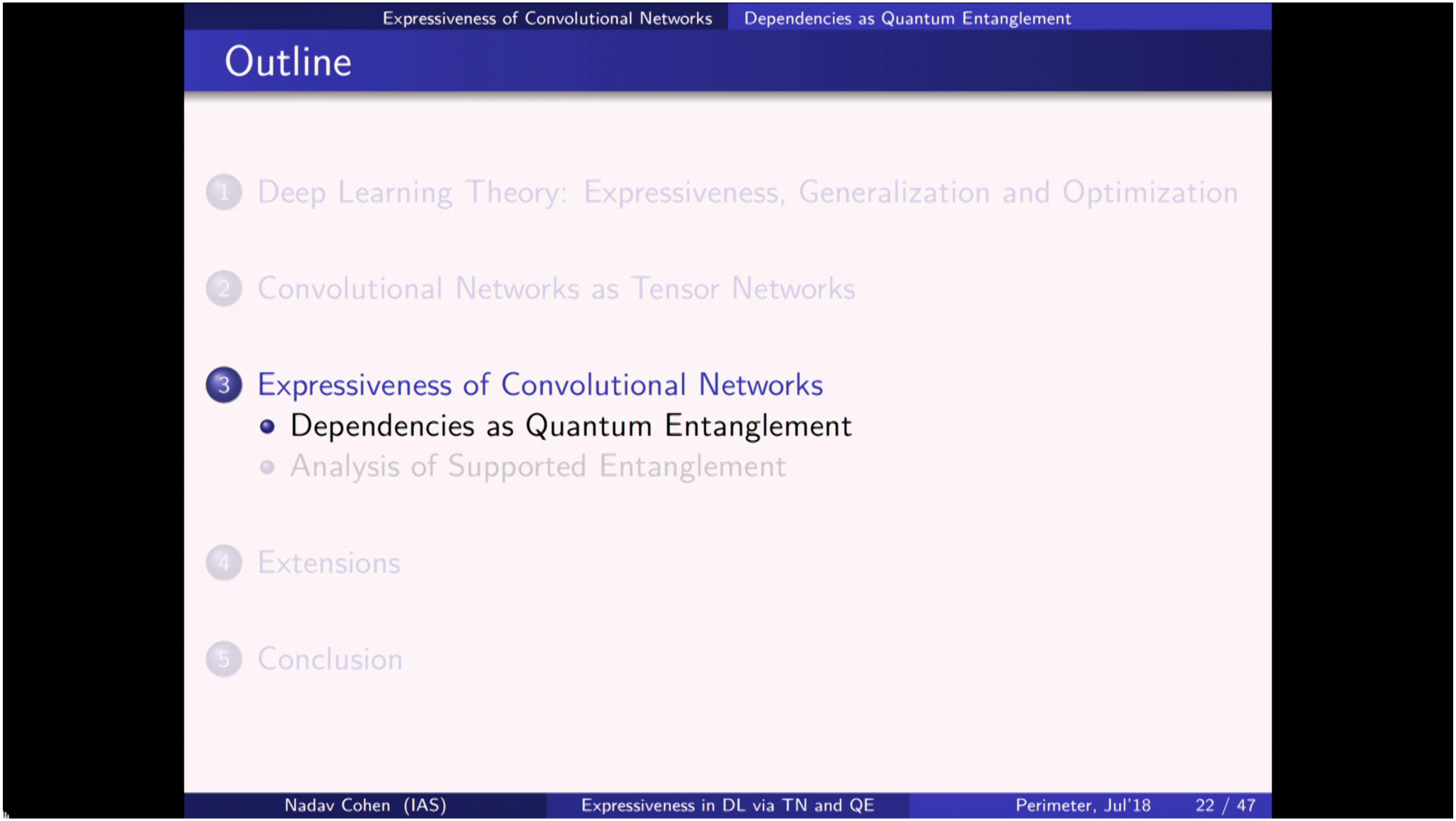


$f^*_{\mathcal{D}}$ – ground truth ($\text{argmin}_{f \in \mathcal{Y}^{\mathcal{X}}} L_{\mathcal{D}}(f)$)

$h^*_{\mathcal{D}}$ – 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


Expressiveness of Convolutional Networks
Dependencies as Quantum Entanglement
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1 Deep Learning Theory: Expressiveness, Generalization and Optimization
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Nadav Cohen (IAS)
Expressiveness in DL via TN and QE
Perimeter, Jul'18
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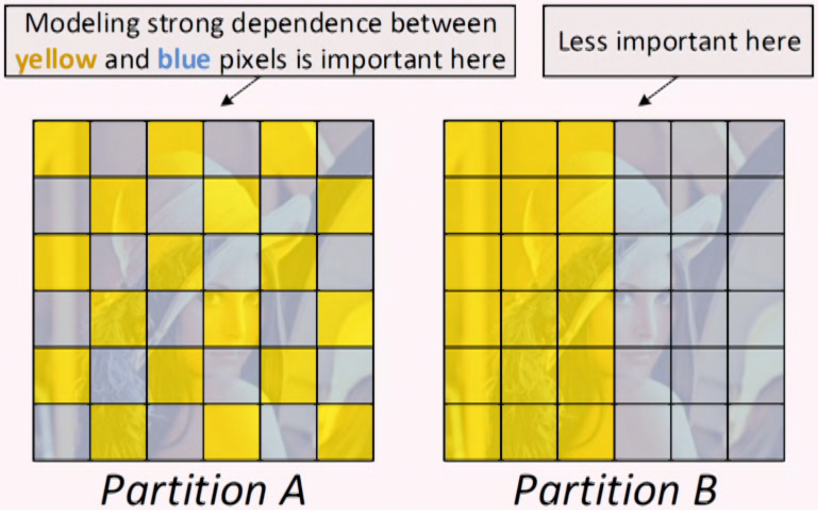
Modeling Dependencies in Data

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

Key property of such func:

dependencies modeled between sets of input elements



Q: What kind of dependencies do ConvNets model?

Q: How do these relate to network arch?

Quantum Entanglement

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

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

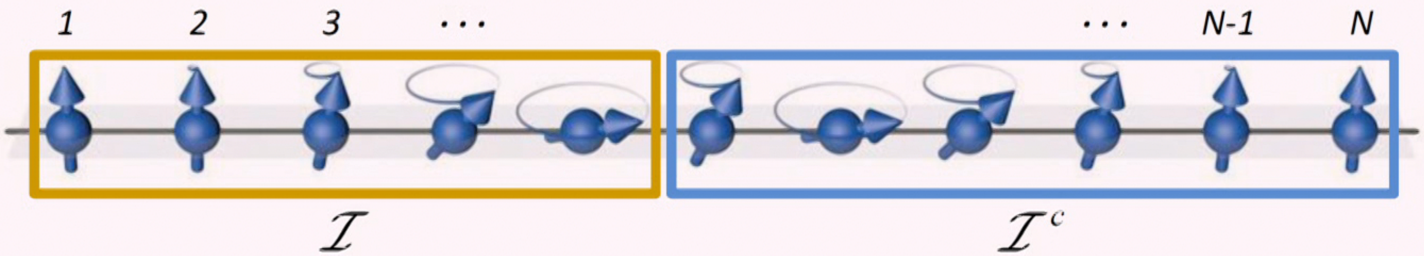
System of N particles is represented as vec in tensor product space:

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

Quantum entanglement measures quantify "dependencies" that system state models between sets of particles

Quantum Entanglement (cont'd)

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

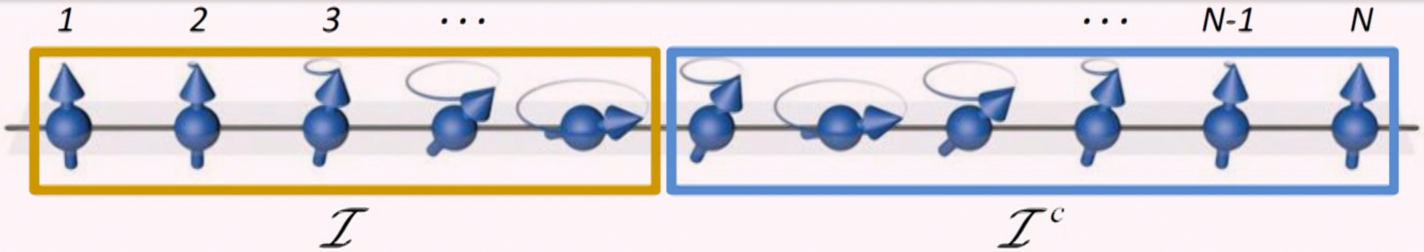


Consider partition of the N particles into sets $\mathcal{I}$ and $\mathcal{I}^c$

$[\![\mathcal{A}]\!]_{\mathcal{I}}$ – 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)



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

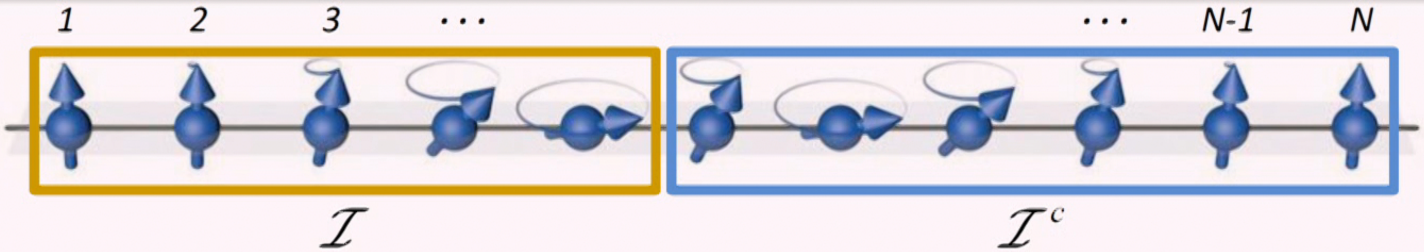
$[\![\mathcal{A}]\!]_{\mathcal{I}}$ – matricization of $\mathcal{A}$ w.r.t. $\mathcal{I}$

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 $(\sigma_1^2, \ldots, \sigma_R^2) / \|\boldsymbol{\sigma}\|_2^2$

Quantum Entanglement (cont'd)



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

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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**: $\|\boldsymbol{\sigma}\|_0 = rank[\![\mathcal{A}]\!]_{\mathcal{I}}$

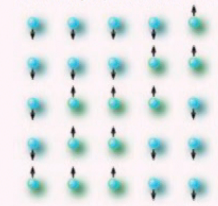
Measuring Dependence with Entanglement

Structural equivalence:

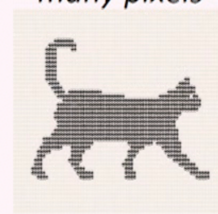
quantum many-body state

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

state of many particles



func over many pixels



func over many local elements

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

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

Measuring Dependence with Entanglement – Interpretation

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

When func $h(\cdot)$ is separable w.r.t. input sets $\mathcal{I}/\mathcal{I}^c$:

$$\exists g, g' \text{ s.t. } h(\mathbf{x}_1, \ldots, \mathbf{x}_N) = g\left((\mathbf{x}_i)_{i \in \mathcal{I}}\right) \cdot g'\left((\mathbf{x}_{i'})_{i' \in \mathcal{I}^c}\right)$$

it does not model any dependence between $\mathcal{I}/\mathcal{I}^c$

(In probabilistic setting, this means $\mathcal{I}/\mathcal{I}^c$ are stat independent)

Entanglement measures on $\mathcal{A}$ quantify dist of $h(\cdot)$ from separability:

- $\mathcal{A}$ has high (low) entanglement w.r.t. $\mathcal{I}/\mathcal{I}^c$
  $\Longrightarrow$ $h(\cdot)$ is far from (close to) separability w.r.t. $\mathcal{I}/\mathcal{I}^c$
- Choice of entanglement measure determines dist metric

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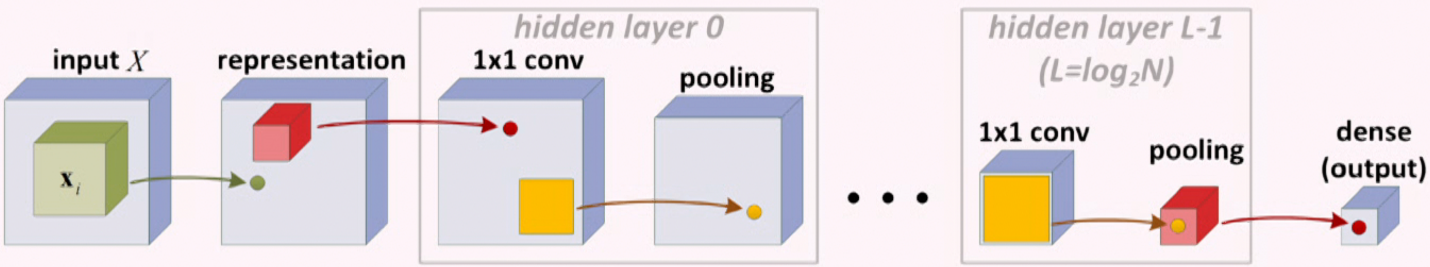
5. Conclusion

Convolutional Arithmetic Circuits $\longleftrightarrow$ Tensor Networks

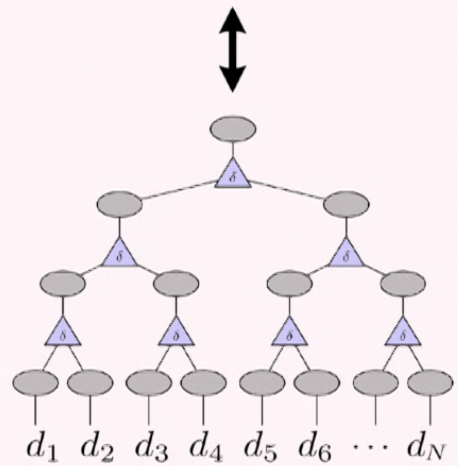
Recap

Func realized by ConvAC may be represented via tree TN



structural correspondence

ConvAC	TN
input elements	terminal nodes
# of layers	tree depth
layer widths	bond dims
pool geometry	connectivity
overlaps	duplications
...	...



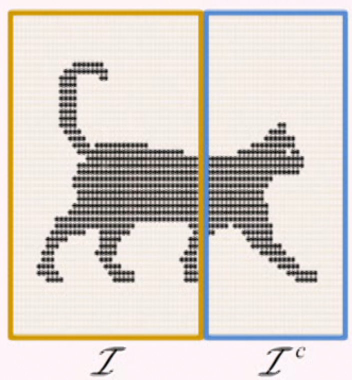
Entanglement via Minimal Cuts

Theorem (Quantum Max Flow/Min Cut)

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

ConvAC entanglement between input sets

TN min cut separating respective node sets



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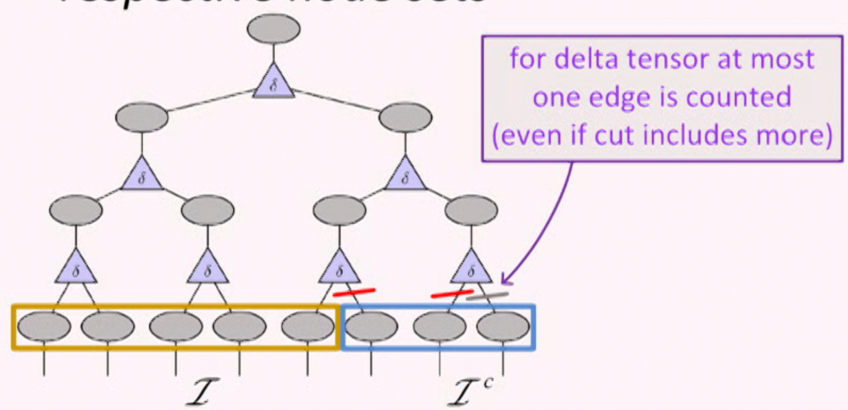
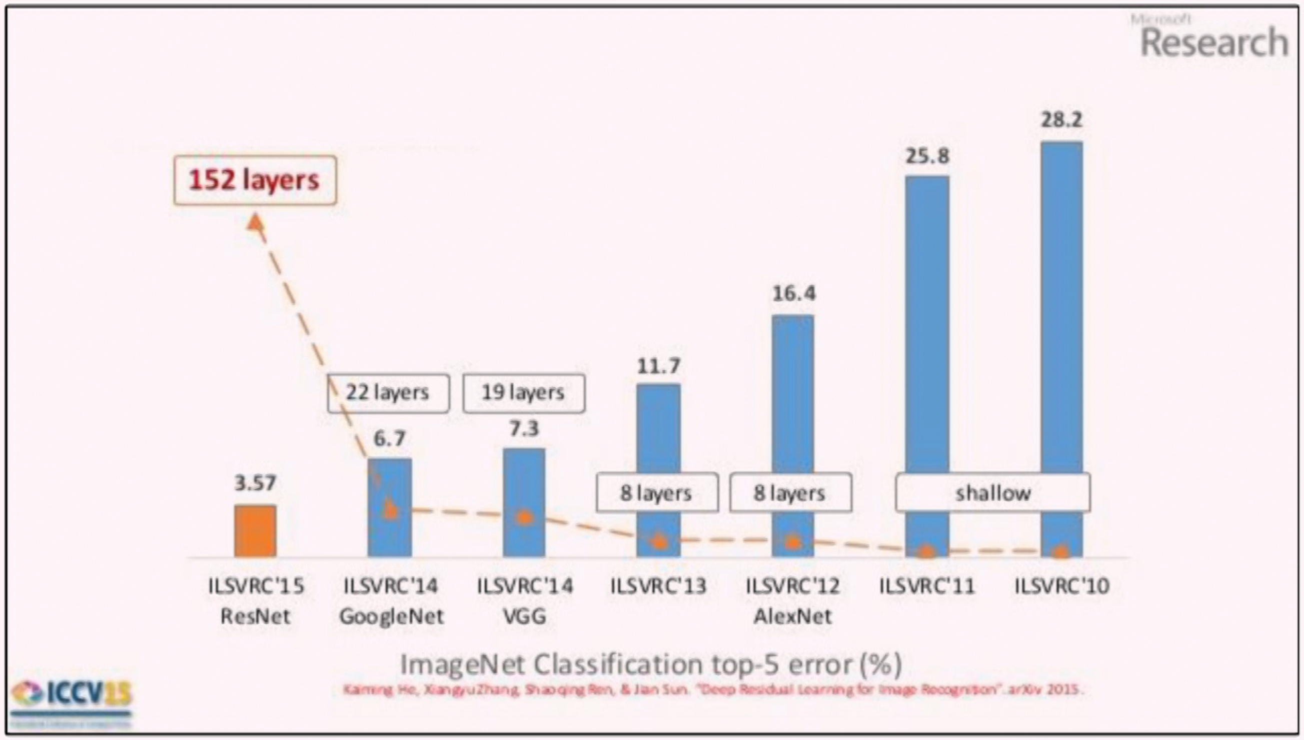


We may analyze the effect of ConvAC arch on the dependencies (entanglement) it can model!

Depth

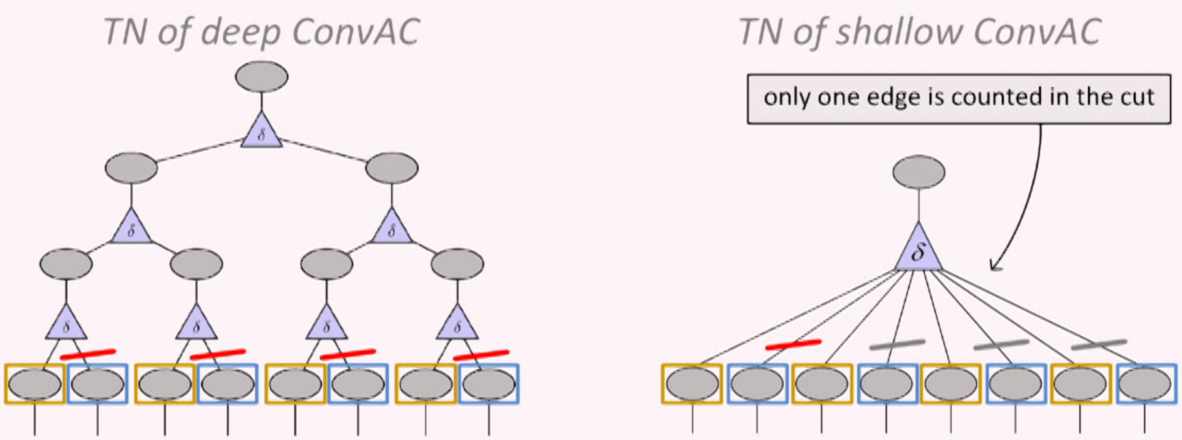
Conjecture – depth efficiency

Deep ConvNets realize func requiring shallow ConvNets to grow unfeasibly



Depth (cont'd)

For certain partitions of terminal nodes, min cut in TN of deep ConvAC is exponentially larger than in TN of shallow ConvAC



This implies:

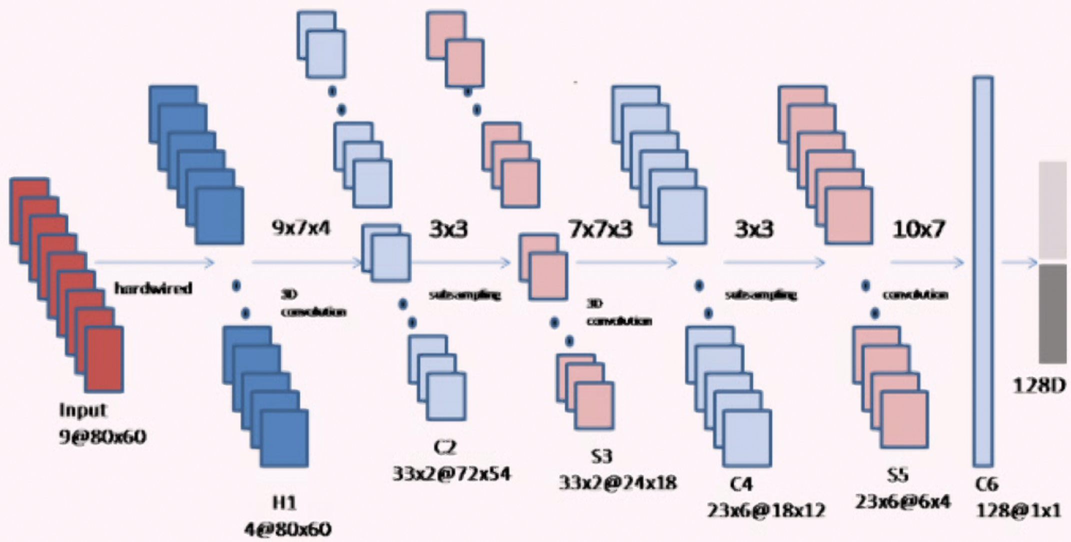
Claim

Deep ConvAC can model dependencies (entanglements) requiring shallow ConvAC to have exponential width

Depth efficiency proven for ConvAC!

Layer Widths

Currently no principle for setting widths (# of channels) of ConvNet layers



Q: *What are the implications of widening one layer vs. another?*

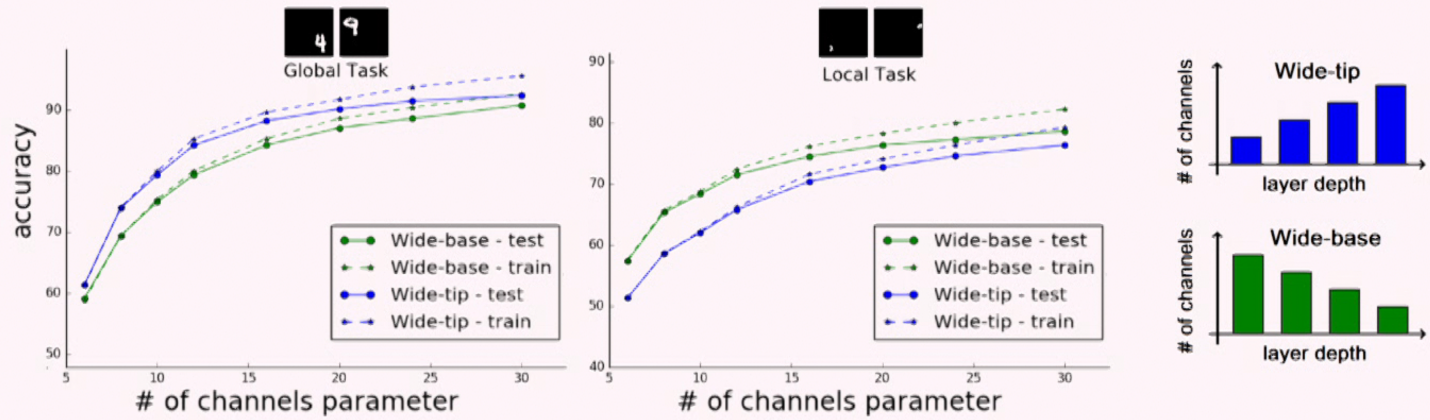
Q: *Can the widths be tailored for a given task?*

Layer Widths (cont'd)

Claim

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

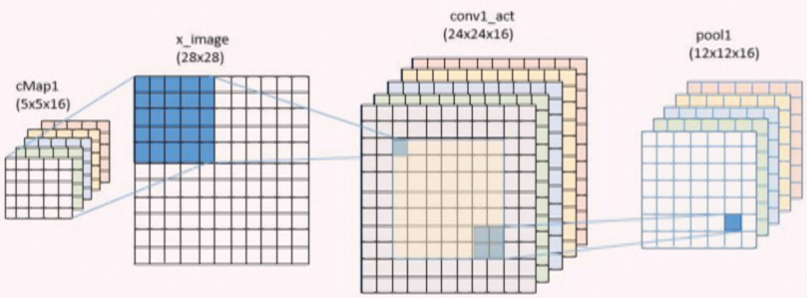
Experiment



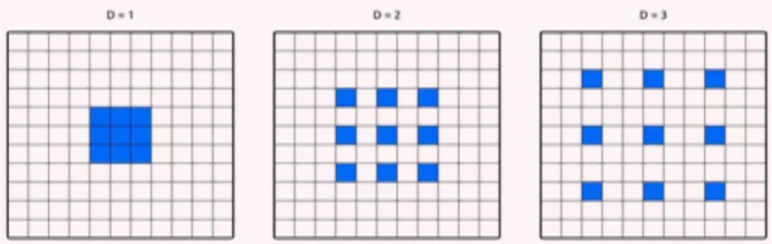
ConvAC layer widths can be tailored to maximize dependencies (entanglements) required for given task!

Pooling Geometry

ConvNets typically employ square conv/pool windows



Recently, dilated windows have also become popular



Q: *What are the implications of one window geometry vs. another?*

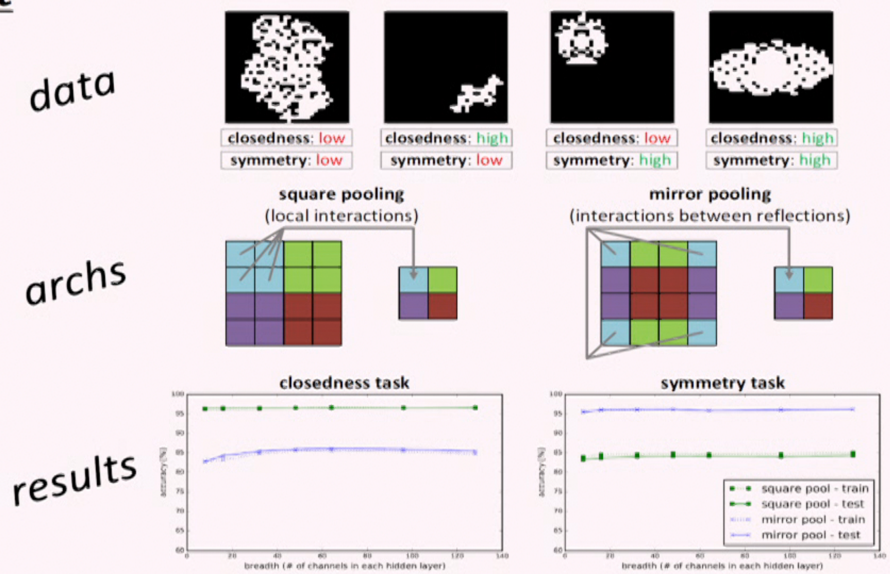
Q: *Can the geometries be tailored for a given task?*

Pooling Geometry (cont'd)

Claim

Input elements pooled together early have stronger dependence

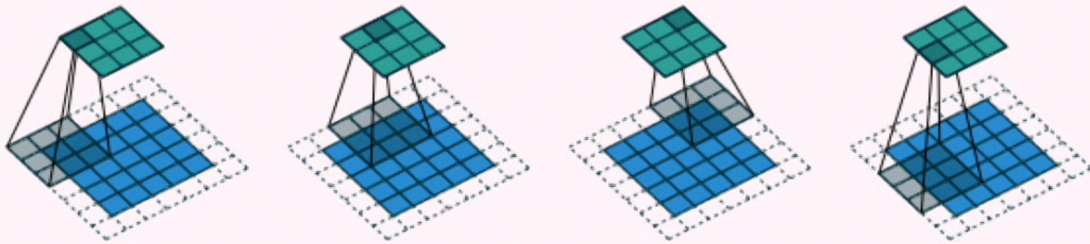
Experiment

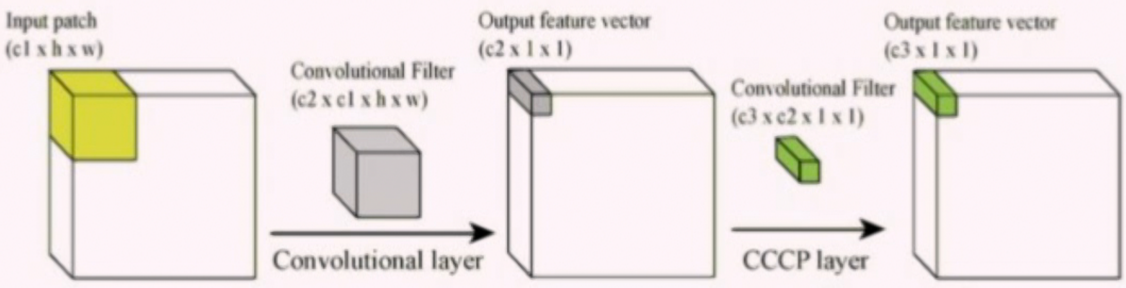


ConvAC pooling geometry can be tailored to maximize dependencies (entanglements) required for given task!

Overlapping Operations

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





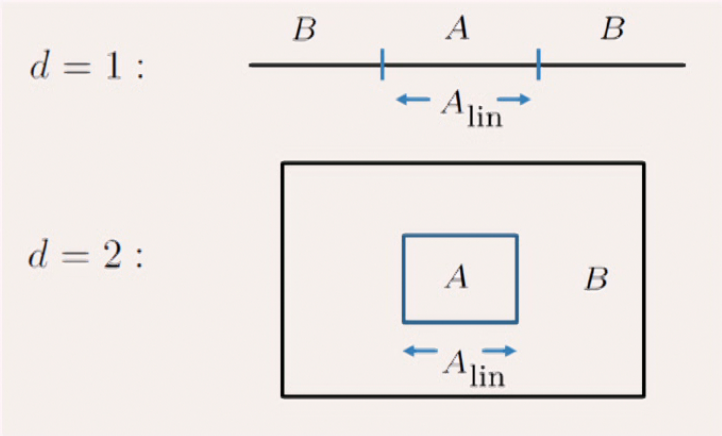
Q: *What are the implications of introducing overlaps?*

Overlapping Operations (cont'd)

Claim

Overlaps in conv/pool operations allow modeling dependencies that otherwise require exponential size

Area/volume law:



area law

entanglement $\propto A_{\text{lin}}^{d-1}$

volume law

entanglement $\propto A_{\text{lin}}^{d}$

ConvAC w/overlaps supports volume law entanglement!

Outline

1. Deep Learning Theory: Expressiveness, Generalization and Optimization
2. Convolutional Networks as Tensor Networks
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   - Dependencies as Quantum Entanglement
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Other Types of Convolutional Networks

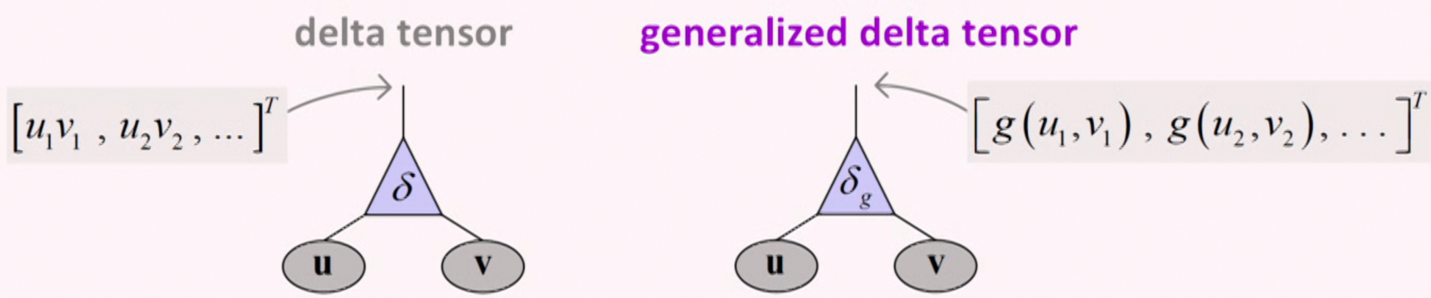
We established equivalence:

$$\text{ConvAC} \longleftrightarrow \text{TN}$$

and used it to analyze dependencies (entanglement) ConvAC can model

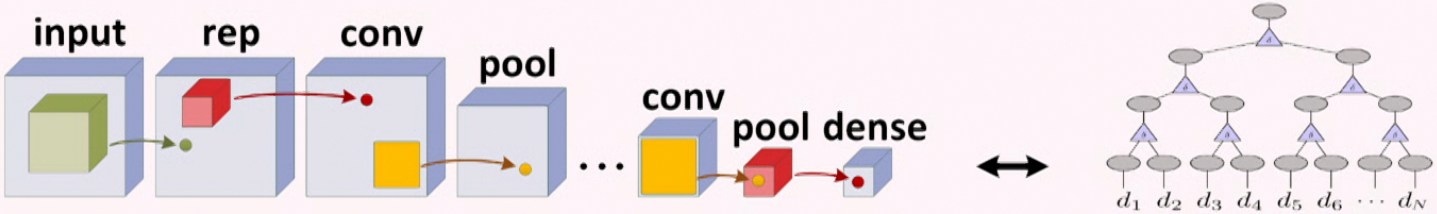
ConvAC delivers promising results in practice, but other types of ConvNets (e.g. w/ReLU activation and max/ave pooling) are more common

Our analysis extends to other types of ConvNets if we generalize the notion of a delta tensor:

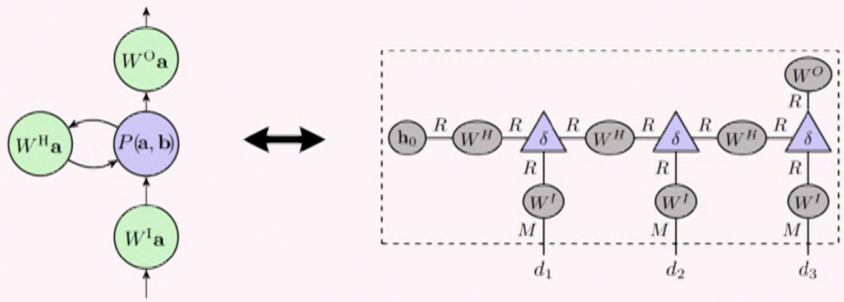


Recurrent Networks

We analyzed **convolutional** nets via equivalence to TN w/**tree** arch



Analysis extends to **recurrent** nets via equivalence to TN w/**chain** arch



Recurrent nets process data sequentially; ability to model dependencies (entanglement) quantifies memory

Outline

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Recap

- Three pillars of statistical learning theory:

  Expressiveness   Generalization   Optimization

Recap

- Three pillars of statistical learning theory:

  Expressiveness Generalization Optimization

  - Well developed theory for classical ML
  - Limited understanding for DL

- State of the art DL arch can be represented as TN:

  convolutional nets $\longleftrightarrow$ tree TN

  recurrent nets $\longleftrightarrow$ chain TN

- Quantum entanglement quantifies dependencies modeled by DL arch

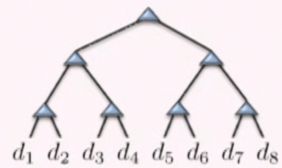
- Quantum max flow/min cut theorem

  $\Longrightarrow$ new results on expressiveness in DL!

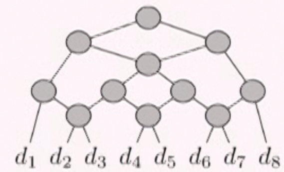
Convolutional Networks for Simulating Quantum States?

For quantum sim, expressiveness of tree TN typically enhanced via loops:

tree TN

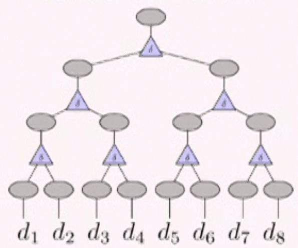


MERA TN

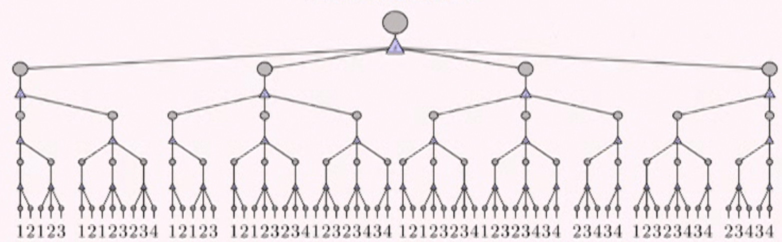


Overlaps in ConvAC give rise to new form of enhancement – duplications:

TN of ConvAC w/no overlaps



TN of ConvAC w/overlaps



Provides volume law entanglement w/efficient calc of wave func amplitude

Useful for quantum sim?