# Expressiveness in Deep Learning via Quantum Entanglement

**Nadav Cohen**

Tel Aviv University

*From Quantum Computing to Quantum Chemistry:*
*Theory, Platforms, and Practical Applications (TAU, CECAM, ISF)*

15 September 2019

# 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*

**Quantum Entanglement in Deep Learning Architectures**
Levine + Sharir + *C* + Shashua
*Physical Review Letters (PRL) 2019*

# Collaborators

Yoav Levine

Or Sharir

Amnon Shashua

Ronen Tamari

David Yakira

# EVERY INDUSTRY WANTS DEEP LEARNING

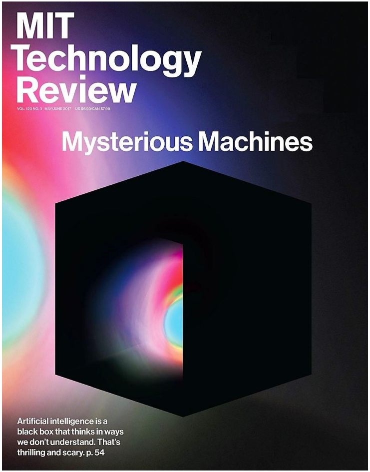
| Cloud Service Provider | Medicine | Media & Entertainment | Security & Defense | Autonomous Machines |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| ➢ Image/Video classification | ➢ Cancer cell detection | ➢ Video captioning | ➢ Face recognition | ➢ Pedestrian detection |
| ➢ Speech recognition | ➢ Diabetic grading | ➢ Content based search | ➢ Video surveillance | ➢ Lane tracking |
| ➢ Natural language processing | ➢ Drug discovery | ➢ Real time translation | ➢ Cyber security | ➢ Recognize traffic sign |

Source

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

# Limited Formal Understanding




**Intelligent Machines**

## The Dark Secret at the Heart of AI

No one really knows how the most advanced algorithms do what they do. That could be a problem.

by Will Knight April 11, 2017

**Last year, a strange self-driving car was released onto the quiet** roads of Monmouth County, New Jersey. The experimental vehicle, developed by researchers at the chip maker Nvidia, didn't look different from other autonomous cars, but it was unlike anything demonstrated by Google, Tesla, or General Motors, and it showed the rising power of artificial intelligence. The car didn't follow a single instruction provided by an engineer or programmer. Instead, it relied entirely on an algorithm that had taught itself to drive by watching a human do it.

# 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

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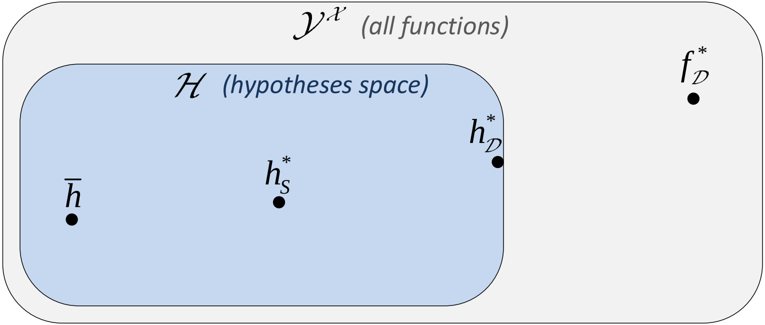
**Approach**

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

$$L_S(h) := \frac{1}{m}\sum\nolimits_{i=1}^{m} \ell(y_i, h(X_i))$$

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

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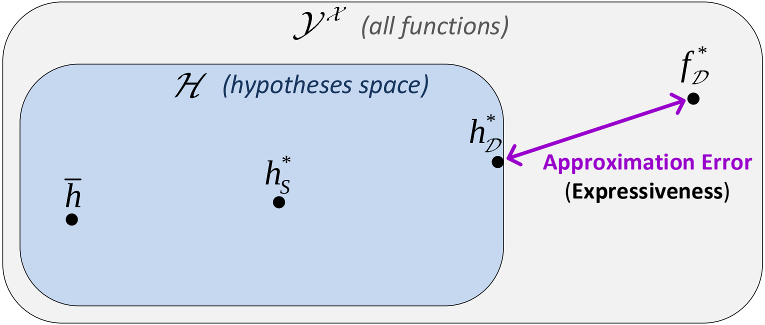


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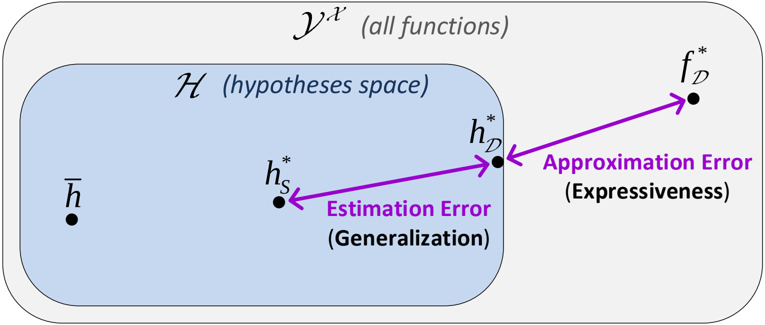


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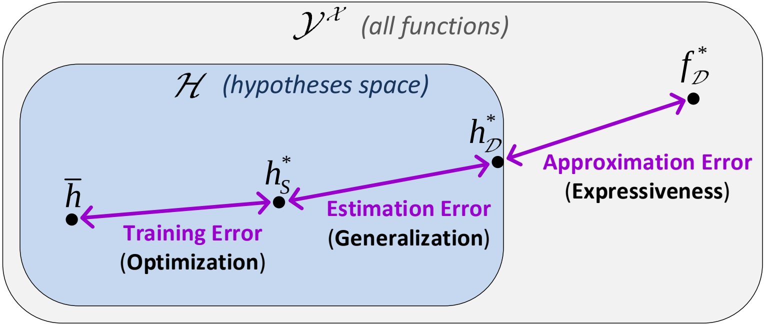


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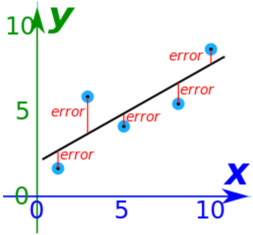
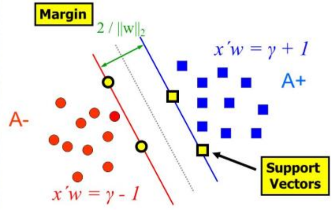
# Classical Machine Learning

- 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*

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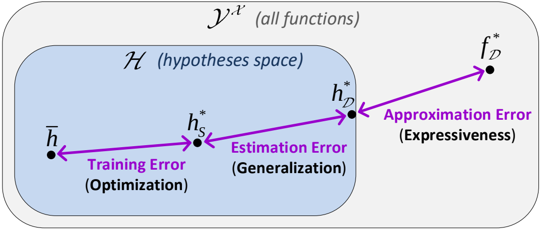

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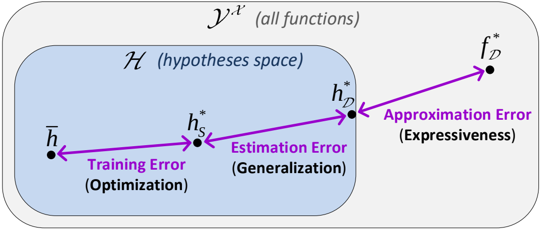


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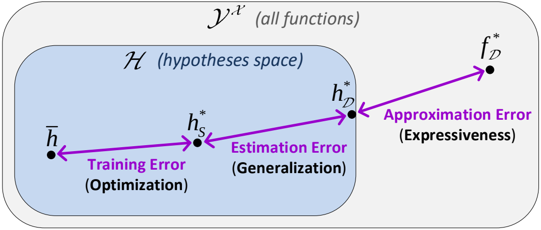


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Bias-variance trade-off:

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| *expands* | $\searrow$ | $\nearrow$ |
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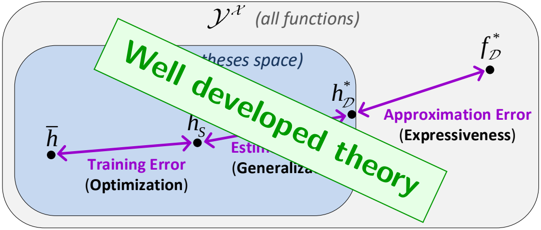


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- Euclidean instance/label spaces
- Composite (non-linear) hypotheses space

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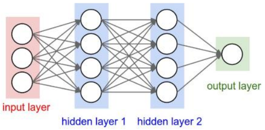
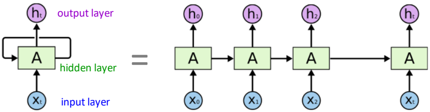
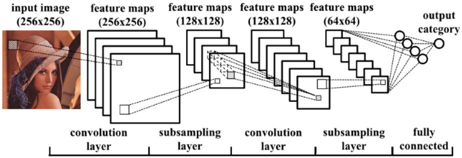



**Recurrent Networks**




**Convolutional Networks**



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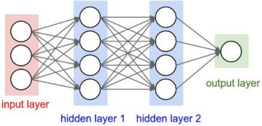


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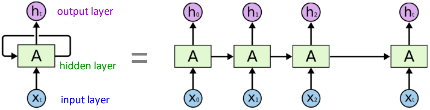


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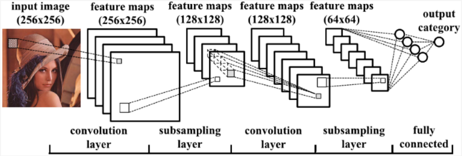

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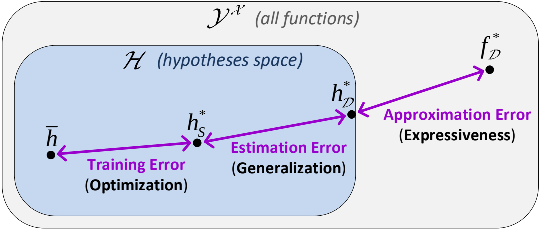

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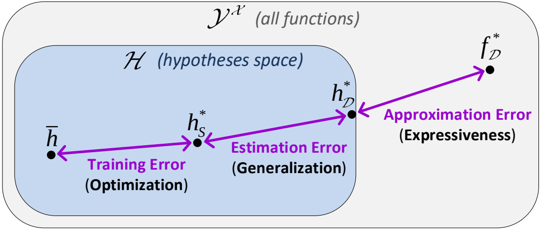


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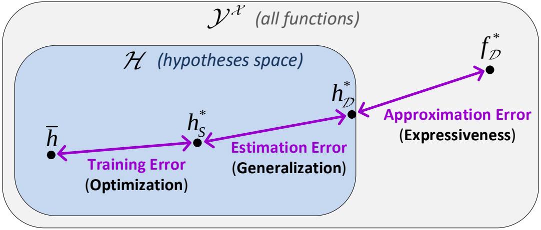


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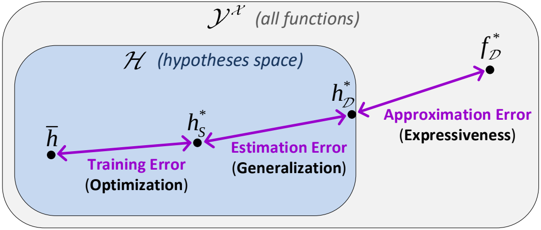


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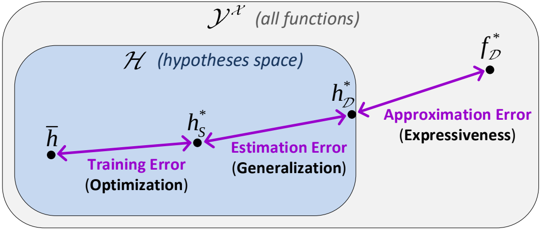


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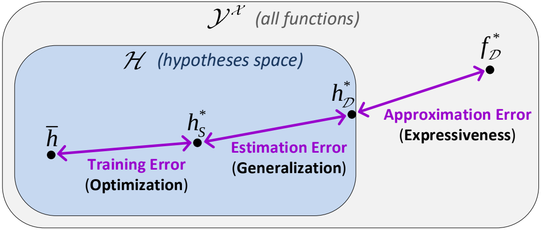


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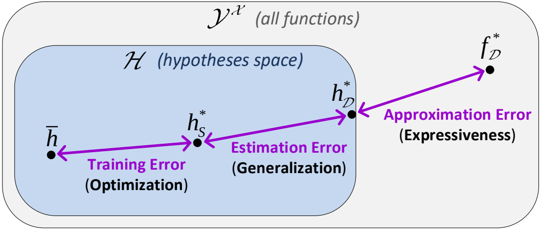


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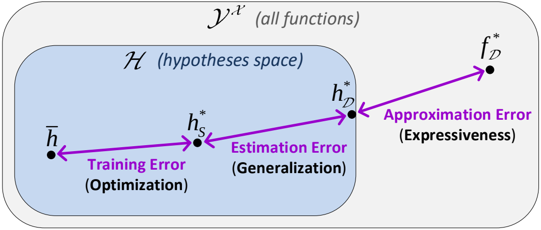


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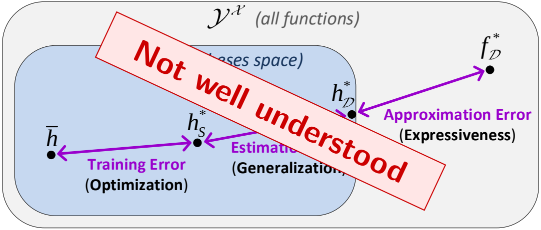


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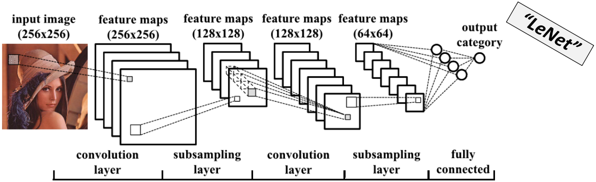
# Outline

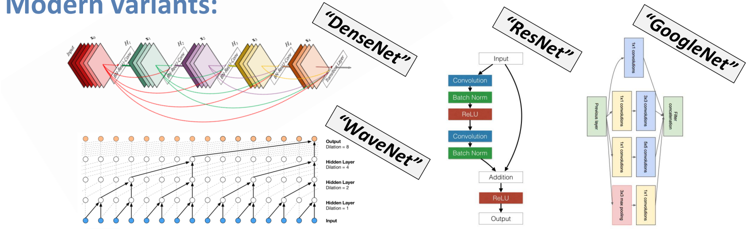
# Convolutional Networks

Most successful deep learning arch to date!

## Classic structure:




## Modern variants:




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

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

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

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

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

# Tensor Networks

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

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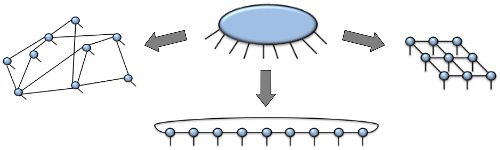

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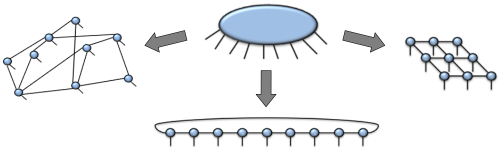

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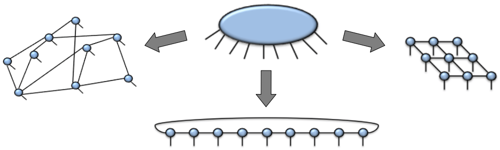

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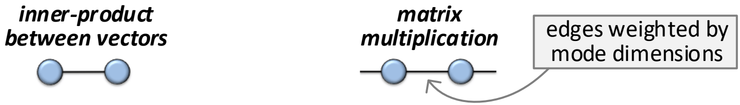
- Graphs in which: vertices $\longleftrightarrow$ tensors edges $\longleftrightarrow$ modes


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



# Tree Tensor Network $\longrightarrow$ Convolutional Arithmetic Circuit

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

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TN topology $\longleftrightarrow$ ConvAC arch

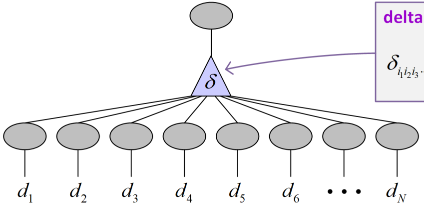
TN tensors $\longleftrightarrow$ ConvAC weights

# 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:

$\mathcal{A} \;=$




**delta tensor**:

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

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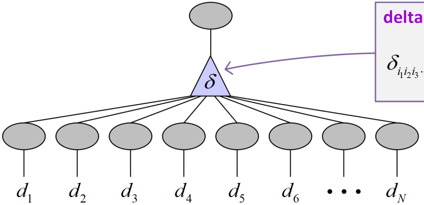


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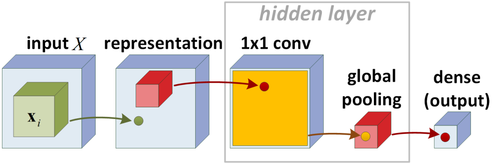
func is computed by shallow ConvAC (single hidden layer, global pooling):



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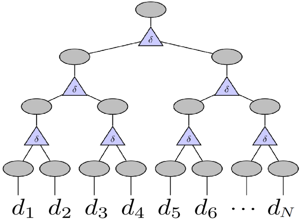

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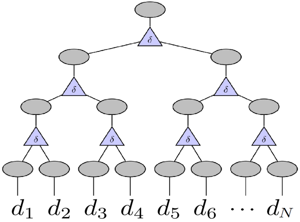
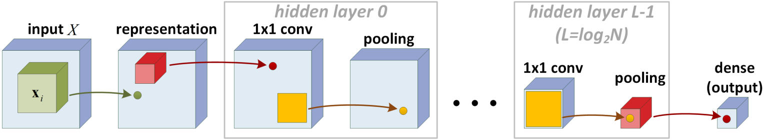



func is computed by deep ConvAC (size-2 pooling windows):



# Example 3: Deep Model with Overlaps

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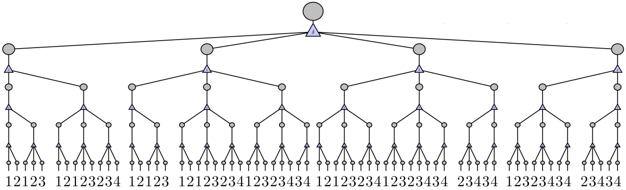

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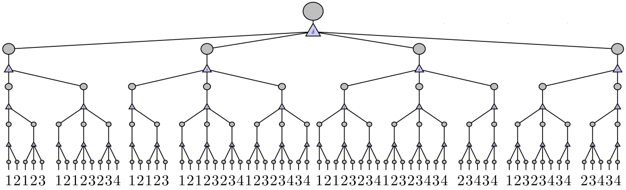


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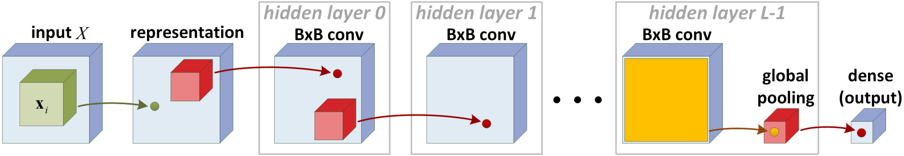
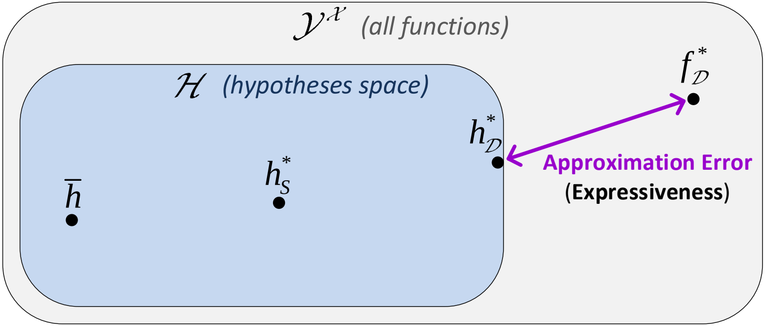


# Outline

# Expressiveness




$f^*_{\mathcal{D}}$ – ground truth (minimizer of population loss over all func)

$h^*_{\mathcal{D}}$ – optimal hypothesis (minimizer of population loss over $\mathcal{H}$)

$h^*_S$ – empirically optimal hypothesis (minimizer of empirical loss over $\mathcal{H}$)

$\bar{h}$ – returned hypothesis

# Outline

# Modeling Dependencies in Data

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

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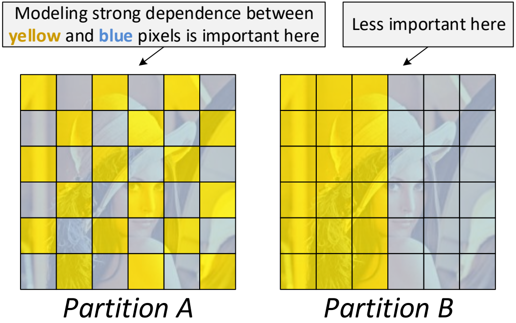

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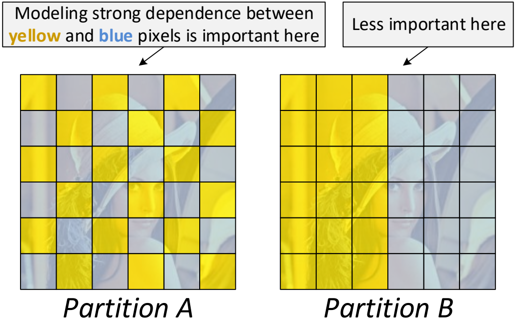


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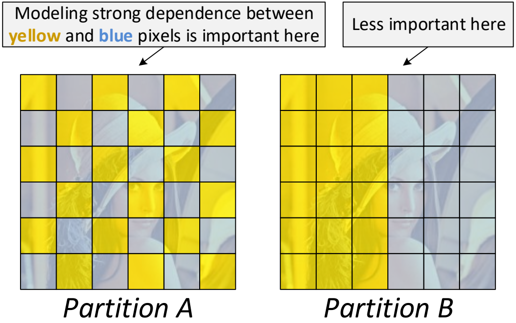


***Q:*** What kind of dependencies do ConvNets model?

***Q:*** How do these relate to network arch?

# Quantum Entanglement

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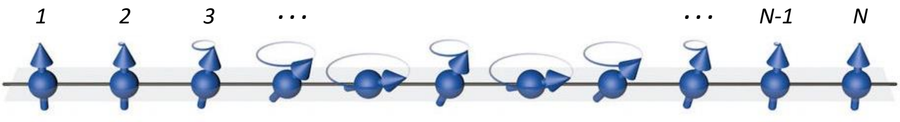


In quantum physics, particle is represented as vec in Hilbert space:

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

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

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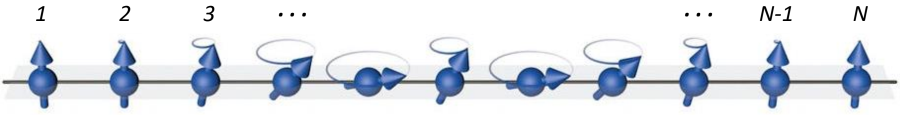


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**Quantum entanglement** quantifies "dependencies" that system state models between sets of particles

# Quantum Entanglement (cont'd)

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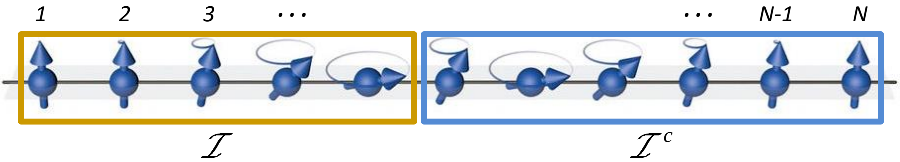


Consider partition of particles into sets $\mathcal{I}$ and $\mathcal{I}^c$

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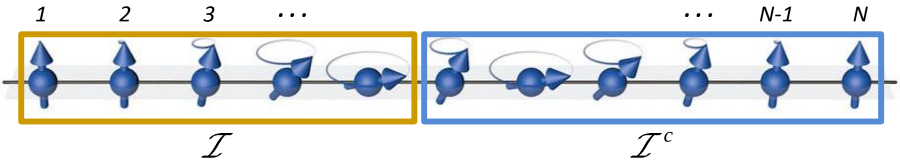


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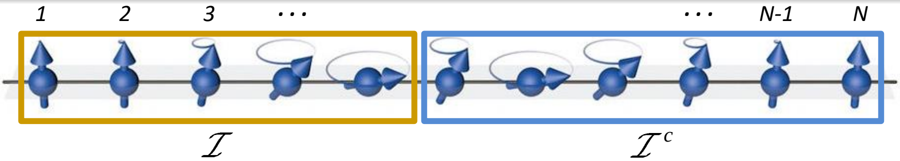
$[\![\mathcal{A}]\!]_{\mathcal{I}}$ – matricization of coeff tensor $\mathcal{A}$ w.r.t. $\mathcal{I}$:

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

# Quantum Entanglement (cont'd)

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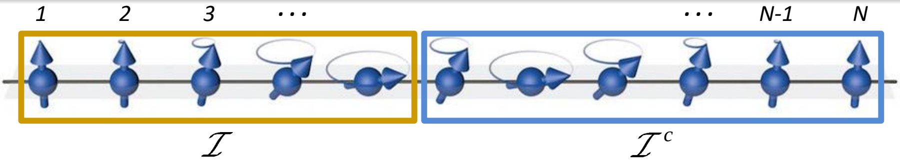


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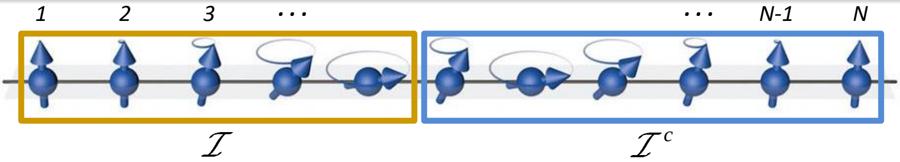


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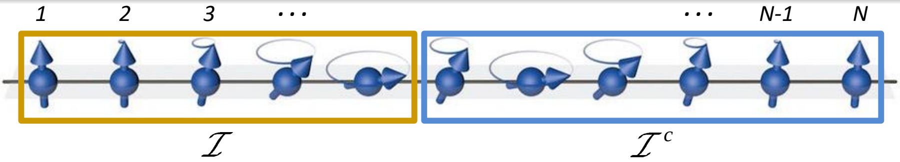


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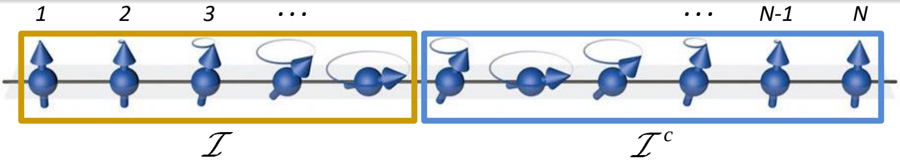


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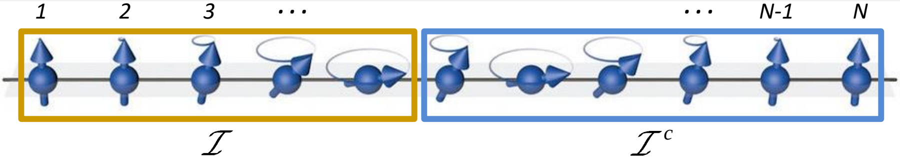


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- **Schmidt Number**: $\|\boldsymbol{\sigma}\|_0 = \mathit{rank}[\![\mathcal{A}]\!]_{\mathcal{I}}$

# Measuring Dependence with Entanglement

Structural equivalence:

quantum many-body state

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

func over many local elements

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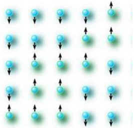
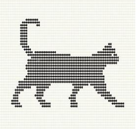


*func over many pixels*



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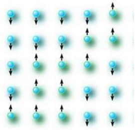

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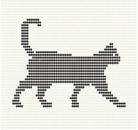

**We may quantify dependencies func models between input sets by applying entanglement measures to its coeff tensor!**

# Measuring Dependence with Entanglement – Interpretation

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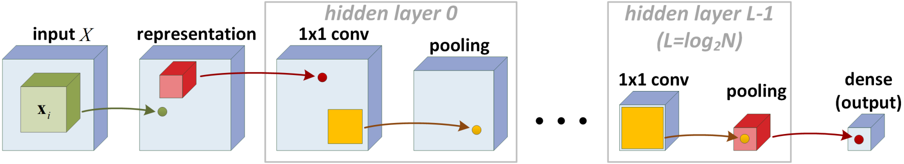
- Choice of entanglement measure determines dist metric

# Outline

# Convolutional Arithmetic Circuits $\longleftrightarrow$ Tensor Networks

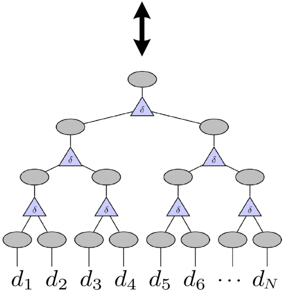
**Recap**

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*

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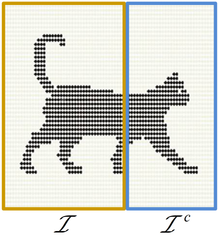


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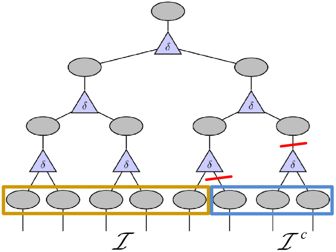

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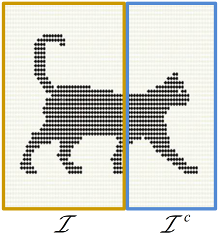


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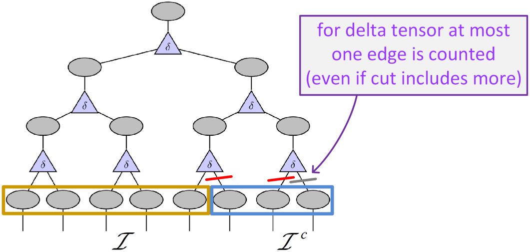

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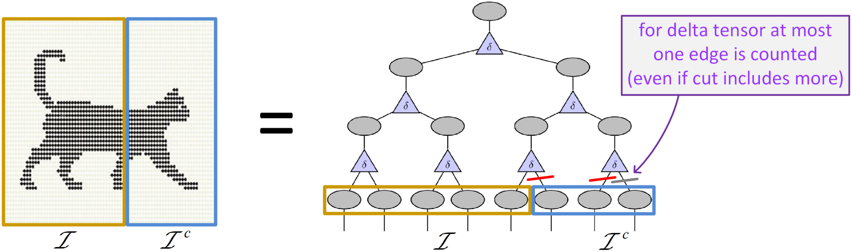


**We may analyze the effect of ConvAC arch on the dependencies (entanglement) it can model!**

# Depth

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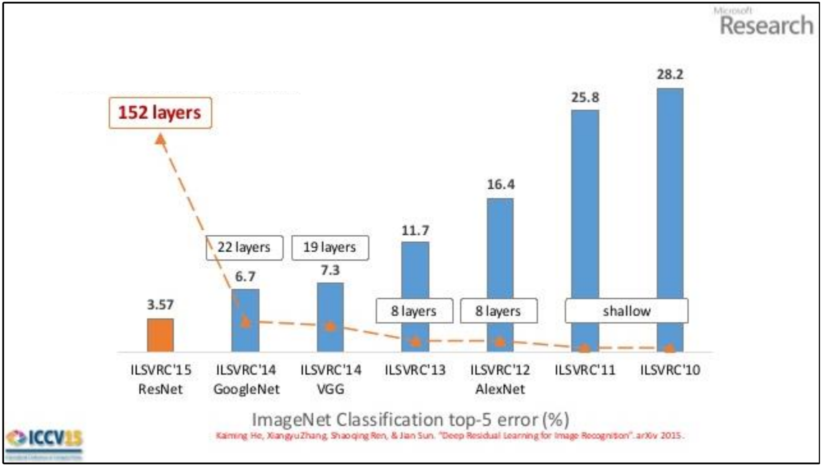
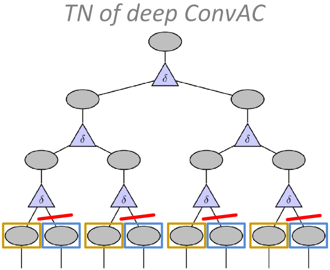
**Conjecture – depth efficiency**

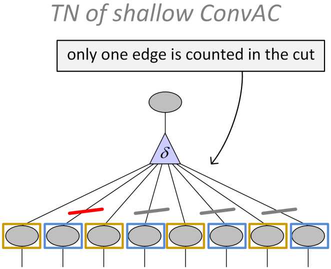
Deep ConvNets realize func requiring shallow ConvNets to grow unfeasibly



# Depth (cont'd)

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



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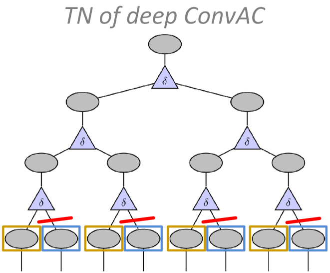


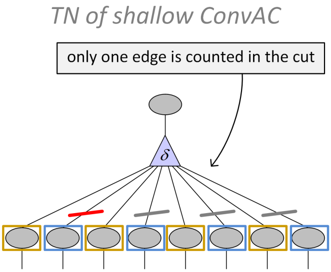


This implies:

**Claim**

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

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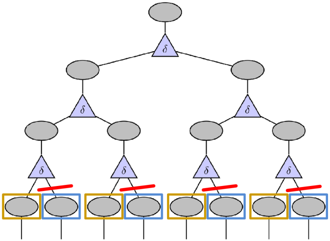


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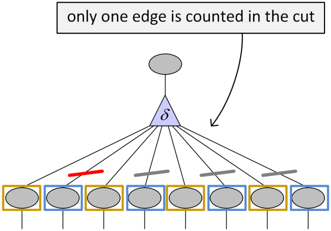


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**Depth efficiency proven for ConvAC!**

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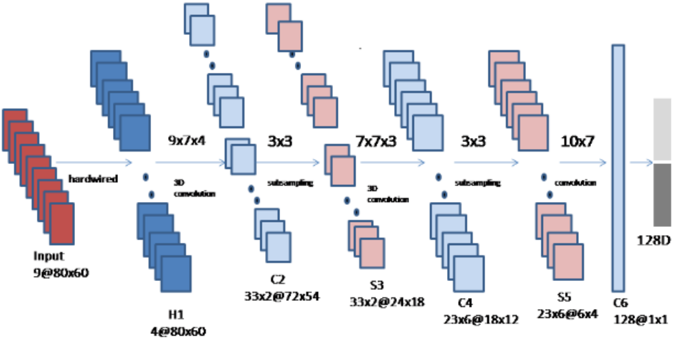

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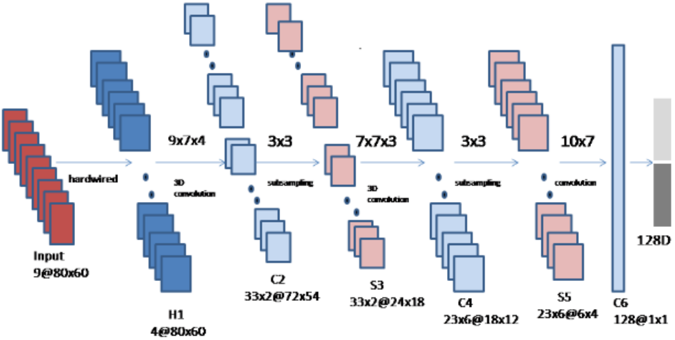


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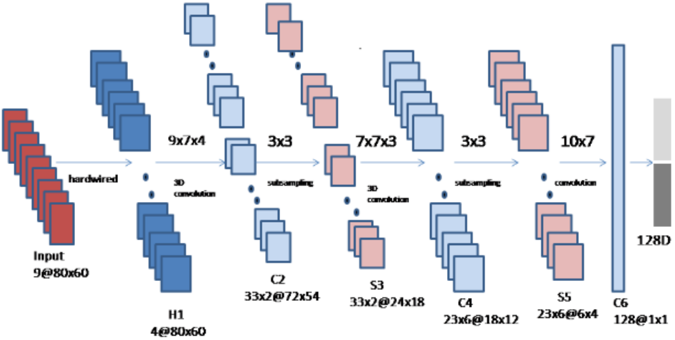


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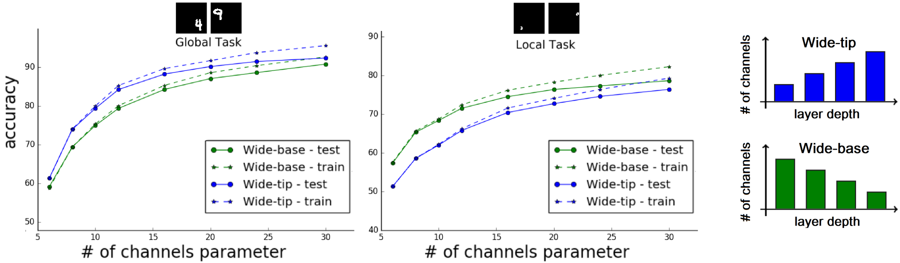

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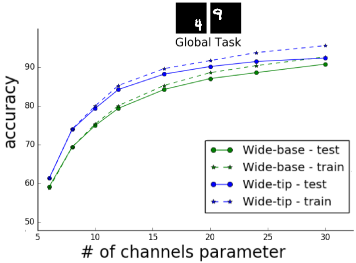


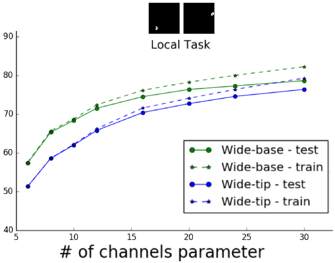


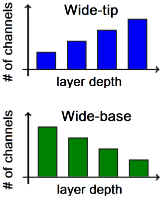


**ConvAC layer widths can be tailored to maximize dependencies (entanglements) required for given task!**

# Pooling Geometry

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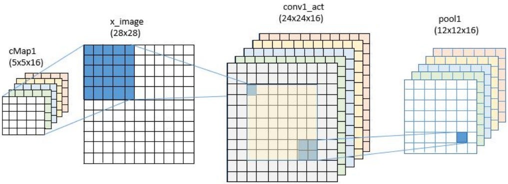
ConvNets typically employ square conv/pool windows



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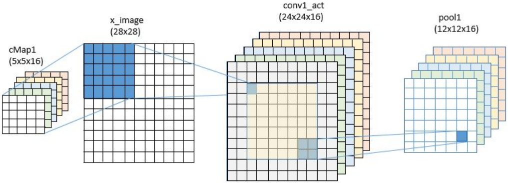


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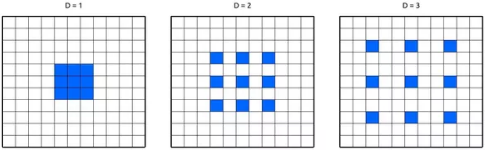

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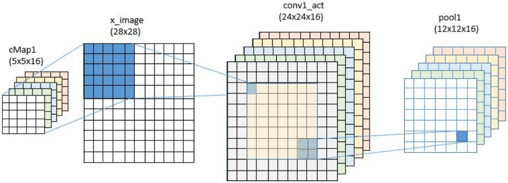


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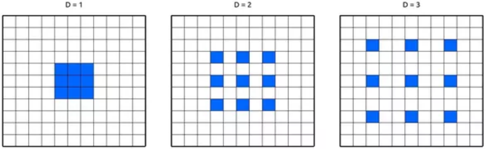


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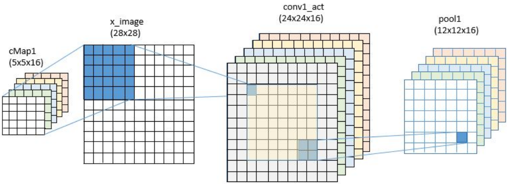


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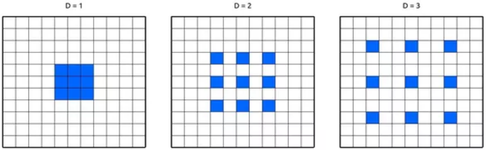


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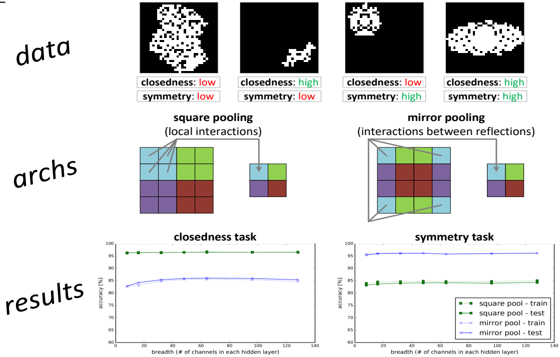

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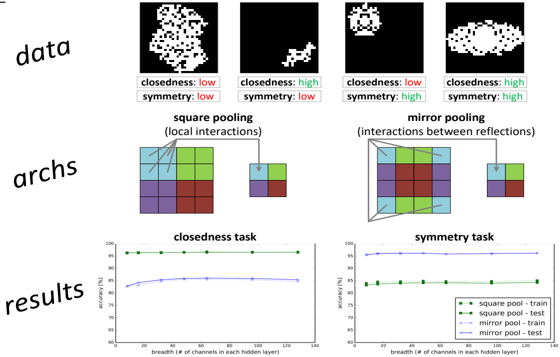


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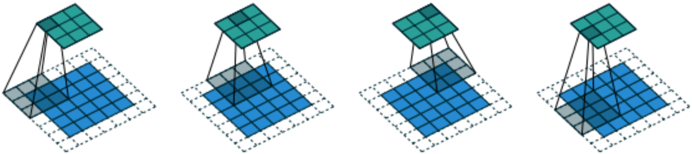
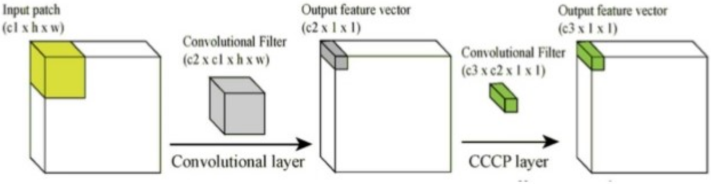
Modern ConvNets employ both overlapping and non-overlapping conv/pool operations





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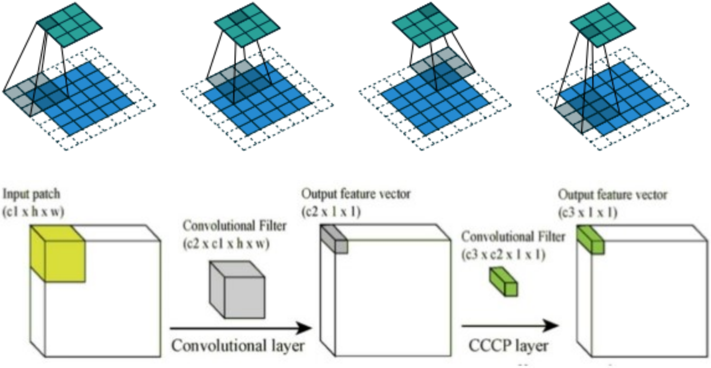


***Q:*** *What are implications of introducing overlaps?*

# Overlapping Operations (cont'd)

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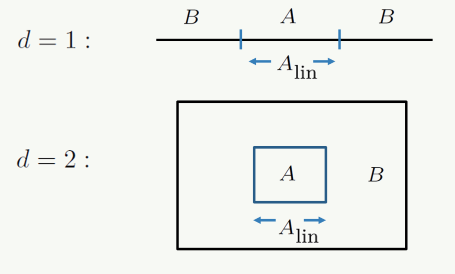


**area law**

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

**volume law**

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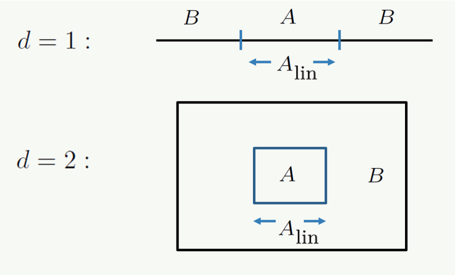


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**ConvAC w/overlaps supports volume law entanglement!**

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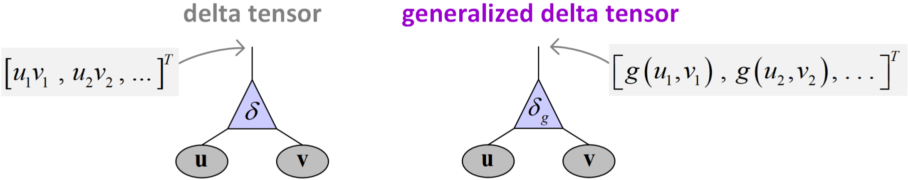
Our analysis extends to other ConvNets if we generalize delta tensor:



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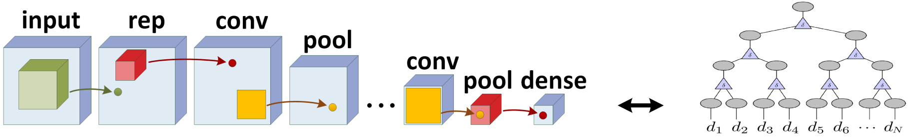

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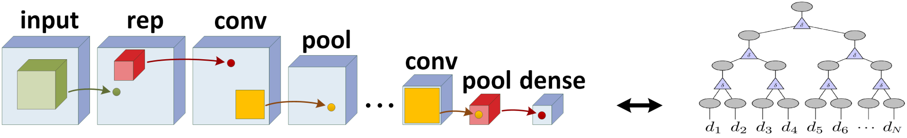


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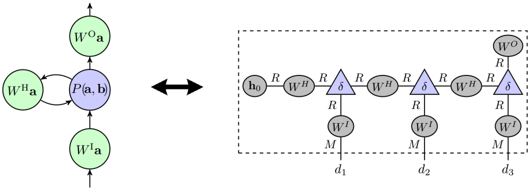

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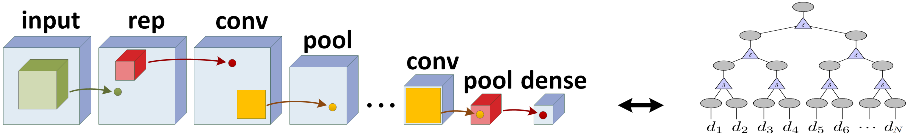


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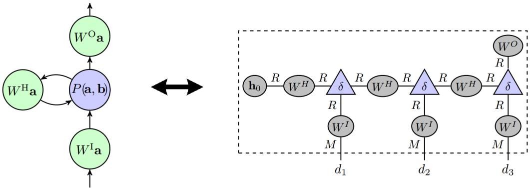


Recurrent nets process data sequentially; ability to model dependencies (entanglement) quantifies memory

# 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**

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- Quantum max flow/min cut theorem

  $\Longrightarrow$ new results on expressiveness in DL!

# Perspective

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Understanding deep learning calls for natural sciences

# Outline

# Thank You