

Matrix-Mimetic Tensor Algebra: A Unified Framework for Optimal Decomposition and Equivariant Learning

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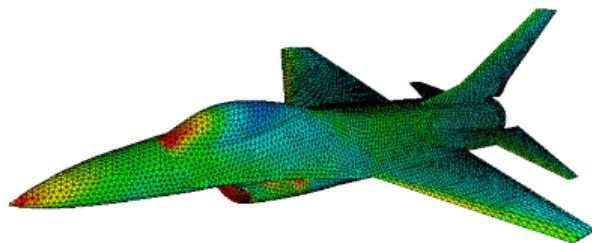


Introduction

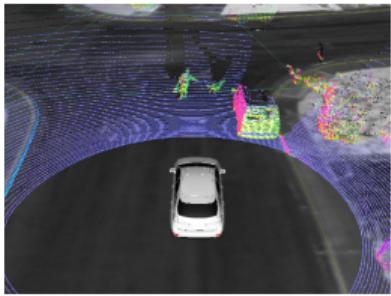
- Much of real-world **data** is inherently **multidimensional**



- Many **operators** and **models** are natively **multi-way**



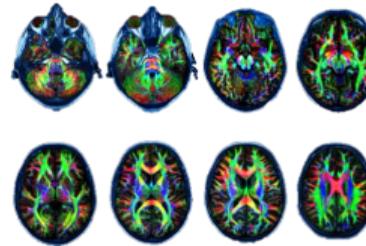
Tensor Applications



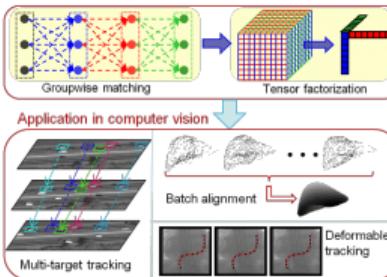
Machine vision

$$\begin{matrix} \text{Parts} \\ \text{Entries} \\ \text{Terms} \end{matrix} \begin{matrix} D \\ \text{ } \\ \text{ } \end{matrix} = U_{Entry} \times_1 \begin{matrix} U_{Part} \\ \times_2 \\ \text{ } \end{matrix} \times_3 U_{Term}$$

Latent semantic tensor indexing



Medical imaging



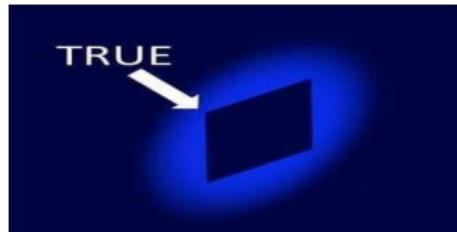
Video surveillance, streaming

Ivanov, Mathies, Vasilescu, **Tensor subspace analysis for viewpoint recognition**, ICCV, 2009

Shi, Ling, Hu, Yuan, Xing, **Multi-target tracking with motion context in tensor power iteration**, CVPR, 2014

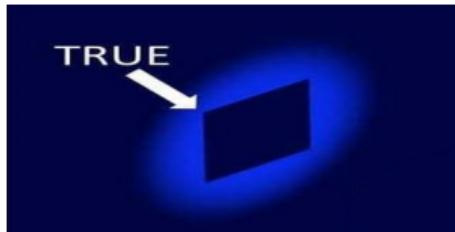
Where the Truth Lies ?

- If this is true

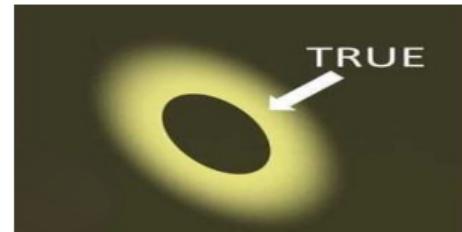


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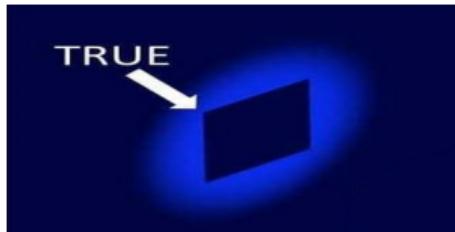


- But also this is true...

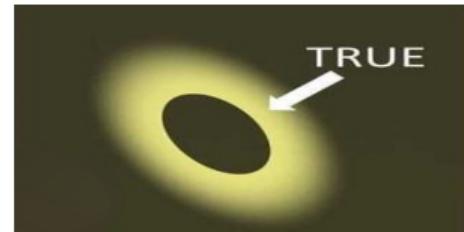


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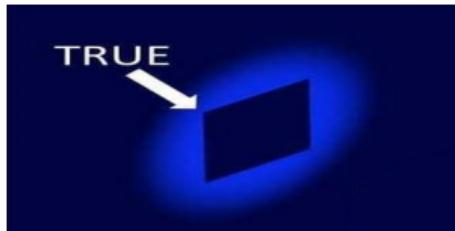
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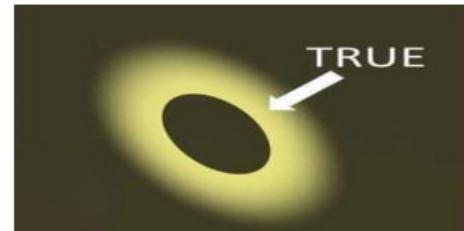
- Where the truth lies ?

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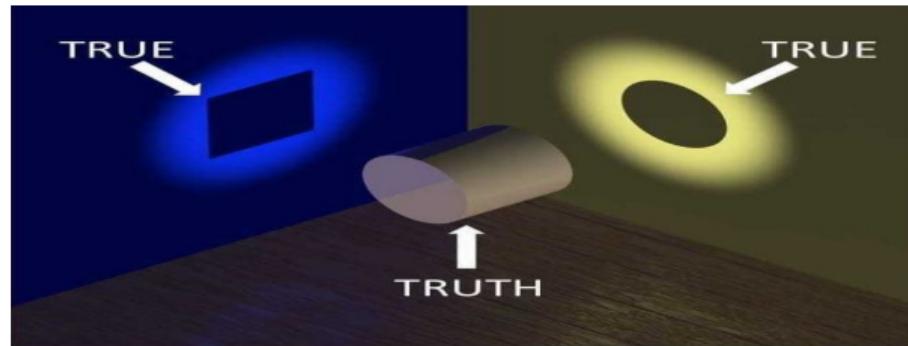
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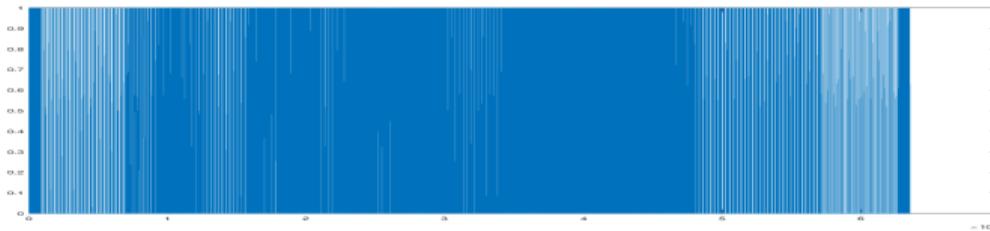


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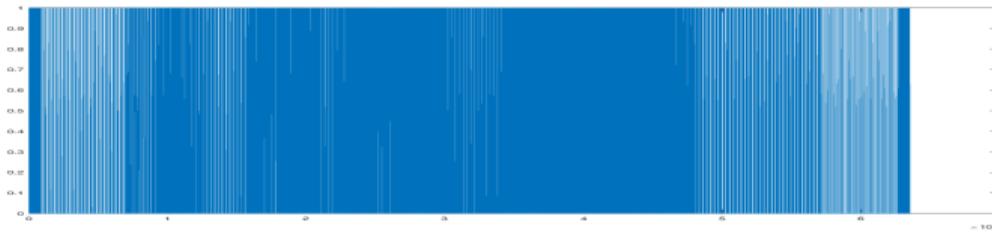
The Power of Representation

- Traditional **matrix-based** methods assuming data **vectorization** are generally **agnostic** to possible **high dimensional correlations**
- What is that ?



The Power of Representation

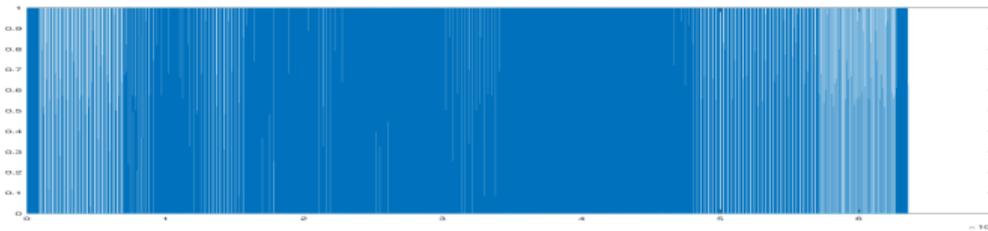
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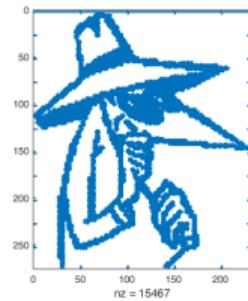
- Observe the same data but in a different (matrix rather than vector) representation

The Power of Representation

- Traditional **matrix-based** methods assuming data **vectorization** are generally **agnostic** to possible **high dimensional correlations**
- What is that ?



- Observe the same data but in a different (matrix rather than vector) representation



- **Representation matters!** some correlations can only be **realized** in appropriate representation

Background and Notation

- **Notation** : $\mathcal{A}^{n_1 \times n_2 \dots \times n_d}$ - d^{th} order tensor
 - ▶ 0^{th} order tensor - **scalar**



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- ▶ 1^{st} order tensor - **vector**



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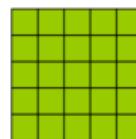
- ▶ 0^{th} order tensor - **scalar**



- ▶ 1^{st} order tensor - **vector**



- ▶ 2^{nd} order tensor - **matrix**



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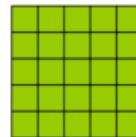
- ▶ 0^{th} order tensor - **scalar**



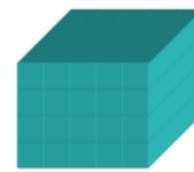
- ▶ 1^{st} order tensor - **vector**



- ▶ 2^{nd} order tensor - **matrix**

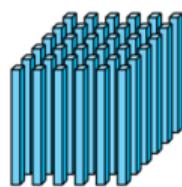


- ▶ 3^{rd} order tensor ...



Inside the Box

- *Tube (Fiber)* - a **vector** defined by fixing all **but one** index while varying the rest



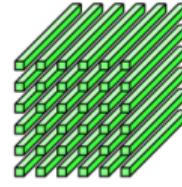
mode-1

$$\mathcal{A}_{:,j,k}$$



mode-2

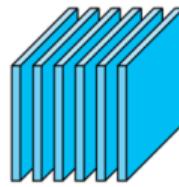
$$\mathcal{A}_{i,:,:}$$



mode-3

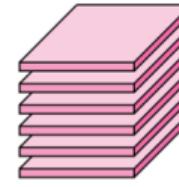
$$\mathcal{A}_{i,j,:}, a_{ij}$$

- *Slice* - a **matrix** defined by fixing all **but two** indices while varying the rest



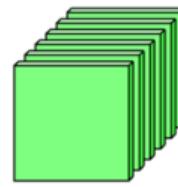
lateral

$$\mathcal{A}_{:,j,:}, \vec{\mathcal{A}}_j$$



horizontal

$$\mathcal{A}_{i,:,:}$$



frontal

$$\mathcal{A}_{:, :, k}, A^{(k)}$$

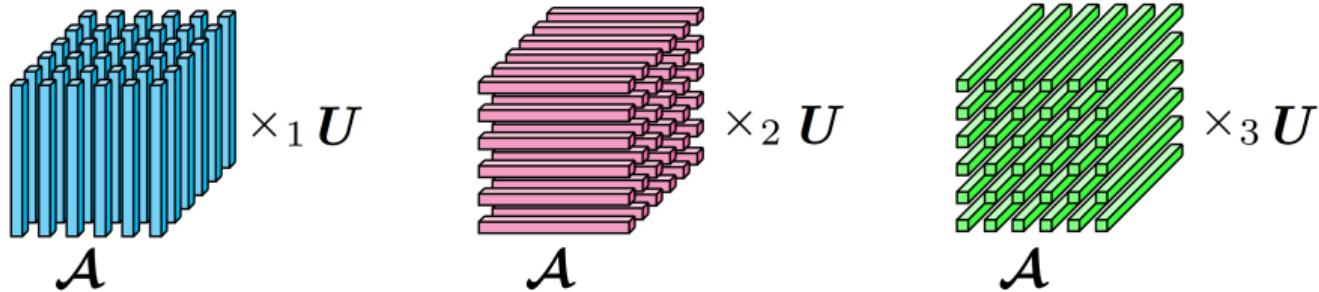
Tensor Multiplication

Definition

- The k - mode multiplication of a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ with a matrix $U \in \mathbb{R}^{j \times n_k}$ is denoted by $\mathcal{A} \times_k U$ and is of size $n_1 \times \cdots \times n_{k-1} \times j \times n_{k+1} \times \cdots \times n_d$
- Element-wise

$$(\mathcal{A} \times_k U)_{i_1 \cdots i_{k-1} j i_{k+1} \cdots i_d} = \sum_{i_k=1}^{n_k} a_{i_1 i_2 \cdots i_d} u_{j i_k}$$

- k-mode multiplication



Tensor Network / Diagram Notation

- Tensor networks invariants / isomorphism offers means to analyze and identify (space and time complexity) structure in high dimensional computation

vector v_j					$= \sum_j M_{ij} v_j$		$= A_{ij} B_{jk}$	$= AB$		$= \sum_k T_{ijkl} V_{km}$
matrix M_{ij}						$= \sum_k T_{ijkl} V_{km}$			$= \sum_{\alpha_1, \alpha_2, \alpha_3} A_{\alpha_1}^{s_1} B_{\alpha_1 \alpha_2}^{s_2} C_{\alpha_2 \alpha_3}^{s_3} D_{\alpha_3}^{s_4}$	
3-index tensor T_{ijk}		<td></td> <td></td> <td></td> <td>$= \sum_k T_{ijkl} V_{km}$</td> <td></td> <td></td> <td>$= \sum_{\alpha_1, \alpha_2, \alpha_3} A_{\alpha_1}^{s_1} B_{\alpha_1 \alpha_2}^{s_2} C_{\alpha_2 \alpha_3}^{s_3} D_{\alpha_3}^{s_4}$</td>				$= \sum_k T_{ijkl} V_{km}$			$= \sum_{\alpha_1, \alpha_2, \alpha_3} A_{\alpha_1}^{s_1} B_{\alpha_1 \alpha_2}^{s_2} C_{\alpha_2 \alpha_3}^{s_3} D_{\alpha_3}^{s_4}$	

- Tensors are notated by **nodes**, while indices are represented by **edges**
- Connecting index **edges** implies **contraction** / summation over connected indices

How Powerful are Tensor Networks ?

MENU ▾

nature

Article | Published: 23 October 2019

Quantum supremacy using a programmable superconducting processor

Frank Arute, Kunal Arya, [...] John M. Martinis 

Nature 574, 505–510(2019) | Cite this article

661k Accesses | 26 Citations | 6016 Altmetric | Metrics

Abstract

The promise of quantum computers is that certain computational tasks might be executed exponentially faster on a quantum processor than on a classical processor¹. A fundamental challenge is to build a high-fidelity processor capable of running quantum algorithms in an exponentially large computational space. Here we report the use of a processor with programmable superconducting qubits^{2,3,4,5,6,7} to create quantum states on 53 qubits, corresponding to a computational state-space of dimension 2^{53} (about 10^{16}). Measurements from repeated experiments sample the resulting probability distribution, which we verify using classical simulations. Our Sycamore processor takes about 200 seconds to sample one instance of a quantum circuit a million times—our benchmarks currently indicate that the equivalent task for a state-of-the-art classical supercomputer would take approximately 10,000 years. This dramatic increase in speed compared to all known classical algorithms is an experimental realization of quantum supremacy^{8,9,10,11,12,13,14} for this specific computational task, heralding a much-anticipated computing paradigm.

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Google researchers in Santa Barbara, California, say their advance may lead to near-term applications of quantum computers. ISTOCK.COM/JHVEPHOTO

IBM casts doubt on Google's claims of quantum supremacy

By Adrian Cho | Oct. 23, 2019, 5:40 AM

Pareto-Efficient Quantum Circuit Simulation Using Tensor Contraction Deferral*

Edwin Pednault^{†1}, John A. Gunnels^{†1}, Giacomo Nannicini^{†1}, Lior Horesh¹, Thomas Magerlein², Edgar Solomonik³, Erik W. Draeger⁴, Eric T. Holland⁴, and Robert Wisniewski⁴

¹IBM T.J. Watson Research Center, Yorktown Heights, NY

²Tufts University, Medford, MA

³Dept. of Computer Science, University of Illinois at Urbana-Champaign, Champaign, IL

⁴Lawrence Livermore National Laboratory, Livermore, CA

Low Rank Structure

Low Rank Property

- Express a d^{th} -order tensor \mathcal{A} as the sum of rank-1 tensors,

$$\mathcal{A} \approx \sum_{i=1}^r \sigma_i \cdot u_i^{(1)} \circ u_i^{(2)} \circ \dots \circ u_i^{(d)}$$

- We seek a d^{th} -order tensor \mathcal{B} of rank $k \leq r$ to optimize:

$$\begin{aligned} \operatorname{argmin}_{\mathcal{B}} \quad & \|\mathcal{A} - \mathcal{B}\|_F \\ \text{s.t.} \quad & \mathcal{B} \text{ has rank } k \leq r \end{aligned}$$

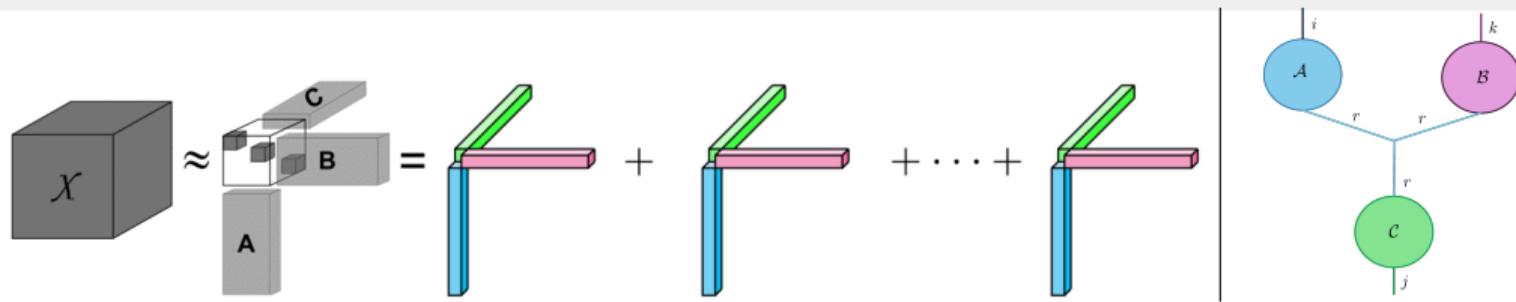
- When $d = 2$, \mathcal{B} is the matrix SVD truncated to k terms (Eckart-Young)
- Is there is a similar theoretical result for higher order tensors ?

Theorem (Schmidt 1907; Eckart & Young 1936; Mirsky 1960)

Let $\mathbf{A} \in \mathbb{C}^{n_1 \times n_2}$ be a matrix with $\operatorname{rank}(\mathbf{A}) = r$. The truncated Singular Value Decomposition (SVD) yields the **best low-rank approximation**; i.e., for $k \leq r$,

$$\mathbf{A}_k = \sum_{i=1}^k \sigma_i \mathbf{u}_i \mathbf{v}_i^H = \operatorname{argmin}_{\operatorname{rank}(\mathbf{B}) \leq k} \|\mathbf{A} - \mathbf{B}\|_F$$

Tensor Decompositions - CP (CANDECOMP-PARAFAC)²



- Find the best **tensor rank- r** fit¹:

$$\min_{a_i, b_i, c_i} \left\| \mathcal{X} - \sum_{i=1}^r \sigma_i \cdot a_i \circ b_i \circ c_i \right\|_F$$

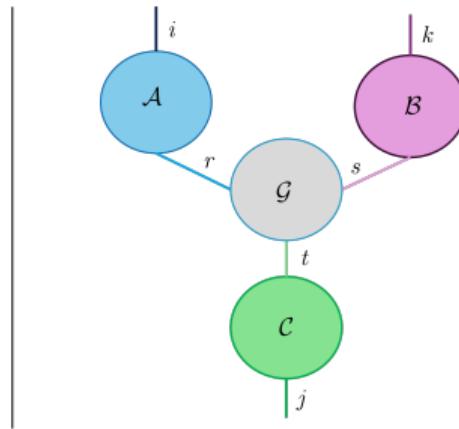
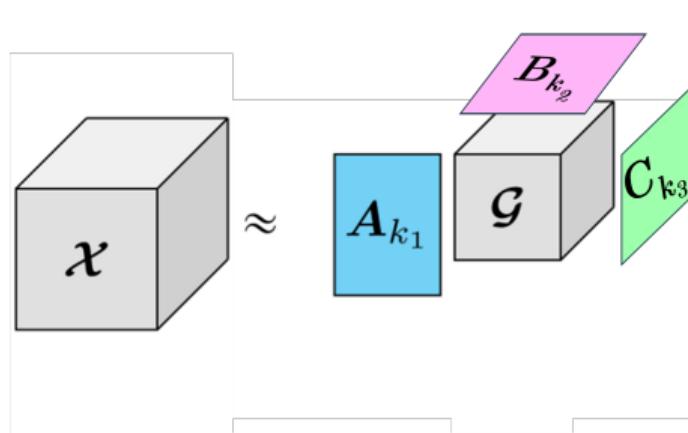
- Extension of matrix rank
- Interpretable
- Summing k factors is sub-optimal
- Determining rank is NP-hard

- The set of tensors of a given size that **do not** have a best rank- k approximation has **positive volume** (i.e., positive Lebesgue measure) for at least some values of k , implying that **lack of best approximation** is rather common

¹ de Silva, Lim, Tensor rank and ill-posedness of the best low-rank approximation problem, 2008

² Hitchcock, J Math Phys, 1927; Harshman, 1970; Carroll, Chang, 1970

Tensor Decompositions - Tucker⁴



- Find the best **multi-linear rank- (k_1, k_2, k_3)** fit³:

$$\min_{\mathbf{A}_{k_1}, \mathbf{B}_{k_2}, \mathbf{C}_{k_3}} \|\mathcal{X} - \mathcal{G} \times_1 \mathbf{A}_{k_1} \times_2 \mathbf{B}_{k_2} \times_3 \mathbf{C}_{k_3}\|_F$$

- Higher-order PCA
- Compressible
- Truncation of full orth. sub-optimal
- Hard to interpret

³ De Lathauwer, De Moor, Vandewalle, HOSVD, 2000; Cichocki, Zdunek, Phan, Amari, Nonnegative T&M Factorizations, 2009

⁴ Tucker, Problems in Measuring Change, 1963

Tensor Train Decomposition

Tensor Train format of a tensor \mathcal{A}

$$\mathcal{A}(i_1, \dots, i_d) = \sum_{\alpha_0, \dots, \alpha_d} \mathcal{G}_1(\alpha_0, \textcolor{green}{i_1}, \alpha_1) \mathcal{G}_2(\alpha_1, \textcolor{red}{i_2}, \alpha_2), \dots, \mathcal{G}_d(\alpha_{d-1}, \textcolor{blue}{i_d}, \alpha_d)$$

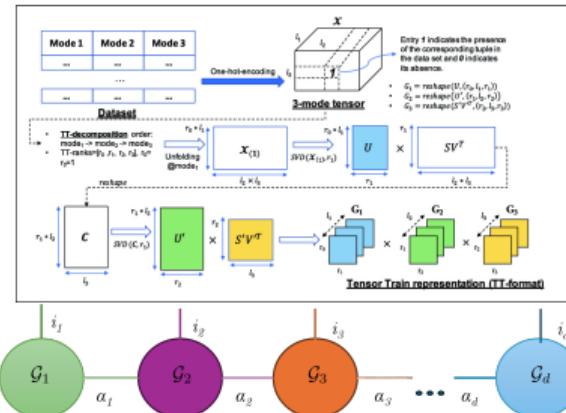
Can be represented compactly as a matrix product:

$$\mathcal{A}(i_1, \dots, i_d) = \underbrace{\mathcal{G}_1[\textcolor{green}{i_1}]}_{1 \times r_1} \underbrace{\mathcal{G}_2[\textcolor{red}{i_2}]}_{r_1 \times r_2} \dots \underbrace{\mathcal{G}_d[\textcolor{blue}{i_d}]}_{r_{d-1} \times 1}$$

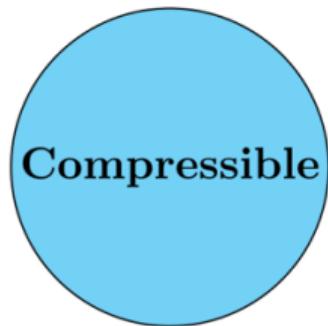
- \mathcal{G}_i : TT-cores (collections of matrices)
- r_i : TT-ranks
- $r = \max r_i$: the maximal TT-rank

TT uses $\mathcal{O}(dn r^2)$ memory to store $\mathcal{O}(nd)$ elements

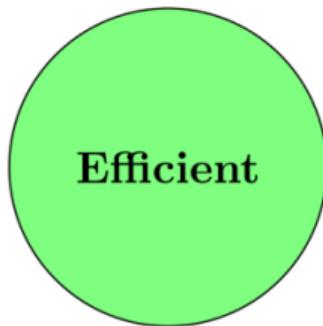
Efficient **only** when all **ranks** are **small**



Tensor Algebra Desired Properties

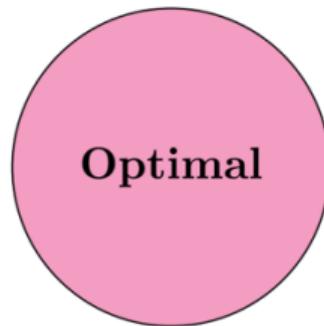


Compressible



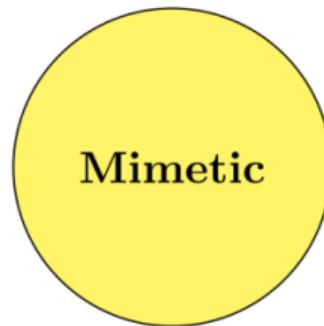
Efficient

Powerful
representation



Optimal

Provable
superiority



Mimetic

Matrix property
preservation

Groups and Representations

A **group** is a set G with a binary operation $\circ : G \times G \rightarrow G$ satisfying the following axioms:

Group Axioms

- **Closure:** For all $a, b \in G$, $a \circ b \in G$
- **Associativity:** For all $a, b, c \in G$, $(a \circ b) \circ c = a \circ (b \circ c)$
- **Identity:** There exists $e \in G$ such that for all $a \in G$, $e \circ a = a \circ e = a$
- **Inverses:** For each $a \in G$, there exists $a^{-1} \in G$ such that $a \circ a^{-1} = a^{-1} \circ a = e$

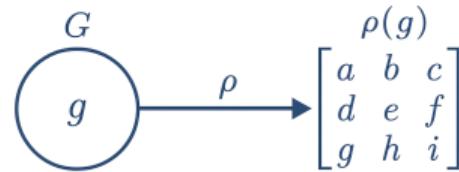
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A group **representation** is a homomorphism $\rho : G \rightarrow \text{GL}(V)$ mapping a group G to the general linear group of a vector space V , preserving the group operation: i.e.



$$\rho(g_1 \circ g_2) = \rho(g_1)\rho(g_2), \quad \forall g_1, g_2 \in G$$

$g \in G \rightarrow \rho(g) \rightarrow [\text{Matrix}]$

Rings

A **ring** is a set R with two binary operations $+$: $R \times R \rightarrow R$ and \cdot : $R \times R \rightarrow R$ satisfying:

Ring Axioms

- **Abelian Group under $+$:** $(R, +)$ forms an abelian group with identity 0
- **Associative Multiplication:** For all $a, b, c \in R$, $(a \cdot b) \cdot c = a \cdot (b \cdot c)$
- **Distributivity:** For all $a, b, c \in R$:
 - ▶ $a \cdot (b + c) = a \cdot b + a \cdot c$ (left distributivity)
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Additional properties may include:

- **Unity:** Multiplicative identity $1 \in R$ with $1 \cdot a = a \cdot 1 = a$ for all $a \in R$
- **Commutativity:** $a \cdot b = b \cdot a$ for all $a, b \in R$

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Examples: \mathbb{Z} , $\mathbb{Q}[x]$, $M_n(\mathbb{R})$, $\mathbb{Z}/n\mathbb{Z}$

Modules

Let \mathcal{R} be a ring. A **left \mathcal{R} -module** is an abelian group $(M, +)$ with scalar multiplication $\cdot : \mathcal{R} \times M \rightarrow M$ satisfying:

Module Axioms

- **Distributivity over module addition:** $r \cdot (m + n) = r \cdot m + r \cdot n$
- **Distributivity over ring addition:** $(r + s) \cdot m = r \cdot m + s \cdot m$
- **Associativity:** $(rs) \cdot m = r \cdot (s \cdot m)$
- **Unity** (if \mathcal{R} has 1): $1 \cdot m = m$

for all $r, s \in \mathcal{R}$ and $m, n \in M$.

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When \mathcal{R} is a **field**, an \mathcal{R} -module is precisely a **vector space** over \mathcal{R} .

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Module Axioms

- **Distributivity over module addition:** $r \cdot (m + n) = r \cdot m + r \cdot n$
- **Distributivity over ring addition:** $(r + s) \cdot m = r \cdot m + s \cdot m$
- **Associativity:** $(rs) \cdot m = r \cdot (s \cdot m)$
- **Unity** (if \mathcal{R} has 1): $1 \cdot m = m$

for all $r, s \in \mathcal{R}$ and $m, n \in M$.

When \mathcal{R} is a **field**, an \mathcal{R} -module is precisely a **vector space** over \mathcal{R} .

Examples: Abelian groups (as \mathbb{Z} -modules), \mathbb{R}^n (as \mathbb{R} -module), $\mathbb{Z}/n\mathbb{Z}$ (as \mathbb{Z} -module)

Algebra over Tubes

Definition

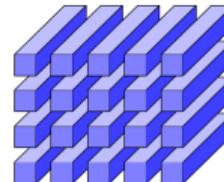
A tensor $\mathcal{X} \in \mathbb{F}^{m \times p \times n}$ is an $m \times p$ matrix of tubes - \mathbb{F}_n elements



$x \in \mathbb{F}_n$ - tube



$X \in \mathbb{F}_n^p$ - slice



$\mathcal{X} \in \mathbb{F}_n^{m \times p}$ - tensor

where \mathbb{F}_n^p is a free-module over the ring \mathbb{F}_n

Tubal Operation

- Let $\mathbf{M} \in \mathbb{F}^{n \times n}$ be invertible. \mathbb{F}_n denotes the ring $(\mathbb{F}^{1 \times 1 \times n}, +, \star_M)$.

$$\mathbf{a} \star_M \mathbf{b} = \mathbf{M}^{-1}(\mathbf{M} \mathbf{a} \odot \mathbf{M} \mathbf{b}) = \mathbf{M}^{-1} \operatorname{diag}(\mathbf{M} \mathbf{a}) \mathbf{M} \mathbf{b}$$

$$\begin{array}{ccc} \text{a} & \star_M & \text{b} \\ \text{---} & & \text{---} \\ 1 \times 1 \times n_3 & & 1 \times 1 \times n_3 \end{array} = \begin{array}{c} \text{c} \\ \text{---} \\ 1 \times 1 \times n_3 \end{array}$$

- Tube fiber interpretation:

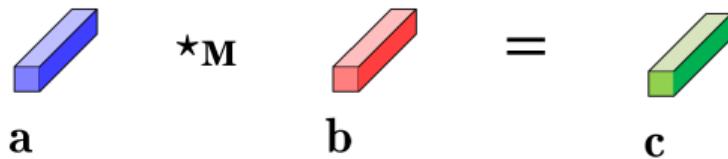
$$\begin{aligned} \mathbf{c} &= \operatorname{fold}((\mathbf{M}^{-1} \operatorname{diag}(\mathbf{a}) \mathbf{M}) \operatorname{vec}(\mathbf{b})) \\ &= \operatorname{fold}((\mathbf{M}^{-1} \operatorname{diag}(\mathbf{b}) \mathbf{M}) \operatorname{vec}(\mathbf{a})) \end{aligned}$$

- Commutativity, and characterization using set of diagonal matrices diagonalized by \mathbf{M} and its inverse

Tubal Operation

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$$\begin{array}{ccc} \text{a} & \star_M & \text{b} \\ \text{---} & & \text{---} \\ 1 \times 1 \times n_3 & & 1 \times 1 \times n_3 \end{array} = \begin{array}{c} \text{c} \\ \text{---} \\ 1 \times 1 \times n_3 \end{array}$$


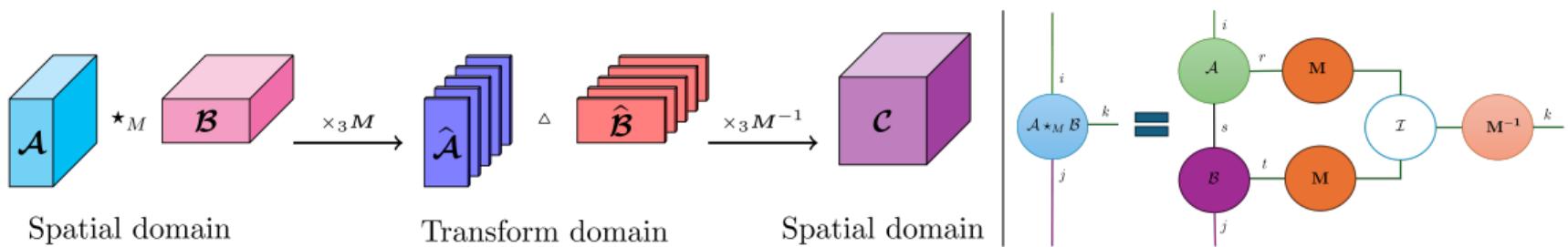
- $T : \mathbb{F}_n^p \rightarrow \mathbb{F}_n^m$ is a module homomorphism $(T(\mathbf{a} \star_M \mathbf{b}) = \mathbf{b} \star_M T(\mathbf{a}))$ if and only if $T\mathcal{B} = \mathcal{A} \star_M \mathcal{B}$ for some $\mathcal{A} \in \mathbb{F}_n^{m \times p}$

The \star_M -Product Algebra

Given $\mathcal{A} \in \mathbb{R}^{\ell \times p \times n}$, $\mathcal{B} \in \mathbb{R}^{p \times m \times n}$, and an invertible $n \times n$ matrix M , then

$$\mathcal{C} = \mathcal{A} \star_M \mathcal{B} = (\hat{\mathcal{A}} \triangle \hat{\mathcal{B}}) \times_3 M^{-1}$$

where $\mathcal{C} \in \mathbb{R}^{\ell \times m \times n}$, $\hat{\mathcal{A}} = \mathcal{A} \times_3 M$, and \triangle multiplies the frontal slices in parallel



Useful properties: tensor conjugate transpose, unitarity invariance, identity tensor, connection to Fourier transform, circulant shifts invariance, ...

\star_M SVD and Truncation Optimality

Theorem (Kilmer, Horesh, Avron, Newman, 2021)

Let the t -SVD of $\mathcal{A} \in \mathbb{R}^{\ell \times m \times n}$ be given by $\mathcal{A} = \mathcal{U} \star_M \mathcal{S} \star_M \mathcal{V}^\top$, with $\ell \times \ell \times n$ orthogonal tensor \mathcal{U} , $m \times m \times n$ orthogonal tensor \mathcal{V} , and $\ell \times m \times n$ *f-diagonal* tensor \mathcal{S}

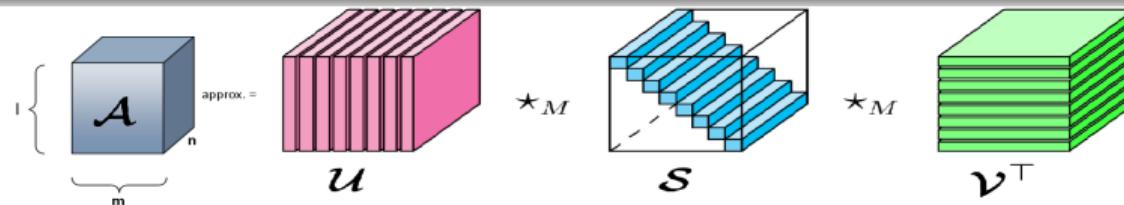
- For $k < \min(l, m)$, define

$$\mathcal{A}_k = \mathcal{U}(:, 1:k, :) \star_M \mathcal{S}(1:k, 1:k, :) \star_M \mathcal{V}^\top(:, 1:k, :) = \sum_{i=1}^k \mathcal{U}(:, i, :) \star_M \mathcal{S}(i, i, :) \star_M \mathcal{V}(:, i, :)^\top$$

- Then

$$\mathcal{A}_k = \operatorname{argmin}_{\hat{\mathcal{A}} \in \mathcal{M}} \|\mathcal{A} - \hat{\mathcal{A}}\|$$

where $\mathcal{M} = \{\mathcal{C} = \mathcal{X} \star_M \mathcal{Y} \mid \mathcal{X} \in \mathbb{R}^{\ell \times k \times n}, \mathcal{Y} \in \mathbb{R}^{k \times m \times n}\}$



Tensor Representation Superiority

- Why might we expect the **tensor** representation to be more **informative** than matrix representation?

Tensor Representation Superiority

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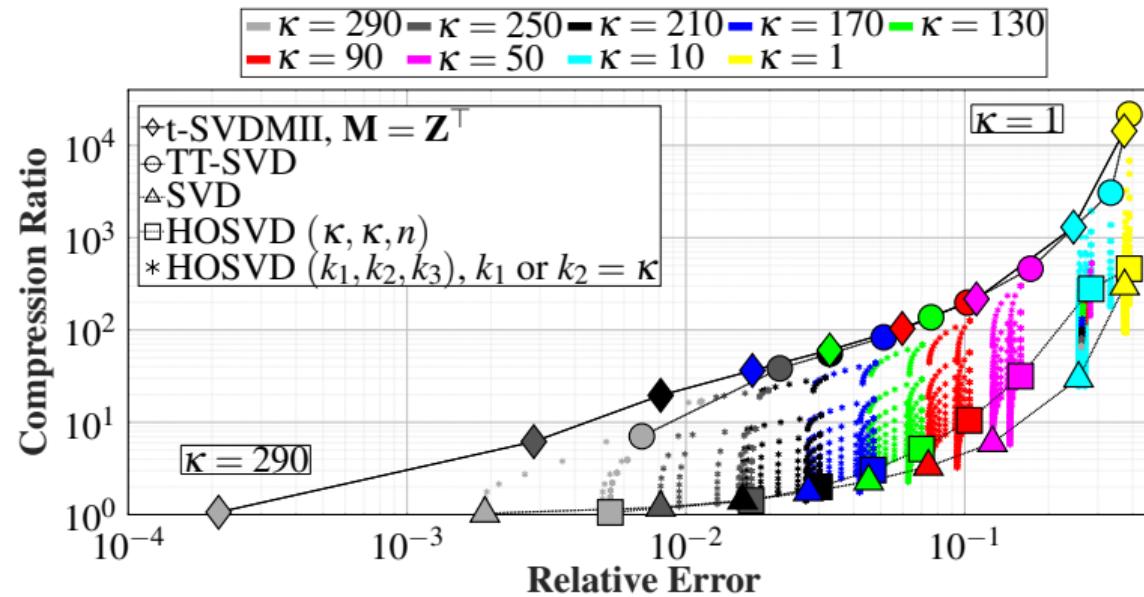
Theorem (Kilmer, Horesh, Avron, Newman, 2021)

Let $X(:, i) = \text{unfold}(\mathcal{A}(:, i, :))$. Let \mathcal{A}_k denote the optimal k -term truncated \star_M tensor-SVD approximation to \mathcal{A} , and let A_k denote the optimal k -term (i.e. rank- k) matrix SVD approximation to A . Then

$$\|\mathcal{A} - \mathcal{A}_k\|_F \leq \|A - A_k\|_F$$

How it Compares to Other Tensorial Frameworks?

- **Theoretically**, similar superiority results are proved over HOSVD and TT-SVD
- Possible to **interpret** decompositions of the new tensor in **CP** form



De Lathauwer, De Moor, J. Vandewalle, **A multilinear singular value decomposition**, SIMAX 2000

Oseledets, **Tensor-train decomposition**, SISC 2011

Kilmer, Horesh, Avron, Newman, **Tensor-tensor products for optimal representation and compression**, PNAS 2021

Tensor-Tensor Applications - Proper Orthogonal Decomposition

Proper Orthogonal Decomposition (POD)

Motivation: Solving large-scale dynamical systems is computationally expensive

- Dynamic system: $\frac{\partial \bar{a}(t)}{\partial t} = L\bar{a}(t) + f(\bar{a}(t)) + \bar{q}(t)$
- For 2D grid $n_x \times n_y$: state size is $n_x n_y \times 1$, operator L is $n_x n_y \times n_x n_y$

Matrix-based POD:

- Collect snapshots $\{\bar{a}^1, \dots, \bar{a}^{\mu_s}\}$ into matrix $A \in \mathbb{R}^{n_x n_y \times \mu_s}$
- Compute SVD $A = USV^\top$
- Use first k left singular vectors as projection basis U_k
- Galerkin projection: $U_k^\top U_k \frac{\partial \tilde{a}}{\partial t} = \underbrace{U_k^\top L U_k}_{k \times k} \tilde{a} + U_k^\top f(U_k \tilde{a}) + U_k^\top \bar{q}$

Tensor Proper Orthogonal Decomposition (t-POD)

Key Idea: Preserve spatial structure using tensors

- Form snapshot **tensor** $\mathcal{A} \in \mathbb{R}^{n_x \times \mu_s \times n_y}$ instead of matrix
- Compute k -term truncated t-SVD: $\mathcal{A}_k = \mathcal{U}_k \star_M \mathcal{S}_k \star_M \mathcal{V}_k^\top$
- Use $\mathcal{U}_k \in \mathbb{R}^{n_x \times k \times n_y}$ for projection

Advantages:

- t-POD basis better captures spatial structure of solutions
- Significantly lower relative error vs. matrix POD for same number of snapshots
- Orders of magnitude error reduction observed in diffusion equation experiments

Zhang, Kilmer, Horesh, Avron (2021); Zhang, Tufts PhD thesis, 2017

Tensor Proper Orthogonal Decomposition - Example

Diffusion Equation: $\frac{\partial a(\mathbf{r},t)}{\partial t} - \nabla \cdot \kappa \nabla a(\mathbf{r},t) = 0$

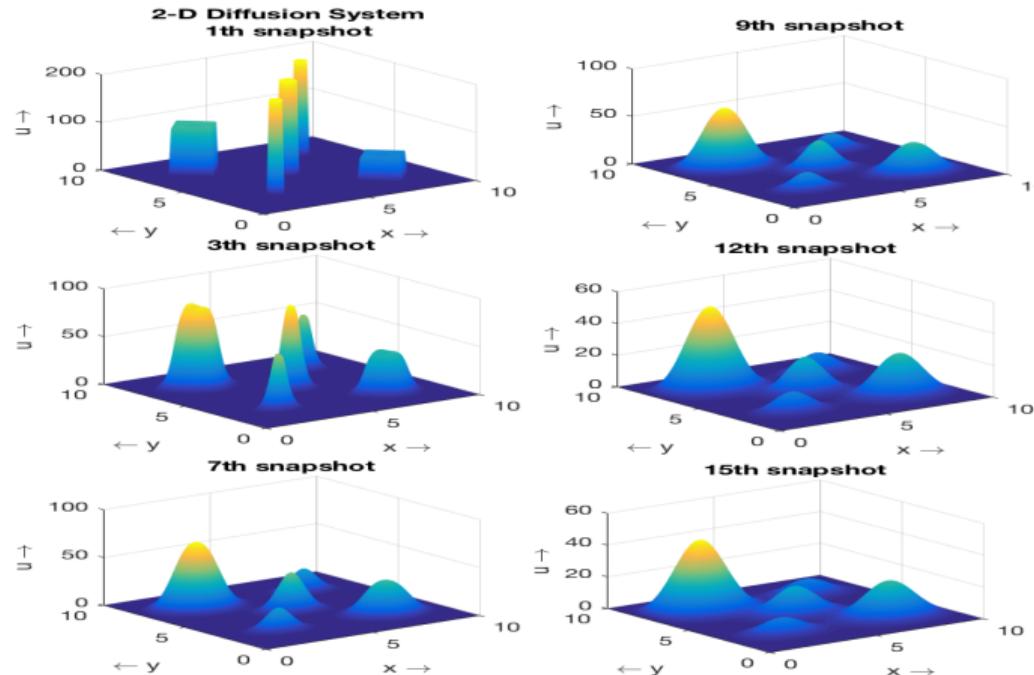


Figure: Sample snapshots of solution $\bar{\mathbf{a}}^j$, $j = 1, 3, 7, 9, 12, 15$

Better Basis? - Numerical Support

Diffusion Equation: $\frac{\partial a(\mathbf{r},t)}{\partial t} - \nabla \cdot \kappa \nabla a(\mathbf{r},t) = 0$

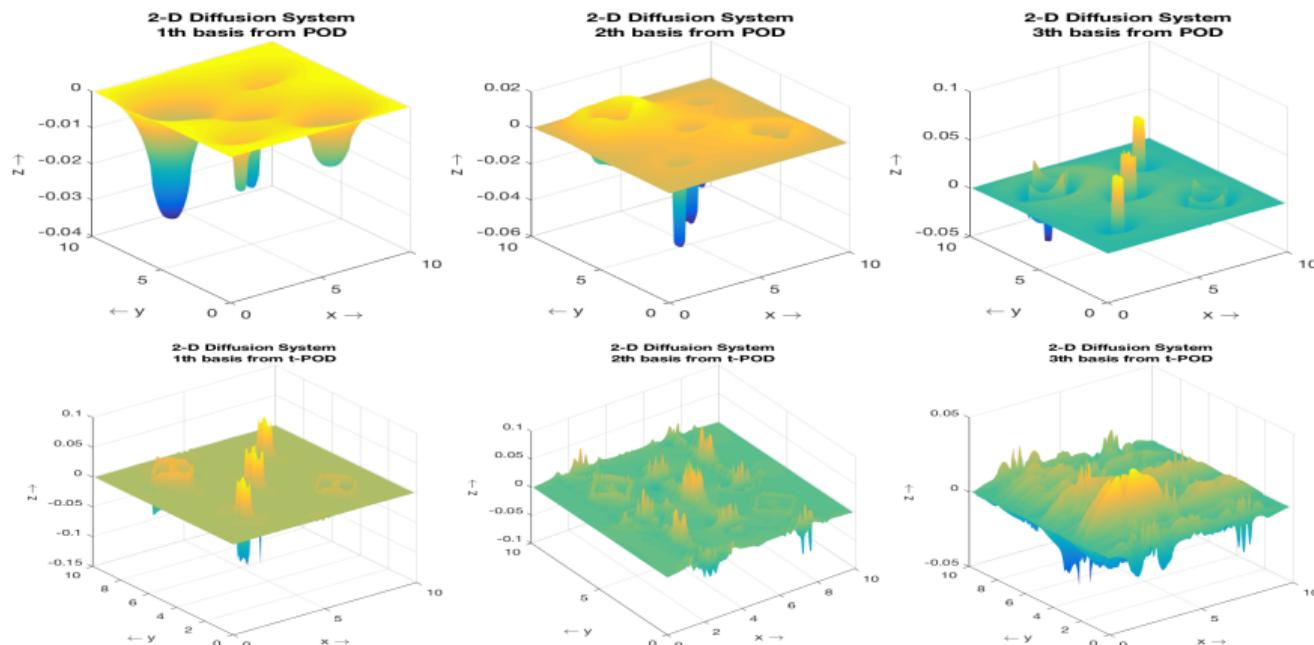
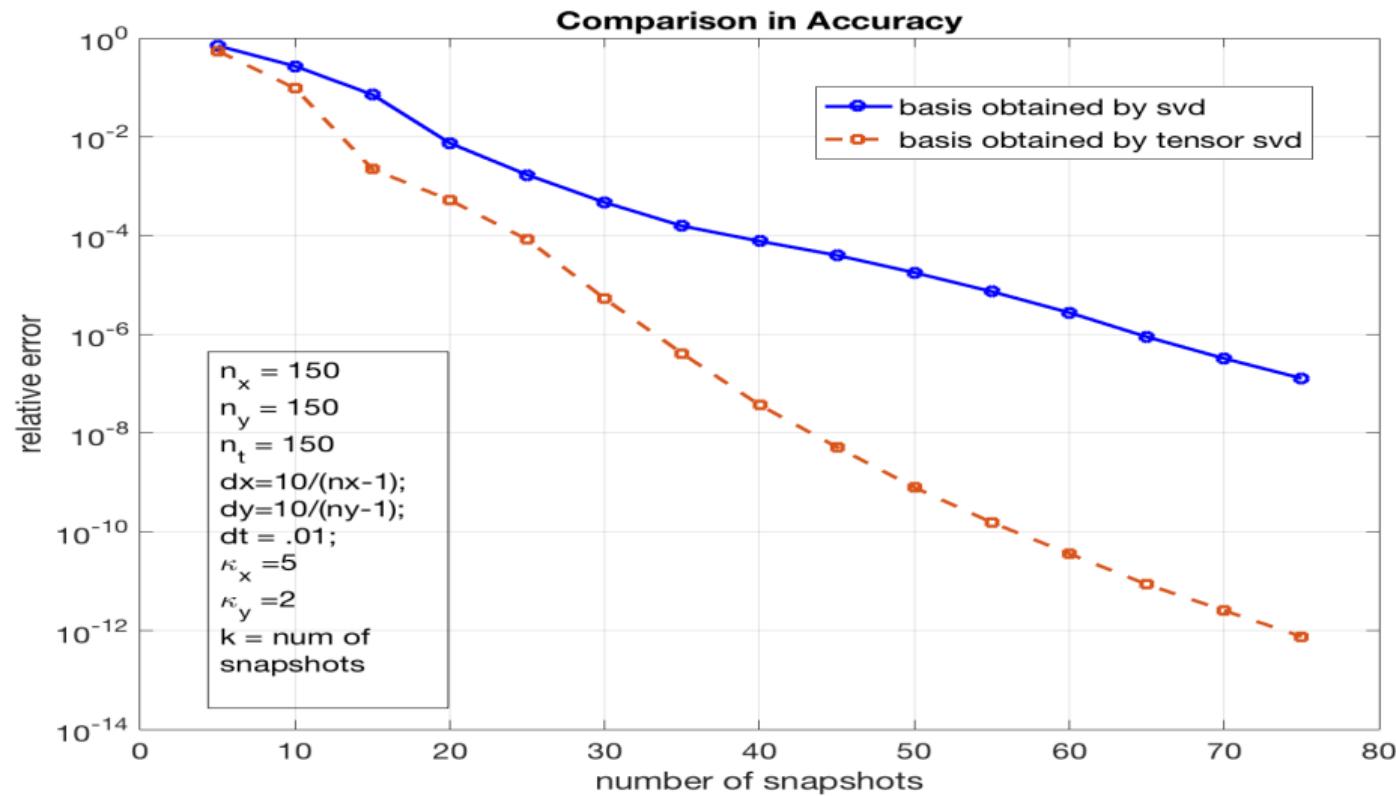


Figure: First 3 basis slices from **matrix POD** (top) and **t-POD** (bottom)

Tensor Proper Orthogonal Decomposition - Error vs. Snapshots Count



Tensor-Tensor Neural Networks

Tensor Neural Networks: Motivation

Key Idea: Replace matrix operations with tensor operations in neural networks

Standard Neural Network (Matrix):

$$\mathbf{a}_{j+1} = \sigma(W_j \cdot \mathbf{a}_j + \mathbf{b}_j) \quad \text{for } j = 0, \dots, N-1$$

Tensor Neural Network:

$$\vec{\mathcal{A}}_{j+1} = \sigma(\mathcal{W}_j \star_M \vec{\mathcal{A}}_j + \vec{\mathcal{B}}_j)$$

Benefits of Tensor Formulation:

- **Reduced parameters:** $n^4 + n^2 \rightarrow n^3 + n^2$ for $n \times n$ images
- Preserves multi-dimensional structure of data
- Mimetic structure: tensors are M-linear operators (analogous to matrices)

Stable Architectures via Hamiltonian Framework

Dynamic Perspective: Network layers = discrete time steps

$$\frac{d}{dt} \mathbf{a}(t) = \sigma(W(t) \mathbf{a}(t) + \mathbf{b}(t)) \quad \text{for } t \in [0, T]$$

Well-Posed Learning requires stability conditions on eigenvalues of Jacobian

Hamiltonian-Inspired System: Antisymmetric \Rightarrow inherently stable

$$\frac{d}{dt} \begin{bmatrix} \vec{\mathcal{A}}(t) \\ \vec{\mathcal{Z}}(t) \end{bmatrix} = \sigma \left(\begin{bmatrix} 0 & \mathcal{W}(t) \\ -\mathcal{W}(t)^\top & 0 \end{bmatrix} \star_M \begin{bmatrix} \vec{\mathcal{A}}(t) \\ \vec{\mathcal{Z}}(t) \end{bmatrix} + \begin{bmatrix} -\vec{\mathcal{B}}(t) \\ \vec{\mathcal{B}}(t) \end{bmatrix} \right)$$

Leapfrog Integration: Stable for purely imaginary eigenvalues

$$\vec{\mathcal{Z}}_{j+\frac{1}{2}} = \vec{\mathcal{Z}}_{j-\frac{1}{2}} - h \sigma(\mathcal{W}_j^\top \star_M \vec{\mathcal{A}}_j + \vec{\mathcal{B}}_j), \quad \vec{\mathcal{A}}_{j+1} = \vec{\mathcal{A}}_j + h \sigma(\mathcal{W}_j \star_M \vec{\mathcal{Z}}_{j+\frac{1}{2}} + \vec{\mathcal{B}}_j)$$

Tensor Neural Network Training

Forward Propagation: $\vec{\mathcal{A}}_{j+1} = \sigma(\mathcal{W}_j \star_M \vec{\mathcal{A}}_j + \vec{\mathcal{B}}_j)$

Objective Function:

$$E = \frac{1}{2} \|W_N \cdot \text{unfold}(\vec{\mathcal{A}}_N) - \mathbf{c}\|_F^2$$

Backward Propagation:

$$\delta \vec{\mathcal{A}}_j = \mathcal{W}_j^\top \star_M (\delta \vec{\mathcal{A}}_{j+1} \odot \sigma'(\vec{\mathcal{Z}}_{j+1}))$$

Parameter Updates (Gradient Descent):

$$\delta \mathcal{W}_j = (\delta \vec{\mathcal{A}}_{j+1} \odot \sigma'(\vec{\mathcal{Z}}_{j+1})) \star_M \vec{\mathcal{A}}_j^\top$$

$$\delta \vec{\mathcal{B}}_j = \delta \vec{\mathcal{A}}_{j+1} \odot \sigma'(\vec{\mathcal{Z}}_{j+1})$$

where $\vec{\mathcal{Z}}_{j+1} = \mathcal{W}_j \star_M \vec{\mathcal{A}}_j + \vec{\mathcal{B}}_j$ and \odot is pointwise product

Mimetic Structure

- **Update relations** are **analogous** to their matrix counterparts by **no coincidence**
- In the **M-product** framework, tensors are **M-linear** operators just as **matrices** are **linear** operators

Experimental Results

MNIST (28×28 grayscale, 60K train / 10K test)

- Tensor networks achieve **comparable accuracy** with **$28 \times$ fewer parameters**
- Parameters: Matrix $28^4 N$ vs. Tensor $28^3 N$

CIFAR-10 ($32 \times 32 \times 3$ RGB, 50K train / 10K test)

- Tensor networks **outperform** matrix networks at same depth
- Better accuracy with **$32 \times$ fewer parameters**

Key Findings:

- Hamiltonian + Leapfrog: stable even with large step sizes ($h = 1$)
- Standard ResNet: unstable, requires small h (≤ 0.25)
- Tensor formulation preserves spatial structure \Rightarrow better generalization

Newman, Horesh, Avron, Kilmer, **Stable tensor neural networks for rapid deep learning**,
Frontiers in Big Data, 2024

Stability in Motion

Data: 1200 train, concentric spheres (417 black, 466 red, 317 blue)

Parameters: $\alpha = 0.01$, $\sigma = \tanh$, 50 epochs, batch size = 10, $N = 32$

Regularized: $\frac{1}{2h} \|\mathbf{w}_{j+1} - \mathbf{w}_j\|_F^2$ for $1 \times 1 \times 3$ tubes \mathbf{w}_j

Resnet with $h = 0.5$

$$\mathbf{a}_{j+1} = \mathbf{a}_j + h \sigma(\mathbf{w}_j * \mathbf{a}_j + \mathbf{b}_j)$$

Stability in Motion

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Leapfrog with $h = 1$

$$\begin{cases} \mathbf{z}_{j+\frac{1}{2}} = \mathbf{z}_{j-\frac{1}{2}} - h \sigma(\mathbf{w}_j^\top * \mathbf{a}_j + \mathbf{b}_j) \\ \mathbf{a}_{j+1} = \mathbf{a}_j + h \sigma(\mathbf{w}_j * \mathbf{z}_{j+\frac{1}{2}} + \mathbf{b}_j) \end{cases}$$

Tensor-Tensor Graph Convolutional Neural Networks

TensorGCN: Motivation and Method

Motivation

- Graphs – popular data structures to effectively represent interactions
- Real world applications involve time evolving graphs; learning representations of dynamic graphs essential

Proposed Approach

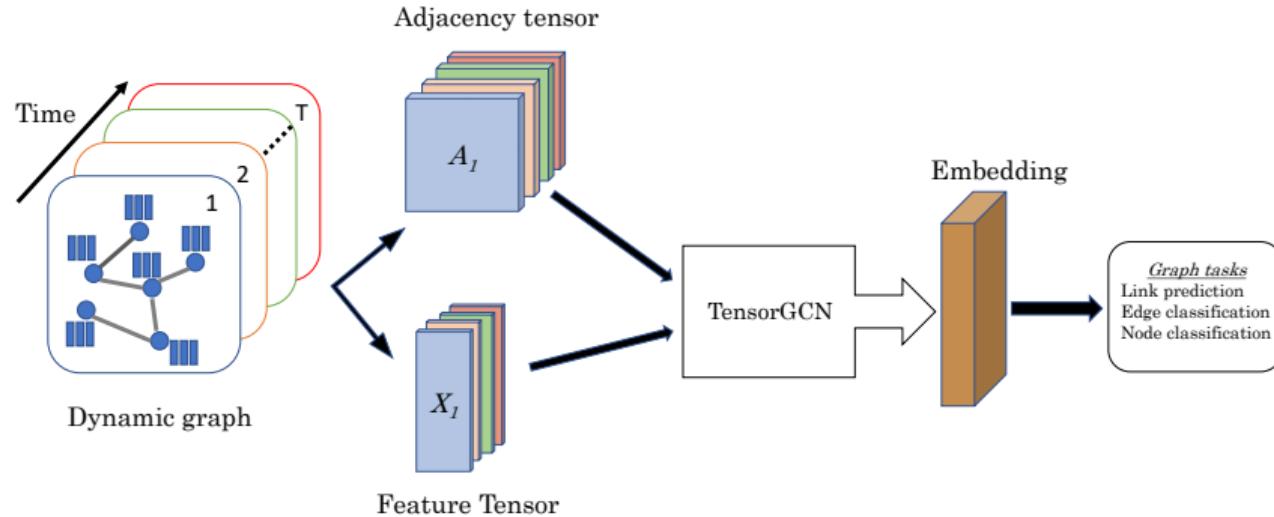
- Novel *tensor variant* of graph convolutional network (GCN)
- Captures correlation over time via tensor M-product framework

Two-Layer TensorGCN Model:

$$\mathcal{Z} = \text{softmax} \left(\mathcal{L} \star_M \sigma \left(\mathcal{L} \star_M \mathcal{X} \star_M \mathcal{W}^{(0)} \right) \star_M \mathcal{W}^{(1)} \right)$$

Graph Tasks: Link prediction, Edge classification, Node classification

TM-GCN



$$\mathbf{M} \cdot \text{unfolded tensor} = \text{output}$$

Diagram illustrating the matrix multiplication of a matrix \mathbf{M} with an **unfolded tensor** to produce an **output**. The **unfolded tensor** is shown as a sequence of vertical columns, and the **output** is shown as a sequence of vertical columns.

TensorGCN: Experimental Results (Edge Classification)

Table 1: Results without symmetrizing adjacency matrices (higher is better)

Method	Bitcoin OTC	Bitcoin Alpha	Reddit	Chess
WD-GCN	0.2062	0.1920	0.2337	0.4311
EvolveGCN	0.3284	0.1609	0.2012	0.4351
GCN	0.3317	0.2100	0.1805	0.4342
TensorGCN (Ours)	0.3529	0.2331	0.2028	0.4708

Table 2: Results with symmetrized adjacency matrices (higher is better)

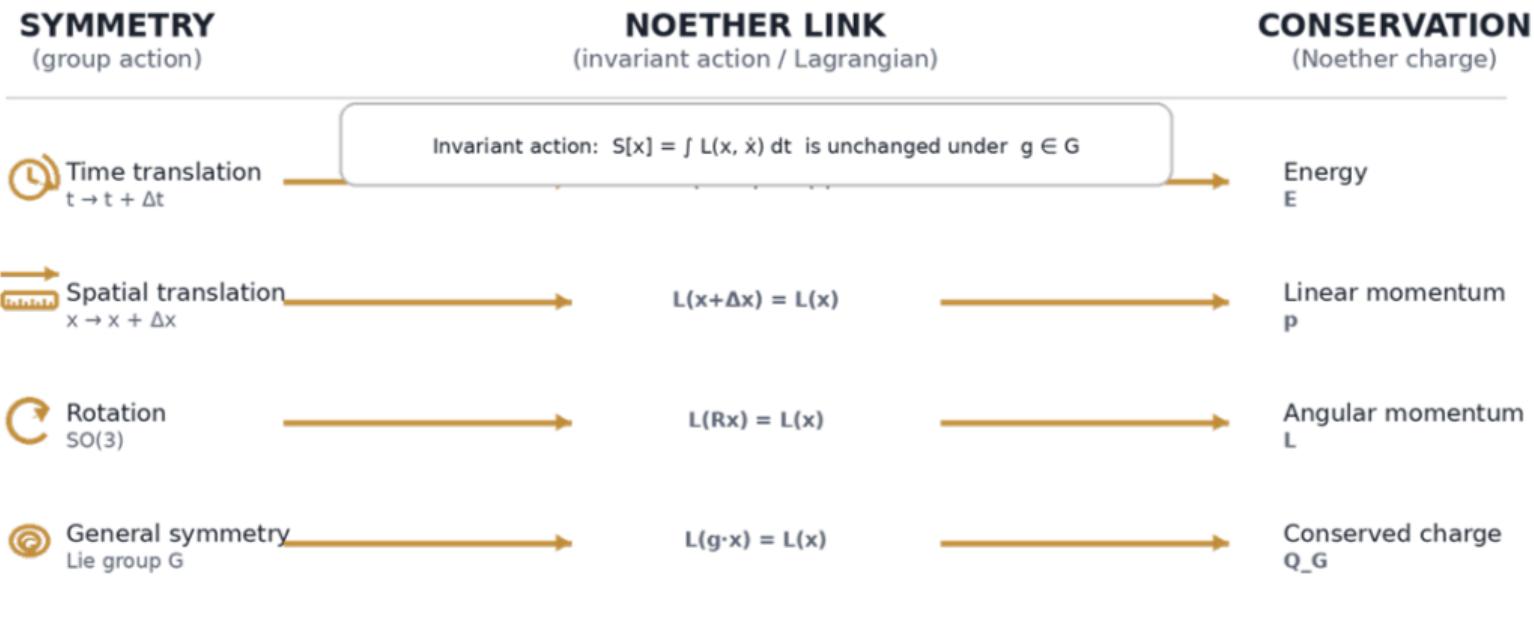
Method	Bitcoin OTC	Bitcoin Alpha	Reddit	Chess
WD-GCN	0.1009	0.1319	0.2173	0.4321
EvolveGCN	0.0913	0.2273	0.1942	0.4091
GCN	0.0769	0.1538	0.1966	0.4369
TensorGCN (Ours)	0.3103	0.2207	0.2071	0.4713

Malik, Ubaru, Horesh, Kilmer, Avron, **Dynamic graph convolutional networks using the tensor M-Product**, SIAM SDM, 2021

Optimal Symmetry-Aware Compression of Multiway Data

The Universal Importance of Symmetry

Noether's Theorem: Symmetry \Leftrightarrow Conservation



Implication for ML

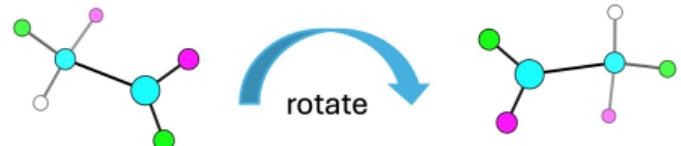
Models that respect symmetry inherit conservation properties automatically

Symmetries in Data

- Real-world data exhibit fundamental symmetries:

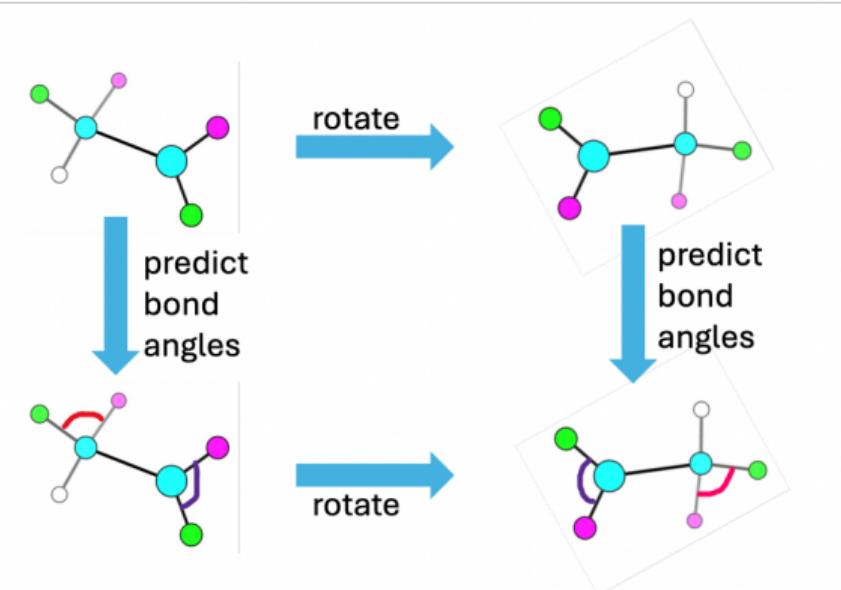
- ▶ **Graphs:** Permutation symmetry
- ▶ **Molecules:** 3D rotational symmetry
- ▶ **Images/Videos:** Translational symmetry
- ▶ **Time series:** Temporal invariance
- ▶ **Crystals/Fingerprints:** Reflection symmetry
- ▶ **Financial/Medical data:** Scale invariance

- **Groups** mathematically model data symmetries:
A set closed under an associative operation, with identity and inverse elements



Equivariant Models

- **Equivariant models** respect data symmetries
- **Definition:** A function f is equivariant to group G if:
$$f(g \cdot x) = g \cdot f(x) \quad \forall g \in G$$
- If we transform the input, the output transforms *consistently*



Translating Physical Symmetries into Machine Learning Language

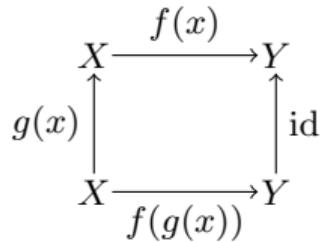
We express symmetry in models through two primary properties: Invariance and Equivariance

Invariance (The prediction doesn't change)

A function f is **invariant** to a transformation g if the output remains identical:

$$f(g(x)) = f(x)$$

Example: Classifying a 3D object. The label (“airplane”) should not change if the object is rotated

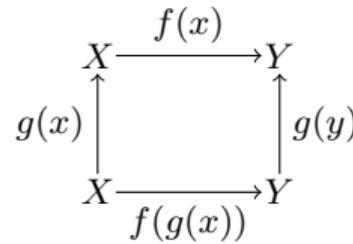


Equivariance (The prediction transforms with the input)

A function f is **equivariant** if transforming the input and then applying the function is the same as applying the function and then transforming the output:

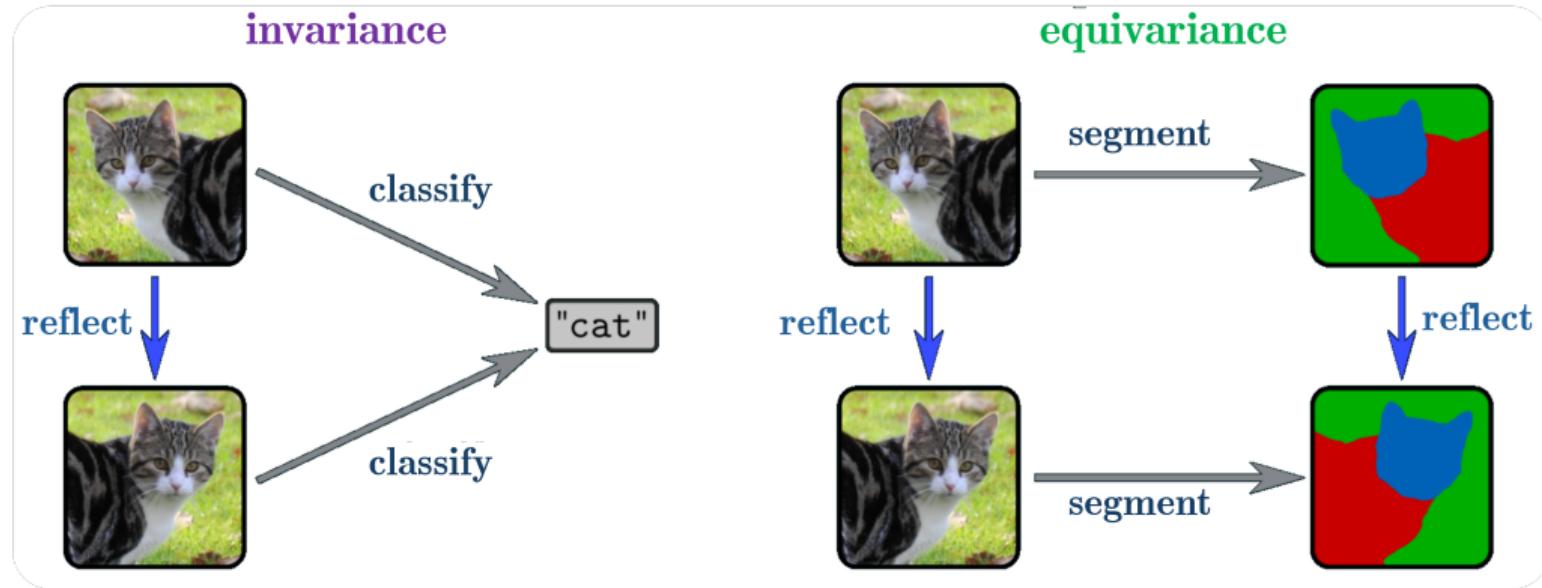
$$f(g(x)) = g(f(x))$$

Example: Predicting a force field on a molecule. If the molecule rotates, the force vectors must rotate with it



Translating Physical Symmetries into Machine Learning Language

We express symmetry in models through two primary properties: Invariance and Equivariance



The Brute-Force Approach vs. Principled Design

How can a model learn to respect symmetries?



Learning by Rote (Data Augmentation)

Present the model with the same data in many different transformed states (e.g., rotated, translated)

- **Computationally Expensive:** Requires massive datasets and long training times.
- **Incomplete:** Can never cover the full continuum of transformations (e.g., all possible rotations).
- **Not Robust:** Only achieves approximate invariance/equivariance

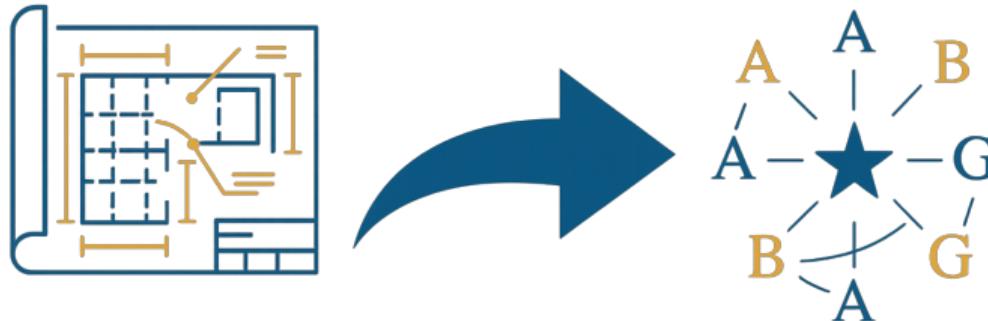


Generalizing by Design (Equivariant Architecture)

Constrain the model's hypothesis space to functions that are *guaranteed* to be equivariant

- The model does not need to *learn* the symmetry; it is an inherent property of its operations
- This ‘bakes in’ the equivariance, leading to automatic generalization across all transformations within the group

A Paradigm Shift: From Architectural Constraint to Intrinsic Property



The Old Question: “How can we design a *network architecture* that is equivariant to group G ?”

ENNs: Symmetry by Design

The New Question: “How can we define an *algebra* where group symmetry is an inherent property of multiplication itself?”



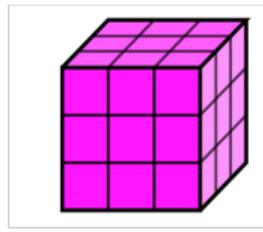
\star_G Algebra: Symmetry by Definition

Two Paths to Symmetry: A Comparison

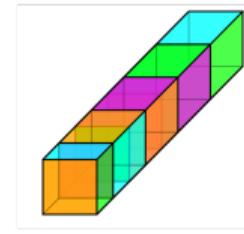
Feature	Equivariant Neural Networks (ENNs)	\star_G Algebra
Symmetry Handling	An architectural constraint , <i>enforced</i> layer by layer	An algebraic property , <i>intrinsic</i> to the features
Flexibility	Architectures are often group-specific	Universal . Any finite group G can define an algebra
Composition	Complex ; may require framework redesign	Seamless via direct product groups $(G_1 \times G_2 \times \dots \times G_m)$
Underlying Math	Constrained function approximation	Group representation theory
Analogy	Building a house from a specific blueprint	Writing sentences in a universal language

Structure-Aware Tensor Compression

- We look for tensor approximation that preserves
 - ➊ Symmetries in data
 - ➋ Number of modes of the original tensor
- **Why symmetries matter:** Enable simpler models, better sample efficiency, and improved generalization
- **Why preserve modes:** Maintain higher-order correlations lost in the matricization / vectorization process



order 3 tensor



Higher-order tensors

Definition: Convolution Tensor

Definition (Convolution Tensor)

Given a finite group G of order n , its corresponding **convolution tensor** $\mathcal{T} \in \mathbb{R}^{n \times n \times n}$ is defined by

$$\mathcal{T}(a, b, c) = \begin{cases} 1 & \text{if } ab = c \\ 0 & \text{otherwise} \end{cases}$$

for all $a, b, c \in G$

Key Property: For each $a \in G$, $\mathcal{T}(a, :, :)^\top = \rho(a)$

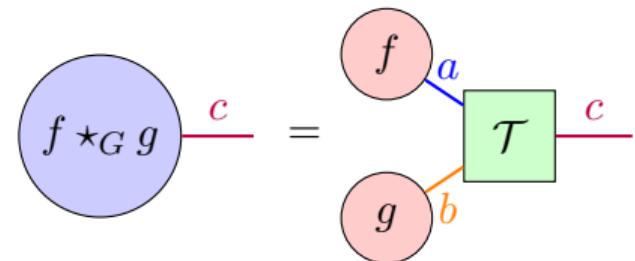
The horizontal slices of \mathcal{T} give the regular representation of group G

Convolution as Tensor Contraction

The convolution of functions $f, g: G \rightarrow \mathbb{R}$ satisfies

$$(f \star_G g)(c) = \sum_{a \in G} \sum_{b \in G} f(a)g(b)\mathcal{T}(a, b, c)$$

for all $c \in G$

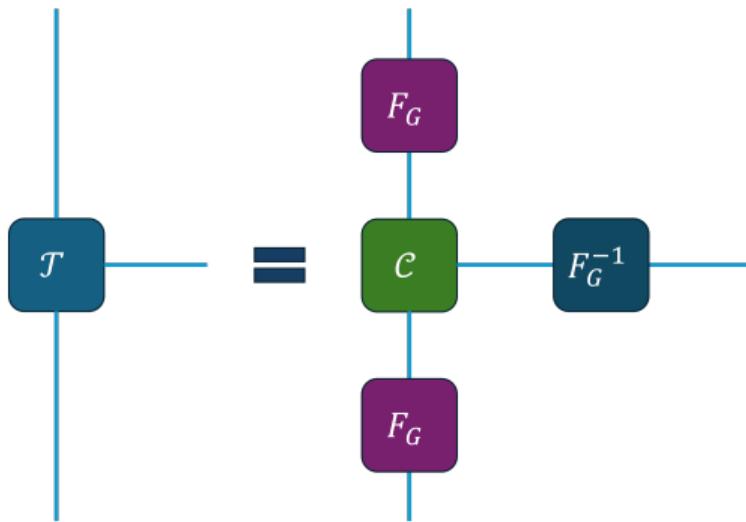


Proof idea: The condition $ab = c$ is equivalent to $b = a^{-1}c$, so $\mathcal{T}(a, b, c) = \delta_{b, a^{-1}c}$

- Reduces the double sum to the standard convolution definition
- The convolution tensor \mathcal{T} acts as a **multiplication table** in tensor form, enabling efficient computation of group convolutions through tensor contractions

Decomposing the Engine with the Peter-Weyl Theorem

The Peter-Weyl theorem allows us to decompose the convolution tensor \mathcal{T} into its fundamental algebraic components:



- **Factor Matrices (F_G):** Generalized Fourier Transforms that map data from the group domain into a new ‘symmetry basis’. For any finite group, $F(a, :) = \text{rvec}(\rho(a))$
- **Core Tensor (\mathcal{C}):** The **Peter-Weyl Tensor**: The algebraic “heart” of the group convolution tensor

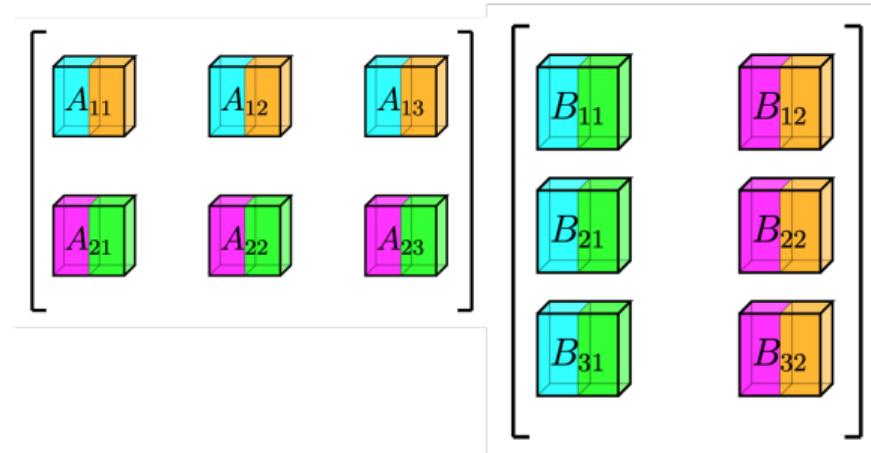
New Equivariant Tensor Algebra

- View order p tensors as matrices whose entries are order $d = p - 2$ tensors with entry-wise addition and multiplication given by convolution along each mode:

$$(\mathcal{A}_{ik} \star_G \mathcal{B}_{kj})(c_1, \dots, c_d) = \sum_{(a_1, \dots, a_d) \in G} \mathcal{A}_{ik}(a_1, \dots, a_d) \mathcal{B}_{kj}(a_1^{-1} c_1, \dots, a_d^{-1} c_d),$$

- Equivariant** product of two of these matrices is defined by:

$$(\mathcal{A} \star_G \mathcal{B})_{ij} = \sum_{k=1}^m \mathcal{A}_{ik} \star_G \mathcal{B}_{kj}$$



Useful properties: Notions of conjugate transpose, identity tensor, unitary tensor.
Connection to Fourier analysis

Tensor \star_G -SVD

- The SVD decomposition of a tensor \mathcal{A} is

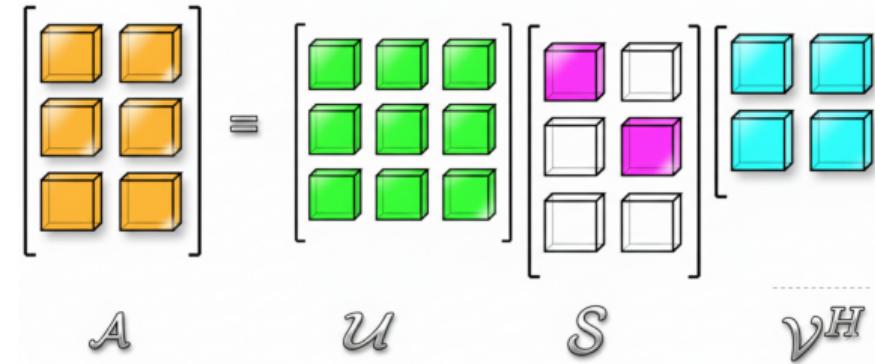
$$\mathcal{A} = \mathcal{U} \star_G \mathcal{S} \star_G \mathcal{V}^H$$

$$= \sum_{i=1}^r \mathcal{U}(:, i, :) \star_G \mathcal{S}(i, i, :) \star_G \mathcal{V}^H(:, i, :)$$

with \mathcal{U}, \mathcal{V} unitary and \mathcal{S} f -diagonal.

- The t-rank k approximation is

$$\mathcal{A}_k = \mathcal{U}(:, 1:k, :) \star_G \mathcal{S}(1:k, 1:k, :) \star_G \mathcal{V}^H(:, 1:k, :)$$



Optimal Compression Guarantee

- Eckart-Young-like equivariant result for tensors:

Theorem (Hoyos, Ubaru, Huh, Clarkson, Kilmer, Horesh (2025))

Given a finite group G , let $\mathcal{A} = \mathcal{U} \star_G \mathcal{S} \star_G \mathcal{V}^H$ be an SVD decomposition for the tensor $\mathcal{A} \in \mathbb{K}_G^{\ell \times m}$. Define $\mathcal{A}_k = \mathcal{U}(:, 1:k, :) \star_G \mathcal{S}(1:k, 1:k, :) \star_G \mathcal{V}^H(:, 1:k, :)$. Then \mathcal{A}_k is the best t -rank k approximation of the tensor \mathcal{A} . The squared error is

$$\|\mathcal{A} - \mathcal{A}_k\|_F^2 = \sum_{i=k+1}^r \|\mathbf{s}_i\|_F^2,$$

where r is the t -rank of \mathcal{A} .

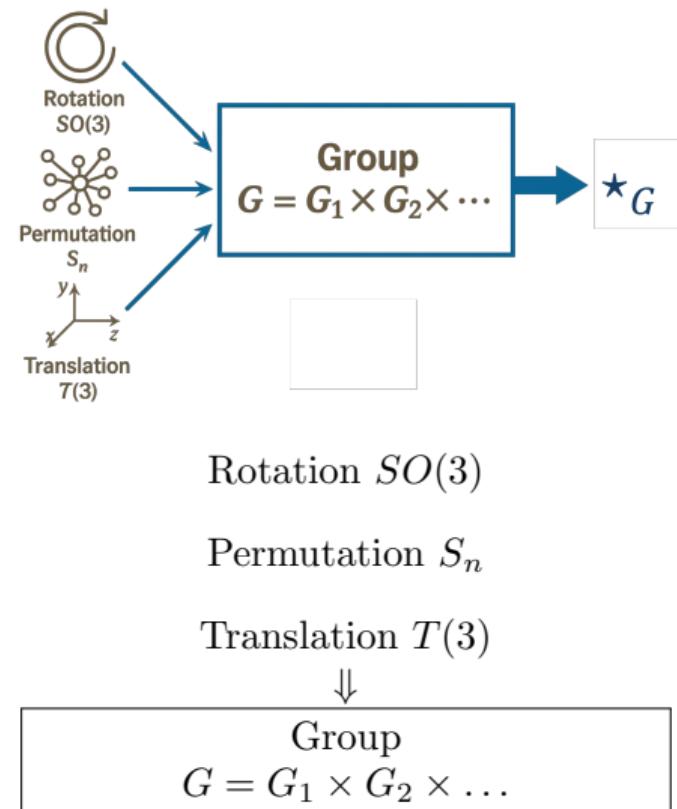
- For any t -rank k tensor \mathcal{B} , we have that

$$\|\mathcal{A} - \mathcal{A}_k\|_F^2 \leq \|\mathcal{A} - \mathcal{B}\|_F^2$$

Benefit 1: Seamless Composition of Symmetries

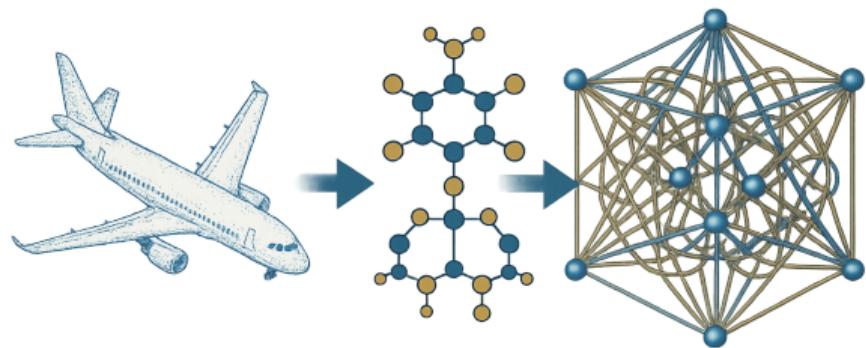
- The \star_G algebra naturally handles **direct product groups**: $G = G_1 \times G_2 \times \dots \times G_d$
- Allows the creation of a **single algebraic system** that is simultaneously equivariant to **multiple**, distinct symmetry groups

Example: An algebra defined by the group $G = SO(3) \times S_n$ can natively handle data that is both rotatable ($SO(3)$) and contains permutable parts (S_n). This is achieved without re-engineering network layers



Benefit 2: The Native Language of High-Order Symmetries

- Built upon **group representation theory**, the mathematical language of quantum mechanics and field theory
- Can **natively** represent symmetries beyond simple geometric transformations, such as the $SU(N)$ gauge symmetries crucial in Lattice QCD
- Provides a **principled**, first-principles way to incorporate deep **physical/geometrical priors** directly into machine learning models



$SO(3) \rightarrow$ Point Groups $\rightarrow SU(2, SU3)$

Benefit 3: Optimal Equivariant Compression

$$\mathcal{A} = \mathcal{U} \mathcal{S} \mathcal{V}^H$$

- The \star_G algebra offers a Singular Value Decomposition, and an Eckart-Young-like theorem holds:

$$A = U \star_G S \star_G V^H$$

where U and V are \star_G -unitary

- **The truncated \star_G -SVD provides the provably best low-rank approximation** to a tensor within the space of G -equivariant structures
- This is not possible with standard SVD or Tucker decompositions, which are blind to symmetry

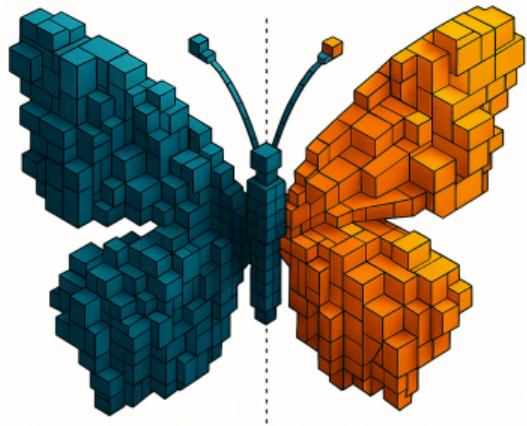
Summary

\star_M Algebra:

- Elementary units are *tubes*, not scalars
- Matrix-mimetic with optimal representations
- Preserves operator/data structure duality
- Scalable algorithms with seamless retrofit

\star_G Algebra:

- Elementary units are $d = p - 2$ tensors
- Extends to general group symmetries
- Reveals hidden equivariants in high-dimensional data



Take Away Message

Instead of forcing our world into a simple math,
we can adapt our math to the shape of the world

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