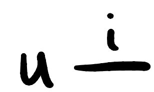
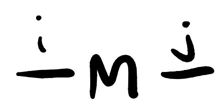
II. Tensor Networks

[Moitra, W '18]
[Ouerfelli, Tamaazousti, Rivasseau '22]
[Kunisky, Moore, W '24]

$u = (u_i) \quad i \in [n] = \{1, \dots, n\}$



$M = (M_{ij}) \quad i, j \in [n]$

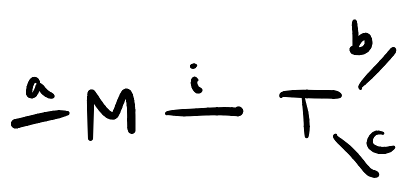


$T = (T_{ijk}) \quad i, j, k \in [n]$

$\vdots$

* Assume M, T symmetric : $T_{ijk} = T_{ikj} = \cdots$

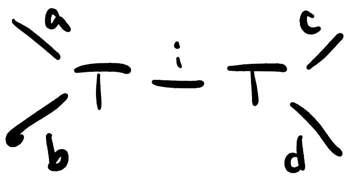
"Contraction" :



* Diagram describes a new tensor
* Indexed by open edges
* Sum over indices on closed edges

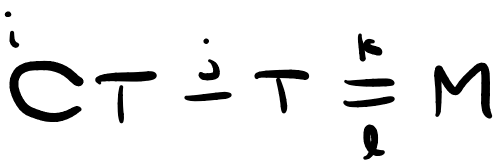
$S \in \mathbb{R}^{n \times n \times n}$

$$S_{abc} = \sum_{i \in [n]} M_{ai} T_{ibc}$$

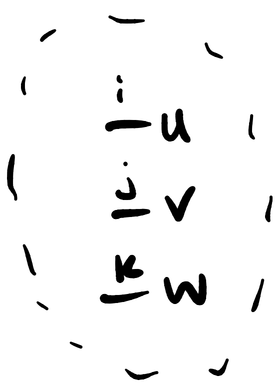


$S \in \mathbb{R}^{n \times n \times n \times n}$

$$S_{abcd} = \sum_i T_{abi} T_{icd}$$



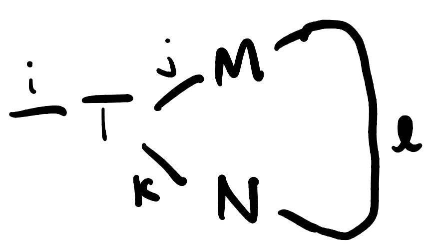
$\leftarrow$ Scalar: $\sum_{i,j,k,l} T_{iij} T_{jkl} M_{kl}$



$\leftarrow$ $u \otimes v \otimes w$

$S \in \mathbb{R}^{n \times n \times n}$

$$S_{ijk} = u_i v_j w_k$$

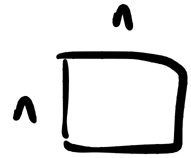


$u \in \mathbb{R}^n$

$$u_i = \sum_{jkl} T_{ijk} M_{jl} N_{kl}$$

Generalizes matrix / vector multiplication :

u, v 

A, B 

$u -$

$v -$

$- A -$

$- B -$

$u \overset{i}{-} v \iff \langle u, v \rangle = \sum_i u_i v_i$

$\overset{i}{-} A \overset{k}{-} B \overset{j}{-} \iff AB$ (matrix mult.)

$$C_{ij} = \sum_k A_{ik} B_{kj}$$

$- A - u \iff Au$ (matrix-vector mult.)

$u - A - B - v \iff u^T A B v$

* Tensors of order ≥ 3 can be "multiplied" in many ways

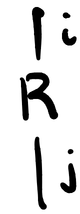
Change of basis (matrix)

$n \times n$ orthogonal matrix R : $RR^T = R^TR = I$

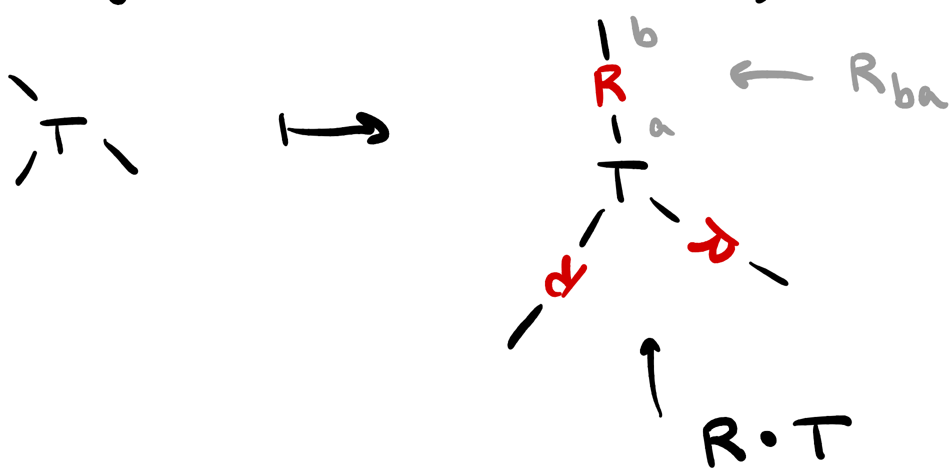
$M \mapsto RMR^T$

$-M- \qquad -R-M-R-$

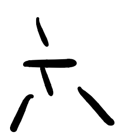
$R = (R_{ij})$



Change of basis (tensor)

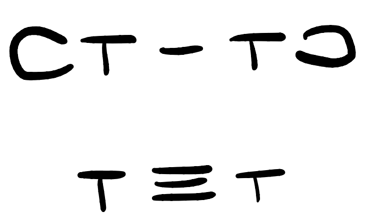


<u>Fact</u> : A closed diagram built from copies

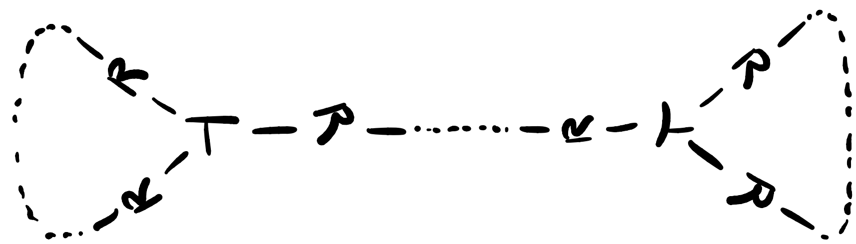
of  defines a <u>rotationally</u>-<u>invariant</u>

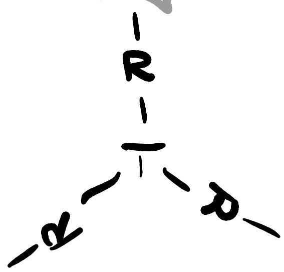
function $f : \mathbb{R}^{n \times n \times n} \to \mathbb{R}$.

$f(T) = f(R \cdot T)$

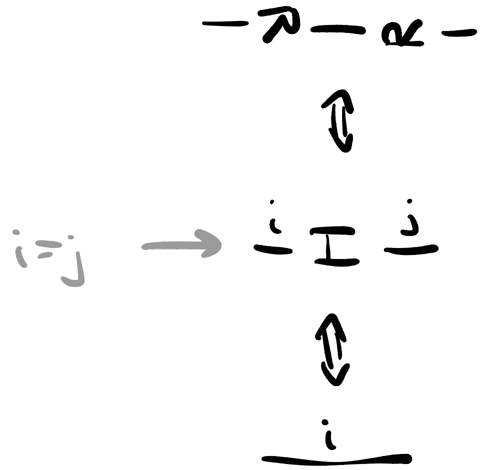


Why: $f(T) =$ 

$f(\underbrace{R \cdot T}) =$ 



$R^T R = I$



$I_{ij} = \mathbb{1}_{i=j}$

* $f(T)$ is a "graph moment" T^G ← graph

* $f(T)$ is a polynomial (in entries of T) of degree d = # vertices

see [KMW '24]

Fact: Graph moments with $\leq D$ vertices form a basis for rotationally invariant polynomials of degree $\leq D$.

* Tensor networks capture "all" invariant functions

* Same is true for tensors of other orders:

<u>Order-1</u>: $f(v) = f(Rv)$

empty diagram $\qquad f(v) \equiv 1$

$v - v \iff f(v) = \|v\|^2$

$$\begin{matrix} v \overset{i}{-} v \\ v \overset{j}{-} v \end{matrix} \iff F(v) = \|v\|^4$$

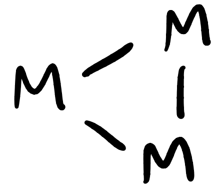
$$\sum_{ij} v_i v_i v_j v_j = \Big(\sum_i v_i^2\Big)\Big(\sum_j v_j^2\Big)$$

<u>Order-2</u>: $f(M) = f(RMR^T)$ $\qquad$ M Symmetric

$\emptyset$ (empty diagram) $\qquad f(M) \equiv 1$

$\overset{i}{(M)} \qquad f(M) = \sum_i M_{ii} = Tr(M)$

$M = M \qquad f(M) = Tr(M^2)$



$\vdots$

cycles

$$f(M) = \mathrm{Tr}(M^3)$$

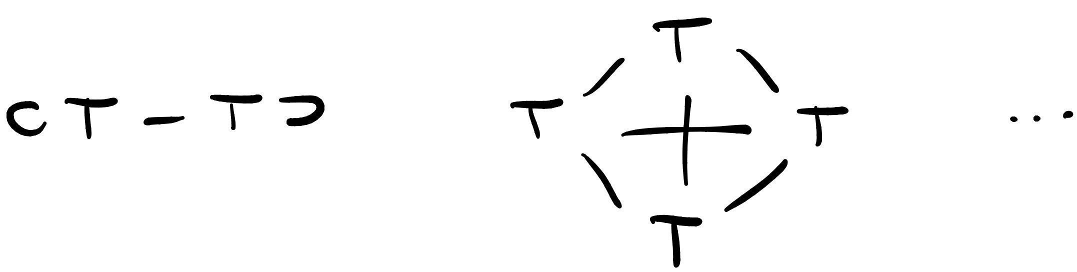
$$\vdots$$

$$\mathrm{Tr}(M^k) = \sum_i \lambda_i^k$$

eigenvalues

* Invariant polynomials are empirical moments of spectrum

* Tensors don't have a spectrum (?) but they do have (the analogue of) "empirical moments" T^G



<u>Fact</u>: Diagrams with one open edge and $\leq D$ vertices form a basis for rotationally <u>equivariant</u> polynomials of degree $\leq D$.

$$f : \mathbb{R}^{n \times n \times n} \to \mathbb{R}^n$$

$$f(R \cdot T) = R\, f(T)$$

$$\begin{tikzcd}
T \arrow[dd, equal] \arrow[dr, dash] & & \\
& T \arrow[r, dash] & {} \\
T \arrow[ur, dash] & &
\end{tikzcd}$$