Four Talks on Tensor Computations

4. Power Iterations, Symmetry, and Tensor Trains

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What is this Lecture About?

Rayleigh Quotients!

The eigenvalues and eigenvectors of a symmetric matrix C can be defined by the quotient

$$\frac{x^T C x}{x^T x}$$

and the singular values and singular vectors of a general matrix A can be defined by the quotient

$$\frac{u^T A v}{\parallel u \parallel \parallel v \parallel}$$

These are called Rayleigh Quotients and they can be generalized to tensors.

What is this Lecture About?

Symmetry

Given a basis $\{\phi_i(\mathbf{r})\}_{i=1}^n$ of atomic orbital functions, we consider the following order-4 tensor:

$$\mathcal{A}(p,q,r,s) \;=\; \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\phi_p(\mathbf{r}_1)\phi_q(\mathbf{r}_1)\phi_r(\mathbf{r}_2)\phi_s(\mathbf{r}_2)}{\|\mathbf{r}_1-\mathbf{r}_2\|} d\mathbf{r}_1 d\mathbf{r}_2.$$

This tensor has these symmetries:

$$\mathcal{A}(p,q,r,s) \;=\; \begin{cases} \mathcal{A}(q,p,r,s) & \text{(i)} \\ \mathcal{A}(p,q,s,r) & \text{(ii)} \\ \mathcal{A}(r,s,p,q) & \text{(iii)} \end{cases}$$

What is this Lecture About?

Data-Sparse Representations

The tensor $\mathcal{A}(1{:}n, 1{:}n, 1{:}n, 1{:}n, 1{:}n)$ involves $O(n^5)$ data but if

$$
\begin{aligned}
\mathcal{G}_1&: \quad n \times r \\
\mathcal{G}_2&: \quad r \times n \times r \\
\mathcal{G}_3&: \quad r \times n \times r \\
\mathcal{G}_4&: \quad r \times n \times r \\
\mathcal{G}_5&: \quad r \times n
\end{aligned}
$$

then the approximation

$$
\mathcal{A}(i_1, i_2, i_3, i_4, i_5) \approx
\sum_{k_1=1}^{r} \sum_{k_2=1}^{r} \sum_{k_3=1}^{r_3} \sum_{k_4=1}^{r} \mathcal{G}_1(i_1, k_1) \cdot \mathcal{G}_2(k_1, i_2, k_2) \cdot \mathcal{G}_3(k_2, i_3, k_3) \cdot \mathcal{G}_4(k_3, i_4, k_4) \cdot \mathcal{G}_5(k_4, i_5)
$$

involves $O(nr^2)$ data. Cool even if $r = O(n)$.

Power Iterations

Rayleigh Quotient: Matrix Case

The Big Connection

The singular values and singular vectors of a general matrix A are related to the stationary values and vectors of

$$\psi_A(u, v) \; = \; \frac{u^T A v}{\| \, u \, \| \| \, v \, \|}.$$

Rayleigh Quotient: Matrix Case

Definition

$$\psi_A(u,v) = \frac{\displaystyle\sum_{i_1=1}^{n_1}\sum_{i_2=1}^{n_2} A(i_1,i_2)u(i_1)v(i_2)}{\| u \|_2 \| v \|_2}$$

$$= \frac{u^T A v}{\| u \|_2 \| v \|_2}$$

$$= \frac{v^T A^T u}{\| u \|_2 \| v \|_2}$$

$$\mathcal{A} \in \mathbb{R}^{n_1 \times n_2}, u \in \mathbb{R}^{n_1}, v \in \mathbb{R}^{n_2}$$

Rayleigh Quotient: Tensor Case

Definition

$$\psi_{\mathcal{A}}(u,v,w) \;=\; \frac{\displaystyle\sum_{i_1=1}^{n_1}\sum_{i_2=1}^{n_2}\sum_{i_3=1}^{n_3} \mathcal{A}(i_1,i_2,i_3)\cdot u(i_1)\,v(i_2)\,w(i_3)}{\parallel u \parallel \parallel v \parallel \parallel w \parallel}$$

$$= \; u^T \mathcal{A}_{(1)}(w \otimes v) \,/\, (\parallel u \parallel\parallel v \parallel\parallel w \parallel)$$

$$= \; v^T \mathcal{A}_{(2)}(w \otimes u) \,/\, (\parallel u \parallel\parallel v \parallel\parallel w \parallel)$$

$$= \; w^T \mathcal{A}_{(3)}(v \otimes u) \,/\, (\parallel u \parallel\parallel v \parallel\parallel w \parallel)$$

$$\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3},\; u \in \mathbb{R}^{n_1},\; v \in \mathbb{R}^{n_2},\; w \in \mathbb{R}^{n_3}$$

Rayleigh Quotient: Matrix Case

The Gradient

If

$$\psi_A(u,v) \;=\; \frac{\displaystyle\sum_{i_1=1}^{n_1}\sum_{i_2=1}^{n_2} A(i_1,i_2)u(i_1)v(i_2)}{\parallel u \parallel_2 \parallel v \parallel_2}$$

and u and v are unit vectors, then

$$\nabla\psi_A(u,v) \;=\; \begin{bmatrix} Av \;-\; \psi_A(u,v)u \\ A^T u \;-\; \psi_A(u,v)v \end{bmatrix}$$

Rayleigh Quotient: Tensor Case

The Gradient

If

$$\psi_{\mathcal{A}}(u,v,w) \;=\; \frac{\displaystyle\sum_{i_1=1}^{n_1}\sum_{i_2=1}^{n_2}\sum_{i_3=1}^{n_3} \mathcal{A}(i_1,i_2,i_3)\cdot u(i_1)\, v(i_2)\, w(i_3)}{\parallel u \parallel \parallel v \parallel \parallel w \parallel}$$

and u, v, and w are unit vectors, then

$$\nabla\psi_{\mathcal{A}} \;=\; \left[\begin{array}{c} \mathcal{A}_{(1)}(w\otimes v) \;-\; \psi_{\mathcal{A}}(u,v,w)u \\ \mathcal{A}_{(2)}(w\otimes u) \;-\; \psi_{\mathcal{A}}(u,v,w)v \\ \mathcal{A}_{(3)}(v\otimes u) \;-\; \psi_{\mathcal{A}}(u,v,w)w \end{array}\right]$$

Rayleigh Quotient: Matrix Case

The SVD Connection

If $\nabla \psi_A(u, v) = 0$, then

$$\begin{aligned} Av &= \psi_A(u, v) \cdot u \\ A^T u &= \psi_A(u, v) \cdot v \end{aligned}$$

Thus, the stationary values (vectors) for ψ_A define the singular values (singular vectors) for A.

Rayleigh Quotient: Tensor Case

The SVD Connection

If $\nabla \psi_A(u, v, w) = 0$, then

$$\begin{aligned} A_{(1)} \cdot (w \otimes v) &= \psi_A(u, v, w) \cdot u \\ A_{(2)} \cdot (w \otimes u) &= \psi_A(u, v, w) \cdot v \\ A_{(3)} \cdot (v \otimes u) &= \psi_A(u, v, w) \cdot w \end{aligned}$$

We **define** the stationary values (vectors) for $\psi_{\mathcal{A}}$ to be the singular values (singular vectors) for $\mathcal{A}$.

Rayleigh Quotient: Matrix Case

The Gradient Equations

$$\begin{aligned} Av &= \psi_A(u,v)\cdot u \\ A^T u &= \psi_A(u,v)\cdot v \end{aligned}$$

Power Method Step

$$\begin{aligned} \tilde{u} &= Av, & u &\leftarrow \tilde{u}/\parallel \tilde{u} \parallel \\ \tilde{v} &= A^T u. & v &\leftarrow \tilde{v}/\parallel \tilde{v} \parallel \\ \sigma &= \psi_A(u,v) \end{aligned}$$

Same as power method applied to $A^T A$.

In the limit, $\sigma u v^T$ converges to the closest rank-1 to A.

Rayleigh Quotient: Tensor Case

The Gradient Equations

$$
\begin{aligned}
A_{(1)} \cdot (w \otimes v) &= \psi_A(u, v, w) \cdot u \\
A_{(2)} \cdot (w \otimes u) &= \psi_A(u, v, w) \cdot v \\
A_{(3)} \cdot (v \otimes u) &= \psi_A(u, v, w) \cdot w
\end{aligned}
$$

Higher-Order Power Method Step

$$
\begin{aligned}
\tilde{u} &= \mathcal{A}_{(1)}(w \otimes v), \quad u_1 = \tilde{u}/\| \tilde{u} \| \\
\tilde{v} &= \mathcal{A}_{(2)}(w \otimes u), \quad u_2 = \tilde{v}/\| \tilde{v} \| \\
\tilde{w} &= \mathcal{A}_{(3)}(v \otimes u), \quad u_3 = \tilde{w}/\| \tilde{w} \| \\
\sigma &= \psi_{\mathcal{A}}(u, v, w)
\end{aligned}
$$

In the limit, $\sigma u \circ v \circ w$ tends to converge to the closest rank-1 to $\mathcal{A}$.

Power Iterations with Symmetry

Rayleigh Quotients: Symmetric Matrix Case

Definition

If $C \in \mathbb{R}^{n \times n}$ is symmetric, then

$$\begin{aligned} \phi_C(x) &= \frac{x^T C x}{x^T x} \\ &= \left(\sum_{i_1=1}^{n} \sum_{i_2=1}^{n} C(i_1, i_2) x(i_1) x(i_2) \right) \Big/ \left(x^T x \right) \end{aligned}$$

is a Rayleigh quotient.

Gradient

If $x \in \mathbb{R}^n$ is a unit vector, then

$$\nabla \phi_C = 2 \left(C x - \phi_C(x) \cdot x \right).$$

Rayleigh Quotients: Symmetric Matrix Case

The Eigenvalue Connection

If $\nabla\phi_C(x) \;=\; 0$ then

$$C\,x \;=\; \phi_C(x)\cdot x$$

Thus, the stationary values (vectors) of ϕ_C define the eigenvalues (eigenvectors) of C.

This has many implications for both analysis and algorithms...

Rayleigh Quotients: Symmetric Matrix Case

Power Method Step

$$\begin{aligned} \tilde{x} &= Cx \\ x &= \tilde{x}/\| \tilde{x} \| \\ \lambda &= x^T C x \end{aligned}$$

To formulate a tensor analog we need to be clear on the notion of a symmnetric tensor

Tensor Transposition: The Order-3 Case

Six possibilities...

If $\mathcal{C} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$, then there are $6 = 3!$ possible transpositions identified by the notation $\mathcal{C}^{<[i\ j\ k]>}$ where $[i\ j\ k]$ is a permutation of $[1\ 2\ 3]$:

$$\mathcal{B} = \left\{ \begin{array}{c} \mathcal{C}^{<[1\ 2\ 3]>} \\ \mathcal{C}^{<[1\ 3\ 2]>} \\ \mathcal{C}^{<[2\ 1\ 3]>} \\ \mathcal{C}^{<[2\ 3\ 1]>} \\ \mathcal{C}^{<[3\ 1\ 2]>} \\ \mathcal{C}^{<[3\ 2\ 1]>} \end{array} \right\} \quad \Longrightarrow \quad \left\{ \begin{array}{c} b_{ijk} \\ b_{ikj} \\ b_{jik} \\ b_{jki} \\ b_{kij} \\ b_{kji} \end{array} \right\} = c_{ijk}$$

for $i = 1{:}n_1,\ j = 1{:}n_2,\ k = 1{:}n_3$.

Symmetric Tensors

The Order-3 Definition: $\mathcal{C} \in \mathbb{R}^{n \times n \times n}$

$$\mathcal{C}(i,j,k) = \begin{cases} \mathcal{C}(i,k,j) \\ \mathcal{C}(j,i,k) \\ \mathcal{C}(i,k,i) \\ \mathcal{C}(k,i,j) \\ \mathcal{C}(k,j,i) \end{cases}$$

Symmetric Tensors

Rank-1 Symmetric Tensors

If $x \in \mathbb{R}^n$, then

$$\mathcal{C} \;=\; x \circ x \circ x$$

is a symmetric rank-1 tensor. This is obvious since

$$\mathcal{C}(i_1, i_2, i_3) \;=\; x(i_1)x(i_2)x(i_3).$$

Note that

$$\text{vec}(x \circ x \circ \circ x) \;=\; x \otimes x \otimes x$$

Symmetric Tensors

Symmetric Rank

An order-3 symmetric tensor $\mathcal{C}$ has symmetric rank r if there exists $x_1, \ldots, x_r \in \mathbb{R}^n$ and $\sigma \in \mathbb{R}^r$ such that

$$\mathcal{C} \;=\; \sum_{k=1}^{r} \sigma_k \cdot x_k \circ x_k \circ x_k$$

and no shorter sum of symmetric rank-1 tensors exists. Symmetric rank is denoted by $\text{rank}_S(\mathcal{C})$.

Note, there may be a shorter sum so

$$\mathcal{C} \;=\; \sum_{k=1}^{\tilde{r}} \tilde{\sigma}_k \cdot \tilde{x}_k \circ \tilde{y}_k \circ \tilde{z}_k$$

Rayleigh Quotients: Symmetric Tensor Case

Definition

$$\phi_{\mathcal{C}}(x) \;=\; \frac{\displaystyle\sum_{i_1=1}^{n}\sum_{i_2=1}^{n}\sum_{i_3=1}^{n} \mathcal{C}(i_1,i_2,i_3)\cdot x(i_1)\,x(i_2)\,x(i_3)}{\parallel x \parallel^3}$$

where $\mathcal{C} \in \mathbb{R}^{n\times n\times n}$ is symmetric and $x \in \mathbb{R}^N$.

Alternative Formulation

$$\phi_{\mathcal{C}}(x) \;=\; \frac{x^T \mathcal{C}_{(k)}(x \otimes x)}{\parallel x \parallel^3} \qquad k \text{ doesn't matter}$$

Easy to get the gradient of $\phi_{\mathcal{C}}$...

Rayleigh Quotients: Symmetric Tensor Case

Gradient of $\phi_{\mathcal{C}}$

If x is a unit vector, then

$$\nabla \phi_{\mathcal{C}}(x) \;=\; \mathcal{C}_{(1)}(x \otimes x) \;-\; \phi_{\mathcal{C}}(x) \cdot x$$

Idea for improving x:

$$\tilde{x} = \mathcal{C}_{(1)}(x \otimes x), \quad x = \tilde{x} / \| \tilde{x} \|$$

Rayleigh Quotients: Symmetric Tensor Case

Symmetric Higher-Order Power Method

Initialize unit vector x.

Repeat

$$\tilde{x} \;=\; \mathcal{C}_{(1)}(x \otimes x)$$

$$x = \tilde{x}/\parallel \tilde{x} \parallel$$

Sample Convergence Result

If the order of $\mathcal{C}$ is even and M is a square unfolding, then the iteration converges if M is positive definite.

The SVD - SymEig Connection

The "Sym" of a Matrix

$$\text{sym}(A) \;=\; \left[\begin{array}{cc} 0 & A \\ A^T & 0 \end{array}\right] \in \mathbb{R}^{(n_1+n_2)\times(n_1+n_2)}$$

The SVD of A Relates to the EVD of sym(A)

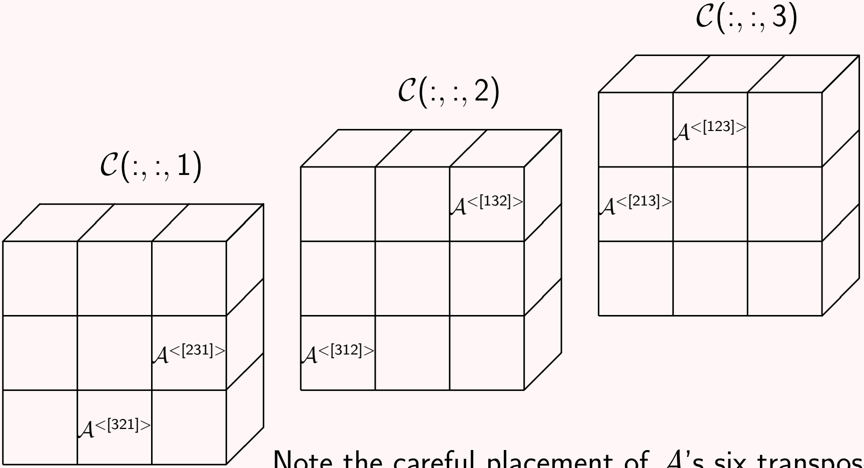
If $A = U \cdot \text{diag}(\sigma_i) \cdot V^T$ is the SVD of $A \in \mathbb{R}^{n_1 \times n_2}$, then for $k = 1{:}\text{rank}(A)$

$$\left[\begin{array}{cc} 0 & A \\ A^T & 0 \end{array}\right] \left[\begin{array}{c} u_k \\ \pm v_k \end{array}\right] \;=\; \pm\sigma_k \left[\begin{array}{c} u_k \\ \pm v_k \end{array}\right]$$

where $u_k = U(:, k)$ and $v_k = V(:, k)$.

The above SVD-related power method was essentially traditional power method applied to finding the largest eigenvector of sym(A).

An Order-3 Example...



Note the careful placement of $\mathcal{A}$'s six transposes

Eigenvalue Rayleigh Quotients For Symmetric Tensors

Equivalence

If $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, then applying the Higher-Order Power Method to $\mathcal{A}$, is "equivalent" to applying the Symmetric Higher order Power Method to $\text{sym}(\mathcal{A})$.

Exiting the former with σ, u_1, u_2 and u_3 is essentially the same as exiting the latter with σ and

$$x = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}.$$

Eigenvalue Rayleigh Quotients For Symmetric Tensors

Theorem

If

$$\left\{ \sigma, \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \right\}$$

is a stationary pair for sym($\mathcal{C}$) then so are

$$\left\{ \sigma, \begin{bmatrix} u_1 \\ -u_2 \\ -u_3 \end{bmatrix} \right\}, \quad \left\{ -\sigma, \begin{bmatrix} u_1 \\ -u_2 \\ u_3 \end{bmatrix} \right\}, \quad \left\{ -\sigma, \begin{bmatrix} u_1 \\ u_2 \\ -u_3 \end{bmatrix} \right\}$$

Recall that for matrices...

$$\begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} u_k \\ \pm v_k \end{bmatrix} = \pm\sigma_k \begin{bmatrix} u_k \\ \pm v_k \end{bmatrix}$$

Symmetric Tensors: Interesting Aside about Rank

Fact

If $\mathcal{C} \in \mathbb{C}^{n\times\cdots\times n}$ is an order-d symmetric tensor, then with probability 1

$$\text{rank}_S(\mathcal{C}) = \begin{cases} f(d,m)+1 & \text{if } (d,n) = (3,5),(4,3),(4,4), \text{ or } (4,5) \\ f(d,n) & \text{otherwise} \end{cases}$$

where

$$f(d,n) = \text{ceil}\left(\frac{\binom{n+d-1}{d}}{n} \right)$$

Symmetric Tensor Rank is "more tractable" than General Tensor Rank.

Symmetric Tensors: Interesting Aside about Rank

Interesting Possible Connection

Easy:

$$d!\ \mathrm{rank}(\mathcal{A}) \ \leq \ \mathrm{rank}_S(\mathrm{sym}(\mathcal{A}))$$

Equality is hard or perhaps not true. But if it could be established, then we would have new insight into the tensor rank problem.

More on Tensor Symmetry

The Two-Electron Integral Tensor (TEI)

Given a basis $\{\phi_i(\mathbf{r})\}_{i=1}^{n}$ of atomic orbital functions, we consider the following order-4 tensor:

$$\mathcal{A}(p,q,r,s) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\phi_p(\mathbf{r}_1)\phi_q(\mathbf{r}_1)\phi_r(\mathbf{r}_2)\phi_s(\mathbf{r}_2)}{\|\mathbf{r}_1 - \mathbf{r}_2\|} d\mathbf{r}_1 d\mathbf{r}_2.$$

The TEI tensor has these symmetries:

$$\mathcal{A}(p,q,r,s) \ = \begin{cases} \mathcal{A}(q,p,r,s) & \text{(i)} \\ \mathcal{A}(p,q,s,r) & \text{(ii)} \\ \mathcal{A}(r,s,p,q) & \text{(iii)} \end{cases}$$

We say that $\mathcal{A}$ is "((12)(34))-symmetric".

The ((12)(34))-Symmetric Multilinear Product where $X \in \mathbb{R}^{n \times n}$

$$\mathcal{B}(j_1, j_2, j_3, j_4)$$

$$=$$

$$\sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \sum_{i_3=1}^{n} \sum_{i_4=1}^{n} \mathcal{A}(i_1, i_2, i_3, i_4) \cdot X(i_1, j_1) \cdot X(i_2, j_2) \cdot X(i_3, j_3) \cdot X(i_4, j_4)$$

and the tensor $\mathcal{B}$ has these symmetries...

$$\mathcal{B}(p, q, r, s) = \begin{cases} \mathcal{B}(q, p, r, s) \\ \mathcal{B}(p, q, s, r) \\ \mathcal{B}(r, s, p, q) \end{cases}$$

In other words $\mathcal{B}$ is also ((12)(34))-symmetric.

The Block Matrix Product Formulation

If $A = (A_{rs})$ and $B = (B_{rs})$ are n-by-n block matrices with n-by-n blocks and

$$\mathcal{A}(p,q,r,s) \quad \leftrightarrow \quad [\, A_{rs} \,]_{pq}$$

$$\mathcal{B}(p,q,r,s) \quad \leftrightarrow \quad [\, B_{rs} \,]_{pq}$$

then the ((12)(34))-symmetric multilinear product is equivalent to

$$B \;=\; (X \otimes X)^T A (X \otimes X)$$

The n^2-by-n^2 matrix A is special. It is positive definite with very low rank. And it has multiple symmetries...

A "Inherits" $\mathcal{A}$'s Structure

Since

$$\mathcal{A}(p,q,r,s) \;\leftrightarrow\; [\,A_{rs}\,]_{pq}$$

and

$$\mathcal{A}(p,q,r,s) \;=\; \begin{cases} \mathcal{A}(q,p,r,s) & \text{(i)} \\ \mathcal{A}(p,q,s,r) & \text{(ii)} \\ \mathcal{A}(r,s,p,q) & \text{(iii)} \end{cases}$$

it follows that

(i) The blocks of A are symmetric ($A_{rs}^T = A_{rs}$) because of (i).

(ii) A is symmetric as a block matrix ($A_{rs} = A_{sr}$) because (ii).

Time to Talk About Unfoldings

The tensor $\mathcal{A} \in \mathbb{R}^{n \times n \times n \times n}$ can be unfolded several ways.

- We have depicted the $[1,3] \times [2,4]$ unfolding $A = \mathcal{A}_{[1,3]\times[2,4]}$ defined by

$$\mathcal{A}(i_1, i_2, i_3, i_4) \;\rightarrow\; A(i_1 + (i_3 - 1)n, i_2 + (i_4 - 1)n)$$

- Also of interest is the $[1,2] \times [3,4]$ unfolding $A = \mathcal{A}_{[1,2]\times[3,4]}$ defined by

$$\mathcal{A}(i_1, i_2, i_3, i_4) \;\rightarrow\; A(i_1 + (i_2 - 1)n, i_3 + (i_4 - 1)n)$$

If $\mathcal{A}$ is ((12)(34))-symmetric, these two unfoldings display different multiple symmetries...

The $[1,3]\times[2,4]$ Unfolding a ((12)(34))-Symmetric $\mathcal{A}$

If $A = \mathcal{A}_{[1,3]\times[2,4]}$, then (as we have seen) A is block symmetric with symmetric blocks.

$$A = \left[\begin{array}{ccc|ccc|ccc} 11 & 12 & 13 & 12 & 17 & 18 & 13 & 18 & 22 \\ 12 & 14 & 15 & 17 & 19 & 20 & 18 & 23 & 24 \\ 13 & 15 & 16 & 18 & 20 & 21 & 22 & 24 & 25 \\ \hline 12 & 17 & 18 & 14 & 19 & 23 & 15 & 20 & 24 \\ 17 & 19 & 20 & 19 & 26 & 27 & 20 & 27 & 29 \\ 18 & 20 & 21 & 23 & 27 & 28 & 24 & 29 & 30 \\ \hline 13 & 18 & 22 & 15 & 20 & 24 & 16 & 21 & 25 \\ 18 & 23 & 24 & 20 & 27 & 29 & 21 & 28 & 30 \\ 22 & 24 & 25 & 24 & 29 & 30 & 25 & 30 & 31 \end{array}\right].$$

The $[1,2] \times [3,4]$ Unfolding of a ((12)(34)) Symmetric $\mathcal{A}$

If $A = \mathcal{A}_{[1,2]\times[3,4]}$, then A is symmetric and (among other things) is "perfect shuffle" symmetric.

$$A = \left[\begin{array}{ccc|ccc|ccc} 11 & 12 & 13 & 12 & 14 & 15 & 13 & 15 & 16 \\ 12 & 17 & 18 & 17 & 19 & 20 & 18 & 20 & 21 \\ 13 & 18 & 22 & 18 & 23 & 24 & 22 & 24 & 25 \\ \hline 12 & 17 & 18 & 17 & 19 & 20 & 18 & 20 & 21 \\ 14 & 19 & 23 & 19 & 26 & 27 & 23 & 27 & 28 \\ 15 & 20 & 24 & 20 & 27 & 29 & 24 & 29 & 30 \\ \hline 13 & 18 & 22 & 18 & 23 & 24 & 22 & 24 & 25 \\ 15 & 20 & 24 & 20 & 27 & 29 & 24 & 29 & 30 \\ 16 & 21 & 25 & 21 & 28 & 30 & 25 & 30 & 31 \end{array}\right]$$

Each column reshapes into a 3x3 symmetric matrix, e.g., $A(:,)$ reshapes to

$$\left[\begin{array}{ccc} 11 & 12 & 13 \\ 12 & 14 & 15 \\ 13 & 15 & 16 \end{array}\right]$$

What is perfect shuffle symmetry?

Perfect Shu□e Symmetry

An n^2-by-n^2 matrix A has perfect shuffle symmetry if

$$A = \Pi_{n,n} A \Pi_{n,n}$$

where

$$\Pi_{n,n} \; = \; I_{n^2}(:, v), \qquad v \; = \; [\, 1{:}n{:}n^2 \mid 2{:}n{:}n^2 \mid \; \cdots \; \mid n{:}n{:}n^2 \,].$$

e.g.,

$$\Pi_{3,3} \; = \; \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right]$$

The Perfect Shu□e Π_{nn}

Because $\Pi_{n,n}$ is symmetric it has just two eigenvalues: $+1$ and -1.

$$\Pi_{3,3} = \left[\begin{array}{ccc|ccc|ccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \begin{bmatrix} x_{11} \\ x_{21} \\ x_{31} \\ \mathbf{x_{12}} \\ x_{22} \\ x_{32} \\ x_{13} \\ x_{23} \\ x_{33} \end{bmatrix} = \pm \begin{bmatrix} x_{11} \\ x_{12} \\ x_{13} \\ \mathbf{x_{21}} \\ x_{22} \\ x_{23} \\ x_{31} \\ x_{32} \\ x_{33} \end{bmatrix}$$

If $\Pi_{n,n}x = x$, then $\texttt{reshape}(x, n, n)$ is symmetric.

If $\Pi_{n,n}x = -x$, then $\texttt{reshape}(x, n, n)$ is skew-symmetric.

Solution Framework:

1. Closed-form block diagonalization with a special highly-structured orthogonal $Q = [Q_1\ Q_2]$:

$$Q^T A Q \;=\; \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix}$$

2. Compute half-sized rank-revealing LDL factorizations:

$$P_i A_i P_i^T \;\approx\; L_i D_i L_i^T, \quad i = 1, 2$$

3. Set

$$\tilde{A} \;=\; Y_1 D_1 Y_1^T \;+\; Y_2 D_2 Y_2^T$$

where $Y_i = Q_i P_i^T L_i$.

4. $B \;\approx\; \tilde{B} \;=\; (X \otimes X)^T \tilde{A} (X \otimes X)$

Tensor Trains

Tensor Train: An Example

Given the "carriages"...

$$
\begin{aligned}
\mathcal{G}_1 &: \quad n_1 \times r_1 \\
\mathcal{G}_2 &: \quad r_1 \times n_2 \times r_2 \\
\mathcal{G}_3 &: \quad r_2 \times n_3 \times r_3 \\
\mathcal{G}_4 &: \quad r_3 \times n_4 \times r_4 \\
\mathcal{G}_5 &: \quad r_4 \times n_5
\end{aligned}
$$

We define the train" $\mathcal{A}(1{:}n_1, 1{:}n_2, 1{:}n_3, 1{:}n_4, 1{:}n_5)$...

$$
\mathcal{A}(i_1, i_2, i_3, i_4, i_5)
$$

$$
=
$$

$$
\sum_{k_1=1}^{r_1} \sum_{k_2=1}^{r_2} \sum_{k_3=1}^{r_3} \sum_{k_4=1}^{r_4} \mathcal{G}_1(i_1, k_1) \cdot \mathcal{G}_2(k_1, i_2, k_2) \cdot \mathcal{G}_3(k_2, i_3, k_3) \cdot \mathcal{G}_4(k_3, i_4, k_4) \cdot \mathcal{G}_5(k_4, i_5)
$$

Think of a graph where the nodes are low-order tensors and the edges are contractions.

Tensor Train: An Example

Given the "carriages"...

$$
\begin{aligned}
\mathcal{G}_1 &: \quad n_1 \times r_1 \\
\mathcal{G}_2 &: \quad r_1 \times n_2 \times r_2 \\
\mathcal{G}_3 &: \quad r_2 \times n_3 \times r_3 \\
\mathcal{G}_4 &: \quad r_3 \times n_4 \times r_4 \\
\mathcal{G}_5 &: \quad r_4 \times n_5
\end{aligned}
$$

We define the train" $\mathcal{A}(1{:}n_1, 1{:}n_2, 1{:}n_3, 1{:}n_4, 1{:}n_5)$...

$$\mathcal{A}(i_1, i_2, i_3, i_4, i_5)$$

$$=$$

$$\sum_{k_1=1}^{r_1} \sum_{k_2=1}^{r_2} \sum_{k_3=1}^{r_3} \sum_{k_4=1}^{r_4} \mathcal{G}_1(i_1, k_1) \cdot \mathcal{G}_2(k_1, i_2, k_2) \cdot \mathcal{G}_3(k_2, i_3, k_3) \cdot \mathcal{G}_4(k_3, i_4, k_4) \cdot \mathcal{G}_5(k_4, i_5)$$

$O(nr^2)$ vs $O(n^5)$

Tensor Train: An Example

Given the "carriages"...

$$\mathcal{G}_1: \quad n_1 \times r_1$$

$$\mathcal{G}_2: \quad r_1 \times n_2 \times r_2$$

$$\mathcal{G}_3: \quad r_2 \times n_3 \times r_3$$

$$\mathcal{G}_4: \quad r_3 \times n_4 \times r_4$$

$$\mathcal{G}_5: \quad r_4 \times n_5$$

We define the train" $\mathcal{A}(1{:}n_1, 1{:}n_2, 1{:}n_3, 1{:}n_4, 1{:}n_5)$...

$$\mathcal{A}(i_1, i_2, i_3, i_4, i_5)$$

$$=$$

$$\sum_{k_1=1}^{r_1} \sum_{k_2=1}^{r_2} \sum_{k_3=1}^{r_3} \sum_{k_4=1}^{r_4} \mathcal{G}_1(i_1, k_1) \cdot \mathcal{G}_2(k_1, i_2, k_2) \cdot \mathcal{G}_3(k_2, i_3, k_3) \cdot \mathcal{G}_4(k_3, i_4, k_4) \cdot \mathcal{G}_5(k_4, i_5)$$

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$$\mathcal{G}_2: \quad r_1 \times n_2 \times r_2$$
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$$\mathcal{A}(i_1, i_2, i_3, i_4, i_5)$$
$$=$$
$$\sum_{k_1=1}^{r_1}\sum_{k_2=1}^{r_2}\sum_{k_3=1}^{r_3}\sum_{k_4=1}^{r_4} \mathcal{G}_1(i_1, k_1)\cdot\mathcal{G}_2(k_1, i_2, k_2)\cdot\mathcal{G}_3(k_2, i_3, k_3)\cdot\mathcal{G}_4(k_3, i_4, k_4)\cdot\mathcal{G}_5(k_4, i_5)$$

$O(nr^2)$ vs $O(n^5)$

Tensor Train: An Example

Given the "carriages"...

$$\begin{array}{ll} \mathcal{G}_1: & n_1 \times r_1 \\ \mathcal{G}_2: & r_1 \times n_2 \times r_2 \\ \mathcal{G}_3: & r_2 \times n_3 \times r_3 \\ \mathcal{G}_4: & r_3 \times n_4 \times r_4 \\ \mathcal{G}_5: & r_4 \times n_5 \end{array}$$

We define the train" $\mathcal{A}(1{:}n_1, 1{:}n_2, 1{:}n_3, 1{:}n_4, 1{:}n_5)$...

$$\mathcal{A}(i_1, i_2, i_3, i_4, i_5)$$
$$=$$
$$\sum_{k_1=1}^{r_1}\sum_{k_2=1}^{r_2}\sum_{k_3=1}^{r_3}\sum_{k_4=1}^{r_4} \mathcal{G}_1(i_1, k_1)\cdot\mathcal{G}_2(k_1, i_2, k_2)\cdot\mathcal{G}_3(k_2, i_3, k_3)\cdot\mathcal{G}_4(k_3, i_4, k_4)\cdot\mathcal{G}_5(k_4, i_5)$$

$O(nr^2)$ vs $O(n^5)$

Computing a Tensor Train Representation

Main Idea

A sequence of unfoldings is produced.

The unfoldings get narrower and narrower.

A rank-revealing SVD $U(\Sigma V^T) = UZ$ is computed each time.

The "carriages" are reshaped U-matrices.

Computing a Tensor Train Representation

1(a) Rank-revealing SVD: $\texttt{reshape}(A, [n_1\ ,\ n_2 n_3 n_4 n_5]) \ = \ U_1 Z_1.$

$\mathcal{G}_1 = \texttt{reshape}(U_1, [n_1, r_1]).$

Computing a Tensor Train Representation

1(a) Rank-revealing SVD: $\texttt{reshape}(A, [n_1\ ,\ n_2 n_3 n_4 n_5]) \ = \ U_1 Z_1.$

$\mathcal{G}_1 = \texttt{reshape}(U_1, [n_1, r_1]).$

2(a) Rank-revealing SVD: $\texttt{reshape}(Z_1, [r_1 n_2, n_3 n_4 n_5]) \ = \ U_2 Z_2.$

$\mathcal{G}_2 = \texttt{reshape}(U_2, [r_1, n_2, r_2]).$

Computing a Tensor Train Representation

1(a) Rank-revealing SVD: $\texttt{reshape}(A, [n_1\ ,\ n_2 n_3 n_4 n_5]) \;=\; U_1 Z_1.$

$\mathcal{G}_1 = \texttt{reshape}(U_1, [n_1, r_1]).$

2(a) Rank-revealing SVD: $\texttt{reshape}(Z_1, [r_1 n_2, n_3 n_4 n_5]) \;=\; U_2 Z_2.$

$\mathcal{G}_2 = \texttt{reshape}(U_2, [r_1, n_2, r_2]).$

3(a) Rank-revealing SVD: $\texttt{reshape}(Z_2, [r_2 n_3, n_4 n_5]) \;=\; U_3 Z_3.$

$\mathcal{G}_3 = \texttt{reshape}(U_3, [r_2, n_3, r_3]).$

Computing a Tensor Train Representation

1(a) Rank-revealing SVD: $\texttt{reshape}(A, [n_1\ ,\ n_2 n_3 n_4 n_5]) \;=\; U_1 Z_1.$

$\mathcal{G}_1 = \texttt{reshape}(U_1, [n_1, r_1]).$

2(a) Rank-revealing SVD: $\texttt{reshape}(Z_1, [r_1 n_2, n_3 n_4 n_5]) \;=\; U_2 Z_2.$

$\mathcal{G}_2 = \texttt{reshape}(U_2, [r_1, n_2, r_2]).$

3(a) Rank-revealing SVD: $\texttt{reshape}(Z_2, [r_2 n_3, n_4 n_5]) \;=\; U_3 Z_3.$

$\mathcal{G}_3 = \texttt{reshape}(U_3, [r_2, n_3, r_3]).$

4(a) Rank-revealing SVD: $\texttt{reshape}(Z_3, [r_3 n_4, n_5]) \;=\; U_4 Z_4.$

$\mathcal{G}_4 = \texttt{reshape}(U_4, [r_3, n_4, r_4]).$

$\mathcal{G}_5 = \texttt{reshape}(Z_4, [r_4, n_5]).$

Computing a Tensor Train Representation

Why Do We Emerge With...

$$\mathcal{A}(i_1, i_2, i_3, i_4, i_5)$$
$$=$$
$$\sum_{k_1=1}^{r_1} \sum_{k_2=1}^{r_2} \sum_{k_3=1}^{r_3} \sum_{k_4=1}^{r_4} \mathcal{G}_1(i_1, k_1) \cdot \mathcal{G}_2(k_1, i_2, k_2) \cdot \mathcal{G}_3(k_2, i_3, k_3) \cdot \mathcal{G}_4(k_3, i_4, k_4) \cdot \mathcal{G}_5(k_4, i_5)$$

The reason is because...

1. The rows and columns of an unfolding can be "multi-indexed"

2. The product of two matrices can sometimes be viewed as a contraction between two tensors.

Multi-Indexing Rows and Columns

```
n = [2 3 2 2 3];
A = randn(n);
B = reshape(A,[n(1)*n(2)*n(3) , n(4)*n(5) ]
```

$$
\begin{array}{cc}
 & \begin{array}{cccccc} (1,1) & (2,1) & (1,2) & (2,2) & (1,3) & (2,3) \end{array} \\
B = & \left[\begin{array}{cccccc}
a_{11111} & a_{11121} & a_{11112} & a_{11122} & a_{11113} & a_{11123} \\
a_{21111} & a_{21121} & a_{21112} & a_{21122} & a_{21113} & a_{21123} \\
a_{12111} & a_{12121} & a_{12112} & a_{12122} & a_{12113} & a_{12123} \\
a_{22111} & a_{22121} & a_{22112} & a_{22122} & a_{22113} & a_{22123} \\
a_{13111} & a_{13121} & a_{13112} & a_{13122} & a_{13113} & a_{13123} \\
a_{23111} & a_{23121} & a_{23112} & a_{23122} & a_{23113} & a_{23123} \\
a_{11211} & a_{11221} & a_{11212} & a_{11222} & a_{11213} & a_{11223} \\
a_{21211} & a_{21221} & a_{21212} & a_{21222} & a_{21213} & a_{21223} \\
a_{12211} & a_{12221} & a_{12212} & a_{12222} & a_{12213} & a_{12223} \\
a_{22211} & a_{22221} & a_{22212} & a_{22222} & a_{22213} & a_{22223} \\
a_{13211} & a_{13221} & a_{13212} & a_{13222} & a_{13213} & a_{13223} \\
a_{23211} & a_{23221} & a_{23212} & a_{23222} & a_{23213} & a_{23223}
\end{array}\right]
\begin{array}{c}
(1,1,1) \\ (2,1,1) \\ (1,2,1) \\ (2,2,1) \\ (1,3,1) \\ (2,3,1) \\ (1,1,2) \\ (2,1,2) \\ (1,2,2) \\ (2,2,2) \\ (1,3,2) \\ (2,3,2)
\end{array}
\end{array}
$$

Matrix Multiplication with Multi-indexing

Suppose B is $(n_1 n_2 n_3) \times r$ and C is $r \times (n_4 n_5)$

$A = BC$ as a Matrix Product

$$A(i,j) \;=\; \sum_{k=1}^{r} B(i,k)C(k,j)$$

$1 \le i \le n_1 n_2 n_3, \;\; 1 \le j \le n_4 n_5$

$A = BC$ as a tensor contraction

$$A(i_1,i_2,i_3,j_1,j_2) \;=\; \sum_{k=1}^{r} B(i_1,i_2,i_3,k)C(k,j_1,j_2)$$

$1 \le i_1 \le n_1, \;\; 1 \le i_2 \le n_2, \;\; 1 \le i_3 \le n_3, \;\; 1 \le j_1 \le n_4, \;\; 1 \le j_2 \le n_5$

Summary of Lecture

Key Words

- Symmetric tensors have the property that the value of $\mathcal{A}(\mathbf{i})$ does not depend upon the order the indices. They arise in many settings and special properties.
- Setting to zero the gradient of a multilinear Rayleigh quotient leads to the idea of eigenvalues and singular value of tensors.
- Higher-order power methods based on the Rayleigh quotient can be used to find nearest rank-1 approximations to either general or symmetric tensors
- When tensors with multiple symmetries are unfolded, the unfoldings have multiple symmetries that can be exploited.
- Data sparse approximations are critical to the development of tensor methods that scale with d. Tensor Trains are one approach in this direction.

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