CS 598 EVS: Tensor Computations

Tensor Decomposition

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CP Decomposition Rank

- The *canonical polyadic or CANDECOMP/PARAFAC (CP) decomposition* expresses an order d tensor in terms of d factor matrices
  - *For $\boldsymbol{\mathcal{T}} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, a rank R CP decomposition is defined by matrices $\boldsymbol{U}^{(i)} \in \mathbb{R}^{n_i \times R}$ so that*

$$t_{i_1 \dots i_d} = \sum_{r=1}^{R} \prod_{j=1}^{d} u_{i_j r}^{(j)}$$

  - *The CP decomposition is also often denoted by*

$$\boldsymbol{\mathcal{T}} = [\![\boldsymbol{U}^{(1)}, \dots, \boldsymbol{U}^{(d)}]\!]$$

  - *First proposed by Hitchcock in 1927*
  - *Given a tensor, the smallest R for which it has a CP decomposition is the tensor rank, also sometimes referred to as the CP rank or canonical rank*
  - *Finding the CP rank and associated decomposition enables automatic derivation of bilinear algorithms as reviewed in the prior lecture*
  - *Early parts of this lectures mostly follow T. Kolda and B. Bader ”Tensor Decompositions and Applications”, SIAM Review 2009.*

Tensor Rank Properties

- Tensor rank does not satisfy many of the properties of matrix rank
  - *Rank of a real-valued tensor can be different over the complex field, e.g., for*

    $$\mathcal{T} = \left[\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \right]$$

    which is a perfectly conditioned tensor, the rank over $\mathbb{R}$ *is* 3 *but over* $\mathbb{C}$ *it is* 2*,*

    $$\mathcal{T} = [\![\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix}]\!]$$

  - *The maximal possible rank of tensors of particular dimensions is often unequal to the typical tensor rank, which is any rank for which the set of tensors of a given size with that rank has positive volume*
  - $2 \times 2 \times 2$ *tensors have typical ranks* 2 *(79%) and* 3 *(21%) over* $\mathbb{R}$*, and typical rank* 2 *over* $\mathbb{C}$

Typical Rank and Generic Rank

- When there is only a single typical tensor rank, it is the *generic rank*
  - *For decomposition over $\mathbb{C}$, tensors have a generic rank*
  - *For symmetric tensors, the symmetric rank (all CP factors same) is equal to the CP rank if the factor matrices are full rank [Comon, Golub, Lim, Mourrain, 2008]*
  - *If we restrict to symmetric tensors of order $d > 2$ and dimension n, the generic rank over $\mathbb{C}$ is*

    $$R = \left\lceil \binom{n+d-1}{d} / n \right\rceil$$

    except when $(d, n) \in \{(3,5),(4,3),(4,4),(4,5)\}$ in which cases it should be increased by one (Alexander–Hirschowitz theorem)
  - *This rank bound makes sense, as the total amount of information in a single factor matrix is $nR \approx \binom{n+d-1}{d}$, which matches the number of unique entries in the symmetric tensor*
  - *For maximal rank of an $n_1 \times n_2 \times n_3$ tensor, the maximal rank is bounded (weakly) by $R \leqslant \min(n_1n_2, n_1n_3, n_2n_3)$, which follows by the same intuition*

Uniqueness Sufficient Conditions

- Unlike the low-rank matrix case, the CP decomposition can be unique
  - *In the matrix case, given $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{V}^T$, for any invertible $\boldsymbol{M}$ we can obtain a new factorization $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{M}(\boldsymbol{V}\boldsymbol{M}^{-1})^T$*
  - *In CP decomposition, the indeterminacy is generally limited to permutation of the R rank-1 factors and scaling of their components*
  - *Modulo permutation and scaling, strong conditions exist on uniqueness of the CP decomposition*
  - *Define the k-rank of a matrix as the maximum value of k such that any k columns of the matrix are linearly independent*
  - *For an order 3 tensor with CP decomposition $[\![\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}]\!]$ where the factor matrices have k-ranks k_A, k_B, and k_C, a sufficient condition for uniqueness is*

$$k_A + k_B + k_C \geqslant 2R + 2$$

  - *For order d tensors whose CP decomposition is composed of matrices with has k ranks $k_1, \ldots, k_d$, the sufficient condition is*

$$\sum_{i=1}^{d} k_i \geqslant 2R + (d - 1)$$

Uniqueness Necessary Conditions

- Necessary conditions for uniqueness of the CP decomposition also exist
  - *A simple necessary condition for uniqueness is*

$$\min_{l \in \{1,\ldots,d\}} \left(\prod_{i=1, i \neq l}^{d} \operatorname{rank}(\boldsymbol{U}^{(i)}) \right) \geqslant R$$

  - *This condition stems from the more general restriction that*

$$\min_{l \in \{1,\ldots,d\}} \operatorname{rank} \left(\bigodot_{i=1, i \neq l}^{d} \boldsymbol{U}^{(i)} \right) = R$$

  - *When one of the d Khatri-Rao products is rank deficient, multiple (infinite) choices of the lth factor matrices must bring the residual to zero*

Degeneracy

- The best rank-k approximation may not exist, a problem known as *degeneracy* of a tensor
  - *Consider a rank 3 tensor*

$$\boldsymbol{\mathcal{T}} = \boldsymbol{a}_1 \otimes \boldsymbol{b}_1 \otimes \boldsymbol{c}_2 + \boldsymbol{a}_1 \otimes \boldsymbol{b}_2 \otimes \boldsymbol{c}_1 + \boldsymbol{a}_2 \otimes \boldsymbol{b}_1 \otimes \boldsymbol{c}_1$$

  - *The tensor can be approximated arbitrarily closely by*

$$\boldsymbol{\mathcal{W}}^{(\alpha)} = \alpha(\boldsymbol{a}_1 + \frac{1}{\alpha}\boldsymbol{a}_2) \otimes (\boldsymbol{b}_1 + \frac{1}{\alpha}\boldsymbol{b}_2) \otimes (\boldsymbol{c}_1 + \frac{1}{\alpha}\boldsymbol{c}_2) - \alpha \boldsymbol{a}_1 \otimes \boldsymbol{b}_1 \otimes \boldsymbol{c}_1$$

    in particular

$$\lim_{\alpha\to\infty} \|\boldsymbol{\mathcal{W}}^{(\alpha)} - \boldsymbol{\mathcal{T}}\| = 0$$

  - *Consequently, the best rank-2 approximation does not exist for this tensor, as in the limit $\boldsymbol{\mathcal{W}}^{(\alpha)}$ converges to an order 3 tensor*

Border Rank

- Degeneracy motivates an approximate notion of rank, namely *border rank*
  - *The border rank of a tensor $\mathcal{T}$ is defined as the smallest R such that, for any $\epsilon > 0$, there exists a rank R tensor $\mathcal{W}$ such that*

    $$\|\mathcal{T} - \mathcal{W}\| < \epsilon$$

  - *The border rank is always less than the rank of a tensor, but can also be smaller*
  - *The concept of border rank has been intensively used to find fast bilinear algorithms for matrix multiplication*
  - *The border rank and rank of the $4 \times 4 \times 4$ multiplication tensor are both 7, yielding Strassen's algorithm*
  - *For the $9 \times 9 \times 9$ tensor defining multiplication of 3×3 matrices, determining rank and border rank is an open problem, the rank is between 19 and 23, while the border rank is between 14 and 21*

Approximation by CP Decomposition

- Approximation via CP decomposition is a nonlinear optimization problem
  - *Given order d tensor $\boldsymbol{\mathcal{T}}$ with all dimensions equal to n, the rank-R CP approximation problem can be written as*

$$\min_{\boldsymbol{U}^{(1)},\ldots,\boldsymbol{U}^{(n)}\in\mathbb{R}^{n\times R}} \underbrace{\frac{1}{2}\|\boldsymbol{\mathcal{T}} - [\![\boldsymbol{U}^{(1)},\ldots,\boldsymbol{U}^{(d)}]\!]\|_F^2}_{\phi(\boldsymbol{U}^{(1)},\ldots,\boldsymbol{U}^{(d)})}$$

  - *The gradient of this objective function is*

$$\nabla\phi = \left[d\phi/d\boldsymbol{U}^{(1)} \ldots d\phi/d\boldsymbol{U}^{(d)}\right]$$

  - *Each component of the gradient has the form*

$$\frac{d\phi}{d\boldsymbol{U}^{(i)}}(\boldsymbol{U}^{(1)},\ldots,\boldsymbol{U}^{(d)}) = \boldsymbol{U}^{(i)} \ast_{j=1,j\neq i}^{d} \boldsymbol{U}^{(j)^T}\boldsymbol{U}^{(j)} - \underbrace{\boldsymbol{\mathcal{T}}_{(i)} \bigodot_{j=1,j\neq i}^{d} \boldsymbol{U}^{(j)}}_{\textit{MTTKRP}}$$

  - *Unless R is very large, computing $\frac{d\phi}{d\boldsymbol{U}^{(i)}}(\boldsymbol{U}^{(1)},\ldots,\boldsymbol{U}^{(d)})$ is not much cheaper than minimizing ϕ w.r.t. $\boldsymbol{U}^{(i)}$ by solving for $\boldsymbol{U}^{(i)}$ in $\frac{d\phi}{d\boldsymbol{U}^{(i)}}(\boldsymbol{U}^{(1)},\ldots,\boldsymbol{U}^{(d)}) = \mathbf{0}$*

Alternating Least Squares Algorithm

- The standard approach for finding an approximate or exact CP decomposition of a tensor is the *alternating least squares (ALS) algorithm*
  - *Consider rank R decomposition of a tensor $\mathcal{T} \in \mathbb{R}^{n\times n\times n}$ over $\mathbb{R}$*
  - *A sweep takes as input $[\![\boldsymbol{U}^{(k)}, \boldsymbol{V}^{(k)}, \boldsymbol{W}^{(k)}]\!]$ solves 3 quadratic optimization problems to obtain $[\![\boldsymbol{U}^{(k+1)}, \boldsymbol{V}^{(k+1)}, \boldsymbol{W}^{(k+1)}]\!]$, updating each factor matrix in sequence, typically via the normal equations:*

$$\begin{aligned}
(\boldsymbol{V}^{(k)^T}\boldsymbol{V}^{(k)} * \boldsymbol{W}^{(k)^T}\boldsymbol{W}^{(k)})\boldsymbol{U}^{(k+1)} &= \boldsymbol{T}_{(1)}(\boldsymbol{V}^{(k)} \odot \boldsymbol{W}^{(k)}) \\
(\boldsymbol{U}^{(k+1)^T}\boldsymbol{U}^{(k+1)} * \boldsymbol{W}^{(k)^T}\boldsymbol{W}^{(k)})\boldsymbol{V}^{(k+1)} &= \boldsymbol{T}_{(2)}(\boldsymbol{U}^{(k+1)} \odot \boldsymbol{W}^{(k)}) \\
(\boldsymbol{U}^{(k+1)^T}\boldsymbol{U}^{(k+1)} * \boldsymbol{V}^{(k+1)^T}\boldsymbol{V}^{(k+1)})\boldsymbol{W}^{(k+1)} &= \boldsymbol{T}_{(3)}(\boldsymbol{U}^{(k+1)} \odot \boldsymbol{V}^{(k+1)})
\end{aligned}$$

  - *Residual decreases monotonically, since the subproblems in each subset of nR variables are quadratic*
  - *Forming the linear equations has cost $O(dnR^2)$ while forming the right-hand-sides requires an MTTKRP with cost $O(n^dR)$*

Properties of Alternating Least Squares for CP

- *CP-ALS achieves linear local convergence to local minima of our objective* ϕ
  - *this follows from the equivalence of the optimality conditions (vanishing gradient) and the ALS update rule*
  - *no global convergence guarantees are available, and in practice algorithm convergence can stagnate, typically due to the factor matrix iterates becoming ill-conditioned*
- *CP-ALS guarantees monotonic decrease in residual*
  - *the exact minimizer is found for each quadratic subproblem, which cannot be worse than the previous choice*
- *the equations for each subproblem are formed by a Khatri-Rao product, which makes subproblems amenable to fast approximate methods*

Alternating Least Squares for Tucker Decomposition

- For Tucker decomposition, an analogous optimization procedure to ALS is referred to as *high-order orthogonal iteration (HOOI)*
  - *Each component of the derivative of the Tucker approximation objective function with respect to the product of a factor matrix and the core tensor is a TTMc (as opposed to MTTKRP in the CP case)*

$$\psi(\boldsymbol{\mathcal{Z}},\boldsymbol{U},\boldsymbol{V},\boldsymbol{W}) = \frac{1}{2}\Big(t_{ijk} - \sum_{pqr} z_{pqr}u_{ip}v_{jq}w_{kr}\Big)^2$$

$$\frac{d\psi}{d(\boldsymbol{\mathcal{Z}} \times_1 \boldsymbol{U})}(\boldsymbol{\mathcal{Z}},\boldsymbol{U},\boldsymbol{V},\boldsymbol{W}) = \sum_{j,k} t_{ijk}v_{jq}w_{kr} - \sum_{pq'r'} z_{pqr}u_{ip}\underbrace{\Big(\sum_{j} v_{jq'}v_{jq}\Big)}_{\delta(q,q')}\underbrace{\Big(\sum_{k} w_{kr'}w_{kr}\Big)}_{\delta(r,r')}$$

  - *Consequently, we can find the minimizing $\boldsymbol{\mathcal{Z}} \times_1 \boldsymbol{U}$ by SVD of the mode-1 unfolding of the TTMC $\boldsymbol{\mathcal{T}} \times_2 \boldsymbol{V}^T \times_3 \boldsymbol{W}^T$, which is a $s \times R^2$ matrix*
  - *Optimizing for a single factor matrix in this way costs $O(s^d R + sR^d)$*
  - *A sweep of HOOI requires forming N such TTMcs and computing their SVDs*

Dimension Trees for ALS

- The cost of ALS can be reduced by amortizing computation common terms
  - *The cost of ALS is typically dominated by MTTKRPs, d of which are computed for each sweep, for $d = 3$,*

$$\boldsymbol{T}_{(1)}(\boldsymbol{V}^{(k)} \odot \boldsymbol{W}^{(k)}), \boldsymbol{T}_{(2)}(\boldsymbol{U}^{(k+1)} \odot \boldsymbol{W}^{(k)}), \boldsymbol{T}_{(3)}(\boldsymbol{U}^{(k+1)} \odot \boldsymbol{V}^{(k+1)})$$

  - *Note that given $\boldsymbol{\mathcal{Z}} = \boldsymbol{\mathcal{T}} \times_3 \boldsymbol{W}^{(k)^T}$, we can compute the first two MTTKRPs with $O(s^2R)$ cost, since*

$$\sum_{j,l} t_{ijl} v_{jr}^{(k)} w_{lr}^{(k)} = \sum_{j} z_{ijr} v_{jr}^{(k)} \quad \textit{and} \quad \sum_{j,l} t_{ijl} u_{ir}^{(k+1)} w_{lr}^{(k)} = \sum_{i} z_{ijr} u_{ir}^{(k+1)}$$

  - *In general, we can reuse a single TTM to compute the next $d-1$ sets of right-hand-sides (MTTKRPs) in ALS (in this sweep or the next sweep)*
  - *The amortized cost of each ALS sweep (assuming Strassen-like matrix-multiplication algorithms are not used) is then given by $\frac{2d}{d-1}s^dR + O(ds^{d-1}R) + O(dR^3)$ where the final term comes from Cholesky factorization of the matrices $\boldsymbol{G}^{(i)} = \ast_{j=1,j\neq i}^{d} \boldsymbol{U}^{(j)^T}\boldsymbol{U}^{(j)}$*

Gauss-Newton Algorithm

- ALS generally achieves linear convergence, while Newton-based methods can converge quadratically
  - *Derive these by casting CP as a nonlinear least squares problem,*

$$\phi(\boldsymbol{x}) = \frac{1}{2}\| \underbrace{\boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x})}_{\boldsymbol{r}(\boldsymbol{x})} \|^2$$

  - *Newton's method computes* $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \boldsymbol{H}_\phi(\boldsymbol{x})^{-1}\nabla\phi(\boldsymbol{x})$
  - *For nonlinear least squares problems, the gradient and Hessian are*

$$\begin{aligned}\nabla\phi(\boldsymbol{x}) &= \boldsymbol{J}_r^T(\boldsymbol{x})\boldsymbol{r}(\boldsymbol{x}),\\ \boldsymbol{H}_\phi(\boldsymbol{x}) &= \boldsymbol{J}_r^T(\boldsymbol{x})\boldsymbol{J}_r(\boldsymbol{x}) + \sum_i r_i(\boldsymbol{x})\boldsymbol{H}_{r_i}(\boldsymbol{x})\end{aligned}$$

  - *The Gauss-Newton method approximates* $\boldsymbol{H}_\phi(\boldsymbol{x}) \approx \boldsymbol{J}_r^T(\boldsymbol{x})\boldsymbol{J}_r(\boldsymbol{x})$*, so*

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} - \boldsymbol{s}^{(k)}, \quad \boldsymbol{s}^{(k)} = (\boldsymbol{J}_r^T(\boldsymbol{x}^{(k)})\boldsymbol{J}_r(\boldsymbol{x}^{(k)}))^{-1}\boldsymbol{J}_r^T(\boldsymbol{x}^{(k)})\boldsymbol{r}(\boldsymbol{x}^{(k)}),$$

$$\boldsymbol{J}_r(\boldsymbol{x}^{(k)})\boldsymbol{s}^{(k)} \cong \boldsymbol{r}(\boldsymbol{x}^{(k)})$$

Gauss-Newton for CP Decomposition

- CP decomposition for order $d = 3$ tensors ($d > 3$ is similar) minimizes

$$\phi(\boldsymbol{U}^{(1)}, \boldsymbol{U}^{(2)}, \boldsymbol{U}^{(3)}) = \frac{1}{2} \sum_{ijk} \Big(t_{ijk} - \sum_{r=1}^{R} u_{ir}^{(1)} u_{jr}^{(2)} u_{kr}^{(3)}\Big)^2$$

  - *The Gauss-Newton approximate Hessian is $dnR \times dnR$,*

$$\boldsymbol{H} = \begin{bmatrix} \boldsymbol{H}^{(1,1)} & \cdots & \boldsymbol{H}^{(1,d)} \\ \vdots & \ddots & \vdots \\ \boldsymbol{H}^{(d,1)} & \cdots & \boldsymbol{H}^{(d,d)} \end{bmatrix}, \text{ where } \boldsymbol{H}^{(q,q)} = \boldsymbol{G}^{(n,n)} \otimes \boldsymbol{I}$$

while for $q \neq p, \quad h_{krlz}^{(q,p)} = u_{kz}^{(q)} u_{lr}^{(p)} g_{rz}^{(q,p)},$

where in both cases $\quad g_{rz}^{(n,p)} = \prod_{m=1, m \neq q,p}^{d} \left(\sum_i u_{ir}^{(m)} u_{iz}^{(m)} \right)$

Gauss-Newton for CP Decomposition

- A step of Gauss-Newton requires solving a linear system with $\boldsymbol{H}$
  - Cholesky of $\boldsymbol{H}$ requires $O(d^2n^2R^2)$ memory and cost $O(d^3n^3R^3)$
  - Matrix-vector product with $\boldsymbol{H}$ can be computed with cost $O(d^2nR^2)$
  - Can use CG method with implicit matrix-vector product[1]
  - Each product $\boldsymbol{u} = \boldsymbol{H}\boldsymbol{v}$ can be performed using tensor contractions each with cost $O(nR^2)$
  - $\boldsymbol{H}$ admits an effective block-diagonal preconditioner (inverse of each block applies step of ALS)

[1] P. Tichavsky, A. H. Phan, and A. Cichocki, 2013

Alternating Mahalanobis Distance Minimization (AMDM)

- High-order convergence can be achieved for low-rank exact CP using the AMDM algorithm
  - *For an order tensor $\mathcal{T}$, given iterates $\boldsymbol{U}^{(k)}$, $\boldsymbol{V}^{(k)}$, and $\boldsymbol{W}^{(k)}$, AMDM computes*

$$\begin{aligned}\boldsymbol{U}^{(k+1)} &= \boldsymbol{T}_{(1)}(\boldsymbol{V}^{(k)+T} \odot \boldsymbol{W}^{(k)+T})\\ \boldsymbol{V}^{(k+1)} &= \boldsymbol{T}_{(2)}(\boldsymbol{U}^{(k+1)+T} \odot \boldsymbol{W}^{(k)+T})\\ \boldsymbol{W}^{(k+1)} &= \boldsymbol{T}_{(3)}(\boldsymbol{U}^{(k+1)+T} \odot \boldsymbol{V}^{(k+1)+T})\end{aligned}$$

  - *A sketch of the high-order convergence proof is as follows*
  - *Let $\mathcal{T} = [\![\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}]\!]$ then*

$$\begin{aligned}&\boldsymbol{T}_{(1)}((\boldsymbol{V}^{+T} + \boldsymbol{\delta V}) \odot (\boldsymbol{W}^{+T} + \boldsymbol{\delta W}))\\ &\quad = \boldsymbol{U} + \boldsymbol{U}(\boldsymbol{I} * \boldsymbol{\delta V}^T\boldsymbol{V}) + \boldsymbol{U}(\boldsymbol{I} * \boldsymbol{\delta W}^T\boldsymbol{W}) + O(\|\boldsymbol{\delta V}\|\|\boldsymbol{\delta W}\|)\end{aligned}$$

where the first two error terms amount to rescaling of the columns of $\boldsymbol{A}$, while the last term controls convergence and scales with the product of the errors in the other factors.

Computing the CP Rank

Exact algorithms for bounding the CP rank of a tensor can be phrased via methods for polynomial systems of equations[2]

- *A general n-variate polynomial of degree k has the form*

$$f(x_1, \ldots, x_n) = \sum_{i_1,\ldots i_n, i_1+\cdots+i_n \leqslant k} c_{i_1,\ldots,i_n} x_1^{i_1} \cdots x_n^{i_n}$$

- *A CP decomposition of an order d tensor $\mathcal{T}$ corresponds to a set of polynomial equations in the entries of the factor matrices $\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(d)}$,*

$$\forall \boldsymbol{i} = (i_1, \ldots, i_d) \in \{1, \ldots, n\}^d, \quad \underbrace{t_{\boldsymbol{i}} - \sum_{r=1}^{R} \prod_{j=1}^{d} x_{i_j r}^{(j)}}_{f_{\boldsymbol{i}}(\boldsymbol{X}^{(1)},\ldots,\boldsymbol{X}^{(d)})} = 0$$

- *The degree of each $f_{\boldsymbol{i}}$ is d.*

[2] Aliabadi, Mohsen, and Shmuel Friedland. ”On the complexity of finding tensor ranks.” Communications on Applied Mathematics and Computation 3.2 (2021): 281-289.

Effective Nullstellensatz

Hilbert's weak Nullstellensatz is a characterization of polynomial equations[3]

- *Let $f_1, \ldots, f_m$ be k-variate complex polynomials of degree at most d, then exactly one of the following two statements hold*
  1. $\exists \boldsymbol{x} \in \mathbb{C}^k$, *s.t.*, $f_1(\boldsymbol{x}) = \cdots = f_m(\boldsymbol{x}) = 0$
  2. $\exists g_1, \ldots g_m$ *where each* g_i *is a complex polynomial, such that* $\sum_{i=1}^m g_i f_i = 1$
- *in the second case, the degree of each* $f_i g_i$ *is at most* d^k *if* $k \leqslant m$ *and* $d \geqslant 3$ *(such upper bounds are referred to as an 'effective Nullstellensatz')*

This characterization reduces polynomial systems to linear equations

- *The coefficients of* $\sum_{i=1}^m g_i f_i$ *can be computed convolution, or equivalently the product of a structured matrix defined from the coefficients of the* f_i*s and a vector of coefficients of each of the* g_i
- *Using FFT of dimension* d^k *leads to a complexity of* $O(kd^k)$
- *For CP decomposition of rank* R *of an order* d *tensor with all dimension equal to* n*, we have* $k = dnR$

[3] Following Terence Tao's formulation of this theorem `https://terrytao.wordpress.com/2007/11/26/hilberts-nullstellensatz/` (accessed Oct. 2024).

Tensor Completion

- The *tensor completion* problem seeks to build a model (e.g., CP decomposition) for a partially-observed tensor
  - *Completion differs from decomposition of a sparse tensor with zeros for entries that are unobserved, as the CP decomposition would be fitting the zeros*
  - *For an order three tensor $\mathcal{T} \in \mathbb{R}^{n \times n \times n}$, given a set of observed entries t_{ijk} for $(i, j, k) \in \Omega$, we seek to minimize*

$$f(\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}) = \sum_{(i,j,k)\in\Omega} (t_{ijk} - \sum_r u_{ir} v_{jr} w_{kr})^2 + \lambda^2 (\|\boldsymbol{U}\|_2^2 + \|\boldsymbol{V}\|_2^2 + \|\boldsymbol{W}\|_2^2)$$

- The problem generalized matrix completion, a problem partly popularized by the Netflix prize collaborative filtering problem
  - *This problem involved building a model for predicting user ratings of movies, given the set of movies they have already rated, with each rating corresponding to a tuple (user, movie)*
  - *These can be enumerated in a tensor if including additional attributes, such as time of day*

CP Tensor Completion Gradient and Hessian

- The gradient of the tensor completion objective function is sparsified according to the set of observed entries
  - *Lets restrict attention to optimizing for the ith row of the first factor matrix, define Ω_i so that $(j,k) \in \Omega_i$ if s $(i,j,k) \in \Omega$, then*

$$\phi(\boldsymbol{u}_i) = \sum_{(j,k)\in\Omega_i} (t_{ijk} - \langle \boldsymbol{u}_i, \boldsymbol{v}_j, \boldsymbol{w}_k \rangle)^2 + \lambda \|\boldsymbol{u}_i\|_2^2 \quad \textit{where} \quad \langle \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \rangle = \sum_r x_r y_r z_r$$

  - *Consider the derivative with respect to the ith row of the first factor matrix*

$$\nabla\phi(\boldsymbol{u}_i) = \frac{d\phi}{d\boldsymbol{u}_i}(\boldsymbol{u}_i) = 2 \sum_{(j,k)\in\Omega_i} (\boldsymbol{v}_j * \boldsymbol{w}_k)(\langle \boldsymbol{u}_i, \boldsymbol{v}_j, \boldsymbol{w}_k \rangle - t_{ijk}) + 2\lambda \boldsymbol{u}_i$$

- ALS for tensor decomposition solves quadratic optimization problem for each row of each factor matrix, in the completion case, Newton's method on these subproblems yields different Hessians
  - *The Hessian $\boldsymbol{H}_i^{(\phi)}$ depends on the set of entries $\Omega_i = \{(j,k) : \exists (i,j,k) \in \Omega\}$,*

$$\boldsymbol{H}_i^{(\phi)} = \frac{d\phi^2}{d\boldsymbol{u}_i d\boldsymbol{u}_i}(\boldsymbol{u}_i) = \sum_{(j,k)\in\Omega_i} (\boldsymbol{v}_j * \boldsymbol{w}_k)(\boldsymbol{v}_j * \boldsymbol{w}_k)^T + 2\lambda \boldsymbol{I}$$

Methods for CP Tensor Completion

- ALS for tensor completion with CP decomposition incurs additional cost
  - *For each* $(i, j, k) \in \Omega$*, need to accumulate* $(\boldsymbol{v}_j * \boldsymbol{w}_k)(\boldsymbol{v}_j * \boldsymbol{w}_k)^T$ *to* $\boldsymbol{H}_i^{(\phi)}$
  - *While the* n *outer products can be amortized with cost* $O(nR^2)$*, no easy way to do so for their partial sums, leading to cost* $O(|\Omega|R^2)$
- Alternative methods for tensor completion include coordinate descent and stochastic gradient descent
  - *Stochastic gradient descent (SGD) would compute subgradients for each* (i, j, k) *which are summands in the sum over* Ω_i *in* $\nabla\phi(\boldsymbol{u}_i)$
  - *SGD can be implemented efficiently, by computing a sum over a random set of subgradients at a time, via subsampling of* Ω
  - *Coordinate descent optimizes an entry of each factor matrix at a time*
  - *Variants of coordinate descent select different orderings of entries to optimize, e.g., alternating among columns of factor matrices then factor matrices or vice versa*

Coordinate Descent for CP Tensor Completion

- Coordinate descent avoids the need to solve linear systems of equations
  - *The coordinate-wise objective function is*

    $$\psi(u_{ir}) = \sum_{(j,k)\in\Omega_i} (\rho_{ijk}^{(r)} - u_{ir}v_{jr}w_{kr})^2 + \lambda u_{ir}^2 \text{ where } \rho_{ijk}^{(r)} = t_{ijk} - \langle \boldsymbol{u}_i, \boldsymbol{v}_j, \boldsymbol{w}_k \rangle + u_{ir}v_{ir}w_{kr}$$

    above $\rho_{ijk}^{(r)}$ is equal to an entry of the residual tensor with the rth rank-one component of the CP decomposition excluded
  - *Taking its derivative, we obtain*

    $$\psi'(u_{ir}) = -2 \sum_{(j,k)\in\Omega_i} v_{jr}w_{kr}(\rho_{ijk}^{(r)} - u_{ir}v_{jr}w_{kr}) + 2\lambda u_{ir}$$
  - *Setting this derivative to zero, we can solve for u_{ir}*

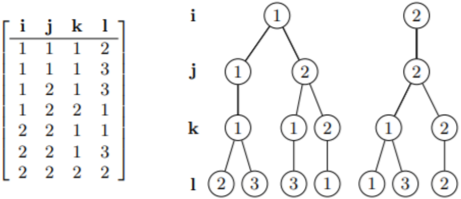
    $$u_{ir}^{(\textit{new})} = \frac{\sum_{(j,k)\in\Omega_i} v_{jr}w_{kr}\rho_{ijk}^{(r)}}{\lambda + \sum_{(j,k)\in\Omega_i} v_{jr}^2 w_{kr}^2}$$
  - *This can be implemented efficiently by keeping track of a residual tensor and obtaining $\rho_{ijk}^{(r)}$ as a modification thereof when working on the rth column*

Sparse Tensor Contractions

- Tensor completion and sparse tensor decomposition require operations on sparse tensors
  - *In many publicly available sparse tensor datasets, the density is extremely low, e.g., 10^{-7}, i.e., there can be $O(n)$ nonzeros in interesting $n \times n \times n$ tensors*
  - *For both decomposition and completion, tensor sparsity does not generally imply sparsity of CP or Tucker factors, and these are typically assumed to be dense*
- Sparse tensor contractions often correspond to products of *hypersparse* matrices, i.e., matrices with mostly zero rows
  - *Consider TTM with a $n \times n \times n$ tensor $\boldsymbol{\mathcal{T}}$ containing $O(n)$ nonzeros, $\boldsymbol{T}_{(1)}^T\boldsymbol{M}$, the matrix $\boldsymbol{T}_{(1)}^T$ has $O(n)$ nonzeros, but n^2 rows, while $\boldsymbol{T}_{(1)}^T\boldsymbol{M}$ has $O(n)$ dense rows and all other $O(n^2)$ rows are zero*
  - *To reduce sparse tensor contractions to sparse matrix multiplication kernels, need support for hypersparse matrix formats (e.g., compressed sparse-row (CSR) format would require $\Theta(n^2)$ storage for $\boldsymbol{T}_{(1)}$) and ideally specialized formats for matrices such as $\boldsymbol{T}_{(1)}^T\boldsymbol{M}$ (e.g., dense matrix consisting of nonzero rows and vector of row indices)*

Sparse Tensor Formats

- The overhead of transposition, and non-standard nature of the arising sparse matrix products, motivates sparse data structures for tensors that are suitable for tensor contractions of interest
  - *Particularly important, especially for tensor decomposition, are MTTKRP (suffices to CP ALS) and TTMc (suffices for HOOI)*
  - *TTM is also prevalent, but is a less attractive primitive in the sparse case than MTTKRP and TTMc, as these yield dense, low-order outputs, while the output of TTM can be sparse and larger than the starting tensor*
- The *compressed sparse fiber (CSF)* format provides an effective representation for sparse tensors
  - *CSF can be visualized as a tree (diagram taken from original CSF paper, by Shaden Smith and George Karpis, IAˆ3, 2015)*



i	j	k	l
1	1	1	2
1	1	1	3
1	2	1	3
1	2	2	1
2	2	1	1
2	2	1	3
2	2	2	2

Operations in Compressed Format

- CSF permits efficient execution of important sparse tensor kernels
  - Analogous to CSR format, which enables efficient implementation of the sparse matrix vector product
  - where `row[i]` stores a list of column indices and nonzeros in the ith row of $\boldsymbol{A}$

```
for i in range(n):
  for (a_ij,j) in row[i]:
    y[i] += a_ij * x[j]
```

  - In CSF format, a multilinear function evaluation $\boldsymbol{f}^{(\boldsymbol{\mathcal{T}})}(\boldsymbol{x},\boldsymbol{y}) = \boldsymbol{T}_{(1)}(\boldsymbol{x} \odot \boldsymbol{y})$ can be implemented as

```
for (i,T_i) in T_CSF:
  for (j,T_ij) in T_i:
    for (k,t_ijk) in T_ij:
      z[i] += t_ijk * x[j] * y[k]
```

MTTKRP in Compressed Format

- MTTKRP and CSF pose additional implementation opportunities and challenges
  - MTTKRP $u_{ir} = \sum_{j,k} t_{ijk} v_{jr} w_{kr}$ can be implemented by adding a loop over r to our code for $\boldsymbol{f}^{(\mathcal{T})}$, but would then require $3mr$ operations if m is the number of nonzeros in $\mathcal{T}$, can reduce to $2mr$ by amortization

```
for (i,T_i) in T_CSF:
  for (j,T_ij) in T_i:
    for r in range(R):
      f_ij = 0
      for (k,t_ijk) in T_ij:
        f_ij += t_ijk * w[k,r]
      u[i,r] = f_ij * v[j,r]
```

  - However, this amortization is harder (requires storage or iteration overheads) if the index i is a leaf node in the CSF tree
  - Similar challenges in achieving good reuse and obtaining good arithmetic intensity arise in implementation of other kernels, such as TTMc

All-at-once Contraction

- When working with sparse tensors, it is often more efficient to contract multiple operands in an all-at-once fashion
  - *Given chain of matrix products* $\boldsymbol{ABC}\cdots$, *dimension of overall iteration space scales with number of matrices, but by contracting pairwise, obtain cubic cost in matrix dimension with linear dependence on number of matrices*
  - *A case when such pairwise contraction is not a good idea, is the sampled dense-dense matrix-multiplication (SDDMM),*

    $$c_{ij} = \sum_{r}^{R} a_{ij} u_{ir} v_{jr} \Leftrightarrow \boldsymbol{C} = \boldsymbol{A} * (\boldsymbol{U}\boldsymbol{V}^T)$$

    where $\boldsymbol{A}$ *is sparse with* m *nonzeros, while* $\boldsymbol{U}$ *and* $\boldsymbol{V}$ *are dense*
  - *Since the sparsity pattern of* $\boldsymbol{C}$ *is the same as of* $\boldsymbol{A}$*, suffices to iterate over nonzeros of* $\boldsymbol{A}$ *and multiply each by inner product of a row of* $\boldsymbol{U}$ *and a row of* $\boldsymbol{V}$*, with cost* $O(mR)$
  - *Pairwise contraction is inefficient, contracting first* $\boldsymbol{A}$ *with* $\boldsymbol{U}$ *would yield a third-order intermediate, while contracting* $\boldsymbol{U}$ *with* $\boldsymbol{V}^T$ *would have cost* $O(n^2R)$
  - *Generalizing SDDMM to higher order gives the tensor-times tensor-product (TTTP), an application of which is computing the residual in tensor completion*

Complexity of Sparse Tensor Contractions

- The cost of a contraction of two sparse tensors depends on the position of the nonzeros
  - *The product of two square matrices with n nonzeros may require n^2 work (outer product)*
  - *The product of two square matrices with $n^2/2$ nonzeros may require no work (consider $\boldsymbol{AB}$ where $\boldsymbol{A} = [\boldsymbol{A}_1, 0]$, $\boldsymbol{B} = [0, \boldsymbol{B}_1]^T$)*
  - *In general, the number of nontrivial products is not easy to infer cheaply from matrix structure*
- The cost of a contraction of a single sparse tensor with dense tensors can be quantified more directly
  - *A simple bound follows from fixing the indices of the sparse tensor for each nonzero, each of which reduces to a dense tensor contraction*
    - *For MTTKRP, this yields $O(\mathrm{nnz}(T)R)$*
    - *For TTMc with $d-1$ matrices of rank R, this yields $O(\mathrm{nnz}(T)R^{d-1})$*

Complexity of Contractions with a Single Sparse Tensor

In general, when contracting a single sparse tensor with many dense tensors partial sums can be amortized

- *Assuming each dense tensor is contracted with exactly one mode of the sparse tensor and the contractions are done starting from the lowest level of a CSF tree format, the cost can be quantified as*

$$C(\boldsymbol{\mathcal{T}}, \boldsymbol{\mathcal{A}}_1, \ldots, \boldsymbol{\mathcal{A}}_k) \sum_{i=1}^{k} C_i(\mathrm{nnz}_i(\boldsymbol{\mathcal{T}}), \boldsymbol{\mathcal{A}}_k)$$

  where $\mathrm{nnz}_i(\boldsymbol{\mathcal{T}})$ is the number of nodes in the i level of the CSF tree starting from the leaves, so $\mathrm{nnz}_1(T) = \mathrm{nnz}(T)$, and C_i is the cost of the ith contraction with the given number of nonzeros in $\boldsymbol{\mathcal{T}}$ (depends on how $\boldsymbol{\mathcal{A}}_k$ is contracted and the order of iteration over the indices)

Constrained Tensor Decomposition

- Many applications of tensor decomposition in data science, feature additional structure, which can be enforced by constraints
  - *A basic and common constraint is nonnegativity of factor matrices, which often makes sense when working with a tensor that is nonnegative (e.g., count data)*
  - *Most of the methods we've discussed can be generalized to handle nonnegativity, e.g., one could perform ALS by solving each subproblem subject to nonnegativity constraints*
  - *Another common constraint is factor matrix orthogonality, which can be incorporated similarly into subproblems*
  - *For symmetric tensors, repeating factors are often desired, which can be formulated via constraints or by using an appropriate method (two good alternatives are ALS with subiterations to converge updates to repeated factors, or Gauss-Newton, which automatically preserves repeating factors when working with a symmetric tensor)*

Nonnegative Tensor Factorization

- *Nonnegative tensor factorization (NTF)*, such as CP decomposition with $\boldsymbol{\mathcal{T}} \geqslant 0$ and $\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W} \geqslant 0$ are widespread and a few classes of algorithms have been developed
  - *Optimization for one of $\boldsymbol{U}$, $\boldsymbol{V}$, or $\boldsymbol{W}$ (while the other two are fixed) is a convex optimization problem*
  - *Many methods based on alternating optimization/updates in the style of ALS*
  - *A basic approach is to 'clip' result of ALS step so that each factor matrix is nonnegative after update*
  - *Block coordinate descent (BCD) methods update on or more columns of $\boldsymbol{U}$, $\boldsymbol{V}$, or $\boldsymbol{W}$ based on a coordinate-descent-like update rule*
  - *Proximal gradient methods are multicolumn BCD methods, which approximately solve each subproblem by minimizing a constrained objective derived based on a proximally projected gradient*
  - *All-at-once methods that update all factor matrices, such as Gauss-Newton with an augmented Lagrangian objective function (sequential quadratic programming)*

Nonnegative Matrix Factorization

- NTF algorithms with alternating updates have a close correspondence with alternating update algorithms for *Nonnegative matrix factorization (NMF)*[4]
  - *The rank-r NMF problem is to find, given matrix $\boldsymbol{A} \in \mathbb{R}_+^{n \times n}$, the minimizer $\boldsymbol{U}, \boldsymbol{V} \in \mathbb{R}_+^{n \times r}$ to*
    $$f^{(\boldsymbol{A})}(\boldsymbol{U}, \boldsymbol{V}) = \|\boldsymbol{A} - \boldsymbol{U}\boldsymbol{V}^T\|_F$$
  - *The NMF hard is NP hard, for exact NMF $O(n^{2r^2})$-time algorithms exist*
  - *Solutions to NMF are generally non-unique, though for low-rank CP NTF uniqueness could hold based on previously described conditions*
  - *Alternating optimization problems for NTF are essentially the same as in NMF, for*
    $$g^{(\boldsymbol{\mathcal{T}})}(\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}) = \|\boldsymbol{\mathcal{T}} - [\![\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}]\!]\|_F$$
    minimizing $\phi^{(\boldsymbol{\mathcal{T}})}_{\boldsymbol{V},\boldsymbol{W}}(\boldsymbol{U}) = g^{(\boldsymbol{\mathcal{T}})}(\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W})$ is the same as the NMF subproblem $\phi^{(\boldsymbol{T}_{(1)})}_{\boldsymbol{V}\odot\boldsymbol{W}}(\boldsymbol{U}) = f^{(\boldsymbol{T}_{(1)})}(\boldsymbol{U}, \boldsymbol{V} \odot \boldsymbol{W})$

[4] Gillis, Nicolas. ”The why and how of nonnegative matrix factorization.” Regularization, optimization, kernels, and support vector machines 12.257 (2014): 257-291.

Optimality Conditions for NMF

- The optimality conditions for NMF are

$$\begin{aligned} \boldsymbol{U}, \boldsymbol{V} \geqslant 0, \frac{df^{(\boldsymbol{A})}}{d\boldsymbol{U}}(\boldsymbol{U}, \boldsymbol{V}) &= \boldsymbol{U}\boldsymbol{V}\boldsymbol{V}^T - \boldsymbol{A}\boldsymbol{V} \geqslant 0 \quad \textit{and} \quad \frac{df^{(\boldsymbol{A})}}{d\boldsymbol{U}}(\boldsymbol{U}, \boldsymbol{V}) * \boldsymbol{U} = 0 \\ \frac{df^{(\boldsymbol{A})}}{d\boldsymbol{V}}(\boldsymbol{U}, \boldsymbol{V}) &= \boldsymbol{V}\boldsymbol{U}\boldsymbol{U}^T - \boldsymbol{A}\boldsymbol{U} \geqslant 0 \quad \textit{and} \quad \frac{df^{(\boldsymbol{A})}}{d\boldsymbol{V}}(\boldsymbol{U}, \boldsymbol{V}) * \boldsymbol{V} = 0. \end{aligned}$$

- These follow from the KKT conditions, including complementarity slackness
  - *The Lagrangian function is*

$$\mathcal{L}^{(A)}(\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{\lambda}_U, \boldsymbol{\lambda}_V) = f^{(\boldsymbol{A})}(\boldsymbol{U}, \boldsymbol{V}) - \langle \boldsymbol{\lambda}_U, \boldsymbol{U} \rangle - \langle \boldsymbol{\lambda}_V, \boldsymbol{V} \rangle$$

  - *Its partial derivatives vanish at any local minima, which gives that*

$$\boldsymbol{\lambda}_U = \frac{df^{(\boldsymbol{A})}}{d\boldsymbol{U}}(\boldsymbol{U}, \boldsymbol{V}), \quad \boldsymbol{\lambda}_V = \frac{df^{(\boldsymbol{A})}}{d\boldsymbol{V}}(\boldsymbol{U}, \boldsymbol{V})$$

  - *Further the KKT conditions give that* $\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{\lambda}_U, \boldsymbol{\lambda}_V \geqslant 0$ *and, by complementarity slackness,* $\langle \boldsymbol{\lambda}_U, \boldsymbol{U} \rangle = 0$*. Since all nonzero terms in this inner product have the same sign, we also then have* $\boldsymbol{\lambda}_U * \boldsymbol{U} = 0$*, and similar for* $\boldsymbol{V}$*.*

Coordinate Descent for NMF and NTF

- Coordinate descent gives optimal closed-form updates for variables in NMF and NTF
  - *We can write an optimization subproblem for a single column $\boldsymbol{u}_i$ as minimizing*

$$\phi_i^{(\boldsymbol{A})}(\boldsymbol{u}_i) = \|\boldsymbol{A} - \sum_{r=1}^{R} \boldsymbol{u}_r \boldsymbol{v}_r^T\|_2 \quad \textit{s.t.} \quad \boldsymbol{u}_i \geqslant 0$$

$$\boldsymbol{u}_i^{\textit{new}} = |\boldsymbol{u}_i + \frac{\boldsymbol{A}\boldsymbol{v}_i - \boldsymbol{U}\boldsymbol{V}^T\boldsymbol{v}_i}{\boldsymbol{v}_i^T\boldsymbol{v}_i}|_+$$

where $\boldsymbol{y} = |\boldsymbol{x}|_+$ gives $y_i = x_i$ if $x_i > 0$ and $y_i = 0$ otherwise

  - *Given $\boldsymbol{\rho}^{(i)} = \boldsymbol{A} - \boldsymbol{U}\boldsymbol{V}^T + \boldsymbol{u}_i\boldsymbol{v}_i^T = \boldsymbol{A} - \sum_{j \neq i} \boldsymbol{u}_j \boldsymbol{v}_j^T$, if columns of $\boldsymbol{V}$ are normalized, we can alternatively write the update as*

$$\boldsymbol{u}_i^{\textit{new}} = \left| \frac{\boldsymbol{\rho}^{(i)}\boldsymbol{v}_i}{\boldsymbol{v}_i^T\boldsymbol{v}_i} \right|_+$$

Alternating Optimization for NMF and NTF

- If all except one factor is fixed, the resulting subproblem is an inequality-constrained convex optimization problem
  - *With* $\boldsymbol{V}$ *fixed the* i*th row of* $\boldsymbol{U}$, $\boldsymbol{u}_i^T$ *gives the subproblem*

$$\phi_i^{(\boldsymbol{A})}(\boldsymbol{u}_i^T) = \|\boldsymbol{V}^T \boldsymbol{a}_i^T - \boldsymbol{u}_i\|_2 \textit{ s.t. } \boldsymbol{u}_i \geqslant 0$$

  - *This constrained quadratic optimization problem can be solved via active set or interior point methods*
  - *A popular method for NMF is based on multiplicative updates, which results in an easy-to-compute alternating update rule*

Generalized Tensor Decomposition

- Aside from addition of constraints, the objective function may be modified by using different elementwise loss functions
  - *The standard loss function is $(x - m)^2$ where x is an element of the tensor and m is its approximation via CP*
  - *For count data, the Poisson loss function $m - x\log(m)$ may be more appropriate, and typically comes along with nonnegativity constraints*
  - *Other distributions and loss functions of interest include Gamma, Rayleigh, Bernoulli, and NegBinom (see D. Hong, T. Kolda, J. Duersch SIAM Review 2020)*
- Some loss function admit ALS-like algorithms, while others may require gradient-based optimization
  - *Can compute (sub-)gradients given any loss function, by differentiating as necessary*
  - *For Poisson, like for the standard loss function, ALS subproblems may be solved explicitly, allowing more robust convergence*