Numerical Multilinear Algebra and Multiway Statistical Models

Lek-Heng Lim

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Overview

- Rudiments of tensors and multilinear algebra
- Multilinear data-fitting models
- Tensorial rank and Eckart-Young problem
- Nonexistence of optimal low-rank approximation
- Fixing the ill-posedness of Eckart-Young problem

Multilinearity

Consider multivariate vector-valued functions.

Linearity: $f : \mathbb{R}^n \to \mathbb{R}^m$, $f(\mathbf{x}) = f(x_1, \dots, x_n)$,

$$f(\alpha\mathbf{x} + \beta\mathbf{y}) = \alpha f(\mathbf{x}) + \beta f(\mathbf{y})$$

Multilinearity: $f : \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_k} \to \mathbb{R}^m$,

$$f(\mathbf{x}^1; \dots; \mathbf{x}^k) = f(x_1^1, \dots, x_{d_1}^1; \dots; x_1^k, \dots, x_{d_k}^k),$$

$$f(\mathbf{x}^1; \dots; \alpha\mathbf{x}^i + \beta\mathbf{y}^i; \dots; \mathbf{x}^k) = \alpha f(\mathbf{x}^1; \dots; \mathbf{x}^i; \dots; \mathbf{x}^k) + \beta f(\mathbf{x}^1; \dots; \mathbf{y}^i; \dots; \mathbf{x}^k)$$

for $i = 1, \dots, k$.

"*Classification of mathematical problems as linear and nonlinear is like classification of the Universe as bananas and non-bananas.*"

Nonlinear: too general. Multilinear: next natural step.

Matrices

$A \in \mathbb{R}^{m\times n}$ may be viewed as either:

Linear map $A : \mathbb{R}^n \to \mathbb{R}^m$, $\mathbf{x} \mapsto A\mathbf{x}$

relevant decompositions are "one-sided": $A = LU$, $A = QR$, etc

Bilinear functional $A : \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$, $(\mathbf{x};\mathbf{y}) \mapsto \mathbf{x}^t A\mathbf{y}$

relevant decompositions are "two-sided": $A = LDU$, $A = U\Sigma V^t$ (Singular value), $A = QRQ^t$ (real Schur, aka Murnaghan-Wintner), $A = SJS^{-1}$ (real Jordan), etc

We will be interested in generalizations of the latter view: tensors are to multilinear functionals what matrices are to bilinear functionals

Matrices as order-2 tensor

Let $\mathbf{x} \in \mathbb{R}^m, \mathbf{y} \in \mathbb{R}^n$. Write $\mathbf{x} \otimes \mathbf{y} = \mathbf{x}\mathbf{y}^t \in \mathbb{R}^{m \times n}$.

$$\mathbb{R}^m \otimes \mathbb{R}^n := \operatorname{span}_{\mathbb{R}}\{\mathbf{x} \otimes \mathbf{y} \mid \mathbf{x} \in \mathbb{R}^m, \mathbf{y} \in \mathbb{R}^n\}.$$

Then $\mathbb{R}^m \otimes \mathbb{R}^n = \mathbb{R}^{m \times n}$, ie. matrices are order-2 tensors.

Lemma. Let $A \in \mathbb{R}^{m \times n}$. Then rank$(A) = r$ if and only if there exists $\mathbf{x}_1, \dots, \mathbf{x}_r \in \mathbb{R}^m$, $\mathbf{y}_1, \dots, \mathbf{y}_r \in \mathbb{R}^n$ such that

$$A = \mathbf{x}_1 \otimes \mathbf{y}_1 + \cdots + \mathbf{x}_r \otimes \mathbf{y}_r$$

and r is minimal over all such decompositions (ie. A cannot be written as $\sum_{i=1}^{s} \mathbf{x}_i' \otimes \mathbf{y}_i'$ for any $s < r$).

Tensors

Tensor product of 3 or more vectors may be defined in the same fashion as the outer product of two vectors.

Order 2: $\mathbf{x} \in \mathbb{R}^m, \mathbf{y} \in \mathbb{R}^n$; $\mathbf{x} \otimes \mathbf{y} := [x_i y_j] \in \mathbb{R}^{m \times n}$
Order 3: $\mathbf{x} \in \mathbb{R}^l, \mathbf{y} \in \mathbb{R}^m, \mathbf{z} \in \mathbb{R}^n$; $\mathbf{x} \otimes \mathbf{y} \otimes \mathbf{z} := [\![x_i y_j z_k]\!] \in \mathbb{R}^{l \times m \times n}$
Order k: $\mathbf{x}^1 \in \mathbb{R}^{d_1}, \dots, \mathbf{x}^k \in \mathbb{R}^{d_k}$; $\mathbf{x}^1 \otimes \cdots \otimes \mathbf{x}^k := [\![x^1_{i_1} \dots x^k_{i_k}]\!] \in \mathbb{R}^{d_1 \times \cdots \times d_k}$

Define $\mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k} := \operatorname{span}_{\mathbb{R}}\{\mathbf{x}^1 \otimes \cdots \otimes \mathbf{x}^k \mid \mathbf{x}^1 \in \mathbb{R}^{d_1}, \dots, \mathbf{x}^k \in \mathbb{R}^{d_k}\}$

Easy to see that $\mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k} = \mathbb{R}^{d_1 \times \cdots \times d_k}$

May think of order-k tensors as k-way arrays: order-0 tensors are scalars, order-1 tensors are vectors, order-2 tensors are matrices, order-3 tensors are "3-dimensional matrices", and so on.

$\otimes$ distributes over $+$

For $\alpha, \beta \in \mathbb{R}$, $\mathbf{x}^1 \in \mathbb{R}^{d_1}, \ldots, \mathbf{x}^i, \mathbf{y}^i \in \mathbb{R}^{d_i}, \ldots, \mathbf{x}^k \in \mathbb{R}^{d_k}$

$$\mathbf{x}^1 \otimes \cdots \otimes (\alpha \mathbf{x}^i + \beta \mathbf{y}^i) \otimes \cdots \otimes \mathbf{x}^k = \\ \alpha \mathbf{x}^1 \otimes \cdots \otimes \mathbf{x}^i \otimes \cdots \otimes \mathbf{x}^k + \beta \mathbf{x}^1 \otimes \cdots \otimes \mathbf{y}^i \otimes \cdots \otimes \mathbf{x}^k.$$

Observation: looks a lot like the definition of multilinear maps.

An alternative way of saying that $\otimes$ distributes over $+$ is to say the map

$$\theta : \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_k} \to \mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k}, \\ (\mathbf{x}_1; \ldots; \mathbf{x}_k) \mapsto \mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k$$

extends linearly to a multilinear map.

Algebraic structure of tensors

Vector space structure: the set of k-way arrays has a vector space structure — for $[\![t_{j_1,\dots,j_k}]\!], [\![s_{j_1,\dots,j_k}]\!] \in \mathbb{R}^{d_1\times\cdots\times d_k}$,

$$\lambda[\![t_{j_1,\dots,j_k}]\!] + \mu[\![s_{j_1,\dots,j_k}]\!] = [\![\lambda t_{j_1,\dots,j_k} + \mu s_{j_1,\dots,j_k}]\!] \in \mathbb{R}^{d_1\times\cdots\times d_k}.$$

$\mathbb{R}^{d_1\times\cdots\times d_k}$ is a vector space of dimension $d_1 d_2 \dots d_k$.

However, $\mathbb{R}^{d_1\times\cdots\times d_k}$ is more than just a vector space.

Tensor product structure: $\mathbb{R}^{d_1\times\cdots\times d_k} = \mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k}$ has an associated multilinear map $\theta : \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_k} \to \mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k}$, $(\mathbf{x}_1; \dots ; \mathbf{x}_k) \mapsto \mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_k$.

Tensor product structure lost when one 'unfolds' or 'matricize':

$$\mathbb{R}^l \otimes \mathbb{R}^m \otimes \mathbb{R}^n \xrightarrow{\text{unfold}} \mathbb{R}^l \otimes \mathbb{R}^{mn}.$$

Moral: one should not 'compress' an order-3 tensor into a matrix (this is just like compressing a matrix into a vector — the bilinear pairing is lost in the process)

Tensors and multilinear functionals

Let $A \in \mathbb{R}^{m\times n}$. Then there are vectors $\mathbf{a}_i \in \mathbb{R}^m$, $\mathbf{b}_j \in \mathbb{R}^n$ so that $A = \mathbf{a}_1 \otimes \mathbf{b}_1 + \cdots + \mathbf{a}_r \otimes \mathbf{b}_r$. Thus the bilinear functional $A : \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}, (\mathbf{x}; \mathbf{y}) \mapsto \mathbf{x}^t A\mathbf{y}$ may be written as

$$\mathbf{x}^t A\mathbf{y} = \langle \mathbf{a}_1, \mathbf{x}\rangle\langle \mathbf{b}_1, \mathbf{y}\rangle + \cdots + \langle \mathbf{a}_r, \mathbf{x}\rangle\langle \mathbf{b}_r, \mathbf{y}\rangle.$$

Likewise, $T \in \mathbb{R}^{d_1\times\cdots\times d_k}$ may be expressed in the form

$$T = \sum_{i=1}^{r} \mathbf{a}_i^1 \otimes \cdots \otimes \mathbf{a}_i^k$$

for some $\mathbf{a}_i^j \in \mathbb{R}^{d_j}$. It defines a multilinear functional $T : \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_k} \to \mathbb{R}, (\mathbf{x}^1, \dots, \mathbf{x}^k) \mapsto T(\mathbf{x}^1; \dots; \mathbf{x}^k)$ in the same manner,

$$T(\mathbf{x}^1; \dots; \mathbf{x}^k) := \sum_{i=1}^{r} \langle \mathbf{a}_i^1, \mathbf{x}^1\rangle \cdots \langle \mathbf{a}_i^k, \mathbf{x}^k\rangle.$$

The multilinearity of T is embodied in the multilinear map $\theta : \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_k} \to \mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k}$, $(\mathbf{a}_i^1; \dots; \mathbf{a}_i^k) \mapsto \mathbf{a}_i^1 \otimes \cdots \otimes \mathbf{a}_i^k$ mentioned earlier.

Where do you find tensors?

Economics, Optimal Control: Taylor expansion of C^r-function $f : \mathbb{R}^n \to \mathbb{R}$ about $\mathbf{a} = (a_1, \ldots, a_n)$,

$$f(\mathbf{x}) = f(\mathbf{a}) + \sum_i f_i(\mathbf{a})(x_i - a_i) + \frac{1}{2}\sum_{i,j} f_{ij}(\mathbf{a})(x_i - a_i)(x_j - a_j) + \frac{1}{3!}\sum_{i,j,k} f_{ijk}(\mathbf{a})(x_i - a_i)(x_j - a_j)(x_k - a_k) + \cdots$$

where $f_i(\mathbf{a}) = \frac{\partial f}{\partial x_i}(\mathbf{a}), f_{ij}(\mathbf{a}) = \frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{a}), f_{ijk}(\mathbf{a}) = \frac{\partial^3 f}{\partial x_i \partial x_j \partial x_k}(\mathbf{a})$, and so on.

- Gradient $[f_1(\mathbf{a}), \ldots, f_n(\mathbf{a})]$ is an order-1 tensor (vector);
- Hessian $[f_{ij}(\mathbf{a})]_{n\times n}$ is an order-2 tensor (matrix);
- $[\![f_{ijk}(\mathbf{a})]\!]_{n\times n\times n}$ is an order-3 tensor (3-way array).

Geometry:

- metric tensor g_{ij} (order 2);
- torsion tensor T^i_{jk} (order 3);
- Riemann curvature tensor R^i_{jkl} (order 4);
- Ricci tensor $R_{ik} = g^{jm} R_{imkj}$ (order 2)

Physics:

- electromagnetic field tensor in Maxwell's equations, $dF = 0, d * F = \mu * \mathbf{j}$ where

$$F = \begin{bmatrix} 0 & -E_1 & -E_2 & -E_3 \\ E_1 & 0 & B_3 & -B_2 \\ E_2 & -B_3 & 0 & B_1 \\ E_3 & B_2 & -B_1 & 0 \end{bmatrix};$$

- Einstein tensor and energy-momentum tensor in gravitational field equation, $G = 8\pi T$,

$$G_{ij} = R_{ij} - \frac{1}{2} R g_{ij}.$$

Engineering:

- moment of inertia tensor (order 2 symmetric);
- stress tensor (order 2 symmetric);
- piezoelectric tensor (order 3);
- elasticity (order 4)

Note: All these are *tensor fields* — the entries in the array are variables. However, they are often referred to as *tensors* — a source of confusion to newcomers.

Computational statistics and data analysis

Examples of k-way (or k-mode) datas:

- Psychometrics: *individual* × *variable* × *time* (3-way); *individual* × *variable* × *group* (3-way); *individual* × *variable* × *group* × *time* (4-way);
- Sensory analysis: *sample* × *attribute* × *judge*
- Batch data: *batch* × *time* × *variable*
- Time-series analysis: *time* × *variable* × *lag*
- Analytical chemistry: *sample* × *elution time* × *wavelength*
- Spectral data: *sample* × *emission* × *excitation* × *decay*
- Facial image: *people* × *view* × *illumination* × *expression* × *pixels*
- Atmospheric science: *location* × *variable* × *time* × *observation*

Model these datas as higher-order tensors

Two-way datas and bilinear models

sample $\times$ *variable*: ith row $\longleftrightarrow$ ith sample, jth column $\longleftrightarrow$ jth variable. Get data matrix $A = [a_{ij}] \in \mathbb{R}^{m\times n}$, m = number of samples, n = number of variables.

Example (Bro). a_{ij} = fluorescence emission intensity at a specific wavelength λ^{em} of ith sample excited with light at wavelength λ_j^{ex}.

Bilinear model:

$$A = \mathbf{x}_1 \otimes \mathbf{y}_1 + \cdots + \mathbf{x}_r \otimes \mathbf{y}_r + E = XY^t + E$$

where E is the error/residual and r is known in advance. This is equivalent to the problem

$$\operatorname*{argmin}_{\text{rank}(B)\leq r} \|A - B\|_F.$$

Note: $\text{argmin}_{\text{rank}(B)=r}\|A - B\|_F$ may not have a solution as the set $\{B \in \mathbb{R}^{m\times n} \mid \text{rank}(B) = r\}$ is not *closed*.

Multiway datas and multilinear models

Same example as previous slide but with emission intensity measured at several wavelengths instead of just one specific wavelength.

Example (Bro). a_{ijk} = fluorescence emission intensity at wavelength λ_j^{em} of ith sample excited with light at wavelength λ_k^{ex}. Get 3-way data $A = [\![a_{ijk}]\!] \in \mathbb{R}^{l\times m\times n}$.

Trilinear model:

$$A = \mathbf{x}_1 \otimes \mathbf{y}_1 \otimes \mathbf{z}_1 + \cdots + \mathbf{x}_r \otimes \mathbf{y}_r \otimes \mathbf{z}_r + E$$

where E is the error/residual and r is known in advance.

Likewise for multiway datas and multilinear models.

Eckart-Young theorem

Theorem. Let $A = U\Sigma V^t = \sum_{i=1}^{\text{rank}(A)} \sigma_i \mathbf{u}_i \mathbf{v}_i^t$ be the singular value decomposition of $A \in \mathbb{R}^{m\times n}$. For $r \leq \text{rank}(A)$, let

$$A_r := \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^t.$$

Then

$$\|A - A_r\|_F = \min_{\text{rank}(B)\leq r} \|A - B\|_F.$$

May use $\mathbf{x}_i = \sigma_i \mathbf{u}_i, \mathbf{y}_j = \mathbf{v}_j$.

Even though SVD is (essentially) unique, bilinear models are not unique. E.g. take $Q \in O(r)$, then

$$XY^t = XQQ^tY^t = (XQ)(YQ)^t.$$

Need additional information (impose additional contraints) to fix X and Y.

Rank of tensors

Tensorial rank may be defined by generalizing the earlier lemma:

Lemma. Let $A \in \mathbb{R}^{m\times n}$. Then $\operatorname{rank}(A) = r$ if and only if there exists $\mathbf{x}_1, \dots, \mathbf{x}_r \in \mathbb{R}^n$, $\mathbf{y}_1, \dots, \mathbf{y}_r \in \mathbb{R}^m$ such that

$$A = \mathbf{x}_1 \otimes \mathbf{y}_1 + \cdots + \mathbf{x}_r \otimes \mathbf{y}_r$$

and r is minimal over all such decompositions (ie. A cannot be written as $\sum_{i=1}^{s} \mathbf{x}'_i \otimes \mathbf{y}'_i$ for any $s < r$).

Definition. If $T \neq 0$, the **rank** of $T \in \mathbb{R}^{d_1} \otimes \cdots \otimes \mathbb{R}^{d_k} = \mathbb{R}^{d_1\times\cdots\times d_k}$, denoted $\operatorname{rank}(T)$, is defined as the minimum $r \in \mathbb{N}$ such that T may be expressed as a sum of r rank-one tensors:

$$T = \sum_{i=1}^{r} \mathbf{x}_i^1 \otimes \cdots \otimes \mathbf{x}_i^k \qquad \text{(Candecomp/Parafac)}$$

with $\mathbf{x}_i^j \in \mathbb{R}^{d_j}$, $j = 1, \dots, k$. We set $\operatorname{rank}(0) = 0$.

Well-defined: ie. there exists a unique $r = \operatorname{rank}(T)$ for every $T \in \mathbb{R}^{d_1\times\cdots\times d_k}$.

Eckart-Young problem

Frobenius norm of $[\![t_{j_1,\dots,j_k}]\!] \in \mathbb{R}^{d_1\times\cdots\times d_k}$ is defined by

$$\|[\![t_{j_1,\dots,j_k}]\!]\|_F^2 := \sum_{j_1=1}^{d_1}\cdots\sum_{j_k=1}^{d_k} t_{j_1,\dots,j_k}^2.$$

Definition. An **optimal rank-r approximation** to a tensor $T \in \mathbb{R}^{d_1\times\cdots\times d_k}$ is a tensor S_{min} with

$$\|S_{\text{min}} - T\|_F = \inf_{\text{rank}(S)\le r} \|S - T\|_F.$$

Eckart-Young problem: find an optimal rank-r approximation for tensors of order k.

Solving the Eckart-Young problem would allow us, at least in theory, to solve the problem of fitting k-way data with rank-r multilinear model (in practice, one still needs a workable algorithm).

Solvability of Eckart-Young problem

It has always been assumed that the Eckart-Young problem is solvable for tensors of any order and there has been continual interests in finding a satisfactory 'Eckart-Young theorem'-like result for tensors of higher order. The view expressed in the conclusion of the following paper is representative of such efforts:

"*An Eckart-Young type of optimal rank-k approximation theorem for tensors continues to elude our investigations but can perhaps eventually be attained by using a different norm or yet other definitions of orthogonality and rank.*"

Source: T.G. Kolda, "Orthogonal tensor decompositions," *SIAM J. Matrix Anal. Appl.*, **23** (1), 2001 , pp. 243–255.

Surprising fact

The Eckart-Young problem has no solution in general!

A simple fact that's often overlooked: in a norm space, the minimum distance of a point T to a non-closed set $\mathcal{S}$ may not be attained by any point in $\mathcal{S}$.

For tensors of order $k \geq 3$, $r \geq 2$, the set

$$\mathcal{S}(k, r) := \{T \in \mathbb{R}^{d_1 \times \cdots \times d_k} \mid \operatorname{rank}(T) \leq r\}$$

is not closed.

An explicit example

$\mathbf{x}, \mathbf{y}$ two linearly independent vectors in $\mathbb{R}^2$. Consider the order-3 tensor in $\mathbb{R}^{2\times2\times2}$,

$$T := \mathbf{x}\otimes\mathbf{x}\otimes\mathbf{x} + \mathbf{x}\otimes\mathbf{y}\otimes\mathbf{y} + \mathbf{y}\otimes\mathbf{x}\otimes\mathbf{y}.$$

T has rank 3: straight forward.

T has no optimal rank-2 approximation: consider sequence $\{S_n\}_{n=1}^{\infty}$ in $\mathbb{R}^{2\times2\times2}$,

$$S_n := \mathbf{x}\otimes\mathbf{x}\otimes(\mathbf{x}-n\mathbf{y}) + \left(\mathbf{x}+\frac{1}{n}\mathbf{y}\right)\otimes\left(\mathbf{x}+\frac{1}{n}\mathbf{y}\right)\otimes n\mathbf{y},$$

Clear that rank(S_n) ≤ 2 for all n. By multilinearity of $\otimes$,

$$S_n = \mathbf{x}\otimes\mathbf{x}\otimes\mathbf{x} - n\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{y} + n\mathbf{x}\otimes\mathbf{x}\otimes\mathbf{y} + \mathbf{x}\otimes\mathbf{y}\otimes\mathbf{y} + \mathbf{y}\otimes\mathbf{x}\otimes\mathbf{y} + \frac{1}{n}\mathbf{y}\otimes\mathbf{y}\otimes\mathbf{y} = T + \frac{1}{n}\mathbf{y}\otimes\mathbf{y}\otimes\mathbf{y}.$$

For any choice of norm on $\mathbb{R}^{2\times2\times2}$,

$$\|S_n - T\| = \frac{1}{n}\|\mathbf{y}\otimes\mathbf{y}\otimes\mathbf{y}\| \to 0 \qquad \text{as } n\to\infty.$$

Eckart-Young problem is ill-posed

An ill-posed problem is usually taken to mean one that doesn't have a *unique* solution.

The Eckart-Young problem is even worse in that for tensors of order 3 or higher, even the *existence* of a solution is in question.

In other words, the ill-posedness of Eckart-Young problem cannot be fixed by *regularization* (ie. imposing additional constraints to ensure uniqueness) alone.

Another example

Let $\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w} \in \mathbb{R}^4$. Define in $\mathbb{R}^{4\times4\times4}$,

$$T := \mathbf{x}\otimes\mathbf{x}\otimes\mathbf{x}+\mathbf{x}\otimes\mathbf{y}\otimes\mathbf{z}+\mathbf{y}\otimes\mathbf{z}\otimes\mathbf{x}+\mathbf{y}\otimes\mathbf{w}\otimes\mathbf{z}+\mathbf{z}\otimes\mathbf{x}\otimes\mathbf{y}+\mathbf{y}\otimes\mathbf{z}\otimes\mathbf{w}$$

and the sequence

$$\begin{aligned} S_n := {} & \left(\mathbf{y}+\frac{1}{n}\mathbf{x}\right)\otimes\left(\mathbf{y}+\frac{1}{n}\mathbf{w}\right)\otimes n\mathbf{z}+\left(\mathbf{y}+\frac{1}{n}\mathbf{x}\right)\otimes n\mathbf{x}\otimes\left(\mathbf{x}+\frac{1}{n}\mathbf{y}\right) \\ & - n\mathbf{y}\otimes\mathbf{y}\otimes\left(\mathbf{x}+\mathbf{z}+\frac{1}{n}\mathbf{w}\right)-n\mathbf{z}\otimes\left(\mathbf{x}+\mathbf{y}+\frac{1}{n}\mathbf{z}\right)\otimes\mathbf{x} \\ & + n(\mathbf{y}+\mathbf{z})\otimes\left(\mathbf{y}+\frac{1}{n}\mathbf{z}\right)\otimes\left(\mathbf{x}+\frac{1}{n}\mathbf{w}\right) \end{aligned}$$

May check that: $\operatorname{rank}(S_n) \le 5$, $\operatorname{rank}(T) = 6$ and $\|S_n - T\| \to 0$.

T is a rank-6 tensor that has no optimal rank-5 approximations.

Norm independence

The choice of norm in the above examples is inconsequential because of the following basic result.

Fact. All norms on finite-dimensional spaces are equivalent and thus induce the same topology (the Euclidean topology).

Since questions of convergence and whether a set is closed depend only on the topology of the space, the results here would all be independent of the choice of norm on $\mathbb{R}^{d_1 \times \cdots \times d_k}$, which is finite-dimensional.

Exceptional cases: order-2 tensors and rank-1 tensors

Set of tensors of rank not more than r,

$$\mathcal{S}(k,r) = \{T \in \mathbb{R}^{d_1\times\cdots\times d_k} \mid \text{rank}(T) \le r\}.$$

When $k = 2$ (matrices) and when $r = 1$ (decomposable tensors), $\mathcal{S}(k,r)$ is closed — Eckart-Young problem solvable in these cases.

Proposition. For any $r \in \mathbb{N}$, the set $\mathcal{S}(2,r) = \{A \in \mathbb{R}^{m\times n} \mid \text{rank}(\mathrm{s}) \le r\}$ is closed in $\mathbb{R}^{m\times n}$ under any norm-induced topology.

Proposition. The set of decomposable tensors, $\mathcal{S}(k,1) = \{S \in \mathbb{R}^{d_1\times\cdots\times d_k} \mid \text{rank}(S) \le 1\}$, is closed in $\mathbb{R}^{d_1\times\cdots\times d_k}$ under any norm-induced topology.

A classification theorem

Theorem (de Silva and L., 2004). Let $d_1, d_2, d_3 \geq 2$. Let $T \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ with rank$(T) = 3$. T is the limit of a sequence $S_n \in \mathbb{R}^{d_1 \times d_2 \times d_3}$ with rank$(S_n) \leq 2$ if and only if

$$T = \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3$$

for some $\mathbf{x}_i, \mathbf{y}_i$ linearly independent vectors in $\mathbb{R}^{d_i}$, $i = 1, 2, 3$.

Note that a rank-3 tensor of this form is defined by 6 linearly independent vectors. On the other hand, we would expect a rank-3 tensor chosen at random to be defined by 9 linearly independent vectors. T is an example of a tensor that has rank 3 but *closed-rank* 2 (to be defined).

Instead of fitting a 3-way data array with a rank-2 model, we fit a 3-way data array with a closed-rank-2 model.

Density of rank-r matrices

Set of tensors of rank exactly r,

$$\mathcal{R}(k,r) := \{T \in \mathbb{R}^{d_1\times\cdots\times d_k} \mid \text{rank}(T) = r\}.$$

$\mathcal{R}(k,r)$ not closed even in the case where $k = 2$ — higher-rank matrices converging to lower-rank ones easily constructed:

$$\begin{bmatrix} 1 & 1+\frac{1}{n} \\ 1 & 1 \end{bmatrix} \to \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \qquad \begin{bmatrix} \frac{1}{n} & 0 \\ 0 & \frac{1}{n} \end{bmatrix} \to \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

This is often a source of numerical instability: the problem of defining matrix rank in a finite-precision context [Golub-Van Loan 1996], the inherent difficulty of computing a Jordan canonical form [Golub-Wilkinson 1976], may all be viewed as consequences of the fact that $\mathcal{R}(2,r)$ is not closed.

However, closure of $\mathcal{R}(2,r)$ may be easily described (next slide).

Density of rank-r tensors

Proposition. With $\mathcal{R}(2,r) = \{A \in \mathbb{R}^{m\times n} \mid \text{rank}(A) = r\}$ and $\mathcal{S}(2,r) = \{A \in \mathbb{R}^{m\times n} \mid \text{rank}(A) \le r\}$, we have

$$\overline{\mathcal{R}(2,r)} = \mathcal{S}(2,r).$$

Here $\overline{\mathcal{R}}$ denotes the topological closure of a non-empty set $\mathcal{R}$.

Immediate Corollary. $\mathcal{S}(2,r)$ is closed.

Since $\mathcal{S}(k,r)$ is in general not closed for $k > 2$ and $r > 1$, the Proposition is not true for tensors of higher order, ie. $\overline{\mathcal{R}(k,r)} \neq \mathcal{S}(k,r)$. Characterizing the closure of $\mathcal{S}(k,r)$ will be important for fixing the ill-posedness of the Eckart-Young problem.

Example. $\overline{\{T \in \mathbb{R}^{2\times 2\times 2} \mid \text{rank}(T) = 3\}} \neq \mathbb{R}^{2\times 2\times 2}$. In fact, both $\{T \in \mathbb{R}^{2\times 2\times 2} \mid \text{rank}(T) = 3\}$ and $\{T \in \mathbb{R}^{2\times 2\times 2} \mid \text{rank}(T) = 2\}$ have positive volumes in $\mathbb{R}^{2\times 2\times 2}$; thus neither of them can be dense. (Contrast with matrices — $\{A \in \mathbb{R}^{m\times n} \mid \text{rank}(A) < \min(m,n)\}$ always have measure 0).

Fixing the ill-posedness of Eckart-Young problem

Definition. An order-k tensor $S \in \mathbb{R}^{d_1\times\cdots\times d_k}$ has **closed-rank** r if $S \in \overline{\mathcal{S}(k,r)}$ and $S \notin \overline{\mathcal{S}(k-1,r)}$.

Note that $\overline{\mathcal{S}(k,r)} = \{S \in \mathbb{R}^{d_1\times\cdots\times d_k} \mid \text{closedrank}(S) \leq r\}$.

The problem

$$\underset{\text{rank}(S)\leq r}{\text{argmin}} \|S - T\|$$

may not have solutions when $r > 1$.

Suppose we solve the problem

$$S_{\text{min}} = \underset{\text{closedrank}(S)\leq r}{\text{argmin}} \|S - T\|,$$

which always have a solution, will we have fixed the ill-posedness Eckart-Young problem?

Question. How do we know that S_{min} is meaningful?

Optimal rank-2 approximations

Order 3 tensor $T \in \mathbb{R}^{d_1 \times d_2 \times d_3}$, $d_i \geq 2$.

Optimal rank-1 approximation:

$$\min_{\mathbf{x}_i \in \mathbb{R}^{d_i}} \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3\|$$

Optimal solutions exist. Can always find $\mathbf{x}_i^* \in \mathbb{R}^{d_i}$ with

$$\|T - \mathbf{x}_1^* \otimes \mathbf{x}_2^* \otimes \mathbf{x}_3^*\| = \min_{\mathbf{x}_i \in \mathbb{R}^{d_i}} \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3\|.$$

Many ways to determine $\mathbf{x}_1^*, \mathbf{x}_2^*, \mathbf{x}_3^*$ explicitly.

Optimal rank-2 approximation:

$$\min_{\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}} \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|$$

Optimal solutions often don't exist, ie. no $\mathbf{x}_i^*, \mathbf{y}_i^* \in \mathbb{R}^{d_i}$ with

$$\|T - \mathbf{x}_1^* \otimes \mathbf{x}_2^* \otimes \mathbf{x}_3^* - \mathbf{y}_1^* \otimes \mathbf{y}_2^* \otimes \mathbf{y}_3^*\| = \min_{\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}} \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|.$$

Quick but flawed fix

Current way to force a solution for the Eckart-Young problem: perturb the problem by small $\varepsilon > 0$ and find approximate solution $\mathbf{x}_i^*(\varepsilon), \mathbf{y}_i^*(\varepsilon) \in \mathbb{R}^{d_i}$ $(i = 1, 2, 3)$ with

$$\begin{aligned}&\|T - \mathbf{x}_1^*(\varepsilon) \otimes \mathbf{x}_2^*(\varepsilon) \otimes \mathbf{x}_3^*(\varepsilon) - \mathbf{y}_1^*(\varepsilon) \otimes \mathbf{y}_2^*(\varepsilon) \otimes \mathbf{y}_3^*(\varepsilon)\| \\ &\qquad = \varepsilon + \min_{\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}} \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|.\end{aligned}$$

Serious numerical problems due to ill-conditioning (a phenomenon often referred to as *degeneracy* or *swamp* in Chemometrics and Psychometrics).

Reason? Rule of thumb in Computational Math:

A well-posed problem near to an ill-posed one is ill-conditioned.

So, even if we may perturb an ill-posed problem slightly to get a well-posed one, the perturbed problem will more often than not be ill-conditioned.

Optimal closed-rank-2 approximations

For $T \in \mathbb{R}^{d_1 \times d_2 \times d_3}$, we define the smooth functions

$$f_T(\mathbf{x}_1, \ldots, \mathbf{y}_3) := \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|_F^2,$$
$$g_T(\mathbf{x}_1, \ldots, \mathbf{y}_3) := \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 - \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3\|_F^2.$$

By the Theorem mentioned earlier, we have

Corollary. Let $d_1, d_2, d_3 \geq 2$. The closure of the set $\{T \in \mathbb{R}^{d_1 \times d_2 \times d_3} \mid \text{rank}(T) \leq 2\}$ is given by

$$\{\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 \mid \mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}\}$$
$$\cup \{\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3 \mid \mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}\}.$$

It then follows that

$$\min_{\text{closedrank}(S) \leq r} \|S - T\|_F^2 = \min_{\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}} \min\{f_T(\mathbf{x}_1, \ldots, \mathbf{y}_3), g_T(\mathbf{x}_1, \ldots, \mathbf{y}_3)\}.$$

Note that this always have a solution. So there exists

$$S_T^* = \operatorname*{argmin}_{\mathbf{x}_i,\mathbf{y}_i\in\mathbb{R}^{d_i}} \min\{f_T(\mathbf{x}_1,\ldots,\mathbf{y}_3), g_T(\mathbf{x}_1,\ldots,\mathbf{y}_3)\}$$

for any $T \in \mathbb{R}^{d_1\times d_2\times d_3}$.

Computation. Finding S_T^* requires no more than a constant multiple of the computational cost in finding approximate solution: two functional evaluations (f_T and g_T) per iteration instead of one functional evaluation (f_T only) per iteration. We do not need to be concerned about the nondifferentiability of $\min\{f_T, g_T\}$.

Interpretation. How do we know that S_T^* is meaningful? Note that S_T^* will take one of the following forms

$$\mathbf{x}_1^*\otimes\mathbf{x}_2^*\otimes\mathbf{x}_3^*+\mathbf{y}_1^*\otimes\mathbf{y}_2^*\otimes\mathbf{y}_3^* \quad \text{or} \quad \mathbf{x}_1^*\otimes\mathbf{x}_2^*\otimes\mathbf{x}_3^*+\mathbf{x}_1^*\otimes\mathbf{y}_2^*\otimes\mathbf{y}_3^*+\mathbf{y}_1^*\otimes\mathbf{x}_2^*\otimes\mathbf{y}_3^*.$$

Both of them require exactly *six* vectors to define. So the 'information content' of S_T^* is the same whichever one of the two forms it takes.

Summary: cause of ill-posedness

Original problem: Given an order-3 tensor $T \in \mathbb{R}^{d_1 \times d_2 \times d_3}$, find the optimal rank-2 approximation, ie. find six vectors $\mathbf{x}_i^*, \mathbf{y}_i^* \in \mathbb{R}^{d_i}$ $(i = 1, 2, 3)$ so that $\|T - \mathbf{x}_1^* \otimes \mathbf{x}_2^* \otimes \mathbf{x}_3^* - \mathbf{y}_1^* \otimes \mathbf{y}_2^* \otimes \mathbf{y}_3^*\|$ is minimal.

Claim: This is the wrong problem to solve (because there is no solution in general). We should not insist on fitting T with a model of the form $\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3$.

Question: What are we really looking for?

Answer: Six vectors $\mathbf{x}_i^*, \mathbf{y}_i^* \in \mathbb{R}^{d_i}$ $(i = 1, 2, 3)$ to fit the data T. There's no reason to require that these six vectors must be combined in the form $\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3$.

Summary: proposed fix

Observation: If the minimum of $\|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|$ cannot be attained by any $\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}$, then there will instead be $\mathbf{x}_i^*, \mathbf{y}_i^* \in \mathbb{R}^{d_i}$ that attain the minimum of $\|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 - \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3\|$. Moreover,

$$\|T - \mathbf{x}_1^* \otimes \mathbf{x}_2^* \otimes \mathbf{x}_3^* - \mathbf{x}_1^* \otimes \mathbf{y}_2^* \otimes \mathbf{y}_3^* - \mathbf{y}_1^* \otimes \mathbf{x}_2^* \otimes \mathbf{y}_3^*\| = \min_{\mathbf{x}_i, \mathbf{y}_i \in \mathbb{R}^{d_i}} \|T - \mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 - \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3\|.$$

That is: T can always be optimally approximated by a six-vector model provided that we are willing to include the 'boundary points' $\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{x}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3 + \mathbf{y}_1 \otimes \mathbf{x}_2 \otimes \mathbf{y}_3$ on top of the usual $\mathbf{x}_1 \otimes \mathbf{x}_2 \otimes \mathbf{x}_3 + \mathbf{y}_1 \otimes \mathbf{y}_2 \otimes \mathbf{y}_3$.

Natural fix: Minimize over a six-vector model that include both forms.