Problems of nonnegative rank for $n \times 4$ matrices

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Definition

Let $V \in \mathbb{R}_+^{m \times n}$ be a $m \times n$ matrix with entries in $\mathbb{R}_+$. The ***nonnegative rank*** *($\mathrm{rank}_+(V)$) is the minimum r such that there is a factorization*

$$V = M \cdot N$$

with $M \in \mathbb{R}_+^{m \times r}$ and $N \in \mathbb{R}_+^{r \times n}$.

If $V \in \mathbb{R}_+^{m \times n}$ and $\mathrm{rank}(V) \leq 2$ then $\mathrm{rank}_+(V) = \mathrm{rank}(V)$.

KRS *Fixed points of the EM algorithm and nonnegative rank boundary*, K. Kubjas, E. Robeva, B. Sturmfels.

EHK *Algebraic boundary of matrices of nonnegative rank at most three*, Eggermont, Horobet, K. Kubjas.

GG *Program in Matlab to compute rank_+ for 4×4 matrices*, N. Gillis and F. Glineur.

Definition

Suppose $V = (v_{ij}) \in \mathbb{R}_+^{m\times n}$. *We say that* v_{ij}, v_{kp} *are* ***independent*** *if*

$$v_{ij} \cdot v_{kp} > 0 \;\; \textit{and} \;\; v_{ip} \cdot v_{kj} = 0$$

Proposition

If V *contains a set of* d *independent elements two by two then* $\mathrm{rank}_+(V) \geq d$.

Example

$$A = \begin{bmatrix} \mathbf{1} & 1 & 0 & 0 \\ 1 & 0 & \mathbf{1} & 0 \\ 0 & \mathbf{1} & 0 & 1 \\ 0 & 0 & 1 & \mathbf{1} \end{bmatrix}$$ has rank 3 and nonnegative rank 4

We focus on $n \times 4$ matrices with rank 3. Let $V \in \mathbb{R}_+^{n\times 4}$:

$$V = \begin{bmatrix} v_{11} & v_{12} & v_{13} & v_{14} \\ v_{21} & v_{22} & v_{23} & v_{24} \\ \vdots & \vdots & \vdots & \vdots \\ v_{n1} & v_{n2} & v_{n3} & v_{n4} \end{bmatrix}$$

The rows of the matrix V represents n points in $\mathbb{R}^4$ $(v_1, v_2, \ldots, v_n)$. Suppose V is stochastic, $\sum_i v_{1i} = 1$, $\sum_i v_{2i} = 1, \ldots, \sum_i v_{ni} = 1$.

Tetrahedron

Let $w_1 = (1,0,0,0)$, $w_2 = (0,1,0,0)$, $w_3 = (0,0,1,0)$, $w_4 = (0,0,0,1)$ be the vertices of the tetrahedron:

$$\mathcal{T} = \{v \in \mathbb{R}^4 \mid v = \sum \lambda_i w_i \,, \sum \lambda_i = 1\}$$

Suppose $V \in \mathbb{R}^{n\times 4}$ with rank 3. This means that there are 3 independent points (rows) that span a plane ($\mathcal{H}$) that cuts $\mathcal{T}$. Since the sum of coordinates of each point is 1 they lie inside $\mathcal{T}$.

Notation

*We denote by $\mathcal{B}$ the **Convex Hull** of the points $v_1, v_2, \ldots, v_n$.*
We denote by $\mathcal{A}$ the intersection of $\mathcal{H}$ with $\mathcal{T}$.

Corolary

The matrix $V \in \mathbb{R}_+^{n\times 4}$ has nonnegative rank 3 if and only if:

- $\mathrm{rank}(V) = 3$ *and there exists a triangle Δ with $\mathcal{B} \subseteq \Delta \subseteq \mathcal{A}$ such that a vertex of Δ coincides with a vertex of $\mathcal{A}$ or*
- $\mathrm{rank}(V) = 3$ *and there exists a triangle Δ with $\mathcal{B} \subseteq \Delta \subseteq \mathcal{A}$ such that an edge of Δ contains an edge of $\mathcal{B}$*

$\mathcal{H}$ cuts $\mathcal{T}$ in a quadrilateral or in a triangle:

- $\mathcal{H}$ cuts only three of the faces of $\mathcal{T} \Rightarrow \mathrm{rank}_+ = 3$ (because $\mathcal{B}$ is inside a triangle).
- $\mathcal{H}$ cuts in four of the faces of $\mathcal{T} \Rightarrow \mathrm{rank}_+ = 3$ or $\mathrm{rank}_+ = 4$ (we have to give more conditions depending on $\mathcal{B}$).

$\mathrm{rank}_+ = 3$ means that there exists a factorization, $V = M \cdot N$ with $M \in \mathbb{R}^{n\times 3}$ and $N \in \mathbb{R}^{3\times 4}$.

$$\begin{bmatrix} -v_1- \\ -v_2- \\ \vdots \\ -v_n- \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ \vdots & \vdots & \vdots \\ b_{n1} & b_{n2} & b_{n3} \end{bmatrix} \cdot \begin{bmatrix} -a_1- \\ -a_2- \\ -a_3- \end{bmatrix}, \quad v_i = \sum_{j=1}^{3} b_{ij} a_j$$

So, a_1, a_2, a_3 are the vertices of the triangle we have constructed.
So, we want $v_1, \ldots, v_n$ inside a triangle.

Notation

Suppose V with rank 3, there are three independent rows. We denote by V' the 3×4 matrix given by these rows. We denote by A, B, C, D the minors of order 3 of V'.

Hence, the equations of $\mathcal{H}$ are the following:

$$\begin{cases} Ax_1 + Bx_2 + Cx_3 + Dx_4 = 0 \\ x_1 + x_2 + x_3 + x_4 = 1 \end{cases}$$

We give the vertices of the quadrilateral or triangle as solutions of these equations:

$$(\mu_1, 1-\mu, 0, 0), (\mu_2, 0, 1-\mu_2, 0), \ldots, (0, 0, \mu_6, 1-\mu_6)$$

At most 4 of the μ_i satisfy $0 \leq \mu_i \leq 1$.
If there are only three μ_i with $0 \leq \mu_i \leq 1 \Rightarrow$ TRIANGLE.
If there are exactly four μ_i with $0 \leq \mu_i \leq 1 \Rightarrow$ QUADRILATERAL

The important thing for this is the signature of (A, B, C, D).

- $(3, 1)$ represents three points on one side of $\mathcal{H}$ and one on the other side.
- $(2, 2)$ represents two points on one side of $\mathcal{H}$ and two on the other side.

Vertices of the quadrilateral

We identify the 4 vertices of the quadrilateral upon affine transformation with the 4 vertices of the square. From the equations of $\mathcal{H}$ we get that the possible vertices are:

- $W_1 = (\frac{-B}{A-B}, \frac{A}{A-B}, 0, 0)$
- $W_2 = (\frac{-C}{A-C}, 0, \frac{C}{A-C}, 0)$
- $W_3 = (\frac{-D}{A-D}, 0, 0, \frac{A}{A-D})$
- $W_4 = (0, \frac{-C}{B-C}, \frac{B}{B-C}, 0)$
- $W_5 = (0, \frac{-D}{B-D}, 0, \frac{B}{B-D})$
- $W_6 = (0, 0, \frac{-D}{C-D}, \frac{C}{C-D})$

Example

$$A, B > 0, \text{ and } C, D < 0 \Rightarrow \mathrm{vertex} = \{\mathrm{W}_2, \mathrm{W}_3, \mathrm{W}_4, \mathrm{W}_5\}$$

Input= $n \times 4$ matrix
Output= rank_+, M, N
Step 1: compute A, B, C, D

- $(3,1) \Rightarrow$ Output: $\mathrm{rank}_+ = 3, M, N$
- $(2,2) \Rightarrow$ Step 2

Step 2: compute the vertices $\{W_1, W_2, W_3, W_4\}$ (quadrilateral $\mathcal{A}$)
Step 3: compute the convex hull of v_i ($\mathcal{B}$)
Step 4: compute the first type of triangle Δ

- if $\mathcal{B} \subseteq \Delta \subseteq \mathcal{A} \Rightarrow$ Output: $\mathrm{rank}_+ = 3, M, N$
- otherwise $\Rightarrow$ Step 5

Step 5: compute the second type of triangle Δ'

- if $\mathcal{B} \subseteq \Delta' \subseteq \mathcal{A} \Rightarrow$ Output: $\mathrm{rank}_+ = 3, M, N$
- otherwise $\Rightarrow$ Output: $\mathrm{rank}_+ = 4, M, N$

We can give a change of coordinates to give the equations that defined the boundary (triangle) between nonnegative rank 3 or 4.

$$(x, y) \mapsto x(W_2 - W_1) + y(W_3 - W_2) + W_1$$

Example

$$W_1 = (1/2, 0, 0, 1/2), W_2 = (0, 0, 1/2, 1/2),$$

$$W_3 = (0, 1/2, 1/2, 0), W_4 = (1/2, 1/2, 0, 0)$$

$$(x, y) \mapsto (\frac{1-x}{2}, \frac{y}{2}, \frac{x}{2}, \frac{1-y}{2})$$

Rank 1

$$V = \begin{bmatrix} 2*5/12 & 2*1/12 & 2*1/12 & 2*5/12 \\ 0 & 0 & 0 & 0 \\ 5/12 & 1/12 & 1/12 & 5/12 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

V has rank 1, hence $\mathrm{rank}_+(V) = 1$ and the factorization is:

$$M = \begin{bmatrix} 2 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \; N = \begin{bmatrix} 5/12 & 1/12 & 1/12 & 5/12 \end{bmatrix}$$

Rank 2

$$V = \begin{bmatrix} 5/12 & 1/12 & 1/12 & 5/12 \\ 2*5/12 & 2*1/12 & 2*1/12 & 2*5/12 \\ 1/12 & 1/12 & 5/12 & 5/12 \\ 3*1/12 & 3*1/12 & 3*5/12 & 3*5/12 \end{bmatrix}$$

V has rank 2, hence $\mathrm{rank}_+(V) = 2$ and the factorization is:

$$M = \begin{bmatrix} 1/6 & 5/6 \\ 1/3 & 5/3 \\ 5/6 & 1/6 \\ 5/2 & 1/2 \end{bmatrix}, \; N = \begin{bmatrix} 0 & 1/2 & 1/2 & 5/12 \\ 1/2 & 1/12 & 0 & 5/12 \end{bmatrix}$$

Rank 3

$$V = \begin{bmatrix} 5/12 & 1/12 & 1/12 & 5/12 \\ 1/12 & 1/12 & 5/12 & 5/12 \\ 1/12 & 5/12 & 5/12 & 1/12 \\ 1/3 & 4/15 & 1/6 & 7/30 \\ 1/6 & 1/4 & 1/3 & 1/4 \end{bmatrix}$$

V has rank 3. The vertices of the quadrilateral are:
$\{(0,0,1/2,1/2),(0,1/2,1/2,0),(1/2,1/2,0,0),(1/2,0,0,1/2)\}$
The convex hull is:
$\{(1/12,1/12,5/12,5/12),(1/12,5/12,5/12,1/12),$
$(1/3,4/15,1/6,7/30),(5/12,1/12,1/12,5/12)\}$

Factorization

There exists a factorization:

$$M = \begin{bmatrix} 0 & 5/6 & 1/6 \\ 5/36 & 5/36 & 13/18 \\ 5/6 & 0 & 1/6 \\ 5/12 & 7/12 & 0 \\ 65/144 & 35/144 & 11/36 \end{bmatrix}, \quad N = \begin{bmatrix} 1/10 & 1/2 & 2/5 & 0 \\ 1/2 & 1/10 & 0 & 2/5 \\ 0 & 0 & 1/2 & 1/2 \end{bmatrix}$$

Hence, $\mathrm{rank}_+(V) = 3$.

Rank 3

$$V = \begin{bmatrix} 5/12 & 1/12 & 1/12 & 5/12 \\ 1/12 & 1/12 & 5/12 & 5/12 \\ 1/12 & 5/12 & 5/12 & 1/12 \\ 1/2 & 2/19 & 0 & 15/38 \\ 2/19 & 1/2 & 15/38 & 0 \end{bmatrix}$$

V has rank 3. The vertices of the quadrilateral are:
$\{(0,0,1/2,1/2),(0,1/2,1/2,0),(1/2,1/2,0,0),(1/2,0,0,1/2)\}$
The convex hull is:
$\{(1/12,1/12,5/12,5/12),(1/12,5/12,5/12,1/12),$
$(2/19,1/2,15/38,0),(1/2,2/19,0,15/38),(5/12,1/12,1/12,5/12)\}$
There does not exist factorization. Hence, $\mathrm{rank}_+(V) = 4$.

Rank 3

$$V = \begin{bmatrix} 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 \\ 1/12 & 0 & 0 & 1/12 \\ 0 & 1/2 & 1/2 & 0 \\ 1/12 & 1/12 & 5/12 & 5/12 \end{bmatrix}$$

V has rank 3. The vertices of the quadrilateral are:
$\{(0,0,1/2,1/2),(0,1/2,1/2,0),(1/2,1/2,0,0),(1/2,0,0,1/2)\}$
The convex hull is:
$\{(0,0,1/2,1/2),(0,1/2,1/2,0),(1/2,1/2,0,0),(1/2,0,0,1/2)\}$
There does not exist factorization. Hence, $\mathrm{rank}_+(V) = 4$.

If $\mathrm{rank}(V) = 4$ then $\mathrm{rank}_+(V) = 4$.

¡Muchas gracias!