Extreme copositive matrices and periodic dynamical systems

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Optimization without borders
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Outline

Copositive cone

Definition

A real symmetric $n \times n$ matrix A such that $x^T Ax \geq 0$ for all $x \in \mathbb{R}^n_+$ is called copositive.

the set of all such matrices is a regular convex cone, the copositive cone $\mathcal{C}_n$

related cones

- *completely positive* cone $\mathcal{C}_n^* = \text{conv}\{xx^T \,|\, x \geq 0\}$
- sum $\mathcal{N}_n + \mathcal{S}_n^+$ of nonnegative and positive semi-definite cone
- *doubly nonnegative* cone $\mathcal{N}_n \cap \mathcal{S}_n^+$

$$\mathcal{C}_n^* \subset \mathcal{N}_n \cap \mathcal{S}_n^+ \subset \mathcal{N}_n + \mathcal{S}_n^+ \subset \mathcal{C}_n$$

NP-hardness

Theorem (Murty, Kabadi 1987)

Checking whether an $n \times n$ integer matrix is not copositive is NP-complete.

Theorem (Burer 2009)

Any mixed binary-continuous optimization problem with linear constraints and (non-convex) quadratic objective function can be written as a copositive program

$$\min_{x \in \mathcal{C}_n} \langle c, x \rangle : \qquad Ax = b$$

Description in low dimensions

Theorem (Diananda 1962)

Let $n \leq 4$. Then the copositive cone $\mathcal{C}_n$ equals the sum of the nonnegative cone $\mathcal{N}_n$ and the positive semi-definite cone $\mathcal{S}_n^+$.

the Horn form (discovered by Alfred Horn)

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}$$

is an example of a matrix in $\mathcal{C}_5 \setminus (\mathcal{N}_5 + \mathcal{S}_5^+)$

matrices in $\mathcal{C}_n \setminus (\mathcal{N}_n + \mathcal{S}_n^+)$ are called exceptional

Dimension 5

Theorem (Dickinson, Dür, Gijben, H. 2013)

The linear affine section $D_{5,1} = \{A \in \mathcal{C}_5 \mid \operatorname{diag}(A) = \mathbf{1}\}$ possesses a semi-definite description:
$A \in D_{5,1}$ if and only if the 6-th order polynomial on $\mathbb{R}^5$ given by

$$p_A(x) = \left(\sum_{i,j=1}^{5} A_{ij} x_i^2 x_j^2\right) \cdot \left(\sum_{k=1}^{5} x_k^2\right)$$

is a sum of squares.

- every copositive matrix A with $\operatorname{diag} A > 0$ can be diagonally scaled to a copositive matrix $A' = DAD$ with $\operatorname{diag} A' = \mathbf{1}$
- for every matrix $A \in \mathcal{C}_5 \setminus (\mathcal{N}_5 + \mathcal{S}_5^+)$ there exists a positive definite diagonal matrix D such that p_{DAD} is not SOS

Extreme rays

Definition

Let $K \subset \mathbb{R}^n$ be a regular convex cone. An nonzero element $u \in K$ is called extreme if it cannot be decomposed into a non-trivial sum of linearly independent elements of K.

in [Hall, Newman 63] the extreme rays of $\mathcal{C}_n$ belonging to $\mathcal{N}_n + \mathcal{S}_n^+$ have been described:

- the extreme rays of $\mathcal{N}_n$, generated by E_{ii} and $E_{ij} + E_{ji}$
- rank 1 matrices $A = xx^T$ with x having both positive and negative elements

in [Hoffman, Pereira 1973] the extreme elements of $\mathcal{C}_n$ with elements in $\{-1, 0, +1\}$ have been described

Dimension 5

Theorem (H. 2012)

The extreme elements $A \in \mathcal{C}_5 \setminus (\mathcal{N}_5 + \mathcal{S}_5^+)$ of $\mathcal{C}_5$ are exactly the matrices $DPMP^TD$, where D is a diagonal positive definite matrix, P is a permutation matrix, and M is either the Horn form H or is given by a matrix

$$T = \begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & \cos(\psi_2+\psi_3) & -\cos\psi_3 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) & \cos(\psi_3+\psi_4) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ \cos(\psi_2+\psi_3) & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 & -\cos\psi_2 \\ -\cos\psi_3 & \cos(\psi_3+\psi_4) & \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{pmatrix},$$

where $\psi_k > 0$ for $k = 1, \dots, 5$ and $\sum_{k=1}^5 \psi_k < \pi$.

Definition (Baumert 1965)

let $A \in \mathcal{C}_n$ be a copositive matrix

- a non-zero vector $x \geq 0$ is called a zero of A if $x^T A x = 0$
- the set $\operatorname{supp} x = \{i \,|\, x_i > 0\}$ is called the support of x
- the set $\mathcal{V}_A = \{\operatorname{supp} x \,|\, x \text{ is a zero of } A\}$ is called the zero pattern of A

Example: Horn form

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}: \qquad x = \begin{pmatrix} a \\ a+b \\ b \\ 0 \\ 0 \end{pmatrix}, \quad \begin{matrix} a, b \geq 0, \\ a+b > 0 \end{matrix}$$

and cyclically permuted vectors
$\mathcal{V}_H$ consists of $\{1,2\},\{1,2,3\}$ and cyclically permuted sets

Example: T-matrix

$$T = \begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & \cos(\psi_2+\psi_3) & -\cos\psi_3 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) & \cos(\psi_3+\psi_4) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ \cos(\psi_2+\psi_3) & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 & -\cos\psi_2 \\ -\cos\psi_3 & \cos(\psi_3+\psi_4) & \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{pmatrix}$$

has zeros given by the columns of the matrix

$$\begin{pmatrix} \sin\psi_5 & 0 & 0 & \sin\psi_2 & \sin(\psi_3+\psi_4) \\ \sin(\psi_4+\psi_5) & \sin\psi_1 & 0 & 0 & \sin\psi_3 \\ \sin\psi_4 & \sin(\psi_1+\psi_5) & \sin\psi_2 & 0 & 0 \\ 0 & \sin\psi_5 & \sin(\psi_1+\psi_2) & \sin\psi_3 & 0 \\ 0 & 0 & \sin\psi_1 & \sin(\psi_2+\psi_3) & \sin\psi_4 \end{pmatrix}$$

and homothetic images

the zero pattern is $\{\{1,2,3\},\{2,3,4\},\{3,4,5\},\{4,5,1\},\{5,1,2\}\}$

Properties

Theorem (Diananda 1962)

Let $A \in \mathcal{C}_n$ be a copositive matrix, let x be a zero of A, and let $I = \operatorname{supp} x$. Then the principal submatrix $A_{I,I}$ is positive semi-definite.

Theorem (Baumert 1966)

Let A be a copositive matrix and let x be a zero of A. Then $Ax \geq 0$.

- if $A, B \in \mathcal{C}_n$ and x is a zero of $A + B$, then x is a zero of A and B
- (Baumert 1965) if x is a zero of $A \in \mathcal{C}_n$ and $|\operatorname{supp} x| \geq n - 1$, then $A \in \mathcal{N}_n + \mathcal{S}_n^+$

Outline

Framework

scalar discrete-time time-variant dynamical system

$$x_{t+d} + \sum_{i=0}^{d-1} c_{t,i} x_{t+i} = 0, \qquad t \geq 0$$

coefficients n-periodic, $c_{t+n,i} = c_{t,i}$

- solution space $\mathcal{L}$ is d-dimensional, $n > d$
- $\mathcal{L}$ can be parameterized by initial values $x_0, \dots, x_{d-1}$
- if $c_{t,0} \neq 0$ for all t, then the system is reversible

Monodromy

let $x = (x_t)_{t\geq 0}$ be a solution

then $y = (x_{t+n})_{t\geq 0}$ is also a solution

Definition

The linear map $\mathfrak{M} : \mathcal{L} \to \mathcal{L}$ taking x to y is called the monodromy of the periodic system.
Its eigenvalues are called Floquet multipliers.

- x is periodic if and only if it is an eigenvector of $\mathfrak{M}$ with eigenvalue 1
- $\det \mathfrak{M} = (-1)^{nd} \prod_{t=0}^{n-1} c_{t,0}$

Evaluation functionals

let $x = (x_t)_{t \geq 0}$ be a solution

for every t, define a linear map $\mathbf{e}_t$ by $\mathbf{e}_t(x) = x_t$

- $\mathbf{e}_t$ belongs to the dual space $\mathcal{L}^*$
- $\mathbf{e}_{t+n} = \mathfrak{M}^* \mathbf{e}_t$
- $\mathbf{e}_0, \dots, \mathbf{e}_{d-1}$ span $\mathcal{L}^*$

$\mathbf{e}_t$ evolves according to

$$\mathbf{e}_{t+d} + \sum_{i=0}^{d-1} c_{t,i} \mathbf{e}_{t+i} = 0$$

Shift-invariant forms

Definition

A symmetric bilinear form B on $\mathcal{L}^*$ is called shift-invariant if

$$B(\mathbf{e}_{t+n}, \mathbf{e}_{s+n}) = B(\mathbf{e}_t, \mathbf{e}_s) \qquad \forall\, t, s \geq 0$$

- B is shift-invariant if and only if $B(w, w') = B(\mathfrak{M}^* w, \mathfrak{M}^* w')$ for all $w, w' \in \mathcal{L}^*$
- $B = x \otimes x$ for x periodic are shift-invariant
- a positive semi-definite form B is shift-invariant if and only if $\mathfrak{M}[(\ker B)^\perp] = (\ker B)^\perp$ and the restriction of $\mathfrak{M}$ to $(\ker B)^\perp$ is similar to a unitary operator

in particular, $n - \dim \ker B$ eigenvalues of $\mathfrak{M}$ lie on the unit circle

Vector sets with circulant supports

let $n \geq 5$ and let $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}^n_+$ with

$$\begin{aligned} \operatorname{supp} u^1 &= \{1, 2, \dots, n-2\} =: I_1 \\ \operatorname{supp} u^2 &= \{2, 3, \dots, n-1\} =: I_2 \\ &\vdots \\ \operatorname{supp} u^n &= \{n, 1, \dots, n-3\} =: I_n \end{aligned}$$

- supports form an orbit under circular shift
- a copositive matrix having such zeros might not exist

Associated dynamical system

to a collection $\mathbf{u}$ of nonnegative vectors $u^1, \dots, u^n$ with $\operatorname{supp} u^k = I_k$ associate an n-periodic dynamical system

$$\sum_{i=0}^{d} c_{t,i} x_{t+i} = 0$$

with $c_t = (u^t)_{I_t}$, $t = 1, \dots, n$

- order $d = n - 3$
- system is reversible
- all coefficients are positive
- $\det \mathfrak{M} = \prod_{j=1}^n u_j^j / \prod_{j=1}^n u_{j+d}^j > 0$

Periodic solutions

let $\mathcal{L}_{per}$ be the subspace of periodic solutions

Lemma

An n-periodic infinite sequence $x = (x_0, x_1, \dots)$ is a solution if and only if the vector $(x_1, \dots, x_n)^T \in \mathbb{R}^n$ is orthogonal to all zeros u^j, $j = 1, \dots, n$.
In particular, $\dim \mathcal{L}_{per}$ equals the corank of the matrix U composed of $u^1, \dots, u^n$.

corank of U = multiplicity of Floquet multiplier 1

Example: zeros of T-matrix

$n = 5$, $d = 2$, $\mathbf{u}$ given by columns of

$$\begin{pmatrix} \sin\psi_5 & 0 & 0 & \sin\psi_2 & \sin(\psi_3+\psi_4) \\ \sin(\psi_4+\psi_5) & \sin\psi_1 & 0 & 0 & \sin\psi_3 \\ \sin\psi_4 & \sin(\psi_1+\psi_5) & \sin\psi_2 & 0 & 0 \\ 0 & \sin\psi_5 & \sin(\psi_1+\psi_2) & \sin\psi_3 & 0 \\ 0 & 0 & \sin\psi_1 & \sin(\psi_2+\psi_3) & \sin\psi_4 \end{pmatrix}$$

linearly independent solutions of the associated dynamical system are given by

$$x^1 = (1, -\cos\psi_4, \cos(\psi_4+\psi_5), -\cos(\psi_4+\psi_5+\psi_1), \cos(\psi_4+\psi_5+\psi_1+\psi_2), \dots)$$
$$x^2 = (0, \sin\psi_4, -\sin(\psi_4+\psi_5), \sin(\psi_4+\psi_5+\psi_1), -\sin(\psi_4+\psi_5+\psi_1+\psi_2), \dots)$$

Main correspondence

let $\mathcal{A}_{\mathbf{u}} \subset \mathcal{S}_n$ be the linear subspace of symmetric $n \times n$ matrices A satisfying $(Au^k)_{I_k} = 0$

to every $A \in \mathcal{A}_{\mathbf{u}}$ associate a symmetric bilinear form B on the dual solution space $\mathcal{L}^*$ by

$$B(\mathbf{e}_t, \mathbf{e}_s) = A_{ts}, \qquad t, s = 1, \dots, d$$

let $\Lambda : A \mapsto B$ be the corresponding linear map

- for A being copositive $Au^k \geq 0$ is a necessary condition
- Λ maps quadratic forms on $\mathbb{R}^n$ to quadratic forms on $\mathbb{R}^d$

Image of Λ

Lemma

The linear map Λ is injective and its image consists of those shift-invariant symmetric bilinear forms B which satisfy

$$B(\mathbf{e}_t, \mathbf{e}_s) = B(\mathbf{e}_{t+n}, \mathbf{e}_s) \qquad \forall\, t, s \geq 0 : \; 3 \leq s - t \leq n - 3$$

- the image of Λ may be $\{0\}$
- effectively finite number of linear conditions

Copositive matrices with zeros $\mathbf{u}$

Theorem

Let $\mathcal{F}_{\mathbf{u}}$ be the set of positive semi-definite shift-invariant symmetric bilinear forms B on $\mathcal{L}_{\mathbf{u}}^*$ satisfying the linear equality relations

$$B(\mathbf{e}_t, \mathbf{e}_s) = B(\mathbf{e}_{t+n}, \mathbf{e}_s), \qquad 0 \leq t < s < n: \ 3 \leq s - t \leq n - 3$$

and the linear inequalities

$$B(\mathbf{e}_t, \mathbf{e}_{t+2}) \geq B(\mathbf{e}_{t+n}, \mathbf{e}_{t+2}), \qquad t = 0, \dots, n-1.$$

Then the face of $\mathcal{C}^n$ defined by the zeros u^j, $j = 1, \dots, n$, is given by $F_{\mathbf{u}} = \Lambda^{-1}[\mathcal{F}_{\mathbf{u}}]$.

Consequences

the face of $\mathcal{C}_n$ defined by $\mathbf{u}$ is given by linear equality and inequality constraints and a semi-definite constraint

Corollary

Given a vector set $\mathbf{u} = \{u^1, \dots, u^n\} \subset \mathbb{R}^n_+$, we can compute the face $F_{\mathbf{u}}$ of the copositive cone $\mathcal{C}_n$ which consists of matrices having $u^1, \dots, u^n$ as zeros by a semi-definite program.

- matrices in $F_{\mathbf{u}}$ might have also other zeros
- a generic vector set will yield only the trivial solution set $\{0\}$

Periodic solutions

Lemma

Let x be an n-periodic solution, then the form $B = x \otimes x$ is contained in the image of Λ and $A = \Lambda^{-1}(B)$ is positive semi-definite and given by $A = (B(\mathbf{e}_t, \mathbf{e}_s))_{t,s=1,\dots,n}$.

let $\mathcal{P}_\mathbf{u}$ be the convex hull of all forms $x \otimes x$, x an n-periodic solution

- the subset $P_\mathbf{u} \subset F_\mathbf{u}$ of positive semi-definite matrices equals $\Lambda^{-1}[\mathcal{P}_\mathbf{u}]$
- the maximal rank achieved by positive semi-definite matrices in $F_\mathbf{u}$ equals the geometric multiplicity of the Floquet multiplier 1

Maximal rank of bilinear forms

Theorem

- *if the maximal rank $r_{\max}$ of the bilinear forms in the feasible set $\mathcal{F}_{\mathbf{u}}$ does not exceed $d-2$, then $F_{\mathbf{u}} = P_{\mathbf{u}} \sim \mathcal{S}_+^{r_{\max}}$*
- *if $r_{\max} = d-1$, then either $F_{\mathbf{u}} = P_{\mathbf{u}} \sim \mathcal{S}_+^{r_{\max}}$, or $\dim F_{\mathbf{u}} = 1$ and $F_{\mathbf{u}}$ is an exceptional extreme ray*
- *if $r_{\max} = d$, then $F_{\mathbf{u}} = P_{\mathbf{u}} \sim \mathcal{S}_+^{r_{\max}}$ if and only if $\mathfrak{M} = Id$ if and only if $u^1, \dots, u^n$ span a 3-dimensional space*

the exceptional extreme matrices in the case $r_{\max} = d-1$ are generalizations of the Horn form

Full rank, even n

Theorem

Let n be even, suppose the face $F_{\mathbf{u}}$ contains an exceptional copositive matrix and the feasible set $\mathcal{F}_{\mathbf{u}}$ contains a positive definite form.
Then $F_{\mathbf{u}} \simeq \mathbb{R}_+^2$, one boundary ray is generated by a rank 1 positive semi-definite matrix, and the other boundary ray is generated by an extreme exceptional copositive matrix.

examples of this kind appear for $n \geq 6$

Full rank, n odd

Theorem

Let n be odd, suppose the face $F_{\mathbf{u}}$ contains an exceptional matrix and the feasible set $\mathcal{F}_{\mathbf{u}}$ contains a positive definite form. Then $F_{\mathbf{u}}$ does not contain non-zero positive semi-definite matrices.
If $F_{\mathbf{u}}$ is 1-dimensional, then it is generated by an extreme exceptional copositive matrix. This matrix has no zeros other than the multiples of $u^1, \dots, u^n$.
If $\dim F_{\mathbf{u}} > 1$, then the monodromy $\mathfrak{M}$ possesses the eigenvalue -1, and all boundary rays of $F_{\mathbf{u}}$ are generated by extreme exceptional copositive matrices.

the case $\dim F_{\mathbf{u}} = 1$ generalizes the T-matrices

Existence of submanifolds of extreme rays

Theorem

- *For arbitrary $n \geq 5$ there exists a submanifold $M_{2n} \subset \mathcal{C}_n$ of codimension $2n$, consisting of exceptional extreme matrices A each of which has zeros $u^1, \dots, u^n$ with supports $I_1, \dots, I_n$, and such that the submatrices A_{I_k, I_k} have rank $n - 4$.*
- *Let $n \geq 5$ be odd. Then there exists a submanifold $M_n \subset \mathcal{C}_n$ of codimension n, consisting of exceptional extreme matrices A each of which has zeros $u^1, \dots, u^n$ with supports $I_1, \dots, I_n$, and such that the submatrices A_{I_k, I_k} have rank $n - 3$.*

Thank you!