



On some matrix operator and its applications

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Abstract. The paper focuses on a matrix operator, which maps a square real matrix to a block matrix (called the saddle point matrix), where the left-up block represents the given matrix, the right-down block is zero, and two other blocks are vectors of ones. The operator transforms any symmetric matrix into the Karush-Kuhn-Tucker matrix of standard quadratic program on the standard simplex, which is the intersection of a hyperplane with the positive orthant. There are shown some properties of this matrix operator, connections with game theory and necessary and sufficient conditions for existence of unique interior optimizer of standard quadratic program.

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Introduction.

Optimization is very rich source of algebra problems, and constrained optimization is the concept most central to economics that is inherently a framework for studying a world in which individuals or firms make decisions that are best for them with respect to given the inherent limitations, like time or money. Since the constraint imposes restrictions on the domain of the objective function, so the solution to a constrained optimization problem is the optimum value that the function takes on over the restricted part of the domain that is consistent with the constraint. It is the reason that unconstrained minimum and maximum is typically smaller and larger, respectively, and the constrained and unconstrained solutions often do not match up.

Quadratic forms and standard quadratic problem have many applications in such different fields as, for instance, graph theory [2], [6], [13], [14], modeling and simulations of dynamical systems [15], knot theory [1], [8] or game theory [5].

In the paper will be used standard notation; if $\mathbf{A} = (a_{ij}) \in \mathbb{R}^{n \times n}$ is a symmetric matrix ($\mathbf{A} = \mathbf{A}^T$) and \mathbf{x} denotes a column n -vector, then the quadratic form associated to \mathbf{A} is the mapping $F: \mathbf{x} \rightarrow \mathbf{x}^T \mathbf{A} \mathbf{x}$, which produces a quadratic polynomial in the n variables of \mathbf{x} . Any applicability and generality is not lost by symmetric assumption, because if \mathbf{A} is not symmetric, then the matrix $\mathbf{M} = \frac{\mathbf{A} + \mathbf{A}^T}{2}$ is symmetric, and for any \mathbf{x} we have $F(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x} = \mathbf{x}^T \mathbf{M} \mathbf{x}$.

Let Δ be the standard simplex of \mathbb{R}^n , which is the intersection of the $(n-1)$ -dimensional hyperplane with the positive orthant:

$$\Delta = \{\mathbf{x} \in \mathbb{R}^n: \mathbf{e}^T \mathbf{x} = 1, x_i \geq 0 \text{ for all } i = 1, \dots, n\},$$

where $\mathbf{e} = [1, \dots, 1]^T \in \mathbb{R}^n$.

The standard quadratic program is written as

$$\text{Optimize } \{F(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x} \mid \mathbf{x} \in \Delta\} \quad (1)$$

Since we consider the standard quadratic program as a nonlinear constrained program, where the objective function is a quadratic form and the constraint is a linear function of the design variables, then the side constraint $g(\mathbf{x}) = \mathbf{e}^T \mathbf{x}$ is both quasi-convex and quasi-concave, simultaneously convex and concave. Convexity (concavity, respectively) is important in optimization because a convex (concave, respectively) function has no local minima (maxima, respectively) that are not global. When the objective $F(\mathbf{x})$ is strictly convex (concave, respectively) for all feasible points then the problem (1) has a unique local minimum (maximum, respectively) which is also global. Recall that a sufficient condition to guarantee strictly convexity (concavity, respectively) is for A to be positive (negative, respectively) definite.

It is known that the second-order characterization of convexity states that if the function $f(x)$ is twice differentiable on an open set S , then

$$\nabla^2 f(x) > 0 \iff f(x) \text{ is convex for any } x \in S.$$

Recall specialization the first-order necessary conditions to the standard quadratic program. These conditions are sufficient for a global minimum when A is positive definite (eigenvalues are all positive). Otherwise, the most one can said is that they are necessary. The KKT conditions characterize a multiplier λ , called often the KKT multiplier at a feasible optimum \mathbf{x}^* by

1. $g(\mathbf{x}^*) = 1$ (feasibility)
2. $\nabla F(\mathbf{x}^*) = \lambda \nabla g(\mathbf{x}^*)$ (stationarity)

where $g(\mathbf{x}^*) = \mathbf{e}^T \mathbf{x}^*$.

The first condition states that \mathbf{x}^* has to be a feasible solution. The second condition in geometric interpretation states that the gradients of $F(\mathbf{x})$ and the bound $g(\mathbf{x})$ must point in the same direction at \mathbf{x}^* . This means that the gradient vectors of $F(\mathbf{x})$ and $g(\mathbf{x})$ must be parallel, though they may have different lengths. Since $F(\mathbf{x}^*) = \lambda g(\mathbf{x}^*)$ it is equivalent to saying that the gradient $\nabla F(\mathbf{x}^*)$ of the objective function is normal to the tangent surface $g(\mathbf{x}) = 1$ at an optimal \mathbf{x}^* .

From optimization point of view the value of the multiplier at the solution \mathbf{x}^* of the problem is equal to the rate of change in the optimal value of the objective function as the constraint is relaxed. In mathematical economics the value of the multiplier is interpreted as the shadow price of the constraint. This means that if the constraint is changed by one unit, the multiplier informs how much the objective function will change by. Thus, for instance, the multiplier measures the marginal utility of income (more precisely, the rate of increase in maximized utility as income is increased) in the case of a customer choice problem. Obviously, functions $F(\mathbf{x})$, $g(\mathbf{x})$ have in (1) continues second-order partial derivatives at any point.

The KKT rule is very familiar to Lagrange rule. But KKT conditions are surprisingly strong. They distinguish minima from maxima as well. It is the reason they can be said to be more powerful then their Lagrange counterparts.

KKT point is called a feasible point that satisfies the KKT conditions. A point is called regular if the Jacobian of the binding constraints at that point is of full rank. In (1) we have $J(\mathbf{x}) = \nabla g(\mathbf{x}) = \mathbf{e}$, and the point \mathbf{x}^* always is regular.

Results

A convenient way of checking the sufficient condition is to construct a KKT matrix, also referred to as bordered Hessian, and defined as the block matrix

$$\begin{bmatrix} \mathbf{H}(\mathbf{x}) & \mathbf{J}(\mathbf{x}) \\ \mathbf{J}^T(\mathbf{x}) & 0 \end{bmatrix},$$

where $\mathbf{J}(\mathbf{x})$ is the Jacobian of the given constraints and $\mathbf{H}(\mathbf{x})$ is the partial of the gradient of the objective function (Hessian). Young's Theorem which establishes symmetry of the Hessian is valid for the KKT matrix as well. If the objective function has the form $F(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x}$, and the constraint $g(\mathbf{x}) = \mathbf{e}^T \mathbf{x}$, where $\mathbf{e}^T \mathbf{x} = 1$, then the matrix operator

$$\mathbf{A} \in \mathbf{M}^{n,n} \rightarrow (\mathbf{A}, \mathbf{e}) = \begin{bmatrix} \mathbf{A} & \mathbf{e} \\ \mathbf{e}^T & 0 \end{bmatrix} \in \mathbf{M}^{n+1, n+1}$$

leads to the KKT matrix.

It is well known that the second conditions for a minimum (maximum) of (1) states that the border-preserving principal minors of order r of the KKT matrix (\mathbf{A}, \mathbf{e}) are negative (have the sign $(-1)^{r+1}$, respectively) for $r = 2, 3, \dots, n + 1$.

Let \mathbf{A}_i stands for the matrix of \mathbf{A} with the i -th column replaced by the vector \mathbf{e} and \mathbf{M}/\mathbf{A} denotes the Schur complement of \mathbf{A} in \mathbf{M} . Recall that the inertia of any symmetric matrix \mathbf{A} , denoted by $\text{Inertia}(\mathbf{A})$, is an ordered triple

$$\text{Inertia}(\mathbf{A}) = (i_+, i_-, i_0),$$

where i_+ , i_- and i_0 mean, respectively, the number of positive, negative and zero eigenvalues of \mathbf{A} .

It is known that the KKT matrix (\mathbf{A}, \mathbf{e}) is inevitable indefinite, i.e. it must have at least one positive and one negative eigenvalue.

The lemma below establishes some properties of the matrix (\mathbf{A}, \mathbf{e}) , especially whenever it contains a linear combination of \mathbf{A} and $\mathbf{E} = \mathbf{e}\mathbf{e}^T$. Note that in the lemma it is not assumed that the matrix \mathbf{A} is symmetric, except in (5).

Lemma. If $\mathbf{A}, \mathbf{E} \in \mathbb{R}^{n, n}$, then for any real number α the following equalities hold

$$\det(\mathbf{A} + \alpha\mathbf{E}, \mathbf{e}) = \det(\mathbf{A}, \mathbf{e}), \tag{2}$$

$$\det(\mathbf{A} + \alpha\mathbf{E}) = \det\mathbf{A} - \alpha \cdot \det(\mathbf{A}, \mathbf{e}), \tag{3}$$

and if \mathbf{A} is nonsingular

$$\det(\mathbf{A}, \mathbf{e}) = -\mathbf{e}^T \mathbf{A}^{-1} \mathbf{e} \cdot \det\mathbf{A} = (\mathbf{A}, \mathbf{e})/\mathbf{A} \det\mathbf{A}, \tag{4}$$

and if \mathbf{A} is symmetric and nonsingular

$$(\mathbf{A}, \mathbf{e}) \sim \begin{bmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & -\mathbf{e}^T \mathbf{A}^{-1} \mathbf{e} \end{bmatrix} \tag{5}$$

where, by (4), determinants of both congruent matrices have the same value.

Proof (2). The equality is obtained immediately if from the i -th row ($i = 1, \dots, n$) of the matrix $(\mathbf{A} + \alpha\mathbf{E}, \mathbf{e})$ we subtract the last row multiplied by α .

Proof (3). The equality trivially holds for $\alpha = 0$.

The derivative of $\det(\mathbf{A} + \alpha\mathbf{E})$ with respect to α gives

$$\frac{d[\det(\mathbf{A} + \alpha\mathbf{E})]}{d\alpha} = \sum_{i=1}^n \det(\mathbf{A} + \alpha\mathbf{E})_i = \sum_{i=1}^n \det \mathbf{A}_i = -\det(\mathbf{A}, \mathbf{e}).$$

Since then, we have

$$\det(\mathbf{A} + \alpha\mathbf{E}) = - \int \det(\mathbf{A}, \mathbf{e}) d\alpha = -\alpha \det(\mathbf{A}, \mathbf{e}) + C.$$

Putting $\alpha = 0$, we get $C = \det\mathbf{A}$, which gives (3).

Proof (4). The formula follows at once from Banachiewicz inversion formula and from Schur determinant formula (see [16] for more details).

Proof (5). In fact, we have

$$\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{e}^T \mathbf{A}^{-1} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{A} & \mathbf{e} \\ \mathbf{e}^T & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{e} \\ \mathbf{0} & -\mathbf{e}^T \mathbf{A}^{-1} \mathbf{e} \end{bmatrix},$$

and on the other hand

$$\begin{bmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & -\mathbf{e}^T \mathbf{A}^{-1} \mathbf{e} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{A}^{-1} \mathbf{e} \\ \mathbf{0} & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{A} & \mathbf{e} \\ \mathbf{0} & -\mathbf{e}^T \mathbf{A}^{-1} \mathbf{e} \end{bmatrix}. \quad \blacksquare$$

If (\mathbf{A}, \mathbf{e}) is full rank then the rank of \mathbf{A} is one or two less than the rank of (\mathbf{A}, \mathbf{e}) . Converse is not true, but if \mathbf{A} is symmetric and positive definite, then it follows from (4) that (\mathbf{A}, \mathbf{e}) is nonsingular. So it can be written:

$$(\text{rank}(\mathbf{A}, \mathbf{e}) = n + 1) \Rightarrow (n - 1 \leq \text{rank}\mathbf{A} \leq n),$$

$$\mathbf{A} \succ 0 \Rightarrow \det(\mathbf{A}, \mathbf{e}) \neq 0.$$

Moreover, in the last case, the nonsingular (\mathbf{A}, \mathbf{e}) has one negative eigenvalue and n positive ones ([4]):

$$\mathbf{A} \succ 0 \Rightarrow \text{Inertia}(\mathbf{A}, \mathbf{e}) = (n, 1, 0).$$

More properties of saddle point matrices can be found in [10], [11].

Recall also that Gould Theorem [7] states that in quasi-Newton methods for the linear-equality constrained problem (1) it is desirable that the Hessian approximation \mathbf{A} satisfy the “second order sufficiency” condition

$$\mathbf{p}^T \mathbf{A} \mathbf{p} > 0 \text{ for all nonzero } \mathbf{p} \text{ such that } \mathbf{A} \mathbf{p} = 0$$

holds if and only if $\text{Inertia}(\mathbf{A}, \mathbf{e}) = (n, 1, 0)$.

Let $\mathbf{C} = [c_{ij}] \in \mathbb{R}^{(n-1), (n-1)}$ stands for the matrix which entries are obtained from A as follows

$$c_{ik} = -\det(\mathbf{C}_{ik}, \mathbf{e}), \text{ where } \mathbf{C}_{ik} = \begin{bmatrix} a_{ik} & a_{in} \\ a_{nk} & a_{nn} \end{bmatrix}; i, k = 1, \dots, n-1.$$

The matrix \mathbf{C} allows to avoid the constraint. Since \mathbf{A} is symmetric, therefore \mathbf{C} is symmetric as well. Furthermore, the entries of \mathbf{C} can be interpreted as second partial derivatives of an unconstrained function $F_n(\mathbf{x})$ of $(n-1)$ -variables and given as follows

$$F_n(\mathbf{x}) = F(x_1, \dots, x_{n-1}, 1 + x_n - \mathbf{e}^T \mathbf{x}).$$

To construct \mathbf{C} one can apply any function $F_m(\mathbf{x})$ for fixed $m = 1, \dots, n$, and the choice of $F_n(\mathbf{x})$ seems only the most convenient. Therefore in this case we have

$$c_{ik} = \frac{1}{2} \frac{\partial^2 F_n}{\partial x_i \partial x_k} \quad (i, k = 1, \dots, n-1).$$

Really, for any fixed $k = 1, \dots, n-1$, we may write

$$F_n(\mathbf{x}) = \sum_{i=1}^{n-1} a_{ii} x_i^2 + a_{nn} (1 - \sum_{i=1}^{n-1} x_i)^2 + 2 \sum_{\substack{i,j=1 \\ i < j}}^{n-1} a_{ij} x_i x_j + 2 \sum_{i=1}^{n-1} a_{in} x_i (1 - \sum_{i=1}^{n-1} x_i).$$

Since by Leibniz rule is

$$\frac{\partial}{\partial x_k} \left[\sum_{i=1}^{n-1} a_{in} x_i (1 - \sum_{i=1}^{n-1} x_i) \right] = a_{kn} (1 - \sum_{i=1}^{n-1} x_i) - \sum_{i=1}^{n-1} a_{in} x_i,$$

therefore we obtain the following equality

$$\frac{\partial F_n}{\partial x_k} = 2 \left[\sum_{i=1}^{n-1} (a_{ki} - a_{in}) x_i + (a_{kn} - a_{nn}) (1 - \sum_{i=1}^{n-1} x_i) \right].$$

Derivating the expression above with respect to x_h ($h = 1, \dots, n-1$), we have

$$\frac{\partial^2 F_n}{\partial x_k \partial x_h} = -2 \det(\mathbf{C}_{kh}, \mathbf{e}) = 2c_{kh}.$$

Applying the Lemma and remarks above we can give now necessary and sufficient condition for the existence and uniqueness of an interior KKT point and strict local optimizer for (1).

Theorem. If (\mathbf{A}, \mathbf{e}) is non-singular then λ at an interior KKT point of (1) satisfies

$$\lambda \cdot \det(\mathbf{A}, \mathbf{e}) + \det \mathbf{A} = 0, \tag{6}$$

and coefficients x_i ($i = 1, 2, \dots, n$) of this KKT point hold

$$x_i \cdot \det(\mathbf{A}, \mathbf{e}) + \det \mathbf{A}_i = 0, \tag{7}$$

where \mathbf{A}_i denotes the matrix of \mathbf{A} with the i -th row replaced by \mathbf{e} .

A necessary and sufficient condition for the existence and uniqueness of an interior KKT point for (1) is

$$\det \mathbf{A}_i \cdot \det \mathbf{A}_j > 0 \text{ for all } i, j = 1, \dots, n. \tag{8}$$

A necessary and sufficient condition for the existence and uniqueness of an interior strict local solution to (1) is

$$\begin{cases} \det \mathbf{A}_i \cdot \det \mathbf{A}_j > 0 \text{ for all } i, j = 1, \dots, n, \\ \text{definiteness of } \mathbf{C}. \end{cases} \quad (9)$$

If both conditions (9) are fulfilled then

- $\mathbf{C} \prec 0$ for the local maximum,
- $\mathbf{C} \succ 0$ for the local minimum.

Proof. Let \mathbf{x}^* be a stationary point of the given form $F(\mathbf{x})$. By KKT conditions, the point \mathbf{x}^* is such that $\mathbf{A}\mathbf{x}^* = \lambda\mathbf{e}$.

Since elements of \mathbf{x}^* sum to one, then $\lambda\mathbf{e} = \lambda\mathbf{E}\mathbf{x}^*$.

Therefore the equality $\mathbf{A}\mathbf{x}^* = \lambda\mathbf{e}$ can be rewritten as

$$(\mathbf{A} - \lambda\mathbf{E})\mathbf{x}^* = \mathbf{0},$$

and this implies that

$$\det(\mathbf{A} - \lambda\mathbf{E}) = 0.$$

So, by (2) and (3), putting $\alpha = -\lambda$, this leads to equality (6).

To prove (7), note that KKT conditions can be written as

$$(\mathbf{A}, \mathbf{e}) \begin{bmatrix} \mathbf{x} \\ -\lambda \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ 1 \end{bmatrix}. \quad (10)$$

This system of equations expresses stationarity and feasibility conditions for standard quadratic program (1). By (6) and under assumption of non-singularity of (\mathbf{A}, \mathbf{e}) , it follows immediately that the system above has solution

$$x_i = -\frac{\det \mathbf{A}_i}{\det(\mathbf{A}, \mathbf{e})} \quad (i = 1, \dots, n).$$

The sufficiency of (8): the assumption implies that $\det(\mathbf{A}, \mathbf{e}) \neq 0$ and that (7) defines \mathbf{x} as strictly positive vector. The vector \mathbf{x} and the scalar λ , defined by (7), satisfy (10). Thus, the double condition of a KKT point holds. It proves that \mathbf{x} is both interior and the only KKT point with the value $F(\mathbf{x}) = \lambda$.

It remains to prove the necessity of (8). If (1) has a unique KKT point with the value $F(\mathbf{x}) = \lambda$, then \mathbf{x} and λ satisfy the double condition expressed by (10). Moreover, they constitute an isolated solution of (10), because replacing them with any other strictly positive vector $\tilde{\mathbf{x}}$ and scalar $\tilde{\lambda}$ satisfying (10) would give a different KKT point, which by assumption does not exist. The existence of an isolated solution to (11) implies that $\det(\mathbf{A}, \mathbf{e}) \neq 0$. Since the vector \mathbf{x} is strictly positive, the condition (8) now follows from (7).

The condition (9) is obvious, because \mathbf{C} states for Hessian of the unconstrained function $F_n(\mathbf{x})$. As it is known, the composition of a convex quadratic form with an affine constraint is convex. Therefore eliminating equality constraint preserves convexity of the standard quadratic program. ■

Conclusions.

It follows from the Theorem that a quadratic form $F(\mathbf{x})$ such that \mathbf{A} and (\mathbf{A}, \mathbf{e}) are non-singular has at most one interior optimizer.

If the KKT matrix (\mathbf{A}, \mathbf{e}) is singular then multiple interior optimizers may exist. However, multiplicity of interior KKT

points is possible only if \mathbf{A} is also singular. For instance, when $\mathbf{A} = \begin{bmatrix} a & a \\ a & a \end{bmatrix}$, then $(\mathbf{A}, \mathbf{e}) = \begin{bmatrix} a & a & 1 \\ a & a & 1 \\ 1 & 1 & 0 \end{bmatrix}$ ($a \neq 0$),

then $\det \mathbf{A} = \det(\mathbf{A}, \mathbf{e}) = 0$, and $F(\mathbf{x}) = \mathbf{x}^T \mathbf{A} \mathbf{x} = a$ for any $\mathbf{x} = [p, 1-p]^T$, where $p \in (0, 1)$.

If (\mathbf{A}, \mathbf{e}) is singular but \mathbf{A} is non-singular, then (6) cannot possibly hold, and therefore an interior KKT point does not exist.

Generally, a local optimal solution not always is a KKT point, but it must be if either the constraints are linear or the gradients of the binding constraints are linearly independent. Formulas (2) and (7) imply well known property, (see for instance [3]), that the optimizer remains the same if \mathbf{A} is replaced with $\alpha\mathbf{A} + \beta\mathbf{E}$.

From the evolutionary game theory (EGT) point of view (see [9] for more details) the entry a_{ij} of the matrix \mathbf{A} can be interpreted as the amount by which an individual increases its fitness when plays the i -th pure strategy in a contest against another individual that plays the j -th pure strategy. In this case, \mathbf{A} is the resulting fitness matrix, termed also payoff matrix. A point $\mathbf{p} \in \Delta$ is said to be a symmetric Nash equilibrium (NE) strategy if and only if

$$\mathbf{p}^T \mathbf{A} \mathbf{p} \geq \mathbf{x}^T \mathbf{A} \mathbf{p} \text{ for all } \mathbf{x} \in \Delta.$$

NE strategy \mathbf{p} is said to be an evolutionarily stable strategy (ESS) if and only if

$$\mathbf{p}^T \mathbf{A} \mathbf{p} = \mathbf{x}^T \mathbf{A} \mathbf{p} \Rightarrow \mathbf{p}^T \mathbf{A} \mathbf{x} > \mathbf{x}^T \mathbf{A} \mathbf{x}.$$

Note that (4), (9) implies well known Owen's formula [12] for the game value

$$v(\mathbf{A}) = \frac{1}{\mathbf{e}^T \mathbf{A}^{-1} \mathbf{e}}$$

Some of the characterization results of the standard quadratic program (1) which link quadratic forms, optimization theory and EGT, (see [2]), state that if $\mathbf{A} = \mathbf{A}^T$ and $\mathbf{A} \in \mathbb{R}^{n,n}$, $\mathbf{x} \in \Delta$, then:

- a_1 : \mathbf{x} is an ESS $\Leftrightarrow a_2$: \mathbf{x} is a strict local solution to (1),
- b_1 : \mathbf{x} is a NE $\Leftrightarrow b_2$: \mathbf{x} is a KKT point for (1),
- and $a_i \Rightarrow b_i$ ($i = 1, 2$).

This result, by the Theorem given in the paper, for any evolutionary symmetric games can be reformulated and detailed as follows:

- 1) Profile \mathbf{x} is a completely mixed NE iff (8) holds.
- 2) Profile \mathbf{x} is a completely mixed ESS iff (9) holds.
- 3) Payoff of the game with completely mixed NE is expressed by (6).
- 4) Completely mixed NE and ESS profile are given by (7).

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Abbreviations

KKT – Karush-Kuhn-Tucker\

EGT – Evolutionary Game Theory

NE – Nash Equilibrium

ESS – Evolutionary Stable Strategy