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1 ANALYSIS OF TWO DIMENSIONAL NON CONVEX VARIATIONAL PROBLEMS

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Abstract: The purpose of this work is to carry out the analysis of twodimensional scalar variational problems by the method of moments. This method is indeed shown to be useful for treating general cases in which the Lagrangian is a separable polynomial in the derivative variables. In these cases, it follows that the discretization of these problems can be reduced to a single large scale semidefinite program.

Key words: calculus of variations, young measures, the method of moments, semidefinite programming, microstructure, non linear elasticity

1 INTRODUCTION

The classical theory of variational calculus does not provide any satisfactory methods to analyze non-convex variational problems expressed in the form

$$\min_{u} I(u) = \int_{\Omega} f\left(\vec{\nabla} u(x, y)\right) \, dx \, dy \qquad s.t. \qquad u|_{\partial\Omega} = g \tag{1.1}$$

where f is a coercive non-convex Lagrangian function, and u the family of all admissible scalar functions defined on Ω . For a review on recent methods in the calculus of variations see [1].

In order to analyze this class of non-convex variational problems, we must appeal to a new formulation with respect to *Young measures*. For these problems we introduce the *generalized functional*

$$\widetilde{I}(\nu) = \int_{\Omega} \left(\int_{R^2} f(s,t) \, d\mu_{x,y}(s,t) \right) \, dx \, dy$$
with $\nabla u(x,y) = \int_{R^2} (s,t) \, d\mu_{x,y}(s,t)$
and the boundary condition $u|_{\partial\Omega} = g$

$$(1.2)$$

where

$$\nu = \{\mu_{x,y} : (x,y) \in \Omega\}$$

is a parametrized family of probability measures supported on the plane. Each one of these sets ν is called a Young measure, hence the generalized functional \tilde{I} is defined in the family of all Young measures ν .

Young measures theory predicts that the generalized functional (1.2) has a Young measure minimizer

$$\nu^* = \{\bar{\mu}_{x,y} : (x,y) \in \Omega\}$$

which provides information about the limit behavior of the minimizing sequences of the functional I given in (1.1). Thus,

$$\nabla u_n\left(x,y\right) \to d\bar{\mu}_{x,y}$$
(1.3)

in measure, whenever u_n is a minimizing sequence for the functional I. One immediate conclusion is that functional I has a unique minimizer if and only if the generalized functional \tilde{I} has a minimizer ν^* composed only of Dirac measures. In this case

$$\bar{\mu}_{x,y} = \delta_{\vec{\nabla}\bar{u}(x,y)}$$

where \bar{u} is a minimizer for *I*. For a thorough study on Young measures and calculus of variations see [2].

In the present work, we will study the particular case in which the Lagrangian function f takes the polynomial separable form

$$f(s,t) = \sum_{i=0}^{2n} a_i s^i + \sum_{j=0}^{2r} b_j t^j \quad with \quad c_{2n}, \ b_{2r} > 0 \ . \tag{1.4}$$

 $\mathbf{2}$

Under this assumption, Problem (1.2) may be reduced to a single semidefinite program using the theory of the classical problem of moments and elementary convex analysis.

The present paper is organized as follows: in Section 2 we will see a short review on the use of the Method of Moments for treating one dimensional non convex variational problems. In Section 3 we will see how the Method of Moments is used for analyzing the convex envelope of one-dimensional algebraic polynomials. Section 4 describes the general analysis of two dimensional non convex variational problems by the Method of Moments. Section 5 shows how transform the analytical formulation into a particular mathematical program. In Section 6 we will see some examples in detail and finally Section 7 gives some comments about the interplay of this work with pure and applied mathematics.

2 THE METHOD OF MOMENTS

The generalized formulation in Young measures is valid for one-dimensional non convex variational problems like

$$\min_{u} \int_{0}^{1} f(u'(x)) \, dx \qquad s.t. \qquad u(0) = 0, \, u(1) = \alpha$$

Assuming that f is a one-dimensional polynomial in the form

$$f(t) = \sum_{k=0}^{2n} c_k t^k \qquad c_{2n} > 0$$
(2.1)

the generalized problem in Young measures

$$\min_{\nu} I(\nu) = \int_{0}^{1} \int_{R} f(\lambda) d\mu_{x}(\lambda) dx
with u'(x) = \int_{R} \lambda d\mu_{x}(\lambda)
u(0) = 0, u(1) = \alpha$$

$$(2.2)$$

can be recast as

$$\min_{m} \int_{0}^{1} \sum_{k=0}^{2n} c_{k} m_{k}(x) dx
with u'(x) = m_{1}(x)
u(0) = 0, u(1) = \alpha$$
(2.3)

where $m_k(x)$ are the algebraic moments of the parametrized measures μ_x which form the one-dimensional Young measure

$$\nu = \{\mu_x : 0 \le x \le 1\}.$$

The theory of moments provides a good characterization for the algebraic moments of positive measures supported on the real line. Therefore we can study the one-dimensional generalized problem (2.2) by solving the optimization problem (2.3). Here we will study two-dimensional problems defined by separable polynomials in the form (1.4).

For a short review on applications of the method of moments for onedimensional non-convex variational problems see [3]. The essential facts about the characterization of one-dimensional algebraic moments are exposed in [4]. The difficulties about the characterization of two-dimensional algebraic moments are explained in [5].

3 CONVEX ENVELOPES

Given a one-dimensional polynomial (2.1), its convex envelope may be defined as

$$f_c(t) = \min_{\mu} \int_R f(\lambda) \ d\mu(\lambda)$$
(3.1)

where μ represents the family of all probability measures with mean t. In this approach, every probability measure represents a convex combination of points on the real line. Therefore, the measure

$$\bar{\mu} = \lambda_1 \delta_{t_1} + \lambda_2 \delta_{t_2} \tag{3.2}$$

which solves (3.1), represents the convex combination which satisfies

$$\lambda_1 (t_1, f(t_1)) + \lambda_2 (t_2, f(t_2)) = (t, f_c(t)) .$$

From this point of view, it is clear that optimal measure $\bar{\mu}$ has a very precise geometric meaning. Here we have assumed that $\bar{\mu}$ is supported in two points at the most, because of Caratheodory's theorem in convex analysis.

Since f is a polynomial function in the form (2.1), every integral in (3.1) can be written as

$$\sum_{k=0}^{2n} c_k \, m_k$$

where values m_0, \ldots, m_{2n} are the algebraic moments of measure μ . So we can express the convex envelope of f using the next semidefinite program

$$\begin{cases} f_c(t) = c_0 + c_1 t + \min_{m_k} \sum_{k=2}^{2n} c_k m_k & s.t. \\ 1 & t & m_2 & \cdots & m_n \\ t & m_2 & m_3 & \cdots & m_{n+1} \\ m_2 & m_3 & & \cdots & m_{n+2} \\ & & & & & \\ m_n & m_{n+1} & m_{n+2} & \cdots & m_{2n} \end{cases} \succeq 0$$

$$(3.3)$$

where we have used the classical representation of one-dimensional algebraic moments: The convex cone of positive definite Hankel matrices $H = (m_{k+l})_{k,l=0}^{n}$ is the interior of the convex cone of algebraic moments (m_0, \ldots, m_{2n}) of positive measures supported on the real line. For more details we refer the reader to [4].

By using an elementary algebraic procedure, we can obtain the optimal measure $\bar{\mu}$ for problem (3.1) from the optimal values $\bar{m}_2, \ldots, \bar{m}_{2n}$ of the semidefinite program (3.3). Indeed, if $\bar{m}_2 = t^2$, take

$$\lambda_1 = 1, \ \lambda_2 = 0, \ t_1 = t_2 = t$$

4

so the optimal measure $\bar{\mu}$ is equal to the Dirac measure

$$\bar{\mu} = \delta_t.$$

Otherwise, take t_1 and t_2 as the roots of the polynomial

$$P(x) = \begin{vmatrix} 1 & t & \bar{m}_2 \\ t & \bar{m}_2 & \bar{m}_3 \\ 1 & x & x^2 \end{vmatrix}$$

and denote by λ_1, λ_2 the quantities

$$\lambda_1 = \frac{t_2 - t}{t_2 - t_1}$$
 $\lambda_2 = \frac{t - t_1}{t_2 - t_1}$

where $t_1 < t < t_2$. Using these values in the expression (3.2), we obtain the optimal measure $\bar{\mu}$. It is remarkable that only three moments are needed for recovering the optimal measure $\bar{\mu}$. Finally, we conclude that Problem (3.1) and Problem (3.3) are equivalent. For additional details see [6]

When f is a two-dimensional separable polynomial with the form (1.4), its convex envelope is defined as

$$f_c(s,t) = \min_{\mu} \int_{R^2} f(\sigma,\gamma) \, d\mu(\sigma,\gamma) \tag{3.4}$$

where μ represents the family of all probability measures supported in the plane satisfying

$$(s,t) = \int_{R^2} \left(\sigma,\gamma\right) d\mu\left(\sigma,\gamma\right).$$

Note that it is analogous to the definition of convex envelopes for one-dimensional functions.

However, in order to estimate the convex envelope of the separable polynomial f, we must use another well known result of convex analysis: the convex envelope of a separable function is the sum of the convex envelopes of its components. See [1]. From this result and the explanation on convex envelopes of one-dimensional polynomials given above, one observes that the convex envelope of f is given by the semidefinite program

$$f_{c}(s,t) = a_{0} + b_{0} + a_{1}s + b_{1}t + \min_{m_{i},p_{j}} \sum_{i=2}^{2n} a_{i}m_{i} + \sum_{j=2}^{2r} b_{j}p_{j} \quad s.t$$

$$\begin{pmatrix} 1 & s & m_{2} & \cdots & m_{n} \\ s & m_{2} & m_{3} & \cdots & m_{n+1} \\ m_{2} & m_{3} & & \cdots & m_{n+2} \\ & & & \ddots & & \\ m_{n} & m_{n+1} & m_{n+2} & \cdots & m_{2n} \end{pmatrix} \succeq 0$$

$$\begin{pmatrix} 1 & t & p_{2} & \cdots & p_{r} \\ t & p_{2} & p_{3} & \cdots & p_{r+1} \\ p_{2} & p_{3} & \cdots & p_{r+2} \\ & & & \ddots & \\ p_{r} & p_{r+1} & p_{r+2} & \cdots & p_{2r} \end{pmatrix} \succeq 0.$$

$$(3.5)$$

The optimal values $\bar{m}_2, \ldots, \bar{m}_{2n}, \bar{p}_2, \ldots, \bar{p}_{2r}$ for problem (3.5) allow us to determine the optimal probability measure $\bar{\mu}$ which satisfies (3.4).

From a practical point of view, $\bar{\mu}$ is the direct product of two independent one-dimensional distributions $\bar{\mu}_X$ and $\bar{\mu}_Y$, so we have

$$\bar{\mu} = \bar{\mu}_X \times \bar{\mu}_Y$$

where $\bar{\mu}_X$ represents the convex envelope of the first polynomial

$$\sum_{i=0}^{2n} a_i s^i$$

in (1.4) and respectively, $\bar{\mu}_Y$ represents the convex envelope of the second polynomial

$$\sum_{j=0}^{2r} b_j t^j$$

in (1.4). Thus, marginal distributions $\bar{\mu}_X$ and $\bar{\mu}_Y$ are obtained from values s, \bar{m}_2, \bar{m}_3 and t, \bar{p}_2, \bar{p}_3 respectively, in the same way that we did for the onedimensional case. In other words, there is no essential difference between the one-dimensional polynomial case (2.1) and the two-dimensional separable polynomial case (1.4). Finally, it is very important to note that the optimal measure $\bar{\mu} = \bar{\mu}_X \times \bar{\mu}_Y$ determines the convex combination which defines the convex envelope of the separable polynomial f at the point (s, t).

4 PROBLEM ANALYSIS

Our concern here is the analysis of non-convex variational problems like

$$\min_{u} I(u) = \int_{\Omega} f\left(\vec{\nabla}u\left(x,y\right)\right) \, dx \, dy \qquad s.t. \qquad u|_{\partial\Omega} = g \,. \tag{4.1}$$

We will study the case where f is a two-dimensional separable polynomial in the general form (1.4). We first notice that direct discretization of functional Iin (4.1) provides a non-convex optimization problem which is not particularly adequate to be solved by standard numerical optimization software. The reason behind that is the lack of convexity on f, which can cause the search algorithm to stop at some wrong local minima instead of providing the right global minima for the functional I. In addition, we must consider the possibility that Ilacks minimizers on the space of admissible functions. Normally, admissible functions belong to the Sobolev space $W_0^{1,p}(\Omega) + g$ where index p depends on the integrand function f in (4.1).

To overcome this difficulty we study the generalized problem

$$\min_{\nu} I(\nu) = \int_{\Omega} \left(\int_{R^2} f(s,t) \, d\mu_{x,y}(s,t) \right) \, dx \, dy with \quad \vec{\nabla} u(x,y) = \int_{R^2} (s,t) \, d\mu_{x,y}(s,t) and the boundary condition \quad u|_{\partial\Omega} = g$$
 (4.2)

6

whose solution in Young measures provides information about the minimizers of the original functional I. By using the separable polynomial structure of f, we can transform the generalized functional in (4.2) into the functional

$$J(m,p) = \int_{\Omega} \left(\sum_{i=0}^{2n} a_i m_i(x,y) + \sum_{j=0}^{2r} b_j p_j(x,y) \right) \, dx \, dy$$

where $m = (m_i(x, y))_{i=0}^{2n}$ and $p = (p_j(x, y))_{j=0}^{2r}$ represent the algebraic moments of the parametrized measures $\mu_{x,y}$ in the Young measure ν . In this way, we must solve the optimization problem

$$\min_{m,p} J(m,p) = \int_{\Omega} \left(\sum_{i=0}^{2n} a_i m_i(x,y) + \sum_{j=0}^{2r} b_j p_j(x,y) \right) dx dy$$

$$with \quad \vec{\nabla} u(x,y) = (m_1(x,y), p_1(x,y))$$

$$and \quad the \quad boundary \quad condition \quad u|_{\partial\Omega} = g$$

$$(4.3)$$

where the new sets of variables m and p must be characterized as the algebraic moments of one-dimensional probability measure. In order to do so, we impose the linear matrix inequalities

$$\begin{pmatrix} 1 & m_{1}(x,y) & \cdots & m_{n}(x,y) \\ m_{1}(x,y) & m_{2}(x,y) & \cdots & m_{n+1}(x,y) \\ m_{2}(x,y) & m_{3}(x,y) & \cdots & m_{n+2}(x,y) \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & & \\ &$$

for every point $(x, y) \in \Omega$. After an appropriate discretization, this problem can be posed as a single semidefinite program. See [7] and [8] for an introduction to semidefinite programming.

5 DISCRETE AND FINITE MODEL

Here we will transform the optimization problem (4.3) subject to the constraints (4.4), into an equivalent discrete mathematical program. First, we take a finite set of N points on the domain Ω indexed by k, that is

$$(x_k, y_k) \in \Omega \quad for \quad k = 1, \dots, N.$$
 (5.1)

Next, for every discrete point (x_k, y_k) we take the algebraic moments

$$(m_i(x_k, y_k))_{i=1}^{2n} \qquad (p_j(x_k, y_k))_{j=1}^{2r} \tag{5.2}$$

of the respective parametrized measure μ_{x_k,y_k} . Using the $2N \times (n+r)$ variables listed in (5.2), we can express the functional J in the discrete form:

$$J_d(m,p) = \sum_{k=0}^N \left(\sum_{i=0}^{2n} a_i m_i(x_k, y_k) + \sum_{j=0}^{2r} b_j p_j(x_k, y_k) \right) \Delta x_k \, \Delta y_k \,.$$
(5.3)

The constraints (4.4) form a set of linear matrix inequalities for every point in Ω , hence they should keep the same for every point (x_k, y_k) in the mesh (5.1). So we have a set of 2N linear matrix inequalities expressed as

$$[m_{i+j}(x_k, y_k)]_{i,j=0}^n \succeq 0 \qquad [p_{i+j}(x_k, y_k)]_{i,j=0}^r \succeq 0$$
(5.4)

where $m_0 = 1$ and $p_0 = 1$ for every $k = 1, \ldots, N$.

In order to impose the boundary conditions

$$|u|_{\partial\Omega} = g$$

and the constraints

$$\vec{\nabla}u(x,y) = (m_1(x,y), p_1(x,y))$$
 (5.5)

in (4.3), we use the following fact: Given any Jordan curve C inside the domain Ω , the restriction (5.5) implies

$$\int_{\mathcal{C}} (m_1 \, dx + p_1 \, dy) = u \, (x_f, y_f) - u \, (x_0, y_0)$$

where (x_0, y_0) and (x_f, y_f) are two endpoints of curve C.

We shall select a finite collection of M curves C_l with $l = 1, \ldots, M$ which, in some sense, *sweep* the whole domain Ω . It will suffice that each point (x_k, y_k) on the mesh belongs to at least one curve C_l . In order to impose the boundary conditions in (4.3), every curve C_l must link two boundary points of Ω . So we obtain a new set of M constraints in the form

$$\int_{\mathcal{C}_l} (m_1 \, dx + p_1 \, dy) = g\left(x_f^l, y_f^l\right) - g\left(x_0^l, y_0^l\right) \tag{5.6}$$

which can be incorporated as linear equalities in the discrete model.

We can see that optimization problem (4.3) can be transformed into a single semidefinite program after discretization. Note that objective function J_d in (5.3) is a linear function of the variables in (5.2). Those variables are restricted by the set of 2N linear matrix inequalities given in (5.4) and the set of M linear equations given in (5.6). Thus, we have obtained a very large single semidefinite program.

6 EXAMPLES

To illustrate the method proposed in this work, we will analyze the non-convex variational problem

$$\min_{u} \int_{[-1,1]^2} \left\{ \left(1 - \left(\frac{\partial u}{\partial x}\right)^2 \right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 \right\} \, dx \, dy$$

2D NON CONVEX VARIATIONAL PROBLEMS 9

under the following boundary conditions

 $a) \quad g\left(x,y\right)=0 \qquad b) \quad g\left(x,y\right)=1-|x| \qquad c) \quad g\left(x,y\right)=x+1\,.$

The corresponding generalized problem has the form

$$\min_{\nu} \int_{[-1,1]^2} \left\{ \int_{R^2} \left(\left(1 - \sigma^2\right)^2 + \gamma^2 \right) d\mu_{x,y} \left(\sigma,\gamma\right) \right\} dx \, dy$$

under the constraint $\left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = \int_{R^2} \left(\sigma,\gamma\right) d\mu_{x,y} \left(\sigma,\gamma\right)$
and the boundary conditions $u|_{\partial\Omega} = g\left(x\right)$ with $\Omega = \left[-1,1\right]^2$
(6.1)

which transforms into the optimization problem

$$\min_{m,p} \int_{[-1,1]^2} \left\{ 1 - 2m_2(x,y) + m_4(x,y) + p_2(x,y) \right\} dx dy$$

$$under \quad the \quad constraints$$

$$\left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \right) = \left(m_1(x,y), p_1(x,y) \right), \left[m_{i+j}(x,y) \right]_{i,j=0}^2 \succeq 0, \left[p_{i+j}(x,y) \right]_{i,j=0}^1 \succeq 0$$

$$and \quad the \quad boundary \quad conditions \ u |_{\partial\Omega} = g(x) \quad with \quad \Omega = \left[-1, 1 \right]^2.$$

$$(6.2)$$

In order to perform the discretization of this problem, we use the straight lines with slope 1 crossing the square $[-1,1]^2$. With them we can impose the boundary conditions in the finite model. After solving the discrete model, not to be exposed here, we obtain the optimal moments for (6.2), and the Young measure solution for the generalized problem (6.1).

For the three cases studied, we obtain the following optimal parametrized measures $1.5 \times 1.5 \times 1.5 \times 1.5 \times 1.5^{2}$

a)
$$\bar{\mu}_{x,y} = \frac{1}{2}\delta_{(-1,0)} + \frac{1}{2}\delta_{(1,0)} \quad \forall x, y \in [-1,1]$$

b) $\bar{\mu}_{x,y} = \begin{cases} \delta_{(1,0)} & if & -1 \le x \le 0\\ \delta_{(-1,0)} & if & 0 \le x \le 1 \end{cases}$
c) $\bar{\mu}_{x,y} = \delta_{(1,0)} \quad \forall x, y \in [-1,1]^2$

hence we infer that Problem a) does not have minimizers, Problem b) has the minimizer $\bar{u}(x, y) = 1 - |x|$ and Problem c) has the minimizer $\bar{u}(x, y) = x + 1$. Although Problem a) lacks minimizers, the optimal Young measure obtained gives enough information about the limit behavior of the minimizing sequences. Indeed, if u_n is an arbitrary minimizing sequence for Problem a) we have

$$\vec{\nabla}u_n(x,y) \to (\pm 1,0)$$

in measure, where gradient (1,0) is preferred with 50% of possibilities and gradient (-1,0) is preferred with the remaining 50% of possibilities in the minimizing process, for every point $(x, y) \in [-1, 1]^2$.

7 CONCLUDING REMARKS

The major contribution of this work is that it settles the way for studying nonconvex variational problems of the form (4.1). Indeed, the direct method of the calculus of variations does not provide any answer for them if the integrand f is not convex. See [1]. In addition, in this work we propose a method for solving generalized problems like (4.2) when the integrand f has the separable form described in (1.4). In fact to the best knowledge of the author, do not exist other proposals to analyze this kind of generalized problems in two dimensions.

An important remark about this work is that we have reduced the original non convex variational problem (4.1) to the optimization problem (4.3). In addition, the reader should note that Problem (4.3) is a convex problem because the objective function is linear and the feasible set convex. That is a remarkable qualitative difference since numerical implementation of problem (4.1) may provide wrong answers when the search algorithm stops in local minima, whereas a good implementation of Problem (4.3) should yield the global minima of the problem.

Since we can pose Problem (4.3) as a single large scale semidefinite program, we can use existing software for solving non convex variational problems in the form (4.1) whenever the integrand f has the separable form (1.4). This situation prompts further research on large scale semidefinite programming specially suited for generalized problems in the form (4.3).

We should also stress that, although the original non convex variational problem (4.1) may not have a solution, its new formulation (4.3) always has one. In general, this solution is unique and provides information about the existence of minimizers for problem (4.1). If Problem (4.1) has a unique minimizer $\overline{u}(x, y)$, then Problem (4.3) provides the moments of the Dirac measures

$$\left\{ \delta_{\overrightarrow{\nabla}\overline{u}(x,y)}: (x,y)\in \Omega \right\} \, .$$

Moreover, if Problem (4.3) provides the moments of a family of Dirac measures like

$$\left\{\delta_{\overrightarrow{F}(x,y)}:(x,y)\in\Omega\right\}$$

then problem (4.1) has a unique minimizer $\overline{u}(x, y)$ which satisfies $\overrightarrow{\nabla} \overline{u}(x, y) = \overrightarrow{F}(x, y)$.

One fundamental question we feel important to raise is whether the discrete model (5.3) is an adequate representation of the convex problem (4.3). From an analytical point of view, we need to find a particular qualitative feature on the solution of Problem (4.3), that is the Dirac mass condition on all optimal measures. So we can hope that even rough numerical models can provide us with the right qualitative answer about the existence of minimizers for the non convex variational problem (4.1). This has actually been observed in many numerical experiments.

It is also extremely remarkable that we can get a numerical answer to an analytical question. Indeed, we are clarifying the existence of minimizers of one particular variational problem from a numerical procedure. This point is crucial because no analytical method exists which allows to solve this question when we are coping with general non convex variational problems. On the other hand, we really need a fine numerical model because the solution of problem (4.3) contains the information about the oscillatory behavior of minimizing sequences of the non convex problem (4.1). In those cases where Problem (4.1) lacks solution, minimizing sequences show similar oscillatory behavior linked with important features in the physical realm. For example, in elasticity models of solid mechanics such behavior represents the distribution of several solid phases inside some particular body. This information provides the microstructure of the crystalline net of the material.

To discover such phenomena we need a good representation of the optimal Young measure of the generalized problem (4.2), which in turns, is embedded into the solution of the convex formulation in moments (4.3). In conclusion, we feel that it is important to devise a good numerical treatment of problem (4.3) by solving a semidefinite model like (5.3).

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