# ЧИСЛЕННЫЕ МЕТОДЫ ОПТИМИЗАЦИИ

## Оптимизация.
## Построение минимального охватывающего эллипсоида

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# Охватывающий эллипсоид

**Введение. Постановка задачи.**

Пусть в пространстве $R^n$ даны ***m*** точек

$$a_1, a_2, ..., a_m \in R^n$$

Требуется построить эллипсоид минимального объема, содержащий внутри себя все эти точки.

Обозначим через $A$ матрицу размерности $n \times m$ , столбцы которой являются векторами $a_1, a_2, ..., a_m \in R^n$ .

$$A : \left[ a_1 \,|\, a_2 \,|\, ... \,|\, a_m \right].$$

Определение эллипсоида:

Эллипсоид с центром в точке $c$ определяется как

$$E_{Q,c} := \left\{ x \in R^n \,|\, (x-c)^T Q (x-c) \le 1 \right\};$$

# Охватывающий эллипсоид

here $c$ is the center of the ellipsoid and $Q$ determines its general shape. The volume of $\mathbf{E}_{Q,c}$ is given by the formula

$$\frac{\pi^{n/2}}{\Gamma(n/2+1)}\frac{1}{\sqrt{\det Q}};$$

see Grötschel et al. (1998) for example. Here, $\Gamma(\cdot)$ is the standard gamma function of calculus.

Under Assumption 1, a natural formulation of the minimum-volume covering ellipsoid problem is

$$\begin{aligned}(\mathrm{MVCE}^1)\quad & \min_{Q,\,c} \ \det Q^{-1/2} \\ & \text{s.t.}\ (a_i-c)^T Q(a_i-c)\leqslant 1,\quad i=1,\ldots,m, \\ & \quad\ \ Q\succ 0.\end{aligned}$$

# Охватывающий эллипсоид

As written, MVCE[1] is not a convex program. By the change of variables

$$M = Q^{1/2} \quad \text{and} \quad z = Q^{1/2}c,$$

we restate the problem as

$$\begin{aligned}
(\text{MVCE}^2) \quad & \min_{M,z} \quad \psi(M, z) := -\ln\det M \\
& \text{s.t.} \quad (Ma_i - z)^T(Ma_i - z) \leqslant 1, \\
& \qquad\qquad i = 1, \ldots, m, \qquad (1) \\
& \qquad\quad M \succ 0,
\end{aligned}$$

which is now a convex program. If $(\bar{M}, \bar{z})$ is a solution of MVCE[2], we recover the solution of MVCE[1] by setting $(\bar{Q}, \bar{c}) = (\bar{M}^2, \bar{M}^{-1}\bar{z})$.

# Охватывающий эллипсоид

MVCE[2] can be rewritten as a log-determinant maximization problem subject to linear equations and second-order cone constraints:

$$
\begin{aligned}
(\mathrm{MVCE}^3) \quad & \min_{M, z, y, w} \quad -\ln\det M \\
& \text{s.t.} \quad Ma_i - z - y_i = 0, \quad i = 1, \ldots, m, \\
& \qquad w_i = 1, \quad i = 1, \ldots, m, \\
& \qquad (y_i, w_i) \in C_2^n, \quad i = 1, \ldots, m, \\
& \qquad M \succ 0,
\end{aligned}
$$

where $C_2^n$ denotes the second-order cone $\{(y, w) \in \mathbb{R}^{n+1} \mid \|y\| \leqslant w\}$. The format of MVCE[3] is suitable for a solution using a slightly modified version of the software SDPT3 (see Toh et al. 1999, Tütüncü et al. 2003), where the software is modified to handle the parameterized family of barrier functions

# Dual Reduced Newton Algorithm

In this section, we describe and derive our basic algorithm for the minimum-volume covering ellipsoid problem; we call this algorithm the "***dual reduced Newton***" algorithm for reasons that will soon be clear.

**Newton Step**

By adding a logarithmic barrier function to the problem formulation $\text{MVCE}^2$, we obtain the formulation

$$(\text{MVCE}^2_\theta) \quad \min_{M,z,t} \; -\ln\det M - \theta \sum_{i=1}^{m} \ln t_i$$

$$\text{s.t.} \quad (Ma_i - z)^T(Ma_i - z) + t_i = 1, \quad i = 1, \ldots, m,$$

$$M \succ 0,$$

$$t > 0.$$

# Dual Reduced Newton Algorithm

The parameterized solutions to this problem as $\theta$ varies in the interval $(0, \infty)$ define the central trajectory of the problem MVCE$^2$. Identifying dual multipliers $u_i$, $i = 1, \dots, m$, with the equality constraints in MVCE$_\theta^2$, the optimality conditions for (MVCE$_\theta^2$) can be written as

$$\sum_{i=1}^{m} u_i\left[(Ma_i - z)a_i^T + a_i(Ma_i - z)^T\right] - M^{-1} = 0, \quad (4)$$

$$\sum_{i=1}^{m} u_i(z - Ma_i) = 0, \quad (5)$$

$$(Ma_i - z)^T(Ma_i - z) + t_i = 1, \quad i = 1, \dots, m, \quad (6)$$

$$Ut = \theta e, \quad (7)$$

$$u, t \geqslant 0, \quad (8)$$

$$M \succ 0. \quad (9)$$

# Dual Reduced Newton Algorithm

We could attempt to solve (4)–(9) for $(M, z, t, u)$ directly by using Newton's method, which would necessitate forming and factorizing an

$$\left(\frac{n(n+3)}{2} + 2m\right) \times \left(\frac{n(n+3)}{2} + 2m\right)$$

matrix. However, as we now show, the variables $M$ and $z$ can be directly eliminated, and further analysis will result in only having to form and factorize a single $m \times m$ matrix.

# Dual Reduced Newton Algorithm

To see how this is done, note that we can solve (5) for $z$ and obtain

$$z = \frac{MAu}{e^T u}. \qquad (10)$$

Substituting (10) into (4), we arrive at the following equation for the matrix $M$:

$$\left(AUA^T - \frac{Auu^TA^T}{e^Tu}\right)M + M\left(AUA^T - \frac{Auu^TA^T}{e^Tu}\right) = M^{-1}. \qquad (11)$$

# Dual Reduced Newton Algorithm

The following proposition, whose proof is in the appendix, demonstrates an important property of the matrix arising in (11):

PROPOSITION 2. *Under Assumption* 1, *if* $u > 0$, *then* $(AUA^T - Auu^T A^T / e^T u) \succ 0$.

The following remark presents a closed-form solution for the equation system (11); see Lemma 4 of Zhang and Gao (2003):

REMARK 3. For a given $S \succ 0$, $X := S^{-1/2}$ is the unique positive definite solution of the equation system

$$\frac{1}{2}(X^T S + SX) = X^{-1}.$$

# Dual Reduced Newton Algorithm

Utilizing Proposition 2 and Remark 3, the unique solution of (11) is easily derived:

$$M := M(u) := \left[2\left(AUA^T - \frac{Auu^TA^T}{e^Tu}\right)\right]^{-1/2}, \tag{12}$$

and substituting (12) into (10), we conclude:

PROPOSITION 4. *Under Assumption* 1, *if* $u > 0$, *then the unique solution of* (4), (5), *and* (9) *in* $M$, $z$ *is given by*

$$M := M(u) := \left[2\left(AUA^T - \frac{Auu^TA^T}{e^Tu}\right)\right]^{-1/2} \tag{13}$$

*and*

$$z := z(u) := \frac{\left[2\left(AUA^T - \frac{Auu^TA^T}{e^Tu}\right)\right]^{-1/2} Au}{e^Tu}. \tag{14}$$

# Dual Reduced Newton Algorithm

Substituting (13) and (14) into the optimality conditions (4)–(9), we can eliminate the variables $M$ and $z$ explicitly from the optimality conditions, obtaining the following reduced optimality conditions involving only the variables $(u, t)$:

$$h(u) + t = e,$$

$$Ut = \theta e, \tag{15}$$

$$u, t \geqslant 0,$$

# Dual Reduced Newton Algorithm

where $h_i(u)$ is the following nonlinear function of $u$:

$$h_i(u) := (M(u)a_i - z(u))^T(M(u)a_i - z(u))$$
$$= \left(a_i - \frac{Au}{e^Tu}\right)^T \left[2\left(AUA^T - \frac{Auu^TA^T}{e^Tu}\right)\right]^{-1}$$
$$\cdot \left(a_i - \frac{Au}{e^Tu}\right), \tag{16}$$

for $i = 1, \ldots, m$, where $M(u)$ and $z(u)$ are specified by (13) and (14).

# Dual Reduced Newton Algorithm

For a given value of the barrier parameter $\theta$, we will attempt to approximately solve (15) using Newton's method. Let $\nabla_u h(u)$ denote the Jacobian matrix of $h(u)$. The Newton direction $(\Delta u, \Delta t)$ for (15) at the point $(u, t)$ is then the solution of the following system of linear equations in $(\Delta u, \Delta t)$:

$$\begin{aligned} \nabla_u h(u)\Delta u + \Delta t &= r_1 := e - t - h(u), \\ T\Delta u + U\Delta t &= r_2 := \theta e - Ut. \end{aligned} \tag{17}$$

This system will have the unique solution

$$\begin{aligned} \Delta u &= (\nabla_u h(u) - U^{-1}T)^{-1}(r_1 - U^{-1}r_2), \\ \Delta t &= U^{-1}r_2 - U^{-1}T\Delta u, \end{aligned} \tag{18}$$

provided we can show that the matrix $(\nabla_u h(u) - U^{-1}T)$ is nonsingular.

# Dual Reduced Newton Algorithm

To implement the above methodology, we need to explicitly compute $\nabla_u h(u)$, and we also need to show that $(\nabla_u h(u) - U^{-1}T)$ is nonsingular. Towards this end, we define the following matrix function:

$$\Sigma(u) := \left(A - \frac{Aue^T}{e^Tu}\right)^T M^2(u)\left(A - \frac{Aue^T}{e^Tu}\right) \qquad (19)$$

as a function of the dual variables $u$. Let $A \circ B$ denote the Hadamard product of the matrices $A$, $B$, namely $(A \circ B)_{ij} := A_{ij}B_{ij}$ for $i, j = 1, \ldots, m$. The following result conveys an explicit formula for $\nabla_u h(u)$ and also demonstrates other useful properties.

# Dual Reduced Newton Algorithm

PROPOSITION 5. *Under Assumption* 1,

(i) $\nabla_u h(u) = -2(\Sigma(u)/e^T u + \Sigma(u) \circ \Sigma(u))$,

(ii) $\nabla_u h(u) \preceq 0$, *and*

(iii) $h(u) = \text{diag}(\Sigma(u))$.

The proof of this proposition is presented in the appendix. From part (ii) of Proposition 5 and the fact that $U^{-1}T \succ 0$ whenever $u, t > 0$, we then have

COROLLARY 6. *Under Assumption* 1, *if* $u > 0$ *and* $t > 0$, *then* $(\nabla_u h(u) - U^{-1}T) \prec 0$, *and so is nonsingular.*

Now let us put all of this together. To compute the Newton direction $(\Delta u, \Delta t)$ for the reduced optimality conditions (15) at a given point $(u, t)$, we compute according to the following procedure:

# Dual Reduced Newton Algorithm

**Procedure DRN-DIRECTION**$(u, t, \theta)$: Given $(u, t)$ satisfying $u, t > 0$ and given $\theta \geqslant 0$,

*Step* 1. Form and factorize the matrix

$$M^{-2}(u) = \left[ 2\left( AUA^T - \frac{Auu^TA^T}{e^Tu} \right) \right].$$

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$$\Sigma(u) = \left( A - \frac{Aue^T}{e^Tu} \right)^T M^2(u) \left( A - \frac{Aue^T}{e^Tu} \right).$$

*Step* 3. Form

$$\nabla_u h(u) = -2\left( \frac{\Sigma(u)}{e^Tu} + \Sigma(u) \circ \Sigma(u) \right)$$

and factorize $(\nabla_u h(u) - U^{-1}T)$.

*Step* 4. Solve (18) for $(\Delta u, \Delta t)$.

# Dual Reduced Newton Algorithm

Note from (10) that $c = M^{-1}z = Au/e^Tu$, which states that the center of the optimal ellipsoid is a convex weighting of the points $a_1, \ldots, a_m$, with the weights being the normalized dual variables $u_i/e^Tu$, $i = 1, \ldots, m$. It is also easy to see that when $\theta = 0$, the complementarity condition $u_i t_i = \theta = 0$ has a nice geometric interpretation: A point has positive weight $u_i$ only if it lies on the boundary of the optimal ellipsoid. These observations are well-known. Another property is that if one considers the points $a_1, \ldots, a_m$ to be a random sample of $m$ i.i.d. random vectors, then with $u := e/m$ we have that

$$M^{-2}(u) = \frac{2}{m}\left(A - \frac{Aee^T}{m}\right)\left(A - \frac{Aee^T}{m}\right)^T$$

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Based on the Newton step procedure outlined ealier, we construct the following basic interior-point algorithm for solving the MVCE [2] *'formulation of the minimum volume'* covering ellipsoid problem.

We name this algorithm “DRN” for dual reduced Newton algorithm.

***Newton Step***

By adding a logarithmic barrier function to the problem formulation $\mathrm{MVCE}^2$, we obtain the formulation

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and factorize $(\nabla_u h(u) - U^{-1}T)$.

*Step* 4. Solve (18) for $(\Delta u, \Delta t)$.

# Dual Reduced Newton Algorithm

The computational burden of each of the four steps in Procedure DRN-DIRECTION is dominated by the need to factorize the matrices in Steps (1) and (2) above. The matrix $(AUA^T - Auu^T A^T / e^T u)$ in Step (1) is $n \times n$; it requires $mn^2$ operations to form and $n^3$ steps to factorize, while the matrix $(\nabla_u h(u) - U^{-1} T)$ in Step (4) is $m \times m$; it requires $nm^2$ steps to form and $m^3$ steps to factorize.

# Dual Reduced Newton Algorithm

Note from (10) that $c = M^{-1}z = Au/e^T u$, which states that the center of the optimal ellipsoid is a convex weighting of the points $a_1, \ldots, a_m$, with the weights being the normalized dual variables $u_i/e^T u$, $i = 1, \ldots, m$. It is also easy to see that when $\theta = 0$, the complementarity condition $u_i t_i = \theta = 0$ has a nice geometric interpretation: A point has positive weight $u_i$ only if it lies on the boundary of the optimal ellipsoid. These observations are well-known. Another property is that if one considers the points $a_1, \ldots, a_m$ to be a random sample of $m$ i.i.d. random vectors, then with $u := e/m$ we have that

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# Dual Reduced Newton Algorithm

**Algorithm DRN**

Based on the Newton step procedure outlined earlier, we construct the following basic interior-point algorithm for solving the $MVCE_\theta^2$ *' formulation of the minimum volume* covering ellipsoid problem. We name this algorithm "DRN" for dual reduced Newton algorithm.

**Algorithm DRN**

*Step* 0. Initialization. Set $r \leftarrow 0.99$. Choose initial values of $(u^0, t^0)$ satisfying $u^0, t^0 > 0$. Set $(u, t) \leftarrow (u^0, t^0)$.

*Step* 1. Check Stopping Criteria. $\text{OBJ} := -\ln\det[M(u)]$. If $\|e - h(u) - t\| \leqslant \epsilon_1$ and $(u^T t)/\text{OBJ} \leqslant \epsilon_2$, STOP. Return $u$, $Q := [M(u)]^2$, $c := [M(u)]^{-1} z(u)$ and OBJ.

*Step* 2. Compute Direction. Set $\theta \leftarrow (u^T t)/10m$. Compute $(\Delta u, \Delta t)$ using Procedure DRN-DIRECTION$(u, t, \theta)$.

*Step* 3. Step-Size Computation and Step. Compute $\bar{\beta} \leftarrow \max\{\beta \mid (u, t) + \beta(\Delta u, \Delta t) \geqslant 0\}$ and $\tilde{\beta} \leftarrow \min\{r\bar{\beta}, 1\}$. Set $(u, t) \leftarrow (u, t) + \tilde{\beta}(\Delta u, \Delta t)$. Go to *Step* 1.

# Литература

1. Computation of Minimum-Volume Covering Ellipsoids. Peng Sun, Robert M. Freund. OPERATIONS RESEARCH Vol. 52, No. 5, September–October 2004, pp. 690–706