Matrix Optimization: Searching between the First and Second Order Methods

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We consider the “standard” matrix optimization problem (MOP) and its dual:

\[
(P) \quad \begin{aligned}
\min & \quad \langle c, x \rangle + f(x) \\
\text{s.t.} & \quad Ax = b
\end{aligned}
\]

and

\[
(D) \quad \begin{aligned}
\max & \quad \langle b, y \rangle - f^*(z) \\
\text{s.t.} & \quad A^*y - c = z
\end{aligned}
\]

where \( \mathcal{X} \) is the Cartesian product of several finite dimensional real matrix spaces, symmetric or non-symmetric,

\( A^* \) is the adjoint of the linear operator \( A : \mathcal{X} \to \mathbb{R}^m, \ c \in \mathcal{X}, \ b \in \mathbb{R}^m, \)

\( f : \mathcal{X} \to (-\infty, \infty] \) is a closed proper convex function with its Fenchel conjugate \( f^* \).
The Fenchel conjugate of $f$ is defined by

$$f^*(z) := \sup_{x \in X} \{ \langle z, x \rangle - f(x) \}.$$ 

In standard linear programming, $f(x) = \delta_{\mathbb{R}^n_+}(x)$, the indicator function over $\mathbb{R}^n_+$ and $f^*(x) = \delta_{(-\mathbb{R}^n_+)}(x)$.

In semidefinite programming (SDP), $f(x) = \delta_{S^n_+}$, the indicator function over $S^n_+$ and $f^*(x) = \delta_{(-S^n_+)}(x)$. 
We need conditions on $f$. Specifically, we require

- The Moreau-Yosida regularization of $f$

$$
\psi_f(x) := \min_{z \in X} \left\{ f(z) + \frac{1}{2} \|z - x\|^2 \right\}
$$

has a closed form solution, denoted by $P_f(x)$.

- We can easily compute the directional derivative of

$$
\nabla \psi_f(x) = x - P_f(x).
$$

- The function $\nabla \psi_f$ is (strongly) semismooth.
Let us first look at one simple example with nonsymmetric matrices:

$$\min_{y \in \mathbb{R}^k} \left\| A_0 - \sum_{i=1}^{k} y_i A_i \right\|_2,$$

where $A_i$ are $m$ by $n$ matrices, $\| \cdot \|_2$ is the spectral (operator) norm of matrices (the largest singular value).

Use $\| \cdot \|_*$ to denote the nuclear norm (the sum of all singular values) and $B^1_*$ to denote the unit nuclear norm ball.
We can equivalently write (1) in the form of (D):

\[
\begin{align*}
\max & \quad \langle 0, y \rangle - \| Z \|_2 \\
\text{s.t.} & \quad Ay - A_0 = Z
\end{align*}
\]

and the corresponding form of (P):

\[
\begin{align*}
\min & \quad \langle A_0, X \rangle + \delta_{B^1}(X) \\
\text{s.t.} & \quad A^* X = 0.
\end{align*}
\]
Note that we can write \( t \geq \| X \|_2 \) (here, \( X \in \mathbb{R}^{m \times n} \)) equivalently as

\[
S^{m+n} \ni \begin{bmatrix} tI_m & X \\ X^T & tI_n \end{bmatrix} \succeq 0.
\]

Thus, (1) is equivalent to an SDP problem:

\[
\begin{aligned}
\min & \quad t \\
\text{s.t.} & \quad X + \sum_{i=1}^{k} y_i A_i = A_0, \\
& \quad \begin{bmatrix} tI_m & X \\ X^T & tI_n \end{bmatrix} \succeq 0.
\end{aligned}
\]
Actually, most of the MOPs we are considering are "SDP representable".

However, there are two issues to use the SDP representation (2):

- Can we solve these SDPs when \( m \) or \( n \) is not small?
- Is it necessary to increase the matrix dimension from \( mn \) to \( \frac{1}{2}(m+n)^2 \)?

  — No one is likely to do so if \( m = 1 \) or \( n = 1 \) because in this case we can solve a second order cone programming (SOC) problem instead of an SDP problem?

  — How about \( m \ll n \) or \( n \ll m \)?

  — Shall we do so if \( m = n \)?
Let us consider the widely used optimization model in the finance industry and many others:

\[
\min \| D^{-1/2}(X - G)D^{-1/2}\|_F \\
\text{s.t.} \quad \text{diag}(X) = e, \quad X \succeq 0,
\]

where \( G \) is an estimated matrix which often fails to be positive semi-definite, \( D \) is a symmetric and positive definite matrix (weight matrix), and \( e \) is the vector of all ones.

This problem is known as the nearest correlation matrix (NCM) problem, a terminology coined by Nick Higham in 2002. It is used in many situations: stress testing, VaR computation, asset pricing ...
One may write the NCM as a symmetric cone programming with both SDP cone and SOC cone constraints (assuming $D = I$, the identity matrix for notational convenience):

$$\begin{align*}
\min & \quad t \\
\text{s.t.} & \quad \text{diag}(X) = e, \\
& \quad y + \text{svec}(X) = \text{svec}(G), \\
& \quad X \succeq 0, \quad t \geq \|y\|_2.
\end{align*}$$

This is a perfect formula for employing modern interior point methods (IPMs).
<table>
<thead>
<tr>
<th>n</th>
<th>Time (secs)</th>
<th>Iters</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>1.4</td>
<td>15</td>
</tr>
<tr>
<td>40</td>
<td>3.2</td>
<td>15</td>
</tr>
<tr>
<td>50</td>
<td>6.0</td>
<td>15</td>
</tr>
<tr>
<td>60</td>
<td>13.2</td>
<td>16</td>
</tr>
<tr>
<td>70</td>
<td>24.4</td>
<td>15</td>
</tr>
<tr>
<td>80</td>
<td>44.3</td>
<td>15</td>
</tr>
<tr>
<td>90</td>
<td>102.0</td>
<td>19</td>
</tr>
<tr>
<td>100</td>
<td>142.6</td>
<td>16</td>
</tr>
</tbody>
</table>

Table 1: Numerical results for SDPT3
For $n = 110$, it shows Out of Memory [Dell Laptop: 2.99 GB RAM].

The reason is simple: each step we need to store an $m$ by $m$ matrix at least. Here $m$ is the number of equations

$$m = n + 1 + n(n + 1)/2.$$ 

For $n = 110$, we have $m = 6216$.

One may buy a better Laptop or PC. But even so in each step, the computational cost is

$$O(m^3) = O(n^6).$$

For large $n$, we will just feed wrong problems to IPMs.
In optimization, we always look at the dual when we find a problem difficult to solve. Rewrite the NCM as

\[
\min \quad \frac{1}{2} \|X - G\|_F^2 \\
\text{s.t.} \quad \text{diag}(X) = e, \quad X \succeq 0, \tag{4}
\]

Then the dual of the NCM turns to be an unconstrained problem:

\[
\max \quad -\theta(y) := -\left[ \frac{1}{2} \|\Pi_{S^n_+}(G + \text{Diag}(y))\|^2 - \langle e, y \rangle - \frac{1}{2} \|G\|^2 \right] \\
\text{s.t.} \quad y \in \mathbb{R}^n,
\]
where $\Pi_{S_+^n}(X)$ is the unique optimal solution (projection) to

$$\min \frac{1}{2} \|Y - X\|_F^2$$

s.t. $Y \in S_+^n$. 
The convex function $\theta$ is continuously differentiable with

$$\nabla \theta(y) = \text{diag}(\Pi_{S_n^+}(G + \text{Diag}(y))) - e, \quad y \in \mathbb{R}^n.$$  

Moreover, $\nabla \theta(\cdot)$ is globally Lispchitz continuous with modulus one, i.e.,

$$\|\nabla \theta(y) - \nabla \theta(z)\| \leq \|y - z\| \quad \forall \, y, z \in \mathbb{R}^n.$$

To compute $\theta(y)$ and $\nabla \theta(y)$, one only needs to know how to compute $\Pi_{S_n^+}(X)$. 
Let $X \in \mathcal{S}^n$ have the following spectral decomposition\(^1\)

$$X = P \Lambda P^T,$$

where $\Lambda$ is the diagonal matrix of eigenvalues of $X$ and $P$ is a corresponding orthogonal matrix of orthonormal eigenvectors.

Then

$$X_+ := \Pi_{\mathcal{S}^+_n}(X) = P \Lambda_+ P^T.$$  

\(^1\)Use the divide and conquer algorithm, which is much faster than the shifted QR decomposition based algorithm.
Immediately, one will try the following projected gradient (PG) method:

\[ y^{k+1} := y^k - \nabla \theta(y^k) = y^k - \left[ \text{diag}(\Pi_{S^n}(G + \text{Diag}(y^k))) \right] - e. \]

In 2007, Marc Teboulle suggested to us the accelerated projected gradient (APG) method \((x^0 = z^0 = y^0)\):

\[
\begin{align*}
    z^{k+1} &= z^k - \nabla \theta(y^k); \\
    x^{k+1} &= (1 - 2/(k + 2))x^k + 2/(k + 2)z^k; \\
    y^{k+1} &= [1 - 2/((k + 1) + 2)]x^{k+1} + 2/((k + 1) + 2)z^{k+1}.
\end{align*}
\]
In 2011, He et al considered the augmented Lagrangian alternating direction method (ADM) by writing the NCM as:

$$\min \quad \frac{1}{2} \| X - G \|_F^2 + \frac{1}{2} \| Y - G \|_F^2$$

s.t. $$X - Y = 0,$$

$$\text{diag}(Y) = e,$$

$$X \succeq 0.$$
Testing Case 1): Three first order algorithms are tested for a perturbed true correlation matrix: $G_{true}$ is a 1000 by 1000 true correlation matrix and $E$ is a symmetric random matrix with elements in $[-1, 1]$:

$$E = \text{randn}(1000); E = \text{triu}(E) + \text{triu}(E,1)'$$

and set

$$G := 90\% \times G_{true} + 10\% \times E$$

with its all diagonal being ones. For PG and APG methods, the residue represents the primal feasibility. So, the residue should be at least below $10^{-4}$. 
### Table 2: Results for PG, APG, and ADM with $\varepsilon = 10^{-4}$

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time (secs)</th>
<th>Iters</th>
<th>Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td>PG</td>
<td>124.0</td>
<td>95</td>
<td>$9.5 \times 10^{-5}$</td>
</tr>
<tr>
<td>APG</td>
<td>125.0</td>
<td>93</td>
<td>$9.2 \times 10^{-5}$</td>
</tr>
<tr>
<td>ADM</td>
<td>51.0</td>
<td>36</td>
<td>$9.3 \times 10^{-5}$</td>
</tr>
</tbody>
</table>
### Table 3: Results for PG, APG, and ADM with $\varepsilon = 10^{-6}$

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time (secs)</th>
<th>Iters</th>
<th>Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td>PG</td>
<td>190</td>
<td>145</td>
<td>$9.5 \times 10^{-7}$</td>
</tr>
<tr>
<td>APG</td>
<td>225</td>
<td>168</td>
<td>$9.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>ADM</td>
<td>82</td>
<td>58</td>
<td>$9.5 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

Tables 2 and 3 show that all the tested first order methods work well, in particular ADM [By introducing line searches to PG and APG methods, one can improve the performance of these two algorithms].
Testing Case 2): To see the robustness of the first order methods, set

\[ G := \text{rand}(1000,1000), \quad G = G + G' \]

with its diagonal matrices to be ones.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time (secs)</th>
<th>Iters</th>
<th>Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td>PG</td>
<td>1130.0</td>
<td>1000</td>
<td>3.5 \times 10^{-2}</td>
</tr>
<tr>
<td>APG</td>
<td>1120.0</td>
<td>1000</td>
<td>3.6 \times 10^{-4}</td>
</tr>
<tr>
<td>ADM</td>
<td>305.0</td>
<td>257</td>
<td>1.0 \times 10^{-4}</td>
</tr>
</tbody>
</table>

Table 4: Results for PG, APG, and ADM with \( \varepsilon = 10^{-4} \)
<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time (secs)</th>
<th>Iters</th>
<th>Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td>PG</td>
<td>1130.0</td>
<td>1000</td>
<td>$3.5 \times 10^{-2}$</td>
</tr>
<tr>
<td>APG</td>
<td>1120.0</td>
<td>1000</td>
<td>$3.6 \times 10^{-4}$</td>
</tr>
<tr>
<td>ADM</td>
<td>515.0</td>
<td>434</td>
<td>$9.7 \times 10^{-7}$</td>
</tr>
</tbody>
</table>

Table 5: Results for PG, APG, and ADM with $\varepsilon = 10^{-6}$

Tables 4 and 5 show that the performance of PG and APG worsens a lot while ADM does okay.
Testing Case 3): The weighted case: $G$ is the same as in Case 1) but this time we set the weight matrix $D$ to be:

$$D := \text{diag}(\text{rand}(1000,1)) .$$

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time (secs)</th>
<th>Iters</th>
<th>Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td>PG</td>
<td>$&gt;1000$</td>
<td>1000</td>
<td>$2.9 \times 10^0$</td>
</tr>
<tr>
<td>APG</td>
<td>$&gt;1000$</td>
<td>1000</td>
<td>$5.6 \times 10^{-2}$</td>
</tr>
<tr>
<td>ADM</td>
<td>$&gt;1000$</td>
<td>1000</td>
<td>$1.8 \times 10^{-1}$</td>
</tr>
</tbody>
</table>

Table 6: Results for PG, APG, and ADM with $\varepsilon = 10^{-4}$
We have seen for the NCM: IPMs can be pretty robust for small \( n \) while
the first order methods can only deal with easy cases.

Any other possibility other than the IPMs and first order methods?

Note that the dual of the NCM is:

\[
F(y) := \nabla \theta(y) = \text{diag}(\Pi_{S^+}(G + \text{Diag}(y))) - e, \quad y \in \mathbb{R}^n.
\]

The functions \( F \) is strongly semismooth as \( \Pi_{S^+} \) is [Sun and Sun, 02].
That is, \( F \) is directionally diff. at \( y \) and

\[
F(y + h) - F(y) - \partial F(y + h)h = O(\|h\|^2).
\]
Qi and Sun [06] considered the following Semismooth Newton-CG method:

\[ F(y^k) + W_k(y^{k+1} - y^k) \approx 0, \]

where \( W_k \) is any element from Clarke’s generalized Jacobian \( \partial F(y^k) \).

To get \( W_k \) computed would require \( O(n^4) \) flops. So the exact semismooth Newton method will not be efficient.

However, Qi and Sun shows that \( \partial F(y^*) \) are symmetric and positive definite as the NCM is primal non-degenerate (LICQ holds). That’s the reason to apply a number of conjugate gradient (CG) steps to the semismooth Newton system.
<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Time</th>
<th>Iters</th>
<th>CGs</th>
<th>Residue</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADM (case 1)</td>
<td>82.0</td>
<td>58</td>
<td>9</td>
<td>$9.5 \times 10^{-7}$</td>
</tr>
<tr>
<td>Newton-CG</td>
<td>11.0</td>
<td>6</td>
<td>12/6</td>
<td>$6.0 \times 10^{-8}$</td>
</tr>
<tr>
<td>ADM (case 2)</td>
<td>515.0</td>
<td>434</td>
<td></td>
<td>$9.7 \times 10^{-7}$</td>
</tr>
<tr>
<td>Newton-CG</td>
<td>14.0</td>
<td>9</td>
<td>29/9</td>
<td>$6.5 \times 10^{-7}$</td>
</tr>
<tr>
<td>ADM (case 3)</td>
<td>$&gt;1000.0$</td>
<td>1000</td>
<td>94/21</td>
<td>$1.8 \times 10^{-1}$</td>
</tr>
<tr>
<td>Newton-CG</td>
<td>30.0</td>
<td>21</td>
<td>94/21</td>
<td>$6.7 \times 10^{-8}$</td>
</tr>
</tbody>
</table>

Table 7: Results for ADM and semismooth Newton-CG method with $\varepsilon = 10^{-6}$
As one can see the semismooth Newton-CG method\(^2\) for solving the NCM is robust and fast and the number of CGs used in each iteration of the semismooth Newton-CG method is really small ranging from 2 to 5.

Even a rough approximation to Newton’s direction can be extremely helpful.

What can we say about general matrix optimization problems?

\(^2\)NAG http://www.nag.co.uk/ has both the C and Fortran versions.
Let us start with

\[(P) \quad \max \quad \langle C, X \rangle \]
\[\text{s.t.} \quad A(X) = b, \quad X \succeq 0,\]

where \(A : \mathbb{S}^n \rightarrow \mathbb{R}^m\) is a linear map.

The dual problem of \((P)\) is

\[(D) \quad \min \left\{ b^T y \mid A^* y - C \succeq 0 \right\},\]

where \(A^* : \mathbb{R}^m \rightarrow \mathbb{S}^n\) is the adjoint of \(A\).
Given a penalty parameter \( \sigma > 0 \), the augmented Lagrangian function for problem (D) is defined as

\[
L_\sigma(y, X) = b^T y + \frac{1}{2\sigma} \left( \| \Pi_{S^+_n} (X - \sigma (A^* y - C)) \|_2^2 - \| X \|_2^2 \right),
\]

where \((y, X) \in \mathbb{R}^m \times S^n\) and for any \(X \in S^n\).

The augmented Lagrangian function is continuously differentiable. For any given \(X \in S^n_+\), we have

\[
\nabla_y L_\sigma(y, X) = b - A \Pi_{S_n^+} (X - \sigma (A^* y - C)).
\]
For given $X^0 \in \mathcal{S}^n$, $\sigma_0 > 0$, and $\rho > 1$, the augmented Lagrangian method for solving problem (D) and its dual (P) generates sequences $\{y^k\} \subset \mathbb{R}^m$ and $\{X^k\} \subset \mathcal{S}^n$ as follows:

\[
\begin{aligned}
    y^{k+1} &\approx \arg \min_{y \in \mathbb{R}^m} L_{\sigma_k}(y, X^k), \\
    X^{k+1} &= \Pi_{\mathcal{S}^n_+}(X^k - \sigma_k(A^*y^{k+1} - C)), \quad k = 0, 1, 2, \ldots \\
    \sigma_{k+1} &= \rho \sigma_k \text{ or } \sigma_{k+1} = \sigma_k,
\end{aligned}
\]
The augmented Lagrangian method for convex problems is a gradient ascent method applied to the corresponding augmented Lagrangian dual problems

\[
\max_{X \in S^n} \psi_\sigma(X) := \inf_{y \in \mathbb{R}^m} L_\sigma(y, X) = L_\sigma(y(X), X).
\]

But, recent studies [Sun et al, 07] show that under the constraint nondegenerate conditions for (P) and (D) [LICQs], the augmented Lagrangian method for solving SDPs is actually an approximate semismooth Newton method.
Use the semismooth Newton-CG method for solving inner subproblem we need to solve

\[ \nabla_y L_{\sigma_k}(y, X^k) = b - A\Pi_{S^+}(U^k(y)) = 0. \]

where \( U^k(y) := X^k - \sigma_k(A^*y - C) \).

At a current iterate \( y \), we solve a semismooth Newton equation by a CG method:

\[ \mathcal{H}_y := \sigma_k A\Pi_{S^+}'(U^k(y))A^*, \quad \mathcal{H}_y \Delta y = -\nabla_y L(y, X^k). \]
Practical Newton-CG augmented Lagrangian method [SDPNAL]

- Solve $H_y \Delta y = \text{rhs}$ by CG with a diagonal preconditioner.
  Stop when relative-residual $\leq 0.01$.

- Stop the inner iteration when $\| \nabla y L_{\sigma_k}(y^k, X^k) \| \leq 0.2 \| X^{k+1} - X^k \|$.  
  [Zhao, Sun, Toh, 10].
Comments on numerical results for SDPNAL:

want: \( \text{rel-err} = \max \left\{ \frac{\|R_p\|}{1+\|b\|}, \frac{\|R_d\|}{1+\|C\|}, \frac{|\langle X,Z \rangle|+|b^T y|}{1+|\langle C,X \rangle|+|b^T y|} \right\} \leq 10^{-6} \).

PC: Intel Xeon 3.2GHz with 4G RAM, \texttt{Matlab}

SDPNAL can be efficient as the theory predicted when the primal and dual non-degeneracies hold at the solutions. For example: for \( \theta : \text{theta162} \ (m = 127600, \ n = 800) \), SDPNAL needs 17 outer iterations with total computing time of 173 seconds.

Another example: for \( 1zc.2048 \ (m = 39425, \ n = 2048) \), SDPNAL needs 13 outer iterations with total computing time of 45 minutes and 16 seconds.
On the other hand, when the primal and dual non-degeneracies fail to hold, SDPNAL can perform poorly. For example, $2dc.512 \ (n = 512)$, SDPNAL spends 2 hours 25 minutes and 15 seconds to only get a relative error $1.1 \times 10^{-4}$.

As a general solver, SDPNAL currently does not give up the search for a direction better than a gradient direction even the primal and dual degeneracies are detected. This can be costly and unnecessary if one knows that Newton’s direction is not a good choice or difficult to approximate. Future work on these degenerate problems needs to be done.

SDPNAL can be downloaded from
Final remarks

- Nonsymmetric matrix problems need to be treated in their own formats.

- To exploit Newton’s direction can be beneficial when non-degeneracies hold. $1 + \varepsilon$ order methods can perform very well when the first and second order ones do no work efficiently.

- Variational analysis, in particular non-smooth analysis, can guide us in designing efficient algorithms.

- Degenerate programs call for new theory.