On solving indefinite least squares problems via anti–triangular factorizations

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How I got to work with Michael

- Yurii Nesterov, Vincent Blondel and I invited him to LLN

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$$\min \|\Delta\|_2 : \det\left(\begin{bmatrix} S & R \\ R^* & T \end{bmatrix} - \begin{bmatrix} 0 & \Delta \\ \Delta^* & 0 \end{bmatrix}\right) = 0$$

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$$\min \|\Delta\|_2 : \det(\begin{bmatrix} S & R \\ R^* & T \end{bmatrix} - \begin{bmatrix} 0 & \Delta \\ \Delta^* & 0 \end{bmatrix}) = 0$$

- This requires a solid background in two worlds : optimization and matrix theory

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- The anti-triangular symmetric indefinite factorization of A

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  uses Q orthogonal and yields M anti-triangular such that solving $Mx = b$ costs $O(n^2)$ at most
- It is easy to update/downdate when appending one row and column or adding a rank–one matrix ($=> O(n^3)$ algorithm)

Anti–triangular matrix decomposition [SIMAX '13]

$A \in \mathbb{R}^{n\times n}$, $A = A^T$, $\mathrm{In}(A) = (n_-, n_0, n_+)$, $n_1 = \min(n_-, n_+)$, and $n_2 = \max(n_-, n_+) - n_1$. Then

$$M = Q^T A Q = \left[\begin{array}{cccc} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & Y^T \\ \mathbf{0} & \mathbf{0} & X & Z^T \\ \mathbf{0} & Y & Z & W \end{array}\right] \begin{array}{l} \}n_0 \\ \}n_1 \\ \}n_2 \\ \}n_1 \end{array}, \quad \begin{array}{l} Y = \left[\ \triangle\ \right], \\ Q \in \mathbb{R}^{n\times n} \text{orthogonal}, \end{array}$$

is in proper block anti–triangular form with :
$Z \in \mathbb{R}^{n_1\times n_2}$, $W \in \mathbb{R}^{n_1\times n_1}$ symmetric,
$Y \in \mathbb{R}^{n_1\times n_1}$ nonsingular lower anti–triangular,
$X \in \mathbb{R}^{n_2\times n_2}$ symmetric definite if $n_2 > 0$, , i.e., $X = \varepsilon L L^T$,
L nonsingular lower triangular, $\varepsilon = \begin{cases} 1, & \text{if } n_+ > n_- \\ -1, & \text{if } n_+ < n_- \end{cases}$

Anti–triangular matrix decomposition

- If $A \in \mathbb{R}^{n\times n}$, $A = A^T$, is nonsingular, $\mathrm{In}(A) = (n_-, 0, n_+)$, $n_1 = \min(n_-, n_+)$, and $n_2 = \max(n_-, n_+) - n_1$, then exists $Q \in \mathbb{R}^{n\times n}$, $Q^T Q = I$, such that

$$M = Q^T A Q = \begin{bmatrix} \mathbf{0} & \mathbf{0} & Y^T \\ \mathbf{0} & X & Z^T \\ Y & Z & W \end{bmatrix} \begin{matrix} \}n_1 \\ \}n_2 \\ \}n_1 \end{matrix}$$

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  is in proper block anti–triangular form.
- Moreover, if M is in proper block anti–triangular form, then

$$\mathrm{In}(A) = (n_1, 0, n_1) + \left\{ \begin{array}{lll} (0, 0, n_2), & \text{if} & X \text{ spd}, \\ (n_2, 0, 0), & \text{if} & X \text{ snd}. \end{array} \right.$$

Anti–triangular “system solves” are cheap

- $Ax = b$,

$$\underbrace{\begin{bmatrix} \mathbf{0} & \mathbf{0} & Y^T \\ \mathbf{0} & X & Z^T \\ Y & Z & W \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{bmatrix}}_{\mathbf{b}} \begin{matrix} \}n_1 \\ \}n_2 \\ \}n_1 \end{matrix}$$

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-
$$\begin{aligned} Y^T \mathbf{x}_3 &= \mathbf{b}_1 \\ \varepsilon L L^T \mathbf{x}_2 &= \mathbf{b}_2 - Z^T \mathbf{x}_3 \\ Y \mathbf{x}_1 &= \mathbf{b}_3 - Z \mathbf{x}_2 - W \mathbf{x}_3 \end{aligned}$$

Show Batman movie here

Illustrations of backward stability

A are four 100×100 matrix
(rand, randn and 2 Matrix Market matrices)

MV $\frac{\|QMQ^T - A\|_2}{\|A\|_2}$	LUP $\frac{\|LU - PA\|_2}{\|A\|_2}$	QR $\frac{\|QR - A\|_2}{\|A\|_2}$
2.49e-15	7.27e-16	1.12e-15
1.69e-16	7.55e-17	5.91e-16
1.65e-15	1.43e-16	2.41e-15
2.54e-15	2.90e-16	1.63e-15

Indefinite Least Squares (ILS)

- Given $A \in \mathbb{R}^{(p+q)\times n}$, $\mathbf{b} \in \mathbb{R}^{p+q}$, and

$$\Sigma_{pq} = \begin{bmatrix} I_p & \\ & -I_q \end{bmatrix},$$

compute the solution of the indefinite least squares problem:

$$\min_{\mathbf{x}} (\mathbf{b} - A\mathbf{x})^T \Sigma_{pq} (\mathbf{b} - A\mathbf{x}).$$

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- This is well defined iff $A^T \Sigma_{pq} A \succ 0$

Indefinite Least Squares with equality constraints (ILSE)

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and $B \in \mathbb{R}^{s\times n}$, $\mathbf{d} \in \mathbb{R}^{s}$, $s \leq n$, the ILSE problem amounts to :

$$\min_{\mathbf{x}} (\mathbf{b} - A\mathbf{x})^T \Sigma_{pq} (\mathbf{b} - A\mathbf{x}) \text{ subject to } B\mathbf{x} = \mathbf{d}.$$

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- This is well defined iff (i) $\mathrm{rank} B = s$ and (ii) $A^T \Sigma_{pq} A \succ 0$ on $\ker B$

ILSE: augmented system

- The solution of ILSE satisfies the augmented system

$$\underbrace{\begin{bmatrix} \mathbf{0} & \mathbf{0} & B \\ \mathbf{0} & \Sigma_{pq} & A \\ B^T & A^T & \mathbf{0} \end{bmatrix}}_{M} \underbrace{\begin{bmatrix} \lambda \\ \mathbf{s} \\ \mathbf{x} \end{bmatrix}}_{\mathbf{y}} = \underbrace{\begin{bmatrix} \mathbf{d} \\ \mathbf{b} \\ \mathbf{0} \end{bmatrix}}_{\mathbf{g}},$$

where $\mathbf{s} = \Sigma_{pq}(\mathbf{b} - A\mathbf{x}) = \Sigma_{pq}\mathbf{r}$ and λ is the vector of the Lagrange multipliers.

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  where $\mathbf{s} = \Sigma_{pq}(\mathbf{b} - A\mathbf{x}) = \Sigma_{pq}\mathbf{r}$ and λ is the vector of the Lagrange multipliers.
- The idea is to transform the system into an equivalent one with coefficient matrix in proper block anti–triangular form

Algorithm

Let us choose $\hat{Q}_1$ orthogonal such that

$$\begin{bmatrix} B \\ A \end{bmatrix} \hat{Q}_1 = \begin{bmatrix} 0 & Y \\ A_1 & A_2 \end{bmatrix} = \begin{bmatrix} 0 & \triangle \\ A_1 & A_2 \end{bmatrix},$$

Then with $Q_1 := \begin{bmatrix} I_{p+q+s} & \\ & \hat{Q}_1 \end{bmatrix}$, we have

$$M_1 = Q_1^T M Q_1 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \triangle \\ \mathbf{0} & \Sigma_{pq} & A_1 & A_2 \\ \mathbf{0} & A_1^T & \mathbf{0} & \mathbf{0} \\ \triangle & A_2^T & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{matrix} \}s \\ \}p+q \\ \}n-s \\ \}s \end{matrix} \quad .$$

Since M_1 is anti–triangular in the first s rows and columns we process further the central part of

$$M_1 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & Y \\ \mathbf{0} & \Sigma_{pq} & A_1 & A_2 \\ \mathbf{0} & A_1^T & \mathbf{0} & \mathbf{0} \\ Y^T & A_2^T & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{matrix} \}s \\ \}p+q \\ \}n-s \\ \}s \end{matrix} \quad .$$

We thus need to reduce further

$$\hat{M}_1 = \begin{bmatrix} \Sigma_{pq} & A_1 \\ A_1^T & \mathbf{0} \end{bmatrix} \begin{matrix} \}p+q \\ \}n-s \end{matrix} \quad .$$

to proper block anti-triangular form

Partition A_1 as

$$A_1 = \begin{bmatrix} A_{11} \\ A_{12} \end{bmatrix} \begin{matrix} \}p \\ \}q \end{matrix} \quad .$$

and suppose (for simplicity) that $q \geq n - s$. Then we construct an orthogonal matrix

$$\tilde{Q}_2 := \begin{bmatrix} Q_2 & \\ & Q_3 \end{bmatrix} \begin{matrix} \}p \\ \}q \end{matrix}$$

such that

$$\tilde{Q}_2^T A_1 = \begin{bmatrix} \mathbf{0} \\ L_2 \\ R_3 \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \text{◢} \\ \text{◥} \\ \mathbf{0} \end{bmatrix}.$$

Then with $\hat{Q}_2 := \mathrm{diag}\{\tilde{Q}_2, I_{n-s}\}$ we have

$$\hat{M}_2 = \tilde{Q}_2^T \hat{M}_1 \tilde{Q}_2 = \begin{bmatrix} I_{p-n+s} & & & & \mathbf{0} \\ & I_{n-s} & & & L_2 \\ & & -I_{n-s} & & R_3 \\ & & & -I_{q-n+s} & \mathbf{0} \\ \mathbf{0} & L_2^T & R_3^T & \mathbf{0} & \mathbf{0} \end{bmatrix}$$

$$= \begin{bmatrix} I_{p-n+s} & & & & \mathbf{0} \\ & I_{n-s} & & & \text{◿} \\ & & -I_{n-s} & & \text{◹} \\ & & & -I_{q-n+s} & \mathbf{0} \\ \mathbf{0} & \text{◿} & \text{◺} & \mathbf{0} & \mathbf{0} \end{bmatrix}.$$

The inertia of $\hat{M}_i$ can be predicted $(\mathrm{In}(\hat{M}_i) = (p, 0, q + n - s))$ and the further reduction to proper anti-tiangular form is easy to obtain using a sequence of Givens transformations.

$$\hat{M}_3 = \hat{Q}_3^T \hat{M}_2 \hat{Q}_3 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \hat{Y}^T \\ \mathbf{0} & \hat{X} & \hat{Z}^T \\ \hat{Y} & \hat{Z} & \hat{W} \end{bmatrix}$$

where $\hat{X}$ is symmetric negative definite, i.e.,

$$-\hat{X} = \hat{L}\hat{L}^T$$

Numerical results

We construct the matrices B with matlab as

$$B = \texttt{gallery('randsvd',}s,\kappa) \times \texttt{randn}(s,n),$$

with the condition number κ chosen as $10^k, k = 2, 4, 6, 8$ and $n = 50, s = 20, p = 60, q = 40$.
Let $\mathbf{x}_i$ and $\mathbf{r}_i = \mathbf{b} - A\mathbf{x}_i$, be the solution of the augmented linear system and the residual computed by using "\" of matlab (for $i = 1$) and by using the proposed method (for $i = 2$).

κ	$\frac{\Vert\mathbf{x}_1-\mathbf{x}_2\Vert_2}{\Vert\mathbf{x}_2\Vert_2}$	$\Vert\Sigma_{pq}\mathbf{s}-\mathbf{r}_1\Vert_2$	$\Vert\Sigma_{pq}\mathbf{s}-\mathbf{r}_2\Vert_2$	$\Vert B\mathbf{x}_1-\mathbf{d}\Vert_2$	$\Vert B\mathbf{x}_2-\mathbf{d}\Vert_2$
1e2	6.285e-12	1.392e-09	5.331e-12	6.125e-11	7.016e-14
1e4	6.309e-08	4.941e-06	1.774e-10	1.702e-07	1.651e-12
1e6	1.718e-04	6.080e-03	6.474e-09	3.871e-04	4.176e-11
1e8	8.555e-01	3.233e+1	7.356e-07	1.671e+0	1.554e-09

Discrete–time Optimal Control program

$$
\begin{array}{lll}
\min_{x,q} & \sum_{i=1}^{m} \Psi_i(x_i, q_i) & \\
\text{s.t.} & x_i^{\text{low}} \leq x_i \leq x_i^{\text{up}} & \\
 & q_i^{\text{low}} \leq q_i \leq q_i^{\text{up}} & i \in \{1, \ldots, m\} \\
 & 0 \leq R_i(x_i, q_i) & \\
 & 0 = G_i(x_i, q_i) + P_{i+1}(x_{i+1}, q_{i+1}) &
\end{array}
$$

$x_i \in \mathbb{R}^{n_x}$ are the states and $q_i \in \mathbb{R}^{n_q}$ the control parameters.

The discrete–time process evolves over m points $i \in \{1, \ldots, m\}$ in time and is described by the state propagation law given in terms of
$G_i : \mathbb{R}^{n_x} \times \mathbb{R}^{n_q} \to \mathbb{R}^{n_x}, \quad P_i : \mathbb{R}^{n_x} \times \mathbb{R}^{n_q} \to \mathbb{R}^{n_x}$

The state x and control q are subject to possibly nonlinear constraints containing initial values, boundary conditions, or discretized general path constraints (Kirches, Bock et al, 2011).

Quadratic Optimal Control program

Using a linear–quadratic model of the Lagrangian and a linearization of the constraints, we obtain

$$
\begin{array}{lll}
\min_w & \sum_{i=1}^{m} \left(\frac{1}{2} w_i^T H_i w_i + g_i^T w \right) & \\
\text{s.t.} & l_i \leq w_i \leq u_i & i \in \{1, \ldots, m\} \\
& r_i \leq R_i w_i & \\
& h_i = G_i w_i + P_{i+1} w_{i+1} &
\end{array} \tag{1}
$$

$$
\begin{array}{l}
H_i \in \mathbb{R}^{n \times n} \quad \textit{Hessians} \\
g_i \in \mathbb{R}^n \quad \textit{gradients} \\
w_i = (x_i, q_i)
\end{array}
$$

R_i, G_i and P_i are the linearization matrices of R, G and P.

KKT problem

... Summarizing, at each step of the iterative process, a saddle point problem needs to be solved

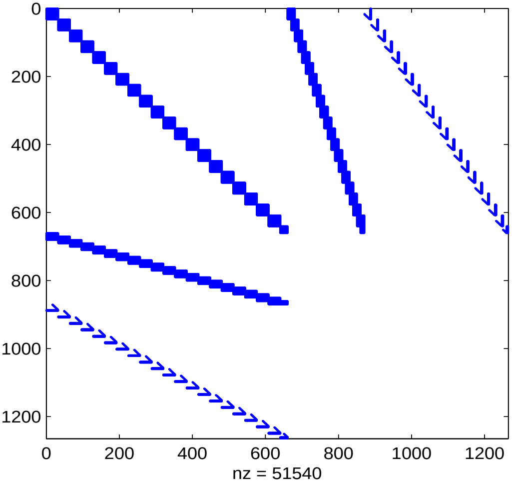
$$\begin{bmatrix} H & M^T & R^T \\ M & \mathbf{0} & \mathbf{0} \\ R & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} w \\ \lambda \\ z \end{bmatrix} = \begin{bmatrix} g \\ h \\ c \end{bmatrix} \tag{2}$$

with

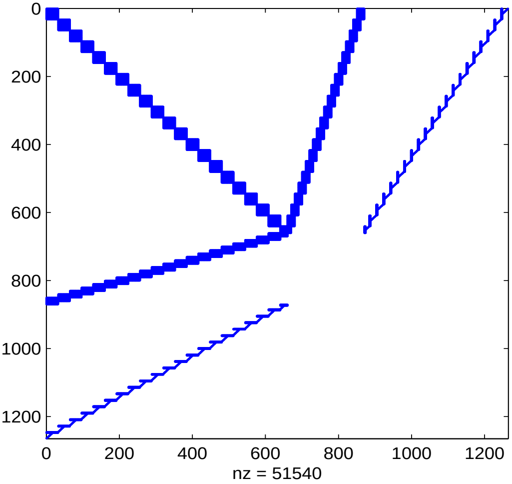
$$H = \begin{bmatrix} H_1 & & \\ & \ddots & \\ & & H_m \end{bmatrix}, M = \begin{bmatrix} G_1 & & & \\ P_1 & \ddots & & \\ & \ddots & G_{m-1} & \\ & & P_{m-1} & G_m \end{bmatrix}, R = \begin{bmatrix} R_1 & & \\ & \ddots & \\ & & R_m \end{bmatrix}.$$

M and C have full row rank due to the choice of a linear independent active set.

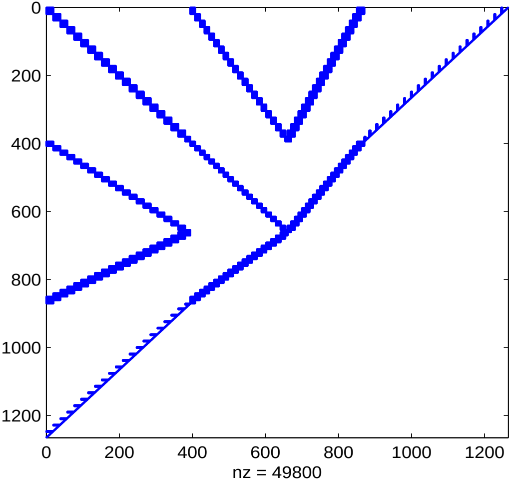
KKT matrix



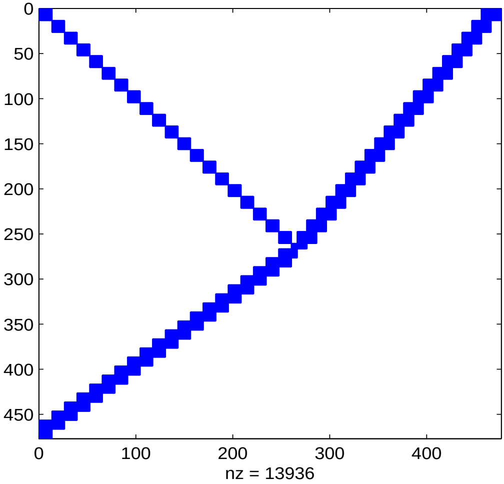
KKT matrix permuted



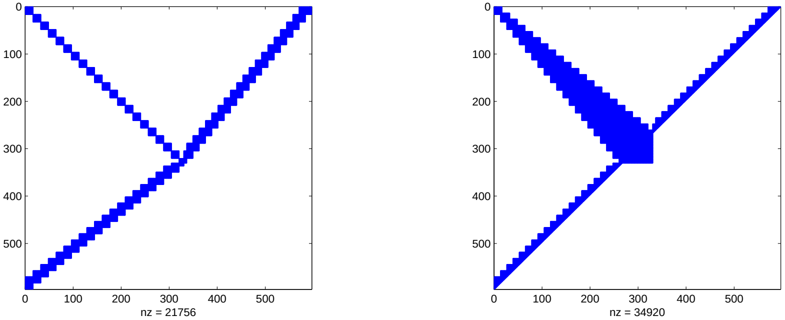
KKT matrix permuted and preprocessed (outer parts)



KKT matrix preprocessed (central part)



KKT matrix further reduction (central part)



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- The solutions presented in the literature require Schur complementation and are potentially unstable
- Scaling the individual matrices in the ILSE problem improves the conditioning estimates for the ILSE problem

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Why Michael gets so much work done ...

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OK, back to real the world,

I'm going to work on my theorems !

Happy birthday, Michael !