Contribution ID: **5** Type: **not specified**

Null space-based approaches for the least squares and symmetric saddle-point problems

Friday, 10 June 2022 15:30 (30 minutes)

Consider saddle-point systems of the following form
A $\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$ $(1) where$A $\in \mathbb{R}^{n\times n}$ is large, sparse and symmetric positive definite and $B \in \mathbb{R}^{k\times n}(n > k)$ has full rank. Such systems arise in various scientific applications, including the finite element approximation of PDEs in which a constraint is enforced on a subset of unknowns via a global scalar Lagrange multiplier, numerical continuation methods for large nonlinear systems of equations, constrained optimization as well as in linear least squares problems [2].

Null-space methods represent one of possible solution approaches to solve such systems. Despite these solution approaches that compute a null-space $Z \in \mathbb{R}^{n\times(n-k)}$ basis of the undetermined block B are traditional in various engineering communities and offer advantages in some situations, general techniques to obtain such bases useful for large and sparse A have not been studied frequently in the past. There are more reasons for this. One of them may be that the resulting transformed system with the matrix Z^TAZ is often dense, or ill-conditioned, or both. Another reason may be that there is a lack of efficient preconditioners for the transformed systems even when the projected matrix Z^TAZ is reasonably sparse. The core of the talk is devoted to discussing various algorithms to find the null-space basis Z. Although in several of the approaches treatment of B that does not have full-rank is not difficult, we do not treat such cases at length.

Initial motivation for studying the null-space approaches in this talk is slightly different from the symmetric saddle-point problem given above. Consider the linear least-squares (LS) problem $\min_x \|Ax-b\|_2, wherethesystemmatrix$A $\in \mathbb{R}^{m\times n}(m \geq n)$ and the right-hand side $b \in \mathbb{R}^m$ are given. Assume that a part of the rows of A is dense and the rows have been initially permuted such that the dense rows are the last rows of A. If we assume a conformal partitioning of the vector b we have A = $\begin{pmatrix} A_s \\ A_d \end{pmatrix}$, $A_s \in \mathbb{R}^{m_s\times n}$, $A_d \in \mathbb{R}^{m_d\times n}$, $b = \begin{pmatrix} b_s \\ b_d \end{pmatrix}$, $b_s \in \mathbb{R}^{m_s}$, $b_d \in \mathbb{R}^{m_d}, where$m$_s$ denotes the number of sparse rows of A, and m_d is the number of dense rows, with $m = m_s + m_d$, $m_s \geq n > m_d \geq 1$ and $m_d \ll m_s$.

The normal equations that describe the solution [3] (not representing always the best way to get the solution) become Cx = (C$_s$+$A_d^TA_d)x = c$, $c = A_s^Tb_s + A_d^Tb_d$, $(2)w$
$A_s^TA_s$ is the reduced normal matrix. The solution of (2) can be obtained from the equivalent $(n+md)\times(n+md)$ system $\begin{pmatrix} C_s & A_d^T \\ A_d & -I \end{pmatrix} \begin{pmatrix} x \\ A_dx \end{pmatrix} = \begin{pmatrix} c \\ 0 \end{pmatrix}$
= m$_d$, $H = C_s, B = A_d$. But the $(2,2)$ block is nonzero and equal to the negative unit matrix of the appropriate dimension. Provided A_s has full column rank, C_s is symmetric positive definite. But the null-space based approach can be extended even if the $(2,2)$ block is nonzero and C_s only positive semidefinite. This positive definiteness is quite common in the LS problems even when the whole A is of full column rank. The approach to solve (3) also in this case for the full rank LS problem (3) is motivated by the following simple lemma.

Lemma: Consider $A = A_sA_d$, $As \in \mathbb{R}^{m_s\times n}$, $A_d \in \mathbb{R}^{m_d\times n}$. If A is of full column rank, then $C_s = A_s^TA_s$ is positive definite on the null space of A_d.

Success of any null-space approach then depends on constructing a suitable null-space basis that keeps the matrix Z^TAZ sufficiently sparse and well-conditioned. Of course, it cannot be an orthogonal null-space basis computed, for example, by pivoted QR factorization of B^T. We will discuss other approaches to find the null-space basis heavily based on the fact that B is wide. That is, it has far fewer rows than columns. The approaches include computing an oblique basis Z computed from more separate QR factorizations and an approach that adds rows of B one by one and extends the basis incrementally. Another approach for constructing Z is the right oblique conjugation. Applied to $B \in \mathbb{R}^{k\times n}$ it yields $V \in \mathbb{R}^{n\times n}$ and lower trapezoidal $L \in \mathbb{R}^{k\times n}$ satisfying BV = L. (4) The null-space basis is then formed by the last $n-k$ columns of V. This approach is directly related to Thesis of Michele Benzi [1]. Techniques implied by this Thesis have motivated the right oblique conjugation, and they may still offer further computational possibilities. Not only for constructing Z but possibly also for preconditioning of the linear systems with the matrix $Z^T AZ$.

Our experimental results show that the null-space bases obtained from the mentioned approaches are of high quality and can push forward further research in optimization and solving constrained least squares. Linear least squares problems that contain a small number of dense rows arising from practical applications are used to illustrate our ideas and to explore their potential for solving large-scale systems. Our work was originally motivated by the paper by Howell [4]. A significant part of the obtained results has been published in [5].

References

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