



Iterative Methods for Symmetric Quasi-Definite Linear Systems

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Overview of talk

- ▶ Symmetric Quasi Positive Definite matrices

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- ▶ G-K bidiagonalization
- ▶ Generalized LSQR and Craig (Stopping criteria)

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- ▶ Generalized LSQR and Craig (Stopping criteria)
- ▶ Numerical examples

Linear operators

Let $\mathbf{M} \in \mathbf{R}^{m \times m}$ and $\mathbf{N} \in \mathbf{R}^{n \times n}$ be symmetric positive definite matrices, and let $\mathbf{A} \in \mathbf{R}^{m \times n}$ be a full rank matrix.

$$\mathcal{M} = \{\mathbf{v} \in \mathbf{R}^m; \|\mathbf{u}\|_{\mathbf{M}}^2 = \mathbf{v}^T \mathbf{M} \mathbf{v}\}, \quad \mathcal{N} = \{\mathbf{q} \in \mathbf{R}^n; \|\mathbf{q}\|_{\mathbf{N}}^2 = \mathbf{q}^T \mathbf{N} \mathbf{q}\}$$

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$$\langle \mathbf{v}, \mathbf{A} \mathbf{q} \rangle_{\mathcal{M}, \mathcal{M}'} = \mathbf{v}^T \mathbf{A} \mathbf{q}, \quad \mathbf{A} \mathbf{q} \in \mathcal{L}(\mathcal{M}) \quad \forall \mathbf{q} \in \mathcal{N}.$$

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The adjoint operator \mathbf{A}^\star of \mathbf{A} can be defined as

$$\langle \mathbf{A}^\star \mathbf{g}, \mathbf{f} \rangle_{\mathcal{N}', \mathcal{N}} = \mathbf{f}^T \mathbf{A}^T \mathbf{g}, \quad \mathbf{A}^T \mathbf{g} \in \mathcal{L}(\mathcal{N}) \quad \forall \mathbf{g} \in \mathcal{M}.$$

Generalized SVD

Given $\mathbf{q} \in \mathcal{M}$ and $\mathbf{v} \in \mathcal{N}$, the critical points for the functional

$$\frac{\mathbf{v}^T \mathbf{A} \mathbf{q}}{\|\mathbf{q}\|_{\mathcal{N}} \|\mathbf{v}\|_{\mathcal{M}}}$$

are the “*generalized singular values and singular vectors*” of \mathbf{A} .

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The saddle-point conditions are

$$\begin{cases} \mathbf{A} \mathbf{q}_i &= \sigma_i \mathbf{M} \mathbf{v}_i & \mathbf{v}_i^T \mathbf{M} \mathbf{v}_j &= \delta_{ij} \\ \mathbf{A}^T \mathbf{v}_i &= \sigma_i \mathbf{N} \mathbf{q}_i & \mathbf{q}_i^T \mathbf{N} \mathbf{q}_j &= \delta_{ij} \end{cases}$$

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n > 0$$

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The generalized singular values are the standard singular values of $\tilde{\mathbf{A}} = \mathbf{M}^{-1/2} \mathbf{A} \mathbf{N}^{-1/2}$. The generalized singular vectors \mathbf{q}_i and \mathbf{v}_i , $i = 1, \dots, n$ are the transformation by $\mathbf{M}^{-1/2}$ and $\mathbf{N}^{-1/2}$ respectively of the left and right standard singular vector of $\tilde{\mathbf{A}}$.

Quadratic programming

The general problem

$$\min_{\mathbf{A}^T \mathbf{w} = \mathbf{r}} \frac{1}{2} \mathbf{w}^T \mathbf{W} \mathbf{w} - \mathbf{g}^T \mathbf{w}$$

where the matrix \mathbf{W} is positive semidefinite and $\ker(\mathbf{W}) \cap \ker(\mathbf{A}^T) = 0$ can be reformulated by choosing

$$\left. \begin{aligned} \mathbf{M} &= \mathbf{W} + \nu \mathbf{A} \mathbf{N}^{-1} \mathbf{A}^T \\ \mathbf{u} &= \mathbf{w} - \mathbf{M}^{-1} \mathbf{g} \\ \mathbf{b} &= \mathbf{r} - \mathbf{A}^T \mathbf{M}^{-1} \mathbf{g}. \end{aligned} \right\}$$

as a projection problem

$$\min_{\mathbf{A}^T \mathbf{u} = \mathbf{b}} \|\mathbf{u}\|_{\mathbf{M}}^2$$

If \mathbf{W} is non singular then we can choose $\nu = 0$.

Augmented system

The augmented system that gives the optimality conditions for the projection problem:

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{b} \end{bmatrix}.$$

Generalized Golub-Kahan bidiagonalization

In Golub Kahan (1965), Paige Saunders (1982), several algorithms for the bidiagonalization of a $m \times n$ matrix are presented. All of them can be theoretically applied to $\tilde{\mathbf{A}}$ and their generalization to \mathbf{A} is straightforward as shown by Bembow (1999). Here, we want specifically to analyse one of the variants known as the "Craig"-variant (see Paige Saunders (1982), Saunders (1995,1997)).

Generalized Golub-Kahan bidiagonalization

$$\begin{cases} \mathbf{A}\tilde{\mathbf{Q}} = \mathbf{M}\tilde{\mathbf{V}} \begin{bmatrix} \tilde{\mathbf{B}} \\ 0 \end{bmatrix} \\ \mathbf{A}^T\tilde{\mathbf{V}} = \mathbf{N}\tilde{\mathbf{Q}} \begin{bmatrix} \tilde{\mathbf{B}}^T; 0 \end{bmatrix} \end{cases} \quad \begin{cases} \tilde{\mathbf{V}}^T\mathbf{M}\tilde{\mathbf{V}} = \mathbf{I}_m \\ \tilde{\mathbf{Q}}^T\mathbf{N}\tilde{\mathbf{Q}} = \mathbf{I}_n \end{cases}$$

where

$$\tilde{\mathbf{B}} = \begin{bmatrix} \tilde{\alpha}_1 & 0 & 0 & \cdots & 0 \\ \tilde{\beta}_2 & \tilde{\alpha}_2 & 0 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & \tilde{\beta}_{n-1} & \tilde{\alpha}_{n-1} & 0 \\ 0 & \cdots & 0 & \tilde{\beta}_n & \tilde{\alpha}_n \\ 0 & \cdots & 0 & 0 & \tilde{\beta}_{n+1} \end{bmatrix}.$$

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where

$$\mathbf{B} = \begin{bmatrix} \alpha_1 & \beta_1 & 0 & \cdots & 0 \\ 0 & \alpha_2 & \beta_2 & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ 0 & \cdots & 0 & \alpha_{n-1} & \beta_{n-1} \\ 0 & \cdots & 0 & 0 & \alpha_n \end{bmatrix}.$$

Algorithm

The augmented system that gives the optimality conditions for $\min_{\mathbf{A}^T \mathbf{u} = \mathbf{b}} \|\mathbf{u}\|_{\mathbf{M}}^2$

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{b} \end{bmatrix}$$

can be transformed by the change of variables

$$\begin{cases} \mathbf{u} = \mathbf{Vz} \\ \mathbf{p} = \mathbf{Qy} \end{cases}$$

Algorithm

$$\begin{bmatrix} \mathbf{I}_n & 0 & \mathbf{B} \\ 0 & \mathbf{I}_{m-n} & 0 \\ \mathbf{B}^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{z}_1 \\ \mathbf{z}_2 \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \mathbf{Q}^T \mathbf{b} \end{bmatrix}.$$

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$$\begin{bmatrix} \mathbf{I}_n & \mathbf{B} \\ \mathbf{B}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{z}_1 \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{Q}^T \mathbf{b} \end{bmatrix}.$$

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$$\begin{bmatrix} \mathbf{I}_n & \mathbf{B} \\ \mathbf{B}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{z}_1 \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{Q}^T \mathbf{b} \end{bmatrix}.$$

$$\mathbf{Q}^T \mathbf{b} = \mathbf{e}_1 \|\mathbf{b}\|_{\mathbf{N}}$$

the value of \mathbf{z}_1 will correspond to the first column of the inverse of \mathbf{B} multiplied by $\|\mathbf{b}\|_{\mathbf{N}}$.

Algorithm

Thus, we can compute the first column of \mathbf{B} and of \mathbf{V} :
 $\alpha_1 \mathbf{M} \mathbf{v}_1 = \mathbf{A} \mathbf{q}_1$, such as

$$\mathbf{w} = \mathbf{M}^{-1} \mathbf{A} \mathbf{q}_1$$

$$\alpha_1 = \mathbf{w}^T \mathbf{M} \mathbf{w} = \mathbf{w} \mathbf{A} \mathbf{q}_1$$

$$\mathbf{v}_1 = \mathbf{w} / \sqrt{\alpha_1}.$$

Algorithm

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Finally, knowing \mathbf{q}_1 and \mathbf{v}_1 we can start the recursive relations

$$\begin{aligned} \mathbf{g}_{i+1} &= \mathbf{N}^{-1} (\mathbf{A}^T \mathbf{v}_i - \alpha_i \mathbf{N} \mathbf{q}_i) \\ \beta_{i+1} &= \mathbf{g}_{i+1}^T \mathbf{N} \mathbf{g}_{i+1} \\ \mathbf{q}_{i+1} &= \mathbf{g}_{i+1} / \sqrt{\beta_{i+1}} \\ \mathbf{w} &= \mathbf{M}^{-1} (\mathbf{A} \mathbf{q}_{i+1} - \beta_{i+1} \mathbf{M} \mathbf{v}_i) \\ \alpha_{i+1} &= \mathbf{w}^T \mathbf{M} \mathbf{w} \\ \mathbf{v}_{i+1} &= \mathbf{w} / \sqrt{\alpha_{i+1}}. \end{aligned}$$

U

Thus, the value of \mathbf{u} can be approximated when we have computed the first k columns of \mathbf{U} by

$$\mathbf{u}^{(k)} = \mathbf{V}_k \mathbf{z}_k = \sum_{j=1}^k \zeta_j \mathbf{v}_j.$$

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The entries ζ_j of \mathbf{z}_k can be easily computed recursively starting with

$$\zeta_1 = -\frac{\|\mathbf{b}\|_{\mathbf{N}}}{\alpha_1}$$

as

$$\zeta_{i+1} = -\frac{\beta_i}{\alpha_{i+1}} \zeta_i \quad i = 1, \dots, n$$

p

Approximating $\mathbf{p} = \mathbf{Q}\mathbf{y}$ by $\mathbf{p}^{(k)} = \mathbf{Q}_k\mathbf{y}_k = \sum_{j=1}^k \psi_j \mathbf{q}_j$, we have that

$$\mathbf{y}_k = -\mathbf{B}_k^{-1} \mathbf{z}_k.$$

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Following an observation made by Paige and Saunders, we can easily transform the previous relation into a recursive one where only one extra vector is required.

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From $\mathbf{p}^{(k)} = -\mathbf{Q}_k\mathbf{B}_k^{-1}\mathbf{z}_k = -\left(\mathbf{B}_k^{-T}\mathbf{Q}_k^T\right)^T \mathbf{z}_k$ and $\mathbf{D}_k = \mathbf{B}_k^{-T}\mathbf{Q}_k^T$

$$\mathbf{d}_i = \frac{\mathbf{q}_i - \beta_i \mathbf{d}_{i-1}}{\alpha_i} \quad i = 1, \dots, n \quad (\mathbf{d}_0 = 0)$$

where \mathbf{d}_j are the columns of \mathbf{D} .

Starting with $\mathbf{p}^{(1)} = -\zeta_1 \mathbf{d}_1$ and $\mathbf{u}^{(1)} = \zeta_1 \mathbf{v}_1$

$$\left. \begin{aligned} \mathbf{u}^{(i+1)} &= \mathbf{u}^{(i)} + \zeta_{i+1} \mathbf{v}_{i+1} \\ \mathbf{p}^{(i+1)} &= \mathbf{p}^{(i)} - \zeta_{i+1} \mathbf{d}_{i+1} \end{aligned} \right\} \quad i = 1, \dots, n$$

Stopping criteria

$$\|\mathbf{u} - \mathbf{u}^{(k)}\|_{\mathbf{M}}^2 = \|\mathbf{e}^{(k)}\|_{\mathbf{M}}^2 = \sum_{j=k+1}^n \zeta_j^2 = \left\| \mathbf{z} - \begin{bmatrix} \mathbf{z}_k \\ 0 \end{bmatrix} \right\|_2^2.$$

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$$\|\mathbf{A}^T \mathbf{u}^{(k)} - \mathbf{b}\|_{\mathbf{N}^{-1}} = |\beta_{k+1} \zeta_k| \leq \sigma_1 |\zeta_k| = \|\tilde{\mathbf{A}}\|_2 |\zeta_k|.$$

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$$\|\mathbf{A}^T \mathbf{u}^{(k)} - \mathbf{b}\|_{\mathbf{N}-1} = |\beta_{k+1} \zeta_k| \leq \sigma_1 |\zeta_k| = \|\tilde{\mathbf{A}}\|_2 |\zeta_k|.$$

$$\|\mathbf{p} - \mathbf{p}^{(k)}\|_{\mathbf{N}} = \left\| \mathbf{QB}^{-1} \left(\mathbf{z} - \begin{bmatrix} \mathbf{z}_k \\ 0 \end{bmatrix} \right) \right\|_{\mathbf{N}} \leq \frac{\|\mathbf{e}^{(k)}\|_{\mathbf{M}}}{\sigma_n}.$$

Error bound

Lower bound We can estimate $\|\mathbf{e}^{(k)}\|_{\mathbf{M}}^2$ by the lower bound

$$\xi_{k,d}^2 = \sum_{j=k+1}^{k+d+1} \zeta_j^2 < \|\mathbf{e}^{(k)}\|_{\mathbf{M}}^2.$$

Given a threshold $\tau < 1$ and an integer d , we can stop the iterations when

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Upper bound Despite being very inexpensive, the previous estimator is still a lower bound of the error. We can use an approach inspired by the Gauss-Radau quadrature algorithm and similar to the one described in Golub-Meurant (2010).

Symmetric Quasi-Definite Systems

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \quad \text{where} \quad \mathbf{M} = \mathbf{M}^T \succ 0, \mathbf{N} = \mathbf{N}^T \succ 0.$$

- ▶ Interior-point methods for LP, QP, NLP, SOCP, SDP, ...
- ▶ Regularized/stabilized PDE problems
- ▶ Regularized least squares
- ▶ How to best take advantage of the structure?

Main Property

Theorem (Vanderbei, 1995)

If \mathbf{K} is SQD, it is **strongly factorizable**, i.e., for *any* permutation matrix \mathbf{P} , there exists a unit lower triangular \mathbf{L} and a diagonal \mathbf{D} such that $\mathbf{P}^T \mathbf{K} \mathbf{P} = \mathbf{L} \mathbf{D} \mathbf{L}^T$.

- ▶ Cholesky-factorizable
- ▶ Used to speed up factorization in regularized least-squares (Saunders) and interior-point methods (Friedlander and O.)
- ▶ Stability analysis by Gill, Saunders, Shinnerl (1996).

Iterative Methods I

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Fact: ... none exploits the SQD structure.

If the system were definite, we would like to use CG.

Related Problems: an example

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix}$$

Related Problems: an example

$$\begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix}$$

are the optimality conditions of

$$\min_{\mathbf{y} \in \mathbf{R}^m} \frac{1}{2} \left\| \begin{bmatrix} \mathbf{A} \\ \mathbf{I} \end{bmatrix} \mathbf{y} - \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} \right\|_{E_+^{-1}}^2 \equiv \min_{\mathbf{y} \in \mathbf{R}^m} \frac{1}{2} \left\| \begin{bmatrix} \mathbf{M}^{-\frac{1}{2}} & 0 \\ 0 & \mathbf{N}^{\frac{1}{2}} \end{bmatrix} \left(\begin{bmatrix} \mathbf{A} \\ \mathbf{I} \end{bmatrix} \mathbf{y} - \begin{bmatrix} \mathbf{b} \\ 0 \end{bmatrix} \right) \right\|_2^2$$

Generalized Least Squares

Normal equations: $(\mathbf{A}^T \mathbf{M}^{-1} \mathbf{A} + \mathbf{N})\mathbf{y} = \mathbf{A}^T \mathbf{M}^{-1} \mathbf{b}$.

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At k -th iteration, seek $y \approx \mathbf{y}_k := \tilde{\mathbf{V}}_k \bar{\mathbf{y}}_k$:

$$(\tilde{\mathbf{B}}_k^T \tilde{\mathbf{B}}_k + \mathbf{I}) \bar{\mathbf{y}}_k = \tilde{\mathbf{B}}_k^T \beta_1 \mathbf{e}_1$$

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i.e.:

$$\min_{\bar{\mathbf{y}} \in \mathbf{R}^k} \frac{1}{2} \left\| \begin{bmatrix} \tilde{\mathbf{B}}_k \\ \mathbf{I} \end{bmatrix} \bar{\mathbf{y}} - \begin{bmatrix} \beta_1 \mathbf{e}_1 \\ 0 \end{bmatrix} \right\|_2^2$$

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or:

$$\begin{bmatrix} \mathbf{I} & \tilde{\mathbf{B}}_k \\ \tilde{\mathbf{B}}_k^T & -\mathbf{I} \end{bmatrix} \begin{bmatrix} \bar{\mathbf{x}}_k \\ \bar{\mathbf{y}}_k \end{bmatrix} = \begin{bmatrix} \beta_1 \mathbf{e}_1 \\ 0 \end{bmatrix}.$$

Generalized LSQR

Solve

$$\min_{\bar{\mathbf{y}} \in \mathbf{R}^k} \frac{1}{2} \left\| \begin{bmatrix} \tilde{\mathbf{B}}_k \\ \mathbf{I} \end{bmatrix} \bar{\mathbf{y}} - \begin{bmatrix} \beta_1 \mathbf{e}_1 \\ 0 \end{bmatrix} \right\|_2^2$$

by specialized Givens Rotations (Eliminate \mathbf{I} first and $\tilde{\mathbf{R}}_k$ will be upper bidiagonal)

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$$\min_{\bar{\mathbf{y}} \in \mathbf{R}^k} \frac{1}{2} \left\| \begin{bmatrix} \tilde{\mathbf{R}}_k \\ 0 \end{bmatrix} \bar{\mathbf{y}} - \begin{bmatrix} \phi_k \\ 0 \end{bmatrix} \right\|_2^2.$$

Generalized LSQR

Solve

$$\min_{\bar{\mathbf{y}} \in \mathbb{R}^k} \frac{1}{2} \left\| \begin{bmatrix} \tilde{\mathbf{B}}_k \\ \mathbf{I} \end{bmatrix} \bar{\mathbf{y}} - \begin{bmatrix} \beta_1 \mathbf{e}_1 \\ 0 \end{bmatrix} \right\|_2^2$$

by specialized Givens Rotations (Eliminate \mathbf{I} first and $\tilde{\mathbf{R}}_k$ will be upper bidiagonal)

$$\min_{\bar{\mathbf{y}} \in \mathbb{R}^k} \frac{1}{2} \left\| \begin{bmatrix} \tilde{\mathbf{R}}_k \\ 0 \end{bmatrix} \bar{\mathbf{y}} - \begin{bmatrix} \phi_k \\ 0 \end{bmatrix} \right\|_2^2.$$

As in Paige-Saunders '82 we can build recursive expressions of \mathbf{y}_k

$$\mathbf{y}_{k+1} = \mathbf{y}_k + \mathbf{d}_k \phi_k \quad (\mathbf{D}_k = \tilde{\mathbf{V}}_k \tilde{\mathbf{R}}_k^{-1})$$

and we have that

$$\|\mathbf{y}\|_{\mathbf{N} + \mathbf{A}^T \mathbf{M}^{-1} \mathbf{A}}^2 = \sum_{j=1}^m \phi_j^2 \quad \text{and} \quad \|\mathbf{y} - \mathbf{y}_k\|_{\mathbf{N} + \mathbf{A}^T \mathbf{M}^{-1} \mathbf{A}}^2 = \sum_{j=k+1}^m \phi_j^2$$

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- ▶ A. and Orban "Iterative methods for symmetric quasi definite systems" in preparation. **WORK IN PROGRESS**