Iterative Methods for Symmetric Quasi-Definite Linear Systems

Mario Arioli[1] Dominique Orban[2]

[1]Rutherford Appleton Laboratory, mario.arioli@stfc.ac.uk

[2]GERAD and École Polytechnique de Montréal, dominique.orban@gerad.ca

Overview of talk

- Symmetric Quasi Definite matrices

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- Why SQD are important?

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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

Symmetric Quasi-Definite Systems

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

- 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).

Centered preconditioning

$$\begin{bmatrix} \mathbf{M}^{-\frac{1}{2}} & \\ & \mathbf{N}^{-\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix} \begin{bmatrix} \mathbf{M}^{-\frac{1}{2}} & \\ & \mathbf{N}^{-\frac{1}{2}} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \end{bmatrix} = \begin{bmatrix} \mathbf{M}^{-\frac{1}{2}}\mathbf{f} \\ \mathbf{N}^{-\frac{1}{2}}\mathbf{g} \end{bmatrix}$$

which is equivalent to

$$\overbrace{\begin{bmatrix} \mathbf{I}_m & \mathbf{M}^{-\frac{1}{2}}\mathbf{A}\mathbf{N}^{-\frac{1}{2}} \\ \mathbf{N}^{-\frac{1}{2}}\mathbf{A}^T\mathbf{M}^{-\frac{1}{2}} & -\mathbf{I}_n \end{bmatrix}}^{\widehat{\mathbf{C}}} \begin{bmatrix} \hat{\mathbf{x}} \\ \hat{\mathbf{y}} \end{bmatrix} = \begin{bmatrix} \mathbf{M}^{-\frac{1}{2}}\mathbf{f} \\ \mathbf{N}^{-\frac{1}{2}}\mathbf{g} \end{bmatrix}$$

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Theorem (Saunders (1995))

Suppose $\tilde{\mathbf{A}} = \mathbf{M}^{-\frac{1}{2}}\mathbf{A}\mathbf{N}^{-\frac{1}{2}}$ *has rank* $p \leq m$ *with nonzero singular values* $\sigma_1, \ldots, \sigma_p$. *The eigenvalues of* $\widehat{\mathbf{C}}$ *are* $+1$, -1 *and* $\pm\sqrt{1+\sigma_k}$, $k = 1, \ldots, p$.

Symmetric spectrum and Iterative methods

A symmetric matrix with a symmetric spectrum can be transform preserving the symmetry of the spectrum in a SQD one. Moreover, Fischer (Theorem 6.9.9 in "Polynomial based iteration methods for symmetric linear systems") Freund (1983), Freund Golub Nachtigal (1992), and Ramage Silvester Wathen (1995) give different poofs that MINRES and CG perform redundant iterations.

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Iterative Methods I

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Fact: . . . none exploits the SQD structure and they are doing redundant iterations

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

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are the optimality conditions of

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

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or of

$$\underset{\mathbf{x},\mathbf{y}}{\text{minimize}} \;\; \tfrac{1}{2}(\|\mathbf{x}\|^2_{\mathbf{M}} + \|\mathbf{y}\|^2_{\mathbf{N}}) \quad \text{subject to} \;\; \mathbf{M}\mathbf{x} + \mathbf{A}\mathbf{y} = \mathbf{b}.$$

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Some properties of SQD matrices

Let us denote the Cholesky factors of **M** and **N** by **R** and **U** (upper triangular matrices).

$$\mathbf{H} = \begin{bmatrix} \mathbf{M} & \\ & \mathbf{N} \end{bmatrix} = \begin{bmatrix} \mathbf{R}^T\mathbf{R} & \\ & \mathbf{U}^T\mathbf{U} \end{bmatrix} = \widetilde{\mathbf{R}}^T\widetilde{\mathbf{R}}$$

We observe that

$$\mathbf{C} = \begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix} = \begin{bmatrix} \mathbf{R}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{U}^T \end{bmatrix} \begin{bmatrix} \mathbf{I}_m & \tilde{\mathbf{A}} \\ \tilde{\mathbf{A}}^T & -\mathbf{I}_n \end{bmatrix} \begin{bmatrix} \mathbf{R} & \mathbf{0} \\ \mathbf{0} & \mathbf{U} \end{bmatrix} = \widetilde{\mathbf{R}}^T\widetilde{\mathbf{C}}\widetilde{\mathbf{R}},$$

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$$\mathbf{H}^{-1}\mathbf{C} = \widetilde{\mathbf{R}}^{-1}\widetilde{\mathbf{C}}\widetilde{\mathbf{R}}$$

Some properties of SQD matrices

By direct computation it is easy to prove that

$$\widetilde{\mathbf{C}}^2 = \begin{bmatrix} \mathbf{I}_m + \tilde{\mathbf{A}}\tilde{\mathbf{A}}^T & \\ & \mathbf{I}_n + \tilde{\mathbf{A}}^T\tilde{\mathbf{A}} \end{bmatrix} = \begin{bmatrix} \widetilde{\mathbf{D}}_1 & \\ & \widetilde{\mathbf{D}}_2 \end{bmatrix} = \widetilde{\mathbf{D}}.$$

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$$\begin{aligned} \widetilde{\mathbf{C}}^{-1} &= \widetilde{\mathbf{D}}^{-1}\widetilde{\mathbf{C}} = \widetilde{\mathbf{C}}\widetilde{\mathbf{D}}^{-1}; \\ \widetilde{\mathbf{C}}\widetilde{\mathbf{D}} &= \widetilde{\mathbf{C}}^3 = \widetilde{\mathbf{D}}\widetilde{\mathbf{C}}; \\ \mathbf{C}\mathbf{H}^{-1}\mathbf{C} &= \widetilde{\mathbf{R}}^T\widetilde{\mathbf{D}}\widetilde{\mathbf{R}} = \mathbf{D} = \begin{bmatrix} \mathbf{M} + \mathbf{A}\mathbf{N}^{-1}\mathbf{A}^T & \\ & \mathbf{N} + \mathbf{A}^T\mathbf{M}^{-1}\mathbf{A} \end{bmatrix}. \end{aligned}$$

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$$\left(\mathbf{H}^{-1}\mathbf{C}\right)^2 = \widetilde{\mathbf{R}}^{-1}\widetilde{\mathbf{C}}^2\widetilde{\mathbf{R}} = \widetilde{\mathbf{R}}^{-1}\widetilde{\mathbf{D}}\widetilde{\mathbf{R}} = \mathbf{H}^{-1}\mathbf{D},$$

$$\left(\mathbf{H}^{-1}\mathbf{C}\right)^3 = \widetilde{\mathbf{R}}^{-1}\widetilde{\mathbf{C}}^3\widetilde{\mathbf{R}} = \mathbf{H}^{-1}\mathbf{C}\mathbf{H}^{-1}\mathbf{D} = \mathbf{H}^{-1}\mathbf{D}\mathbf{H}^{-1}\mathbf{C}$$

$$\mathbf{C}^{-1} = \mathbf{D}^{-1}\mathbf{C}\mathbf{H}^{-1} = \mathbf{H}^{-1}\mathbf{C}\mathbf{D}^{-1}.$$

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Some properties of SQD matrices

$\widetilde{\mathbf{D}}$ and $\widetilde{\mathbf{C}}$ commute.
Both matrices can be simultaneously diagonalized by the generalized eigenvalues of

$$\mathbf{Cz} = \lambda_j \mathbf{Hz},$$

where the $\lambda_j,\ j = 1, \ldots, p = \mathrm{rank}(\bar{\mathbf{A}})$ are the same eigenvalues of $\widehat{\mathbf{C}}$

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Krylov subspaces

Hereafter we will denote by

$$\widetilde{\mathrm{K}}_i(\widetilde{\mathbf{C}}, \mathbf{z}) = \mathrm{Range}\left\{\mathbf{z}, \widetilde{\mathbf{C}}\mathbf{z}, \widetilde{\mathbf{C}}^2\mathbf{z}, \ldots, \widetilde{\mathbf{C}}^{i-1}\mathbf{z}, \widetilde{\mathbf{C}}^i\mathbf{z}\right\}$$

the Krylov subspace generated by $\widetilde{\mathbf{C}}$ and a vector $\mathbf{z}$. We point out that $\widetilde{\mathrm{K}}_i(\widetilde{\mathbf{C}}, \mathbf{z})$ are also the Krylov subspaces used to define the Lanczos algorithm applied to $\mathbf{C}$ symmetrically preconditioned by $\widetilde{\mathbf{R}}$.

$$\widetilde{\mathrm{K}}_i(\mathbf{H}^{-1}\mathbf{C}, \mathbf{w}) = \widetilde{\mathbf{R}}^{-1}\widetilde{\mathrm{K}}_i(\widetilde{\mathbf{C}}, \mathbf{z}), \ \text{where} \qquad \mathbf{w} = \widetilde{\mathbf{R}}\mathbf{z}.$$

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Krylov subspaces

$$\left.\begin{array}{l}\widetilde{\mathbf{C}}^{2k} = \widetilde{\mathbf{D}}^{k} \\ \widetilde{\mathbf{C}}^{2k+1} = \widetilde{\mathbf{C}}\widetilde{\mathbf{D}}^{k} = \widetilde{\mathbf{D}}^{k}\widetilde{\mathbf{C}}\end{array}\right\}.$$

Therefore,

$$\begin{aligned}\widetilde{\mathrm{K}}_k(\widetilde{\mathbf{C}}, \mathbf{z}) &= \widetilde{\mathrm{K}}_{\lfloor k/2 \rfloor}(\widetilde{\mathbf{D}}, \mathbf{z}) + \widetilde{\mathrm{K}}_{\lceil k/2 \rceil - 1}(\widetilde{\mathbf{D}}, \widetilde{\mathbf{C}}\mathbf{z}) \\ &= \widetilde{\mathrm{K}}_{\lfloor k/2 \rfloor}(\widetilde{\mathbf{D}}, \mathbf{z}) + \widetilde{\mathbf{C}}\widetilde{\mathrm{K}}_{\lceil k/2 \rceil - 1}(\widetilde{\mathbf{D}}, \mathbf{z}).\end{aligned}$$

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Krylov subspaces

Finally, denoting by $\widetilde{\mathbf{D}}_1$ and $\widetilde{\mathbf{D}}_2$ the diagonal blocks of $\widetilde{\mathbf{D}}$, i.e. we have:

$$\widetilde{\mathrm{K}}_i(\widetilde{\mathbf{D}}, \begin{bmatrix} \mathbf{z}^1 \\ \mathbf{z}^2 \end{bmatrix}) = \begin{bmatrix} \mathrm{K}_i(\widetilde{\mathbf{D}}_1, \mathbf{z}^1) \\ 0 \end{bmatrix} \oplus \begin{bmatrix} 0 \\ \mathrm{K}_i(\widetilde{\mathbf{D}}_2, \mathbf{z}^2) \end{bmatrix}$$

and

$$\begin{aligned} \widetilde{\mathbf{C}}\widetilde{\mathrm{K}}_i(\widetilde{\mathbf{D}}, \begin{bmatrix} \mathbf{z}^1 \\ \mathbf{z}^2 \end{bmatrix}) &= \begin{bmatrix} \mathrm{K}_i(\widetilde{\mathbf{D}}_1, \mathbf{z}^1) \\ \tilde{\mathbf{A}}^T \mathrm{K}_i(\widetilde{\mathbf{D}}_1, \mathbf{z}^1) \end{bmatrix} \oplus \begin{bmatrix} \tilde{\mathbf{A}} \mathrm{K}_i(\widetilde{\mathbf{D}}_2, \mathbf{z}^2) \\ -\mathrm{K}_i(\widetilde{\mathbf{D}}_2, \mathbf{z}^2) \end{bmatrix} \\ &= \begin{bmatrix} \mathrm{K}_i(\widetilde{\mathbf{D}}_1, \mathbf{z}^1) \\ \mathrm{K}_i(\widetilde{\mathbf{D}}_2, \tilde{\mathbf{A}}^T \mathbf{z}^1) \end{bmatrix} \oplus \begin{bmatrix} \mathrm{K}_i(\widetilde{\mathbf{D}}_1, \tilde{\mathbf{A}} \mathbf{z}^2) \\ -\mathrm{K}_i(\widetilde{\mathbf{D}}_2, \mathbf{z}^2) \end{bmatrix}. \end{aligned}$$

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Intermezzo

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A personal point of view on preconditioning

Hilbert Space Setting

Let $\mathbf{H} \in \mathrm{R}^{k \times k}$ be a SPD non singular matrix. We have that R^k with the scalar product defined by $\mathbf{u}^T\mathbf{H}\mathbf{v}$ is an Hilbert space.

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Vice versa, every finite dimensional Hilbert space $\mathfrak{H}$ of dimension k and scalar product $(u, v)_{\mathfrak{H}}$ is isometric to R^k with a scalar product defined by the matrix $\mathbf{H}$ that is the Gramian matrix (non singular symmetric and positive definite) associated to the basis $\{\phi_j\}_{j=1,\ldots,k}$ of $\mathfrak{H}$:

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The dual space $\mathfrak{H}^\star$ of $\mathfrak{H}$ is itself an Hilbert space with a scalar product induced by $\mathbf{H}^{-1}$.

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Furthermore, we have that the $\{\phi_i\}$ basis is made by the columns of $\mathbf{H}$ and the corresponding $\{\psi_i\}$ basis for $\mathfrak{H}^\star$ is made by the columns of $\mathbf{H}^{-1}$.

Hilbert Space Setting: duality and adjoint.

Given $z \in \mathfrak{H}^\star$, we have

$$\langle z, u \rangle_{\mathfrak{H}^\star,\mathfrak{H}} = \mathbf{z}^T\mathbf{u} = \mathbf{z}^T\mathbf{H}^{-1}\mathbf{H}\mathbf{u} = (\mathbf{u}, \mathbf{H}^{-1}\mathbf{z})_{\mathbf{H}},$$

$\mathbf{w} = \mathbf{H}^{-1}\mathbf{z}$ Riesz vector corresponding to $w = \sum_j w_j \phi_j \in \mathfrak{H}$.

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Let $\mathscr{C} : \mathfrak{H} \mapsto \mathfrak{F}$
$\mathscr{C}^\star : \mathfrak{F}^\star \mapsto \mathfrak{H}^\star$ (adjoint operator)

$$\langle \mathscr{C}^\star v, u \rangle_{\mathfrak{H}^\star,\mathfrak{H}} \triangleq \langle v, \mathscr{C} u \rangle_{\mathfrak{F}^\star,\mathfrak{F}} \quad \forall v \in \mathfrak{F}^\star, u \in \mathfrak{H}.$$

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Therefore, we have

$$\langle \mathscr{C}^\star v, u \rangle_{\mathfrak{H}^\star,\mathfrak{H}} = (\mathbf{C}\mathbf{u}, \mathbf{F}^{-1}\mathbf{v})_{\mathbf{F}} = \mathbf{u}^T\mathbf{C}^T\mathbf{v}.$$

Hilbert Space Setting: normal equations.

If we assume that $\mathfrak{F} = \mathfrak{H}^\star$ then we have that the "normal equations operator" in the Hilbert space is an operator such that

$$\mathscr{C}^\star \circ \mathscr{H}^{-1} \circ \mathscr{C} : \mathfrak{H} \mapsto \mathfrak{H}^\star,$$

and it is represented by the matrix

$$\mathbf{C}^T \mathbf{H}^{-1} \mathbf{C}.$$

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If $\mathbf{C}^T = \mathbf{C}$ then the corresponding operator $\mathscr{C}$ is self-adjoint. Moreover, we have that the operator

$$\mathscr{H}^{-1} \circ \mathscr{C} : \mathfrak{H} \mapsto \mathfrak{H}$$

maps $\mathfrak{H}$ into itself.

$$\left(\mathscr{H}^{-1} \circ \mathscr{C}\right)^i \triangleq (\mathbf{H}^{-1}\mathbf{C})^i.$$

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Linear operators

Let us consider now the Hilbert spaces

$$\mathfrak{M} := (\mathbb{R}^n, \|\cdot\|_{\mathbf{M}}), \qquad \mathfrak{N} := (\mathbb{R}^m, \|\cdot\|_{\mathbf{N}}),$$

and their dual spaces

$$\mathfrak{M}^\star := (\mathbb{R}^n, \|\cdot\|_{\mathbf{M}^{-1}}), \qquad \mathfrak{N}^\star := (\mathbb{R}^m, \|\cdot\|_{\mathbf{N}^{-1}}),$$

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$$\mathscr{A} : \mathfrak{N} \rightarrow \mathfrak{M}^\star$$

$$\langle \mathscr{A} y, u \rangle_{\mathfrak{M}^\star, \mathfrak{M}} \triangleq (\mathbf{u}, \mathbf{M}^{-1}\mathbf{A}\mathbf{y})_{\mathbf{M}} = \mathbf{u}^T\mathbf{A}\mathbf{y}, \quad y \in \mathfrak{N}, \forall u \in \mathfrak{M},$$

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$$\mathscr{A} : \mathfrak{N} \to \mathfrak{M}^\star$$

$$\langle \mathscr{A} y, u \rangle_{\mathfrak{M}^\star, \mathfrak{M}} \triangleq (\mathbf{u}, \mathbf{M}^{-1}\mathbf{A}\mathbf{y})_{\mathbf{M}} = \mathbf{u}^T\mathbf{A}\mathbf{y}, \quad y \in \mathfrak{N}, \forall u \in \mathfrak{M},$$

$$\langle \mathscr{A}^\star u, y \rangle_{\mathfrak{N}^\star, \mathfrak{N}} := (\mathbf{y}, \mathbf{N}^{-1}\mathbf{A}^T\mathbf{u})_{\mathbf{N}} = \mathbf{y}^T\mathbf{A}^T\mathbf{u}, \quad u \in \mathfrak{M}, \forall y \in \mathfrak{N},$$

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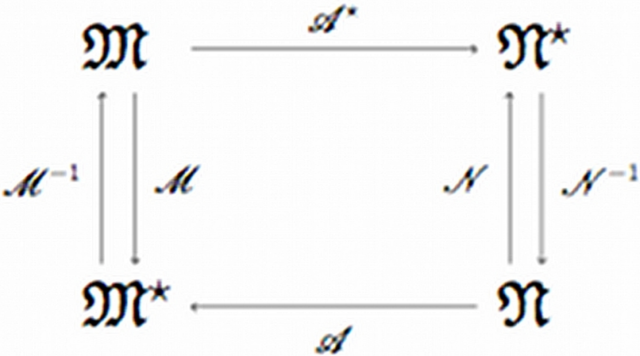
Linear operators



Linear operators

$$\mathbf{C} = \begin{bmatrix} \mathbf{M} & \mathbf{A} \\ \mathbf{A}^T & -\mathbf{N} \end{bmatrix}$$

$$\mathscr{C} : \mathfrak{M} \times \mathfrak{N} \mapsto \mathfrak{M}^\star \times \mathfrak{N}^\star.$$

The scalar product in $\mathfrak{M} \times \mathfrak{N}$ is represented by the matrix

$$\mathbf{H} = \begin{bmatrix} \mathbf{M} & \\ & \mathbf{N} \end{bmatrix}.$$

Generalized SVD

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

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

are the "*elliptic singular values and singular vectors*" of $\mathbf{A}$.

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Generalized SVD

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

are the "*elliptic singular values and singular vectors*" of **A**.
The saddle-point conditions are

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

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

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

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

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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 Benbow (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

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

where

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

Generalized Golub-Kahan bidiagonalization

$$\begin{cases} \mathbf{AQ} = \mathbf{MV}\begin{bmatrix} \mathbf{B} \\ 0 \end{bmatrix} & \mathbf{V}^T\mathbf{MV} = \mathbf{I}_m \\ \mathbf{A}^T\mathbf{V} = \mathbf{NQ}\left[\mathbf{B}^T; 0\right] & \mathbf{Q}^T\mathbf{NQ} = \mathbf{I}_n \end{cases}$$

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

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

$$\begin{aligned} &\mathbf{w} = \mathbf{M}^{-1}\mathbf{A}\mathbf{q}_1 \\ &\alpha_1 = \sqrt{\mathbf{w}^T\mathbf{M}\mathbf{w}} = \sqrt{\mathbf{w}\mathbf{A}\mathbf{q}_1} \\ &\mathbf{v}_1 = \mathbf{w}/\alpha_1. \end{aligned}$$

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Algorithm

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

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

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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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i.e.:

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

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or:

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

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Generalized LSQR

Solve

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

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

Generalized LSQR

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

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

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

Generalized LSQR

Solve

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

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

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

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

and we have that

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

Error bound

Lower bound We can estimate $||\bar{\mathbf{y}} - \mathbf{y}_k||^2_{\mathbf{N}+\mathbf{A}^T\mathbf{M}^{-1}\mathbf{A}}$ by the lower bound

$$\xi^2_{k,d} = \sum_{j=k+1}^{k+d+1} \phi_j^2 < ||\bar{\mathbf{y}} - \mathbf{y}_k||^2_{\mathbf{N}+\mathbf{A}^T\mathbf{M}^{-1}\mathbf{A}}.$$

and $||\bar{\mathbf{y}}||^2_{\mathbf{N}+\mathbf{A}^T\mathbf{M}^{-1}\mathbf{A}}$ by the lower bound $\sum_{j=1}^{k} \phi_j^2$.
Given a threshold $\tau < 1$ and an integer d, we can stop the iterations when

$$\xi^2_{k,d} \leq \tau \sum_{j=1}^{k+d+1} \phi_j^2 < \tau \sum_{j=1}^{k} \phi_j^2 < \tau||\bar{\mathbf{y}}||^2_{\mathbf{N}+\mathbf{A}^T\mathbf{M}^{-1}\mathbf{A}}.$$

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$$\xi^2_{k,d} \leq \tau \sum_{j=1}^{k+d+1} \phi_j^2 < \tau \sum_{j=1}^{k} \phi_j^2 < \tau ||\bar{\mathbf{y}}||^2_{\mathbf{N}+\mathbf{A}^T\mathbf{M}^{-1}\mathbf{A}}.$$

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).

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Generalized CRAIG

$$\min_{\mathbf{y},\mathbf{x}} \ \frac{1}{2}(\|\mathbf{y}\|_{\mathbf{N}}^2 + \|\mathbf{x}\|_{\mathbf{M}}^2) \quad \text{s.t. } \mathbf{A}\mathbf{y} + \mathbf{M}\mathbf{x} = \mathbf{b}.$$

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Generalized CRAIG

$$\min_{\mathbf{y},\mathbf{x}} \ \tfrac{1}{2}(\|\mathbf{y}\|^2_{\mathbf{N}} + \|\mathbf{x}\|^2_{\mathbf{M}}) \quad \text{s.t. } \mathbf{A}\mathbf{y} + \mathbf{M}\mathbf{x} = \mathbf{b}.$$

At step k of GK bidiagonalization, we seek

$$\mathbf{x} \approx \mathbf{x}_k := \mathbf{U}_k\bar{\mathbf{x}}_k, \qquad \text{and} \qquad \mathbf{y} \approx \mathbf{y}_k := \mathbf{V}_k\bar{\mathbf{y}}_k.$$

Generalized CRAIG

$$\min_{\mathbf{y},\mathbf{x}} \ \tfrac{1}{2}(\|\mathbf{y}\|_{\mathbf{N}}^2 + \|\mathbf{x}\|_{\mathbf{M}}^2) \quad \text{s.t. } \mathbf{A}\mathbf{y} + \mathbf{M}\mathbf{x} = \mathbf{b}.$$

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$$\min_{\bar{\mathbf{y}},\bar{\mathbf{x}}} \ \tfrac{1}{2}(\|\bar{\mathbf{y}}\|^2 + \|\bar{\mathbf{x}}\|^2) \quad \text{s.t. } \mathbf{B}_k \bar{\mathbf{y}}_k + \bar{\mathbf{x}}_k = \beta_1 \mathbf{e}_1$$

Generalized CRAIG

$$\min_{\mathbf{y},\mathbf{x}} \ \tfrac{1}{2}(\|\mathbf{y}\|_{\mathbf{N}}^2 + \|\mathbf{x}\|_{\mathbf{M}}^2) \quad \text{s.t. } \mathbf{A}\mathbf{y} + \mathbf{M}\mathbf{x} = \mathbf{b}.$$

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or:

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

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Generalized CRAIG

By contrast with generalized LSQR, we solve the SQD subsystem

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

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Following Saunders (1995) and Paige (1974), we compute an LQ factorization to the k-by-$2k$ matrix $\begin{bmatrix} \mathbf{B}_k & \mathbf{I}_k \end{bmatrix}$ by applying $2k-1$ Givens rotations that zero out the identity block.

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Generalized CRAIG

By contrast with generalized LSQR, we solve the SQD subsystem

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

$$\begin{bmatrix} \mathbf{B}_k & \mathbf{I}_k \end{bmatrix} \mathbf{Q}_k^T = \begin{bmatrix} \hat{\mathbf{B}}_k & 0 \end{bmatrix} \qquad \mathbf{Q}_k^T \mathbf{Q}_k = \mathbf{I}$$

where

$$\hat{\mathbf{B}}_k := \begin{bmatrix} \hat{\alpha}_1 & & & \\ \hat{\beta}_2 & \hat{\alpha}_2 & & \\ & \ddots & \ddots & \\ & & \hat{\beta}_k & \hat{\alpha}_k \end{bmatrix}.$$

Generalized CRAIG

$$\beta_1 \mathbf{e}_1 = \mathbf{B}_k \bar{\mathbf{y}}_k + \bar{\mathbf{x}}_k = \begin{bmatrix} \mathbf{B}_k & I_k \end{bmatrix} \begin{bmatrix} \bar{\mathbf{y}}_k \\ \bar{\mathbf{x}}_k \end{bmatrix} =$$

$$\begin{bmatrix} \hat{\mathbf{B}}_k & 0 \end{bmatrix} \mathbf{Q}_k \begin{bmatrix} \bar{\mathbf{y}}_k \\ \bar{\mathbf{x}}_k \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{B}}_k & 0 \end{bmatrix} \begin{bmatrix} \bar{\mathbf{z}}_k \\ 0 \end{bmatrix} = \hat{\mathbf{B}}_k \bar{\mathbf{z}}_k,$$

for some $\bar{\mathbf{z}}_k \in \mathrm{R}^k$: $\bar{\mathbf{z}}_k = (\zeta_1, \ldots, \zeta_k)$

Generalized CRAIG

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$$\begin{bmatrix} \hat{\mathbf{B}}_k & 0 \end{bmatrix} \mathbf{Q}_k \begin{bmatrix} \bar{\mathbf{y}}_k \\ \bar{\mathbf{x}}_k \end{bmatrix} = \begin{bmatrix} \hat{\mathbf{B}}_k & 0 \end{bmatrix} \begin{bmatrix} \bar{\mathbf{z}}_k \\ 0 \end{bmatrix} = \hat{\mathbf{B}}_k \bar{\mathbf{z}}_k,$$

for some $\bar{\mathbf{z}}_k \in \mathrm{R}^k$: $\bar{\mathbf{z}}_k = (\zeta_1, \ldots, \zeta_k)$

$$\zeta_1 = \beta_1/\hat{\alpha}_1, \quad \zeta_{i+1} = -\hat{\beta}_{i+1}\zeta_i/\hat{\alpha}_{i+1}, \quad (i = 1, \ldots, k-1).$$

Generalized CRAIG: errors bound

Moreover, for $k = 1, \ldots, p := \min(m, n)$,

$$\|\mathbf{x}_k\|^2_{\mathbf{M}} + \|\mathbf{y}_k\|^2_{\mathbf{N}} = \sum_{i=1}^{k} \zeta_i^2,$$

$$\|\mathbf{x}^* - \mathbf{x}_k\|^2_{\mathbf{M}} + \|\mathbf{y}^* - \mathbf{y}_k\|^2_{\mathbf{N}} = \sum_{i=k+1}^{p} \zeta_i^2.$$

Generalized CRAIG: errors bound

Moreover, for $k = 1, \ldots, p := \min(m, n)$,

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$$\|\mathbf{x}^* - \mathbf{x}_k\|^2_{\mathbf{M}} + \|\mathbf{y}^* - \mathbf{y}_k\|^2_{\mathbf{N}} = \sum_{i=k+1}^{p} \zeta_i^2.$$

As for generalized LSQR, we can estimate the error using the windowing technique and we can give a lower bound of the error by

$$\xi^2_{k,d} = \sum_{j=k+1}^{k+d+1} \zeta_i^2 \leq \|\mathbf{x}^* - \mathbf{x}_k\|^2_{\mathbf{M}} + \|\mathbf{y}^* - \mathbf{y}_k\|^2_{\mathbf{N}}$$

and $\|\mathbf{x}_k\|^2_{\mathbf{M}} + \|\mathbf{y}_k\|^2_{\mathbf{N}}$ by the lower bound $\sum_{j=1}^{k} \zeta_j^2$.

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Generalized CRAIG: errors bound

Moreover, for $k = 1, \ldots, p := \min(m, n)$,

$$\|\mathbf{x}_k\|^2_{\mathbf{M}} + \|\mathbf{y}_k\|^2_{\mathbf{N}} = \sum_{i=1}^{k} \zeta_i^2,$$

$$\|\mathbf{x}^* - \mathbf{x}_k\|^2_{\mathbf{M}} + \|\mathbf{y}^* - \mathbf{y}_k\|^2_{\mathbf{N}} = \sum_{i=k+1}^{p} \zeta_i^2.$$

As for GLSQR. If we know a lower bound of singular values we can use an approach inspired by the Gauss-Radau quadrature algorithm and similar to the one described in Golub-Meurant (2010).

Numerical experiments

We will focus on optimization problems:

$$\underset{\mathbf{x}\in\mathrm{R}^n}{\text{minimize}} \ \mathbf{g}^T\mathbf{x} + \tfrac{1}{2}\mathbf{x}^T\mathbf{H}\mathbf{x} \quad \text{subject to } \ \mathbf{C}\mathbf{x} = \mathbf{d}, \ \mathbf{x} \geq 0,$$

where $\mathbf{g} \in \mathrm{R}^n$ and $\mathbf{H} = \mathbf{H}^T \in \mathrm{R}^{n\times n}$ is positive semi-definite, and result in linear systems with coefficient matrix

$$\begin{bmatrix} \mathbf{H} + \mathbf{X}^{-1}\mathbf{Z} + \rho\mathbf{I} & \mathbf{C}^T \\ \mathbf{C} & -\delta\mathbf{I} \end{bmatrix}$$

where $\rho > 0$ and $\delta > 0$ are regularization parameters.

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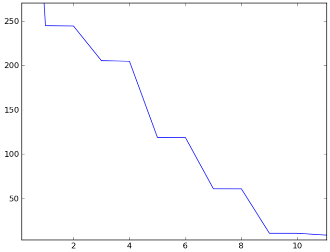
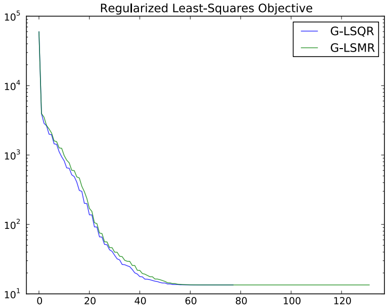
Numerical experiments MINRES

This is a blow-up of some iterations



Numerical experiments GLSQR



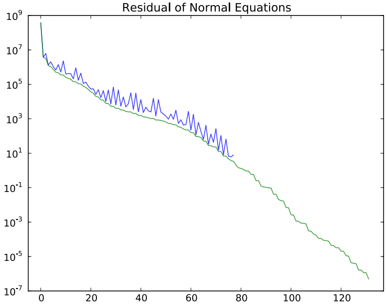


Figure: Problem DUAL1 $(255, 171)$.

Numerical experiments GLSQR

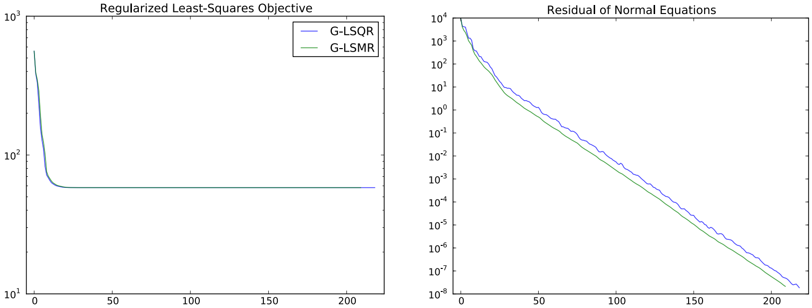


Figure: Problem MOSARQP1 $(5700, 3200)$.

How to choose d?

problem	m	n
dual1	255	171
stcqp1	12291	10246
qpcboei1	1355	980

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Numerical experiments GCraig

$d = 5, 15$

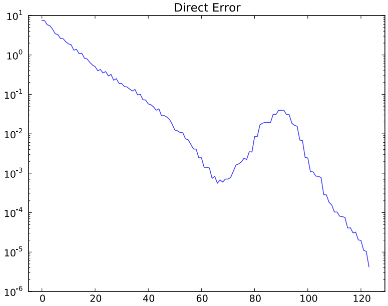

Figure: Problem dual1

Numerical experiments GCraig

$d = 5, 15$

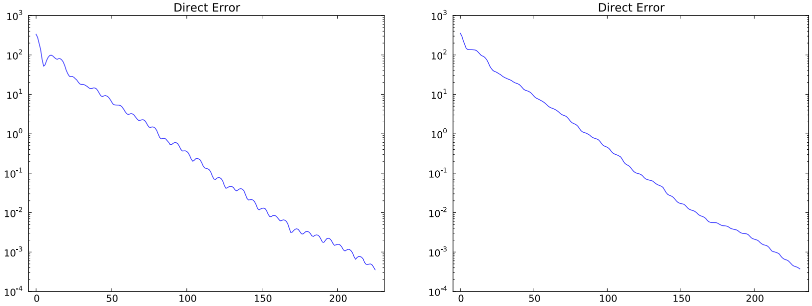

Figure: Problem stcqp1

Numerical experiments GCraig

$d = 5, 15$

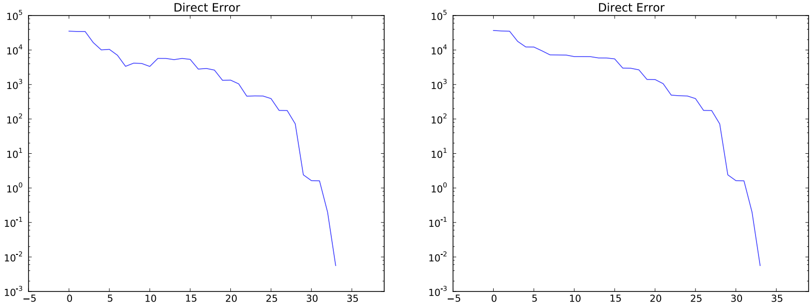

Figure: Problem qpcboei1

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

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