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Generalized Golub-Kahan bidiagonalization and stopping criteria

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Granlibakken 13 June 2011

Overview of talk

- Augmented Systems
- Symmetric Quasi Positive Definite matrices

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- Augmented Systems
  - Generalized singular values and minimization problem
  - G-K bidiagonalization
  - Stopping criteria
  - Numerical examples
- Symmetric Quasi Positive Definite matrices
  - Work in progress in collaboration with Dominique Orban (GERAD and École Polytechnique de Montréal)

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Linear operators

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

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

$$\mathcal{M}' = \{\mathbf{w} \in \mathbf{R}^m; \|\mathbf{w}\|^2_{\mathbf{M}^{-1}} = \mathbf{w}^T\mathbf{M}^{-1}\mathbf{w}\},$$
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$$\langle \mathbf{v}, \mathbf{A}\mathbf{q}\rangle_{\mathcal{M},\mathcal{M}'} = \mathbf{v}^T\mathbf{A}\mathbf{q}, \quad \mathbf{A}\mathbf{q} \in \mathcal{L}(\mathcal{M})\ \forall \mathbf{q} \in \mathcal{N}.$$

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

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

Generalized SVD

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

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

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

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are the "*generalized singular values and singular vectors*" of $\mathbf{A}$.
The saddle-point conditions are

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

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

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Generalized SVD

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

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

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

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

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

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

as a projection problem

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

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)).

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Generalized Golub-Kahan bidiagonalization

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

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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Generalized Golub-Kahan bidiagonalization

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

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

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

can be transformed by the change of variables

$$\begin{cases} \mathbf{u} = \mathbf{V}\mathbf{z} \\ \mathbf{p} = \mathbf{Q}\mathbf{y} \end{cases}$$

Algorithm

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

Algorithm

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

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Algorithm

$$\left[\begin{array}{cc} \mathbf{I}_n & \mathbf{B} \\ \mathbf{B}^T & 0 \end{array}\right]\left[\begin{array}{c} \mathbf{z}_1 \\ \mathbf{y} \end{array}\right]=\left[\begin{array}{c} 0 \\ \mathbf{Q}^T\mathbf{b} \end{array}\right].$$

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

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

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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

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

Algorithm

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

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

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

$\mathbf{u}$

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

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

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

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

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 $\mathbf{D}_k = \mathbf{B}_k^{-T}\mathbf{Q}_k^T$

$$\mathbf{d}_i = \frac{\mathbf{q}_i - \beta_i \mathbf{d}_{i-1}}{\alpha_i} \qquad i = 1, \ldots, n \ \left(\mathbf{d}_0 = 0\right)$$

where $\mathbf{d}_j$ are the columns of $\mathbf{D}$.
Starting with $\mathbf{p}^{(1)} = -\zeta_1 \mathbf{d}_1$ and $\mathbf{u}^{(1)} = \zeta_1 \mathbf{v}_1$

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

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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Stopping criteria

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

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

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Stopping criteria

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

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

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

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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

$$\xi_{k,d}^2 \leq \tau \sum_{j=1}^{k+d+1} \zeta_j^2 < \tau \|\mathbf{u}\|_{\mathbf{M}}^2.$$

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Error bound

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

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

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

$$\xi^2_{k,d} \leq \tau \sum_{j=1}^{k+d+1} \zeta_j^2 < \tau \|\mathbf{u}\|^2_{\mathbf{M}}.$$

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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Two examples

Stokes

The Stokes problems have been generated using the software provided by **ifiss3.0** package (Elman, Ramage, and Silvester). We use the default geometry of "Step case" and the **Q2-Q1** approximation described in **ifiss3.0** manual and in Elman, Silvester, and Wathen (2005).

name	m	n	nnz(**M**)	nnz(**A**)
Step1	418	61	2126	1603
Step2	1538	209	10190	7140
Step3	5890	769	44236	30483
Step4	23042	2945	184158	126799
Step5	91138	11521	751256	518897

(nnz(**M**) is only for the symmetric part)

Two examples

name	# Iter.s	$\|\mathbf{e}^{(k)}\|_2$	$\|\mathbf{A}^T\mathbf{u}^{(k)} - \mathbf{b}\|_2$	$\|\mathbf{p} - \mathbf{p}^{(k)}\|_2$	$\kappa(\mathbf{B})$
Step1	30	6.8e-16	5.1e-16	1.1e-13	7.6
Step2	32	5.4e-14	5.4e-14	5.0e-12	7.7
Step3	34	3.8e-14	2.7e-14	1.0e-11	7.8
Step4	34	5.0e-13	1.3e-13	1.4e-10	7.8
Step5	35	1.8e-13	3.1e-14	1.7e-10	7.8

Stokes (Step) problems results ($d = 5$, $\tau = 10^{-8}$).

Two examples

Poisson with mixed b.c. Problems The Poisson problem is casted in its dual form as a Darcy's problem:

$$\begin{cases} \text{Find} \quad w \in \mathcal{H} = \{\vec{q} \mid \vec{q} \in H_{div}(\Omega),\ \vec{q} \cdot \mathbf{n} = 0 \ \text{ on } \partial_N(\Omega)\},\ u \in L^2(\Omega) \\ \int_\Omega \vec{w} \cdot \vec{q} + \int_{\Omega)} div(\vec{q})u = \int_{\partial_D(\Omega)} u_D \vec{q} \cdot \mathbf{n} \ \ \forall \vec{q} \in \mathcal{H} \\ \int_\Omega div(\vec{w})v = \int_\Omega fv \ \ \forall v \in L^2(\Omega). \end{cases}$$

We approximated the spaces $\mathcal{H}$ and $L^2(\Omega)$ by RT0 and by piecewise constant functions respectively The matrix $\mathbf{N}$ is the mass matrix for the piecewise constant functions and it is a diagonal matrix with diagonal entries equal to the area of the corresponding triangle. The matrix $\mathbf{M}$ has been chosen such that each approximation $\mathcal{H}_h$ of $\mathcal{H}$ is

$$\mathcal{H}_h = \left\{ \mathbf{q} \in \mathrm{R}^m \ \|\mathbf{q}\|^2_{\mathcal{H}_h} = \mathbf{q}^T \mathbf{M} \mathbf{q} \right\}.$$

Therefore, denoting by $\mathbf{W}$ the mass matrix for $\mathcal{H}_h$, we have

$$\mathbf{M} = \mathbf{W} + \mathbf{A}\mathbf{N}^{-1}\mathbf{A}^T.$$

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Two examples

Poisson with mixed b.c. Problems

$h = 2^{-k}$	m	n	nnz($\mathbf{M}$)	nnz($\mathbf{A}$)
2^{-6}	12288	8192	36608	24448
2^{-7}	49152	32768	146944	98048
2^{-8}	196608	131072	588800	392704
2^{-9}	786432	524288	2357248	1571840

(nnz($\mathbf{M}$) is only for the symmetric part)

With the chosen boundary conditions, it is easy to verify that the continuous solution u is $u(x, y) = x$.
We point out that the pattern of $\mathbf{W}$ is structurally equal to the pattern $\mathbf{A}\mathbf{N}^{-1}\mathbf{A}^T$.

Two examples

name	# Iter.s	$\|\mathbf{e}^{(k)}\|_2$	$\|\mathbf{A}^T\mathbf{u}^{(k)} - \mathbf{b}\|_2$	$\|\mathbf{p} - \mathbf{p}^{(k)}\|_2$	$\kappa(\mathbf{B})$
$h = 2^{-6}$	10	2.8e-12	2.9e-16	4.1e-11	1.05
$h = 2^{-7}$	10	9.7e-12	3.0e-16	2.6e-10	1.05
$h = 2^{-8}$	10	2.5e-11	3.0e-16	7.9e-10	1.05
$h = 2^{-9}$	10	2.9e-10	2.8e-16	1.3e-08	1.05

Poisson with mixed b.c. data and RT0 problem results ($d = 5$, $\tau = 10^{-8}$).

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).

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Iterative Methods I

Facts: SQD systems are symmetric, non-singular, square and indefinite.

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- MINRES
- SYMMLQ
- (F)GMRES??
- QMRS????

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Fact: ... none exploits the SQD structure.

Iterative Methods I

Facts: SQD systems are symmetric, non-singular, square and indefinite.

- MINRES
- SYMMLQ
- (F)GMRES??
- QMRS????

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

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

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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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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

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

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

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

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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$\mathbf{R}_k$ will be upper bidiagonal)

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

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

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

and we have that

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

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Conclusions

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

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