Numerical Computations of the Singular Values by the Inverse Iteration

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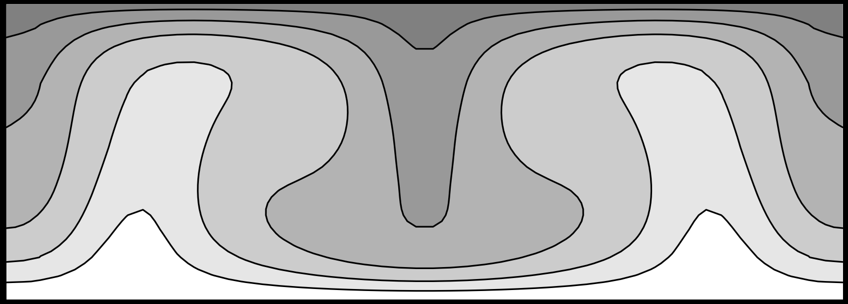
Motivation

In numerical verified computations of stationary solutions for the Rayleigh-Bénard convection, the linear equations account for the most part of all calculation.



2001 RIMS Workshop:
“Discretization Methods and Numerical Algorithms for Differential Equations”
Organizer: KAKO, Takashi
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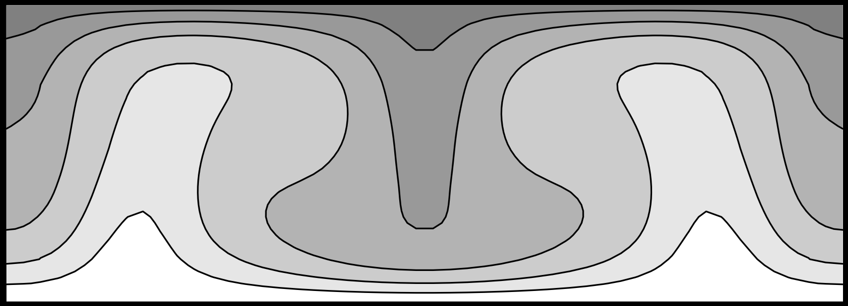

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$\Downarrow$

matrices: large scale and unsymmetry

Linear Equations

$$\boxed{A\boldsymbol{x} = \boldsymbol{b}}$$

- $A \in \boldsymbol{R}^{n\times n},\ \boldsymbol{x}, \boldsymbol{b} \in \boldsymbol{R}^n$
- $\hat{\boldsymbol{x}} \in \boldsymbol{R}^n$: approximate solution of $\boldsymbol{x} = A^{-1}\boldsymbol{b}$
- $\boldsymbol{r} := \boldsymbol{b} - A\hat{\boldsymbol{x}} \in \boldsymbol{R}^n$: residual
- $\|\boldsymbol{x}\|_p = \left(\sum_{k=1}^{n} |x_k|^p\right)^{1/p}$, $\quad \|\boldsymbol{x}\|_\infty = \max_{1\le i\le n} |x_i|$
- $\|A\|_p = \max_{\boldsymbol{x}\neq 0} \frac{\|A\boldsymbol{x}\|_p}{\|\boldsymbol{x}\|_p}$

Verification Algorithm

Krawczyk Operator

Let $R \in \boldsymbol{R}^{n\times n}$ be an approximation of A^{-1},

$$K(X) := \hat{\boldsymbol{x}} - R(A\hat{\boldsymbol{x}} - \boldsymbol{b}) + (I - RA)(X - \hat{\boldsymbol{x}}) \subset \boldsymbol{R}^n.$$

If for $X \subset \boldsymbol{R}^n$

$$K(X) \subset \mathrm{int}(X)$$

holds then A is nonsingular and the unique solution $\boldsymbol{x} = A^{-1}\boldsymbol{b}$ satisfies

$$\boldsymbol{x} \in \hat{\boldsymbol{x}} + K(X)$$

Verification Algorithm

Krawczyk Operator $\Rightarrow$ stable but slow

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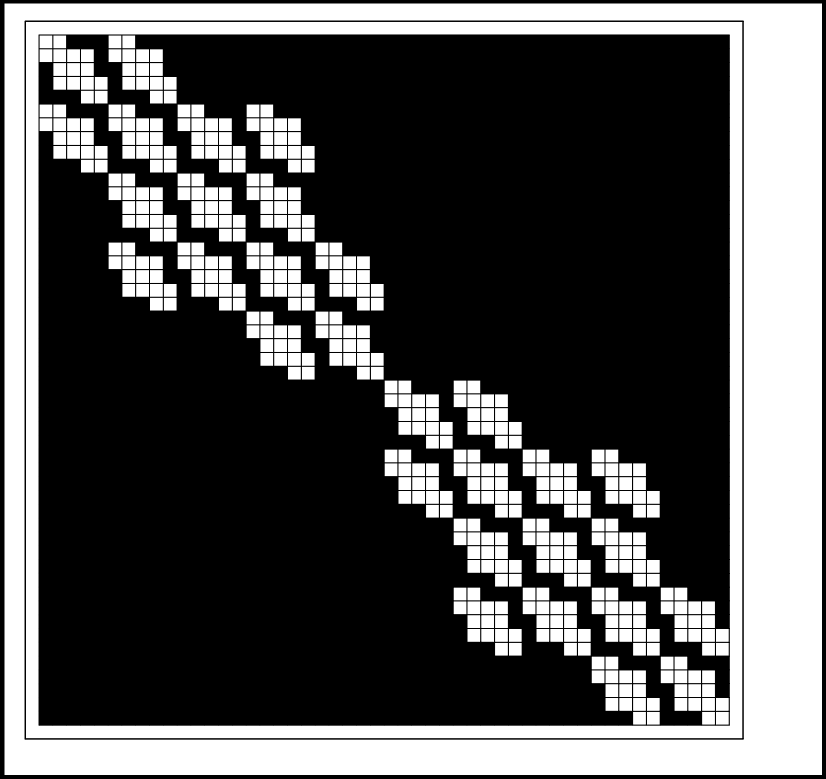
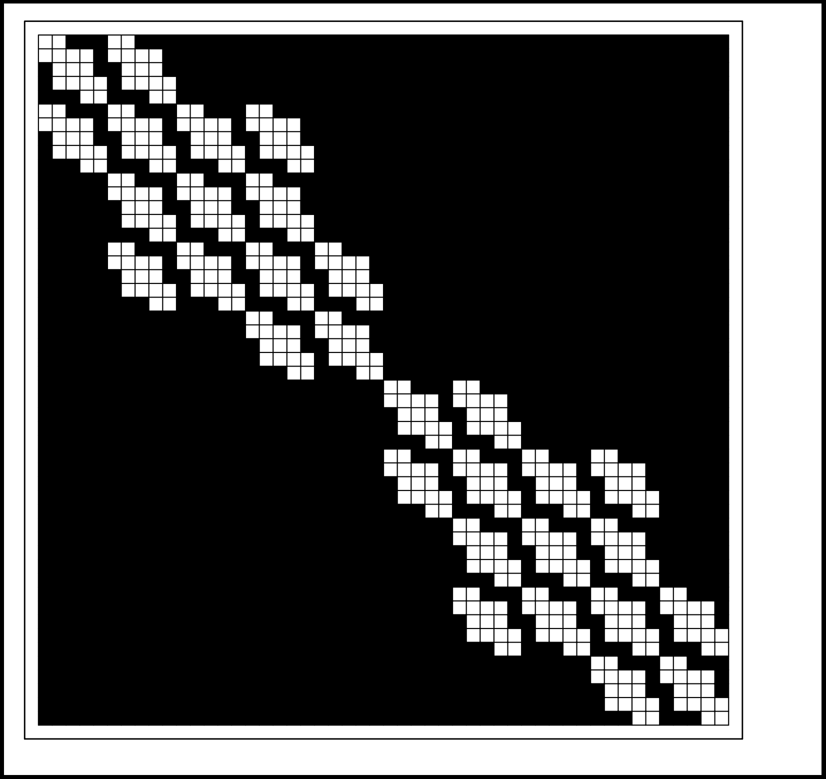
LU Decomposition for Band Matrices

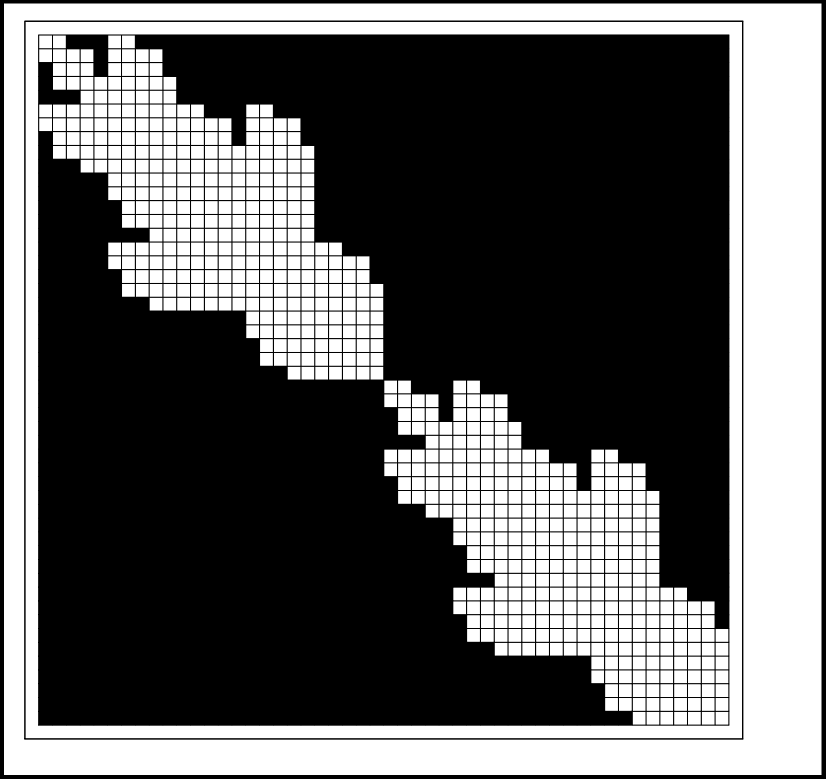


before LU decomposition

black: zero, white: non-zero

LU Decomposition for Band Matrices





before LU decomposition after LU decomposition

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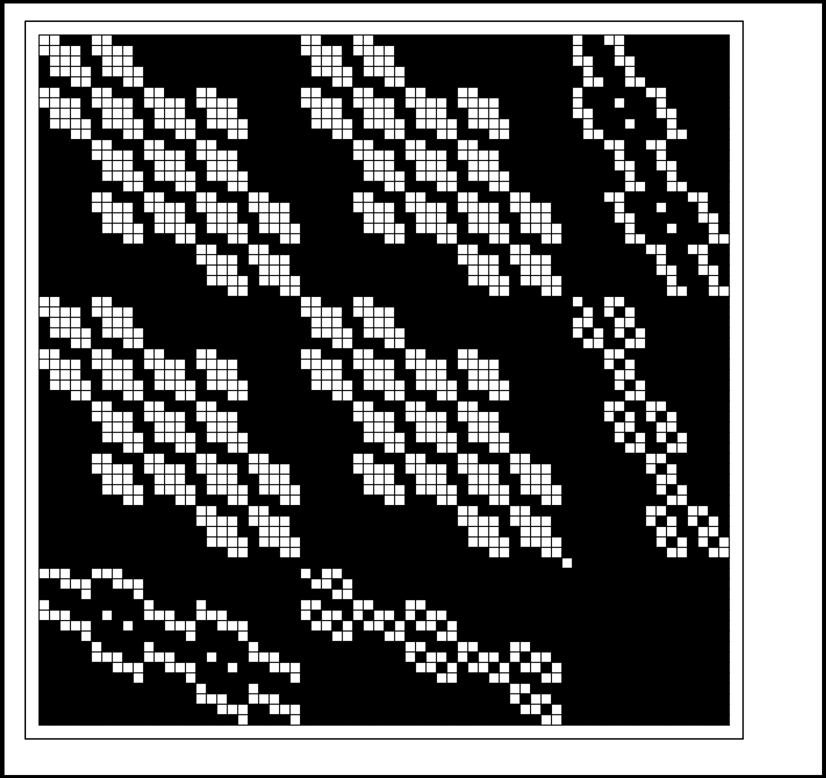
Fill-in



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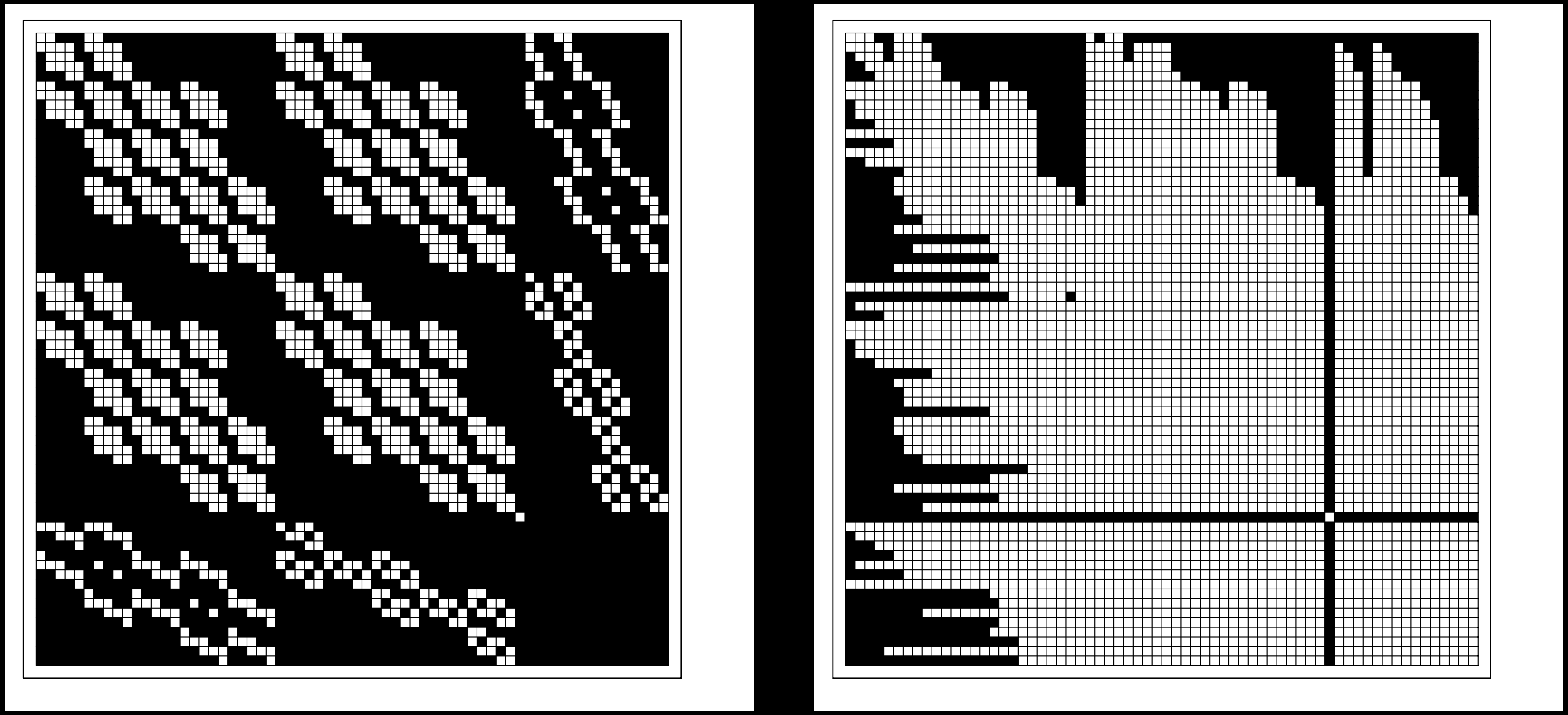

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Aim

When A is unsymmetric or indefinite matrix, is there any guaranteed accuracy method obtaining the solution of the linear system *without matrix decomposition* (LU, LDL^T, LDM, CC^T, QR, etc.)?

$$\|\boldsymbol{x} - \hat{\boldsymbol{x}}\| < \varepsilon, \quad \frac{\|\boldsymbol{x} - \hat{\boldsymbol{x}}\|}{\|\hat{\boldsymbol{x}}\|} < \varepsilon, \quad \frac{\|\boldsymbol{x} - \hat{\boldsymbol{x}}\|}{\|\boldsymbol{x}\|} < \varepsilon$$

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conclusion

difficult!

Validated Solution of Linear Systems

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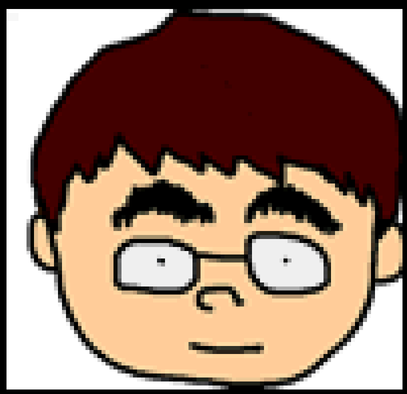

Oishi-Rump

$$A \approx LU$$

$$\|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_\infty \le \frac{\|(U^{-1}L^{-1})(A\hat{\boldsymbol{x}} - \boldsymbol{b})\|_\infty}{1 - \|(U^{-1}L^{-1})A - I\|_\infty}$$

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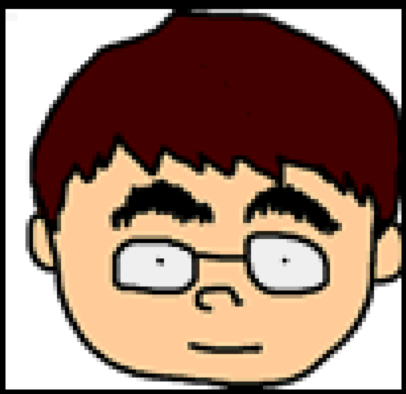

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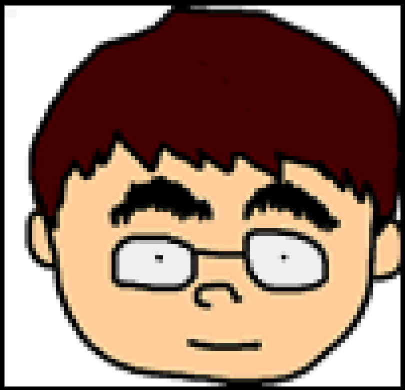
$$\|\boldsymbol{x} - \hat{\boldsymbol{x}}\|_\infty \le \frac{n^{1/2}\|A\hat{\boldsymbol{x}} - \boldsymbol{b}\|_\infty}{\sigma_{\min}(LU) - n^{1/2}\|LU - A\|_\infty}$$

$$\sigma_{\min}(LU) \ge \sigma_{\min}(L)\,\sigma_{\min}(U)$$

Validated Solution of Linear Systems



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Yamamoto. N

$$A \approx LDL^T$$

smallest singular value
for symmetric matrix

Smallest Singular Values

Let $L, \tilde{G} \in \boldsymbol{R}^{n\times n}$, $\tilde{\lambda} \in \boldsymbol{R}$

$$E := \tilde{G}\tilde{G}^T - (LL^T - \tilde{\lambda}I).$$

If $\tilde{\lambda} \geq \|E\|$ for some consistent matrix norm then

$$\sigma_{\min}(L) \geq (\tilde{\lambda} - \|E\|)^{1/2}.$$

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END! ...but still have time

Singular Value Decomposition

$$\boxed{A = U \Sigma V^T}$$

$$UU^T = VV^T = I, \quad \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n),$$
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for $1 \le i \le n$

- $\sigma_i \ge 0$
- λ_i: eigenvalue of $A^T A \quad \longrightarrow \quad \sigma_i = \sqrt{\lambda_i}$ (by renumbering)

Rayleigh Quotient

$$A^T A \boldsymbol{x} = \lambda \boldsymbol{x}$$

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a test using random matrix and vector

$A \in \boldsymbol{R}^{n\times n}$, $\boldsymbol{x}_k \in \boldsymbol{R}^n$, $k = 1, \ldots, 1000000$, $n = 100$.

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↑ as we say in Japanese, “TOHOHO”

Approximation of $\|A^{-1}\|_1$

Computes γ and $\boldsymbol{y} = A^{-1}\boldsymbol{x}$ such that $\gamma \le \|A^{-1}\|_1$ with $\|\boldsymbol{y}\|_1/\|\boldsymbol{x}\|_1 = \gamma$

$\boldsymbol{x} = (1, 1, \ldots, 1)^T/n$

repeat

solve $A\boldsymbol{y} = \boldsymbol{x}$

$\boldsymbol{\xi} =$ sign$(\boldsymbol{y})$ and solve $A^T\boldsymbol{z} = \boldsymbol{\xi}$

if $\|\boldsymbol{z}\|_\infty \le \boldsymbol{z}^T\boldsymbol{x}$

$\gamma = \|\boldsymbol{y}\|_1$ and quit

end if

$\boldsymbol{x} = \boldsymbol{e}_j$, where $|z_j| = \|\boldsymbol{z}\|_\infty$ (smallest such j)

end

W.W.Hager, *Condition Estimates*,
SIAM J. Sci. Comput., Vol.5, No.2 (1984), pp.311–316.

Inverse Iteration

Compute an approximation γ of the smallest singular value of A

set an initial guess $\boldsymbol{x}$ such that $\|\boldsymbol{x}\|_2 = 1$

repeat

solve $A\boldsymbol{y} = \boldsymbol{x}$

solve $A^T\boldsymbol{z} = \boldsymbol{y}$

$\boldsymbol{\xi} = \boldsymbol{z}/\|\boldsymbol{z}\|_2$

if $\|\boldsymbol{\xi} - \boldsymbol{x}\|_\infty / \|\boldsymbol{\xi}\|_\infty \le \varepsilon$ (other norms or criterions are available)

$\gamma = 1/\sqrt{\|\boldsymbol{z}\|_2}$ and quit

end if

$\boldsymbol{x} = \boldsymbol{\xi}$

end

Inverse Iteration

Compute an approximation γ of the smallest singular value of A

set an initial guess $\boldsymbol{x}$ such that $\|\boldsymbol{x}\|_2 = 1$

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solve $A\boldsymbol{y} = \boldsymbol{x}$ Linear Equation

solve $A^T\boldsymbol{z} = \boldsymbol{y}$ Linear Equation

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end if

$\boldsymbol{x} = \boldsymbol{\xi}$

end

Solvers

- "SVD"

  Singular value decomposition $A = U\Sigma V^T$ by Householder transformation and implicit QR method with origin shift

- "$A^T A$"

  Compute $A^T A$ and obtain the smalleset eigenvalue for the symmetric matrix by Householder's method and the bisection method

- Systems of linear equations for general matrices (direct method)

GEPP	LU decomposition with the *partial* pivoting
GECP	LU decomposition with the *complete* pivoting

Iterative Linear Solvers

Systems of linear equations with an unsymmetric or indefinite matrix (iterative method)

MGCR	Modified Generalized Conjugate Residuals method
BICGSTAB(l)	Bi-Conjugate Gradient Stabilized(l) method
QMR	Quasi-Minimal Residual method
TFQMR	Tanspose-Free Quasi-Minimal Residual method

stopping criterion: (0=) $\boldsymbol{x}^{(0)} \to \boldsymbol{x}^{(1)} \to \boldsymbol{x}^{(2)} \to \cdots$

$$\|A\boldsymbol{x}^{(k)} - \boldsymbol{b}\|_2 / \|A\boldsymbol{x}^{(0)} - \boldsymbol{b}\|_2 < \delta$$

*)all solvers are selected in subroutine library FUJITSU SSL II V5.1 except GECP with 64bit precision

Example 1 (problem)

The elliptic partial differential operators:

$$
\begin{aligned}
Lu &= -\Delta u + a_1 \frac{\partial u}{\partial x} + a_2 \frac{\partial u}{\partial y} + a_3 \frac{\partial u}{\partial z} + cu \\
\Omega &= [0, l_x] \times [0, l_y] \times [0, l_z] \\
u &= 0 \text{ on } \partial\Omega
\end{aligned}
$$

Discretization

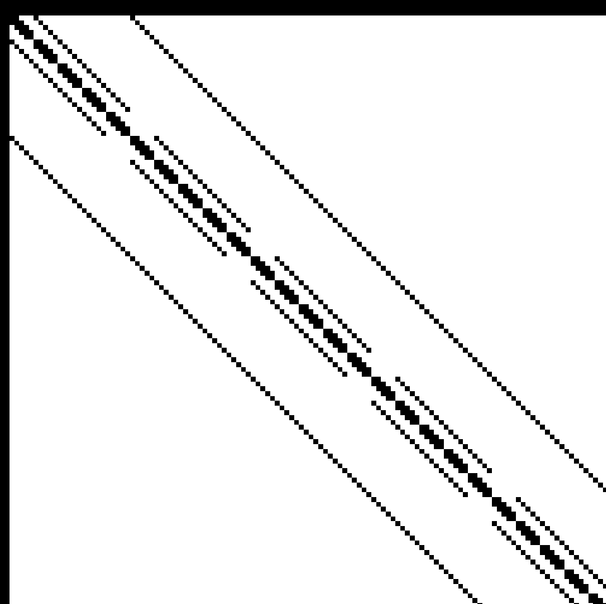
- each dimension of Ω is divided into $n_x + 1$, $n_y + 1$ and $n_z + 1$ in equal subintervals, respectively
- the $n := n_x \times n_y \times n_z$ grid points exist inside Ω.
- $u_{i,j,k} = u(x_i, y_j, z_k)$

Example 1 (discretization)

$$\frac{\partial u}{\partial x}(x_i, y_j, z_k) \simeq \quad (u_{i+1,j,k} - u_{i-1,j,k})(n_x + 1)/(2l_x)$$

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_j, z_k) \simeq \quad (u_{i+1,j,k} - u_{i,j,k} + u_{i-1,j,k})(n_x + 1)^2/{l_x}^2$$

$$\Rightarrow Lu \simeq A\boldsymbol{v}, \qquad A \in \boldsymbol{R}^{n\times n},\ \boldsymbol{v} \in \boldsymbol{R}^n$$



The diagonal storage format

$A \in \boldsymbol{R}^{n\times n} \longrightarrow \tilde{A} \in \boldsymbol{R}^{n\times 7}$

Example1 (part1)

$a_1 = a_2 = a_3 = c = l_x = l_y = l_z = 1$, $n_x = n_y = n_z = 10$,
$n = 1000$, $\delta = \varepsilon = 10^{-6}$.

method	approximation	rel.error	No.	time(sec.)
SVD	30.64520351314805	(assume exact)	—	23.86
$A^T A$	30.64520351315623	2.66×10^{-13}	—	9.28
GEPP	30.64520351315346	1.76×10^{-13}	9	5.60
GECP	30.64520351315355	1.79×10^{-13}	9	21.61
MGCR	30.64520351317838	9.89×10^{-13}	9	0.150
BICGSTAB(l)	30.64520351315359	1.80×10^{-13}	9	0.099
QMR	30.64520351315866	3.46×10^{-13}	9	0.177
TFQMR	30.64520351319651	1.58×10^{-12}	9	0.220

Example1 (part2)

$a_1 = a_2 = a_3 = c = l_x = l_y = l_z = 1,\ n_x = n_y = n_z = 10,$

$n = 1000$, BICGSTAB(l)

$$\longrightarrow \quad \|A\boldsymbol{x}^{(n)} - \boldsymbol{b}\|_2 / \|A\boldsymbol{x}^{(0)} - \boldsymbol{b}\|_2 < \delta$$

ε	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}	10^{-11}	10^{-12}	10^{-13}	10^{-14}	10^{-15}
10^{-1}	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2
10^{-2}	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3
10^{-3}	6	44	4	4	4	4	4	4	4	4	4	4	4	4	4
10^{-4}	113	*	6	6	6	6	6	6	6	6	6	6	6	6	6
10^{-5}	3937	*	17	7	7	7	7	7	7	7	7	7	7	7	7
10^{-6}	*	*	*	9	9	9	9	9	9	9	9	9	9	9	9
10^{-7}	*	*	*	11	12	11	11	11	11	11	11	11	11	11	11
10^{-8}	*	*	*	*	*	15	13	13	13	13	13	13	13	13	13
10^{-9}	*	*	*	*	21	18	14	14	14	14	14	14	14	14	14
10^{-10}	*	*	*	*	*	*	*	24	16	16	16	16	16	16	16
10^{-11}	*	*	*	*	*	*	*	34	23	18	18	18	18	18	18
10^{-12}	*	*	*	*	*	*	*	*	4137	20	20	20	20	20	20
10^{-13}	*	*	*	*	*	*	*	*	*	21	22	21	21	21	21
10^{-14}	*	*	*	*	*	*	*	*	*	26	26	23	23	23	23
10^{-15}	*	*	*	*	*	*	*	*	*	*	*	192	3149	361	69

inverse iteration $\boldsymbol{u}^{(0)} \to \boldsymbol{u}^{(1)} \to \boldsymbol{u}^{(2)} \cdots$

$$\|\boldsymbol{u}^{(m)} - \boldsymbol{u}^{(m-1)}\|_\infty / \|\boldsymbol{u}^{(m-1)}\|_\infty < \varepsilon$$

Example1 (part3)

$a_1 = a_2 = a_3 = 0$, $l_x = l_y = l_z = 1$, $c = -29.4081$,
$n_x = n_y = n_z = 10$, $n = 1000$, $\delta = \varepsilon = 10^{-6}$.

method	approximation	rel.error	No.	time(sec.)
SVD	$7.326361297367409 \times 10^{-9}$	(assume exact)	—	23.49
$A^T A$	$\sqrt{-5.791468462355041 \times 10^{-11}}$	—	—	10.56
GEPP	$7.326403401427804 \times 10^{-9}$	5.74×10^{-6}	2	5.58
GECP	$7.326355667100872 \times 10^{-9}$	7.68×10^{-7}	2	22.71
MGCR	$7.326414257098979 \times 10^{-9}$	7.22×10^{-6}	2	5.57
BICGSTAB(l)	$7.326411417040010 \times 10^{-9}$	6.84×10^{-6}	7	0.337
QMR	$7.326412216218347 \times 10^{-9}$	6.95×10^{-6}	2	0.057
TFQMR	$1.467167322152596 \times 10^{-8}$	1.0025	2	13.37

Example2 (problem)

A sample matrix which the growth factor increases in the process of the Gaussian elimination.

Solve

$$x(s) - \int_0^s k(s,t)x(t)\,dt + \beta(s)x(L) = G(s)$$

with Newton-Cotes and Simpson rule.

Foster, Leslie V.,
Gaussian Elimination with Partial Pivoting Can Fail in Practice,
SIAM Journal on Matrix Analysis and Applications, Vol.15, No.4, pp.1354–1362 (1994).

Example2 (result)

$n = 1000$, $\delta = \varepsilon = 10^{-6}$.

method	approximation	rel.error	No.	time(sec.)
SVD	0.1583383270951388	(assume exact)	—	23.89
$A^T A$	0.1583383270962595	7.07×10^{-12}	—	9.48
GEPP	(failed)	—	—	—
GECP	0.1583383270951446	3.66×10^{-14}	12	22.96
MGCR	0.1583383270951908	3.28×10^{-13}	12	46.29
BICGSTAB(l)	0.1583383270811897	8.80×10^{-11}	12	113.8
QMR	0.1583383272836202	1.19×10^{-9}	12	179.0
TFQMR	0.1583383270658000	1.85×10^{-10}	12	222.8

Example3 (Hilbert Matrix)

$A_{ij} = 1/(i+j-1)$, $\delta = \varepsilon = 10^{-6}$.

dimension	8×8	9×9	10×10	11×11	12×12
$\sigma_{\min}$	1.11×10^{-10}	3.49×10^{-12}	1.09×10^{-13}	3.39×10^{-15}	1.04×10^{-16}

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$\sigma_{\min}$	1.11×10^{-10}	3.49×10^{-12}	1.09×10^{-13}	3.39×10^{-15}	1.04×10^{-16}
$A^T A$	*	*	*	*	*
GEPP	1.27×10^{-8}	1.05×10^{-6}	5.62×10^{-7}	8.11×10^{-4}	5.81×10^{-2}
GECP	4.93×10^{-8}	4.47×10^{-7}	8.06×10^{-6}	3.07×10^{-4}	2.05×10^{-4}
MGCR	1.46×10^{-8}	3.97×10^{-7}	6.71×10^{-6}	2.83×10^{-4}	*
BICGSTAB(l)	7.29×10^{-9}	4.56×10^{-8}	*	*	*
QMR	2.92×10^{-8}	2.98×10^{-6}	1.94×10^{-6}	6.72×10^{13}	4.78×10^{14}
TFQMR	2.28	*	19.58	30.76	5805

Example4 (Random Matrices)

Generate 100 dense matrices. $\delta = \varepsilon = 10^{-6}$.

method	succeed	average precision	average time(sec.)
SVD	100	(assume exaxt)	0.0131
$A^T A$	100	0.215×10^{-6}	0.0966
GEPP	100	0.539×10^{-12}	0.0924
GECP	100	0.452×10^{-12}	0.0158
MGCR	100	0.201×10^{-8}	0.551
BICGSTAB(l)	100	0.586×10^{-9}	3.36
QMR	95	0.240×10^{11}	31.6
TFQMR	99	0.858×10^{-7}	21.8

Example5 (Rayleigh-Bénard Convection)

$$\begin{cases} \mathcal{P}\Delta^2\Psi = \sqrt{\mathcal{P}\mathcal{R}}\,\Theta_x - \Psi_z\Delta\Psi_x + \Psi_x\Delta\Psi_z & \text{in} \quad \Omega, \\ -\Delta\Theta = -\sqrt{\mathcal{P}\mathcal{R}}\,\Psi_x + \Psi_z\Theta_x - \Psi_x\Theta_z & \text{in} \quad \Omega. \end{cases}$$

$$\Omega := \{0 < x < 2\pi/a,\ 0 < z < \pi\}, \quad a > 0.$$

$$\Psi \in \left\{ \sum_{m=1}^{M} \sum_{n=1}^{N} A_{mn} \sin(amx) \sin(nz) \right\}$$

$$\Theta \in \left\{ \sum_{m=0}^{M} \sum_{n=1}^{N} B_{mn} \cos(amx) \sin(nz) \right\}$$

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$$\Uparrow$$

Fourier-Galerkin method combined Newton-Raphson method

Example5 (result)

$N = M = 10$, $n = 110$, $\delta = 10^{-5}$, $\varepsilon = 10^{-6}$.

Inverse iteration is until 100 times.

method	approximation	rel.error	No.	time(sec.)
SVD	131.8910693467725	(assume exact)	—	0.015
A^TA	131.8910681091155	9.38×10^{-9}	—	0.029
GEPP	131.8910693472682	3.75×10^{-12}	6	0.007
GECP	131.8910693472684	3.75×10^{-12}	6	0.018
MGCR	(not converged)	—	100	606
BICGSTAB(l)	(not converged)	—	100	136
QMR	(not converged)	—	100	842
TFQMR	(not converged)	—	100	1136

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How about your matrices and linear solvers ?

We can provide high performance computers and software to estimate singular values!

(9.6Gflops/CPU $\times$ 32)

Problems to be Solve

- other matrices and solvers
  - large scale or parallel computing
  - reordering or DM decomposition
- acceleration
  - Rayleigh-quotient iteration
  - preconditioning and initial value
- guaranteed accuracy
  - information in iterative process
  - stopping criterion / extrapolate error
- benchmarks for linear solvers