On the resolution of linear systems

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Preconditioning

Direct methods Stationary iterative methods Non-Stationary iterative methods

1 Direct methods

2 Stationary iterative methods

3 Non-Stationary iterative methods

Preconditioning

Purpose

- Solve AX = b.
- A is a squared matrix,
- *b* is a given righthand side, or a family of given righthand sides

$$Ax = b \iff Ux : MAx = Mb$$

M is a preconditioner

$$M = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -3 & 1 & 1 \end{pmatrix} \longrightarrow L := M^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & -1 & 1 \end{pmatrix}$$
$$U = MA \iff A = LU, Ax = b \iff LUx = b$$

• LU decomposition $\mathcal{O}(\frac{2n^3}{3})$ elementary operations.

2 Solve Ly = b $O(n^2)$ elementary operations.

3 Solve Ux = y $O(n^2)$ elementary operations.

For *P* values of the righthand side, $N_{op} \sim \frac{2n^3}{3} + P \times 2n^2$.

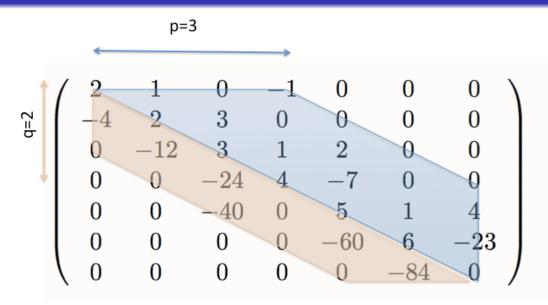


Theorem 1 Let A be an invertible matrix, with principal minors $\neq 0$. Then there exists a unique matrix L lower triangular with $I_{ii} = 1$ for all i, and a unique matrix U upper triangular, such that A = LU. Furthermore $det(A) = \prod_{i=1}^{n} u_{ii}$.

Theorem 2 Let A be an invertible matrix. There exist a permutation matrix P, a matrix L lower triangular with $I_{ii} = 1$ for all i, and a matrix U upper triangular, such that

$$PA = LU$$

Sparse and banded matrices



A banded matrix, upper bandwidth p = 3 and lower bandwidth q = 2, in total p + q + 1 nonzero diagonals.

Direct methods Stationary iterative methods Non-Stationary iterative methods Preconditioning Sparse and banded matrices $U = \begin{pmatrix} 2 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 4 & 3 & -2 & 0 & 0 & 0 \\ 0 & 0 & 12 & -5 & 2 & 0 & 0 \\ 0 & 0 & 0 & 12 & -5 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 20 & 1 & 4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 9 & -11 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -3 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -3 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -3 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -3 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -3 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -3 & 1 & 0 \end{pmatrix}$

Sparse and banded matrices with pivoting

$$L = \left(\begin{array}{cccccccccccccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.6 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ -0.5 & -0.17 & -0.05 & -0.21 & 0.025 & 0.0027 & 1 \end{array}\right)$$

$$U = \left(\begin{array}{cccccccc} -4 & 2 & 3 & 0 & 0 & 0 & 0 \\ 0 & -12 & 3 & 1 & 2 & 0 & 0 \\ 0 & 0 & -40 & 0 & 5 & 1 & 4 \\ 0 & 0 & 0 & 4 & -10 & -0.6 & -2.4 \\ 0 & 0 & 0 & 0 & -60 & 6 & -23 \\ 0 & 0 & 0 & 0 & 0 & -84 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.275 \end{array}\right)$$

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$$P = \left(\begin{array}{cccccccc} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right)$$

Stationary iterative methods

$$AX = b$$
; $A = M - N$; $MX = NX + b$,
 $MX^{m+1} = NX^m + b$.

Use A = D - E - F.

- **1** Jacobi : M = D diagonal part of A.
- **2** Gauss-Seidel : M = D E lower part of A.
- 3 Relaxation : \hat{U}^{m+1} obtained by Gauss-Seidel,

$$X^{m+1} = \omega \hat{U}^{m+1} + (1-\omega)X^m.$$

 $M = \frac{1}{\omega}D - E, \ N = F + \frac{1-\omega}{\omega}D - E$

④ Richardson algorithm

$$X^{m+1} = X^m - \rho r^m = X^m - \rho (AX^m - b)$$
$$M = \frac{1}{\rho} I \quad \rho_{opt} = \frac{2}{\lambda_1 + \lambda_n}$$

Direct methods	Stationary iterative methods	Non-Stationary iterative methods	Preconditioning
Stationary	methods, continue		

$$MX^{m+1} = NX^m + b \iff MX^{m+1} = (M - A)X^m + b$$

$$\iff X^{m+1} = (I - M^{-1}A)X^m + M^{-1}b$$

$$\iff \text{fixed point algorithm to solve } M^{-1}AX = M^{-1}b$$

Preconditioning

$$AX = b \iff M^{-1}AX = M^{-1}b$$

 $\iff X = (I - M^{-1}A)X + M^{-1}b$

Stationary methods, continue

Error
$$e^m := X - X^m$$
,
Residual $r^m := b - AX^m = AX - AX^m = Ae^m$.
 $MX^{m+1} = NX^m + b$
 $MX = NX + b$
 $Me^{m+1} = Ne^m$
 $e^{m+1} = M^{-1}Ne^m$
 $R = M^{-1}N$ is the iteration matrix

Useful alternative formula $R = I - M^{-1}A$.

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Direct methods	Stationary iterative methods	Non-Stationary iterative methods	Preconditioning
Fundament	als tools		

$$X^{m+1} = RX^m + \tilde{b}, \quad e^{m+1} = Re^m, \ R = M^{-1}N.$$

Theorem The sequence is convergent for any initial guess X^0 if and only if $\rho(R) < 1$.

 $\rho(R) = \max\{|\lambda|, \lambda \text{ eigenvalue of } A\}$: convergence factor. To reduce the initial error by a factor ϵ , we need

$$\frac{\|e^m\|}{\|e^0\|} \leq \sim (\rho(R))^m \sim \epsilon$$

So we have $M \sim \frac{\ln \epsilon}{\ln \rho(R)}$. Convergence rate= $-\ln \rho(R)$ digits per iteration.

Symmetric positive definite matrices

Householder-John theorem : Suppose A is positive. If $M + M^T - A$ is positive definite, then $\rho(R) < 1$.

Corollary

- If D + E + F is positive definite, then Jacobi converges.
- 2 If $\omega \in (0, 2)$, then SOR converges.



Tridiagonale matrices

- $\rho(\mathcal{L}_1) = (\rho(J))^2$: Jacobi Gauss-Seidel converge or diverge simultaneously. If convergent, Gauss-Seidel is twice as fast.
- Suppose the eigenvalues of J are real. Then Jacobi and SOR convergent ou converge or diverge simultaneously for ω ∈]0,2[.
- Same assumptions, SOR has an optimal parameter

$$\omega^{*} = \frac{2}{1 + \sqrt{1 - (\rho(J))^{2}}}, \quad \rho(\mathcal{L}_{\omega^{*}}) = \omega^{*} - 1.$$

Descent methods

The descent directions p_m are given. Define

$$X^{m+1} = X^m + \alpha_m p^m, \quad e^{m+1} = e^m - \alpha_m p^m, \quad r^{m+1} = r^m - \alpha_m A p^m.$$

Theorem X is the solution of $AX = b \iff$ it minimizes over \mathbb{R}^N the functional $J(y) = \frac{1}{2}(Ay, y) - (b, y)$. This is equivalent to minimizing $G(y) = \frac{1}{2}(A(y - X), y - X)$ At each step minimize J in the direction of p_m

$$\alpha_m = \frac{(p^m, r^m)}{(Ap^m, p^m)}, \quad (p^m, r^{m+1}) = 0$$

$$G(x^{m+1}) = G(x^m)(1-\mu_m), \quad \mu_m = \frac{(r^m, p^m)^2}{(Ap^m, p^m)(A^{-1}r^m, r^m)}$$

Direct methods	Stationary iterative methods	Non-Stationary iterative methods	Preconditioning
Steepest d	lescent		

$$p^m = r^m$$
.

$$X^{m+1} = X^m + \alpha_m r^m, \quad e^{m+1} = e^m - \alpha_m r^m, \quad r^{m+1} = (I - \alpha_m A) p^m.$$

$$\alpha_m = \frac{\|r^m\|^2}{(Ar^m, r^m)}, \quad (r^m, r^{m+1}) = 0$$

$$G(x^{m+1}) = G(x^m) \left(1 - \frac{\|r^m\|^4}{(Ar^m, r^m)(A^{-1}r^m, r^m)} \right) \le \left(\frac{\kappa(A) - 1}{\kappa(A) + 1} \right)^2 G(x^m)$$

Conjugate gradient

$$X^{m+1} = X^m + \alpha_m p^m, \quad (r^m, p^{m-1}) = 0.$$

Search p^m as $p^m = r^m + \beta_m p^{m-1}$
 $G(x^{m+1}) = G(x^m)(1 - \mu_m)$
 $\mu_m = \frac{(r^m, p^m)^2}{(Ap^m, p^m)(A^{-1}r^m, r^m)} = \frac{\|r^m\|^4}{(Ap^m, p^m)(A^{-1}r^m, r^m)}$
Maximize μ_m , or minimize
 $(Ap^m, p^m) = \beta_m^2(Ap^{m-1}, p^{m-1}) + 2\beta_m(Ap^{m-1}, r^m) + (Ar^m, r^m)$

$$\beta_m = -\frac{(Ap^{m-1}, r^m)}{Ap^{m-1}, p^{m-1}} \quad \Rightarrow (Ap^{m-1}, p^m) = 0$$
$$(r^m, r^{m+1}) = 0, \quad \beta_m = \frac{\|r^m\|^2}{\|r^{m-1}\|^2}.$$

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Direct methods	Stationary iterative methods	Non-Stationary iterative methods	Preconditioning
Other prop	erties		

Choose
$$p^0 = r^0$$
. Then $\forall m \ge 1$, if $r^i \ne 0$ for $i < m$.
(r^m, p^i) = 0 for $i \le m - 1$.
($vec(r^0, ..., r^m) = vec(r^0, Ar^0, ..., A^m r^0)$.
($vec(p^0, ..., p^m) = vec(r^0, Ar^0, ..., A^m r^0)$.
(p^m, Ap^i) = 0 for $i \le m - 1$.
(r^m, r^i) = 0 for $i \le m - 1$.
Definition Krylov space $\mathcal{K}_m = vec(r^0, Ar^0, ..., A^{m-1}r^0)$.

Theorem
$$G(x^m) = \inf_{y \in x^0 + \mathcal{K}_m} G(y).$$

Final properties

Theorem Convergence in at most *N* steps (size of the matrix)

Theorem
$$G(x^m) \le 4\left(\frac{\sqrt{\kappa(A)}-1}{\sqrt{\kappa(A)}+1}\right)^2 G(x^m)$$

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$$X^0$$
chosen, $p^0 = r^0 = b - AX^0$.

While m < Niter or $||r^m|| \ge tol$, do

$$\begin{array}{rcl}
\alpha_{m} &=& \frac{\|r^{m}\|^{2}}{(Ap^{m},p^{m})}, \\
X^{m+1} &=& X^{m} + \alpha_{m}p^{m}, \\
r^{m+1} &=& r^{m} - \alpha_{m}Ap^{m}, \\
\beta_{m+1} &=& \frac{\|r^{m+1}\|^{2}}{\|r^{m}\|^{2}}, \\
p^{m+1} &=& r^{m+1} - \beta_{m+1}p^{m}
\end{array}$$

1-D Poisson problem

Poisson equation -u'' = f on (0, 1), Dirichlet boundary conditions $u(0) = g_g$, $u(1) = g_d$. Second order finite difference stencil.

$$(0,1) = \cup (x_j, x_{j+1}), \quad x_{j+1} - x_j = h = \frac{1}{n+1}, \quad j = 0, \dots, n.$$

$$-rac{u(x_{i+1})-2u(x_i)+u(x_{i-1})}{h^2}\sim f(x_i), \quad i=1,\ldots n$$

$$u_0=g_g,\quad u_{n+1}=g_d.$$

$$|u_i - u(x_i)| \le h^2 \frac{\sup_{x \in [a,b]} |u^{(4)}(x)|}{12}$$

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Direct methods	Stationary iterative methods	Non-Stationary iterative methods	Preconditioning
1-D Poissor	n problem		

Discrete unknowns $U = t (u_1, \ldots, u_n)$.

$$A = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & 0 & \\ & \ddots & \ddots & \ddots & \\ 0 & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \quad b = \begin{pmatrix} f_1 - \frac{g_g}{h^2} \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n - \frac{g_d}{h^2} \end{pmatrix}$$

The matrix A is symmetric definite positive.

Discrete problem to be solved is

AX = b

Condition number and error

$$AX = b, \quad A\hat{X} = \hat{b}$$

Define $\kappa(A) = ||A||_2 ||A^{-1}||_2$. If A is symmetric > 0, $\kappa(A) = \frac{\max \lambda_i}{\min \lambda_i}$.

Theorem

$$\frac{\|\hat{X} - X\|_2}{\|X\|_2} \le \kappa(A) \frac{\|\hat{b} - b\|_2}{\|b\|_2}$$

and there is a b such that it is equal.

Eigenvalues of A $(h \times (n+1) = 1)$.

$$\lambda_k = \frac{2}{h^2} (1 - \cos \frac{k\pi}{n+1}) = \frac{4}{h^2} \sin^2 \frac{k\pi h}{2}, \quad V_k = (\sin \frac{jk\pi}{n+1})_{1 \le i \le n},$$

$$\kappa(A) = \frac{\sin^2 \frac{n\pi h}{2}}{\sin^2 \frac{\pi h}{2}} = \frac{\cos^2 \frac{\pi h}{2}}{\sin^2 \frac{\pi h}{2}} \sim \frac{4}{\pi^2 h^2}$$

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Direct methods

Stationary iterative methods

Non-Stationary iterative methods

Preconditioning

Comparison of the iterative methods

spectral radius $ ho(R)$	<i>n</i> = 5	<i>n</i> = 30
$\cos \pi h$	0.81	0.99
$(\rho(J))^2 = \cos^2 \pi h$	0.65	0.98
$\frac{1-\sin\pi h}{1+\sin\pi h}$	0.26	0.74
$\frac{K(A)-1}{K(A)+1}$	0.81	0.99
$\frac{\sqrt{\mathcal{K}(\mathcal{A})}-1}{\sqrt{\mathcal{K}(\mathcal{A})}+1}$	0.51	0.86
	$cos \pi h$ $(\rho(J))^2 = cos^2 \pi h$ $\frac{1 - sin \pi h}{1 + sin \pi h}$ $\frac{K(A) - 1}{1 + sin \pi h}$	$ \begin{array}{cccc} \cos \pi h & 0.81 \\ (\rho(J))^2 = \cos^2 \pi h & 0.65 \\ \frac{1 - \sin \pi h}{1 + \sin \pi h} & 0.26 \\ \frac{K(A) - 1}{K(A) + 1} & 0.81 \\ \sqrt{K(A)} - 1 \end{array} $

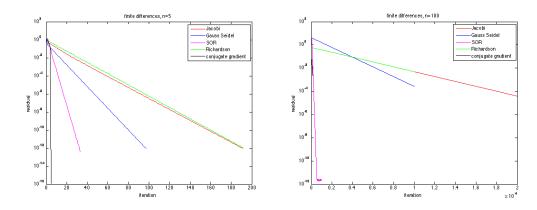
Reduction factor for one digit $M \sim -\frac{1}{\log_{10}\rho(R)}$. For n = 30,

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n	Jacobi	Gauss-Seidel	SOR	St Des	CG
10	56	28	4	56	8
100	4759	2380	37	4759	74

Asymptotic behavior

Algorithm	spectral radius
Jacobi	$1-rac{\pi^2}{2}h^2$,
Gauss-Seidel	$1-\pi^2 h^2$,
SOR	$1-2\pi h$
gradient	$1-\pi h$,
conjugate gradient	$1-\frac{\pi h}{2}$.





Number of elementary operations

Gauss elimination	n ²
optimal overrelaxation	n ^{3/2}
FFT	$n \ln_2(n)$
conjugate gradient	n ^{5/4}
multigrid	n

Asymptotic order of the number of elementary operations needed to solve the 1 - D problem as a function of the number of grid points



Take the system AX = b, with A symmetric definite positive, and the conjugate gradient algorithm. The speed of convergence of the algorithm deteriorates when $\kappa(A)$. The purpose is to replace the problem by another system, better conditioned. Let M be a symmetric regular matrix. Multiply the system on the left by M^{-1} .

$$AX = b \iff M^{-1}AX = M^{-1}b \iff (M^{-1}AM^{-1})MX = M^{-1}b$$

Define

 $\tilde{A} = M^{-1}AM^{-1}, \quad \tilde{X} = MX, \quad \tilde{b} = M^{-1}b,$

and the new problem to solve $\tilde{A}\tilde{X} = \tilde{b}$. Since *M* is symmetric, \tilde{A} is symmetric definite positive. Write the conjugate gradient algorithm for this "tilde" problem.

The algorithm for \tilde{A}

$$ilde{X}^0$$
 given, $ilde{p}^0 = ilde{r}^0 = ilde{b} - ilde{A} ilde{X}^0$.

While m < Niter or $\|\tilde{r}^m\| \ge tol$, do

$$\alpha_{m} = \frac{\|\tilde{r}^{m}\|^{2}}{(\tilde{A}\tilde{p}^{m}, \tilde{p}^{m})},$$

$$\tilde{X}^{m+1} = \tilde{X}^{m} + \alpha_{m}\tilde{p}^{m},$$

$$\tilde{r}^{m+1} = \tilde{r}^{m} - \alpha_{m}\tilde{A}\tilde{p}^{m},$$

$$\beta_{m+1} = \frac{\|\tilde{r}^{m+1}\|^{2}}{\|\tilde{r}^{m}\|^{2}},$$

$$\tilde{p}^{m+1} = \tilde{r}^{m+1} - \beta_{m+1}\tilde{p}^{m}$$

Now define

$$p^m = M^{-1}\tilde{p}^m, \quad X^m = M^{-1}\tilde{X}^m, \quad r^m = M\tilde{r}^m,$$

and replace in the algorithme above.

Direct methods	Stationary iterative methods	Non-Stationary iterative methods	Preconditioning
The algor	ithm for A		

$$\begin{split} Mp^{0} &= M^{-1}r^{0} = M^{-1}b - M^{-1}AM^{-1}MX^{0} \iff \begin{cases} p^{0} &= M^{-2}r^{0}, \\ r^{0} &= b - AX^{0}. \end{cases} \\ & \|\tilde{r}^{m}\|^{2} = (M^{-1}r^{m}, M^{-1}r^{m}) = (M^{-2}r^{m}, r^{m}) \\ \end{split} \\ \text{Define } \boxed{z^{m} = M^{-2}r^{m}}. \text{ Then } \boxed{\beta_{m+1} = \frac{(z^{m+1}, r^{m+1})}{(z^{m}, r^{m})}}. \\ & (\tilde{A}\tilde{p}^{m}, \tilde{p}^{m}) = (M^{-1}AM^{-1}Mp^{m}, Mp^{m}) = (Ap^{m}, p^{m}) \\ & \Rightarrow \boxed{\alpha_{m} = \frac{(z^{m}, r^{m})}{(Ap^{m}, p^{m})}}. \\ MX^{m+1} &= MX^{m} + \alpha_{m}Mp^{m} \iff \boxed{X^{m+1} = X^{m} + \alpha_{m}p^{m}}. \\ M^{-1}r^{m+1} &= M^{-1}r^{m} - \alpha_{m}M^{-1}AM^{-1}Mp^{m} \iff \boxed{r^{m+1} = r^{m} - \alpha_{m}Ap^{m}}. \end{split}$$

$$Mp^{m+1} = M^{-1}r^{m+1} - \beta_{m+1}Mp^m \iff p^{m+1} = z^{m+1} - \beta_{m+1}p^m.$$

The algorithm for A

Define $C = M^2$.

$$X^0$$
 given, $r^0 = b - AX^0$, solve $Cz^0 = r^0$, $p^0 = z^0$.

While m < Niter or $||r^m|| \ge tol$, do

$$\begin{array}{rcl} \alpha_{m} & = & \frac{(z^{m}, r^{m})}{(Ap^{m}, p^{m})}, \\ X^{m+1} & = & X^{m} + \alpha_{m}p^{m}, \\ r^{m+1} & = & r^{m} - \alpha_{m}Ap^{m}, \\ \beta_{m+1} & = & \frac{(z^{m+1}, r^{m+1})}{(z^{m}, r^{m})}, \\ \text{solve } Cz^{m+1} & = & r^{m+1}, \\ p^{m+1} & = & z^{m+1} - \beta_{m+1}p^{m}. \end{array}$$

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Direct methods	Stationary iterative methods	Non-Stationary iterative methods	Preconditioning
How to ch	oose C		

C must be chosen such that

- \tilde{A} is better conditioned than A,
- **2** C is easy to invert.

Use an iterative method such that A = C - N with symmetric C. For instance it can be a symmetrized version of SOR, named SSOR, defined for $\omega \in (0, 2)$ by

$$C = \frac{1}{\omega(2-\omega)}(D-\omega E)D^{-1}(D-\omega F).$$

Notice that if A is symmetric definite positive, so is D and its coefficients are positive, then its square root \sqrt{D} is defined naturally as the diagonal matrix of the square roots of the coefficients. Then C can be rewritten as

$$C = SS^T$$
, with $S = \frac{1}{\sqrt{\omega(2-\omega)}}(D-\omega E)D^{-1/2}$,

yielding a natural Cholewski decomposition of C.

How to choose C, continue

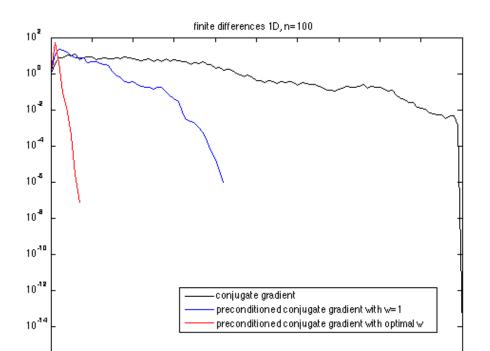
Define furthermore M as the square root of C (M will never been use), *i.e.* diagonalize C as $P\Lambda P^{T}$, with $\Lambda_{ii} > 0$ the eigenvalues of C, then define the symmetric square root of C as $M = P\sqrt{\Lambda}P^{T}$. Notice that $\tilde{\lambda}$ is an eigenvalue of \tilde{A} associated to the eigenvector \tilde{z} if and only if

$$M^{-1}AM^{-1}\tilde{z} = \tilde{\lambda}\tilde{z} \iff M^{-2}AM^{-1}\tilde{z} = \tilde{\lambda}M^{-1}\tilde{z}$$

if and only if $\tilde{\lambda}$ is an eigenvalue of $C^{-1}A$ associated to the eigenvector $M^{-1}\tilde{z}$. The speed of convergence of the iterative method is measured by the spectral radius of $C^{-1}N$, $\rho(C^{-1}N) < 1$. Note μ_i the eigenvalues of $C^{-1}N$. Since $C^{-1}N = I - C^{-1}A$, the eigenvalues of $C^{-1}A$ are equal to $1 - \mu_i \in [1 - \rho(C^{-1}N), 1 + \rho(C^{-1}N)]$. Therefore $\kappa(\tilde{A}) \leq \frac{1 + \rho(C^{-1}N)}{1 - \rho(C^{-1}N)}$, and the smallest $\rho(C^{-1}N)$, the smallest the condition number of \tilde{A} .

Comparison

For the 1-D finite differences matrix and n = 100, we compare the convergence of the conjugate gradient and the preconditioning by SSOR with $\omega = 1$ and with the optimal parameter. The gain even with $\omega = 1$ is striking.



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