Iterative methods for positive definite linear systems with a complex shift

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Outline

1. Numerical solution of the heat equation
2. Richardson iteration
3. Conjugate gradients
4. Preconditioning

Part I

Numerical solution of the heat equation

Initial-boundary value problem

Spatial domain $\Omega \subseteq \mathbb{R}^d$.

Seek $u = u(x,t)$ such that

$$\begin{aligned} \partial_t u - \nabla \cdot (a \nabla u) &= f(x,t) && \text{for } x \in \Omega \text{ and } t > 0, \\ u(x,0) &= u_0(x) && \text{for } x \in \Omega, \\ u(x,t) &= 0 && \text{for } x \in \partial\Omega \text{ and } t > 0. \end{aligned}$$

L_2 inner product

$$(u,v) = \int_\Omega u\bar{v}\,dx.$$

Weak formulation: seek $u : [0,T] \to H_0^1(\Omega)$ such that

$$(u_t, v) + (a\nabla u, \nabla v) = \big(f(t), v\big) \quad \text{for all } v \in H_0^1(\Omega),$$

with $u(0) = u_0$.

Laplace transformation

Write

$$w(z) \equiv \hat{u}(z) = \mathcal{L}\{u(t)\} = \int_0^\infty e^{-zt} u(t)\, dt, \quad \Re z > 0.$$

Since

$$\mathcal{L}\{(\partial_t u, v)\} = \big(z\hat{u}(z) - u(0), v\big) = z\big(w(z), v\big) - (u_0, v),$$

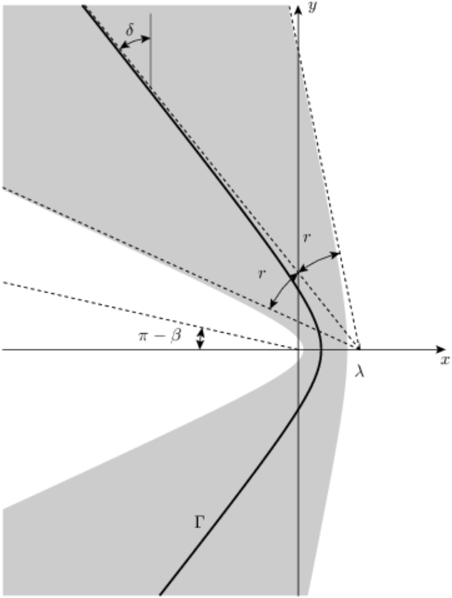
define $g(z) = u_0 + \hat{f}(z)$ then $w(z) \in H_0^1(\Omega)$ satisfies

$$z\big(w(z), v\big) + \big(a\nabla w(z), \nabla v\big) = \big(g(z), v\big) \quad \text{for all } v \in H_0^1(\Omega).$$

Spectrum $\sigma(A)$ on positive real axis, so if $0 < \delta < \pi$ then

$$\|w(z)\| \le \frac{C_\delta \|g(z)\|}{1 + |z|} \quad \text{for } |\arg z| > \pi - \delta.$$

The contour Γ



Laplace inversion formula

For simplicity, choose

$$\Gamma = \{\, x + iy : (x-1)^2 - y^2 = 1 \text{ and } x \le 0 \,\}.$$

Assume $\hat{f}(z)$ bounded and analytic, on and to the right of Γ, then

$$u(t) = \frac{1}{2\pi i} \int_\Gamma e^{zt} w(z)\, dz \quad \text{for } t > 0, \qquad w = \hat{u}.$$

Parametric representation

$$z(\xi) = 1 - \cosh\xi + i \sinh\xi \quad \text{for } -\infty < \xi < \infty,$$

gives

$$u(t) = \int_{-\infty}^{\infty} v(\xi, t)\, d\xi \quad \text{where} \quad v(\xi, t) = \frac{e^{z(\xi)t}}{2\pi i} w\bigl(z(\xi)\bigr) z'(\xi).$$

Quadrature

Step size $k = \log q / q > 0$. For $|j| \leq q$,

$$\xi_j = jk, \quad z_j = z(\xi_j), \quad z_j' = z'(\xi_j).$$

Equal-weight quadrature approximation

$$u(t) = \int_{-\infty}^{\infty} v(\xi, t)\, d\xi \approx U_q(t) = k \sum_{j=-q}^{q} v(\xi_j, t),$$

that is,

$$U_q(t) = \frac{k}{2\pi i} \sum_{j=-q}^{q} e^{z_j t} w(z_j) z_j'.$$

Points furthest from 0:

$$z_{\pm q} = 1 - \tfrac{1}{2}(q + q^{-1}) \pm \tfrac{1}{2} i (q - q^{-1}) \approx \tfrac{1}{2}(-1 \pm i) q.$$

Spatial discretization

Weak solution $u(t) \in H_0^1(\Omega)$ satisfies

$$(u_t, v) + (a\nabla u, \nabla v) = \big(f(t), v\big) \quad \text{for all } v \in H_0^1(\Omega),$$

with $u(0) = u_0$.

Conforming, piecewise-linear finite element space $V_h \subseteq H_0^1(\Omega)$.

Spatially discrete solution $u_h(t) \in V_h$ satisfies

$$(u_{h,t}, \chi) + (a\nabla u_h, \nabla \chi) = \big(f(t), \chi\big) \quad \text{for all } \chi \in V_h,$$

subject to $u_h(0) = L_2$-projection of u_0 onto V_h, so

$$\big(u_h(0), \chi\big) = (u_0, \chi) \quad \text{for all } \chi \in V_h.$$

Fully-discrete solution

Recall

$$z\big(w(z),v\big)+\big(a\nabla w(z),\nabla v\big)=\big(g(z),v\big)\quad \text{for all } v\in H_0^1(\Omega).$$

Similarly, $w_h(z)=\hat{u}_h(z)\in V_h$ satisfies

$$z\big(w_h(z),\chi\big)+\big(a\nabla w_h(z),\nabla\chi\big)=\big(g(z),\chi\big)\quad \text{for all } \chi\in V_h.$$

Put

$$U_{q,h}(t)=\frac{k}{2\pi i}\sum_{j=-q}^{q}e^{z_j t}w_h(z_j)z_j'.$$

Linear system

Interior (free) nodes: P_1, P_2, $\ldots$, P_N.

Nodal basis functions: Φ_1, Φ_2, $\ldots$, Φ_N satisfying $\Phi_n(P_m) = \delta_{mn}$. Then

$$w_h(x, z_j) = \sum_{n=1}^{N} w_n(z_j)\Phi_n(x) \quad \text{with} \quad w_n(z_j) = w_h(P_n, z_j).$$

Mass matrix, stiffness matrix, load vector:

$$\mathcal{M}_{mn} = (\Phi_n, \Phi_m), \quad \mathcal{S}_{mn} = (a\nabla\Phi_n, \nabla\Phi_m), \quad g_m = \big(g(z_j), \Phi_m\big).$$

Need to solve

$$(z_j\mathcal{M} + \mathcal{S})\mathbf{w} = \mathbf{g} \quad \text{or} \quad (z_j I + \mathcal{M}^{-1}\mathcal{S})\mathbf{w} = \mathcal{M}^{-1}\mathbf{g},$$

where $\mathbf{w} = [w_n] \in \mathbb{C}^N$ and $\mathbf{g} = [g_n] \in \mathbb{C}^N$.

Accuracy required for an iterative solver

Iterative solver computes $\widetilde{w}_h(z_j) \approx w_h(z_j)$, leading to

$$\widetilde{U}_{q,h}(t) = \frac{k}{2\pi i} \sum_{j=-q}^{q} e^{z_j t} \widetilde{w}_h(z_j) z_j'.$$

The error is

$$\begin{aligned}
\widetilde{U}_{q,h}(t) - u(t) &= \big[\widetilde{U}_{q,h}(t) - U_{q,h}(t)\big] \\
&\qquad + \big[U_{q,h}(t) - u_h(t)\big] + \big[u_h(t) - u(t)\big] \\
&= \frac{k}{2\pi i} \sum_{j=-q}^{q} e^{z_j t} \big[w_h(z_j) - \widetilde{w}_h(z_j)\big] z_j' \\
&\qquad + O(e^{-cq/\log q}) + O(h^2),
\end{aligned}$$

so we desire $\|\widetilde{w}_h(z_j) - w_h(z_j)\| \le \epsilon_j$ with

$$\frac{k}{2\pi} \sum_{j=-q}^{q} e^{x_j t} \epsilon_j |z_j'| \simeq e^{-cq/\log q} \simeq h^2.$$

Part II

Richardson iteration

The setting

Finite dimensional complex vector space V with inner product $(\cdot, \cdot)$.
Hermitian positive-definite operator $A : V \to V$,

$$(Av, w) = (v, Aw).$$

Equation with complex shift,

$$A_z w = b \quad \text{where} \quad A_z = zI + A \quad \text{and} \quad |\arg z| < \pi - \delta.$$

In our example, $V = \mathbb{C}^N$ with

$$A = \mathcal{M}^{-1}\mathcal{S}, \qquad b = \mathcal{M}^{-1}\mathbf{g},$$

and

$$(\mathbf{v}, \mathbf{w}) = \langle \mathcal{M}\mathbf{v}, \mathbf{w} \rangle, \qquad \langle \mathbf{v}, \mathbf{w} \rangle = \sum_{l=1}^{N} v_l \bar{w}_l,$$

so

$$(A\mathbf{v}, \mathbf{w}) = \langle \mathcal{S}\mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{v}, \mathcal{S}\mathbf{w} \rangle = (\mathbf{v}, A\mathbf{w}).$$

The basic iteration

Sheen, Sloan and Thomée (2003).
For any $\alpha \in \mathbb{C}$, exact solution satisfies

$$w = (I - \alpha A_z)w + \alpha b,$$

Initial guess w^0.
Richardson iteration

$$w^{n+1} = (I - \alpha A_z)w^n + \alpha b \quad \text{for } n = 0, 1, 2, \ldots.$$

Optimal choice of the acceleration parameter α?
Error $e^n = w^n - w$ satisfies

$$e^{n+1} = (I - \alpha A_z)e^n,$$

so choose $\alpha = \alpha^*$ to minimise the error reduction ratio

$$\|I - \alpha A_z\|_{V \to V} = \max_{\lambda \in \sigma(A)} \bigl|1 - \alpha(z + \lambda)\bigr|.$$

Slow convergence

Order the eigenvalues of A as $0 < \lambda_1 < \lambda_2 < \cdots < \lambda_N$.

Classical case $z = 0$:

$$\epsilon_0 = \|I - \alpha^* A_0\| = \frac{\lambda_N - \lambda_1}{\lambda_N + \lambda_1} \quad \text{if } \alpha^* = \frac{2}{\lambda_1 + \lambda_N}.$$

For general z with $|\arg z| < \pi$, can compute

$$\alpha^* = \alpha^*(z, \lambda_1, \lambda_N)$$

and find

$$\epsilon_z = \|I - \alpha^* A_z\| \le 1 - c\lambda_N^{-1}, \qquad c = c(z, \lambda_1).$$

In our case, $\lambda_N(\mathcal{M}^{-1}\mathcal{S}) = O(h^{-2})$ so

$$\epsilon_z = \|I - \alpha^*(zI + \mathcal{M}^{-1}\mathcal{S})\| \le 1 - ch^2.$$

Preconditioning

Hermitian positive-definite operator $B_z : V \to V$; mimics A_z^{-1}.

Preconditioned equation

$$B_z A_z w = B_z b.$$

Preconditioned Richardson iteration

$$w^{n+1} = (I - \alpha B_z A_z) w^n + \alpha B_z b.$$

Again seek optimal acceleration parameter α^* to minimize

$$\tilde{\epsilon}_z \equiv \| I - \alpha B_z A_z \|.$$

Implementation without preconditioning

Recall

$$(z\mathcal{M} + \mathcal{S})\mathbf{w} = \mathbf{g},$$

or equivalently,

$$(zI + A)\mathbf{w} = \mathcal{M}^{-1}\mathbf{g}, \qquad A = \mathcal{M}^{-1}\mathcal{S},$$

or equivalently,

$$\mathcal{A}_z\mathbf{w} = \mathbf{g}, \qquad \mathcal{A}_z = \mathcal{M}A_z = \mathcal{M}(zI + A) = z\mathcal{M} + \mathcal{S}.$$

Residual $\mathbf{r}^n = \mathbf{g}_z - \mathcal{A}_z\mathbf{w}^n$.

Richardson iteration:

$$\mathbf{w}^{n+1} = (I - \alpha\mathcal{M}^{-1}\mathcal{A}_z)\mathbf{w}^n + \alpha\mathcal{M}^{-1}\mathbf{g}_z = \mathbf{w}^n + \alpha\mathcal{M}^{-1}\mathbf{r}^n,$$

Implementation with preconditioning

Let

$$B_z = \mathcal{B}_z \mathcal{M},$$

with $\mathcal{B}_z$ positive-definite and Hermitian with respect to the standard inner product $\langle \cdot, \cdot \rangle$ on $\mathbb{C}^N$, so B_z is Hermitian with respect to $(\cdot, \cdot)$:

$$(B_z \mathbf{v}, \mathbf{w}) = \langle \mathcal{B}_z \mathcal{M} \mathbf{v}, \mathcal{M} \mathbf{w} \rangle = (\mathbf{v}, B_z \mathbf{w}),$$

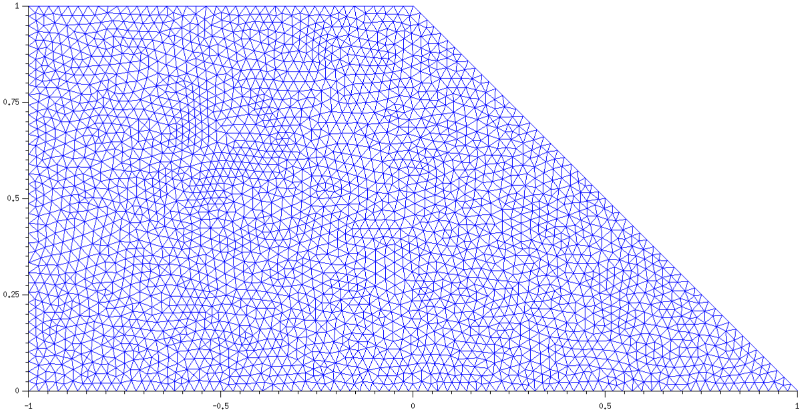
Residual $r^n = \mathbf{g} - \mathcal{A}_z \mathbf{w}^n$.

Preconditioned Richardson iteration

$$\begin{aligned} \mathbf{w}^{n+1} &= (I - \alpha B_z A_z)\mathbf{w}^n + \alpha B_z \mathcal{M}^{-1}\mathbf{g} \\ &= (I - \alpha \mathcal{B}_z \mathcal{M} A_z)\mathbf{w}^n + \alpha \mathcal{B}_z \mathcal{M} \mathcal{M}^{-1}\mathbf{g} \\ &= (I - \alpha \mathcal{B}_z \mathcal{A}_z)\mathbf{w}^n + \alpha \mathcal{B}_z \mathbf{g} \\ &= \mathbf{w}^n + \alpha \mathcal{B}_z \mathbf{r}^n. \end{aligned}$$

Model problem — finite element mesh

Triangulation of Ω has $N = 2663$ free nodes, with maximum element diameter $h = 0.035$.



Model problem — other details

Constant diffusivity $a = 1/15$ chosen to normalize the minimum eigenvalue of $A = \mathcal{M}^{-1}\mathcal{S}$:

$$\lambda_1(A) = 1.01380 \quad \text{and} \quad \lambda_N(A) = 4006.79.$$

Errors $\|U_{h,q}(t) - u(t)\|_h$ using a direct solver:

t	$q = 10$	$q = 20$	$q = 30$	$\|u(t)\|_h$
0.25	1.3436e-02	4.3778e-04	4.1747e-04	0.4452
0.50	6.1232e-04	1.6260e-04	1.7541e-04	0.4623
1.00	2.2024e-04	2.1088e-04	2.1114e-04	0.4206
2.00	1.9403e-04	1.9411e-04	1.9411e-04	0.2579

Effect of special preconditioner $B_z = (\mu_z I + A)^{-1}$

Using optimal acceleration parameter $\alpha = \rho e^{-i\varphi}$.

			Without B_z			With B_z			
j	x_j	y_j	ρ	φ	ϵ_z	ρ	φ	μ_z	$\widetilde{\epsilon}_z$
0	0.0	0.0	5.0e-4	0.0	0.9995	1.0	0.0	0.0	0.00
2	-0.0	0.3	4.9e-4	0.2	0.9995	1.0	0.2	0.0	0.15
4	-0.2	0.6	4.7e-4	0.3	0.9995	1.0	0.3	0.0	0.32
6	-0.4	1.0	4.3e-4	0.5	0.9996	0.9	0.5	0.2	0.50
8	-0.8	1.5	3.8e-4	0.7	0.9996	0.8	0.7	0.5	0.66
10	-1.4	2.1	3.2e-4	0.9	0.9995	0.7	0.9	1.1	0.76
12	-2.1	2.9	2.9e-4	1.0	0.9995	0.6	1.0	2.1	0.82
14	-3.1	4.0	2.6e-4	1.0	0.9994	0.5	1.0	3.5	0.86
16	-4.5	5.5	2.4e-4	1.1	0.9993	0.5	1.1	5.5	0.88
18	-6.5	7.4	2.2e-4	1.1	0.9991	0.5	1.1	8.2	0.89
20	-9.0	10.0	2.2e-4	1.1	0.9988	0.4	1.1	11.8	0.90
	-20.0	20.0	2.0e-04	1.2	0.9978	0.4	1.1	26.9	0.92

Related literature

Freund (1990): Krylov methods for $(zI + A)w = b$ with A Hermitian and possibly indefinite. Motivated by the Helmholtz equation

$$-\omega^2 u + i\sigma u - \nabla^2 u = f.$$

Benzi and Bertaccini (2003), Bellavia et al. (2011): preconditioners in the special case of real $z = x > 0$, with efficient updates for different x. Motivated by implicit finite difference timestepping for parabolic PDEs.

Simoncini (2003): full orthogonalization method for $z = x \in \mathbb{R}$ and $xI + A$ nonsingular.

Meerbergen (2003), Meerbergen and Bai (2010): Krylov methods for $\mathcal{S} - \alpha\mathcal{M}$, $\alpha \in [\alpha_{\text{min}}, \alpha_{\text{max}}]$.

Part III

Conjugate gradients

The setting

Finite dimensional complex Hilbert space V with inner product (v, w).

Positive-definite Hermitian linear operator $A : V \to V$.

Seek $w \in V$ satisfying

$$A_z w = b,$$

where

$$A_z = zI + A, \qquad z = x + iy, \qquad |\arg z| < \pi.$$

Krylov subspaces

Initial guess w_0.

Initial residual $r_0 = b - A_z w_0 \neq 0$.

Krylov subspace

$$V_n = \text{span}\{r_0, A_z r_0, \ldots, A_z^{n-1} r_0\} \quad \text{for } n \geq 1.$$

Notice

$$V_n = \text{span}\{r_0, A r_0, \ldots, A^{n-1} r_0\},$$

but r_0 still depends on z.

Galerkin method

Exact solution satisfies

$$(A_z w, \varphi) = (b, \varphi) \quad \text{for all } \varphi \in V.$$

Conjugate gradient (CG) solution

$$w_n = w_0 + v_n, \qquad v_n \in V_n,$$

determined by

$$(A_z w_n, \varphi) = (b, \varphi) \quad \text{for all } \varphi \in V_n.$$

Thus,

$$\big(A_z(w_n - w_0), \varphi\big) = (b - A_z w_0, \varphi),$$

or

$$v_n \in V_n \quad \text{and} \quad (A_z v_n, \varphi) = (r_0, \varphi) \quad \text{for all } \varphi \in V_n.$$

Uniqueness and existence

If $(A_z v_n, \varphi) = 0$ for all $\varphi \in V_n$, then taking $\varphi = v_n$ gives

$$(A_z v_n, v_n) = z\|v_n\|^2 + (Av_n, v_n) = 0,$$

or in other words,

$$x\|v_n\|^2 + (Av_n, v_n) = 0 \quad \text{and} \quad y\|v_n\|^2 = 0,$$

so $v_n = 0$, by our assumption $|\arg z| < \pi$.

Hence, v_n is unique.

Hence, v_n exists (because V is finite dimensional).

Key tools

Put

$$|||v|||^2 = |z| \|v\|^2 + (Av, v) \quad \text{for } v \in V.$$

Sesquilinear form $(A_z v, w)$ not an inner product if $\Re z \neq 0$, but ...

Lemma

If $\theta_z = \arg z \in (-\pi, \pi)$ then, for all $v, \varphi \in V$,

$$|(A_z v, \varphi)| \leq |||v||| \, |||\varphi||| \quad \textit{and} \quad |(A_z v, v)| \geq \cos(\tfrac{1}{2}\theta_z) |||v|||^2$$

Lemma (Galerkin orthogonality)

The CG error $e_n = w_n - w$ satisfies

$$(A_z e_n, \varphi) = 0 \quad \textit{for all } \varphi \in V_n.$$

CG solution is quasi-optimal

Theorem

The CG solution w_n satisfies

$$|||w_n - w||| \leq \sec(\tfrac{1}{2}\theta_z) \inf_{v \in w_0 + V_n} |||v - w|||.$$

Proof.

Error $e_n = w_n - w$ satisfies

$$\begin{aligned}
\cos(\tfrac{1}{2}\theta_z)|||e_n|||^2 &\leq \left|\left(A_z e_n, w_n - w\right)\right| \\
&= \left|\left(A_z e_n, (w_n - v) + (v - w)\right)\right| \\
&= \left|(A_z e_n, \underbrace{w_n - v}_{\in V_n}) + (A_z e_n, v - w)\right| \\
&= \left|0 + (A_z e_n, v - w)\right| \leq |||e_n||| \, |||v - w|||
\end{aligned}$$

□

Error reduction ratio

Theorem

The CG error satisfies

$$\|e_n\| \le \frac{2\sec(\frac{1}{2}\theta_z)}{|\eta_z^n + \eta_z^{-n}|}\|e_0\|$$

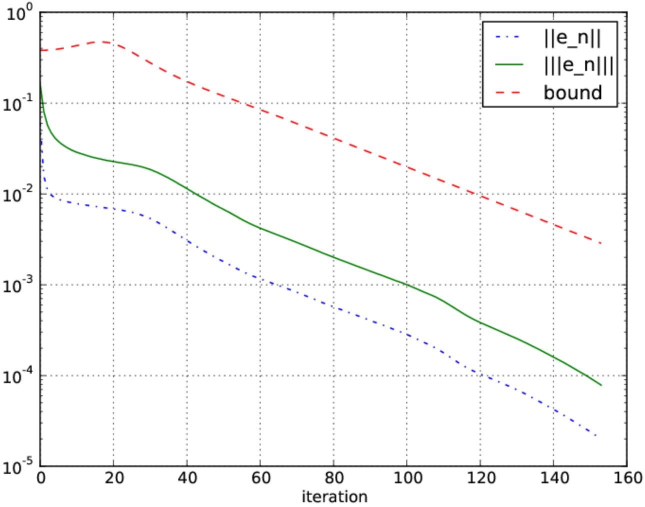
where

$$\eta_z = -\frac{\sqrt{\lambda_N + z} - \sqrt{\lambda_1 + z}}{\sqrt{\lambda_N + z} + \sqrt{\lambda_1 + z}} \quad \textit{and} \quad |\eta_z| \le 1 - c(z, \lambda_1)\lambda_N^{-1/2}.$$

Thus, for $A = \mathcal{M}^{-1}\mathcal{S}$,

$$\|e_n\| \le 2\sec(\tfrac{1}{2}\theta_z)|\eta_z|^n\|e_0\| \quad \text{with} \quad |\eta_z| \le 1 - ch.$$

Model problem ($z = z_{15}$)



Orthogonal basis of residuals

Residual $r_n = b - A_z w_n$.

There exists $N^* \leq N = \dim V$ such that

$$r_n \neq 0 \quad \text{for } 0 \leq n < N^* \qquad \text{but} \qquad r_n = 0 \quad \text{for } n \geq N^*.$$

Furthermore

$$r_n \in V_{n+1} \qquad \text{and} \qquad (r_n, \varphi) = 0 \quad \text{for all } \varphi \in V_n \text{ and } n \geq 0.$$

so $r_0, r_1, \ldots, r_{n-1}$ form an orthogonal basis for V_n if $n \leq N^*$.

Thus,

$$V_0 \subsetneq V_1 \subsetneq \cdots \subsetneq V_{N^*} = V_{N^*+1} = \cdots .$$

Conjugate search directions

Put $p_0 = r_0$ and, for $0 \le n < N^*$,

$$p_{n+1} = r_{n+1} + \sum_{k=0}^{n} \beta_{nk} p_k \quad \text{where} \quad \beta_{nk} = -\frac{(A_z r_{n+1}, p_k)}{(A_z p_k, p_k)}.$$

In this way,

$$p_n \in V_{n+1} \quad \text{and} \quad (A_z p_n, p_j) = 0 \quad \text{for } 0 \le j < n.$$

If $n \le N^*$ then $p_0, p_1, \ldots, p_{n-1}$ form a basis for V_n.

Find $\beta_{nk} = 0$ for $0 \le k < n$ so

$$p_{n+1} = r_{n+1} + \beta_n p_n, \qquad \beta_n = \beta_{nn}.$$

If $\Im z \ne 0$ and $0 \le j < n$, then

$$(A_z p_j, p_n) = (A_z p_j, p_n) - (p_j, A_z p_n) = (z - \bar{z})(p_j, p_n) \ne 0.$$

Abstract CG algorithm

$p_0 = r_0 = b - A_z w_0$
for $n = 0, 1, 2, \ldots$ **do**
  if *converged* **then**
    break
  end if
  $\alpha_n = \|r_n\|^2/(A_z p_n, p_n)$
  $w_{n+1} = w_n + \alpha_n p_n$
  $r_{n+1} = r_n - \alpha_n A_z p_n$
  $\beta_n = -(r_{n+1}, A_z p_n)/(A_z p_n, p_n)$
  $p_{n+1} = r_{n+1} + \beta_n p_n$
end for

In the classical CG algorithm, α_n is real and

$$-\alpha_n(r_{n+1}, A_z p_n) = (r_{n+1}, r_n - \alpha_n A_z p_n) = \|r_{n+1}\|^2$$

so $\beta_n = \|r_{n+1}\|^2/\|r_n\|^2$.

Concrete CG algorithm

Recall

$$\mathcal{A}_z = \mathcal{M}A_z = z\mathcal{M} + \mathcal{S}, \quad \mathcal{A}_z \mathbf{w} = \mathbf{g}, \quad (\mathbf{v}, \mathbf{w}) = \langle \mathcal{M}\mathbf{v}, \mathbf{w} \rangle.$$

$\mathbf{p}_0 = \mathbf{r}_0 = \mathcal{M}^{-1}(\mathbf{g} - \mathcal{A}_z \mathbf{w}_0)$
for $n = 0, 1, 2, \ldots$ **do**
  if *converged* **then**
    break
  end if
  $\alpha_n = \langle \mathcal{M}\mathbf{r}_n, \mathbf{r}_n \rangle / \langle \mathcal{A}_z p_n, p_n \rangle$
  $\mathbf{w}_{n+1} = \mathbf{w}_n + \alpha_n \mathbf{p}_n$
  $\mathbf{r}_{n+1} = \mathbf{r}_n - \alpha_n \mathcal{M}^{-1} \mathcal{A}_z \mathbf{p}_n$
  $\beta_n = -\langle \mathbf{r}_{n+1}, \mathcal{A}_z \mathbf{p}_n \rangle / \langle \mathcal{A}_z \mathbf{p}_n, \mathbf{p}_n \rangle$
  $\mathbf{p}_{n+1} = \mathbf{r}_{n+1} + \beta_n \mathbf{p}_n$
end for

Can use lumped mass approximation $\mathcal{M} \approx \mathcal{D}$, with $\mathcal{D}$ diagonal.

Part IV

Preconditioning

Special preconditioner

Consider

$$B_z = (\mu_z I + A)^{-1}, \qquad \mu_z > -\lambda_1(A).$$

Since

$$A_z = zI + A = (z - \mu_z)I + (\mu_z I + A)$$

the equation

$$(zI + A)w = b$$

is equivalent to one of the same form:

$$(\tilde{z}I + B_z)w = \tilde{z}B_z b, \qquad \tilde{z} = (z - \mu_z)^{-1}.$$

Error reduction ratio

Norm

$$|||v|||_{\sim}^2 = |\tilde{z}|\|v\|^2 + (B_z v, v).$$

Error $e_n = w_n - w$ satisfies

$$|||e_n|||_{\sim} \le \frac{2\sec(\frac{1}{2}\theta_z)}{|\tilde{\eta}_z^n + \tilde{\eta}_z^{-n}|} |||e_0|||_{\sim} \le 2\sec(\tfrac{1}{2}\theta_z)|\tilde{\eta}_z|^n |||e_0|||_{\sim},$$

with

$$|\tilde{\eta}_z| \le c(z, \lambda_1, \mu_z) < 1 \quad \text{uniformly as } \lambda_N \to \infty.$$

Optimal choice for preconditioner parameter

$$\mu_z = -\lambda_1 + \frac{q_z}{1 - q_z}(\lambda_N - \lambda_1) > -\lambda_1, \qquad q_z = \left|\frac{z + \lambda_1}{z + \lambda_N}\right|,$$

$$\to |z + \lambda_1| - \lambda_1 \quad \text{as } \lambda_N \to \infty.$$

Results for model problem

j	x_j	y_j	$\lvert\eta_z\rvert$	$\lvert\tilde{\eta}_z\rvert$	μ_z	$\lvert\tilde{\eta}_z\rvert$	μ_z
0	0.00	0.00	0.97	0.00	0.00	0.00	0.00
2	-0.05	0.30	0.97	0.08	0.00	0.08	0.00
4	-0.18	0.64	0.97	0.17	0.03	0.17	0.00
6	-0.43	1.02	0.97	0.27	0.17	0.27	0.00
8	-0.81	1.51	0.97	0.38	0.51	0.39	0.00
10	-1.35	2.12	0.97	0.46	1.14	0.50	0.00
12	-2.10	2.93	0.97	0.52	2.12	0.58	0.00
14	-3.13	4.01	0.97	0.57	3.53	0.66	0.00
16	-4.54	5.45	0.96	0.59	5.49	0.71	0.00
18	-6.45	7.38	0.96	0.61	8.18	0.76	0.00
20	-9.02	9.97	0.95	0.63	11.85	0.80	0.00
	-20.00	20.00	0.94	0.66	26.89	0.86	0.00

General preconditioning

Arbitrary Hermitian positive-definite B_z.

Preconditioned equation

$$B_z A_z w = B_z b.$$

Both B_z and $B_z A$ are Hermitian with respect to

$$[v, w] = (B_z^{-1} v, w),$$

but $B_z A_z = zB_z + B_z A$ is not of the form zI + Hermitian.

Preconditioned residual

$$\tilde{r}_n = B_z b - B_z A_z w_n = B_z(b - A_z w_n) = B_z r_n.$$

Krylov subspaces

$$\tilde{V}_n = \text{span}\{\tilde{r}_0, B_z A_z \tilde{r}_0, \ldots, (B_z A_z)^{n-1} \tilde{r}_0\}.$$

Quasi-optimality

Preconditioned CG iterates $w_n = w_0 + v_n$, with $v_n \in \tilde{V}_n$, defined by

$$(A_z w_n, \varphi) = (b, \varphi) \quad \text{for all } \varphi \in \tilde{V}_n.$$

Equivalently

$$[B_z A_z w_n, \varphi] = [B_z b, \varphi] \quad \text{for all } \varphi \in \tilde{V}_n.$$

Galerkin orthogonality:

$$(A_z e_n, \varphi) = [B_z A_z e_n, \varphi] = 0 \quad \text{for all } \varphi \in \tilde{V}_n.$$

Theorem

$$|||w_n - w||| \le \sec(\tfrac{1}{2}\theta_z) \inf_{v \in w_0 + \tilde{V}_n} |||v - w|||.$$

But no error bound.

Recursion involves all previous iterates

Preconditioned residual $\tilde{r}_n = B_z(b - A_z w_n) = B_z r_n$ satisfies

$$\tilde{r}_n \in \tilde{V}_{n+1} \quad \text{and} \quad [\tilde{r}_n, \varphi] = (r_n, \varphi) = 0 \quad \text{for all } \varphi \in \tilde{V}_n.$$

Set

$$p_0 = \tilde{r}_0 \quad \text{and} \quad p_{n+1} = \tilde{r}_{n+1} + \sum_{k=0}^{n} \beta_{nk} p_k \quad \text{for } n \geq 0,$$

where the β_{nk} satisfy the $(n+1) \times (n+1)$ lower-triangular system

$$\sum_{k=0}^{j} (A_z p_k, p_j) \beta_{nk} = -(A_z \tilde{r}_n, p_j) \quad \text{for } 0 \leq j \leq n,$$

so that

$$0 \neq p_n \in \tilde{V}_{n+1} \quad \text{and} \quad (A_z p_n, p_j) = 0 \quad \text{for } 0 \leq k < n < N^*.$$

Abstract preconditioned CG algorithm

$r_0 = b - A_z w_0$
$p_0 = \tilde{r}_0 = B_z r_0$
for $n = 0, 1, 2, \ldots$ **do**
  if *converged* **then**
    break
  end if
  $\alpha_n = (r_n, \tilde{r}_n)/(A_z p_n, p_n)$
  $w_{n+1} = w_n + \alpha_n p_n$
  $r_{n+1} = r_n - \alpha_n A_z p_n$
  $\tilde{r}_{n+1} = B_z r_n$
  Solve $\sum_{k=0}^{j} (A_z p_k, p_j) \beta_{nk} = -(A_z \tilde{r}_n, p_j)$, $0 \le j \le n$
  $p_{n+1} = \tilde{r}_{n+1} + \sum_{k=0}^{n} \beta_{nk} p_k$
end for

In practice, restart the iteration after every m steps.

Concrete preconditioned CG algorithm

$\mathcal{M}\mathbf{r}_0 = \mathbf{g} - \mathcal{A}_z\mathbf{w}_0$
$\mathbf{p}_0 = \tilde{\mathbf{r}}_0 = \mathcal{B}_z\mathcal{M}\mathbf{r}_0$
for $n = 0, 1, 2, \ldots$ **do**
  if *converged* **then**
    break
  end if
  $\alpha_n = \langle\mathcal{M}\mathbf{r}_n, \tilde{\mathbf{r}}_n\rangle / \langle\mathcal{A}_z\mathbf{p}_n, \mathbf{p}_n\rangle$
  $\mathbf{w}_{n+1} = \mathbf{w}_n + \alpha_n\mathbf{p}_n$
  $\mathcal{M}\mathbf{r}_{n+1} = \mathcal{M}\mathbf{r}_n - \alpha_n\mathcal{A}_z\mathbf{p}_n$
  $\tilde{\mathbf{r}}_{n+1} = \mathcal{B}_z\mathcal{M}\mathbf{r}_n$
  Solve $\sum_{k=0}^{j}\langle\mathcal{A}_z\mathbf{p}_k, \mathbf{p}_j\rangle\beta_{nk} = -\langle\mathcal{A}_z\tilde{\mathbf{r}}_n, \mathbf{p}_j\rangle$, $0 \leq j \leq n$
  $\mathbf{p}_{n+1} = \tilde{\mathbf{r}}_{n+1} + \sum_{k=0}^{n}\beta_{nk}\mathbf{p}_k$
end for

No need to compute the action of $\mathcal{M}^{-1}$.

Iterations for model problem

Stopping criterion $\|\widetilde{w}_h(z_j) - w_h(z_j)\| \le \epsilon_j$.

j	–	INV	IC	AMG(1)	$\|w_j\|$	ϵ_j
0	250	1	52	7	1.14e+00	3.18e-06
2	227	5	48	7	1.13e+00	3.06e-06
4	235	6	50	8	1.03e+00	2.84e-06
6	242	7	51	9	7.67e-01	2.78e-06
8	234	8	50	10	4.39e-01	3.03e-06
10	219	9	46	11	2.21e-01	3.86e-06
12	184	10	40	11	1.19e-01	6.08e-06
14	149	9	32	10	7.41e-02	1.27e-05
16	98	8	22	9	5.11e-02	3.83e-05
18	34	5	11	5	3.69e-02	1.91e-04
20	10	2	3	2	2.71e-02	1.87e-03