Some more comments on the normal equations: With a focus on discretisation of partial differential equations

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Due Giorni Di Algebra Lineare Numerica, 20th January 2025

UNIVERSITY OF OXFORD

Mathematical Institute

Oxford Mathematics

THE NORMAL EQUATION

Let us consider the following linear system of equations

$$\underline{\underline{A}}\,\underline{x} = \underline{b}, \qquad \underline{\underline{A}} \in \mathbb{R}^{n\times n}, \quad \underline{x}, \underline{b} \in \mathbb{R}^n.$$

$$A^T \neq A$$

In order to solve the system, we can consider the normal equation, i.e.

$$B := \underline{\underline{A}}^T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T \underline{b}$$

SIMAX Vol. 13, Iss. 3, 1992 (N. M. Nachtigal, S. C. Reddy, L. N. Trefethen),

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- Unfortunately the condition number of $\underline{\underline{A}}^T \underline{\underline{A}}$ is the square of the condition number of $\underline{\underline{A}}$.
- We now have a symmetric positive definite system, that can be solved using CG (**CGNE**).

HOW CAN WE PRECONDITION THE NORMAL EQUATIONS?

SIREV Vol. 64, Iss. 3, 2022 (A. Wathen),

Good preconditioners – Classical Definition

$\underline{\underline{P}}$ is a good preconditioner if $\underline{\underline{P}}^{-1}\underline{\underline{A}}$ has clustered eigenvalues.

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$$A = \begin{bmatrix} b_0 & & \\ & \ddots & \\ & & b_{n-1} \end{bmatrix}, \qquad P = \begin{bmatrix} & & b_0 \\ & \iddots & \\ b_{n-1} & & \end{bmatrix}.$$

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$$P^{-1}A = \begin{bmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{bmatrix}, \qquad G^{-1}B = \begin{bmatrix} (b_0/b_{n-1})^2 & & \\ & \ddots & \\ & & (b_{n-1}/b_0)^2 \end{bmatrix}.$$

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SIREV Vol. 64, Iss. 3, 2022 (A. Wathen),
QJRMS Vol. 64, Iss. 3, 2022 (S. Gratton, Et Al.).

Gratton–Gürol–Simon–Toint

If the matrix P is such that $\|I - A\,P^{-1}\|_2 \leq \sqrt{2} - 1 - \delta$, then

$$\Lambda(G^{-1}B) \subset (\sqrt{2}\delta + \delta^2, 2 - \sqrt{2}\delta - \delta^2).$$

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If the matrix P is such that $\|I - AP^{-1}\|_2 \leq \sqrt{2} - 1 - \delta$, then

$$\Lambda(G^{-1}B) \subset (\sqrt{2}\delta + \delta^2, 2 - \sqrt{2}\delta - \delta^2).$$

We consider the matrix $T := I - AP^{-1}$, and expand $G^{-1}B$ as

$$G^{-1}B = P^{-1}P^{-T}A^TA \sim P^{-T}A^TAP^{-1} = I - T - T^T + T^TT.$$

Since $\Lambda(G^{-1}B) \subset [-\|G^{-1}B\|_2, \|G^{-1}B\|_2]$, we can easily see that

$$-1 - 2\|T\|_2 - \|T\|_2^2 \leq \lambda \leq 1 + 2\|T\|_2 + \|T\|_2^2.$$

Substituting $\|I - AP^{-1}\|_2 \leq \sqrt{2} - 1 - \delta$ we obtained the desired result.

CROSS PRECONDITIONING

We would like to give a different intuition of good preconditioners for normal equations. To this aim we consider the previously observed similarity,

$$G^{-1}B = P^{-1}P^{-T}A^TA \sim P^{-T}A^TAP^{-1} = (AP^{-1})^T(AP^{-1}).$$

Hence, the closer the matrix AP^{-1} is to an orthogonal matrix, the closer $G^{-1}B$ is to the identity matrix.

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Hence, the closer the matrix AP^{-1} is to an orthogonal matrix, the closer $G^{-1}B$ is to the identity matrix.

Cross preconditioning

We say that the preconditioner P is a good **left** preconditioner for the normal equations if it is a good **right** preconditioner for $\underline{\underline{A}}$, in the sense that $\underline{\underline{AP}}^{-1}$ has clustered singular values.

CROSS PRECONDITIONING

The ideal preconditioner for $\underline{\underline{A}}$ is unique, up to scaling, and it is the inverse of $\underline{\underline{A}}$.

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QR decomposition

We can construct an ideal preconditioner using the QR decomposition of $\underline{\underline{A}}$, i.e.

$$\underline{\underline{P}} = \underline{\underline{R}}, \ \underline{\underline{A}} = \underline{\underline{Q}}_{QR}\underline{\underline{R}}.$$

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Polar decomposition

We can construct an ideal preconditioner using the polar decomposition of $\underline{\underline{A}}$, i.e.

$$\underline{\underline{P}} = (\underline{\underline{A}}^T\underline{\underline{A}})^{\frac{1}{2}}, \ \underline{\underline{A}} = \underline{\underline{Q}}_{P}\underline{\underline{P}}.$$

ADVECTION DIFFUSION ODE – CROSS PRECONDITIONING

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We consider the classical advection-diffusion ODE in one dimension, i.e.

$$-\nu \ddot{u} + \beta \dot{u} = f \text{ in } (a, b) \subset \mathbb{R},$$
$$u(a) = 0,\ u(b) = 1,\ \nu, \beta \in \mathbb{R}_{\geq 0}.$$

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For the moment we will consider neither diffusion nor advection-dominated regimes, i.e. $\nu \approx \beta$, and discretisation over an equi-spaced mesh of step-size h. Such a discretisation results in the matrix

$$\underline{\underline{A}} = \text{tridiag}\left(-\frac{\nu}{h^2} - \frac{\beta}{2h}, \frac{2\nu}{h^2}, -\frac{\nu}{h^2} + \frac{\beta}{2h}\right)$$

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n	QR	RQ	$Q(A^TA)^{1/2}$	$(AA^T)^{1/2}Q$
10	2	12	2	4
100	2	-	2	6
1000	2	-	2	7

Table: Comparison of the number of iterations for different preconditioners for the left preconditioned normal equation. The CGNE method was terminated when the absolute residual was less than 10^{-12}. If the method did not converge in 1000 iterations, we marked the number of iterations with a dash.

ADVECTION DIFFUSION PDE

We consider the classical advection-diffusion PDE in two dimensions, i.e.

$$\mathcal{L}u := -\nu \Delta u + \underline{\beta} \cdot \nabla u = f \text{ in } \Omega \subset \mathbb{R}^d,$$

$$u = g \text{ on } \partial\Omega, \text{ with } \nu \ll \|\beta\|, \ \nabla \cdot \beta = 0.$$

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Finite Element Discretisation

Fix a discrete space $V_h \subset H_0^1(\Omega)$ and look for $u_h \in V_h$ such that

$$(\hat{\mathcal{L}}u_h, v_h) = \nu(\nabla u_h, \nabla v_h)_{L^2(\Omega)} + (\beta \cdot \nabla u_h, v_h)_{L^2(\Omega)} = (f, v_h)_{L^2(\Omega)} \text{ for any } v_h \in V_h.$$

THE NORMAL EQUATIONS

We now need to understand what are the normal equations associated with the linear system,

$$A\,\underline{x} = \underline{b}, \text{ with } A_{ij} = (\hat{\mathcal{L}}\varphi_i, \varphi_j)_{L^2(\Omega)} \text{ and } b_j = (f, \varphi_j)_{L^2(\Omega)}.$$

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The first thing we need to understand is what is $\underline{\underline{A}}^T$, in fact $\underline{\underline{A}}^T$ is neither **Hilbert adjoint** of A nor the **Banach adjoint** seen as the operator $A : V_h \subset H_0^1(\Omega) \to H^{-1}(\Omega) \subset V_h'$.

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In fact, A^T is an operator itself of the form $A^T : V_h \subset H_0^1(\Omega) \to H^{-1}(\Omega) \subset V_h'$ which corresponds to the discretisation of the **Hilbert adjoint** of $\mathcal{L}$, i.e.

$$A^T_{ij} = A_{ji} = (\hat{\mathcal{L}}\varphi_j, \varphi_i)_{L^2(\Omega)} = (\varphi_j, \hat{\mathcal{L}}^*\varphi_i)_{L^2(\Omega)} = (\hat{\mathcal{L}}^*\varphi_i, \varphi_j)_{L^2(\Omega)},$$

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If we consider the classical normal equations, i.e. $\underline{\underline{A}}^T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T \underline{b}$.

Primal Dual Error

We notice that there is a primal dual error in the classical formulation of the normal equations.

$$V_h \subset H_0^1(\Omega) \xrightarrow{A} H^{-1} \subset V_h' \qquad\qquad V_h \subset H_0^1(\Omega) \xrightarrow{A^T} H^{-1} \subset V_h'$$

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To make sense of the normal equations we need to consider a Riesz map $T : V_h' \to V_h$.

$$V_h \subset H_0^1(\Omega) \xrightarrow{A} H^{-1} \subset V_h' \xrightarrow{\quad T \quad} V_h \subset H_0^1(\Omega) \xrightarrow{A^T} H^{-1} \subset V_h'$$

THE NORMAL EQUATIONS

The Riesz map gives rise to a discrete operator $T : V_h' \to V_h$, which is **symmetric and positive definite**. Therefore if we consider the normal equations with respect to the Riesz map, i.e.

$$\boxed{\underline{\underline{A}}^T T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T T \underline{b},}$$

we can rewrite them using a Cholesky factorisation of T, i.e. $T = C^T C$.

$$(CA)^T (CA)\underline{x} = (CA)^T C\underline{b},$$

hence the previous normal equation are associated with the linear system $CA\underline{x} = C\underline{b}$.

- The normal equations are still symmetric and positive definite. Hence we can solve them using CGNE. The cross-preconditioning idea is still applicable.
- The condition number of the normal equations is the square of the condition number of the original system.

THE NORMAL EQUATIONS – L^2-RIESZ MAP

We can consider as Riesz map the L^2-Riesz map, i.e.

$$(Tf, v_h)_{L^2(\Omega)} = \langle f, v_h \rangle \text{ for any } v_h \in V_h,\ f \in V_h'$$

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Using the L^2-Riesz map the new normal is approximating, in the limit $\nu \to 0$, the problem: find $u \in H_0^1(\Omega)$ such that

$$(\beta \otimes \beta \nabla u, \nabla v)_{L^2(\Omega)} = (g, v)_{L^2(\Omega)} \text{ for any } v \in H_0^1(\Omega).$$

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ν	CGNE Iterations
$1 \cdot 10^{-2}$	4231
$5 \cdot 10^{-3}$	3803
$2.5 \cdot 10^{-3}$	3327
$1.25 \cdot 10^{-3}$	2419

Table: The CGNE methods were terminated when the absolute residual was less than 10^{-5}.

Due to the function space involved in the weak form, **we chose the wrong Riesz map**.

$$H_0^1(\Omega) \longrightarrow H^{-1} \subset L^{2\prime} \xrightarrow{T^{-1}} L^2 \not\subset H_0^1(\Omega) \longrightarrow H^{-1}$$

THE NORMAL EQUATIONS – H^1-RIESZ MAP

We can consider as Riesz map the H^1-Riesz map, i.e.

$$(\nabla Tf, \nabla v_h)_{L^2(\Omega)} = \nu^{-1}\langle f, v_h\rangle, \ \forall v_h \in V_h, f \in V_h'.$$

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Using this Riesz map the normal equations $\underline{\underline{A}}^T T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T T \underline{b}$ is approximating the problem: find $u \in H_0^1(\Omega)$ such that

$$\boxed{\nu(\nabla u, \nabla v)_{L^2(\Omega)} + \nu^{-1}(\Pi_\nabla \beta u, \Pi_\nabla \beta v)_{L^2(\Omega)},\ \text{for any } v \in H_0^1(\Omega).}$$

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$$(\nabla Tf, \nabla v_h)_{L^2(\Omega)} = \nu^{-1}\langle f, v_h\rangle, \ \forall v_h \in V_h, f \in V_h'.$$

ν	32×32	64×64	128×128
$1 \cdot 10^{-2}$	2	2	2
$5 \cdot 10^{-3}$	3	3	3
$2.5 \cdot 10^{-3}$	3	3	3
$1.25 \cdot 10^{-3}$	3	3	3

Table: The CGNE methods were terminated when the absolute residual was less than 10^{-5}.

Using this Riesz map the normal equations $\underline{\underline{A}}^T T \underline{\underline{A}}\,\underline{x} = \underline{\underline{A}}^T T \underline{b}$ is approximating the problem: find $u \in H_0^1(\Omega)$ such that

$$\nu(\nabla u, \nabla v)_{L^2(\Omega)} + \nu^{-1}(\Pi_\nabla \beta u, \Pi_\nabla \beta v)_{L^2(\Omega)}, \text{ for any } v \in H_0^1(\Omega).$$

THE NORMAL EQUATIONS – PRECONDITION USING THE MASS MATRIX AND AMG

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Find $u_h \in V_h$ such that $\nu^{-1}(\beta u_h, \beta v_h)_{L^2(\Omega)},$ for any $v_h \in V_h$.

ν	32×32	64×64	128×128	256×256	512×512
$1 \cdot 10^{-2}$	9	14	21	24	26
$5 \cdot 10^{-3}$	13	13	19	28	33
$2.5 \cdot 10^{-3}$	19	17	17	25	37
$1.25 \cdot 10^{-3}$	27	24	21	22	33

Table: Comparison of the number of iterations for the CGNE method preconditioned by the inversion via PETSc GAMG, for different values of ν and different mesh sizes. The wind is fixed to $\beta = (1, 0)$ and as right-hand side we consider the function $f(x, y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

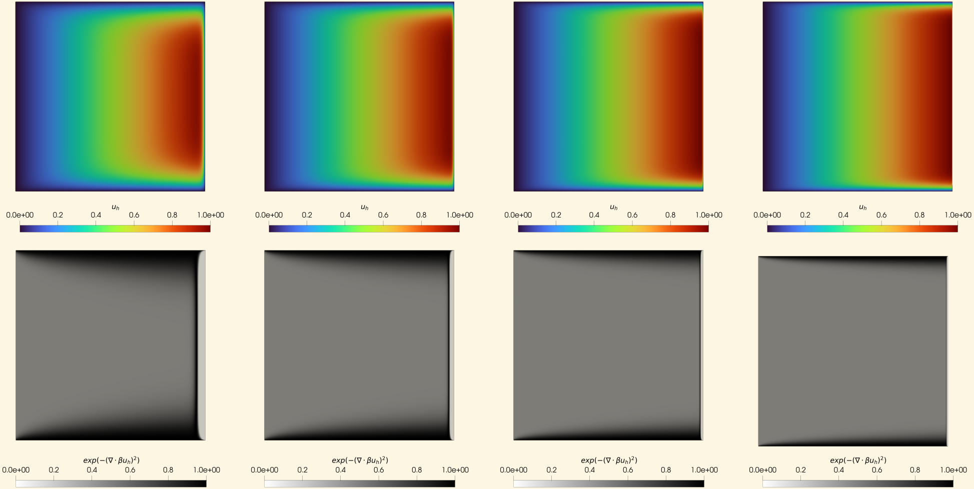

Figure: The discrete solution u_h of the advection-diffusion equation (1) for different value of ν at the finest mesh size 512×512, together with $exp(-|\nabla \cdot \beta u_h|^2)$.

THE NORMAL EQUATIONS – PRECONDITION USING THE MASS MATRIX AND AMG

Find $u_h \in V_h$ such that $\nu^{-1}(\beta u_h, \beta v_h)_{L^2(\Omega)},$ for any $v_h \in V_h$.

ν	32×32	64×64	128×128	256×256
$1 \cdot 10^{-2}$	10	15	20	23
$5 \cdot 10^{-3}$	11	15	22	30
$2.5 \cdot 10^{-3}$	17	16	21	32
$1.25 \cdot 10^{-3}$	26	24	23	30

Table: Comparison of the number of iterations for the CGNE method preconditioned by the inversion via PETSc GAMG, for different values of ν and different mesh sizes. The wind is fixed to $\sqrt{2}\beta = (1, 1)$ and as right-hand side we consider the function $f(x, y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

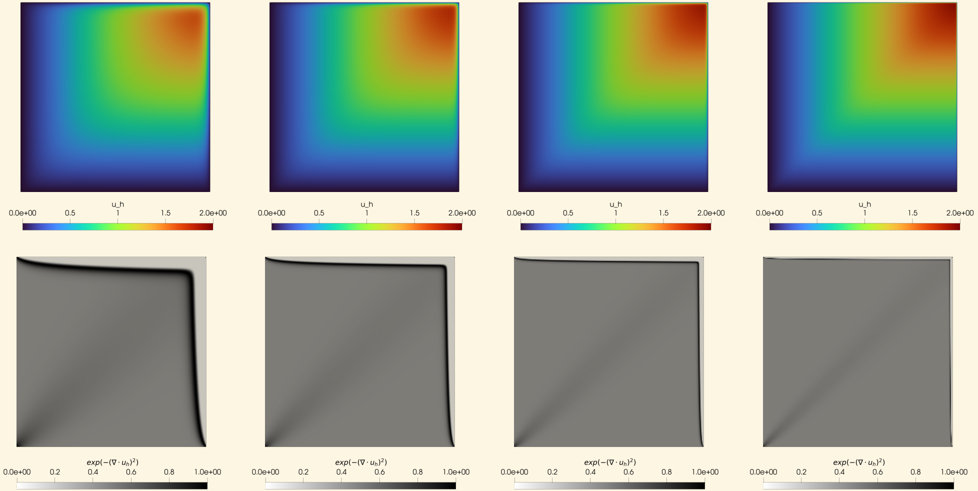

Figure: The discrete solution u_h of the convection-diffusion equation (1), with $\sqrt{2}\underline{\beta} = (1,1)$, for different values of ν at the finest mesh size 512×512, together with $exp(-|\nabla \cdot \beta u_h|^2)$.

Find $u_h \in V_h$ such that $\nu^{-1}(\Pi_\nabla \beta u_h, \Pi_\nabla \beta v_h)_{L^2(\Omega)}$, for any $v_h \in V_h$.

ν	32×32	64×64	128×128
$1 \cdot 10^{-2}$	14	22	40
$5 \cdot 10^{-3}$	16	21	33
$2.5 \cdot 10^{-3}$	22	22	29
$1.25 \cdot 10^{-3}$	30	30	34

Table: Comparison of the number of iterations for the CGNE method preconditioned by symmetric successive over-relaxation, for different values of ν and different mesh sizes. The wind is fixed to $\sqrt{2}\beta = (1, 1)$ and as right-hand side we consider the function $f(x, y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

Find $u_h \in V_h$ such that $\nu^{-1}(\Pi_\nabla \beta u_h, \Pi_\nabla \beta v_h)_{L^2(\Omega)}$, for any $v_h \in V_h$.

ν	32×32	64×64	128×128
$1 \cdot 10^{-2}$	4	5	8
$5 \cdot 10^{-3}$	4	5	7
$2.5 \cdot 10^{-3}$	5	5	7
$1.25 \cdot 10^{-3}$	7	7	7

Table: Comparison of the number of iterations for the CGNE method preconditioned by geometric multigird with SOR smoothing, for different values of ν and different mesh sizes. The wind is fixed to $\sqrt{2}\beta = (1,1)$ and as right-hand side we consider the function $f(x,y) \equiv 1$. The CGNE method was terminated when the absolute residual was less than 10^{-5}.

TAKE AWAY MESSAGE

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Mathematical Institute

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- Understand how to efficiently compute the polar decomposition so that we can construct a good **cross preconditioner** starting from the normal PDE, for LSQR type methods.

THANK YOU!
Lorenzo now accepts questions.

Some more comments on the normal equations: With a focus on discretisation of partial differential equations

L. Lazzarino, Y. Nakatsukasa, Umberto Zerbinati*