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









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.

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



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

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• How to **quickly** access $\underline{\underline{A}}^T$ and $\underline{\underline{B}}$?



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- Unfortunately the condition number of $\underline{\underline{A}}^T\underline{\underline{A}}$ is the square of the condition number of 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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$$A = \begin{bmatrix} b_0 & & & & \\ & \ddots & & \\ & & b_{n-1} \end{bmatrix}, \qquad P = \begin{bmatrix} & & b_0 \\ & \ddots & \\ b_{n-1} & & \end{bmatrix}.$$

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







SIREV Vol. 64, Iss. 3, 2022 (A. Wathen), QJRMS Vol. 64, Iss. 114, 2018 (S. Gratton, Et Al.).

Gratton-Gürol-Simon-Toint

If the matrix P is such that $\|I - AP^{-1}\|_2 \le \sqrt{2} - 1 - \delta$, then $\Lambda(G^{-1}B) \subset (\sqrt{2}\delta + \delta^2, 2 - \sqrt{2}\delta - \delta^2).$

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

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

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

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

Substituing $||I - AP^{-1}||_2 \le \sqrt{2} - 1 - \delta$ 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,

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

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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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**.

ADVECTION DIFFUSION ODE - CROSS PRECONDITIONING



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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$$u(a) = 0, \ u(b) = 1, \ \nu, \beta \in \mathbb{R}_{\geq 0}.$$

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

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



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

$$\begin{split} \mathcal{L}u &:= -\nu \Delta u + \underline{\beta} \cdot \nabla u = f \text{ in } \Omega \subset \mathbb{R}^d, \\ u &= g \text{ on } \partial \Omega, \text{ with } \nu \ll \|\beta\|, \ \nabla \cdot \beta = 0. \end{split}$$



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Finite Element Discretisation

Fix a discrete space $V_h \subset H^1_0(\Omega)$ and look for $u_h \in V_h$ such that

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



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

$$A\underline{x} = \underline{b}$$
, with $A_{ij} = (\hat{\mathcal{L}}\varphi_i, \varphi_j)_{L^2(\Omega)}$ 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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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 $A: V_h \subset H_0^1(\Omega) \to H^{-1}(\Omega) \subset V_h'$.

In fact, A^T is an operator itself of the form $A^T: V_h \subset H^1_0(\Omega) \to H^{-1}(\Omega) \subset V_h'$ which corresponds to the discretisation of the **Hilbert adjoint** of \mathcal{L} , i.e.

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

THE NORMAL EQUATIONS - PRIMAL DUAL ERROR



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

Primal Dual Error

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

$$V_h \subset H^1_0(\Omega) \stackrel{A}{\longrightarrow} H^{-1} \subset V_h'$$

$$V_h \subset H^1_0(\Omega) \xrightarrow{A} H^{-1} \subset V_h'$$
 $V_h \subset H^1_0(\Omega) \xrightarrow{A^T} H^{-1} \subset V_h'$

THE NORMAL EQUATIONS - PRIMAL DUAL ERROR



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Primal Dual Error

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

$$V_h \subset H^1_0(\Omega) \stackrel{A}{\longrightarrow} H^{-1} \subset V'_h \qquad \qquad V_h \subset H^1_0(\Omega) \stackrel{A^T}{\longrightarrow} H^{-1} \subset V'_h$$

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

$$V_h \subset H^1_0(\Omega) \xrightarrow{A} H^{-1} \subset V'_h \xrightarrow{T} V_h \subset H^1_0(\Omega) \xrightarrow{A^T} H^{-1} \subset V'_h$$



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.

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

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

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

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.

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

THE NORMAL EQUATIONS - L2-RIESZ MAP



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Using the L^2 -Riesz map the new normal is approximating, in the limit $\nu \to 0$, the problem: find $u \in H^1_0(\Omega)$ such that

$$(\beta \otimes \beta \nabla u, \nabla v)_{L^2(\Omega)} = (g, v)_{L^2(\Omega)}$$
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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} .

$$(\beta \otimes \beta \nabla u, \nabla v)_{L^2(\Omega)} = (g, v)_{L^2(\Omega)}$$
 for any $v \in H^1_0(\Omega)$.

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

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

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 $\underline{\underline{A}}^T T \underline{\underline{A}} \underline{x} = \underline{\underline{A}}^T T \underline{\underline{b}}$ is approximating the problem: find $u \in H_0^1(\Omega)$ such that

$$\nu(\nabla u, \nabla v)_{L^2(\Omega)} + \nu^{-1}(\Pi_{\nabla}\beta u, \Pi_{\nabla}\beta v)_{L^2(\Omega)}, \text{ for any } v \in H^1_0(\Omega).$$

THE NORMAL EQUATIONS – H¹-RIESZ MAP



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

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

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} .

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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
$1\cdot 10^{-2}$	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} .





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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} .



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- ▶ The correct notion of a good preconditioner for the normal equations is crucial to understand how to precondition the normal equations. We propose the notion of **cross preconditioning**.
- A careful study of the normal equations can suggest a new PDE to use as preconditioner. Often these PDEs are simpler to solve than the original ones. We refer to this idea as normal preconditioning.



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- A careful study of the normal equations can suggest a new PDE to use as preconditioner. Often these PDEs are simpler to solve than the original ones. We refer to this idea as **normal preconditioning**.
- We should reconsider the use of normal equations for solving linear systems arising from PDEs.

FUTURE WORK



▶ There is an intimate connection between the notion of **normal preconditioning** and a method known as **discontinuous Petrov-Galerkin**. We would like to further explore this connection and understand the optimisation problem associated with the normal equations here proposed.

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- Explore the notion of **normal preconditioning** for higher-order finite element discretisation.

FUTURE WORK



- There is an intimate connection between the notion of **normal preconditioning** and a method known as **discontinuous Petrov-Galerkin**. We would like to further explore this connection and understand the optimisation problem associated with the normal equations here proposed.
- Explore the notion of **normal preconditioning** for higher-order finite element discretisation.
- Apply **normal preconditioning** to other PDEs such as the Helmholtz equation, using as Riesz map the T-coercive map. We would also like to study the Oseen equation and C^1 nearly singular problems such as the Helmholtz–Korteweg equation.

THANK YOU! Lorenzo now accepts questions.

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

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