Preconditioning for self-adjointness

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A motivating example – The Bramble-Pasciak CG: consider saddle point problem

$$\mathcal{A} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} \quad \text{with preconditioner} \quad \mathcal{P} = \begin{bmatrix} A_0 & 0 \\ B & -I \end{bmatrix}$$

The (left) preconditioned matrix

$$\widehat{\mathcal{A}} = \mathcal{P}^{-1}\mathcal{A} = \begin{bmatrix} A_0^{-1}A & A_0^{-1}B^T \\ BA_0^{-1}A - B & BA_0^{-1}B^T + C \end{bmatrix}$$

is not symmetric but is self-adjoint and positive definite when

$$\mathcal{H} = \begin{bmatrix} A - A_0 & 0 \\ 0 & I \end{bmatrix}$$

defines an inner product $\langle x, y \rangle_{\mathcal{H}} := x^T \mathcal{H} y$

$\Rightarrow$ CG can be used in this inner product

Conjugate Gradient Method (*Hestenes & Stiefel (1952)*)
for $\widehat{\mathcal{A}}x = b$, $\widehat{\mathcal{A}}$ self-adjoint and positive definite in $\langle\cdot,\cdot\rangle_{\mathcal{H}}$:

Choose x_0, compute $r_0 = b - \widehat{\mathcal{A}}x_0$, set $p_0 = r_0$
`for` $k = 0$ `until` convergence `do`

$\alpha_k = \langle r_k, r_k\rangle_{\mathcal{H}} / \langle \widehat{\mathcal{A}}p_k, p_k\rangle_{\mathcal{H}}$
$x_{k+1} = x_k + \alpha_k p_k$
$r_{k+1} = r_k - \alpha_k \widehat{\mathcal{A}}p_k$
<Test for convergence>
$\beta_k = \langle r_{k+1}, r_{k+1}\rangle_{\mathcal{H}} / \langle r_k, r_k\rangle_{\mathcal{H}}$
$p_{k+1} = r_{k+1} + \beta_k p_k$

`enddo`

computes iterates $\{x_k\}$ such that

$$\langle \widehat{\mathcal{A}}(x - x_k), x - x_k\rangle_{\mathcal{H}} = \langle x - x_k, x - x_k\rangle_{\mathcal{H}\widehat{\mathcal{A}}}$$

is minimal in the relevant Krylov subspace

Self-adjointness: assume

$$\langle \cdot, \cdot \rangle : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$$

is a symmetric bilinear form or an inner product

$\mathcal{A} \in \mathbb{R}^{n \times n}$ is self-adjoint in $\langle \cdot, \cdot \rangle$ iff

$$\langle \mathcal{A}x, y \rangle = \langle x, \mathcal{A}y \rangle \qquad \text{for all } x, y$$

Self-adjointness of $\mathcal{A}$ in $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ $\quad$ ($\langle x, y \rangle_{\mathcal{H}} = x^T \mathcal{H} y$)
thus means

$$x^T \mathcal{A}^T \mathcal{H} y = \langle \mathcal{A}x, y \rangle_{\mathcal{H}} = \langle x, \mathcal{A}y \rangle_{\mathcal{H}} = x^T \mathcal{H} \mathcal{A} y$$

for all x, y $\quad \Rightarrow$

$$\mathcal{A}^T \mathcal{H} = \mathcal{H} \mathcal{A}$$

is the relation for self-adjointness of $\mathcal{A}$ in $\langle \cdot, \cdot \rangle_{\mathcal{H}}$

Basic properties:

LEMMA If $\mathcal{A}_1$ and $\mathcal{A}_2$ are self-adjoint in $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ then for any $\alpha, \beta \in \mathbb{R}$, $\alpha\mathcal{A}_1 + \beta\mathcal{A}_2$ is self-adjoint in $\langle \cdot, \cdot \rangle_{\mathcal{H}}$

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and of relevance when preconditioning:

LEMMA For symmetric $\mathcal{A}$, $\widehat{\mathcal{A}} = \mathcal{P}^{-1}\mathcal{A}$ is self-adjoint in $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ if and only if $\mathcal{P}^{-T}\mathcal{H}$ is self-adjoint in $\langle \cdot, \cdot \rangle_{\mathcal{A}}$

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PROOF

$$(\mathcal{P}^{-T}\mathcal{H})^T\mathcal{A} = \mathcal{H}\mathcal{P}^{-1}\mathcal{A} = (\mathcal{P}^{-1}\mathcal{A})^T\mathcal{H} = \mathcal{A}^T(\mathcal{P}^{-T}\mathcal{H})$$

also combining the above:

LEMMA If $\mathcal{P}_1$ and $\mathcal{P}_2$ are left preconditioners for the symmetric matrix $\mathcal{A}$ for which symmetric matrices $\mathcal{H}_1$ and $\mathcal{H}_2$ exist with $\mathcal{P}_1^{-1}\mathcal{A}$ self-adjoint in $\langle\cdot,\cdot\rangle_{\mathcal{H}_1}$ and $\mathcal{P}_2^{-1}\mathcal{A}$ self-adjoint in $\langle\cdot,\cdot\rangle_{\mathcal{H}_2}$ and if for any α, β

$$\alpha\mathcal{P}_1^{-T}\mathcal{H}_1 + \beta\mathcal{P}_2^{-T}\mathcal{H}_2 = \mathcal{P}_3^{-T}\mathcal{H}_3$$

for some matrix $\mathcal{P}_3$ and some symmetric matrix $\mathcal{H}_3$ then $\mathcal{P}_3^{-1}\mathcal{A}$ is self-adjoint in $\langle\cdot,\cdot\rangle_{\mathcal{H}_3}$.

shows that if we can find such a splitting we have found a new preconditioner and a bilinear form in which the matrix is self-adjoint.

Eigenvalues when $\boldsymbol{\mathcal{A}}$ self-adjoint in $\langle\cdot,\cdot\rangle_{\mathcal{H}}$:

$$\boldsymbol{\mathcal{A}x = \lambda x, \qquad x \neq 0}$$

Multiplying from the left by $\boldsymbol{x^\star\mathcal{H}}$ gives

$$\boldsymbol{x^\star\mathcal{H}\mathcal{A}x = \lambda x^\star\mathcal{H}x}$$

and $\boldsymbol{\mathcal{H}\mathcal{A} = \mathcal{A}^T\mathcal{H} \Rightarrow \lambda} \in \mathbb{R}$

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There is no symmetric bilinear form in which $\boldsymbol{\mathcal{A}}$ is self-adjoint unless $\boldsymbol{\mathcal{A}}$ has real eigenvalues.

LEMMA If $\boldsymbol{\mathcal{A}} = \boldsymbol{R}^{-1}\boldsymbol{\Lambda}\boldsymbol{R}$ is a diagonalization of $\boldsymbol{\mathcal{A}}$ with the diagonal matrix $\boldsymbol{\Lambda}$ of eigenvalues being real, then $\boldsymbol{\mathcal{A}}$ is self-adjoint in $\langle \cdot, \cdot \rangle_{\boldsymbol{R}^T \boldsymbol{\Theta} \boldsymbol{R}}$ for any real diagonal matrix $\boldsymbol{\Theta}$.

PROOF self-adjointness of $\boldsymbol{\mathcal{A}}$ in $\langle \cdot, \cdot \rangle_{\boldsymbol{\mathcal{H}}} \Rightarrow$

$$\boldsymbol{R}^T \boldsymbol{\Lambda} \boldsymbol{R}^{-T} \boldsymbol{\mathcal{H}} = \boldsymbol{\mathcal{H}} \boldsymbol{R}^{-1} \boldsymbol{\Lambda} \boldsymbol{R}$$

clearly satisfied for $\boldsymbol{\mathcal{H}} = \boldsymbol{R}^T \boldsymbol{\Theta} \boldsymbol{R}$ whenever $\boldsymbol{\Theta}$ is diagonal because then $\boldsymbol{\Theta}$ and $\boldsymbol{\Lambda}$ commute.

We remark that this result is not of great use in practice since knowledge of the complete eigensystem of $\boldsymbol{\mathcal{A}}$ is somewhat prohibitive.

Self-adjointness for saddle point systems:

$$\boldsymbol{\mathcal{A}} = \begin{bmatrix} \boldsymbol{A} & \boldsymbol{B}^{\boldsymbol{T}} \\ \boldsymbol{B} & \boldsymbol{0} \end{bmatrix}$$

General preconditioner

$$\boldsymbol{\mathcal{P}}^{-1} = \begin{bmatrix} \boldsymbol{X} & \boldsymbol{Y}^{\boldsymbol{T}} \\ \boldsymbol{Z} & \boldsymbol{W} \end{bmatrix}$$

gives

$$\widehat{\boldsymbol{\mathcal{A}}} = \boldsymbol{\mathcal{P}}^{-1}\boldsymbol{\mathcal{A}} = \begin{bmatrix} \boldsymbol{XA} + \boldsymbol{Y}^{\boldsymbol{T}}\boldsymbol{B} & \boldsymbol{XB}^{\boldsymbol{T}} \\ \boldsymbol{ZA} + \boldsymbol{WB} & \boldsymbol{ZB}^{\boldsymbol{T}} \end{bmatrix}$$

For self-adjointness of

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in

$$\langle \cdot, \cdot \rangle_{\mathcal{H}}, \qquad \mathcal{H} = \begin{bmatrix} \boldsymbol{E} & \boldsymbol{F}^T \\ \boldsymbol{F} & \boldsymbol{G} \end{bmatrix}$$

we require

$$\begin{bmatrix} \boldsymbol{AX}^T + \boldsymbol{BY}^T & \boldsymbol{AZ}^T + \boldsymbol{B}^T\boldsymbol{W}^T \\ \boldsymbol{BX}^T & \boldsymbol{BZ}^T \end{bmatrix} \begin{bmatrix} \boldsymbol{E} & \boldsymbol{F}^T \\ \boldsymbol{F} & \boldsymbol{G} \end{bmatrix} =$$

$$\begin{bmatrix} \boldsymbol{E} & \boldsymbol{F}^T \\ \boldsymbol{F} & \boldsymbol{G} \end{bmatrix} \begin{bmatrix} \boldsymbol{XA} + \boldsymbol{Y}^T\boldsymbol{B} & \boldsymbol{XB}^T \\ \boldsymbol{ZA} + \boldsymbol{WB} & \boldsymbol{ZB}^T \end{bmatrix}$$

Examples: Bramble-Pasciak CG (*Bramble & Pasciak (1988))*
widely used CG technique with preconditioner

$$\mathcal{P}^{-1} = \begin{bmatrix} A_0^{-1} & 0 \\ BA_0^{-1} & -I \end{bmatrix}$$

and inner product matrix

$$\mathcal{H} = \begin{bmatrix} A - A_0 & 0 \\ 0 & I \end{bmatrix}$$

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$$\mathcal{H} = \begin{bmatrix} A - A_0 & 0 \\ 0 & I \end{bmatrix}$$

main drawback: requires

$$A_0 < A$$

involves the computation of an eigenvalue problem in the worst case!

Denote: BP^{-}

Examples: BP with Schur complement preconditioner

(*Klawonn (1998), Meyer et al. (2001), Simoncini (2001)*)

$$\mathcal{P}^{-1} = \begin{bmatrix} A_0^{-1} & 0 \\ S_0^{-1} B A_0^{-1} & -S_0^{-1} \end{bmatrix}$$

Inner product:

$$\mathcal{H} = \begin{bmatrix} A - A_0 & 0 \\ 0 & S_0 \end{bmatrix}$$

Examples: Zulehner (*Zulehner (2001), Schöberl & Zulehner (2007)*

$$\mathcal{P} = \begin{bmatrix} A_0 & B^T \\ B & BA_0^{-1}B^T - S_0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ BA_0^{-1} & I \end{bmatrix} \begin{bmatrix} A_0 & B^T \\ 0 & -S_0 \end{bmatrix}$$

gives $\mathcal{P}^{-1}\mathcal{A}$ self-adjoint in $\langle \cdot, \cdot \rangle_{\mathcal{H}}$,

$$\mathcal{H} = \begin{bmatrix} A_0 - A & 0 \\ 0 & BA_0^{-1}B^T - S_0 \end{bmatrix}$$

if $A_0 > A$ and $S_0 < BA_0^{-1}B^T$

Examples: Benzi-Simoncini *(Benzi and Simoncini (2006))*
extension of CG method of *Fischer, Ramage, Silvester & W (1998)*

$$\mathcal{P}^{-1} = \begin{bmatrix} \boldsymbol{I} & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{I} \end{bmatrix}$$

inner product:

$$\mathcal{H} = \begin{bmatrix} \boldsymbol{A} - \gamma \boldsymbol{I} & \boldsymbol{B}^T \\ \boldsymbol{B} & \gamma \boldsymbol{I} \end{bmatrix}$$

Extension for $\boldsymbol{C} \neq \mathbf{0}$ *(Liesen (2006), Liesen & Parlett (2007))*:

$$\mathcal{H} = \begin{bmatrix} \boldsymbol{A} - \gamma \boldsymbol{I} & \boldsymbol{B}^T \\ \boldsymbol{B} & \gamma \boldsymbol{I} - \boldsymbol{C} \end{bmatrix}$$

Example: Bramble-Pasciak$^+$ method *(Stoll & W(2007))*

$$\mathcal{P}^{-1} = \begin{bmatrix} \boldsymbol{A_0^{-1}} & \mathbf{0} \\ \boldsymbol{B A_0^{-1}} & \boldsymbol{I} \end{bmatrix}$$

and inner product

$$\mathcal{H} = \begin{bmatrix} \boldsymbol{A + A_0} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{I} \end{bmatrix}$$

Note: $\mathcal{H}$ defines an inner product for any symmetric and positive definite preconditioner $\boldsymbol{A_0}$
$\Rightarrow$ can always apply Lanczos, MINRES in this inner product

Example: Bramble-Pasciak^{+} method *(Stoll & W(2007))*

$$\mathcal{P}^{-1} = \begin{bmatrix} A_0^{-1} & 0 \\ BA_0^{-1} & I \end{bmatrix}$$

and inner product

$$\mathcal{H} = \begin{bmatrix} A + A_0 & 0 \\ 0 & I \end{bmatrix}$$

Note: $\mathcal{H}$ defines an inner product for any symmetric and positive definite preconditioner A_0
$\Rightarrow$ can always apply Lanczos, MINRES in this inner product

denote: BP^{+}

Combination preconditioning

Final lemma above shows that if can find $\mathcal{P}_3$ and $\mathcal{H}_3$ with

$$\alpha \mathcal{P}_1^{-1} \mathcal{H}_1 + \beta \mathcal{P}_2^{-1} \mathcal{H}_2 = \mathcal{P}_3^{-T} \mathcal{H}_3$$

this gives a new preconditioner and symmetric bilinear form

Combine Bramble-Pasciak and Benzi-Simoncini:

$$\alpha \mathcal{P}_1^{-1} \mathcal{H}_1 + \beta \mathcal{P}_2^{-1} \mathcal{H}_2 =$$

$$\begin{bmatrix} (\alpha A_0^{-1} + \beta I)A - (\alpha + \beta\gamma)I & (\alpha A_0^{-1} + \beta I)B^T \\ -\beta B & -(\alpha + \beta\gamma)I \end{bmatrix}$$

One possibility for a splitting $\alpha \mathcal{P}_1^{-1} \mathcal{H}_1 + \beta \mathcal{P}_2^{-1} \mathcal{H}_2$ is

$$\mathcal{P}_3^{-T} = \begin{bmatrix} \alpha A_0^{-1} + \beta I & 0 \\ 0 & -\beta I \end{bmatrix}$$

and

$$\mathcal{H}_3 = \begin{bmatrix} A - (\alpha + \beta\gamma)(\alpha A_0^{-1} + \beta I)^{-1} & B^T \\ B & \frac{\alpha + \beta\gamma}{\beta} I \end{bmatrix}$$

Combination preconditioning

Final lemma above shows that if can find $\mathcal{P}_3$ and $\mathcal{H}_3$ with

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Take $\mathcal{P}_1$, $\mathcal{H}_1$ as BP$^-$ and $\mathcal{P}_2$, $\mathcal{H}_2$ as BP$^+$

Combine BP$^-$ and BP$^+$

$$\alpha \mathcal{P}_1^{-T} \mathcal{H}_1 + (1-\alpha) \mathcal{P}_2^{-T} \mathcal{H}_2 =$$

$$\begin{bmatrix} A_0^{-1} A + (1-2\alpha) I & A_0^{-1} B^T \\ 0 & (1-2\alpha) I \end{bmatrix}$$

Combine BP$^-$ and BP$^+$

$$\alpha \mathcal{P}_1^{-T} \mathcal{H}_1 + (1-\alpha) \mathcal{P}_2^{-T} \mathcal{H}_2 =$$

$$\left[\begin{array}{cc} A_0^{-1} A + (1-2\alpha) I & A_0^{-1} B^T \\ 0 & (1-2\alpha) I \end{array} \right]$$

can be split as

$$\mathcal{P}_3^{-T} = \left[\begin{array}{cc} A_0^{-1} & A_0^{-1} B^T \\ 0 & (1-2\alpha) I \end{array} \right], \mathcal{H}_3 = \left[\begin{array}{cc} A + (1-2\alpha) A_0 & 0 \\ 0 & I \end{array} \right]$$

Combine BP$^-$ and BP$^+$

$$\alpha \mathcal{P}_1^{-T}\mathcal{H}_1 + (1-\alpha)\mathcal{P}_2^{-T}\mathcal{H}_2 =$$

$$\begin{bmatrix} A_0^{-1}A + (1-2\alpha)I & A_0^{-1}B^T \\ 0 & (1-2\alpha)I \end{bmatrix}$$

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Recall $\mathcal{P}_3^{-1}\mathcal{A}$ is self-adjoint in $\langle \cdot, \cdot \rangle_{\mathcal{H}_3}$

Combine BP$^-$ and BP$^+$

$$\alpha \mathcal{P}_1^{-T} \mathcal{H}_1 + (1-\alpha)\mathcal{P}_2^{-T}\mathcal{H}_2 =$$

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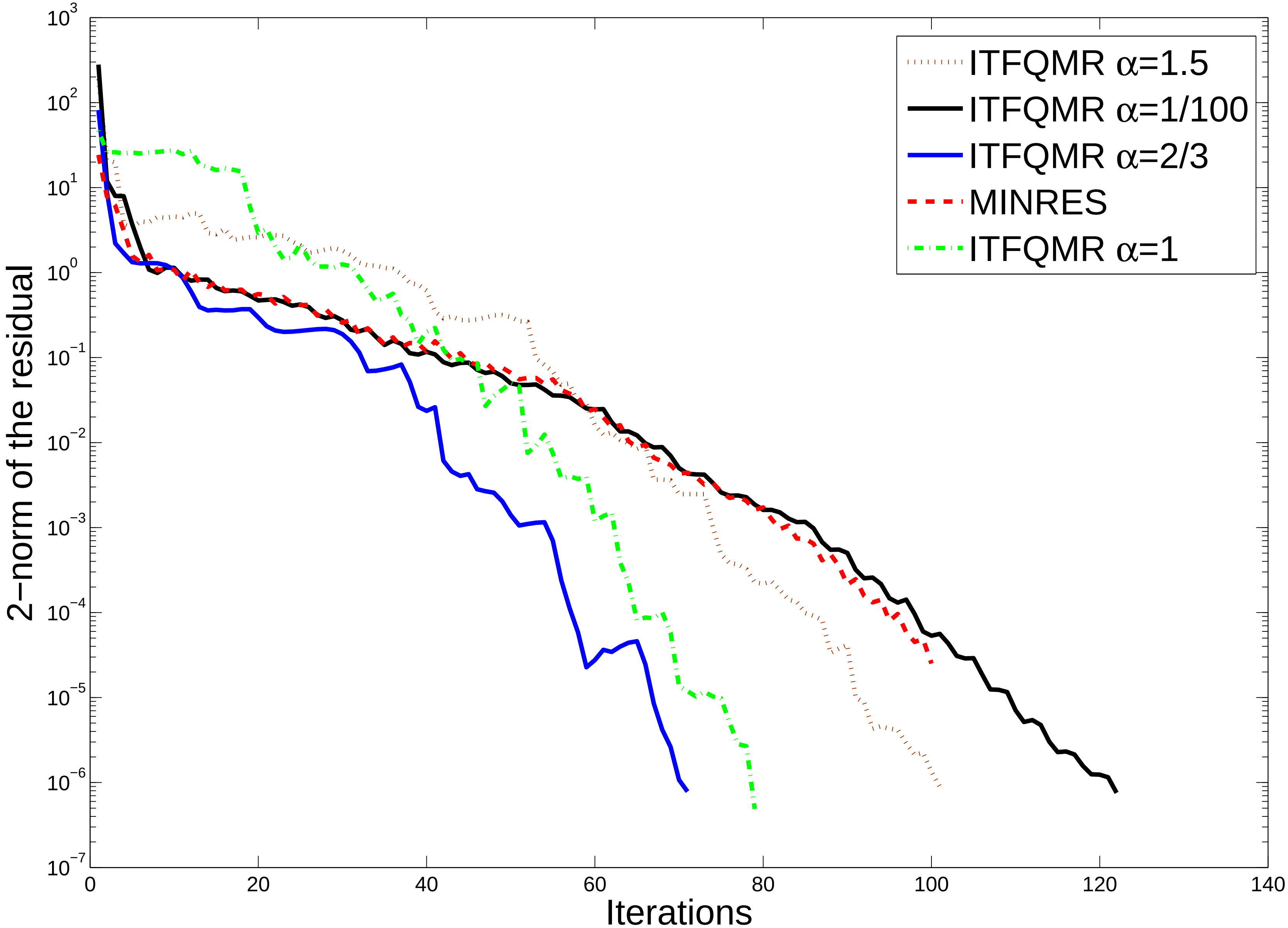
($\alpha = 1 \leftrightarrow$ BP$^-$, $\quad \alpha = 0 \leftrightarrow$ BP$^+$)

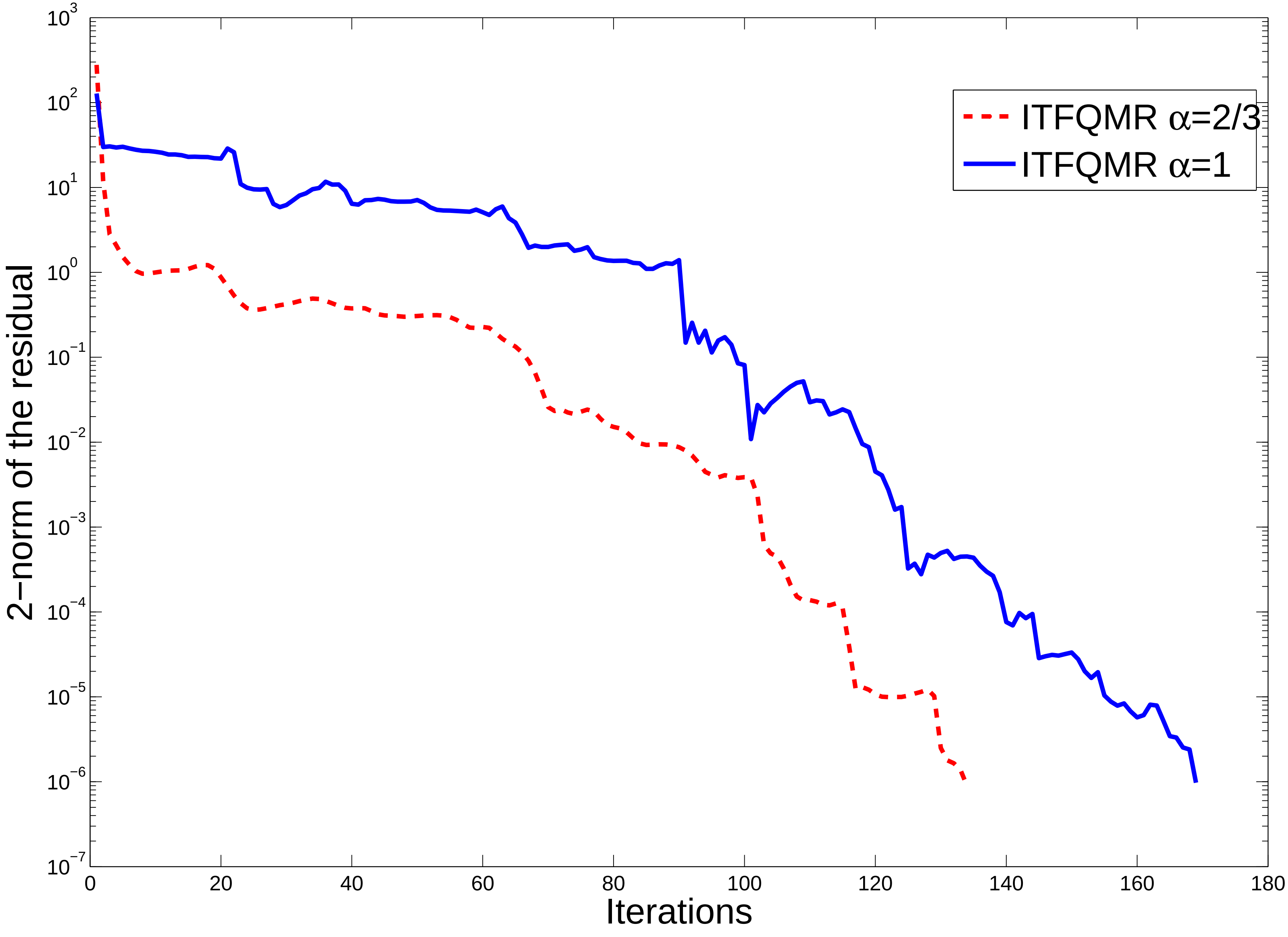
Iterative method?

- MINRES (applicable when $\mathcal{H}_3$ is positive definite)
  (Paige & Saunders (1975))
- ITFQMR — ideal transpose-free Quasi Minimum Residuals
  (Freund & Nachtigal (1995)) (applicable for symmetric nonsingular $\mathcal{H}_3$ and related to BiCG: *Rozloznik (2005)*)



ITFQMR α=1.5
ITFQMR α=1/100
ITFQMR α=2/3
MINRES
ITFQMR α=1
2−norm of the residual
Iterations

Combine BP- and BP+: another IFISS Stokes problem



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- 'isolated' practical examples of self-adjointness in non-standard inner products exist - in particular BP^- and the new BP^+ method
- theory here allow 'interpolation' between such examples, hence broadens the set of possible application of CG or MINRES in non-standard inner products

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- ‘isolated’ practical examples of self-adjointness in non-standard inner products exist - in particular BP^{-} and the new BP^{+} method
- theory here allow ‘interpolation’ between such examples, hence broadens the set of possible application of CG or MINRES in non-standard inner products
- application here to saddle-point matrices, but theory is more general