

IDR(s)ORes and eigenvalue computations

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joint work with Martin Gutknecht
(work in progress)

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ETH Zürich, September 11th, 2009

Outline

Krylov subspace methods

Hessenberg decompositions

QOR/QMR/Ritz-Galärkin

OrthoRes-type methods

LTPM

IDR

IDR(s)ORes

Sonneveld pencil and Sonneveld matrix

Purified pencil

Deflated pencil and deflated matrix

BiORes(s , 1)

Numerical Examples

Hessenberg decompositions

Essential features of Krylov subspace methods can be described by a **Hessenberg decomposition**

$$\mathbf{A}\mathbf{Q}_n = \mathbf{Q}_{n+1}\underline{\mathbf{H}}_n = \mathbf{Q}_n\mathbf{H}_n + \mathbf{q}_{n+1}h_{n+1,n}\mathbf{e}_n^T. \quad (1)$$

Here, \mathbf{H}_n denotes an unreduced Hessenberg matrix.

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In the perturbed case, e.g., in finite precision and/or based on inexact matrix-vector multiplies, we obtain a **perturbed Hessenberg decomposition**

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The matrix \mathbf{H}_n of the perturbed variant will, in general, still be unreduced.

Generalized Hessenberg decompositions

In case of IDR, we have to consider **generalized Hessenberg decompositions**

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Generalized Hessenberg decompositions correspond to a skew projection of the pencil (\mathbf{A}, \mathbf{I}) to the pencil $(\mathbf{H}_n, \mathbf{U}_n)$ as long as \mathbf{Q}_{n+1} has full rank.

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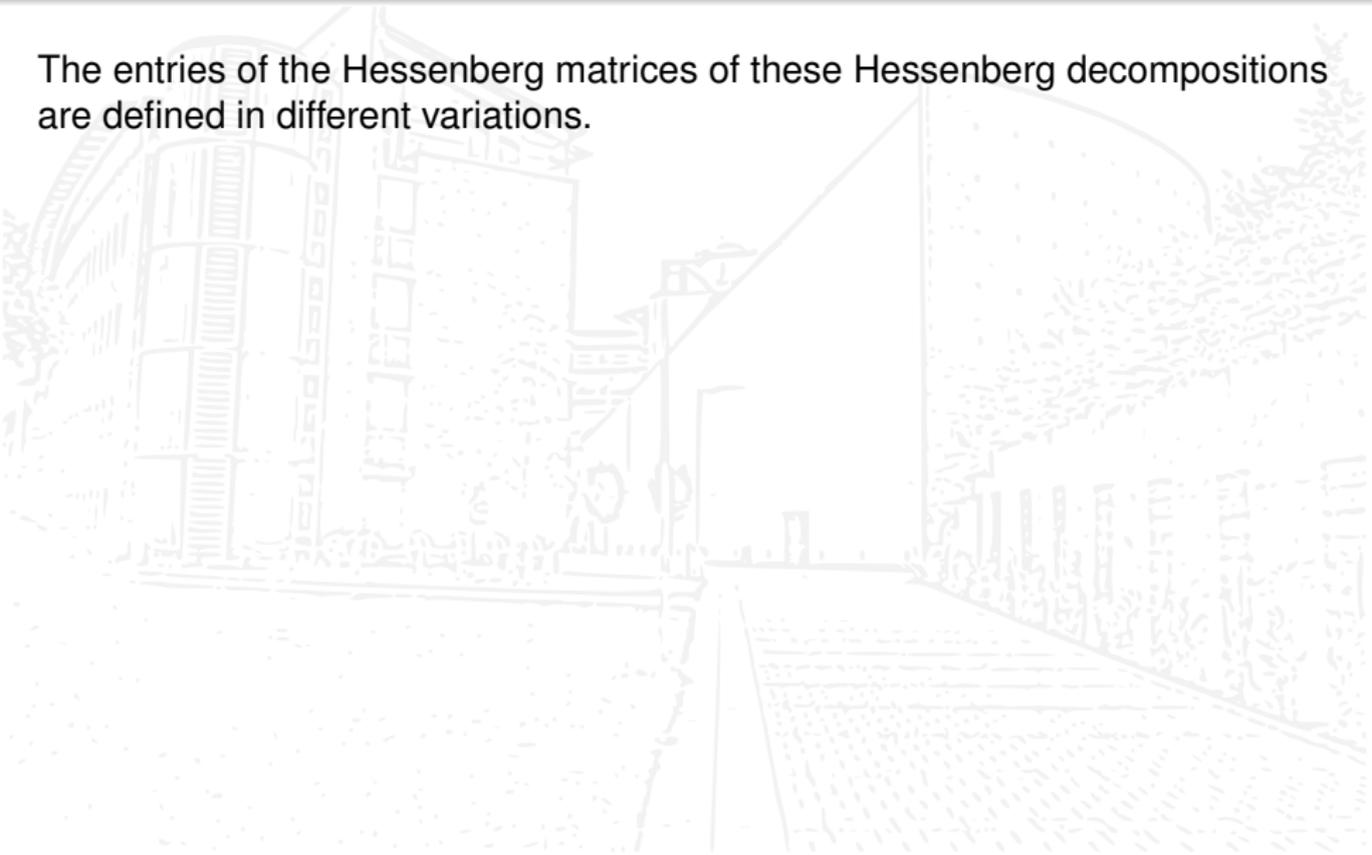
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IDR is of type QOR.

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We show how IDR fits into the LTPM framework.

The prototype IDR(s) (without the recurrences for \mathbf{x}_n , and thus already slightly rewritten)

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compute  $\mathbf{R}_{s+1} = \mathbf{R}_{0:s} = (\mathbf{r}_0, \dots, \mathbf{r}_s)$  using, e.g., ORTHORES
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 $n \leftarrow s + 1, j \leftarrow 1$ 
while not converged
   $\mathbf{c}_n = (\mathbf{P}^H \nabla \mathbf{R}_{n-s:n-1})^{-1} \mathbf{P}^H \mathbf{r}_{n-1}$ 
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A few remarks:

We can start with **any** (simple) **Krylov** subspace method.

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 $\Rightarrow \mathbf{r}_n = (\mathbf{I} - \omega_j \mathbf{A}) \mathbf{v}_{n-1}$ 

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IDR(s)ORes is based on **oblique projections** and $s + 1$ consecutive multiplications with **the same linear factor $\mathbf{I} - \omega_j \mathbf{A}$** .

The underlying Hessenberg decomposition

The IDR recurrences of IDR(s)ORes can be summarized by

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Sonneveld pencil and Sonneveld matrix

The IDR(s)ORes pencil, the so-called **Sonneveld pencil** $(\mathbf{Y}_n^o, \mathbf{Y}_n \mathbf{D}_\omega^{(n)})$, can be depicted by

$$\begin{pmatrix} \times & \times & \times & \times & o & o & o & o & o & o & o & o \\ + & \times & \times & \times & \times & o & o & o & o & o & o & o \\ o & + & \times & \times & \times & \times & o & o & o & o & o & o \\ o & o & + & \times & \times & \times & \times & o & o & o & o & o \\ o & o & o & o & + & \times & \times & \times & \times & o & o & o \\ o & o & o & o & o & + & \times & \times & \times & \times & o & o \\ o & o & o & o & o & o & + & \times & \times & \times & \times & o \\ o & o & o & o & o & o & o & + & \times & \times & \times & \times \\ o & o & o & o & o & o & o & o & + & \times & \times & \times \\ o & o & o & o & o & o & o & o & o & + & \times & \times \\ o & o & o & o & o & o & o & o & o & o & + & \times \\ o & o & o & o & o & o & o & o & o & o & o & + \\ o & o & o & o & o & o & o & o & o & o & o & \times \end{pmatrix}, \begin{pmatrix} \times & \times & \times & \times & o & o & o & o & o & o & o & o \\ o & \times & \times & \times & \times & o & o & o & o & o & o & o \\ o & o & \times & \times & \times & \times & o & o & o & o & o & o \\ o & o & o & \times & \times & \times & \times & o & o & o & o & o \\ o & o & o & o & \times & \times & \times & \times & o & o & o & o \\ o & o & o & o & o & \times & \times & \times & \times & o & o & o \\ o & o & o & o & o & o & \times & \times & \times & \times & o & o \\ o & o & o & o & o & o & o & \times & \times & \times & \times & o \\ o & o & o & o & o & o & o & o & \times & \times & \times & \times \\ o & o & o & o & o & o & o & o & o & \times & \times & \times \\ o & o & o & o & o & o & o & o & o & o & \times & \times \\ o & o & o & o & o & o & o & o & o & o & o & \times \\ o & o & o & o & o & o & o & o & o & o & o & \times \\ o & o & o & o & o & o & o & o & o & o & o & \times \end{pmatrix}.$$

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The upper triangular matrix $\mathbf{Y}_n \mathbf{D}_\omega^{(n)}$ could be inverted, which results in the **Sonneveld matrix**, a **full** unreduced Hessenberg matrix.

Purification

We know the eigenvalues \approx roots of kernel polynomials $1/\omega_j$. We are only interested in the other eigenvalues.

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The **purified IDR(s)ORes pencil** $(\mathbf{Y}_n^\circ, \mathbf{U}_n \mathbf{D}_\omega^{(n)})$, that has only the remaining eigenvalues and some infinite ones as eigenvalues, can be depicted by

$$\begin{pmatrix} \times & \times & \times & \times & \circ \\ + & \times & \times & \times & \times & \circ \\ \circ & + & \times & \times & \times & \times & \circ \\ \circ & \circ & + & \times & \times & \times & \times & \circ \\ \circ & \circ & \circ & + & \times & \times & \times & \times & \circ \\ \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \circ & \circ & \circ & \circ \\ \circ & + & \times & \times & \times & \times & \circ & \circ & \circ \\ \circ & + & \times & \times & \times & \times & \circ & \circ \\ \circ & + & \times & \times & \times & \times & \circ \end{pmatrix}, \begin{pmatrix} \times & \times & \times & \circ \\ \circ & \times & \times & \circ \\ \circ & \circ & \times & \circ \\ \circ & \circ \\ \circ & \circ & \circ & \circ & \times & \times & \times & \circ \\ \circ & \circ & \circ & \circ & \circ & \times & \times & \circ \\ \circ & \circ & \circ & \circ & \circ & \circ & \times & \circ \\ \circ & \circ \\ \circ & \circ \\ \circ & \times & \times & \times & \times & \circ \\ \circ & \times & \times & \times & \times \\ \circ & \times & \times & \times \\ \circ & \times & \times \\ \circ & \times \end{pmatrix}.$$

We get rid of the infinite eigenvalues using a change of basis (**Gauß/Schur**).

Gaussian elimination

The **deflated purified IDR(s)ORes pencil**, after the elimination step ($\mathbf{Y}_n^\circ \mathbf{G}_n, \mathbf{U}_n \mathbf{D}_\omega^{(n)}$), can be depicted by

$$\left(\begin{array}{cccccccccccc} \times & \circ & \circ & \circ & \circ & \circ \\ + & \times & \times & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\ \circ & + & \times & \times & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & + & \circ \\ \circ & \circ & + & + & \times & \circ \\ \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \times & \times & \circ \\ \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times & \times & \times & \circ \\ \circ & \circ & \circ & \circ & \circ & \circ & + & \circ & \circ & \circ & \circ & \circ \\ \circ & + & \circ & \circ & \circ & \circ \\ \circ & + & + & \times & \times & \times \\ \circ & + & \times & \times & \times \\ \circ & + & \times & \times \\ \circ & + \\ \circ & \circ \end{array} \right), \quad \left(\begin{array}{cccccccccccc} \times & \times & \times & \circ \\ \circ & \times & \times & \circ \\ \circ & \circ & \times & \circ \\ \circ & \circ \\ \circ & \circ & \circ & \circ & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \times & \times & \times & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ & \times & \times & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ & \circ & \times & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ \\ \circ & \times & \times & \times \\ \circ & \times & \times & \times \\ \circ & \times & \times \\ \circ & \times \\ \circ & \circ \end{array} \right).$$

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Using Laplace expansion of the determinant of $z\mathbf{U}_n \mathbf{D}_\omega^{(n)} - \mathbf{Y}_n^\circ \mathbf{G}_n$ we can get rid of the trivial constant factors corresponding to infinite eigenvalues. This amounts to a deflation.

Deflation

The **deflated purified IDR(s)ORes pencil**, after the deflation step ($D(\mathbf{Y}_n^\circ \mathbf{G}_n), D(\mathbf{U}_n \mathbf{D}_\omega^{(n)})$), can be depicted by

$$\begin{pmatrix} \times & \times & \times & \times & \times & \times & \circ & \circ & \circ \\ + & \times & \times & \times & \times & \times & \circ & \circ & \circ \\ \circ & + & \times & \times & \times & \times & \circ & \circ & \circ \\ \circ & \circ & + & \times & \times & \times & \times & \times & \times \\ \circ & \circ & \circ & + & \times & \times & \times & \times & \times \\ \circ & \circ & \circ & \circ & + & \times & \times & \times & \times \\ \circ & \circ & \circ & \circ & \circ & + & \times & \times & \times \\ \circ & \circ & \circ & \circ & \circ & \circ & + & \times & \times \end{pmatrix}, \begin{pmatrix} \times & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ \\ \circ & \times & \times & \circ & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \times & \circ & \circ & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \times & \times & \times & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \times & \times & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \times & \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ & \circ & \times & \times & \times & \times \\ \circ & \circ & \circ & \circ & \circ & \circ & \times & \times & \times \\ \circ & \times & \times \\ \circ & \times \end{pmatrix}.$$

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Here, D is an **deflation operator** that removes every $s + 1$ th column and row from the matrix the operator is applied to.

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The block-diagonal matrix $D(\mathbf{U}_n \mathbf{D}_\omega^{(n)})$ has invertible upper triangular blocks and can be inverted to expose the underlying **Lanczos process**.

A Lanczos process with multiple left-hand sides

Inverting the block-diagonal matrix $D(\mathbf{U}_n \mathbf{D}_\omega^{(n)})$ gives an algebraic eigenvalue problem with a block-tridiagonal unreduced upper Hessenberg matrix

$$\mathbf{L}_n := D(\mathbf{Y}_n^\circ \mathbf{G}_n) \cdot D(\mathbf{U}_n \mathbf{D}_\omega^{(n)})^{-1} = \begin{pmatrix} \times \times \times \times \times \times \circ \circ \circ \\ + \times \times \times \times \times \circ \circ \circ \\ \circ + \times \times \times \times \circ \circ \circ \\ \circ \circ + \times \times \times \times \times \times \\ \circ \circ \circ + \times \times \times \times \times \\ \circ \circ \circ \circ + \times \times \times \times \\ \circ \circ \circ \circ \circ + \times \times \times \\ \circ \circ \circ \circ \circ \circ + \times \times \end{pmatrix}.$$

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This is the matrix of the underlying **BiORes(s, 1)** process.

A Lanczos process with multiple left-hand sides

Inverting the block-diagonal matrix $D(\mathbf{U}_n \mathbf{D}_\omega^{(n)})$ gives an algebraic eigenvalue problem with a block-tridiagonal unreduced upper Hessenberg matrix

$$\mathbf{L}_n := D(\mathbf{Y}_n^\circ \mathbf{G}_n) \cdot D(\mathbf{U}_n \mathbf{D}_\omega^{(n)})^{-1} = \begin{pmatrix} \times \times \times \times \times \times \circ \circ \circ \\ + \times \times \times \times \times \times \circ \circ \circ \\ \circ + \times \times \times \times \times \times \circ \circ \circ \\ \circ \circ + \times \times \times \times \times \times \\ \circ \circ \circ + \times \times \times \times \times \times \\ \circ \circ \circ \circ + \times \times \times \times \times \times \\ \circ \circ \circ \circ \circ + \times \times \times \times \\ \circ \circ \circ \circ \circ \circ + \times \times \times \times \\ \circ \circ \circ \circ \circ \circ \circ + \times \times \times \times \end{pmatrix}.$$

This is the matrix of the underlying **BiORes(s, 1)** process.

This matrix (in the extended version) satisfies

$$\mathbf{A} \mathbf{Q}_n = \mathbf{Q}_{n+1} \mathbf{L}_n,$$

where the **reduced residuals** \mathbf{q}_{js+k} , $k = 0, \dots, s-1$, $j = 0, 1, \dots$, with $\Omega_0(z) \equiv 1$ and $\Omega_j(z) = \prod_{k=1}^j (1 - \omega_k z)$ are given by

$$\Omega_j(\mathbf{A}) \mathbf{q}_{js+k} = \mathbf{r}_{j(s+1)+k}.$$

A Lanczos process with multiple left-hand sides

The reduced residuals are defined by

$$\Omega_j(\mathbf{A})\mathbf{q}_{js+k} = \mathbf{r}_{j(s+1)+k} = (\mathbf{I} - \omega_j\mathbf{A})\mathbf{v}_{j(s+1)+k-1}$$

and every $\mathbf{v}_{j(s+1)+k-1}$ is **orthogonal to \mathbf{P}** .

A Lanczos process with multiple left-hand sides

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Thus, $\mathbf{q}_{js+k} \perp \Omega_{j-1}(\mathbf{A}^H)\mathbf{P}$.

A Lanczos process with multiple left-hand sides

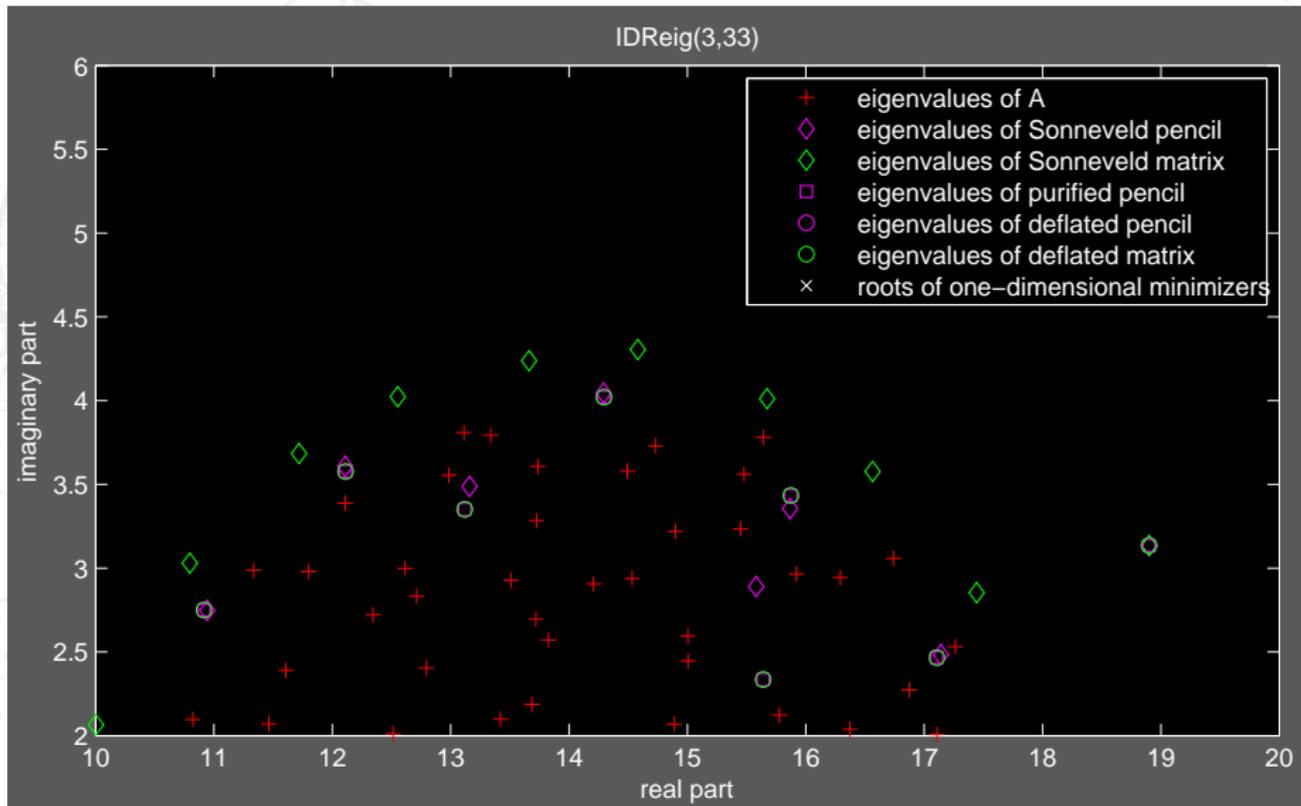
The reduced residuals are defined by

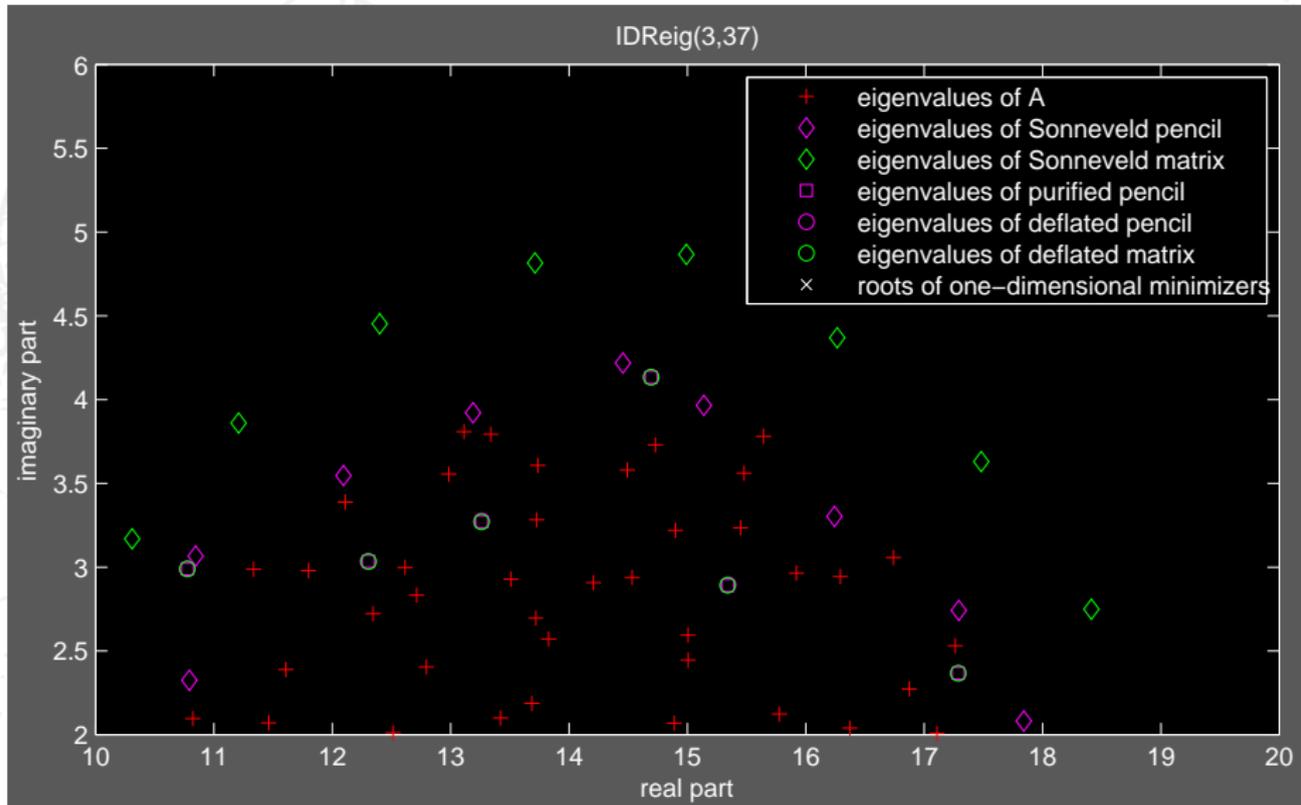
$$\Omega_j(\mathbf{A})\mathbf{q}_{js+k} = \mathbf{r}_{j(s+1)+k} = (\mathbf{I} - \omega_j\mathbf{A})\mathbf{v}_{j(s+1)+k-1}$$

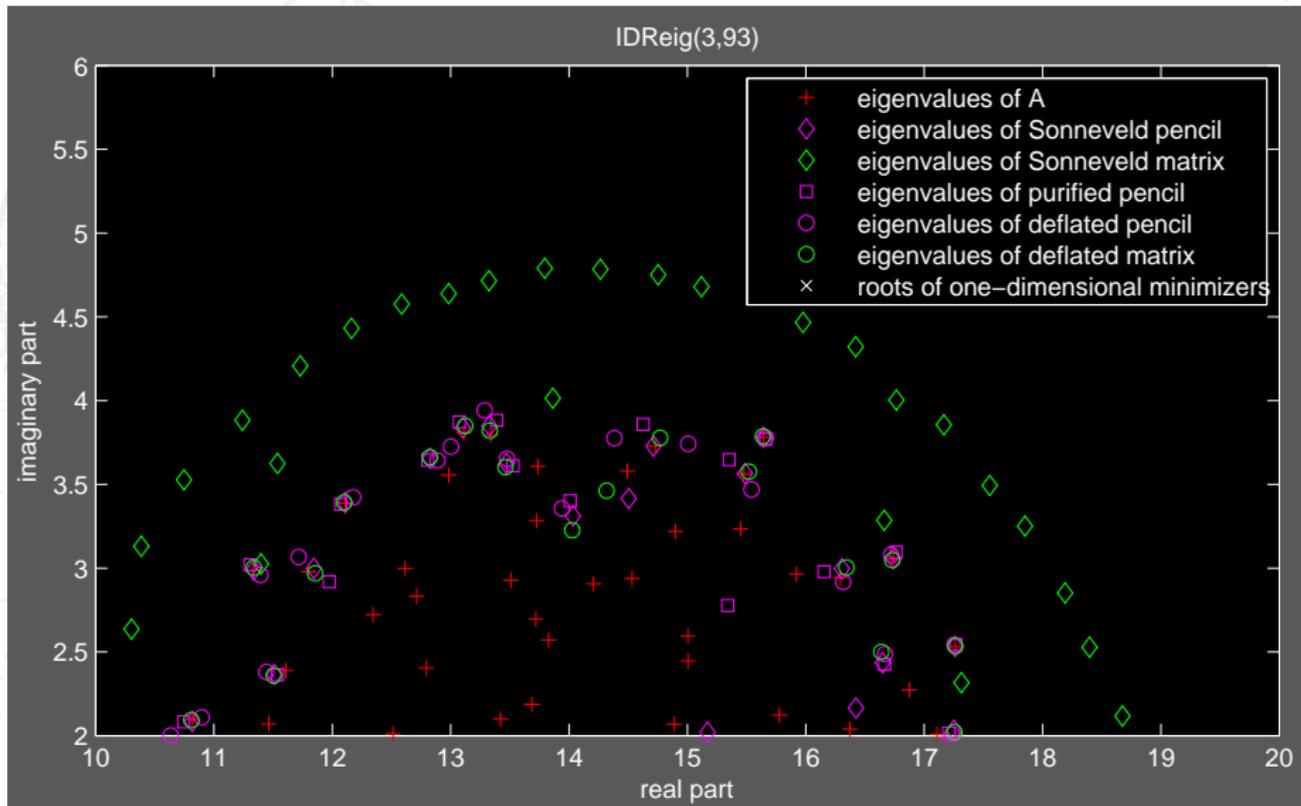
and every $\mathbf{v}_{j(s+1)+k-1}$ is **orthogonal to \mathbf{P}** .

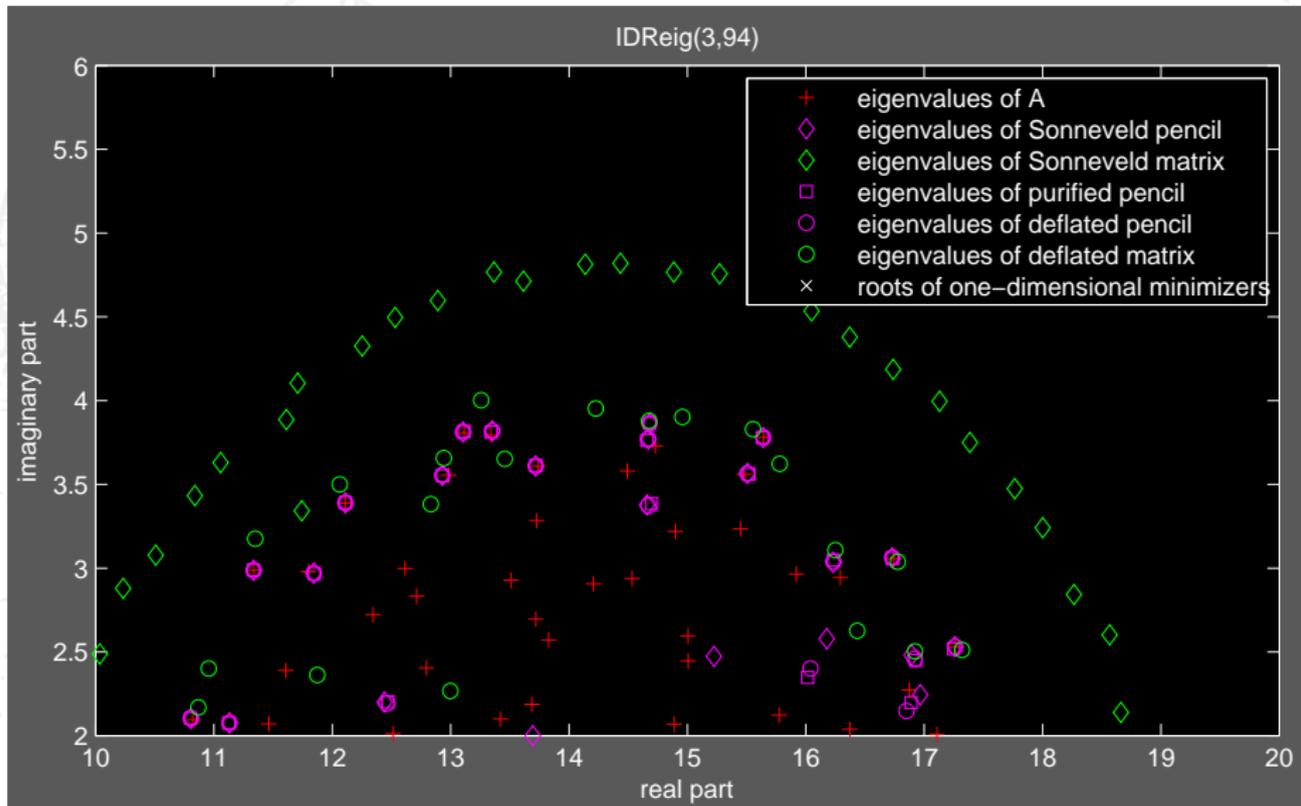
Thus, $\mathbf{q}_{js+k} \perp \Omega_{j-1}(\mathbf{A}^H)\mathbf{P}$.

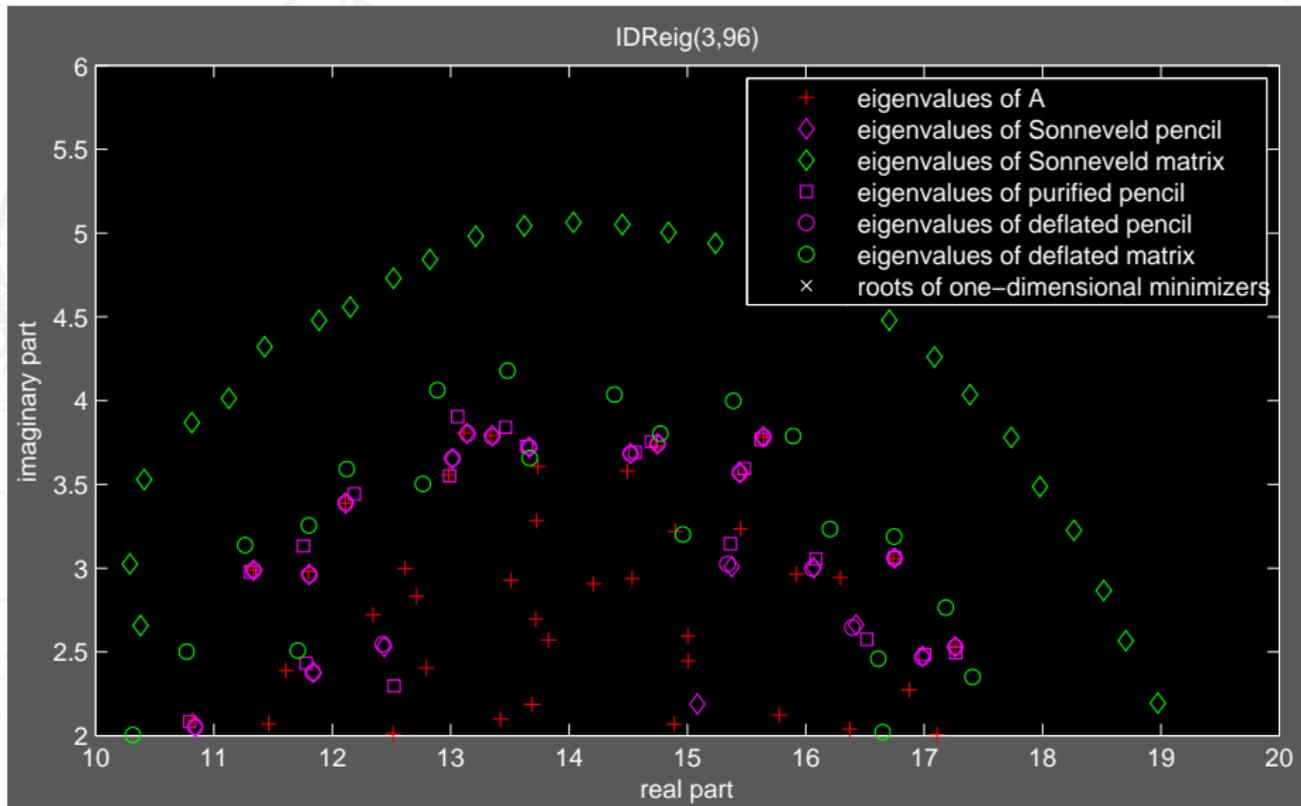
Using induction one can prove that $\mathbf{q}_{js+k} \perp \mathcal{K}_j(\mathbf{A}^H, \mathbf{P})$; thus, this is a two-sided Lanczos process with s left and one right starting vectors.

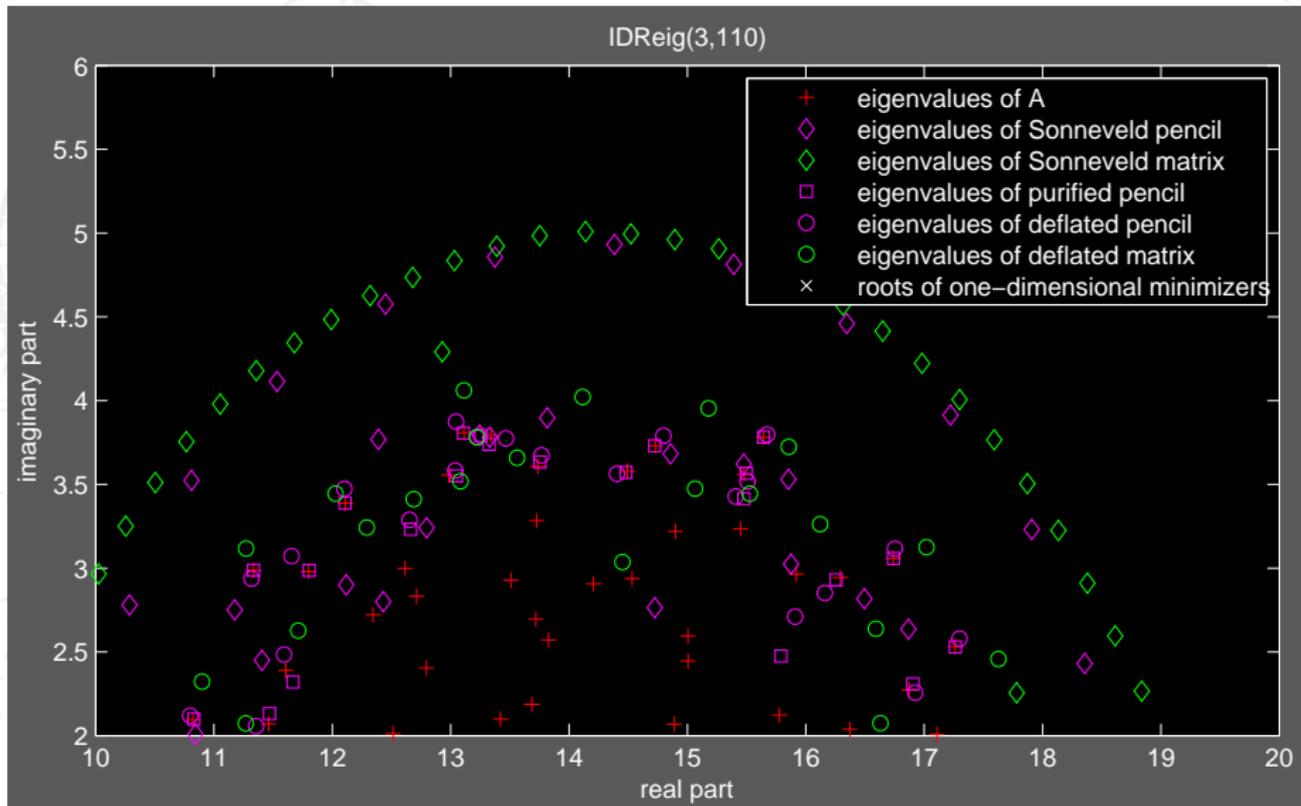
Selected examples for $s = 3$ 

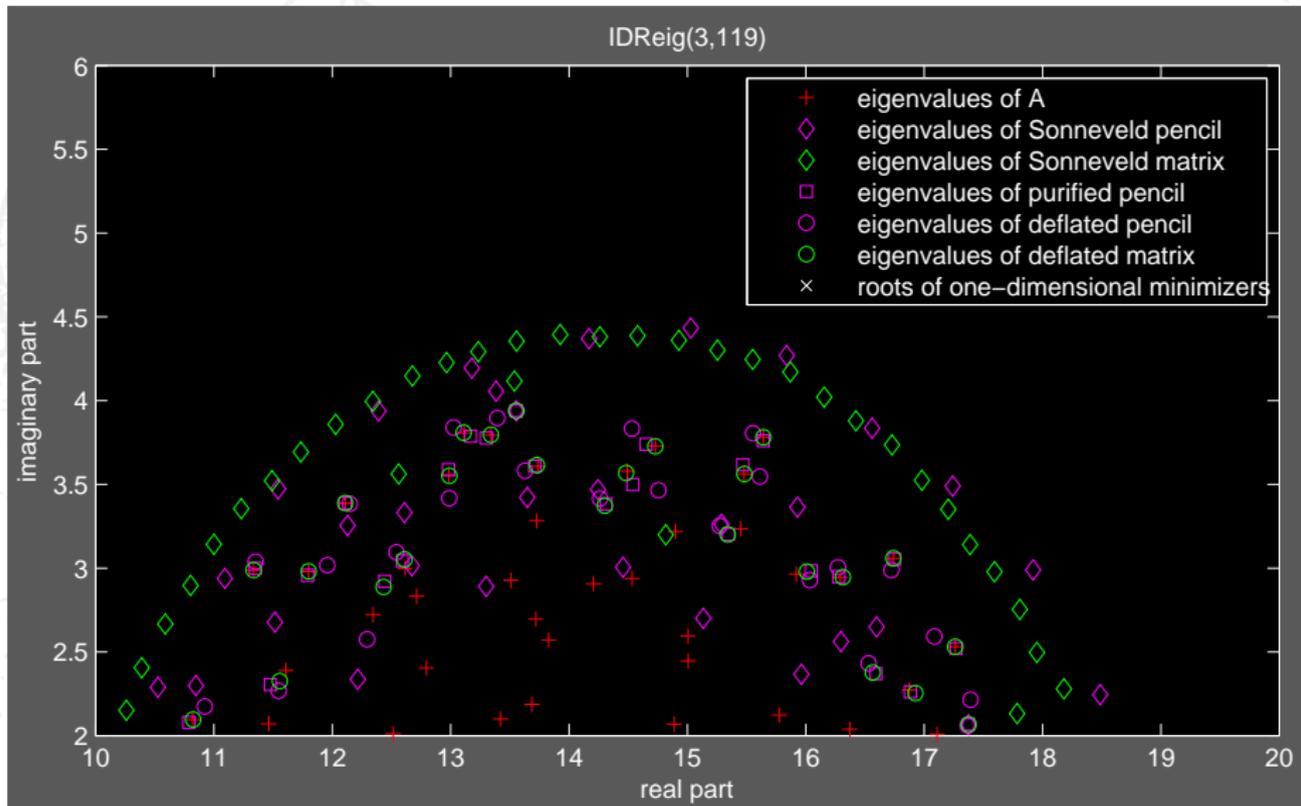
Selected examples for $s = 3$ 

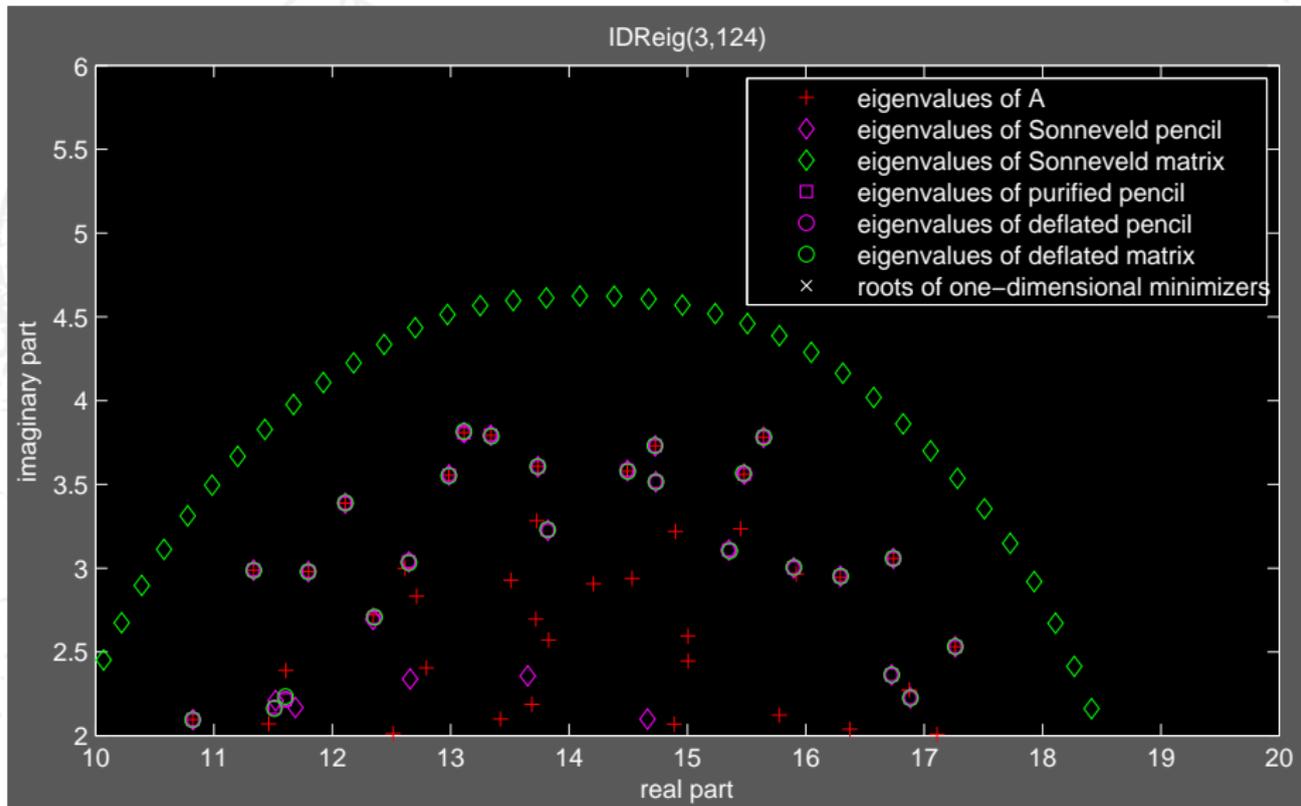
Selected examples for $s = 3$ 

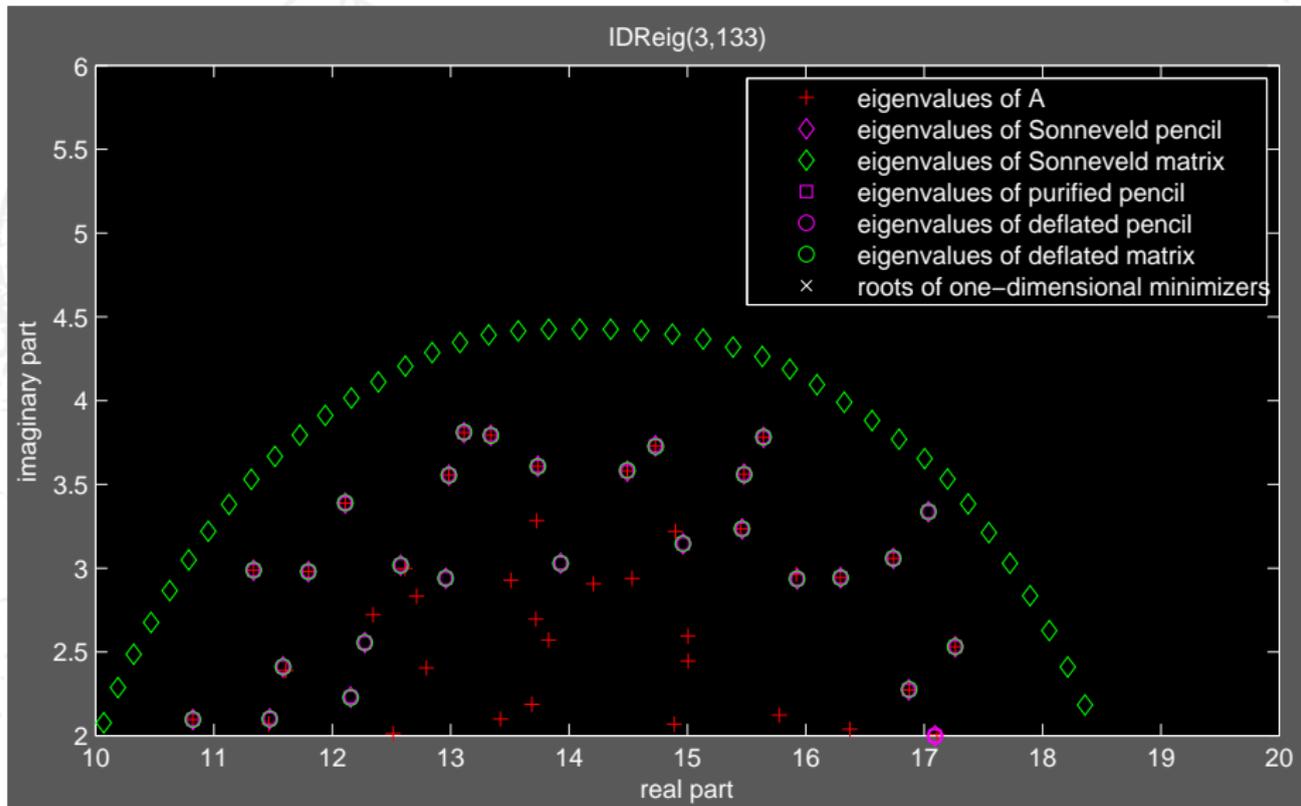
Selected examples for $s = 3$ 

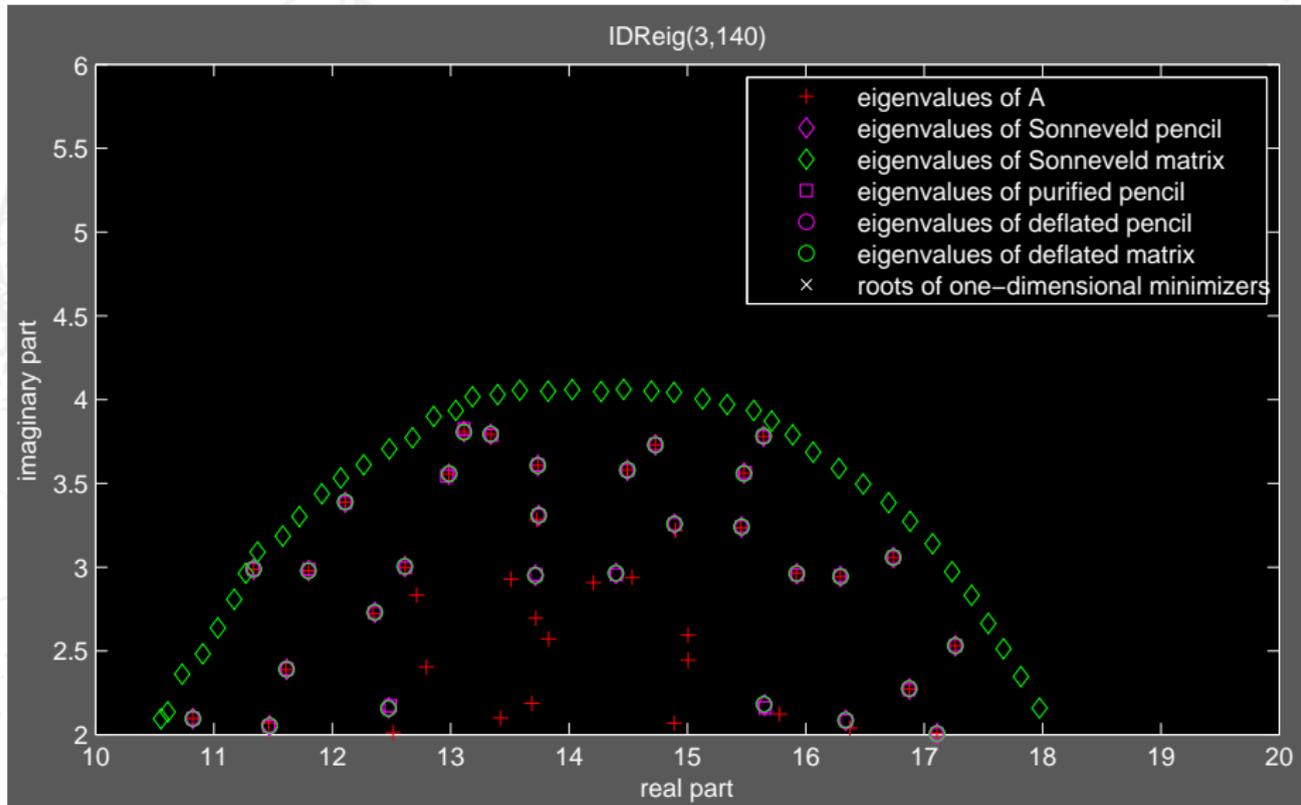
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