# IDR($s$): Finite precision aspects

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joint work with Martin Gutknecht
(work in progress)

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# Outline

## Krylov subspace methods

- origin
- classification
- implementation

## My vision on IDR

- IDR as QOR
- IDR for eigenvalues

## Numerical example

# Origin of Krylov methods

The Krylov matrix $\mathbf{K}_n = \left(\mathbf{q}, \mathbf{A}\mathbf{q}, \mathbf{A}^2\mathbf{q}, \dots, \mathbf{A}^{m-1}\mathbf{q}\right)$ satisfies

$$\left(\mathbf{q}, \mathbf{A}\mathbf{K}_n\right) = \mathbf{K}_{n+1}. \tag{1}$$

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Suppose we choose upper triangular basis transformations $\mathbf{K}_n = \mathbf{Q}_n\mathbf{R}_n$,

$$\left(\mathbf{q}, \mathbf{A}\mathbf{Q}_n\mathbf{R}_n\right) = \mathbf{Q}_{n+1}\mathbf{R}_{n+1} \quad \Rightarrow \quad \left(\mathbf{q}, \mathbf{A}\mathbf{Q}_n\right) = \mathbf{Q}_{n+1}\mathbf{R}_{n+1}\begin{pmatrix} 1 & \mathbf{o}^T \\ \mathbf{o} & \mathbf{R}_n \end{pmatrix}^{-1}. \tag{2}$$

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Then $\underline{\mathbf{C}}_n$ defined by

$$\begin{pmatrix} \star & \underline{\mathbf{C}}_n \\ \mathbf{o} & \end{pmatrix} := \mathbf{R}_{n+1} \begin{pmatrix} 1 & \mathbf{o}^T \\ \mathbf{o} & \mathbf{R}_n \end{pmatrix}^{-1} \tag{3}$$

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We end up with a Hessenberg decomposition

$$\mathbf{A}\mathbf{Q}_n = \mathbf{Q}_{n+1}\underline{\mathbf{C}}_n = \mathbf{Q}_n\mathbf{C}_n + \mathbf{q}_{n+1}c_{n+1,n}\mathbf{e}_n^T, \tag{4}$$

where $\mathbf{C}_n$ is unreduced Hessenberg and measures the “ratio” of the basis transformations.

# Classification of Krylov methods

These Hessenberg decompositions are computed directly (e.g., using the methods of Lanczos or Arnoldi), split (e.g., (Bi)CG-Omin, i.e., using an LDMT decomposition), or implicitly (so-called Lanczos-type product methods, LTPM; e.g., CGS, BiCGStab).

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There are (basically) three well-known approaches based on Hessenberg decompositions, namely

QOR: approximate $\mathbf{x} = \mathbf{A}^{-1}\mathbf{r}_0$ by $\mathbf{x}_n := \mathbf{Q}_n\mathbf{C}_n^{-1}\mathbf{e}_1\|\mathbf{r}_0\|$,

QMR: approximate $\mathbf{x} = \mathbf{A}^{-1}\mathbf{r}_0$ by $\underline{\mathbf{x}}_n := \mathbf{Q}_n\underline{\mathbf{C}}_n^{\dagger}\underline{\mathbf{e}}_1\|\mathbf{r}_0\|$,

Ritz-Galërkin: approximate part of $\mathbf{J} = \mathbf{V}^{-1}\mathbf{A}\mathbf{V}$ by $\mathbf{J}_n := \mathbf{S}_n^{-1}\mathbf{C}_n\mathbf{S}_n$, $\mathbf{V}_n := \mathbf{Q}_n\mathbf{S}_n$.

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To every method from one class corresponds a method of the other.

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The three classes of methods can be described using polynomials and polynomial interpolation:

QOR: $\mathbf{r}_n = \mathcal{R}_n(\mathbf{A})\mathbf{r}_0$, where $\mathcal{R}_n(z) := \det\left(\mathbf{I}_n - z\mathbf{C}_n^{-1}\right)$,

$\mathbf{x}_n = \mathcal{L}_n[z^{-1}](\mathbf{A})\mathbf{r}_0$, where $\mathcal{L}_n[z^{-1}](z) := \frac{\chi_n(0)-\chi_n(z)}{\chi_n(0)} z^{-1}$, $z \neq 0$,

QMR: $\underline{\mathbf{r}}_n = \underline{\mathcal{R}}_n(\mathbf{A})\mathbf{r}_0$, where $\underline{\mathcal{R}}_n(z) := \det\left(\mathbf{I}_n - z\underline{\mathbf{C}}_n^{\dagger}\underline{\mathbf{I}}_n\right)$,

$\underline{\mathbf{x}}_n = \underline{\mathcal{L}}_n[z^{-1}](\mathbf{A})\mathbf{r}_0$, where $\underline{\mathcal{L}}_n[z^{-1}](z)$ interpolates the function $z^{-1}$ at the harmonic Ritz values,

Ritz-Galërkin: $\mathbf{A}\mathbf{V}_n - \mathbf{V}_n\mathbf{J}_n = \frac{\chi_n(\mathbf{A})}{c_{1:n-1}}\mathbf{q}_1\mathbf{e}_n^T\mathbf{S}_n$ (for a specially chosen $\mathbf{S}_n$),

$\mathbf{v}_j^{(m)} = \mathcal{A}_n(\theta, \mathbf{A})\mathbf{q}_1$, where $\mathcal{A}_n(\theta, z) := \frac{\chi_n(\theta)-\chi_n(z)}{\theta - z}$, $\theta \neq z$.

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In finite precision the recurrence will only approximately be satisfied,

$$\mathbf{A}\mathbf{Q}_n + \mathbf{F}_n = \mathbf{Q}_{n+1}\underline{\mathbf{C}}_n = \mathbf{Q}_n\mathbf{C}_n + \mathbf{q}_{n+1}c_{n+1,n}\mathbf{e}_n^T, \tag{5}$$

where the perturbation term $\mathbf{F}_n$ is in some sense “small” and/or structured.

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To analyze the convergence behavior of a perturbed QOR Krylov method one has to figure out the behavior of the Ritz values, i.e., the eigenvalues of the Hessenberg matrices $\mathbf{C}_n$.

# IDR as Krylov subspace method

IDR is a Krylov subspace method, as every step is based on a multiplication with the matrix $\mathbf{A}$ (the iterates lie in a Krylov subspace) and certain linear combinations of previous basis vectors are used to compute new vectors (which defines an upper triangular basis transformation).

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In these methods the columns of the resulting extended Hessenberg matrix sum to zero.

# IDR as Krylov subspace method

The IDR recurrences of the prototype IDR($s$) algorithm can be summarized by

$$\begin{aligned} \mathbf{r}_n &:= (\mathbf{I} - \omega_j \mathbf{A})\, \mathbf{v}_{n-1}\,, \\ \mathbf{v}_n &:= \mathbf{r}_n - \widetilde{\mathbf{R}}_n \Delta \mathbf{c}_n = \widetilde{\mathbf{R}}_n \mathbf{y}_n \\ &= (1 - \gamma_1^{(n)})\mathbf{r}_n + \textstyle\sum_{\ell=1}^{s-1} (\gamma_\ell^{(n)} - \gamma_{\ell+1}^{(n)})\mathbf{r}_{n-\ell} + \gamma_s^{(n)} \mathbf{r}_{n-s}\,. \end{aligned} \tag{6}$$

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Here, $n > s$, and the index of the scalar $\omega_j$ is defined by

$$j := \left\lfloor \frac{n}{s+1} \right\rfloor,$$

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Removing $\mathbf{v}_n$ from the recurrence we obtain the perturbed generalized Hessenberg decomposition

$$\mathbf{A}\mathbf{R}_n \mathbf{Y}_n \mathbf{D}_\omega + \mathbf{F}_n = \mathbf{R}_{n+1} \underline{\mathbf{Y}}_n^\circ . \qquad (7)$$

# IDR as Krylov subspace method

By inspection, the banded Hessenberg matrix $\underline{\mathbf{Y}}_n^\circ$ has zero column sums. Inverting the upper triangular banded matrix $\mathbf{Y}_n\mathbf{D}_\omega$, we obtain the Hessenberg decomposition

$$\mathbf{A}\mathbf{R}_n + \mathbf{F}_n\mathbf{D}_\omega^{-1}\mathbf{Y}_n^{-1} = \mathbf{R}_{n+1}\underline{\mathbf{Y}}_n^\circ\mathbf{D}_\omega^{-1}\mathbf{Y}_n^{-1} =: \mathbf{R}_{n+1}\underline{\mathbf{S}}_n^\circ. \tag{8}$$

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By well-known results the residuals can be expressed in terms of the leading submatrices of the Sonneveld matrix,

$$\mathbf{r}_n = \mathcal{S}_n(\mathbf{A})\mathbf{r}_0, \quad \mathcal{S}_n(z) := \det\left(\mathbf{I}_n - z(\mathbf{S}_n^\circ)^{-1}\right) = \frac{\det\left(\mathbf{S}_n^\circ - z\mathbf{I}_n\right)}{\det\left(\mathbf{S}_n^\circ\right)}.$$

# IDR for eigenvalues

In unperturbed IDR the generalized Hessenberg decomposition is given by

$$\mathbf{A}\mathbf{R}_n\mathbf{Y}_n\mathbf{D}_\omega = \mathbf{R}_{n+1}\underline{\mathbf{Y}}_n^\circ \quad \Rightarrow \quad \mathbf{A}\mathbf{R}_n = \mathbf{R}_{n+1}\underline{\mathbf{S}}_n^\circ. \tag{9}$$

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We can use the leading submatrices of the Sonneveld matrix $\mathbf{S}_n^\circ$ for the computation of Ritz values, the Ritz vectors are the eigenvectors prolonged by the “basis” given by $\mathbf{R}_n$. We can estimate the accuracy similar to Lanczos' method by looking at the last element of the eigenvector and the size of the current residual.

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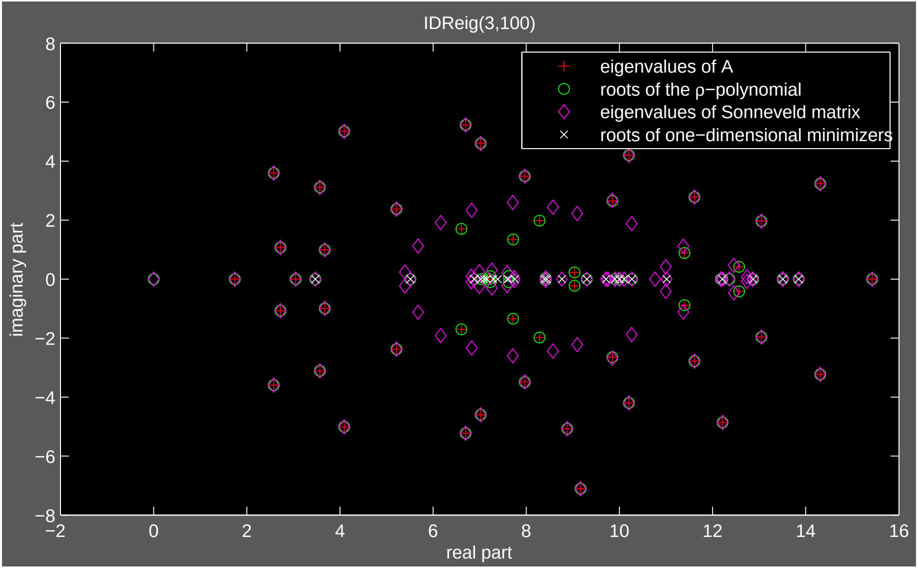
Numerically more stable and more efficient is the use of the Sonneveld pencil $(\mathbf{Y}_n^\circ, \mathbf{Y}_n\mathbf{D}_\omega)$. The stability comes from the fact that we need not be afraid of a large condition of $\mathbf{Y}_n$ and/or $\mathbf{D}_\omega$. The efficiency is due to the structure: The Sonneveld *matrix* is a *full* unreduced Hessenberg matrix, the Sonneveld *pencil* is *banded* upper Hessenberg/triangular and QZ is the method of choice.

# IDR for eigenvalues



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By the manner of construction of the residuals, which is based on the mappings $(\mathbf{I} - \omega_j \mathbf{A}) : \mathcal{G}_{j-1} \to \mathcal{G}_j$, we know that for some $\mathbf{w}_n \in \mathcal{G}_0 = \mathcal{K}(\mathbf{A}, \mathbf{r}_0)$

$$\begin{aligned} \mathbf{r}_n &= \Omega_j(\mathbf{A})\mathbf{w}_n, \\ \mathbf{v}_{n-1} &= \Omega_{j-1}(\mathbf{A})\mathbf{w}_n, \end{aligned} \qquad \Omega_j(z) = \prod_{\ell=1}^{j}(1 - \omega_\ell z), \quad j = \left\lfloor \frac{n}{s+1} \right\rfloor. \tag{10}$$

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The polynomials defined by dividing the residual polynomials by the polynomials $\Omega_j$ are *residual polynomials* in the Krylov subspace $\mathcal{K}(\mathbf{A}, \mathbf{r}_0)$. The polynomials $\Omega_j$ are also residual polynomials, since $\Omega_j(0) = 1$.

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Some thinking results in the wanted purified generalized Hessenberg decomposition

$$\mathbf{A}\mathbf{W}_n\mathbf{U}_n\mathbf{D}_\omega = \mathbf{W}_{n+1}\underline{\mathbf{Y}}_n^\circ, \tag{11}$$

where the change from the original residuals $\mathbf{r}_n$ to the purified residuals $\mathbf{w}_n$ is reflected in the construction of the matrix $\mathbf{U}_n$ from $\mathbf{Y}_n$ by cutting out lower triangles from the band such that $\mathbf{U}_n$ is block-diagonal with alternating $s \times s$ upper triangular blocks and single zero elements at every multiple of $s + 1$.

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We can show based on the properties of unreduced Hessenberg pencils (Z, 2006) and manipulation of equation (11) (Z, 2007) that scalar multiples of the leading determinants of the Hessenberg pencil ${}^z\mathbf{H}_n := (z\mathbf{U}_n\mathbf{D}_\omega - \mathbf{Y}_n^\circ)$ define the purified residual polynomials.

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Both drawbacks can be removed utilizing Schur's determinant formula.

# IDR for eigenvalues

Block-Gauß elimination applied to a typical block of the pencil results in

$$\begin{pmatrix} {}^{z}\mathbf{H}^{\star} & \mathbf{h}_c & \mathbf{L}^{\star} \\ \mathbf{e}_s^T & (\gamma^{\star}-1) & \mathbf{h}_r^T \\ \mathbf{O} & \mathbf{e}_1 & {}^{z}\mathbf{H}_{\star} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{o} & \mathbf{O} \\ -\mathbf{e}_s^T/(\gamma^{\star}-1) & 1/(\gamma^{\star}-1) & -\mathbf{h}_r^T/(\gamma^{\star}-1) \\ \mathbf{O} & \mathbf{o} & \mathbf{I} \end{pmatrix} =$$

$$\begin{pmatrix} {}^{z}\mathbf{H}^{\star} - \mathbf{h}_c\mathbf{e}_s^T/(\gamma^{\star}-1) & \mathbf{h}_c^T/(\gamma^{\star}-1) & \mathbf{L}^{\star} - \mathbf{h}_c\mathbf{h}_r^T/(\gamma^{\star}-1) \\ \mathbf{o}^T & 1 & \mathbf{o}^T \\ -\mathbf{e}_1\mathbf{e}_s^T/(\gamma^{\star}-1) & \mathbf{e}_1^T/(\gamma^{\star}-1) & {}^{z}\mathbf{H}_{\star} - \mathbf{e}_1\mathbf{h}_r^T/(\gamma^{\star}-1) \end{pmatrix}. \quad (12)$$

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$$\begin{pmatrix} {}^z\mathbf{H}^\star & \mathbf{h}_c & \mathbf{L}^\star \\ \mathbf{e}_s^T & (\gamma^\star - 1) & \mathbf{h}_r^T \\ \mathbf{O} & \mathbf{e}_1 & {}^z\mathbf{H}_\star \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{o} & \mathbf{O} \\ -\mathbf{e}_s^T/(\gamma^\star - 1) & 1/(\gamma^\star - 1) & -\mathbf{h}_r^T/(\gamma^\star - 1) \\ \mathbf{O} & \mathbf{o} & \mathbf{I} \end{pmatrix} =$$
$$\begin{pmatrix} {}^z\mathbf{H}^\star - \mathbf{h}_c\mathbf{e}_s^T/(\gamma^\star - 1) & \mathbf{h}_c^T/(\gamma^\star - 1) & \mathbf{L}^\star - \mathbf{h}_c\mathbf{h}_r^T/(\gamma^\star - 1) \\ \mathbf{o}^T & 1 & \mathbf{o}^T \\ -\mathbf{e}_1\mathbf{e}_s^T/(\gamma^\star - 1) & \mathbf{e}_1^T/(\gamma^\star - 1) & {}^z\mathbf{H}_\star - \mathbf{e}_1\mathbf{h}_r^T/(\gamma^\star - 1) \end{pmatrix}. \quad (12)$$

This shows that we can work on a deflated pencil, here depicted block-wise,

$$\begin{pmatrix} {}^z\mathbf{H}^\star - \mathbf{h}_c\mathbf{e}_s^T/(\gamma^\star - 1) & \mathbf{L}^\star - \mathbf{h}_c\mathbf{h}_r^T/(\gamma^\star - 1) \\ -\mathbf{e}_1\mathbf{e}_s^T/(\gamma^\star - 1) & {}^z\mathbf{H}_\star - \mathbf{e}_1\mathbf{h}_r^T/(\gamma^\star - 1) \end{pmatrix}. \quad (13)$$

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$$\begin{pmatrix} {}^z\mathbf{H}^\star - \mathbf{h}_c\mathbf{e}_s^T/(\gamma^\star - 1) & \mathbf{h}_c^T/(\gamma^\star - 1) & \mathbf{L}^\star - \mathbf{h}_c\mathbf{h}_r^T/(\gamma^\star - 1) \\ \mathbf{o}^T & 1 & \mathbf{o}^T \\ -\mathbf{e}_1\mathbf{e}_s^T/(\gamma^\star - 1) & \mathbf{e}_1^T/(\gamma^\star - 1) & {}^z\mathbf{H}_\star - \mathbf{e}_1\mathbf{h}_r^T/(\gamma^\star - 1) \end{pmatrix}. \qquad (12)$$

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This pencil again is of ORTHORES-type as the column sums of the deflated Hessenberg matrix are zero.

# IDR for eigenvalues

As we did remove the infinite eigenvalues, i.e., the zero blocks from the block-diagonal upper triangular matrix $\mathbf{U}_n$, we can now invert the deflated matrix $D(\mathbf{Y}_n\mathbf{D}_\omega\mathbf{G}_n)$ and multiply it from the right to the deflated Hessenberg matrix $D(\mathbf{Y}_n^\circ\mathbf{G}_n)$.

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Here, $\mathbf{G}_n$ denotes the block-Gauß eliminator and $D$ denotes the deflation operator $D(\mathbf{M}) = \mathbf{M}(\mathrm{ind}, \mathrm{ind})$, where ind denotes the set of indices to remain. We remark that $\mathbf{Y}_n\mathbf{D}_\omega$ is not altered by application of $\mathbf{G}_n$.

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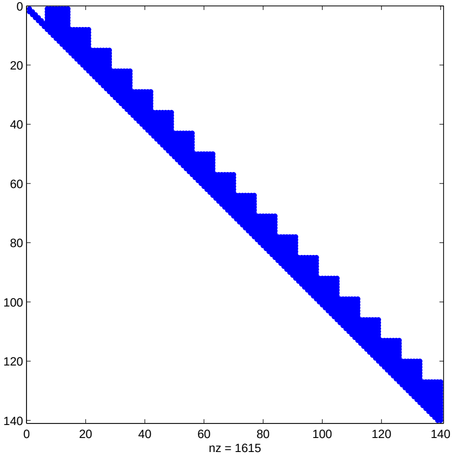
As $D(\mathbf{Y}_n^\circ\mathbf{G}_n)$ is of ORTHORES-type, Hessenberg, and block tridiagonal with blocks of size $s \times s$, and as $D(\mathbf{Y}_n\mathbf{D}_\omega\mathbf{G}_n)$ is block-diagonal upper triangular with blocks of size $s \times s$, the resulting matrix

$$\mathbf{P}_n^\circ := D(\mathbf{Y}_n^\circ\mathbf{G}_n)(D(\mathbf{Y}_n\mathbf{D}_\omega\mathbf{G}_n))^{-1} \tag{14}$$

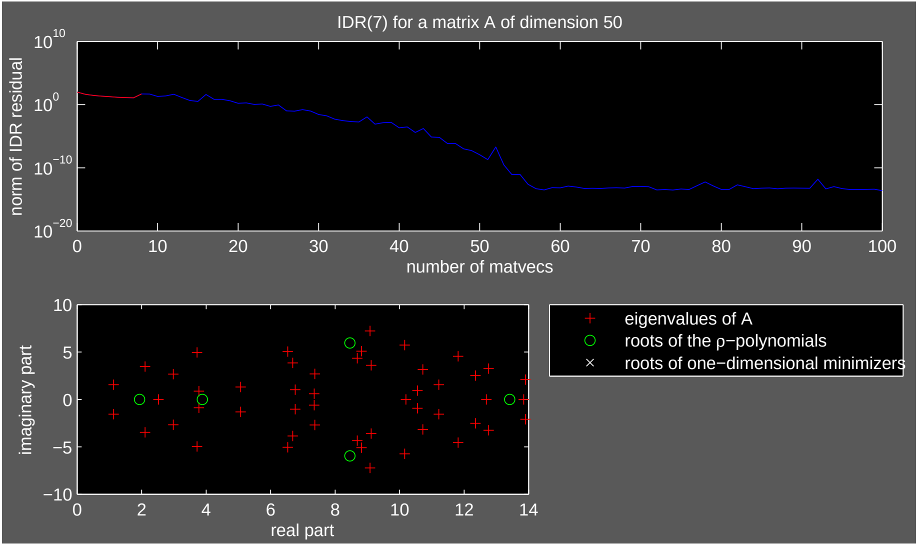
is the matrix of the ORTHORES-form of the underlying two-sided Lanczos' process with $s$ left and one right starting vectors.

# IDR for eigenvalues

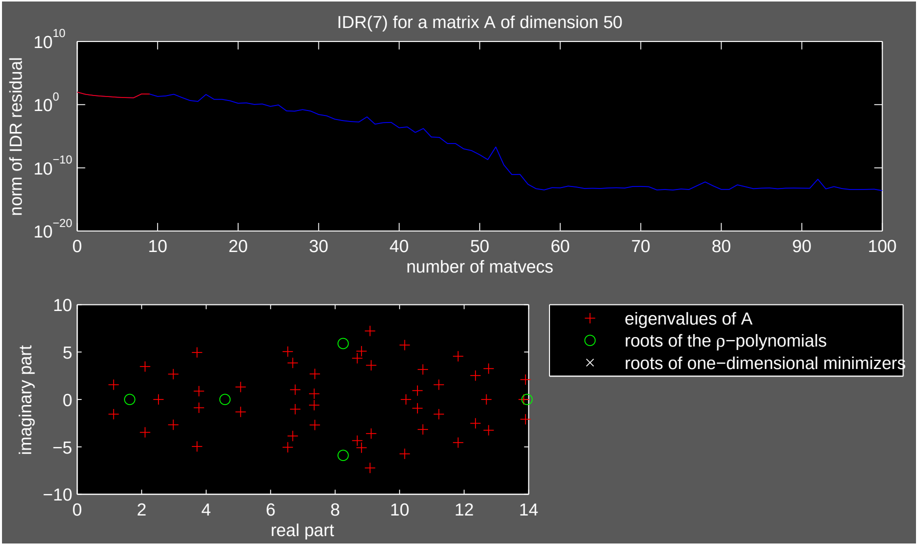
The following picture shows the structure of the resulting matrix $\mathbf{P}_n^\circ$ of the deflated purified process for IDR$(7)$ applied for $160$ steps.



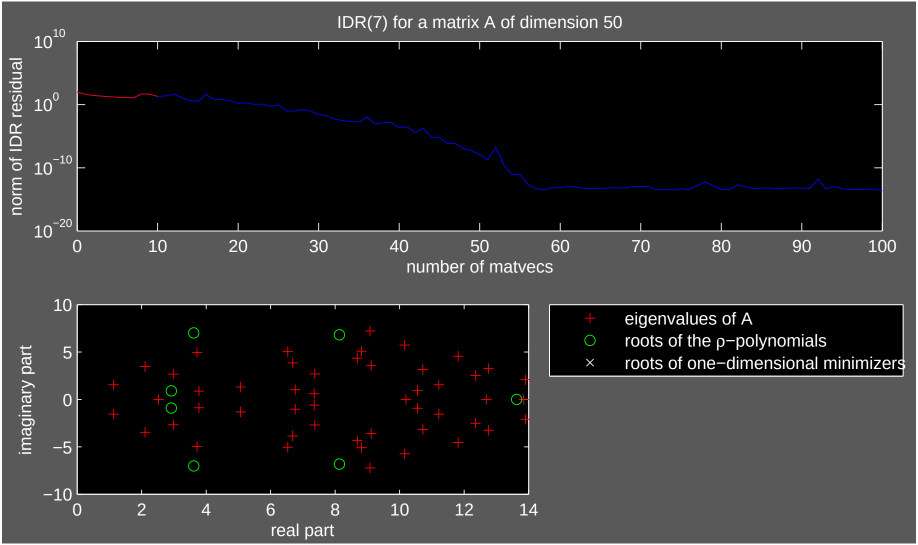
# One run of IDR(7)



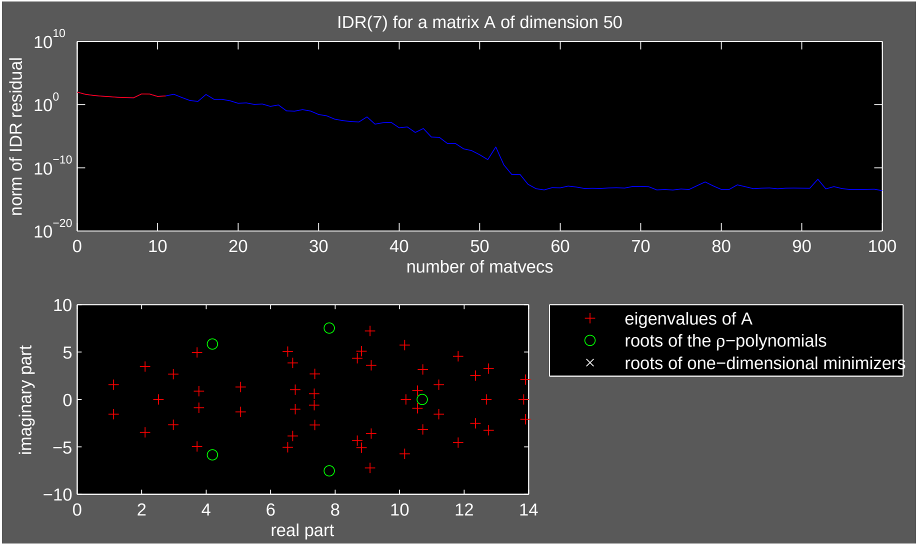
# One run of IDR(7)



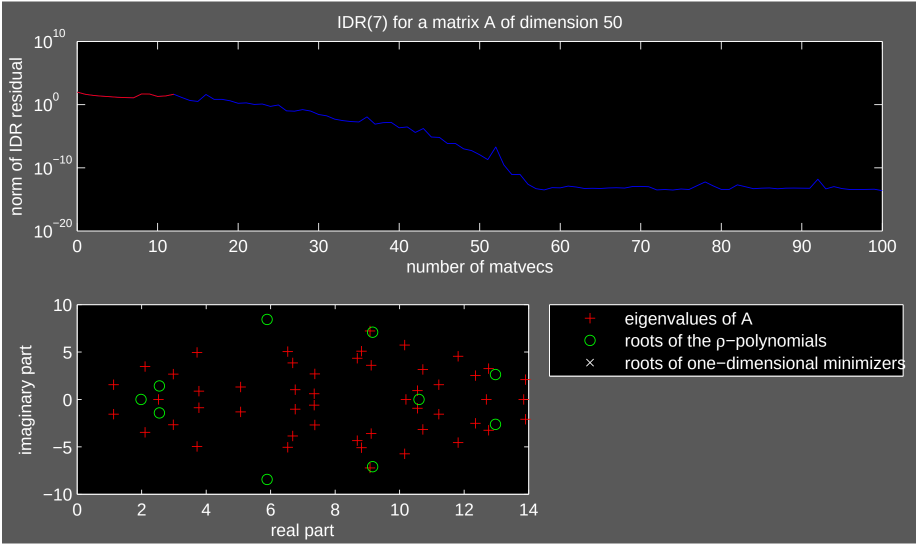
# One run of IDR(7)



# One run of IDR(7)



# One run of IDR(7)



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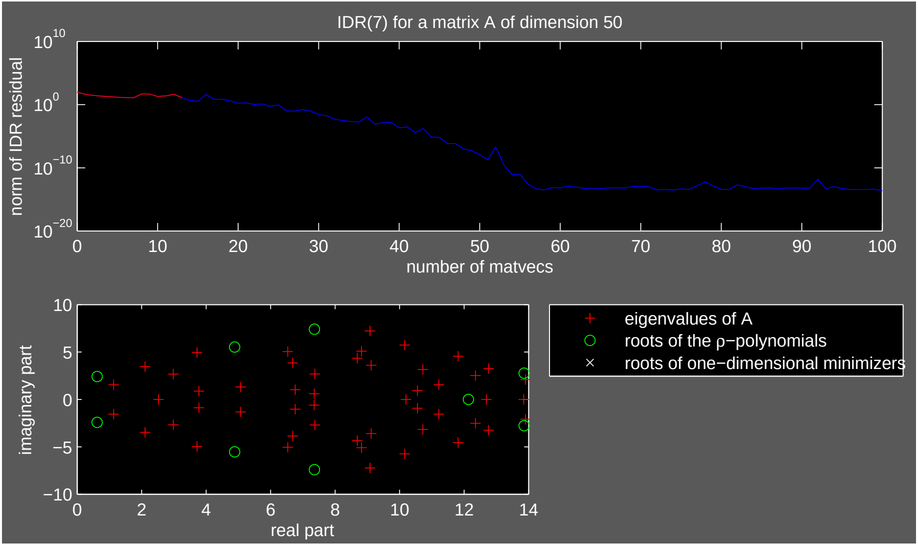

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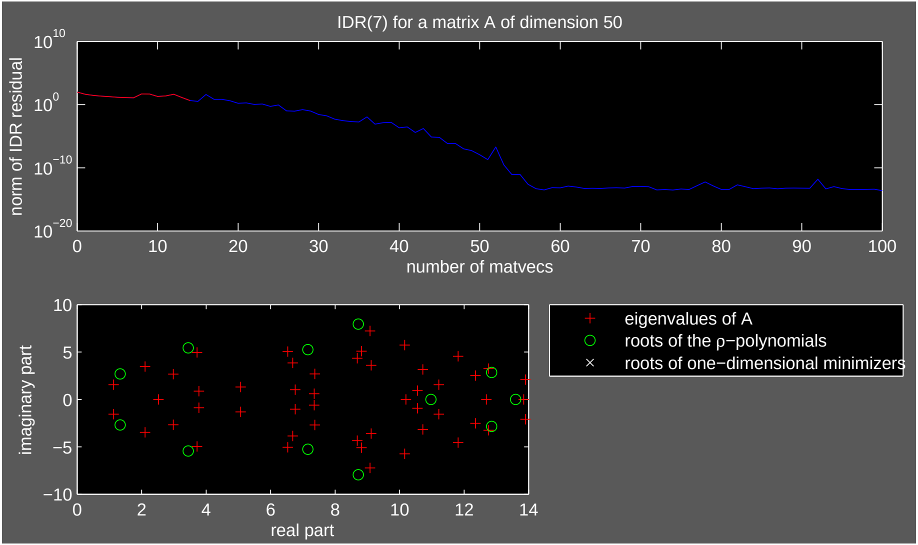

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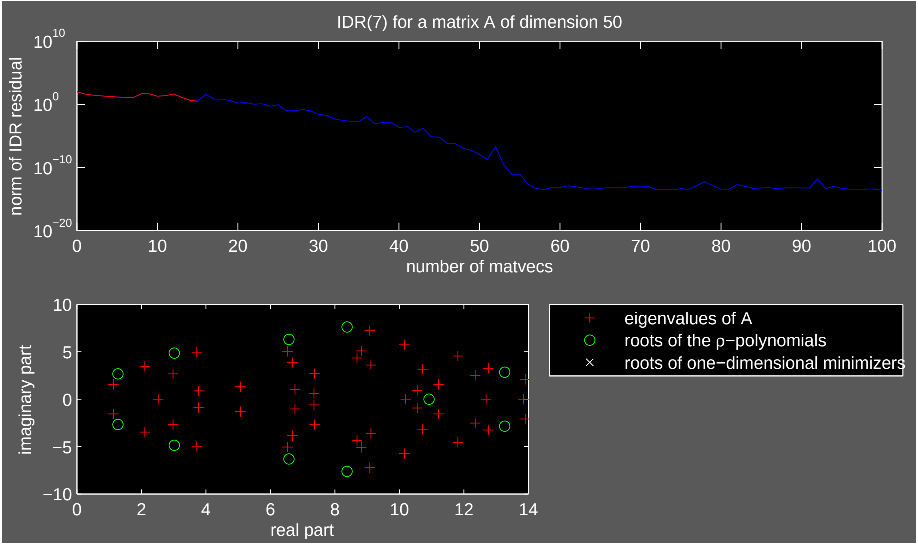

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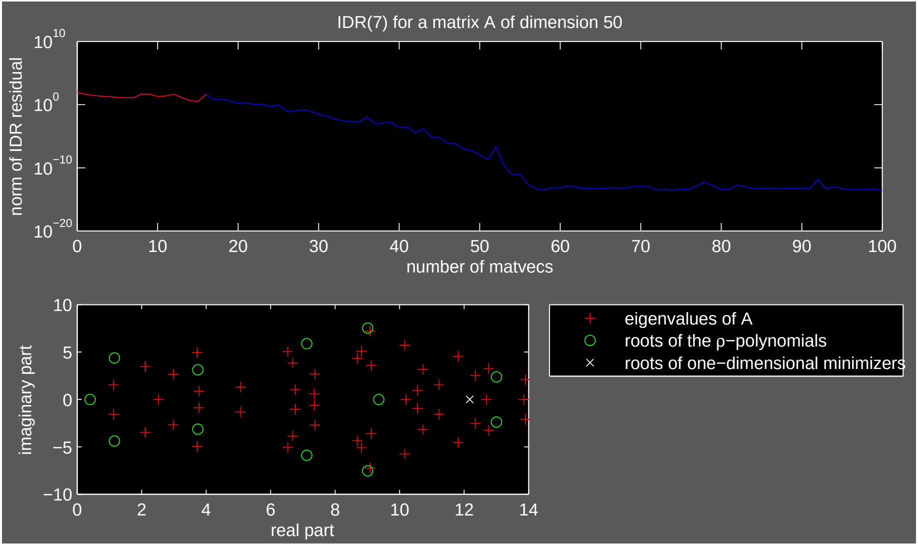

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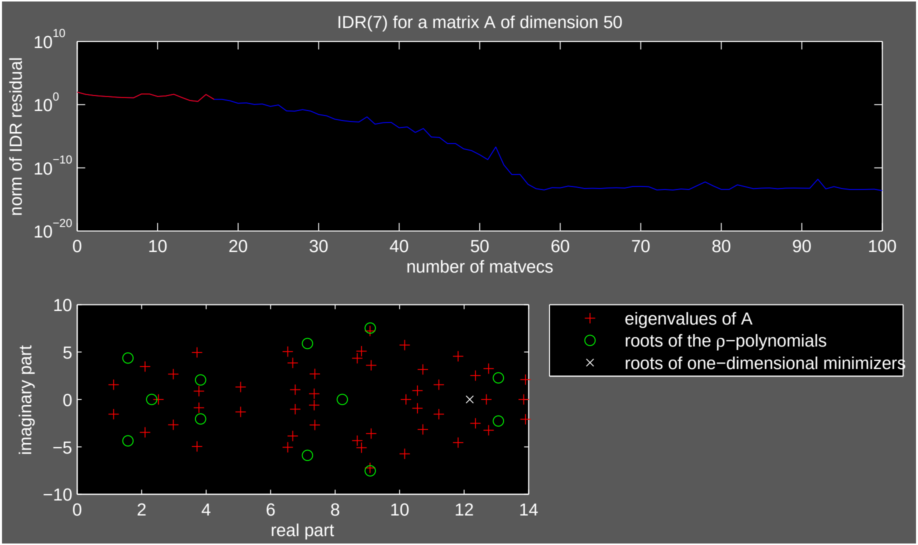

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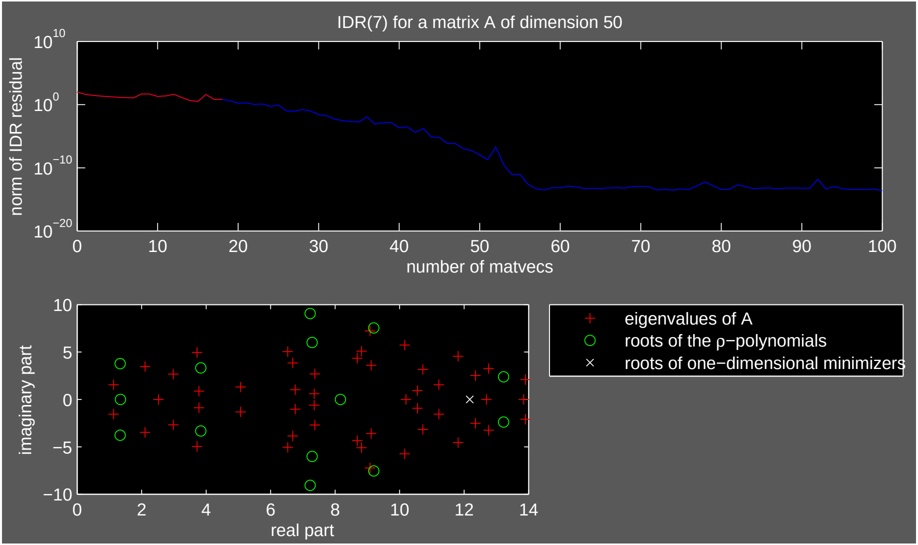

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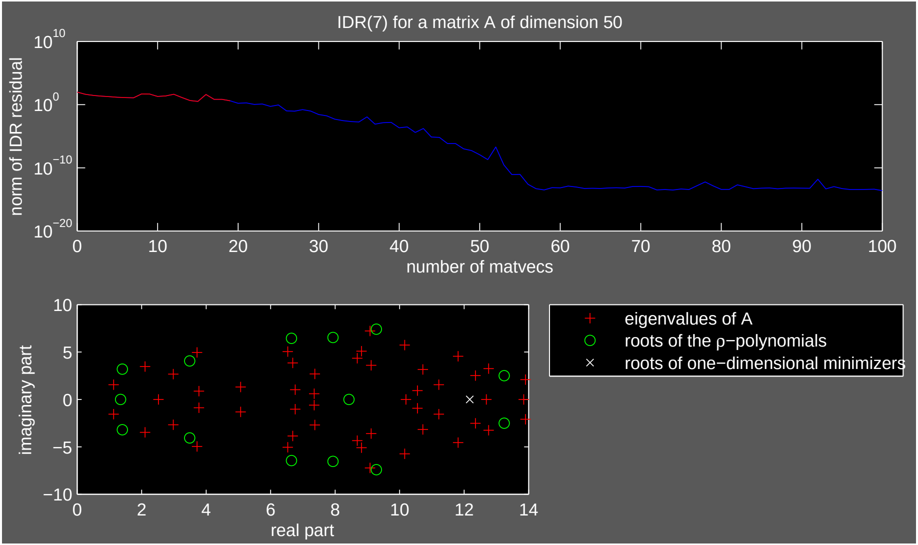

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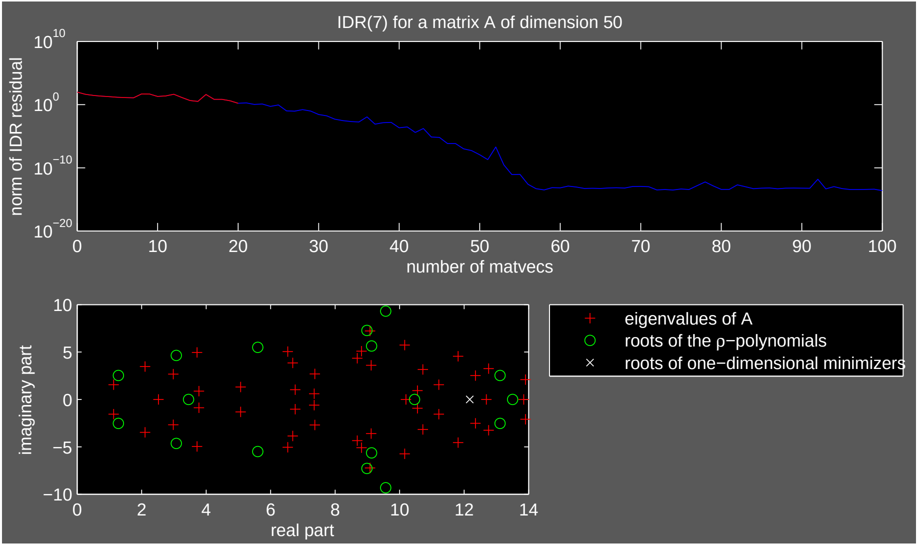

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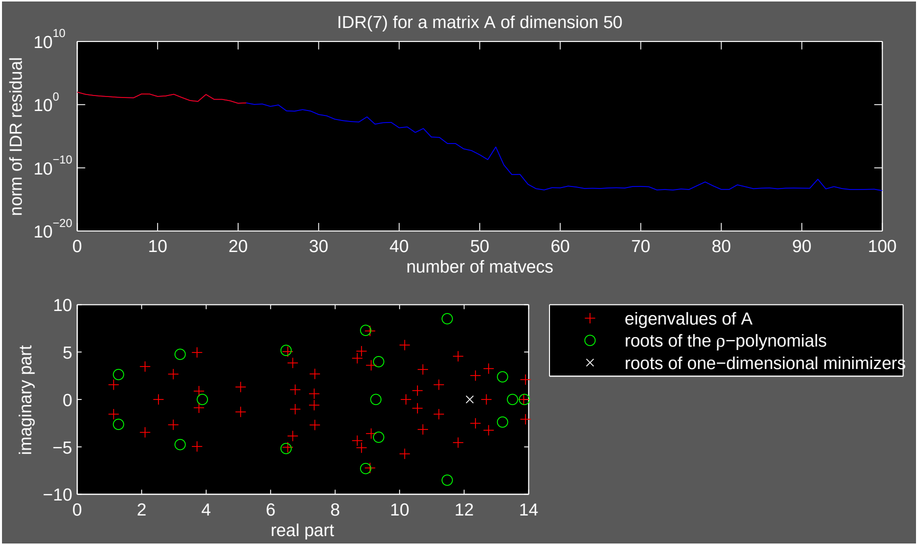

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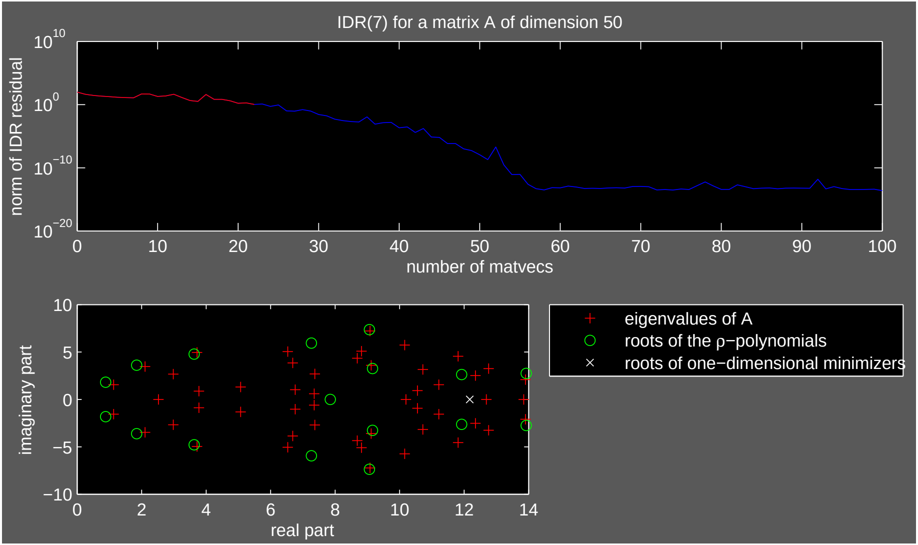

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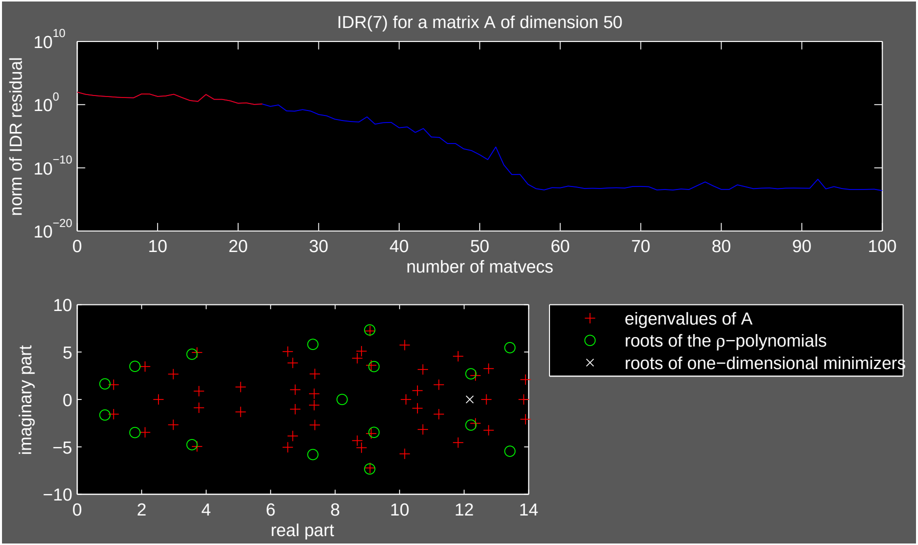

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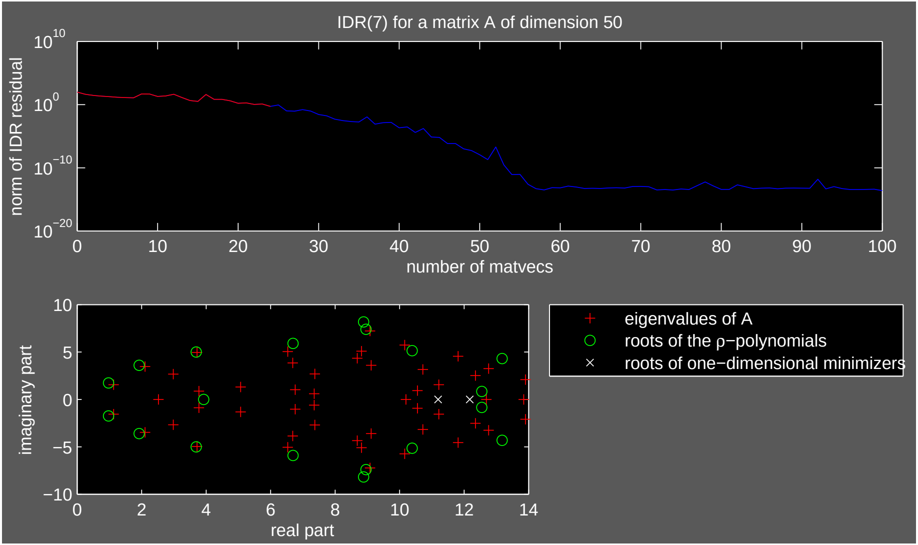

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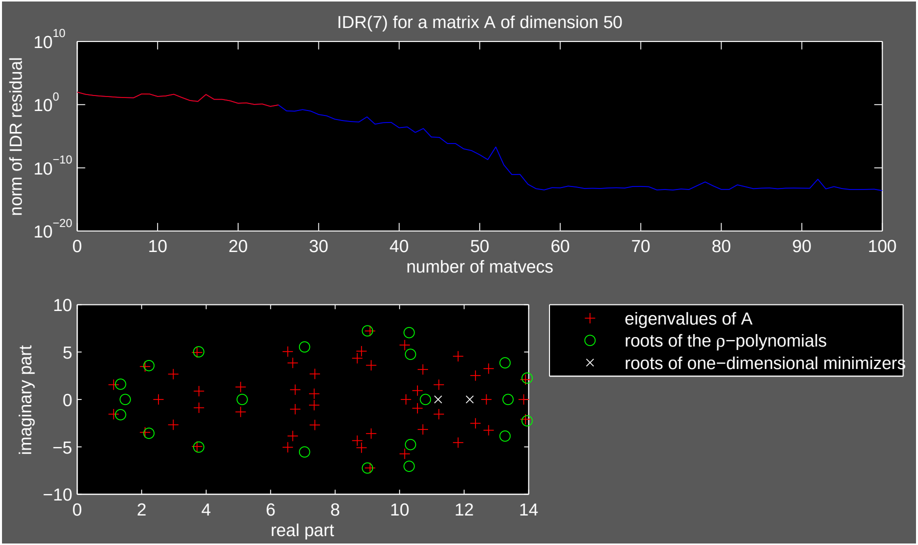

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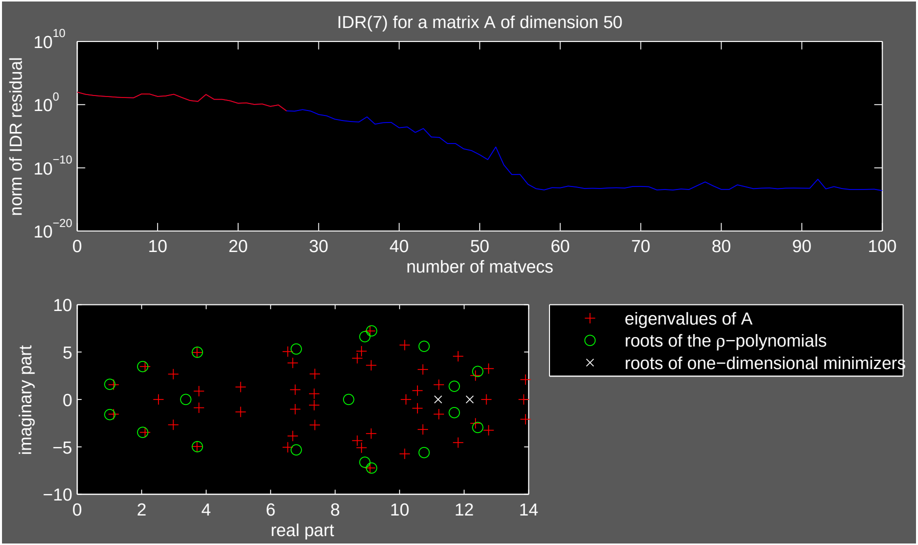

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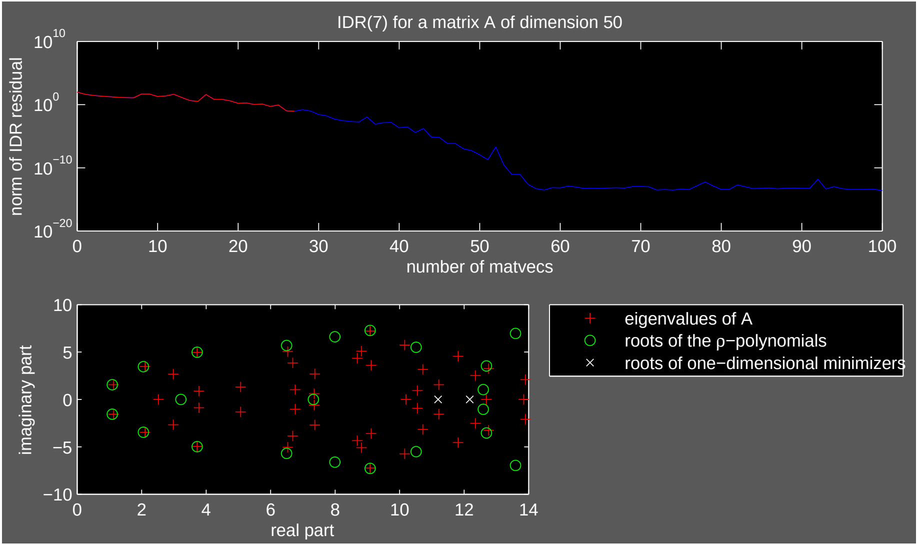

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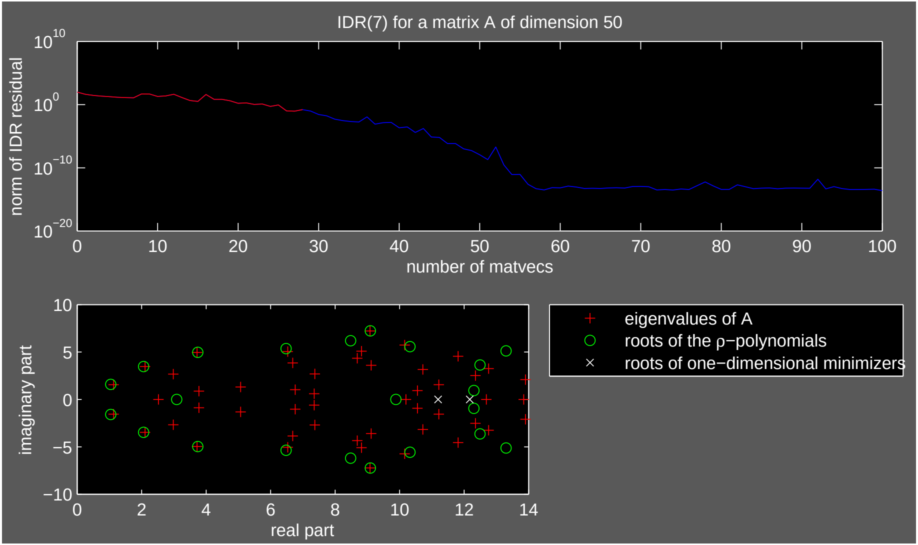

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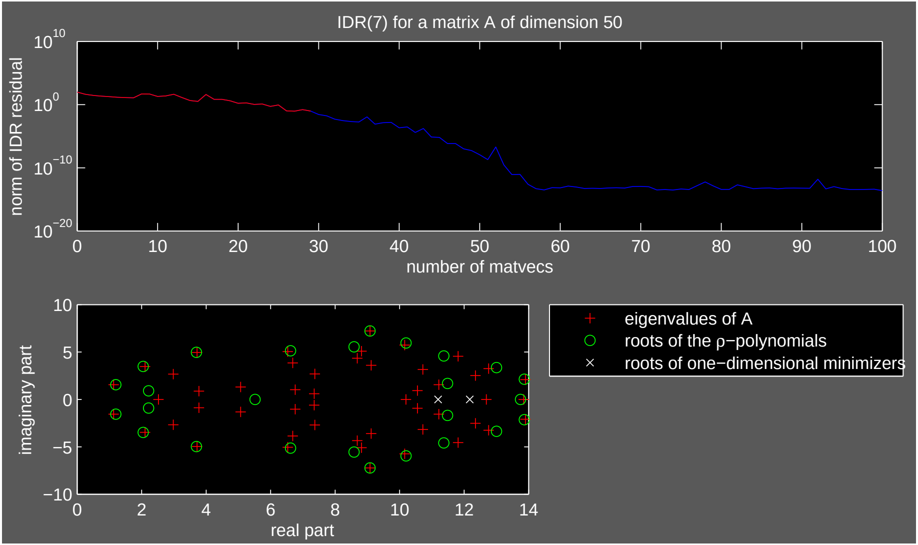

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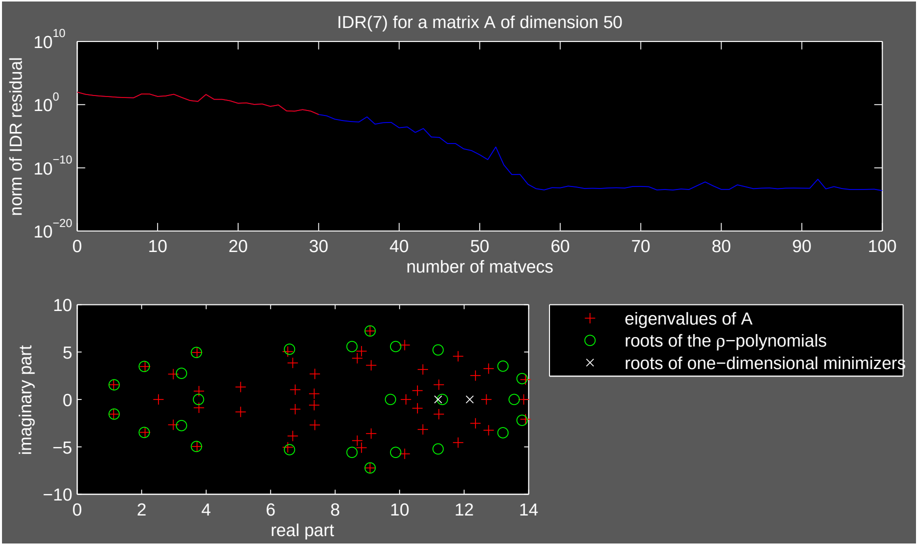

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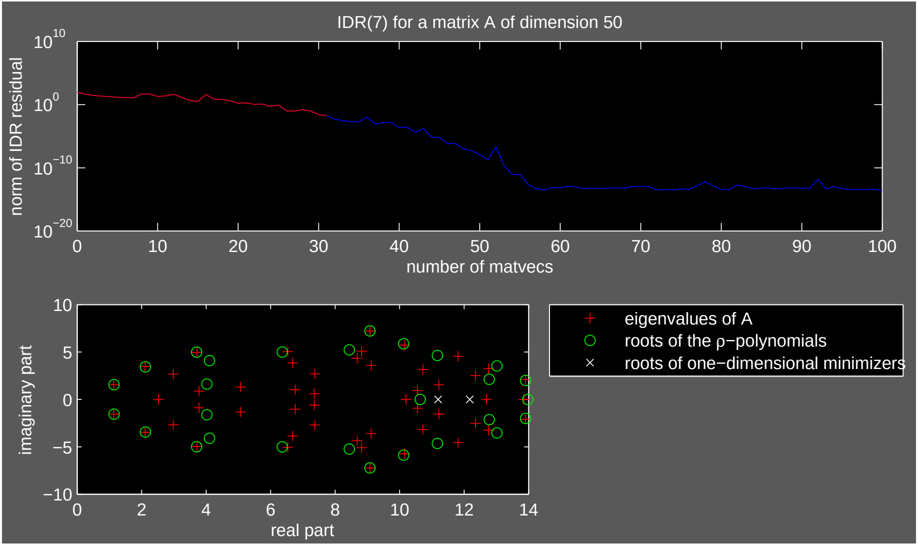

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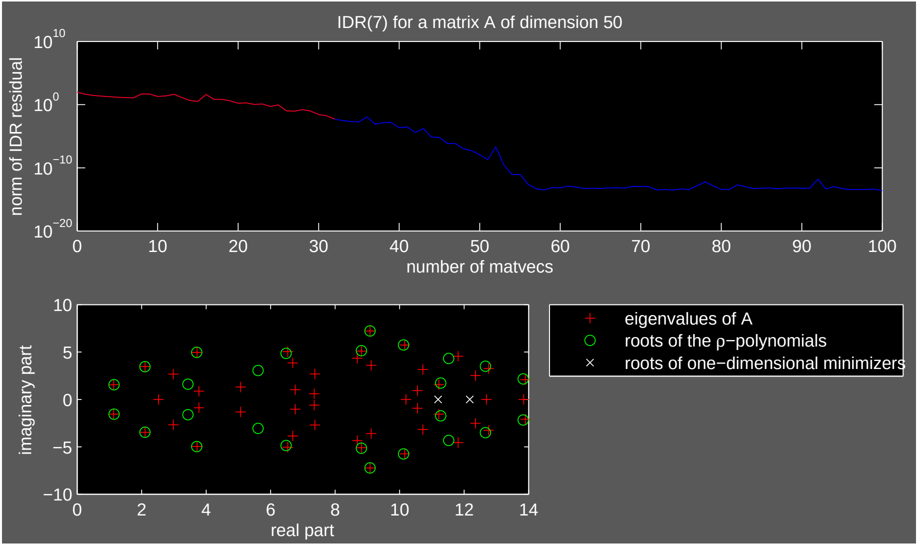

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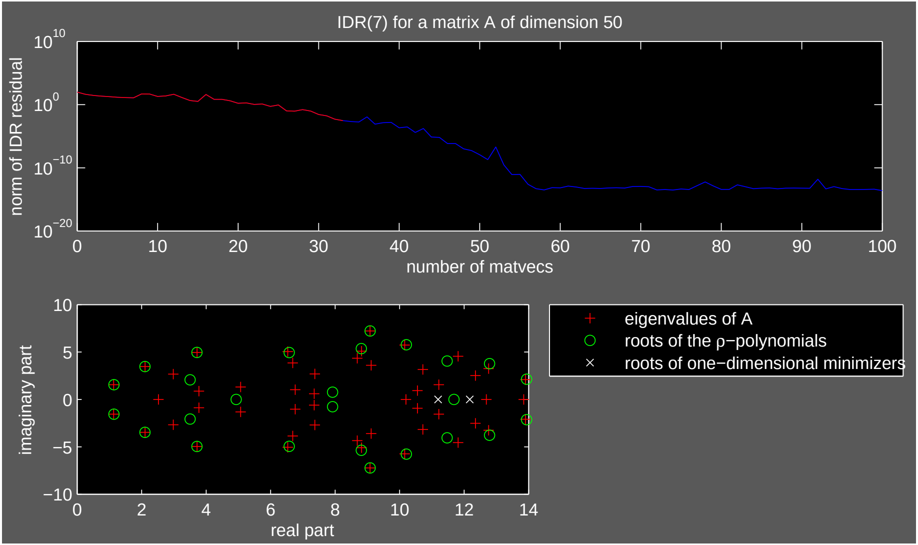

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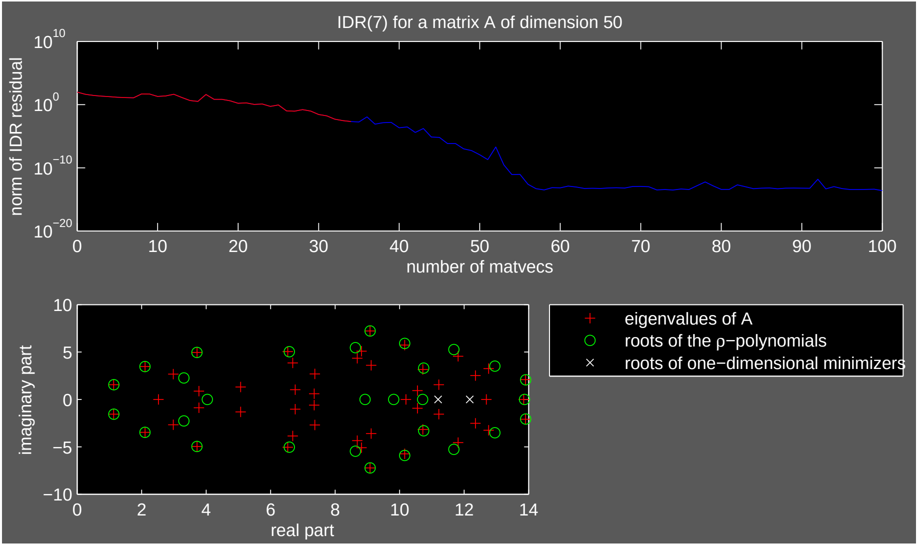

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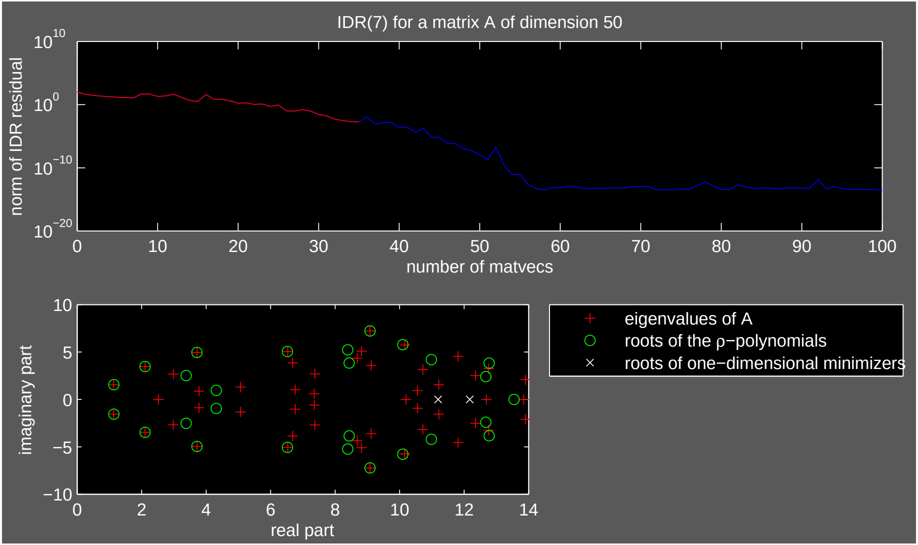

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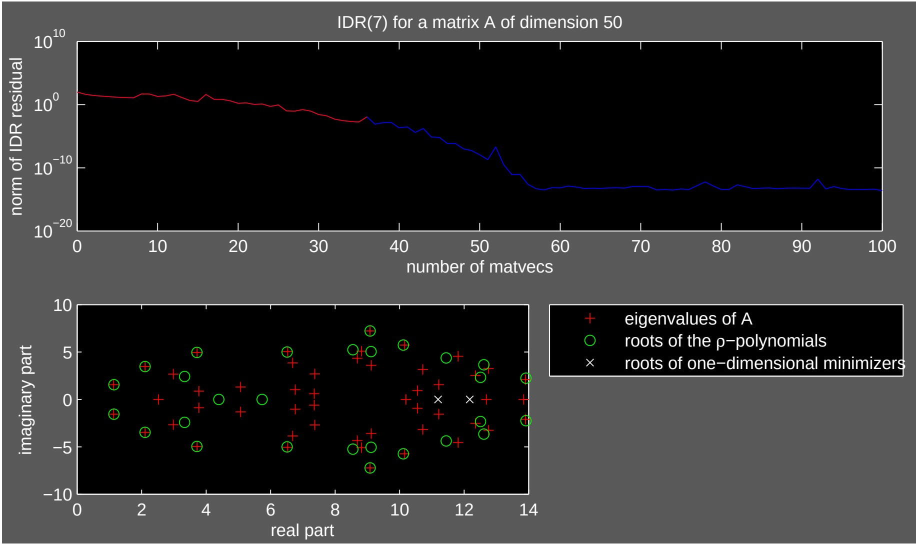

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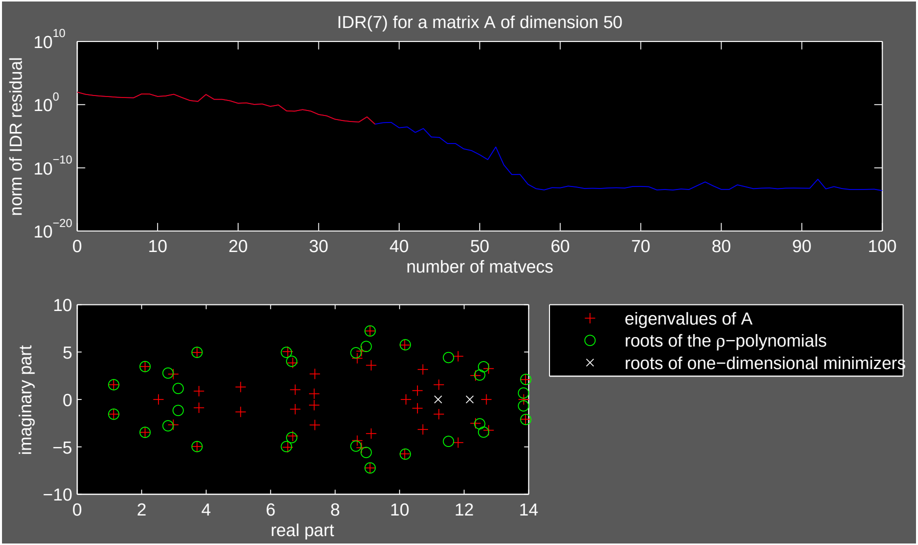

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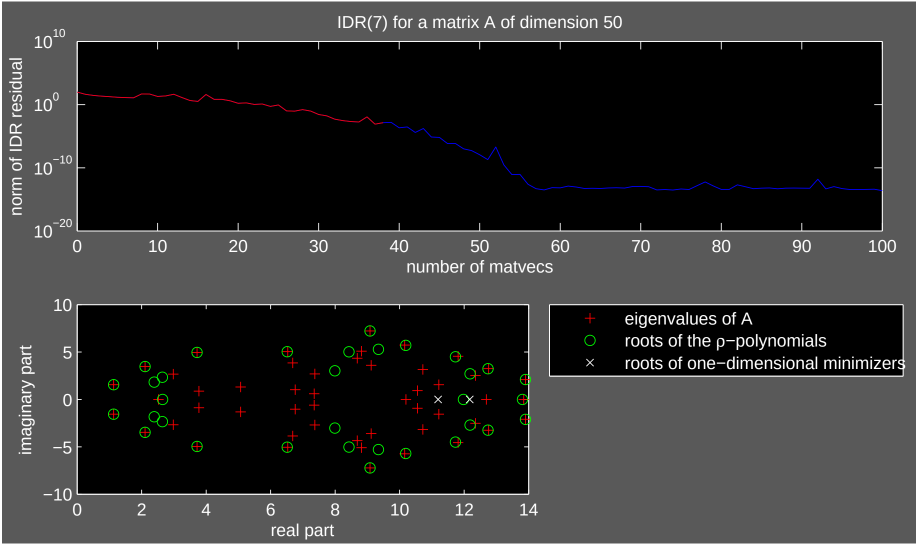

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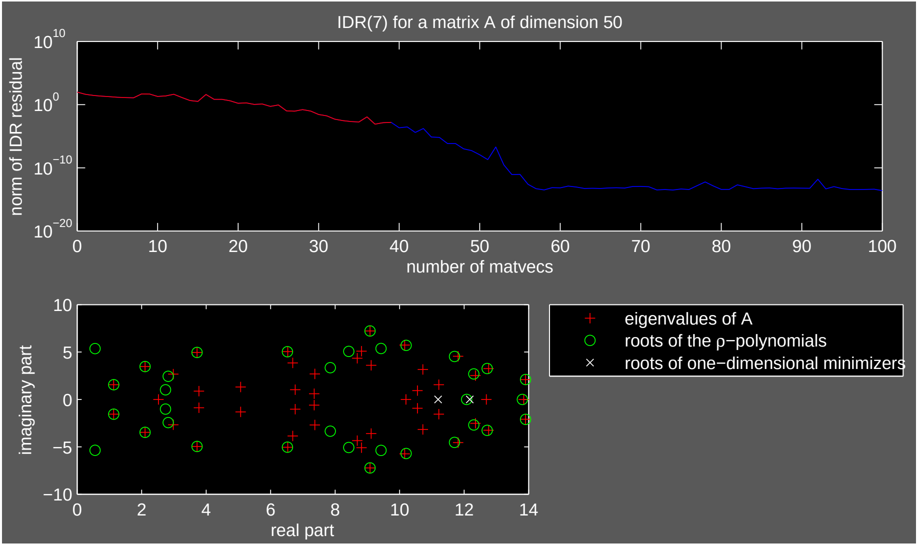

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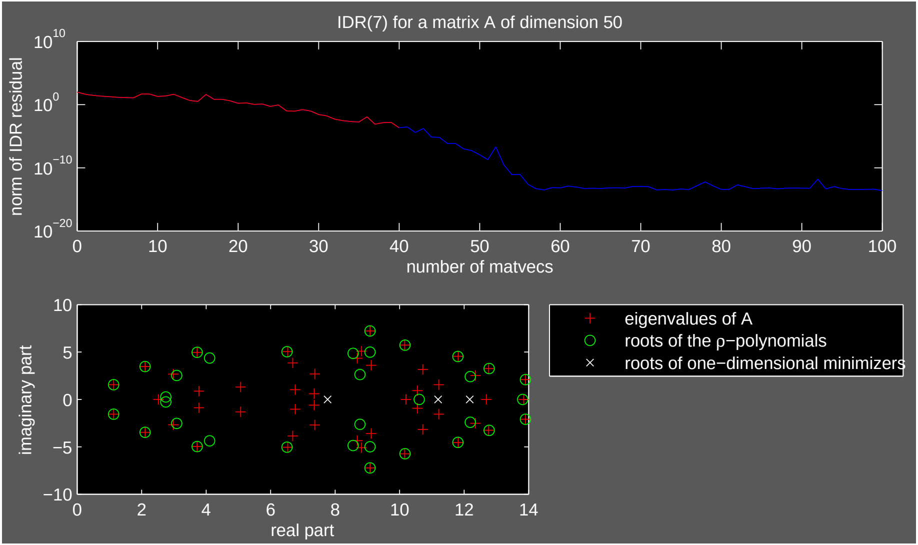

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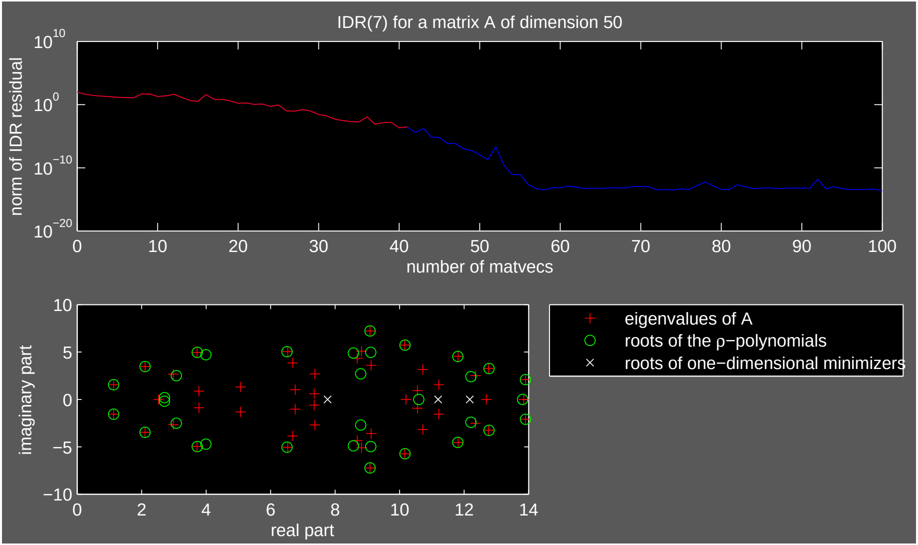

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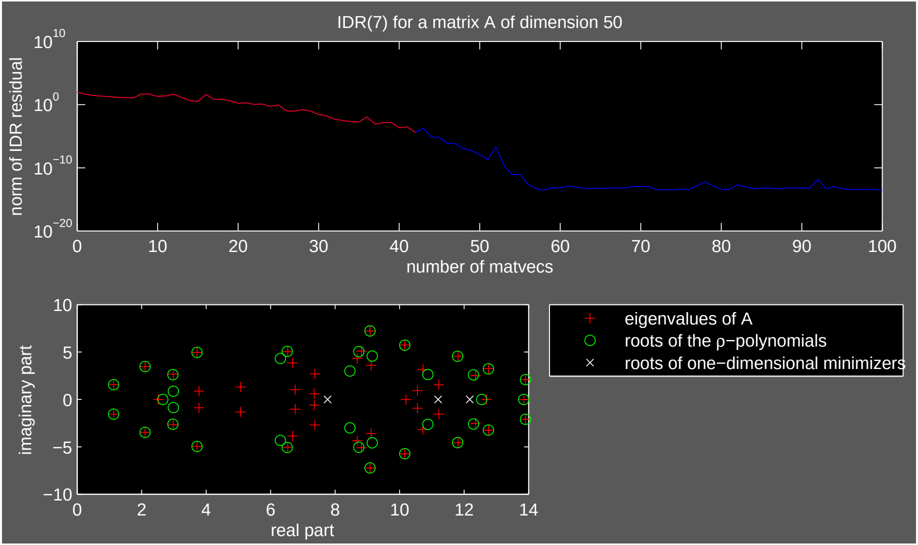

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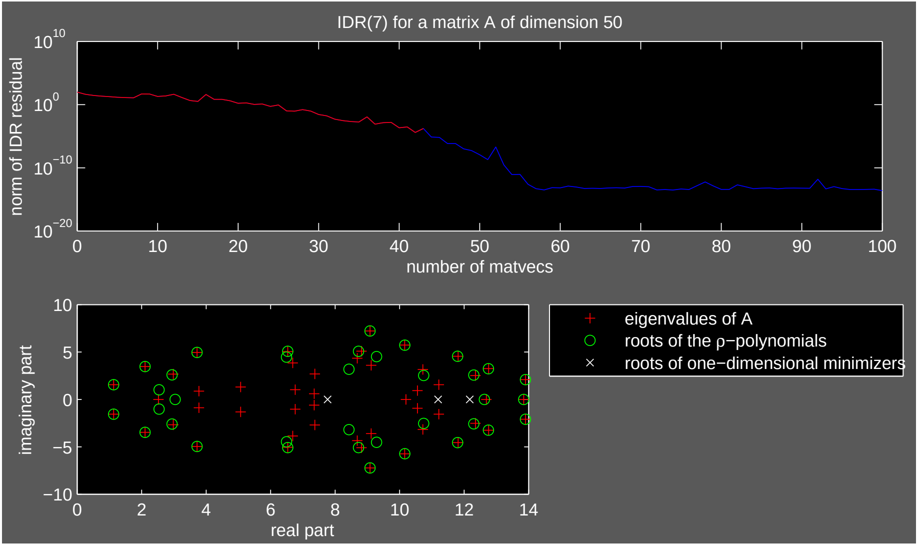

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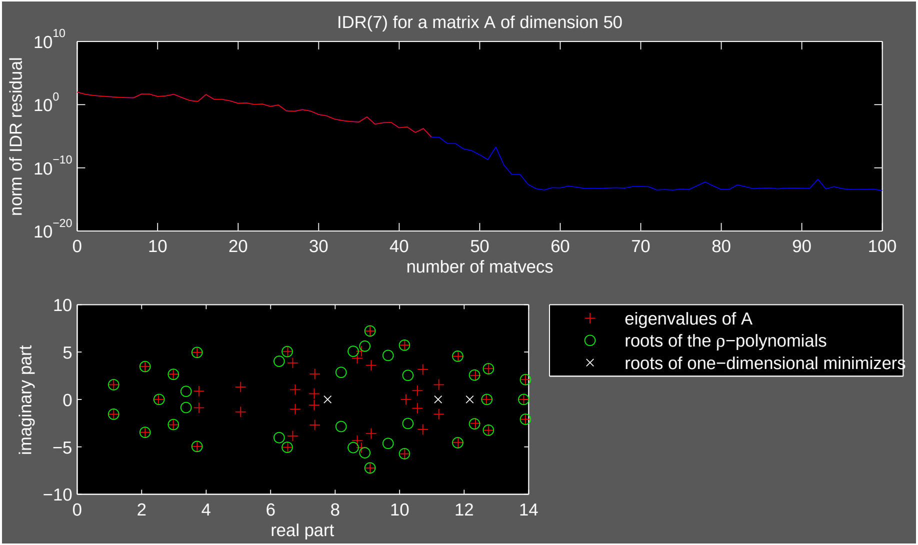

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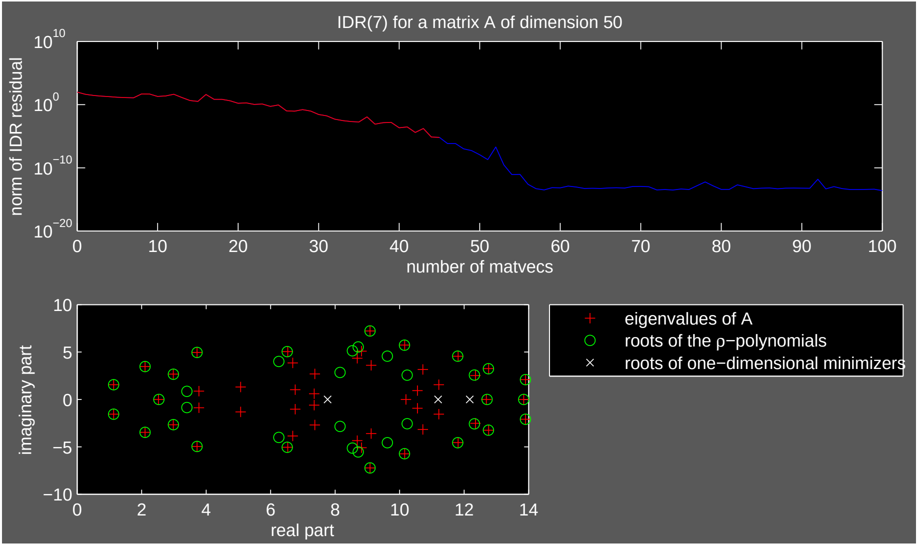

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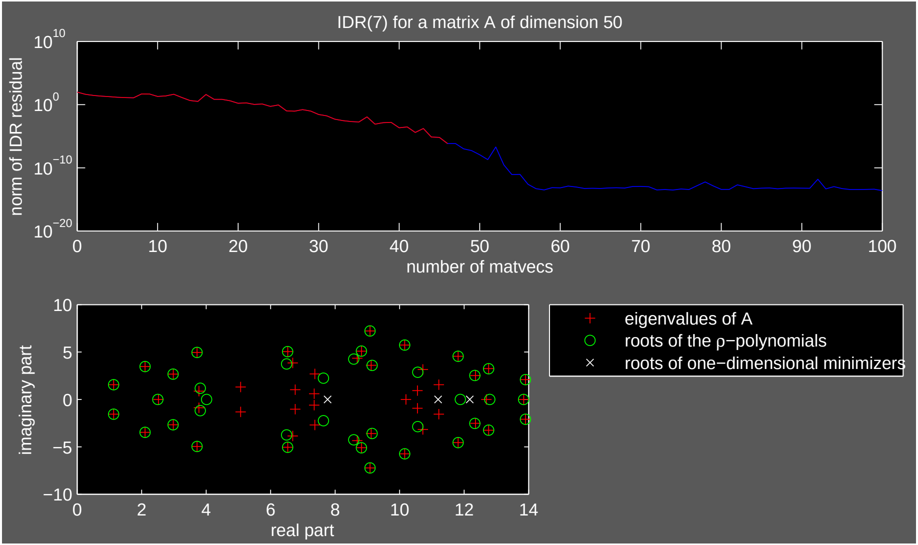

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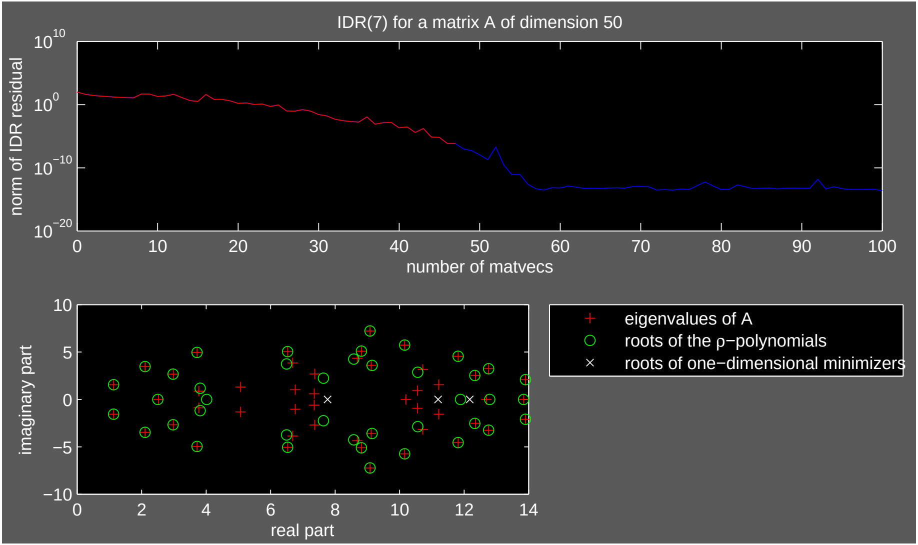

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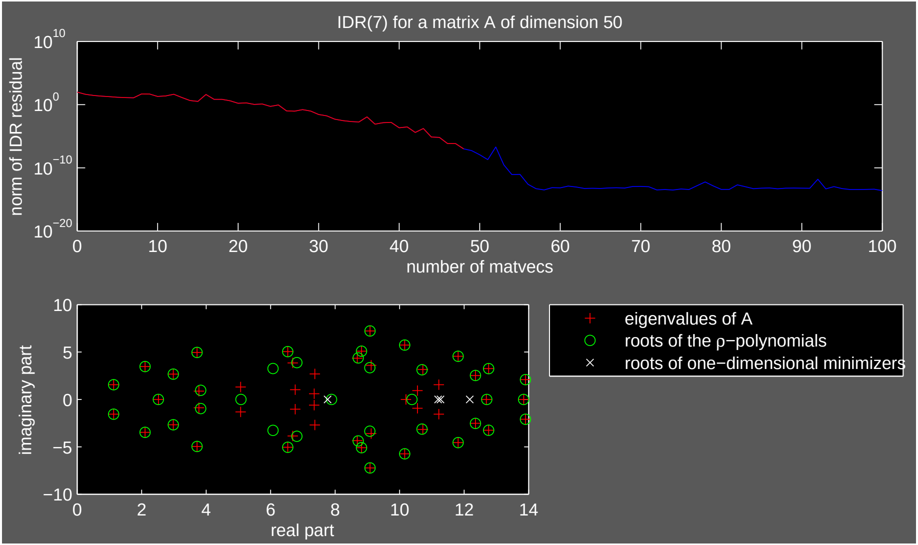

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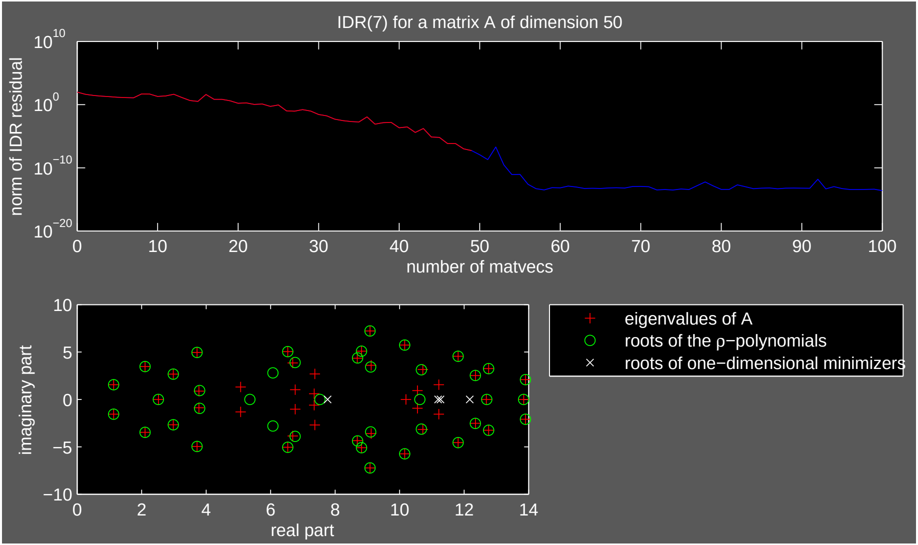

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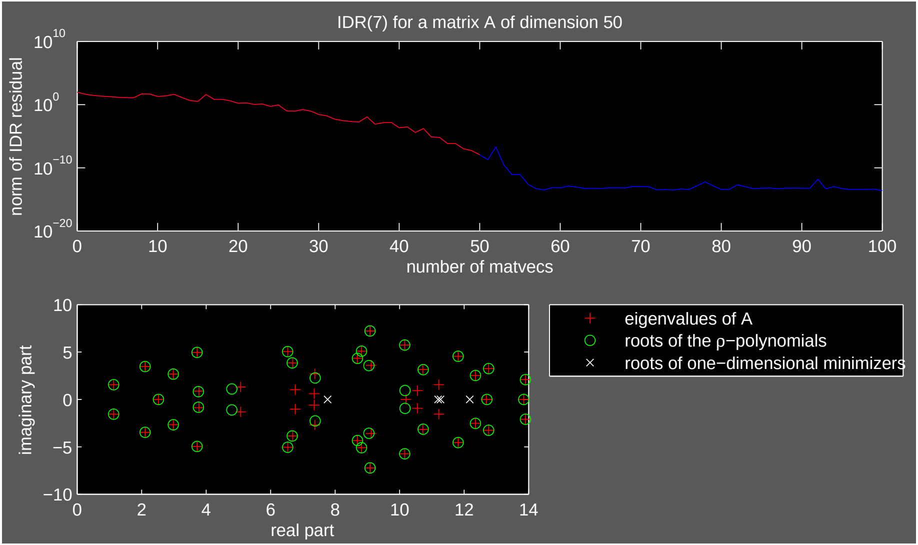

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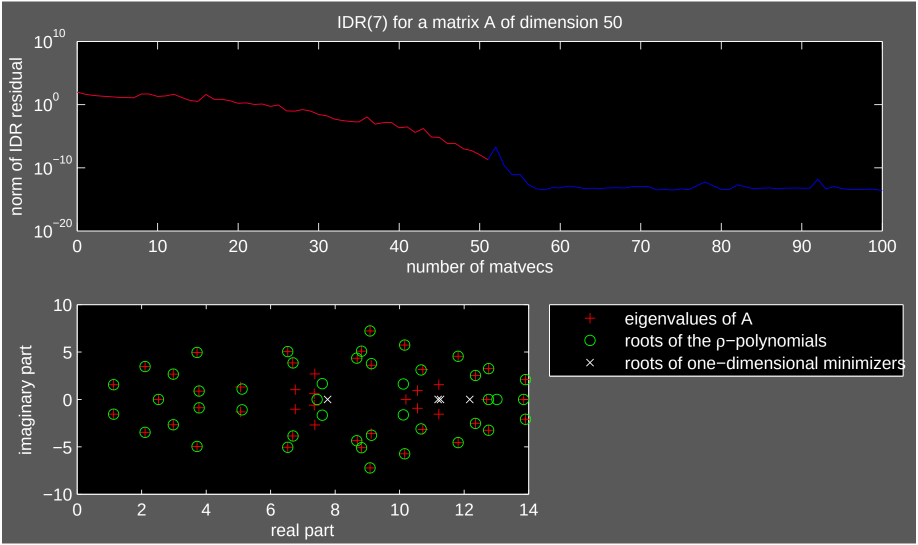

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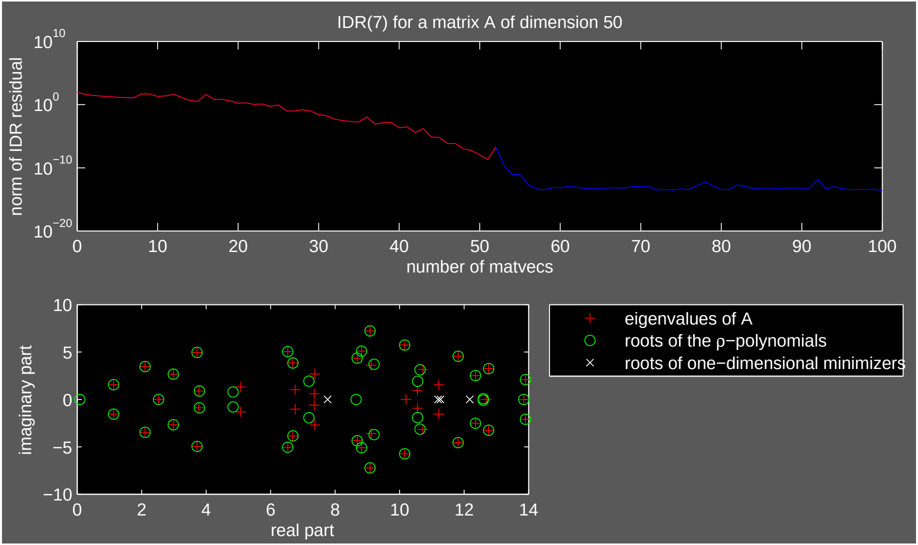

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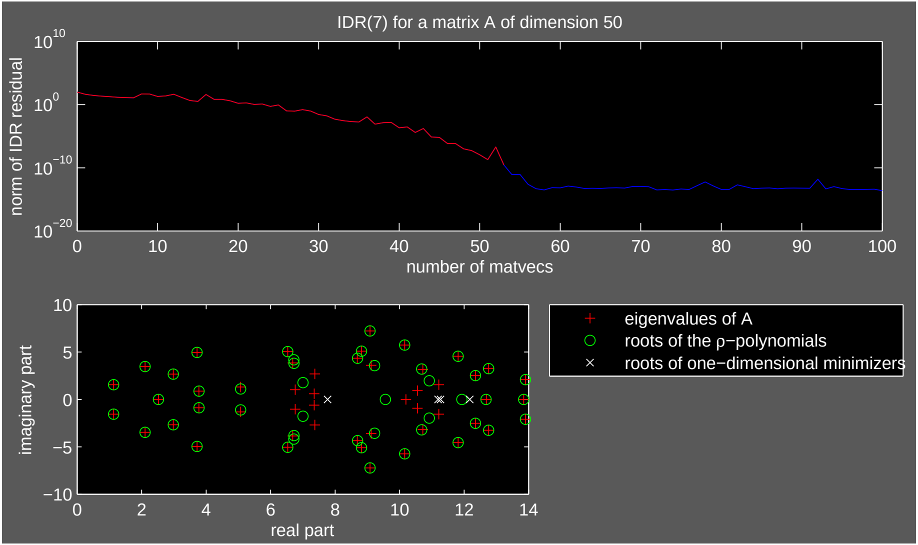

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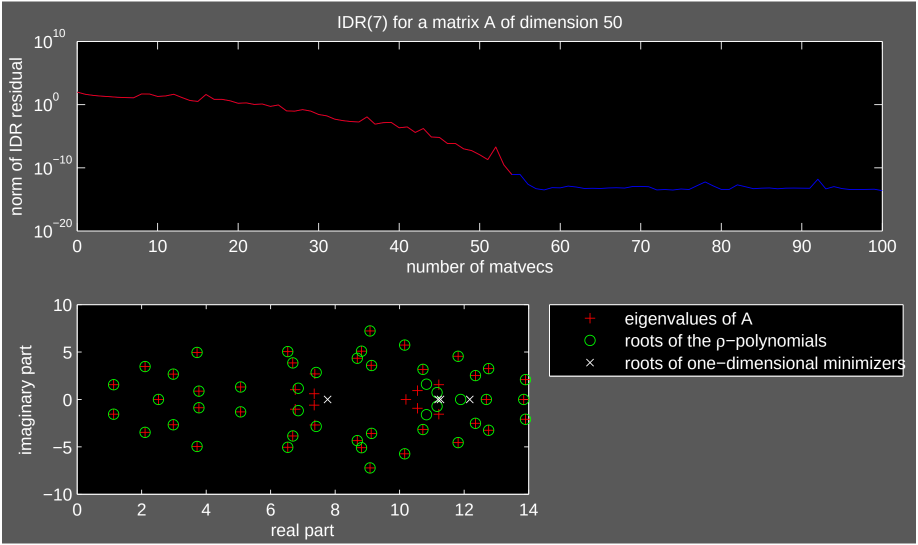

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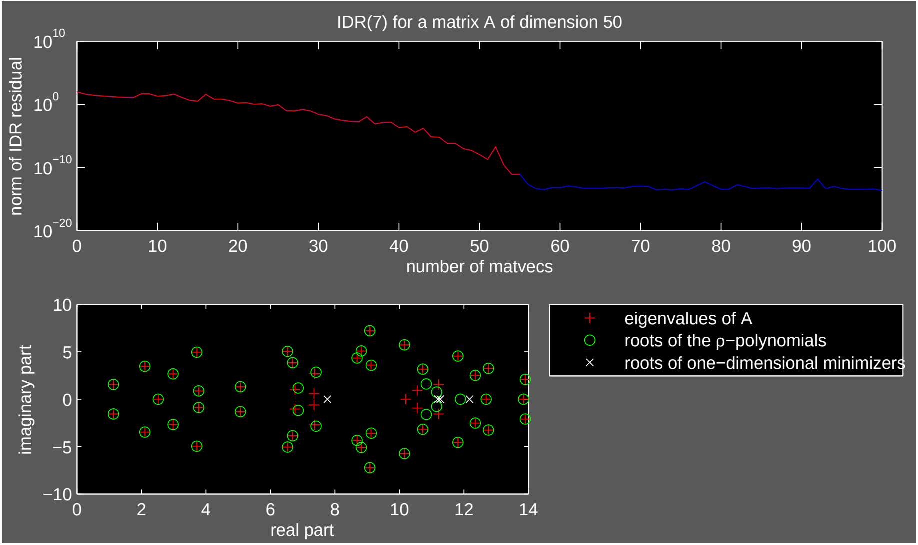

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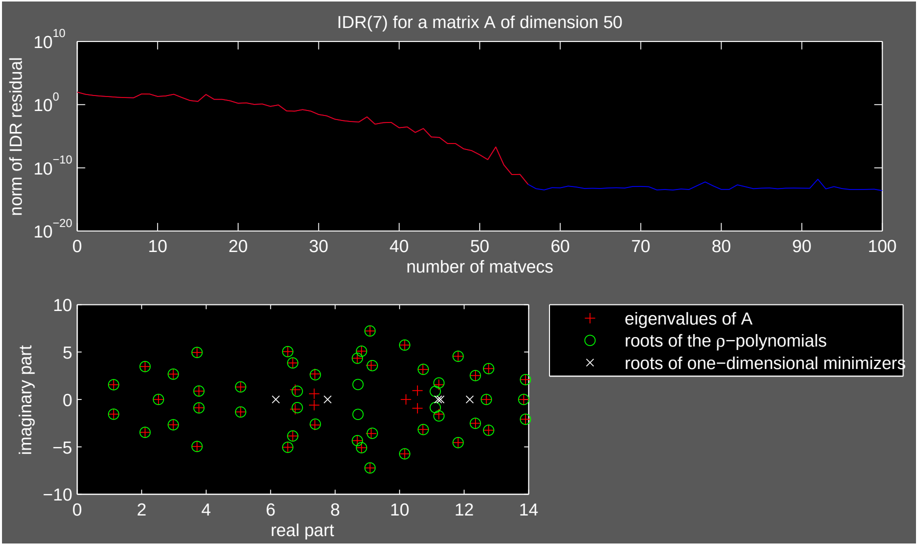

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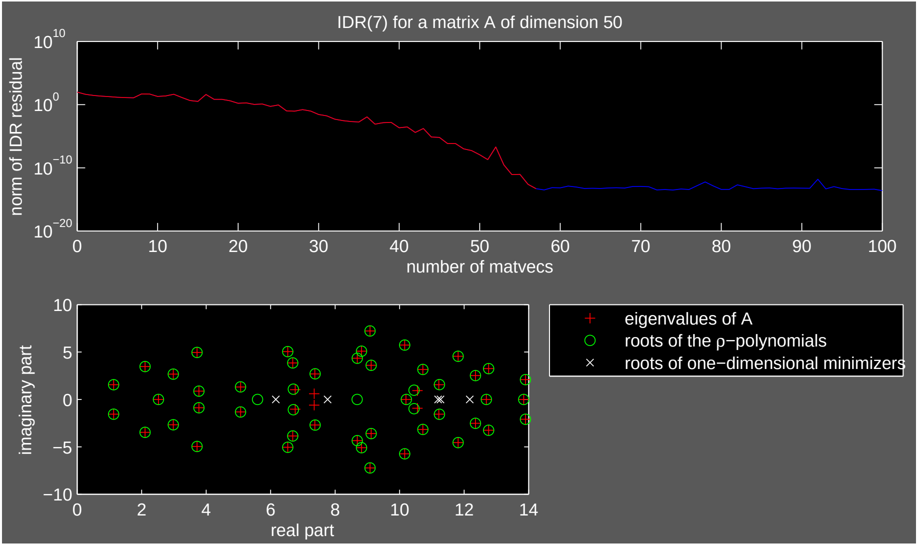

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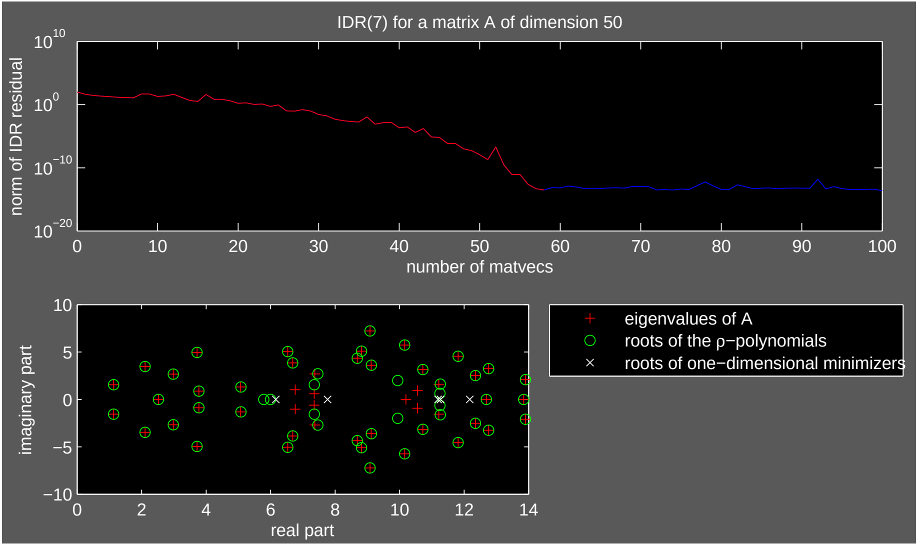

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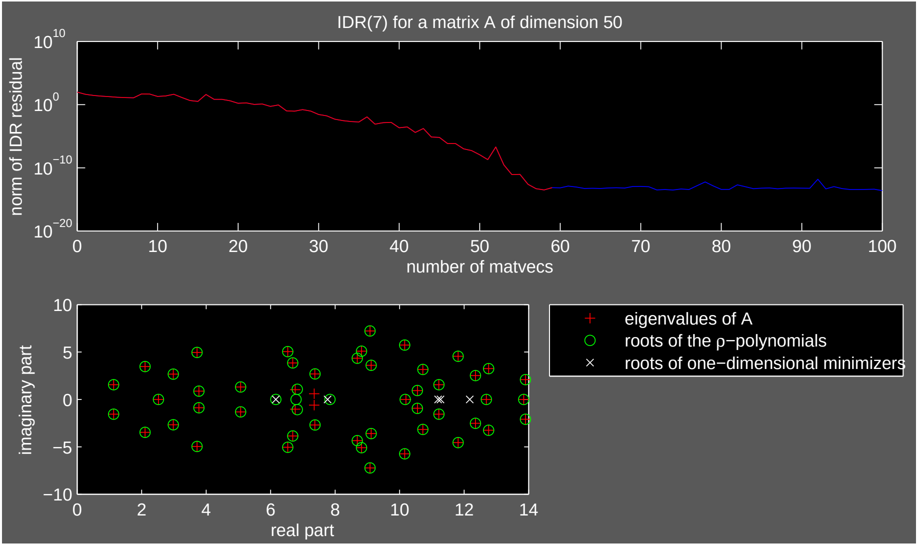

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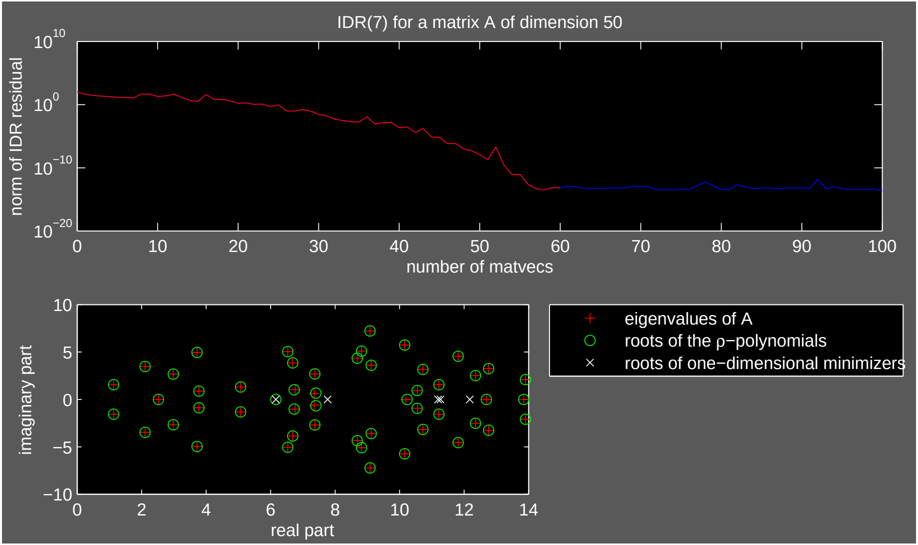

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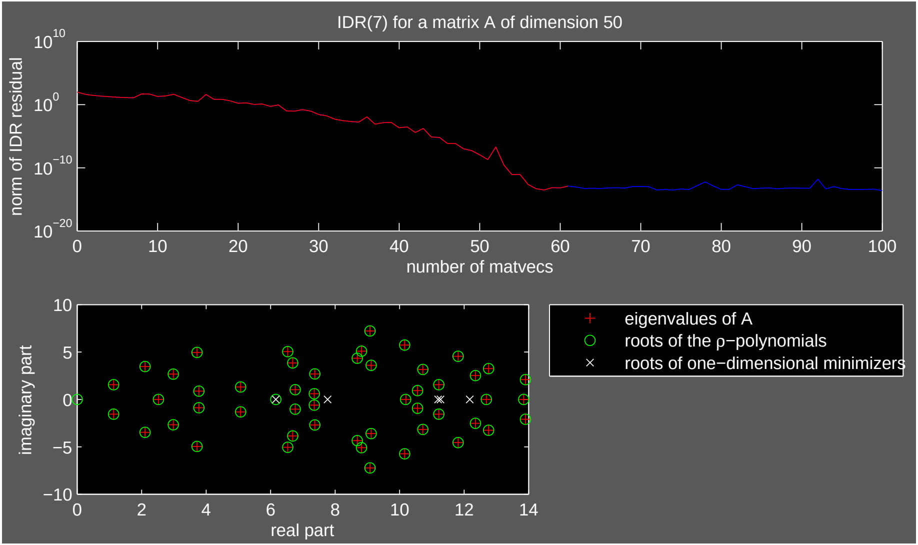

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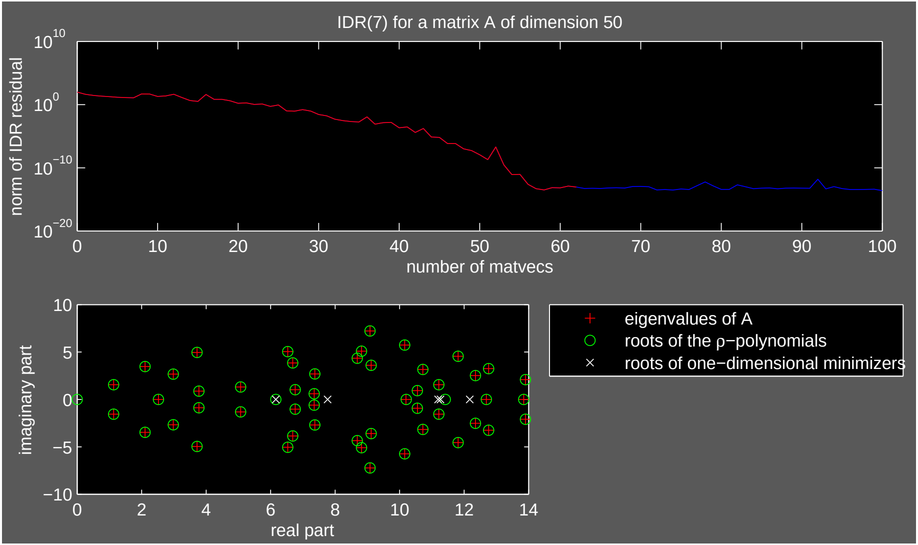

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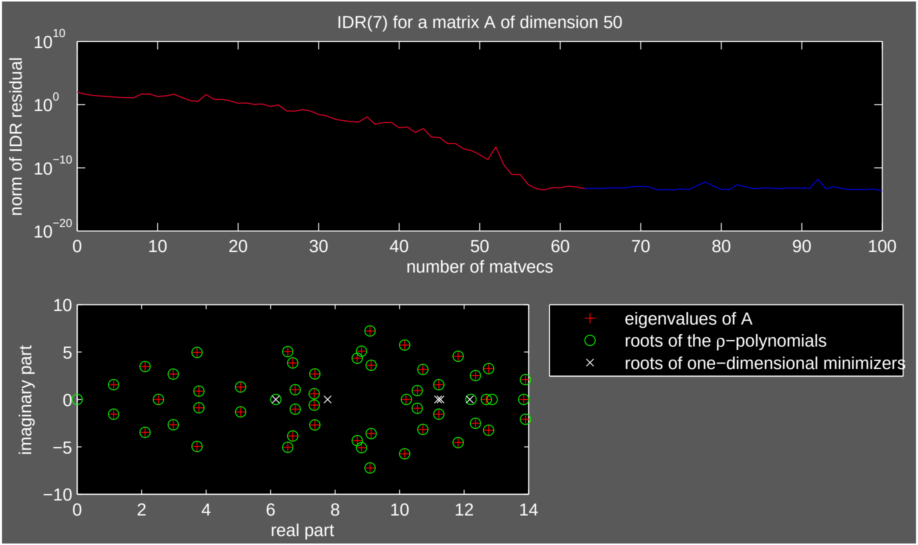

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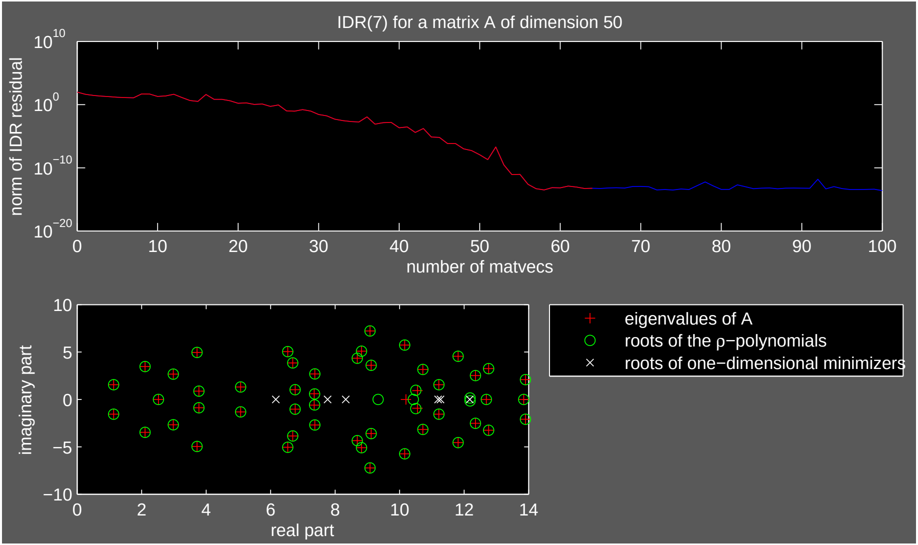

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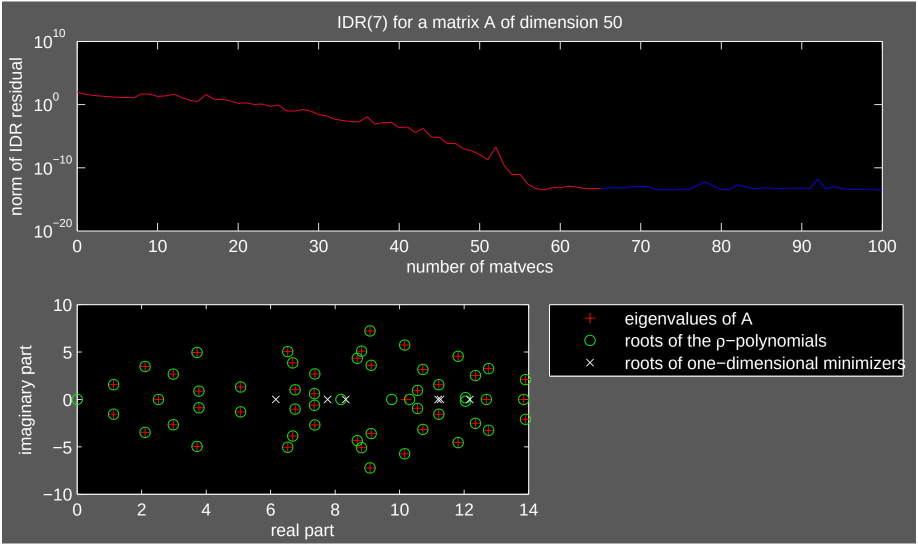

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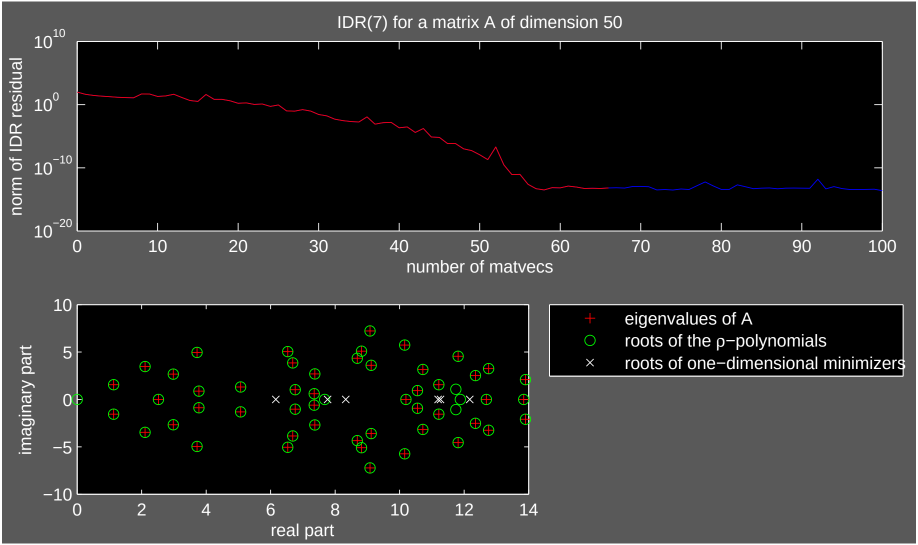

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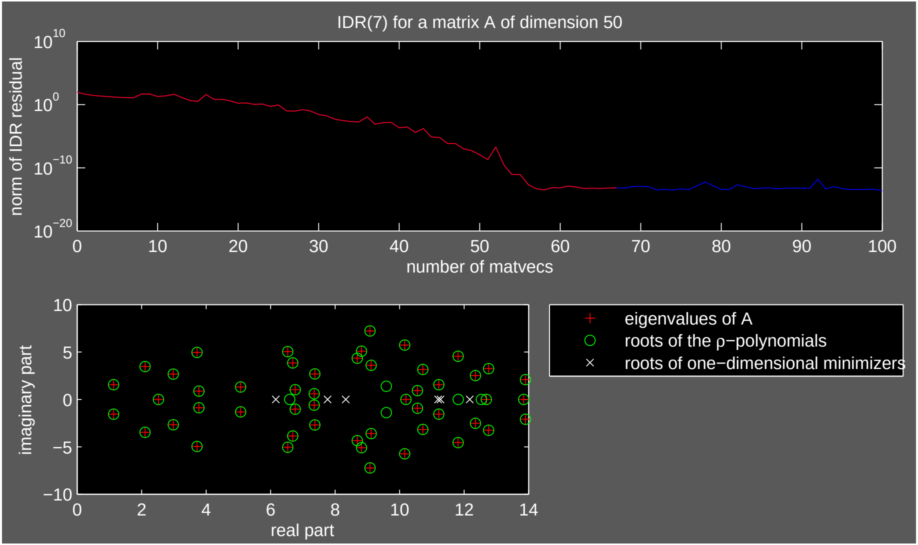

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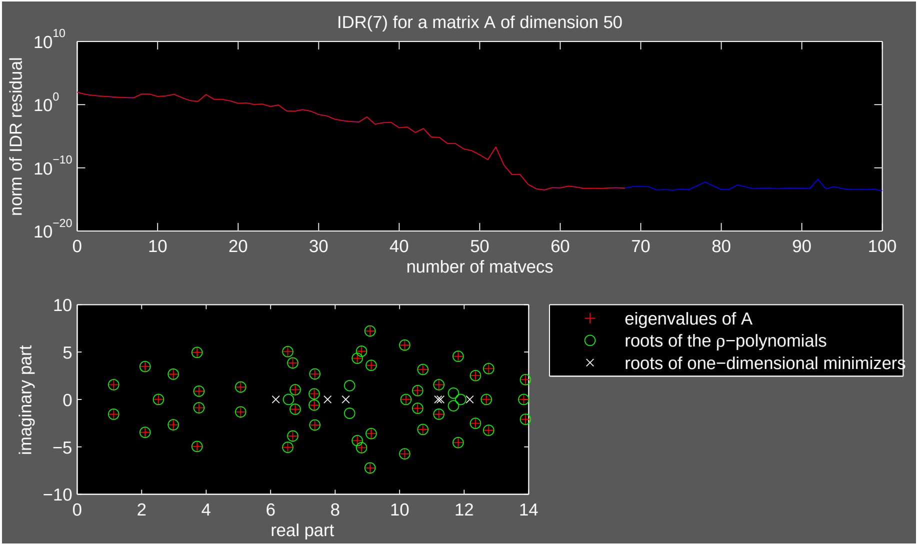

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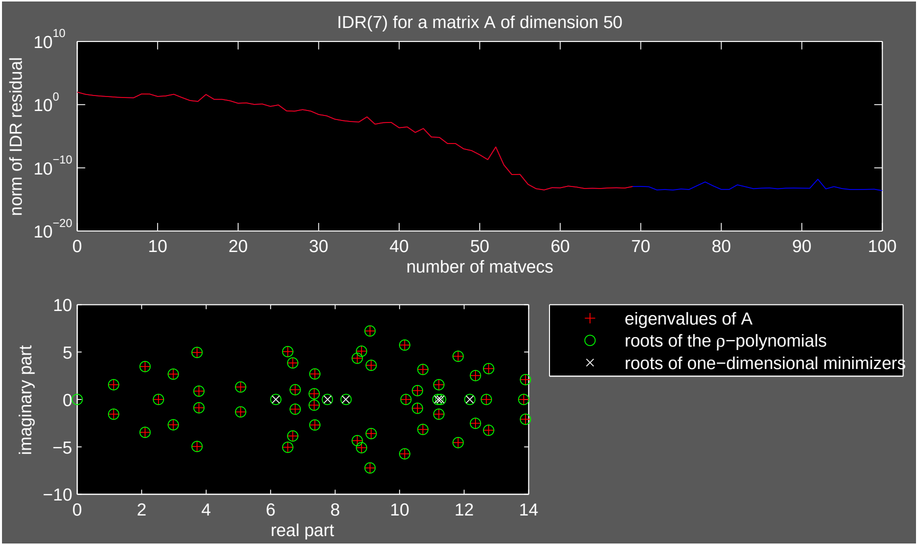

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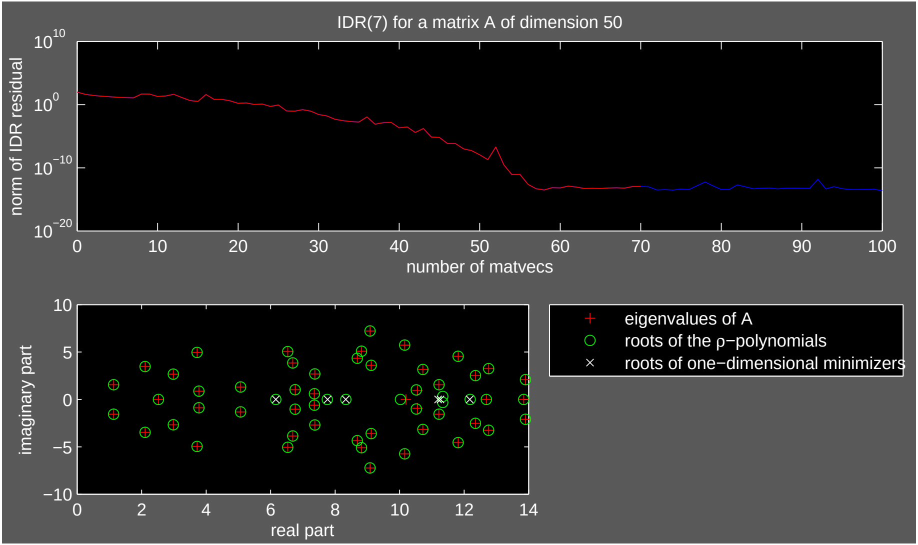

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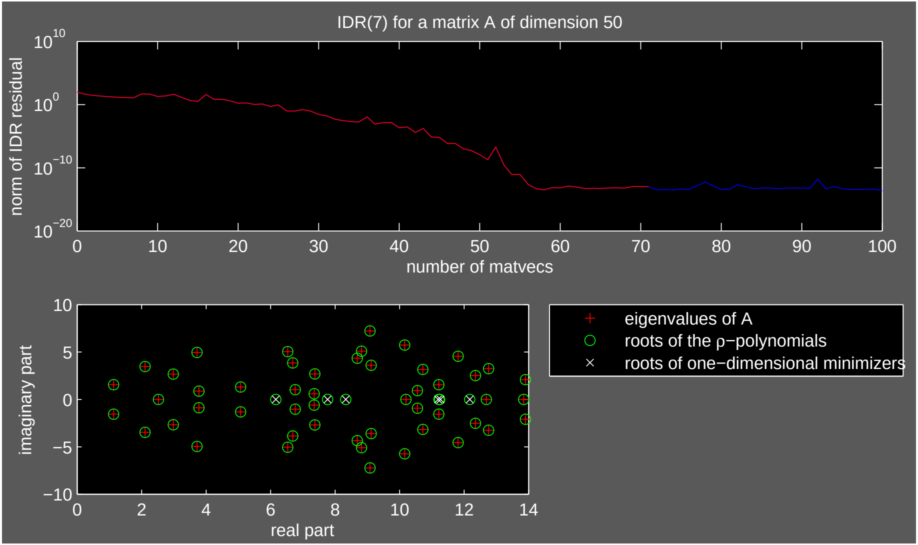

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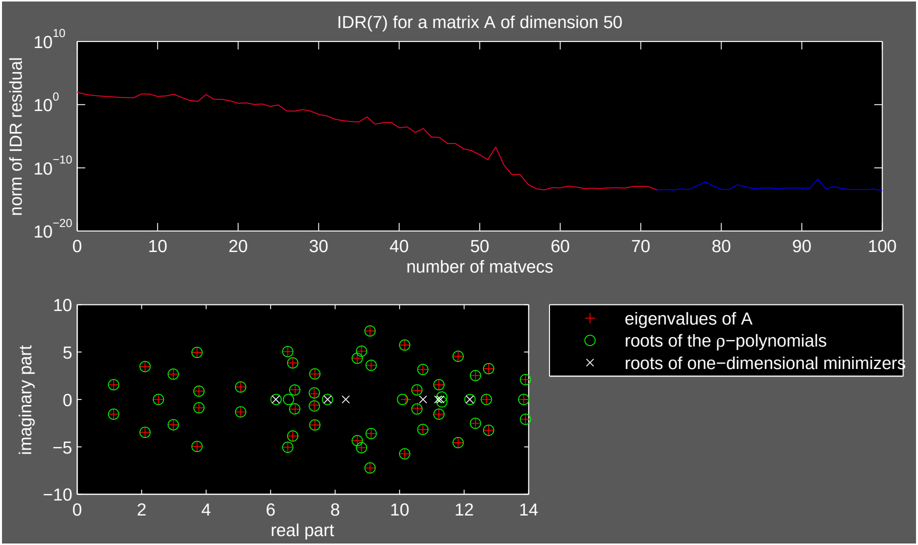

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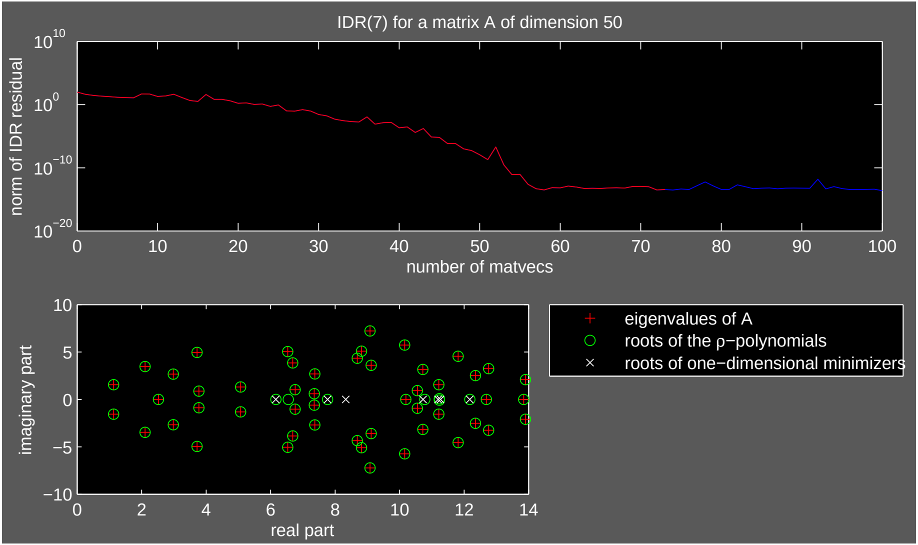

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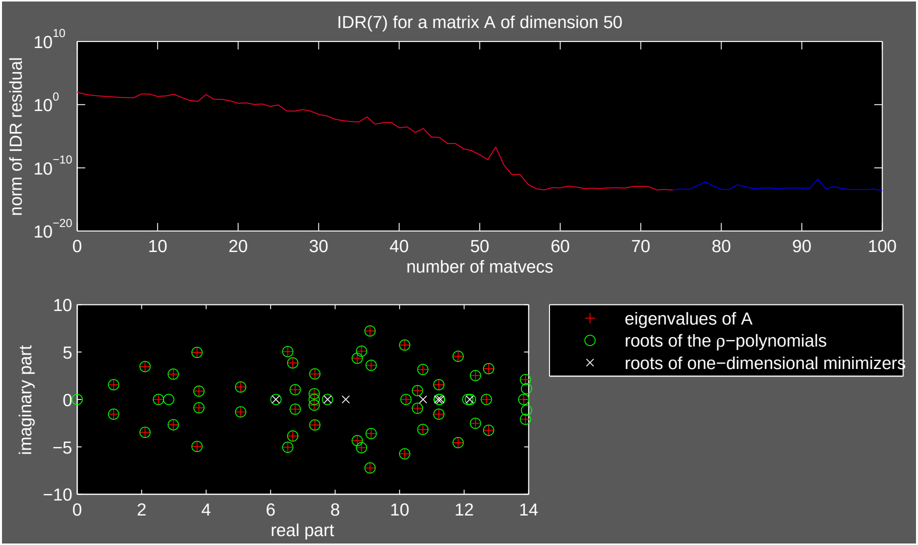

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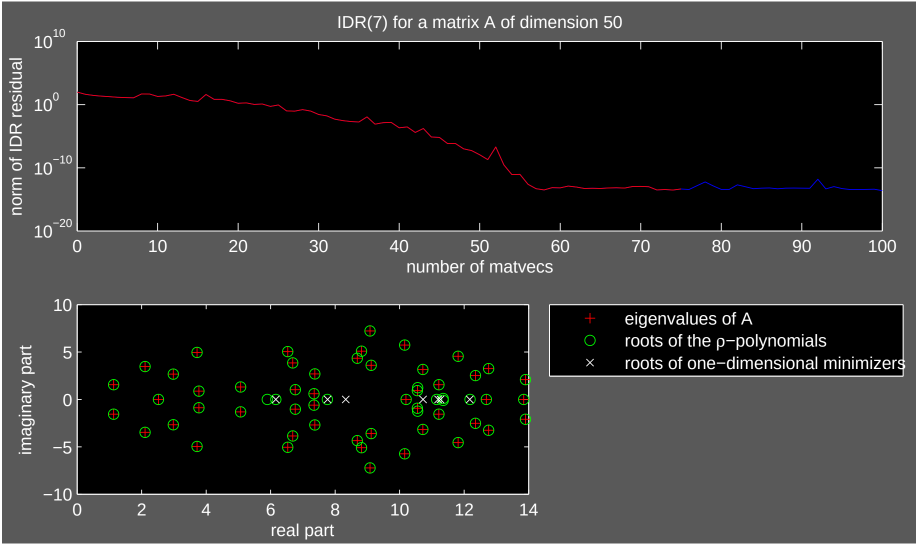

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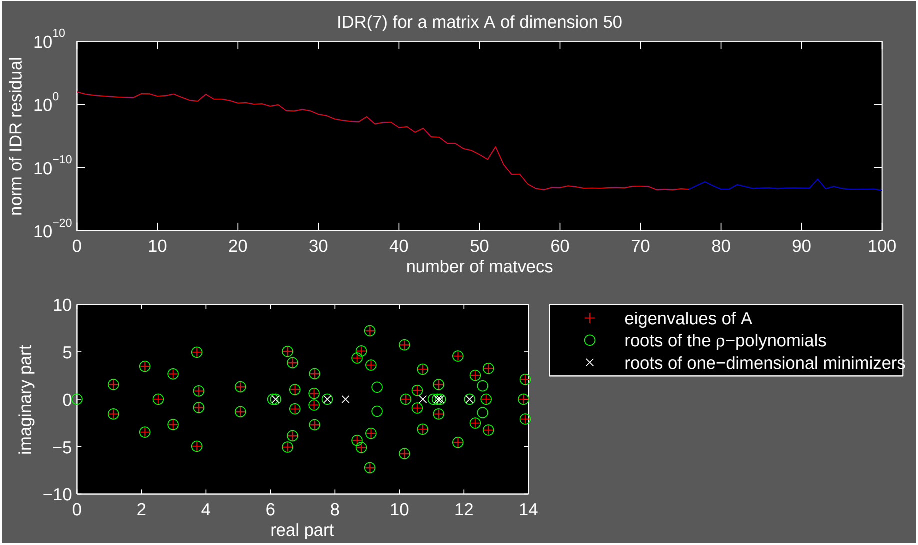

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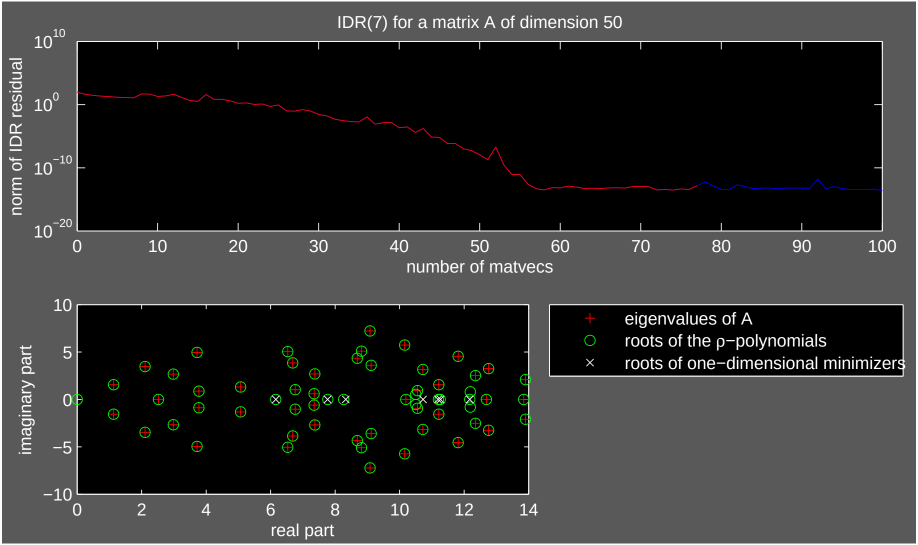

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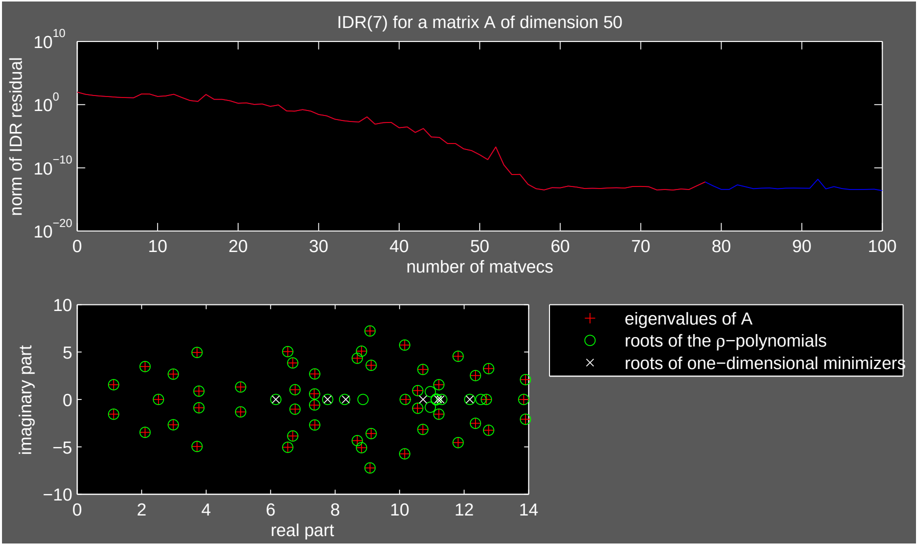

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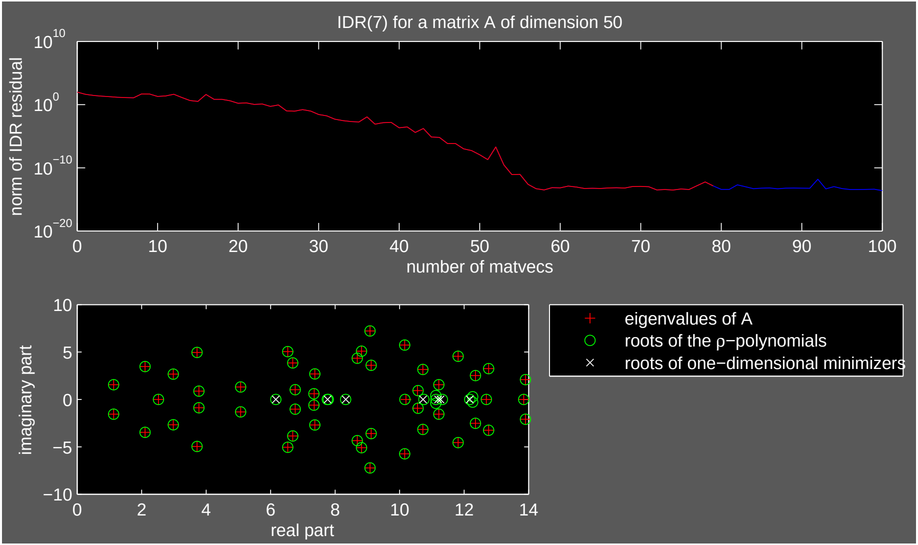

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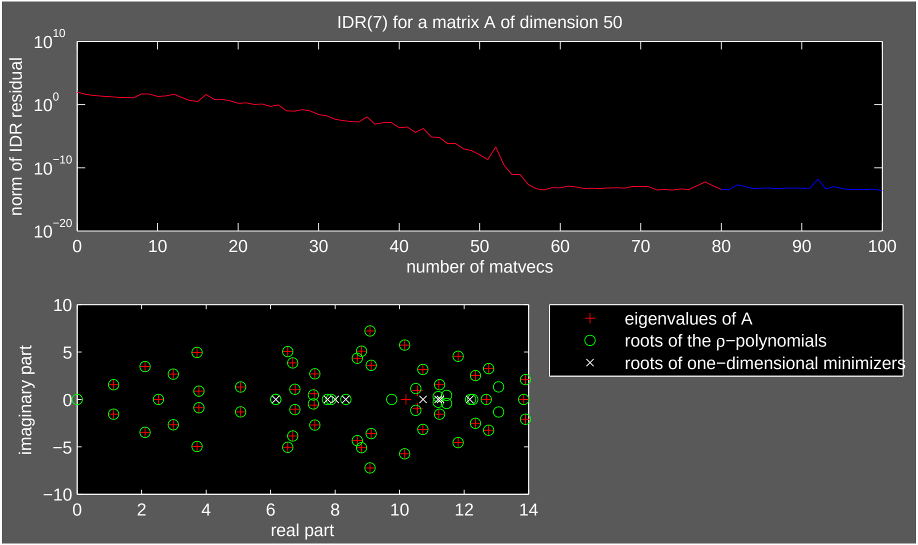

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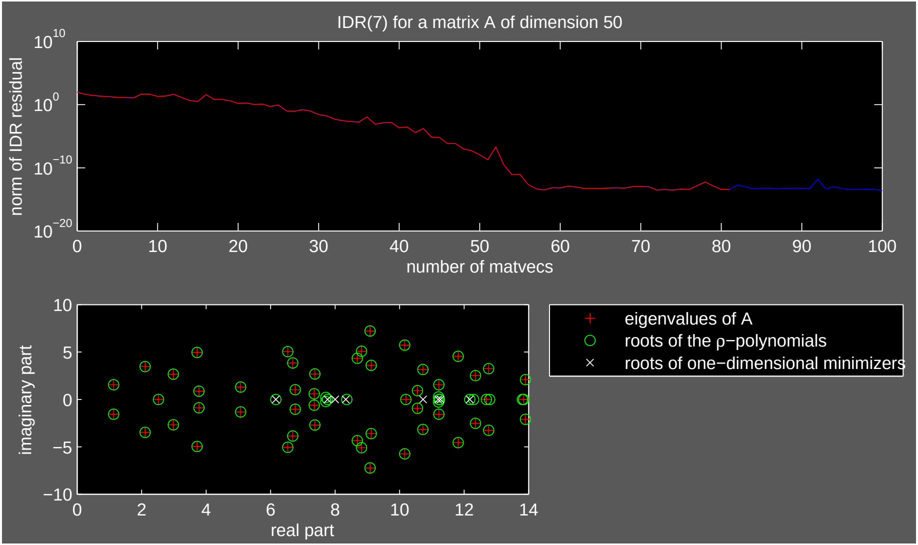

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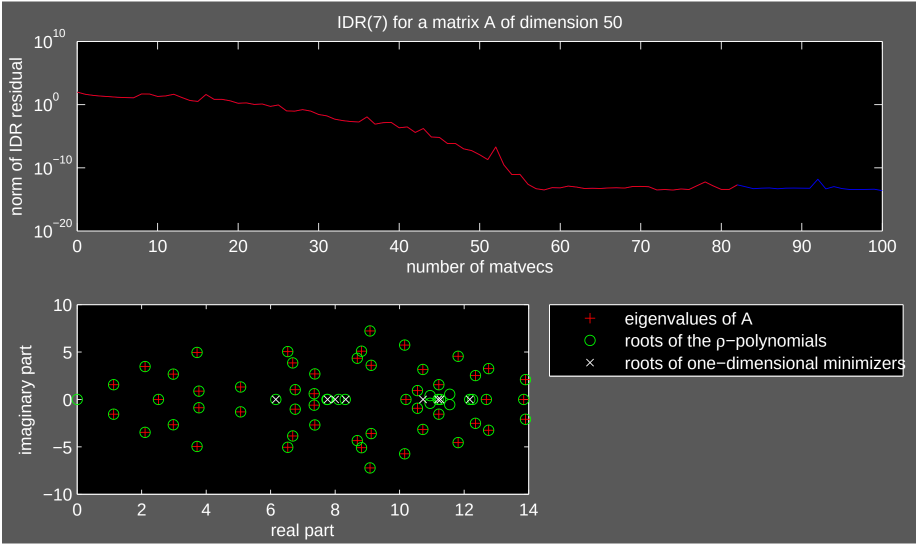

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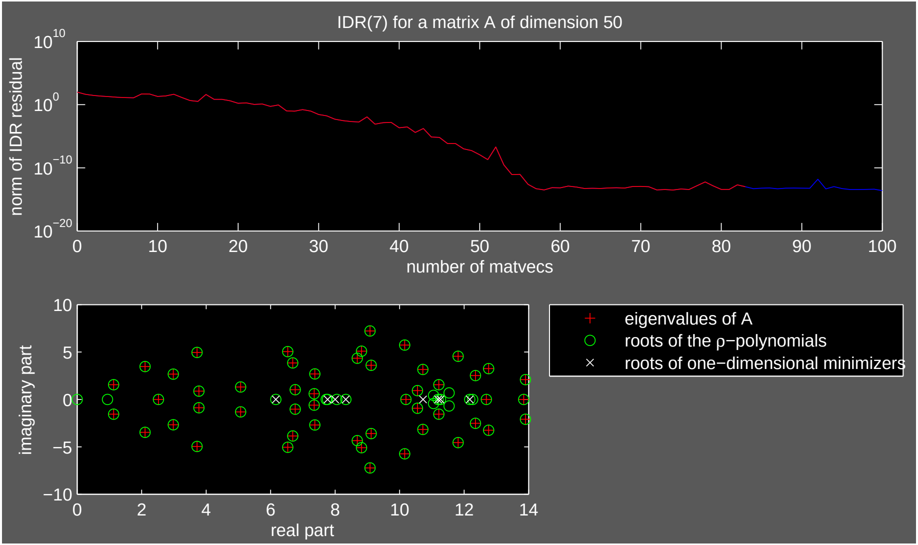

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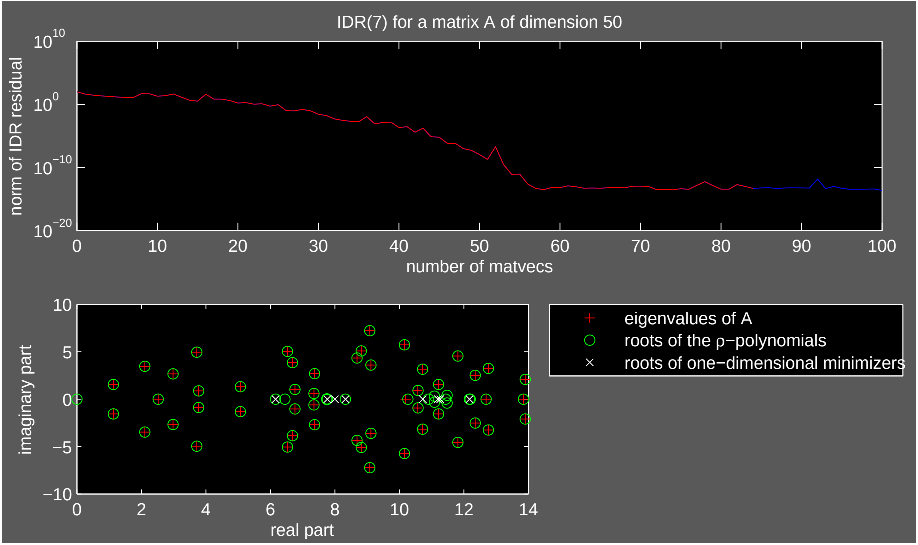

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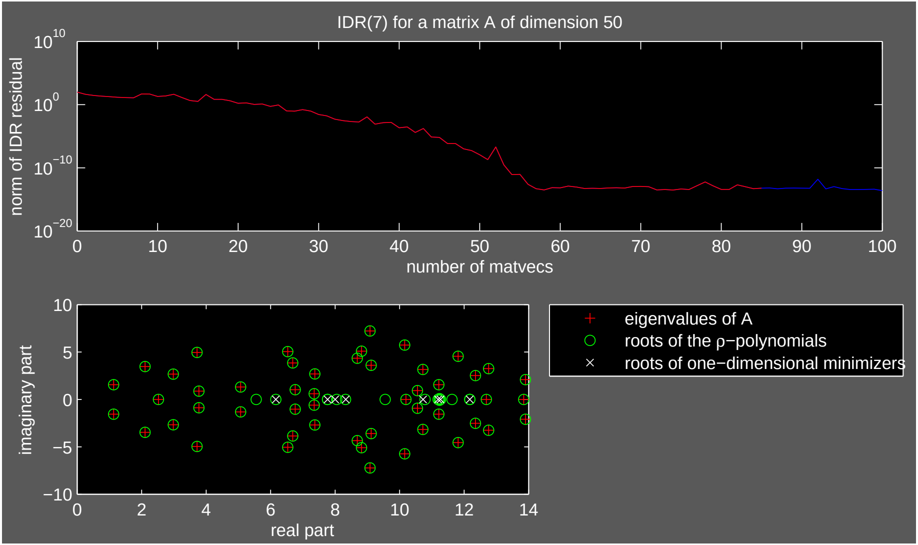

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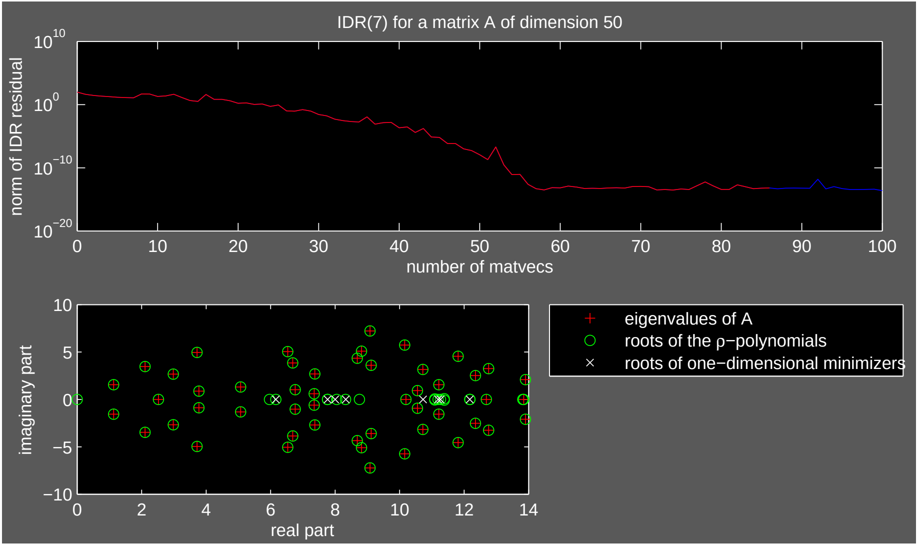

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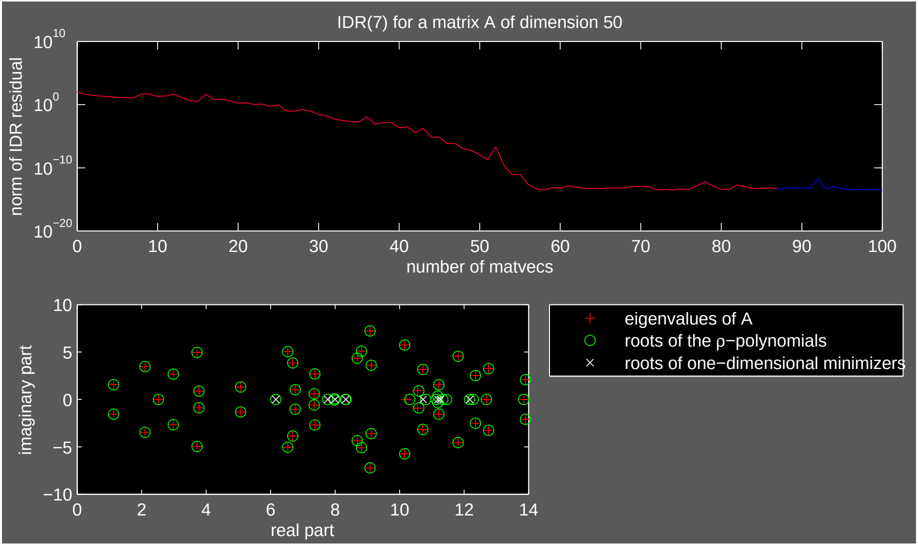

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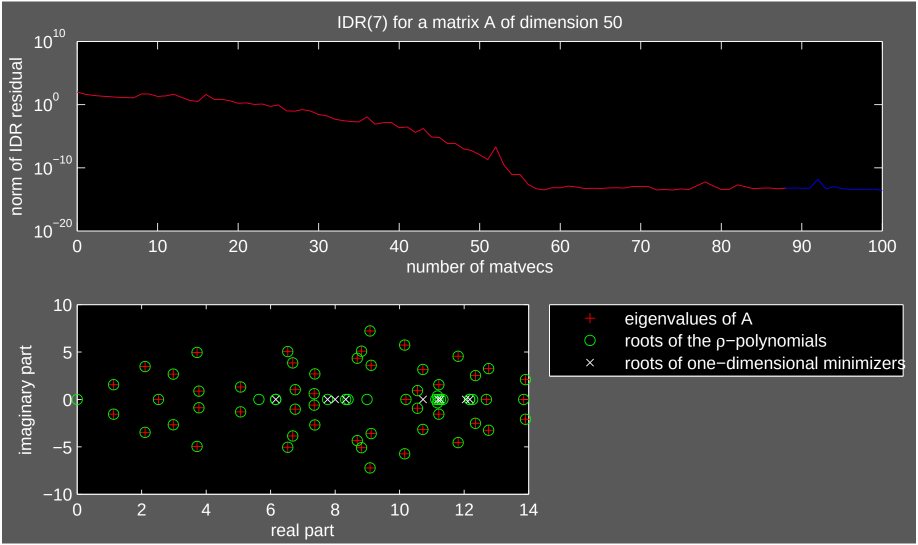

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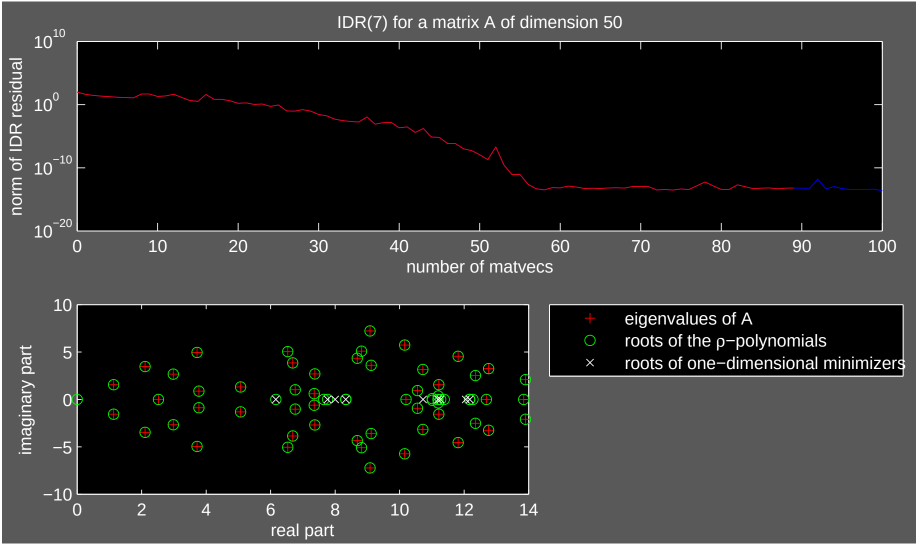

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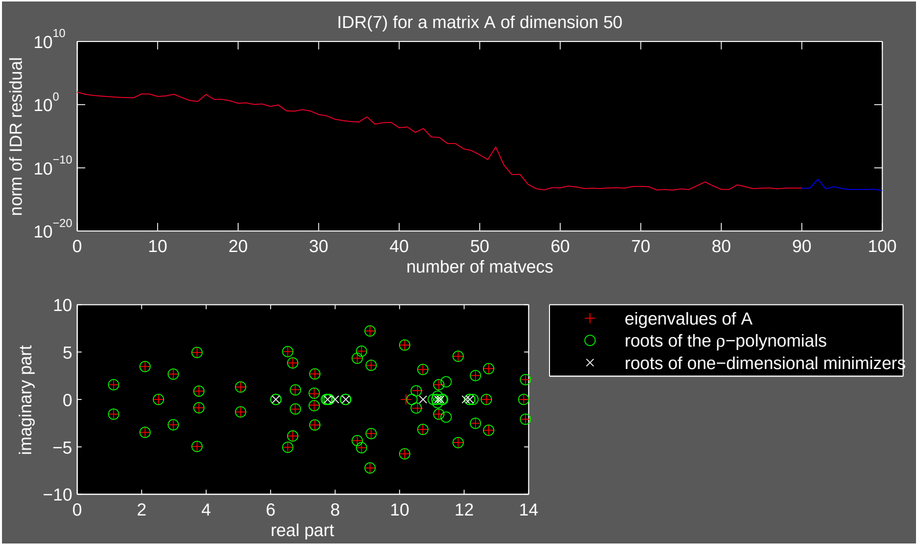

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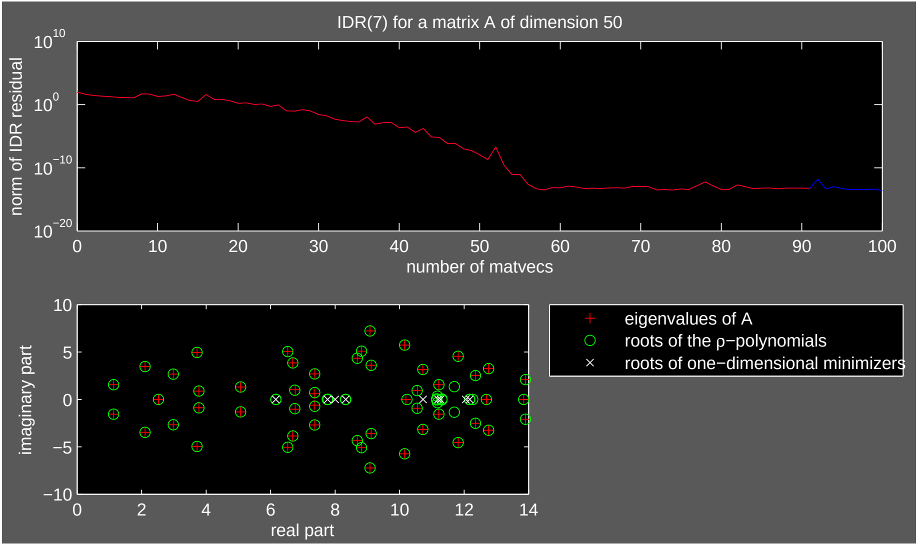

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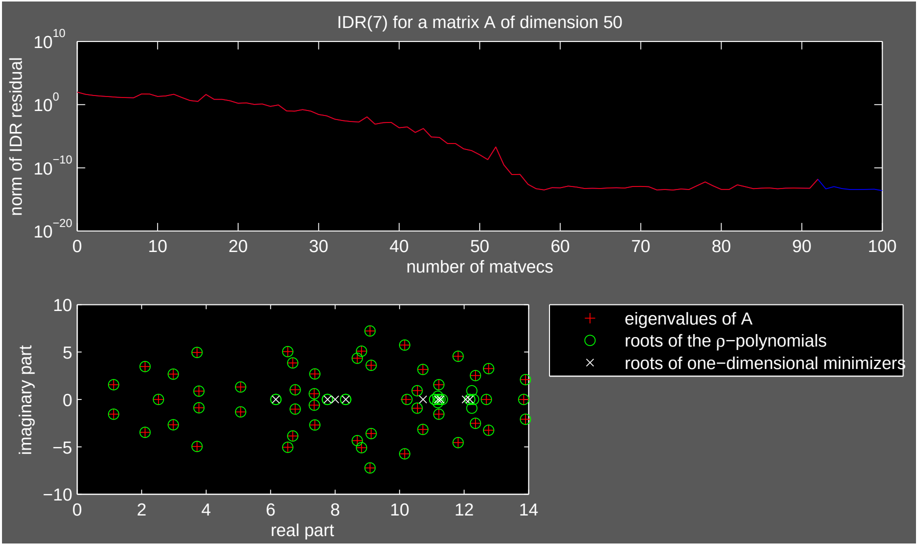

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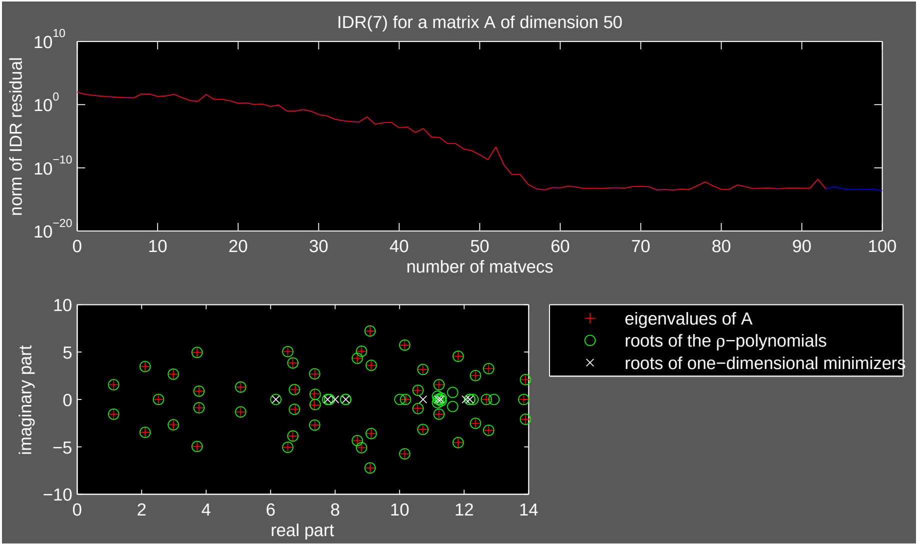

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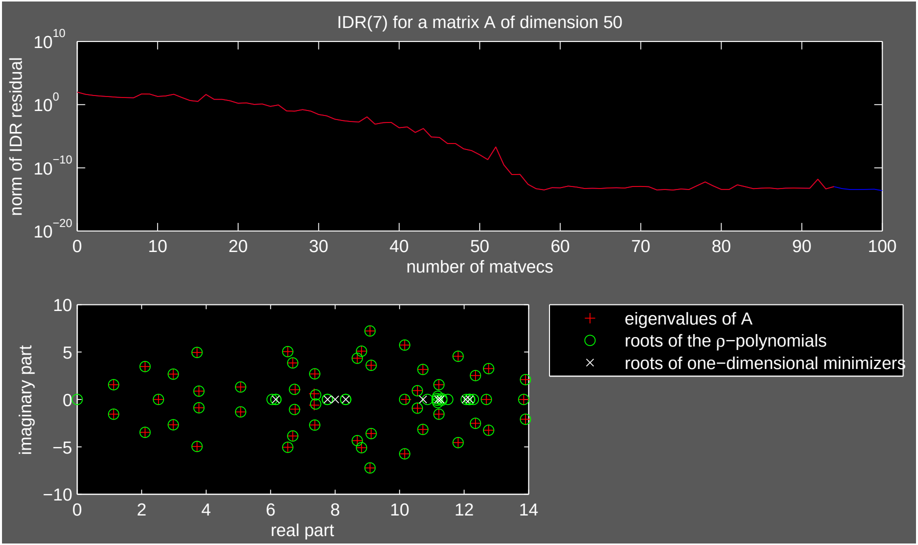

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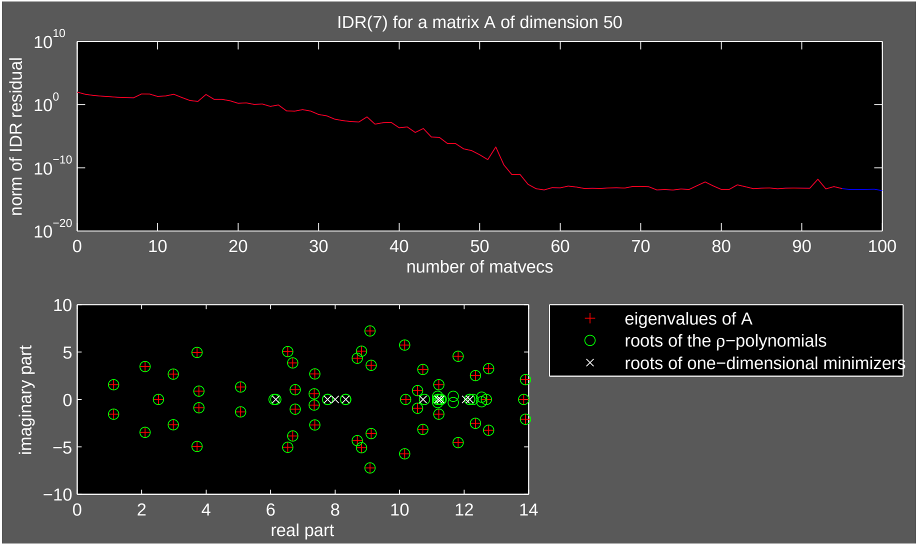

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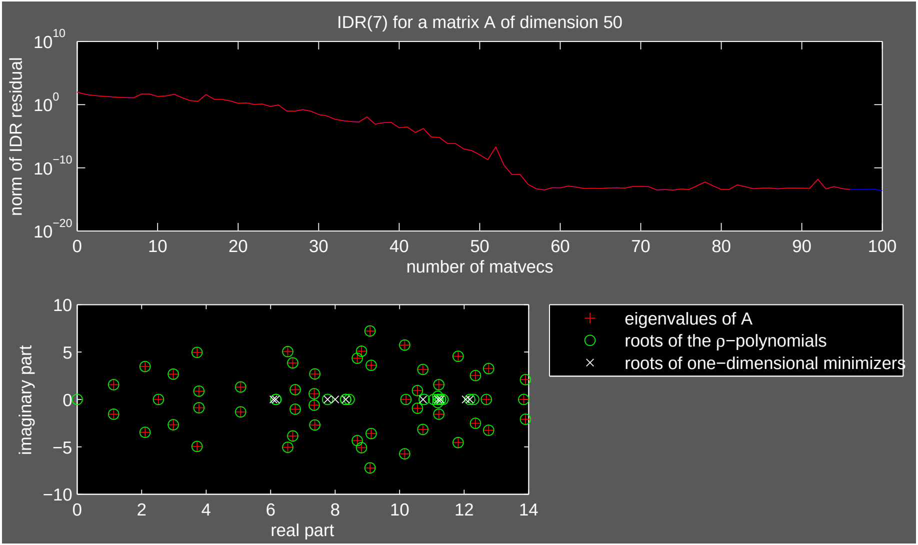

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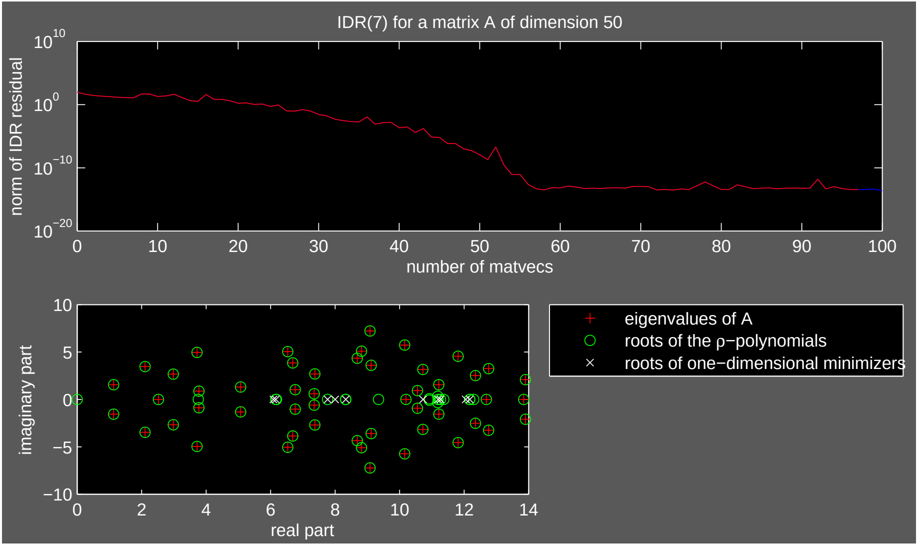

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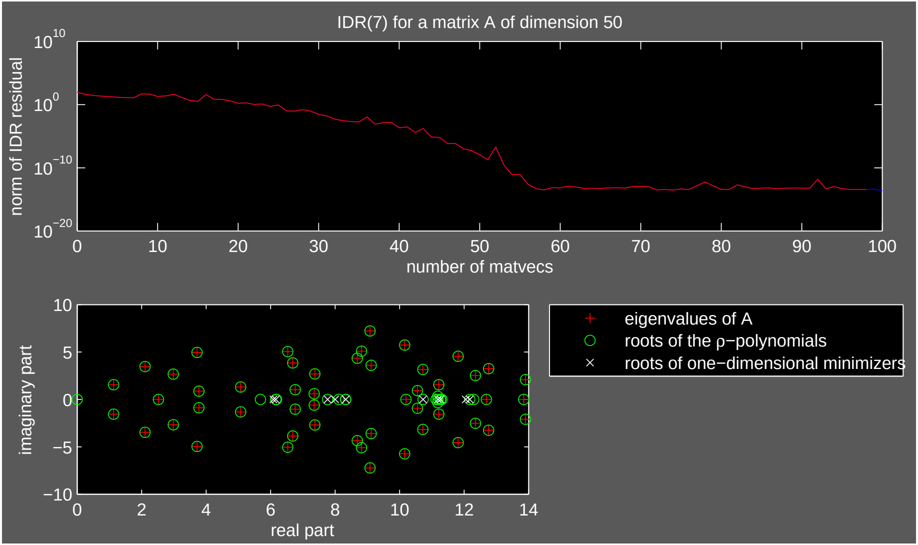

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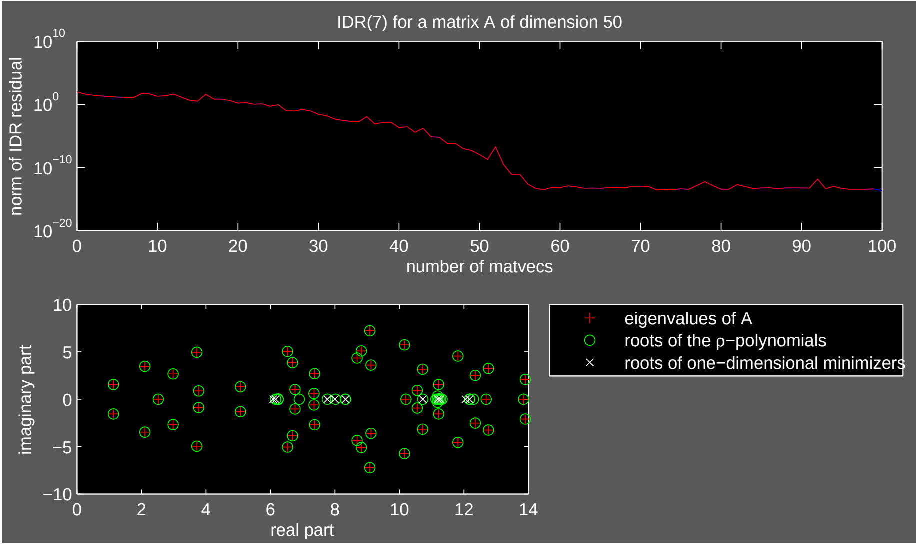

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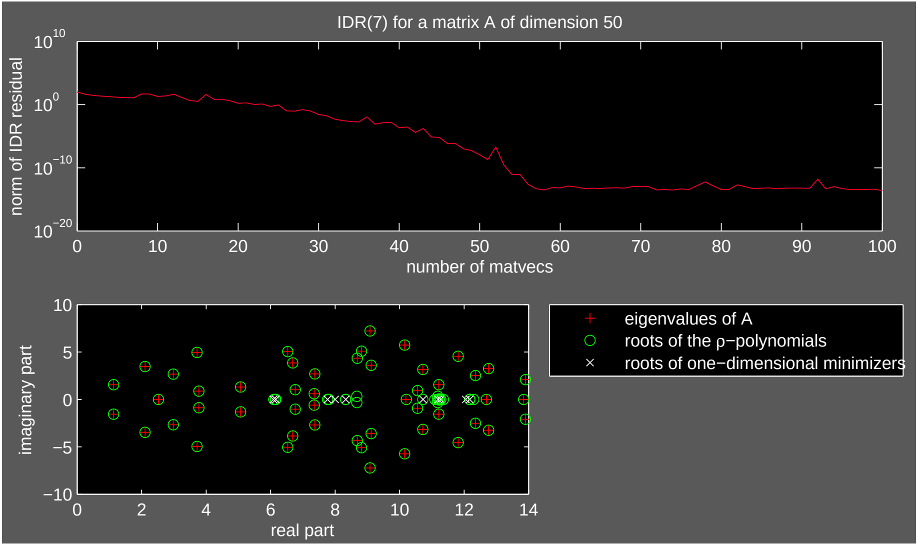

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Many questions, some of them partially attacked, remain:

- How do we compute Ritz vectors? How accurate are the Ritz pairs?
- How are the residual and purified residual decomposition related matrix-wise?
- Are all eigenvalues approximated just once?
- Why does the finite precision Lanczos' process re-compute the minimizers and compute spurious eigenvalues close to zero?
- How does the condition grow when the roots $1/\omega_j$ become (almost) multiple (mostly $s$ fold)?
- How does this affect the convergence rate of finite precision IDR?

Thank you for your attention.