

New ideas on IDR(s)

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joint work with Martin Gutknecht
(work in progress)

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- IDR as QOR

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New ideas on IDR(s)

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Origin of Krylov methods

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

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

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The (columns of the) n th Krylov matrix span(s) a basis of the n th Krylov space \mathcal{K}_n iff n is less or equal to the grade of \mathbf{q} .

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

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

Origin of Krylov methods

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

$$\begin{pmatrix} \star & \underline{\mathbf{C}}_n \\ \mathbf{0} & \end{pmatrix} := \mathbf{R}_{n+1} \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \mathbf{R}_n \end{pmatrix}^{-1} \quad (3)$$

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We end up with a [Hessenberg decomposition](#)

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

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 $\mathbf{x}_n := \mathbf{Q}_n\mathbf{C}_n^\dagger\mathbf{e}_1\|\mathbf{r}_0\|$,

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

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

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

Implementation of Krylov methods

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In finite precision the recurrence will only approximately be satisfied,

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

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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 - \tilde{\mathbf{R}}_n \Delta \mathbf{c}_n = \tilde{\mathbf{R}}_n \mathbf{y}_n \\
 &= (1 - \gamma_1^{(n)}) \mathbf{r}_n + \sum_{\ell=1}^{s-1} (\gamma_\ell^{(n)} - \gamma_{\ell+1}^{(n)}) \mathbf{r}_{n-\ell} + \gamma_s^{(n)} \mathbf{r}_{n-s}.
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Here, $n > s$, and the index of the scalar ω_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

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

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

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

Here, the **Sonneveld matrix** $\underline{\mathbf{S}}_n^\circ$ is defined as long as all $\omega_j \neq 0$ and all $\gamma_1^{(k)} \neq 1$.

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

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

IDR for eigenvalues

In unperturbed IDR the generalized Hessenberg decomposition is given by

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

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We can use the leading submatrices of the Sonneveld matrix \mathbf{S}_n° 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.

IDR for eigenvalues

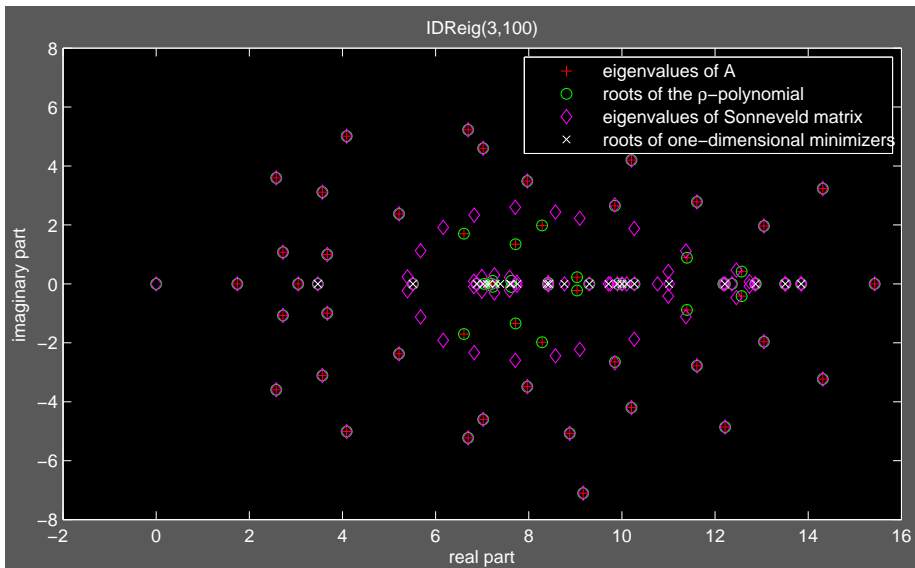
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Numerically more stable and more efficient is the use of the **Sonneveld pencil** ($\mathbf{Y}_n^\circ, \mathbf{Y}_n\mathbf{D}_\omega$). The stability comes from the fact that we need not be afraid of a large condition of \mathbf{Y}_n and/or \mathbf{D}_ω . 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 $(\mathbf{I} - \omega_j \mathbf{A}) : \mathcal{G}_{j-1} \rightarrow \mathcal{G}_j$, we know that for some $\mathbf{w}_n \in \mathcal{G}_0 = \mathcal{K}(\mathbf{A}, \mathbf{r}_0)$

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

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

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We derive the Hessenberg decomposition corresponding to the basis of the **purified residuals** \mathbf{w}_n . This way we only have to compute the unknown eigenvalue approximations instead of computing again the local minimizers.

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Some thinking results in the wanted **purified generalized Hessenberg decomposition**

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

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

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

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

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

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

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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 $D(\mathbf{M}) = \mathbf{M}(\text{ind}, \text{ind})$, 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 .

IDR for eigenvalues

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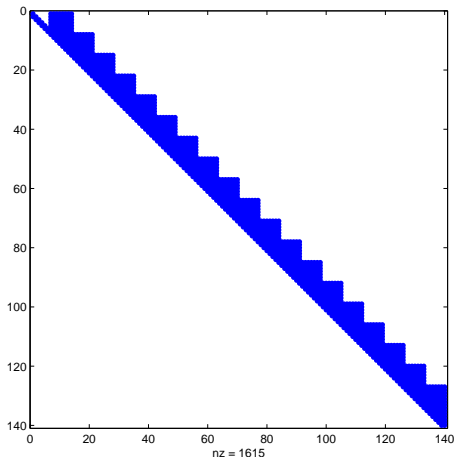
As $D(\mathbf{Y}_n^\circ \mathbf{G}_n)$ is of ORTHORES-type, Hessenberg, and block tridiagonal with blocks of size $s \times s$, and as $D(\mathbf{Y}_n \mathbf{D}_\omega \mathbf{G}_n)$ is block-diagonal upper triangular with blocks of size $s \times s$, the resulting matrix

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

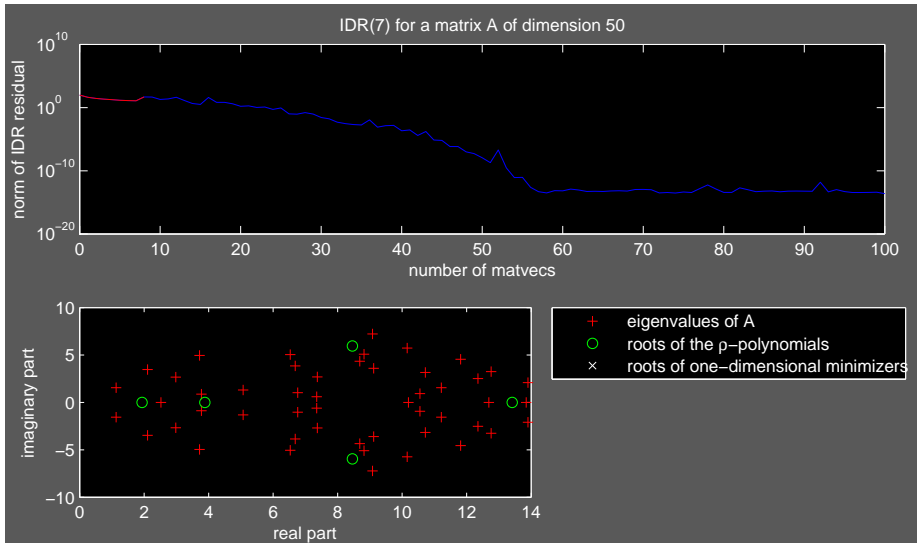
is the matrix of the ORTHORES-form of the underlying two-sided Lanczos' process with s left and one right starting vectors.

IDR for eigenvalues

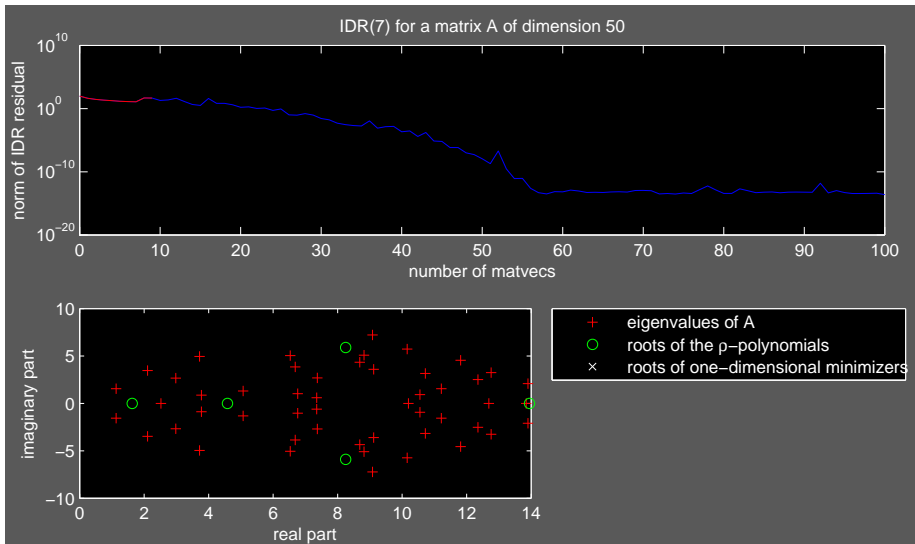
The following picture shows the structure of the resulting matrix \mathbf{P}_n° of the deflated purified process for IDR(7) applied for 160 steps.



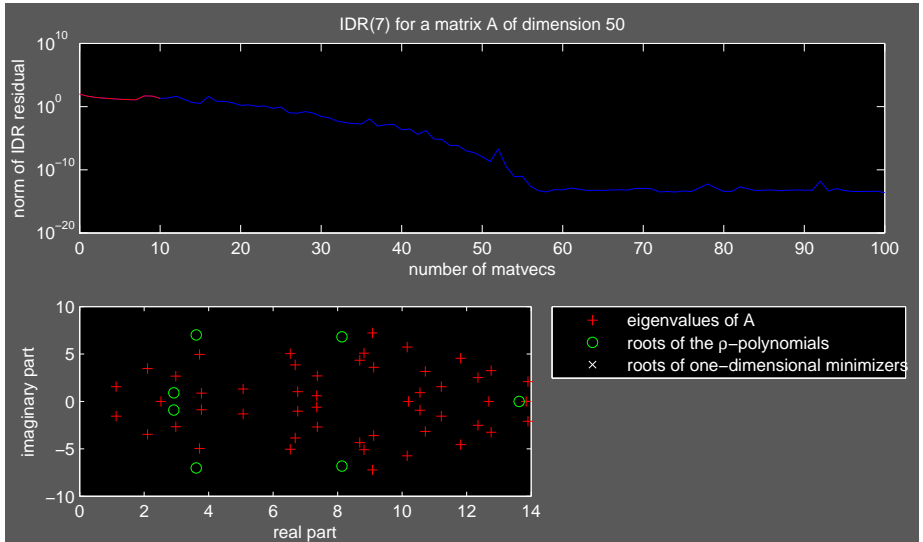
One run of IDR(7)



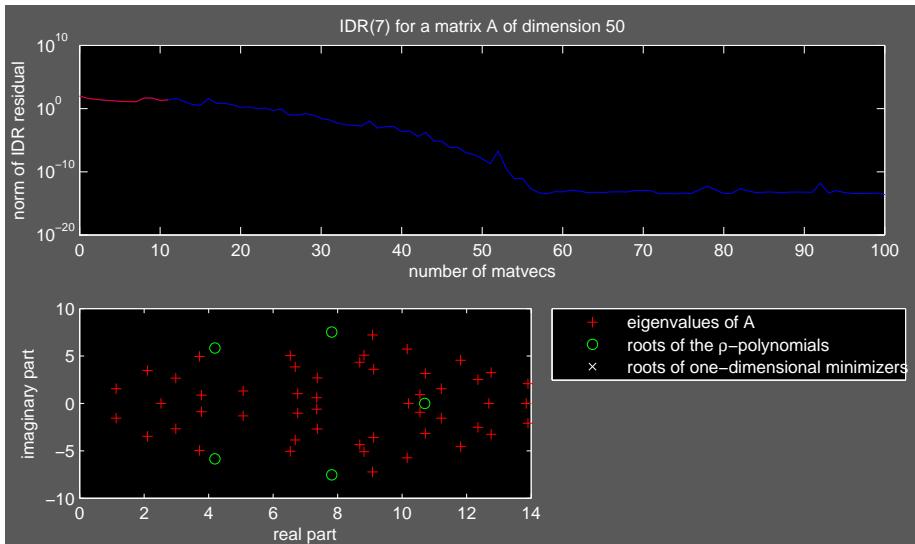
One run of IDR(7)



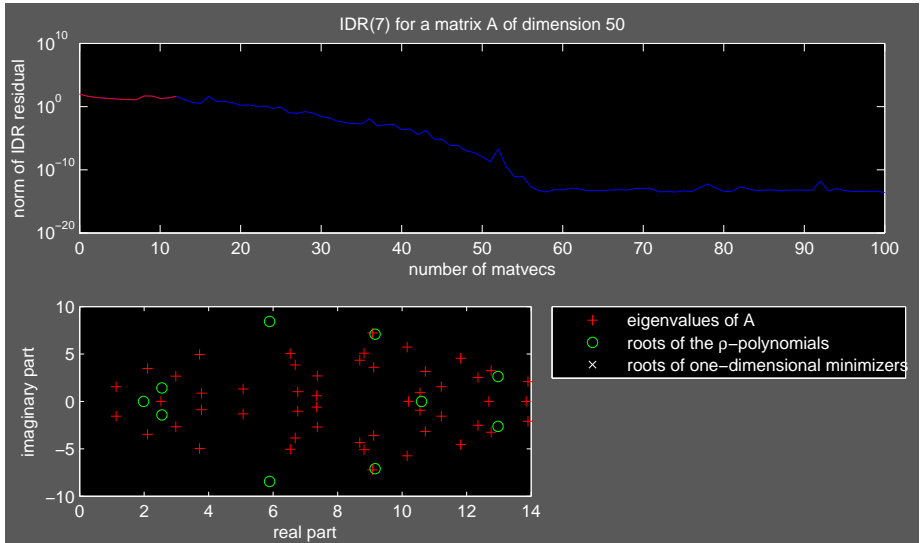
One run of IDR(7)



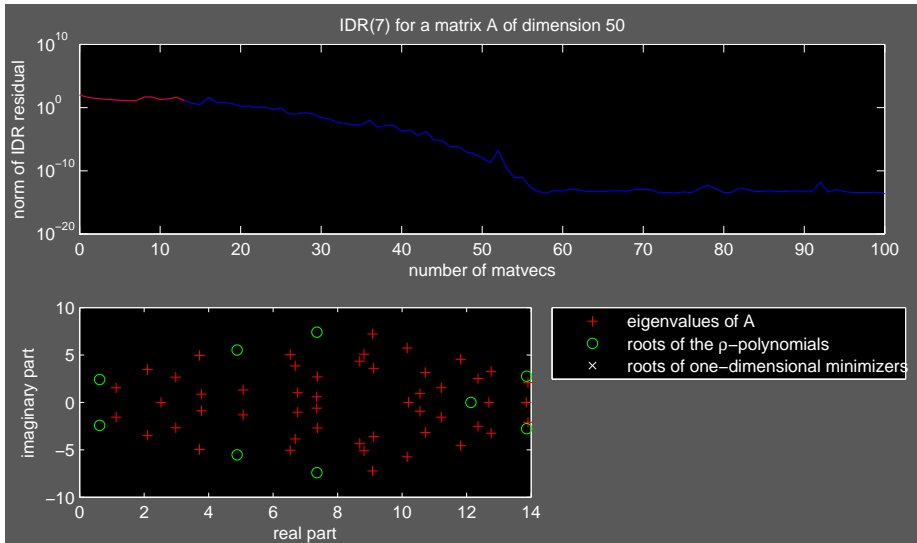
One run of IDR(7)



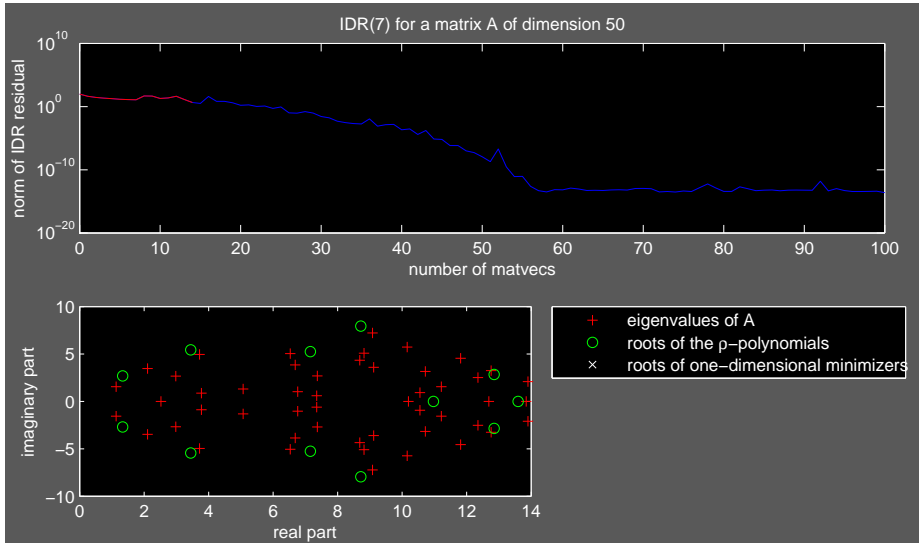
One run of IDR(7)



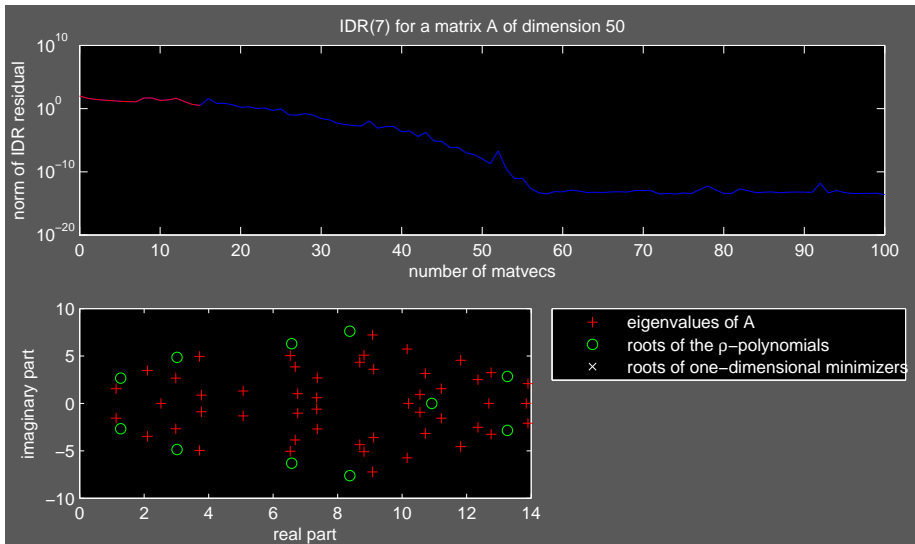
One run of IDR(7)



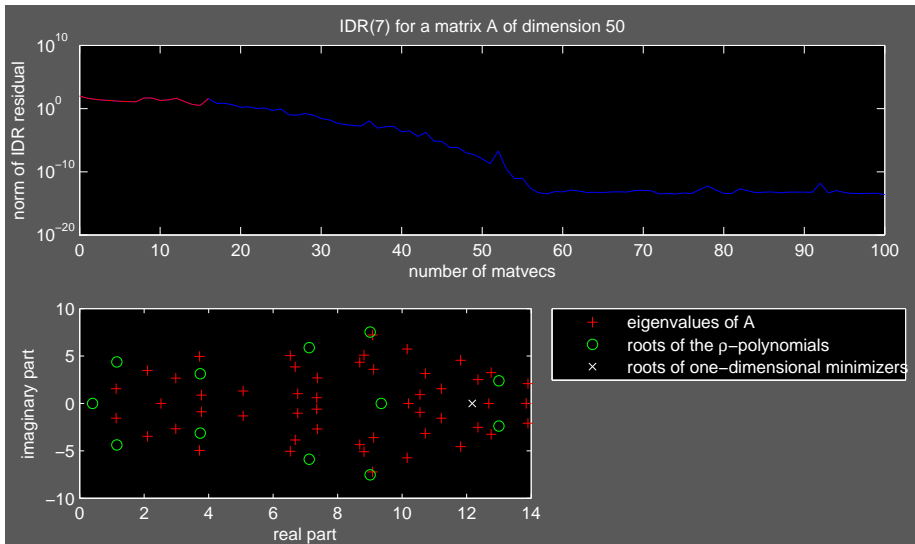
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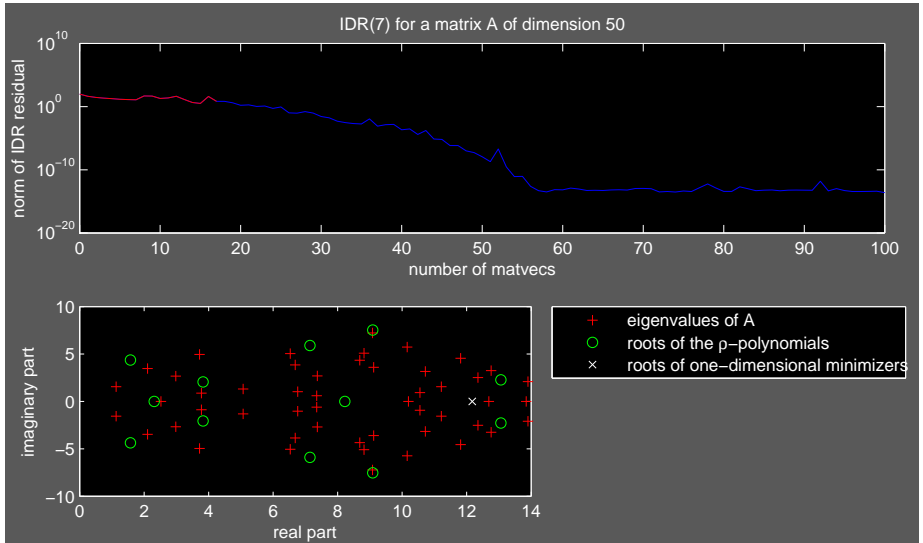
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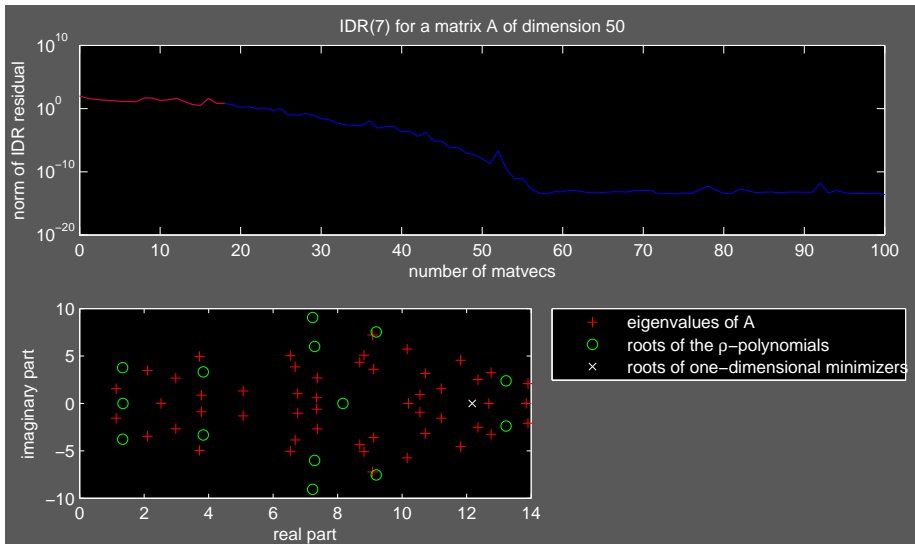
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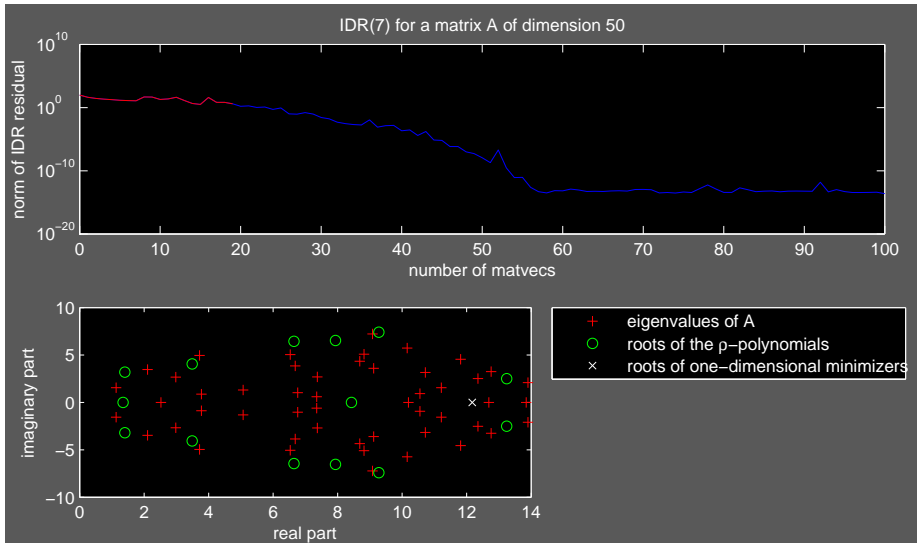
One run of IDR(7)



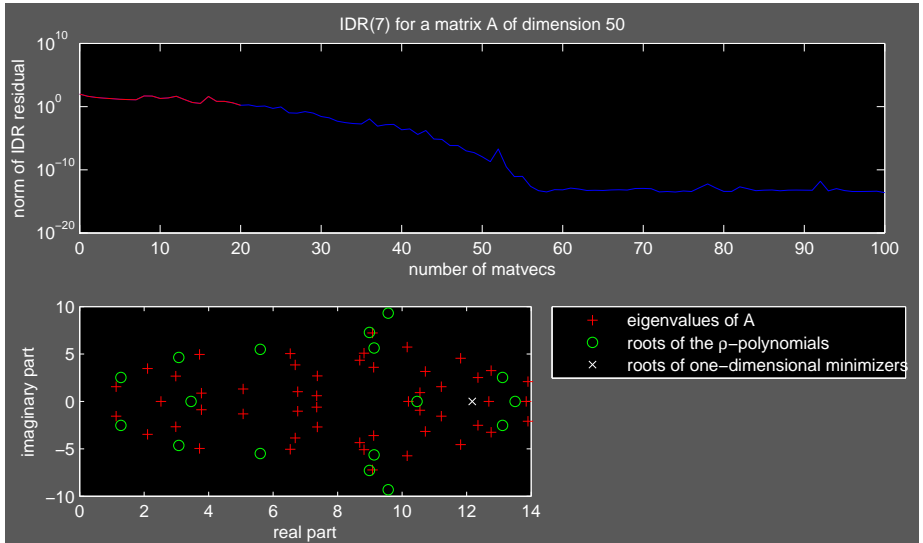
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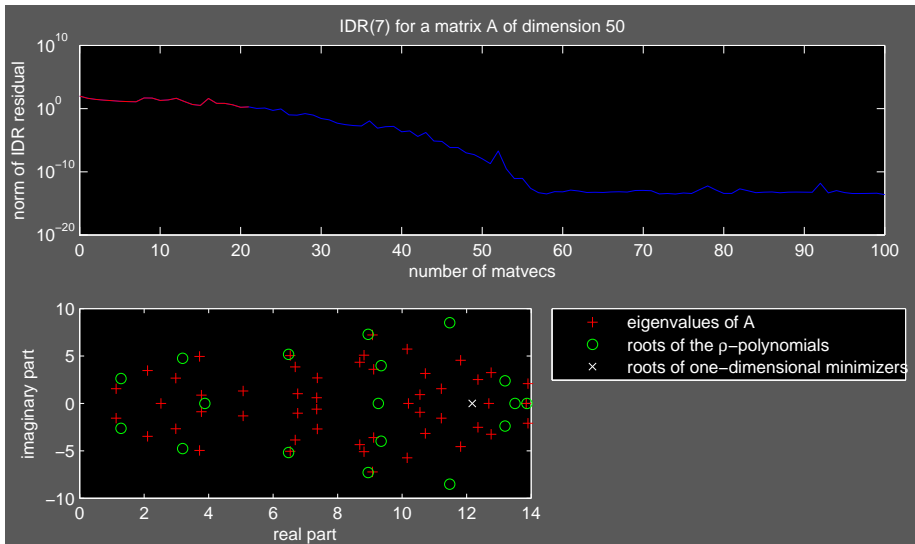
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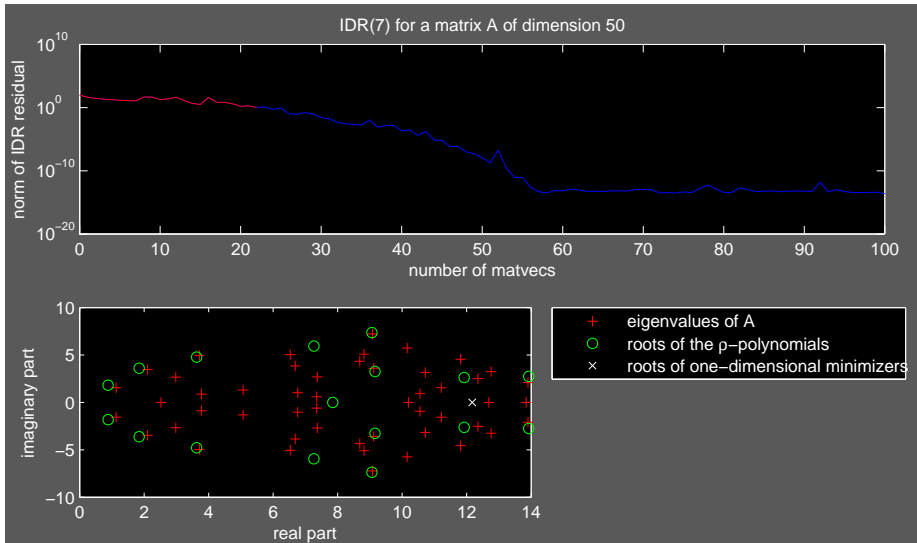
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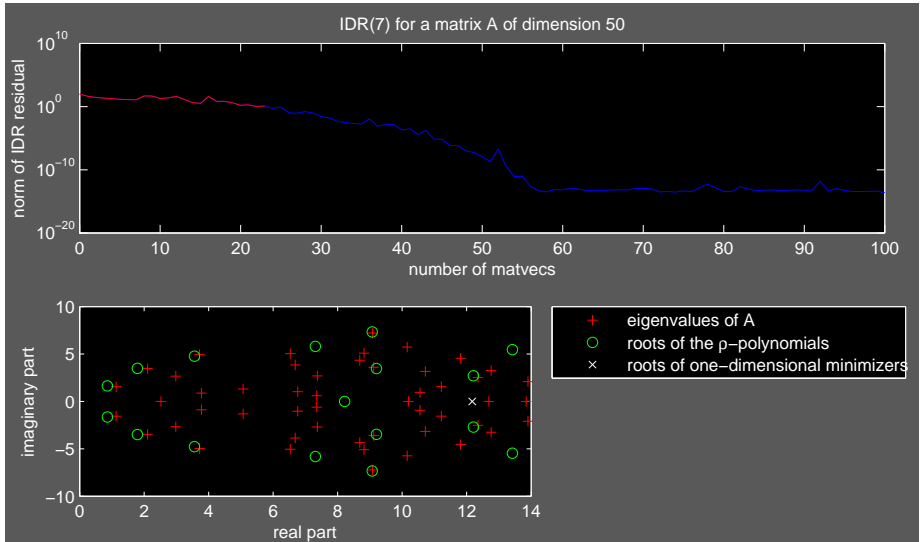
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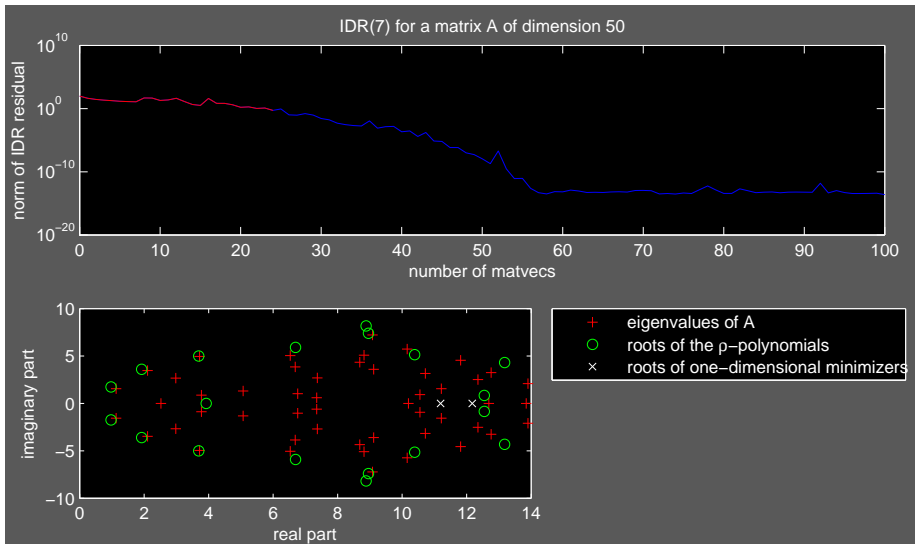
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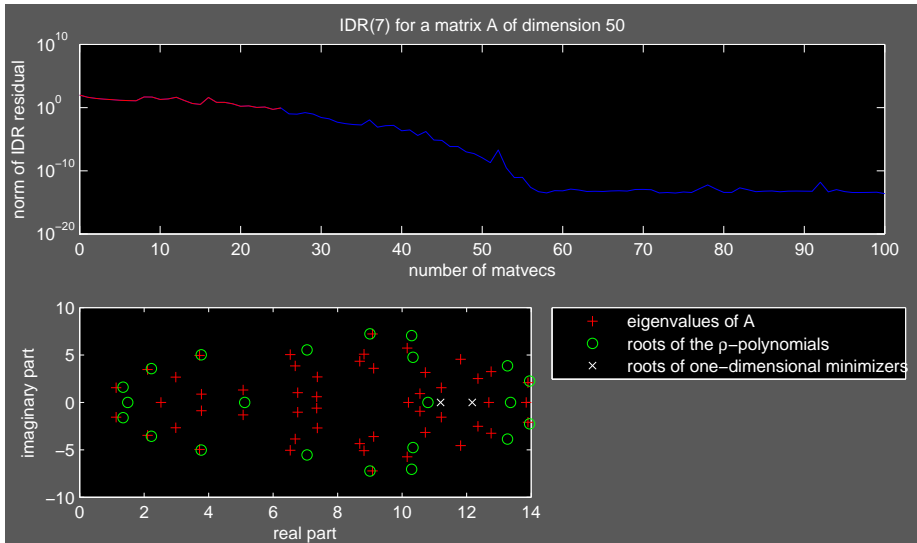
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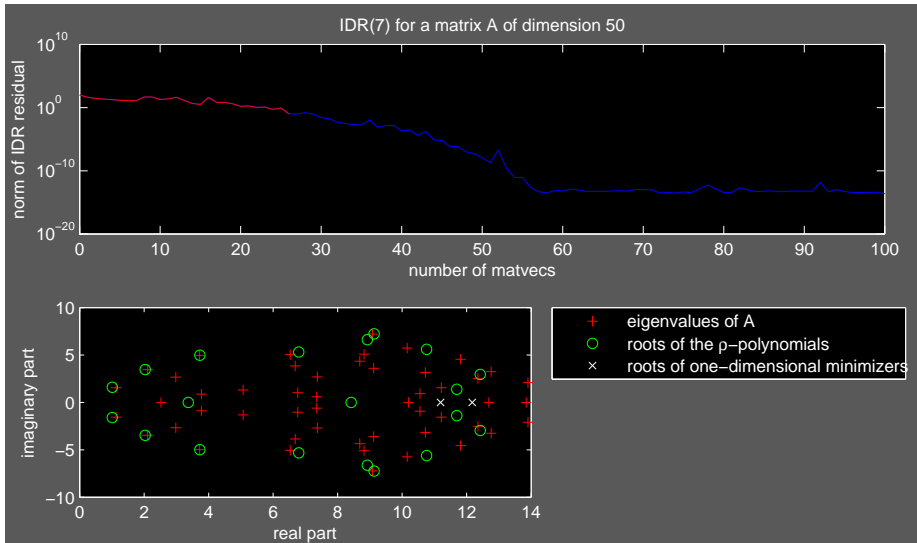
One run of IDR(7)



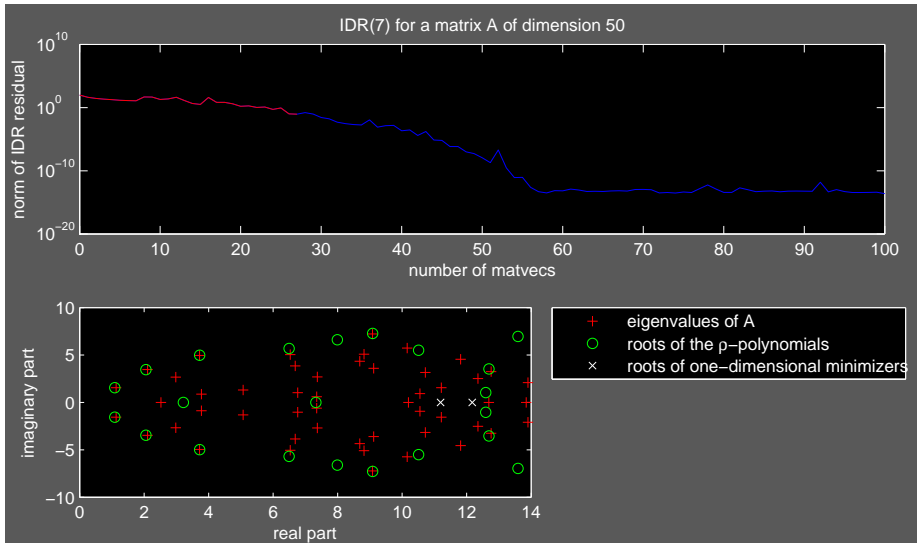
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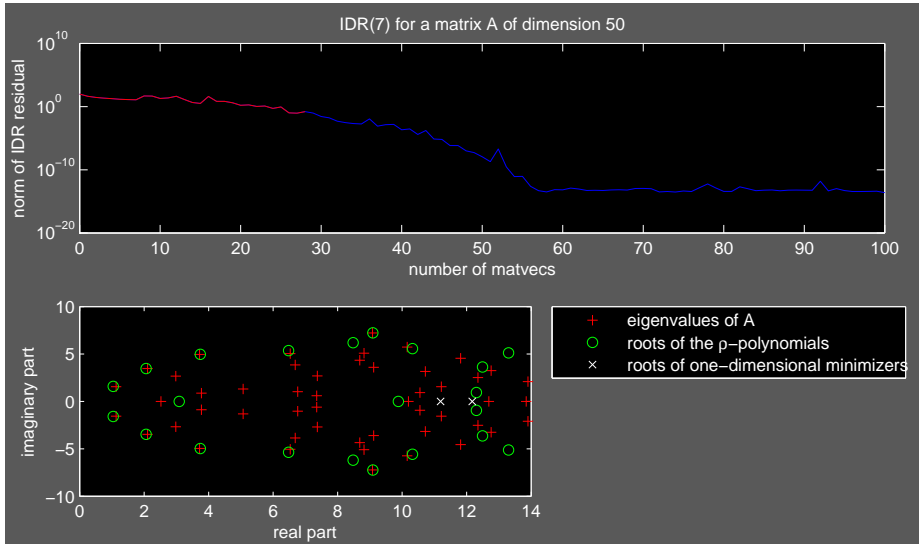
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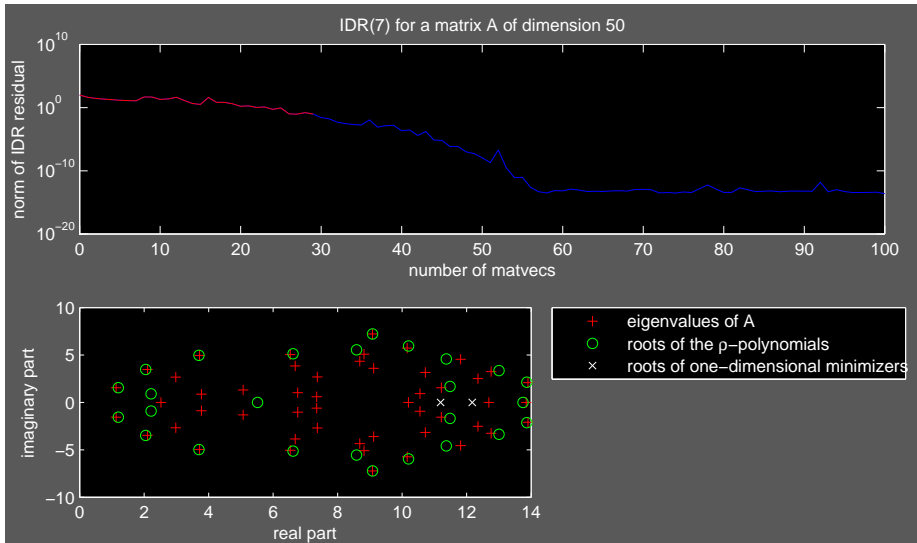
One run of IDR(7)



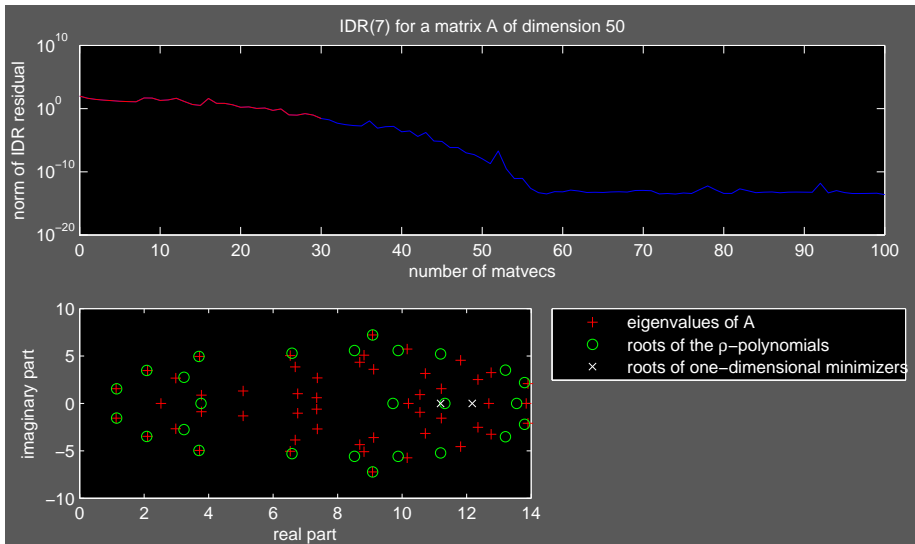
One run of IDR(7)



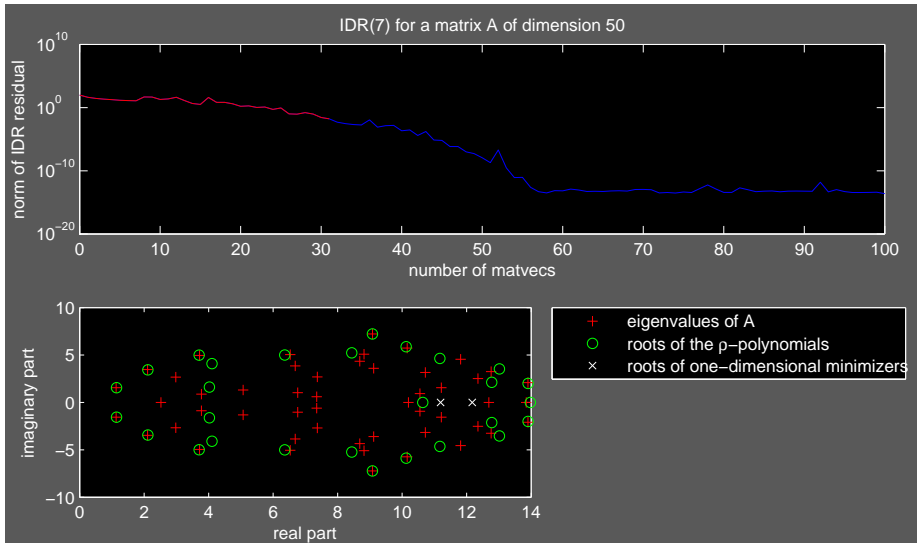
One run of IDR(7)



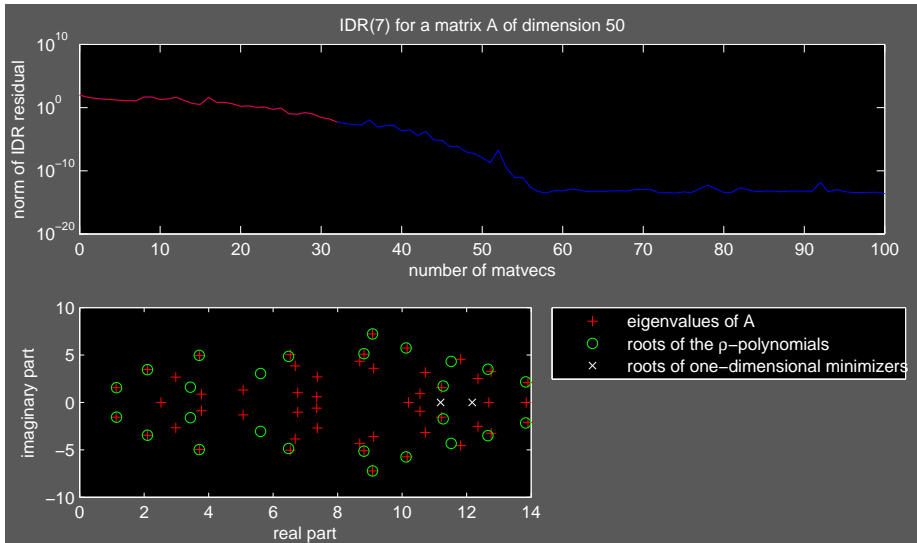
One run of IDR(7)



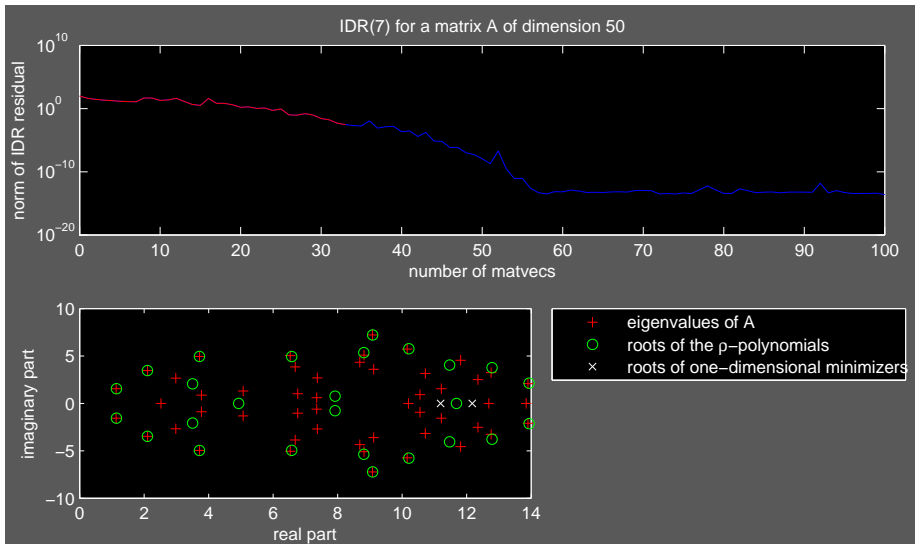
One run of IDR(7)



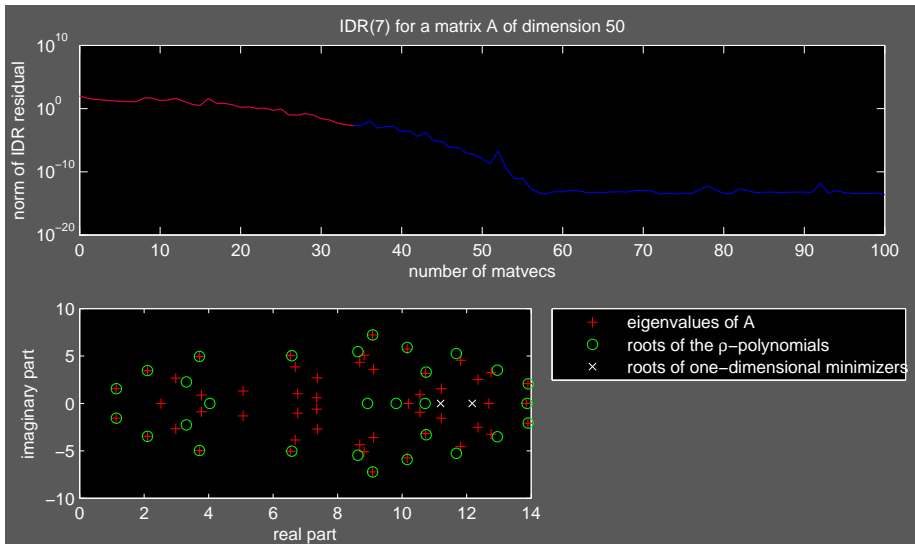
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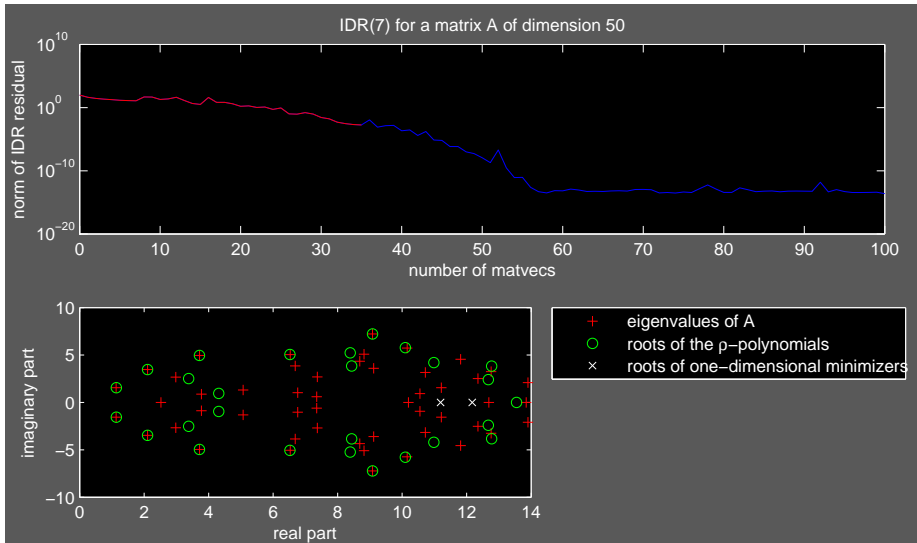
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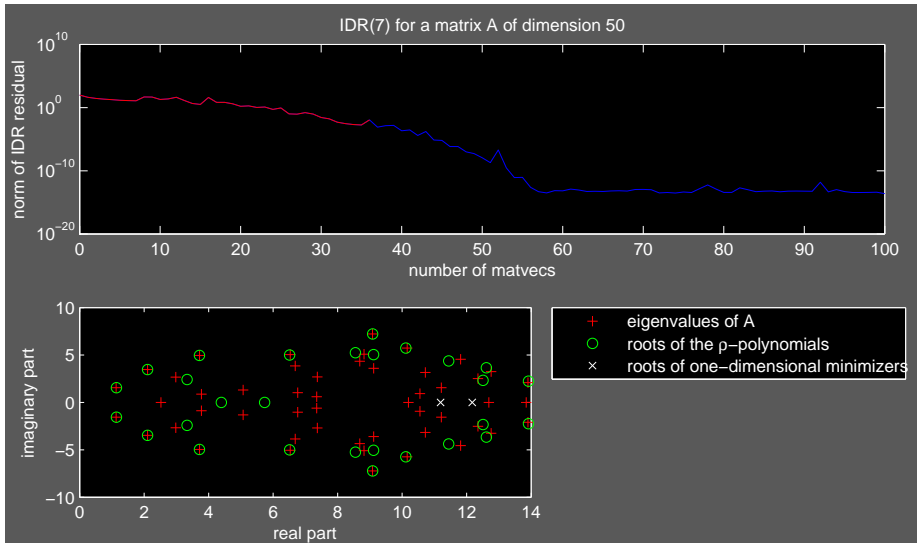
One run of IDR(7)



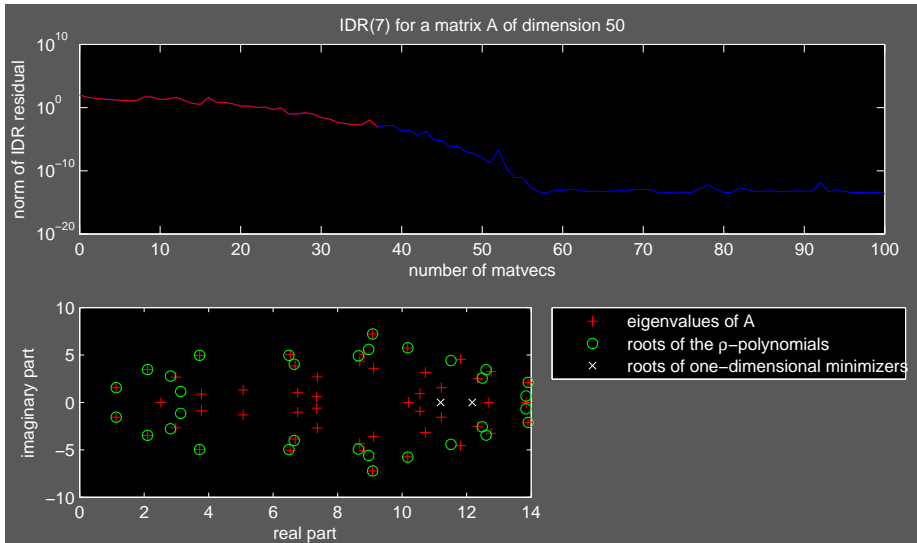
One run of IDR(7)



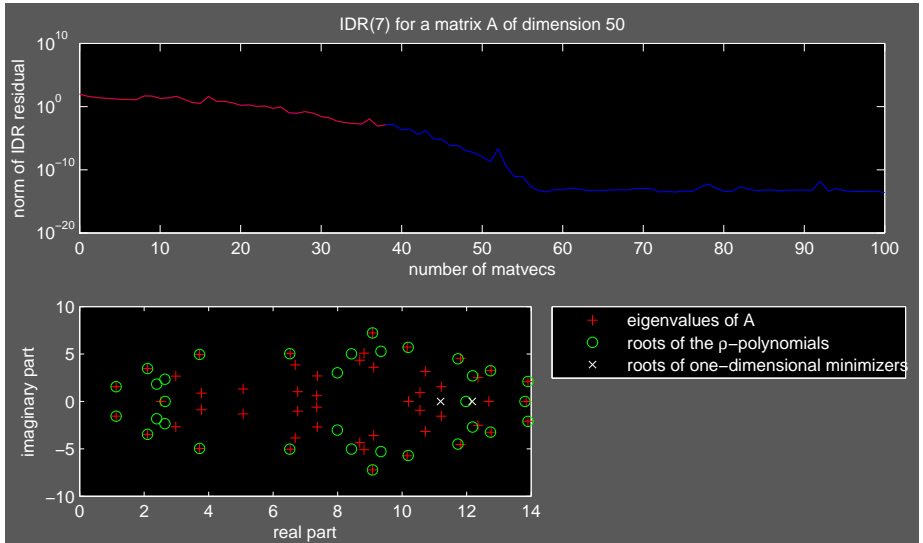
One run of IDR(7)



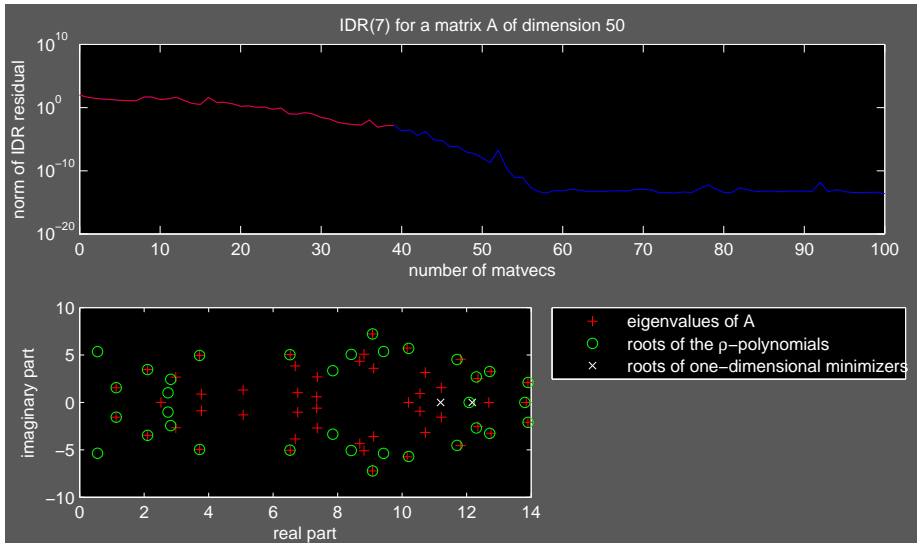
One run of IDR(7)



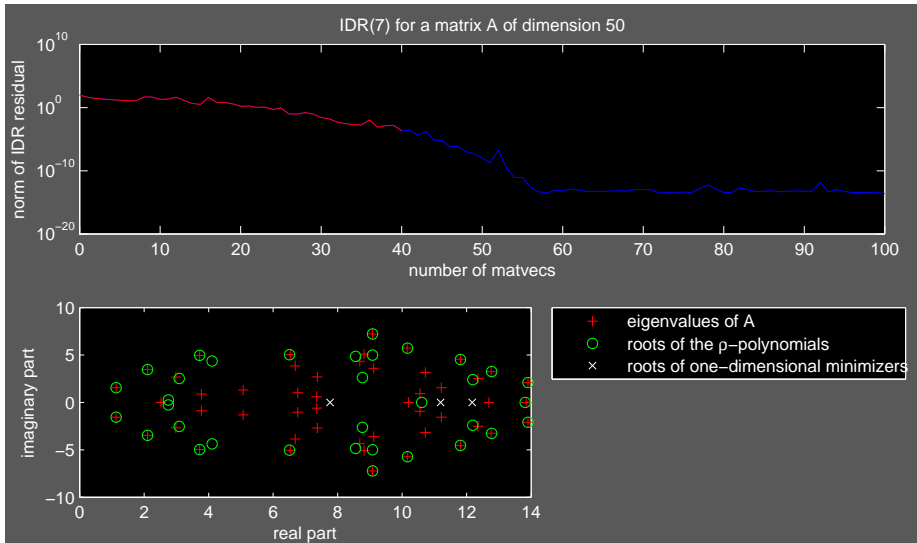
One run of IDR(7)



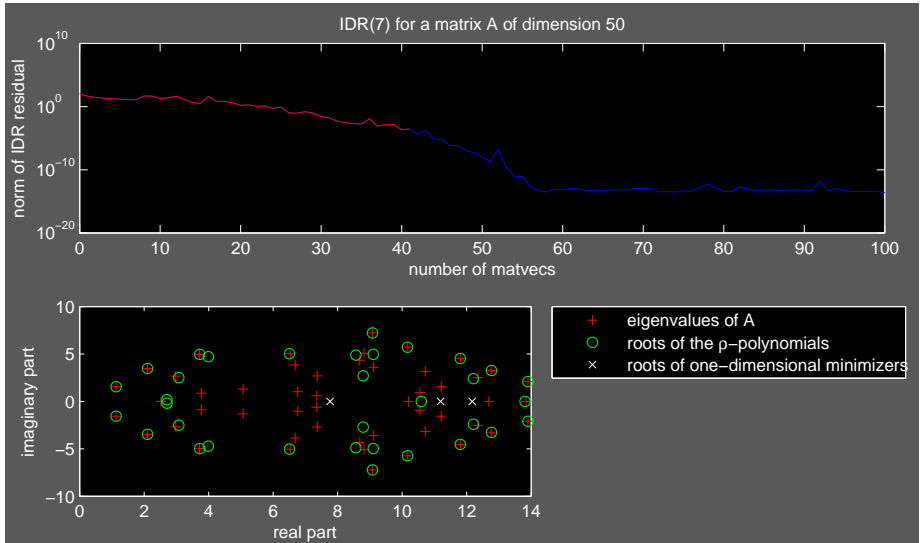
One run of IDR(7)



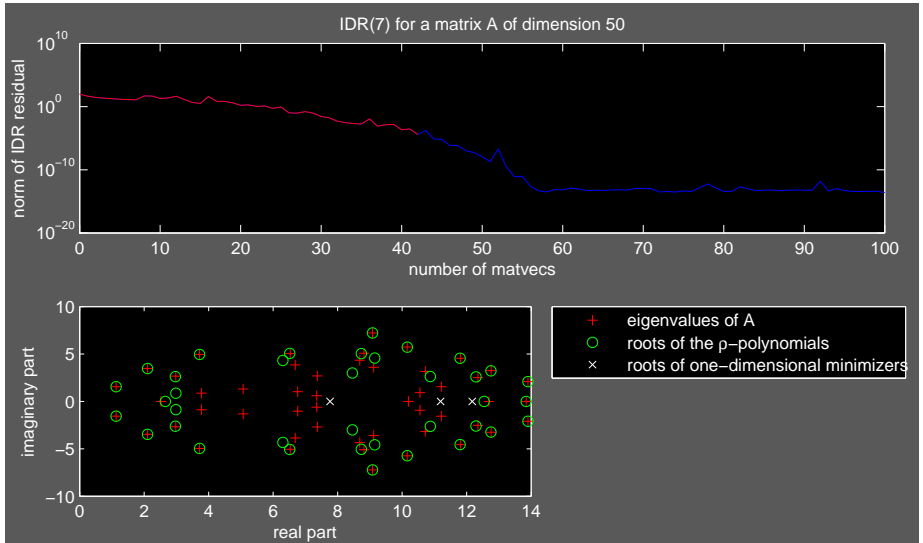
One run of IDR(7)



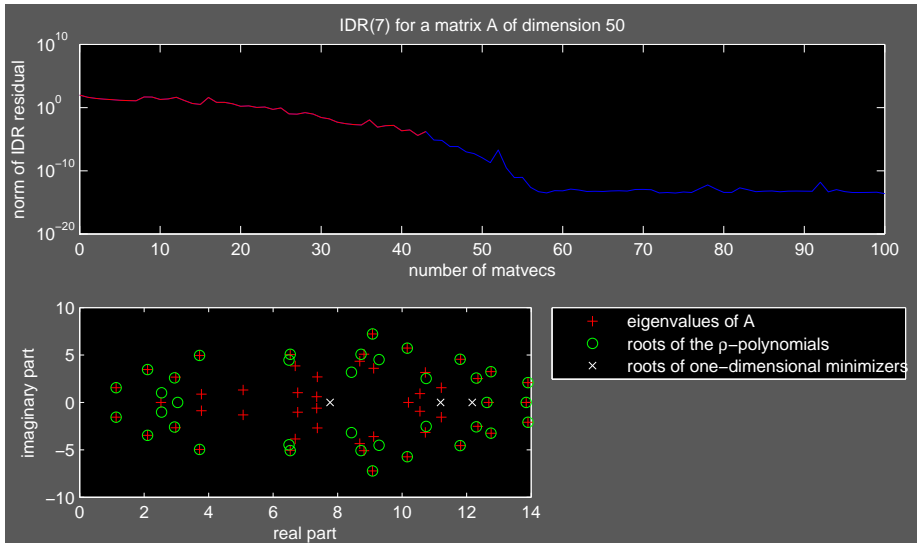
One run of IDR(7)



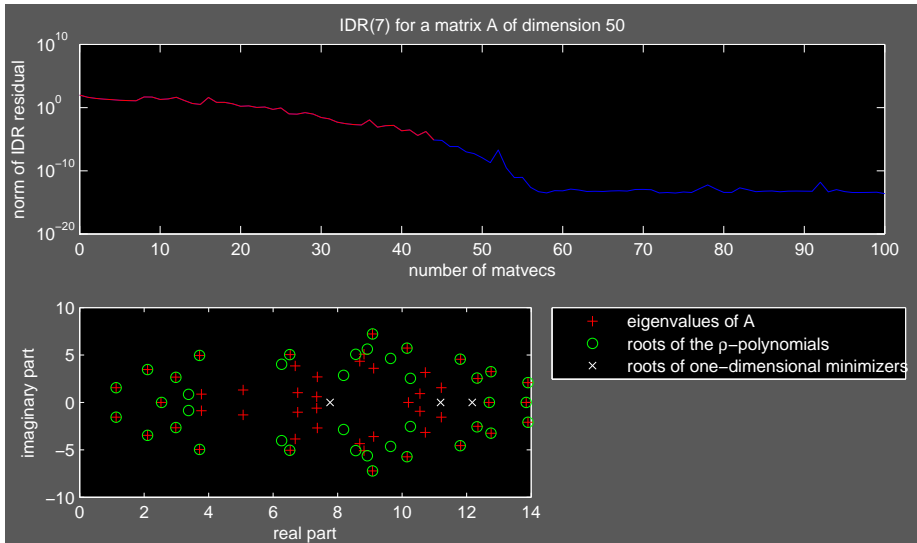
One run of IDR(7)



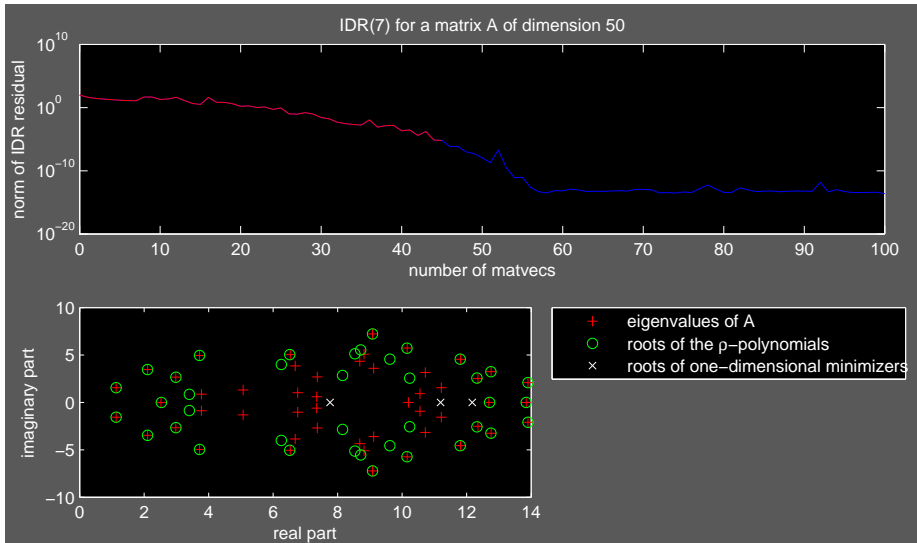
One run of IDR(7)



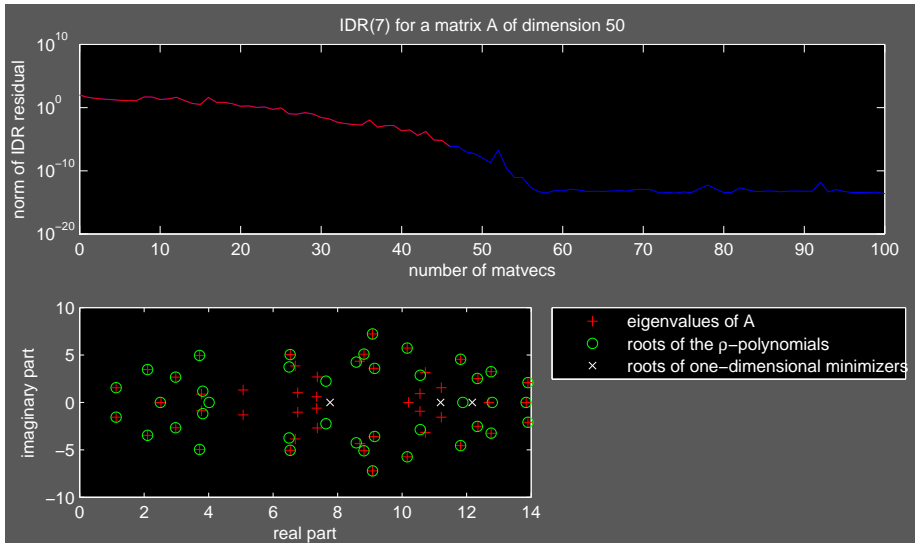
One run of IDR(7)



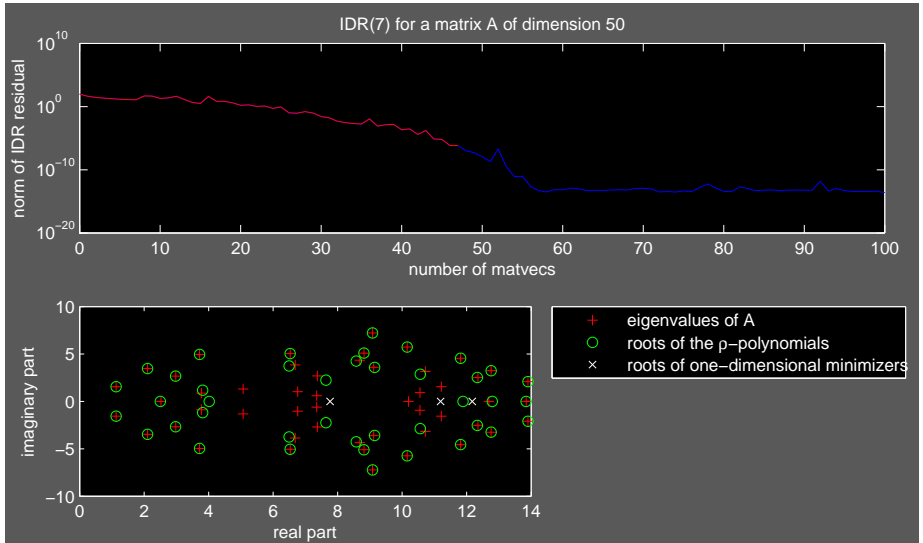
One run of IDR(7)



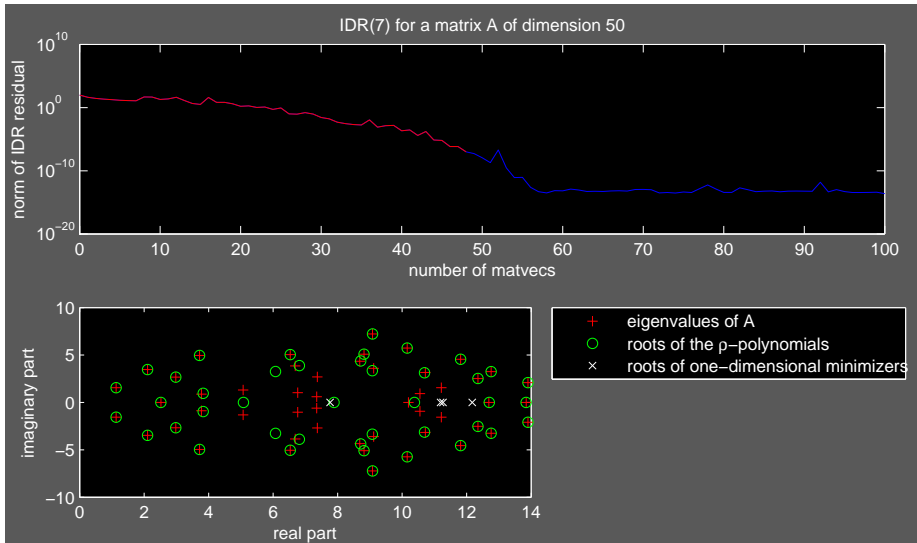
One run of IDR(7)



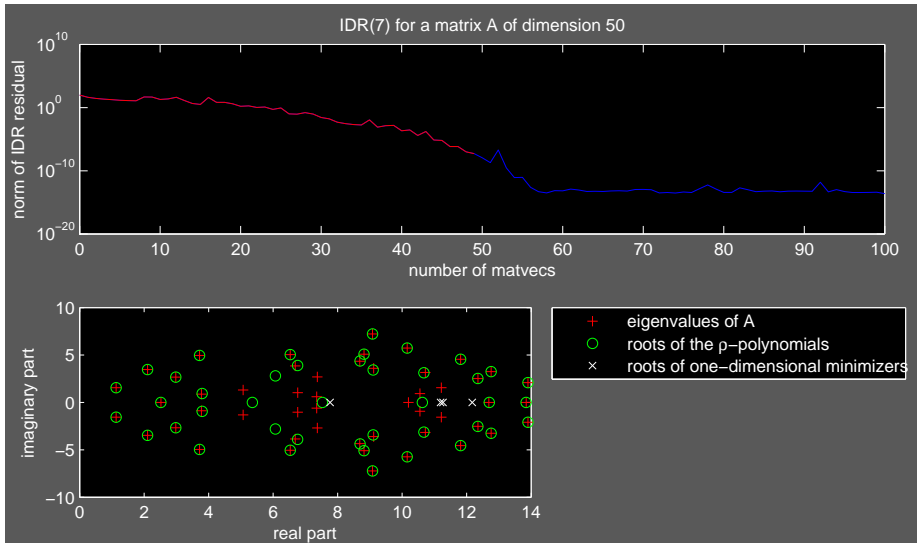
One run of IDR(7)



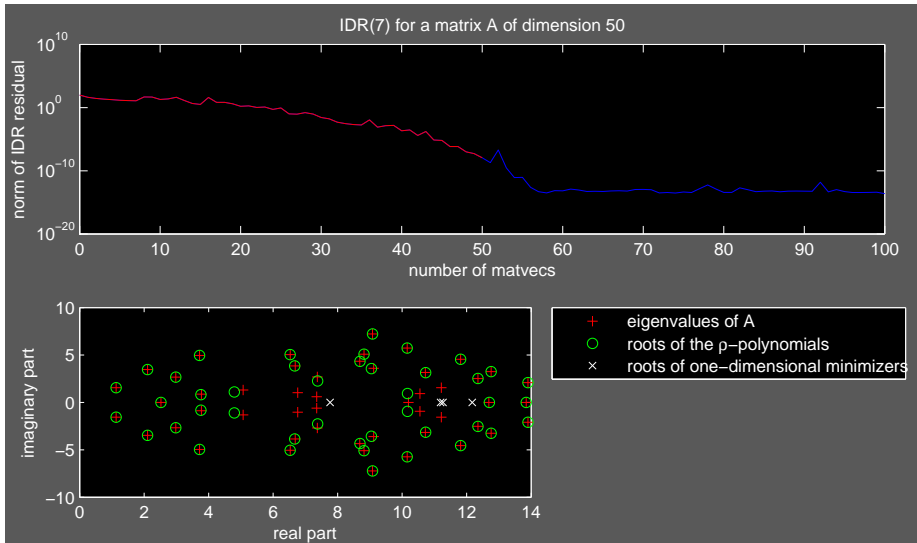
One run of IDR(7)



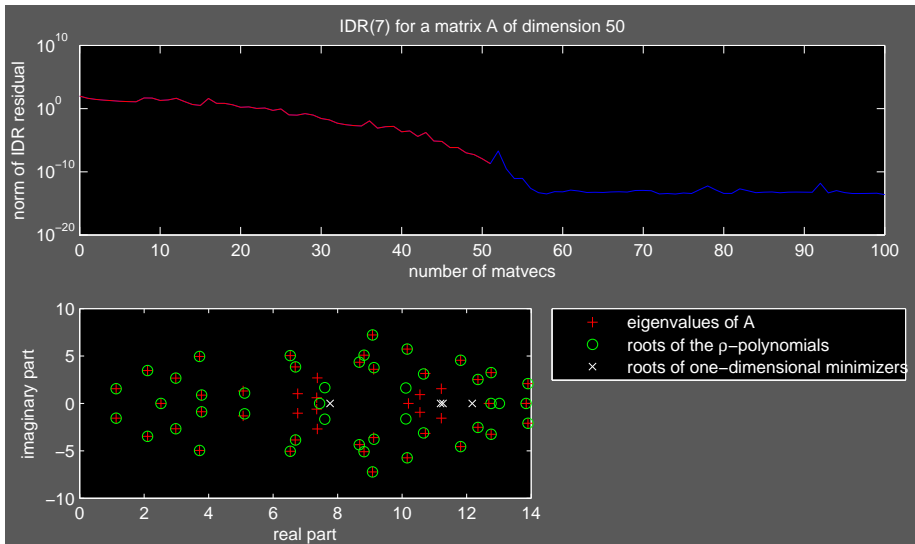
One run of IDR(7)



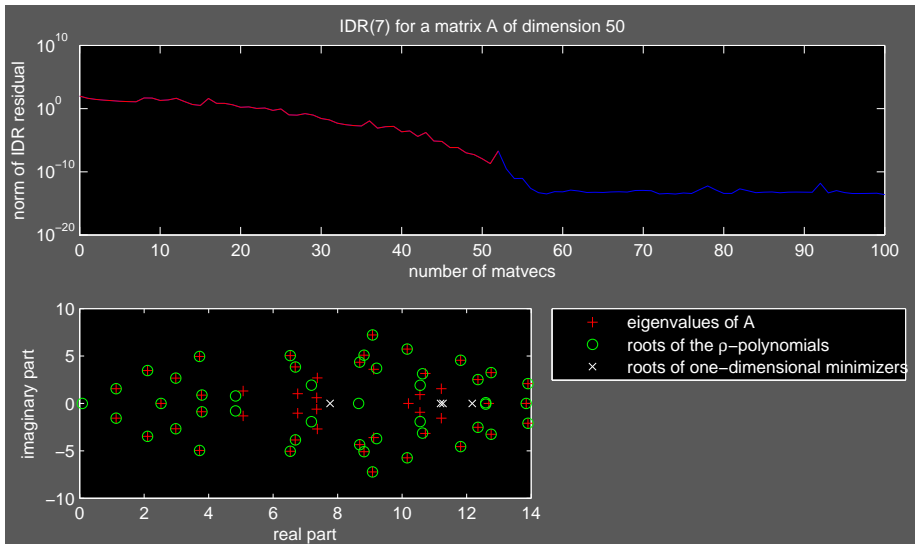
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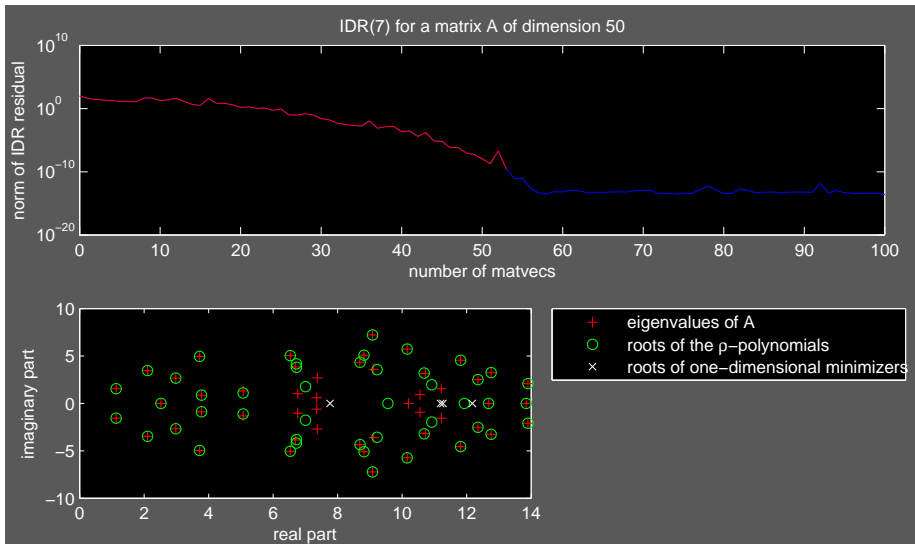
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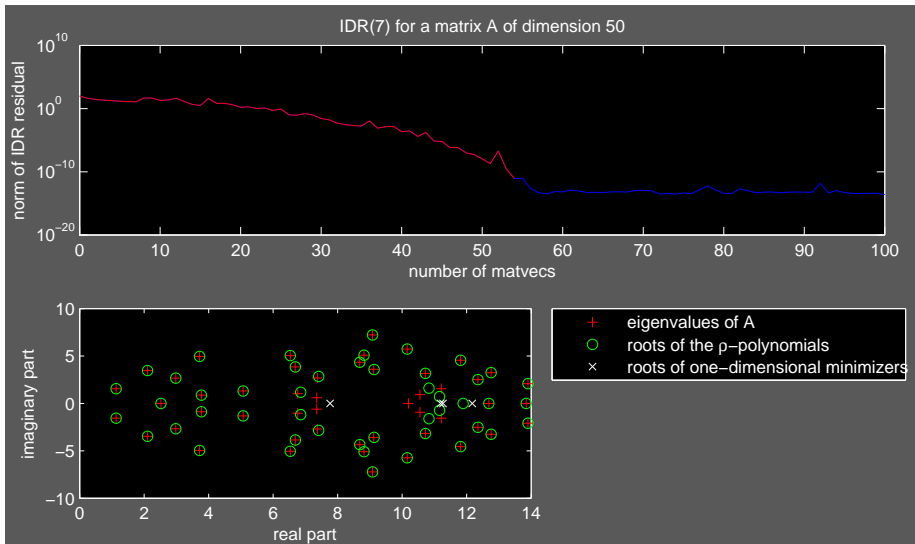
One run of IDR(7)



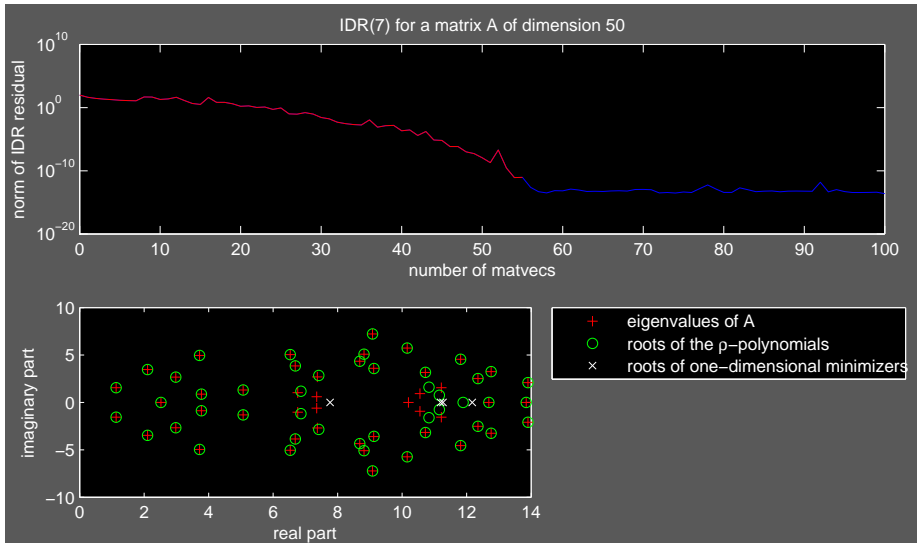
One run of IDR(7)



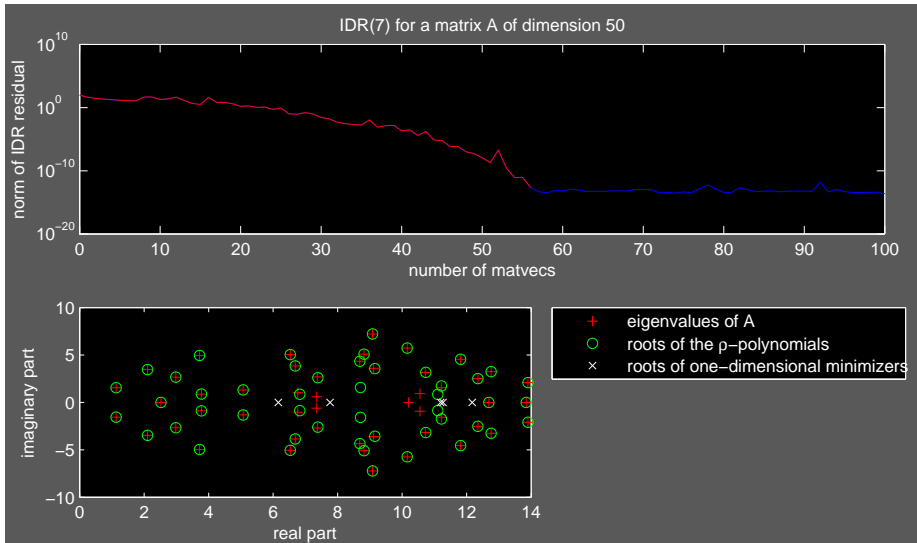
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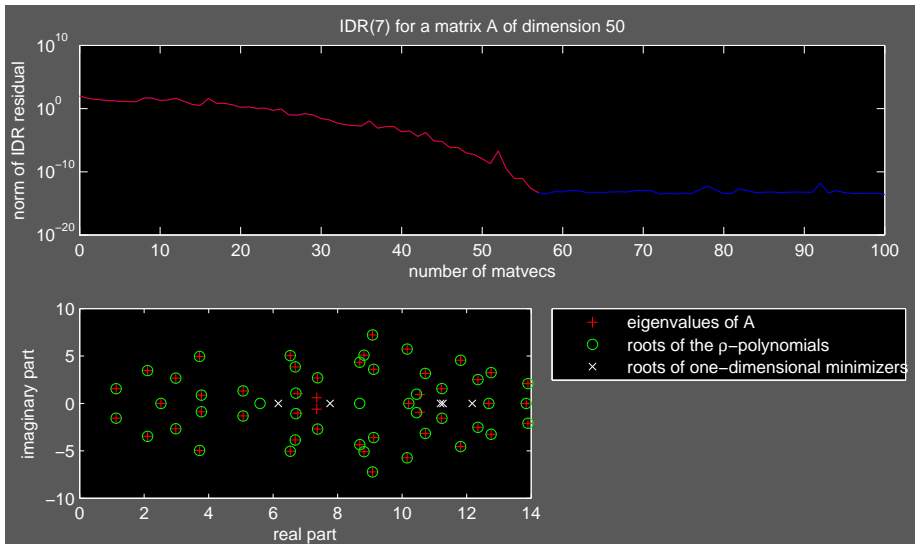
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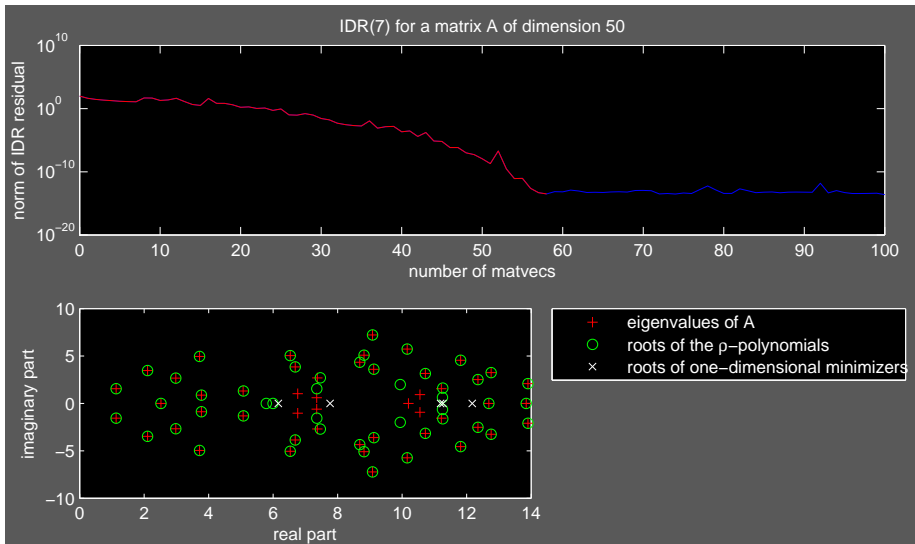
One run of IDR(7)



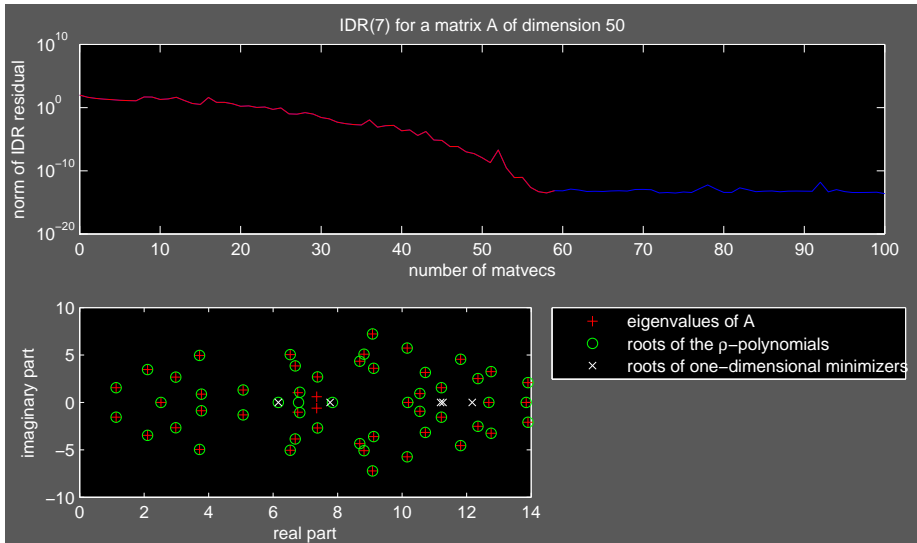
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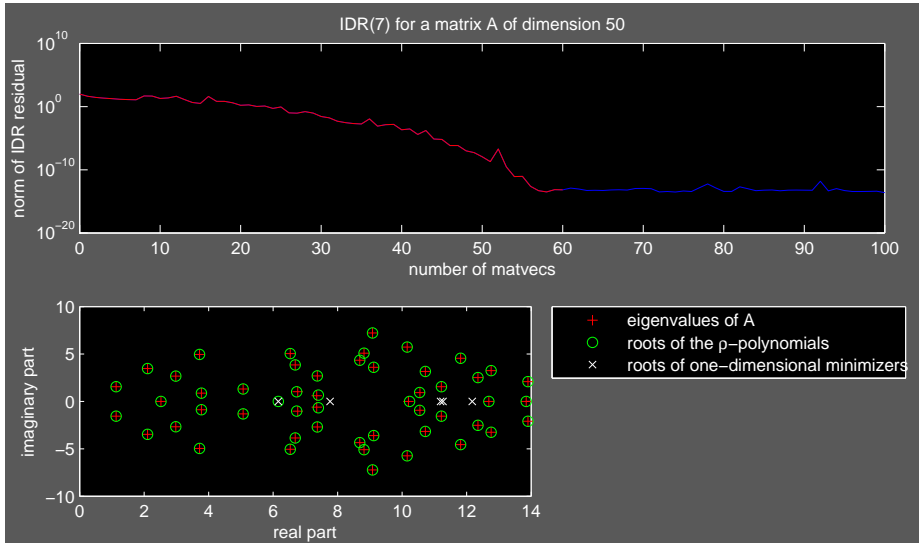
One run of IDR(7)



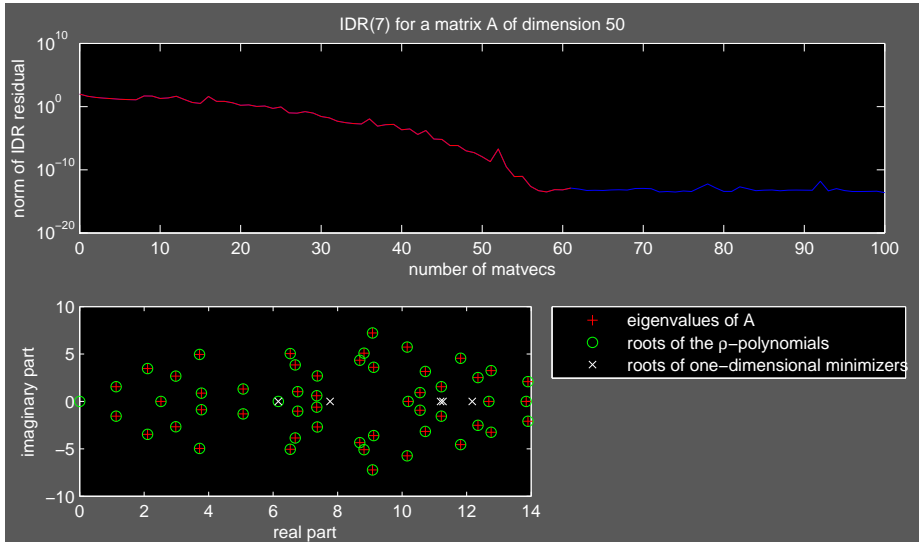
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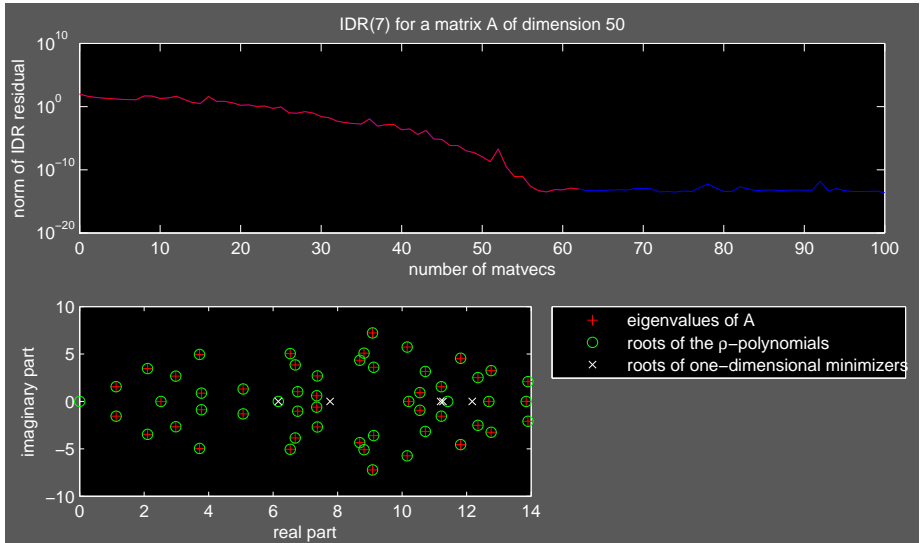
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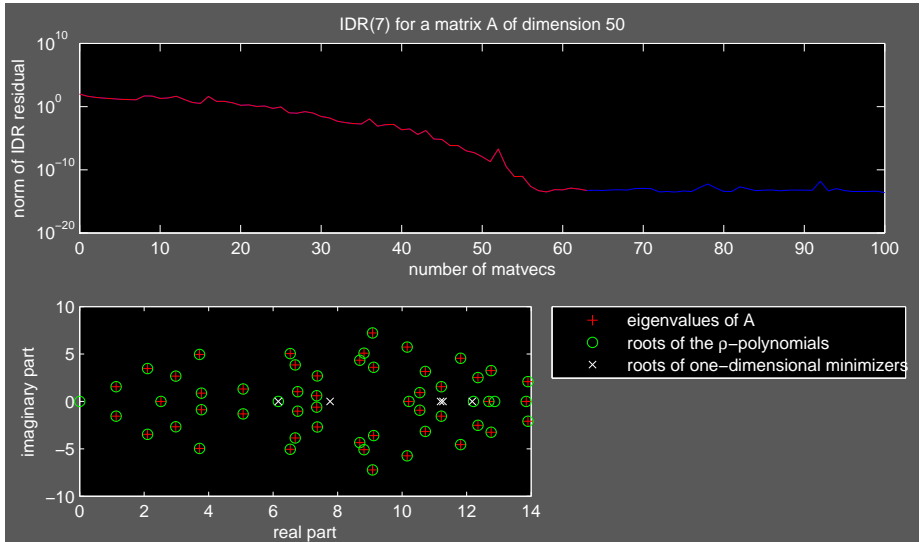
One run of IDR(7)



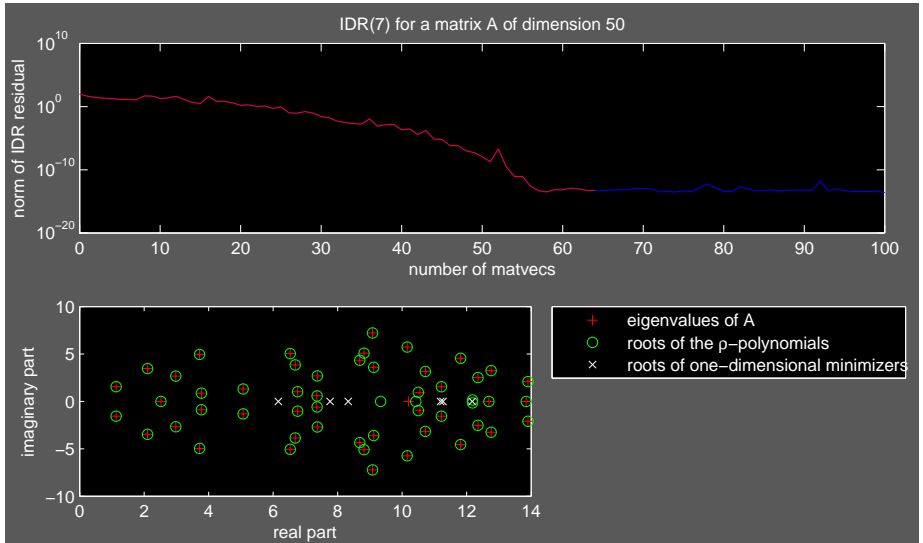
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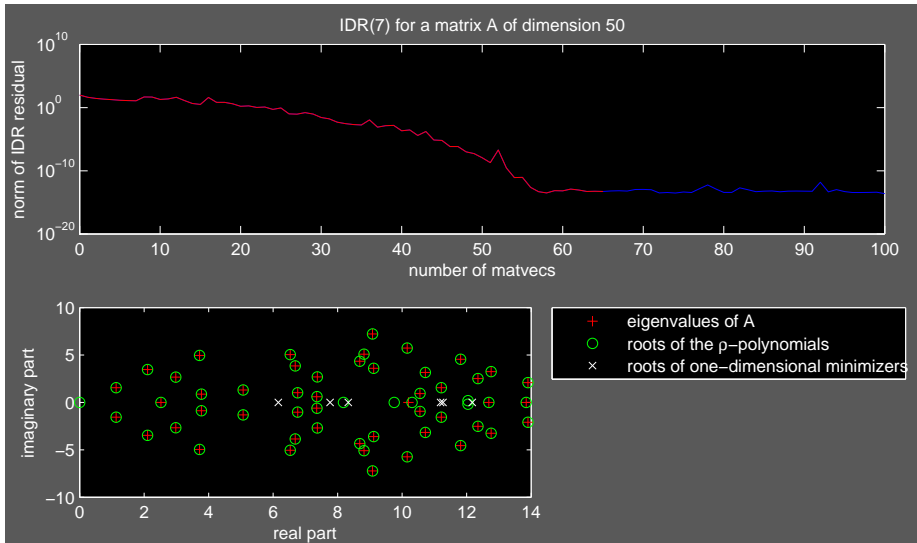
One run of IDR(7)



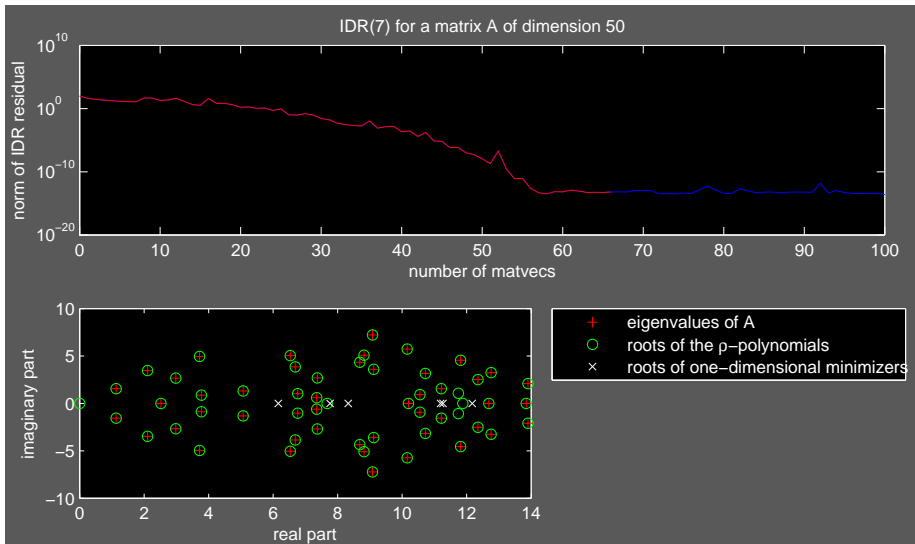
One run of IDR(7)



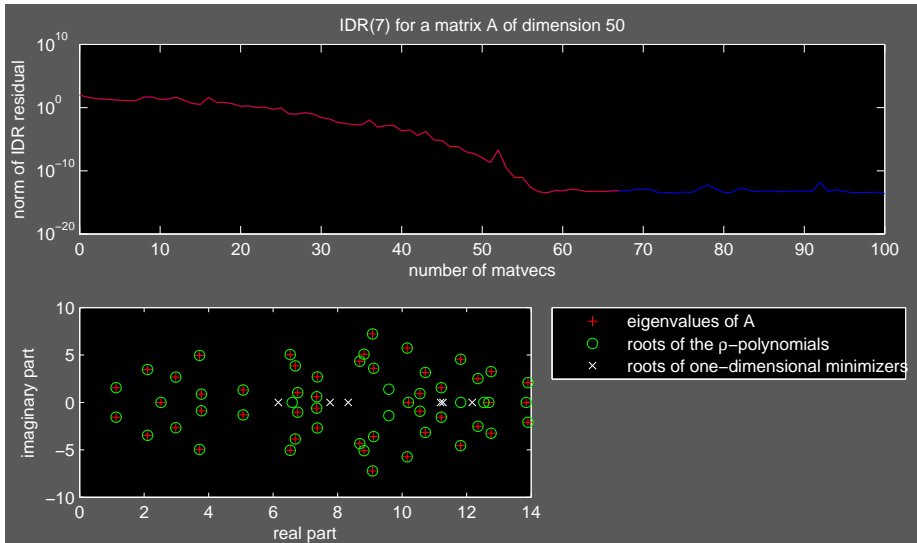
One run of IDR(7)



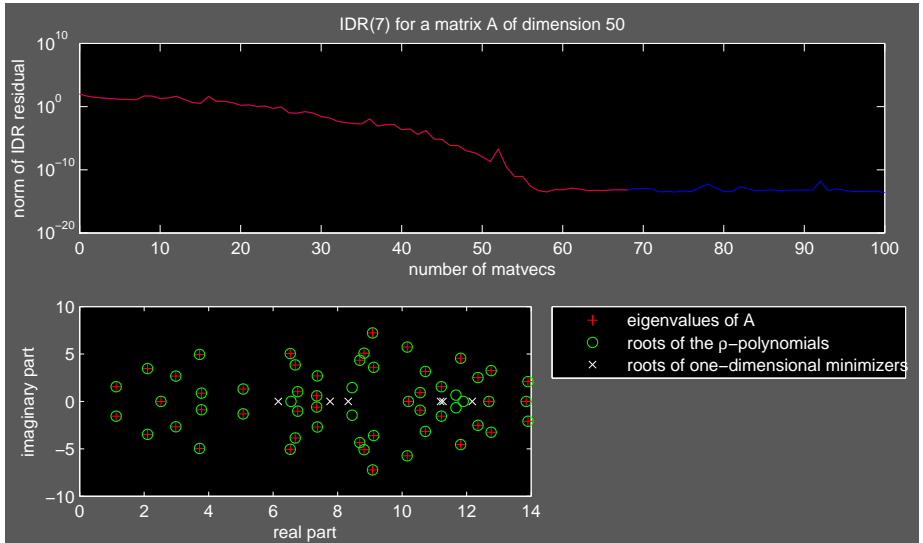
One run of IDR(7)



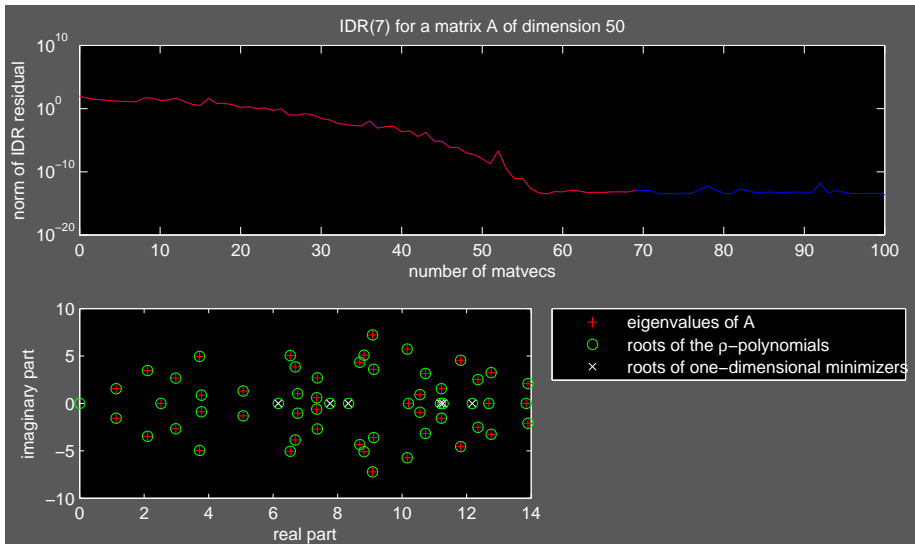
One run of IDR(7)



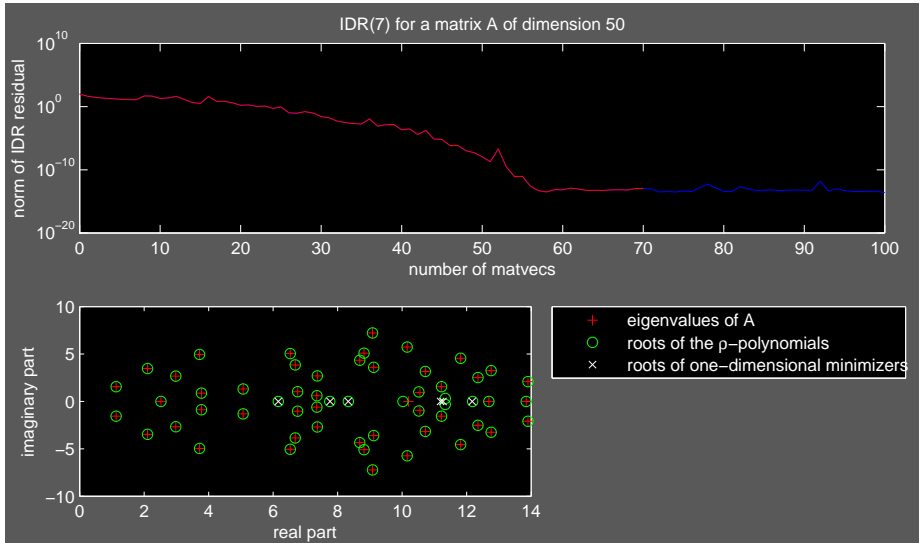
One run of IDR(7)



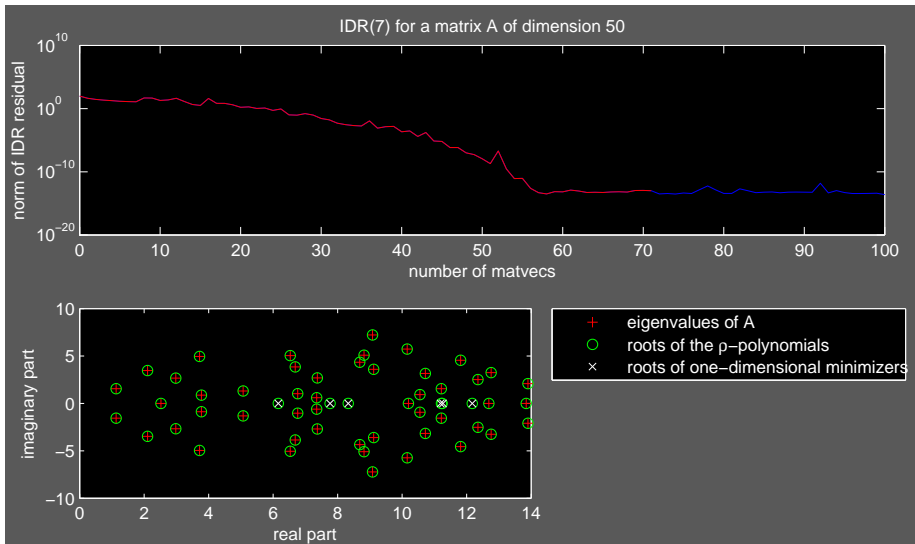
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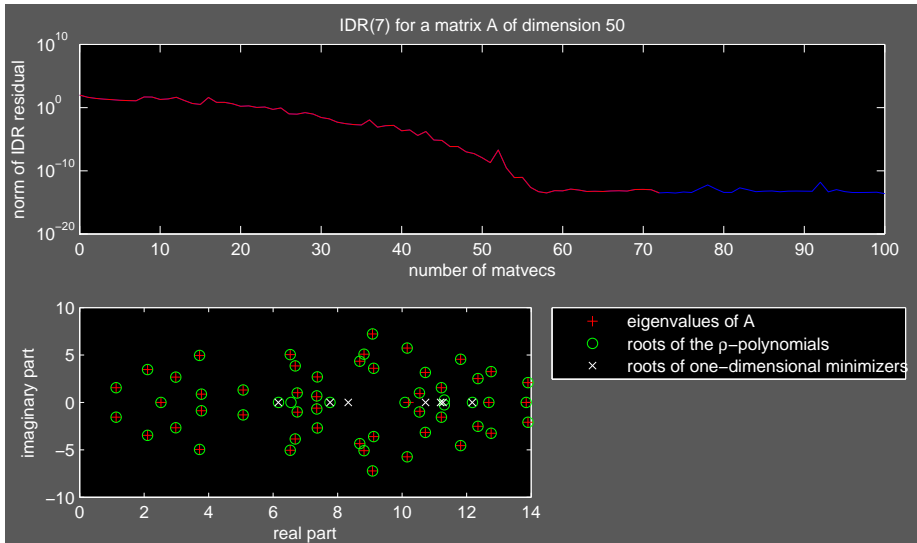
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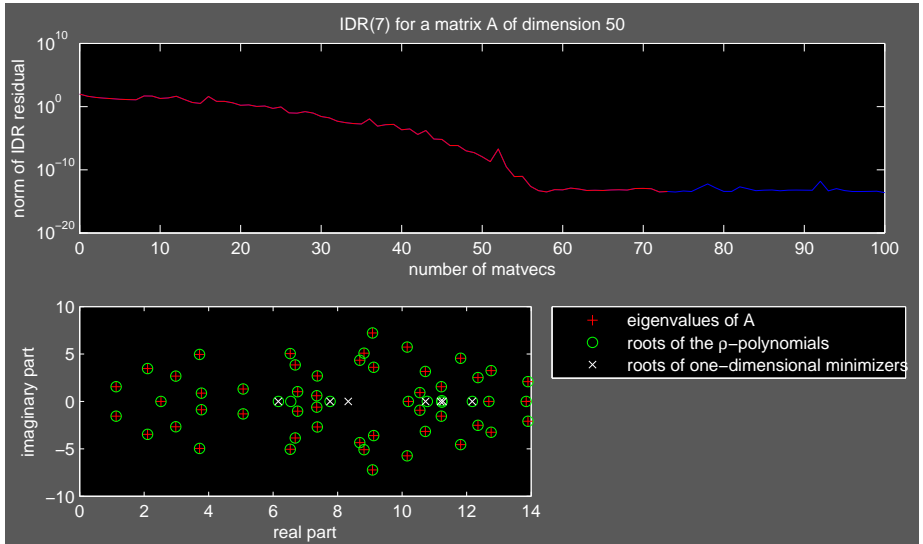
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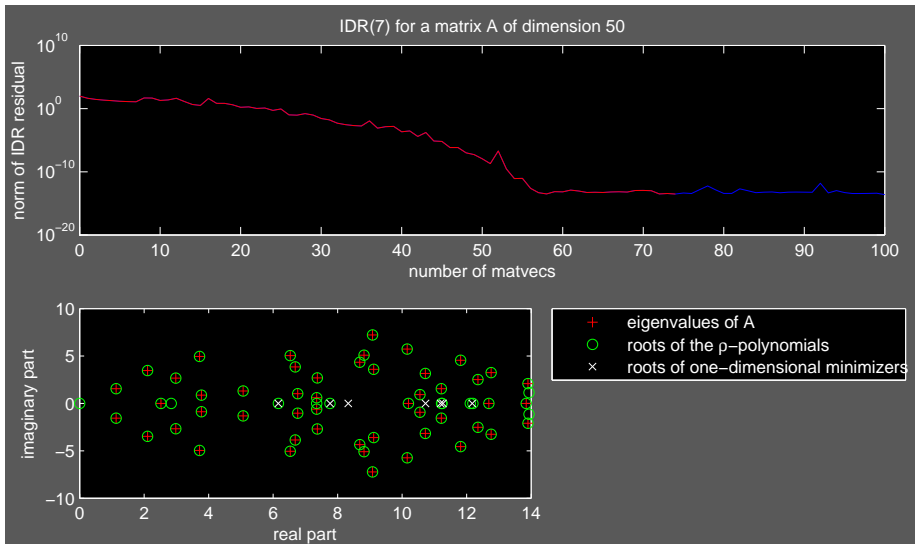
One run of IDR(7)



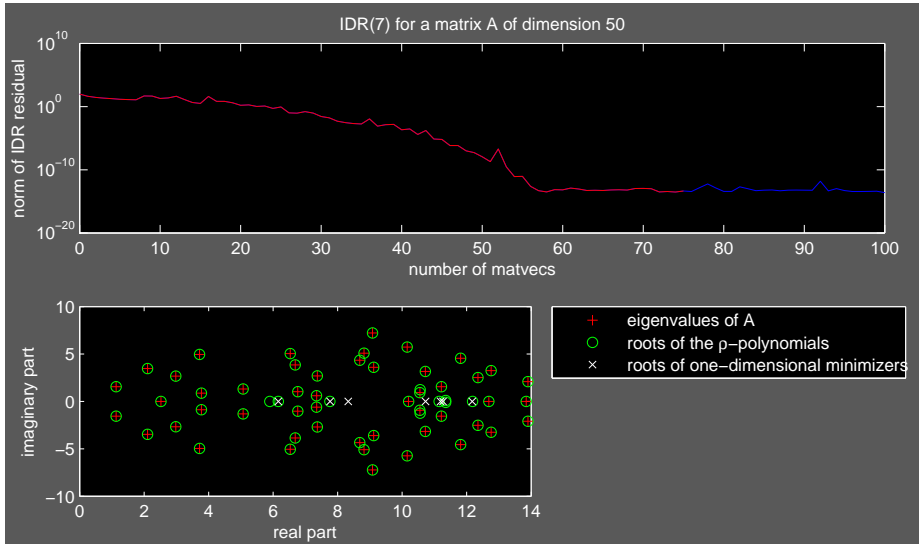
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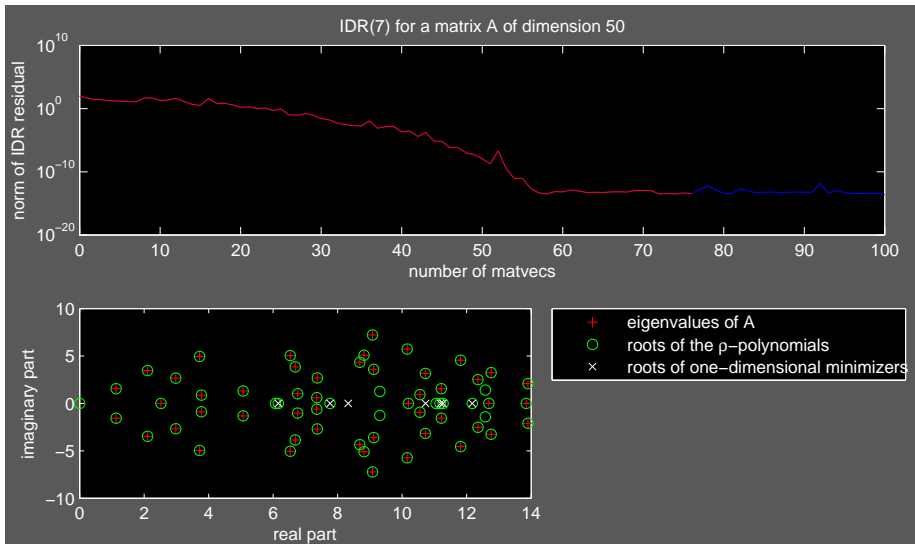
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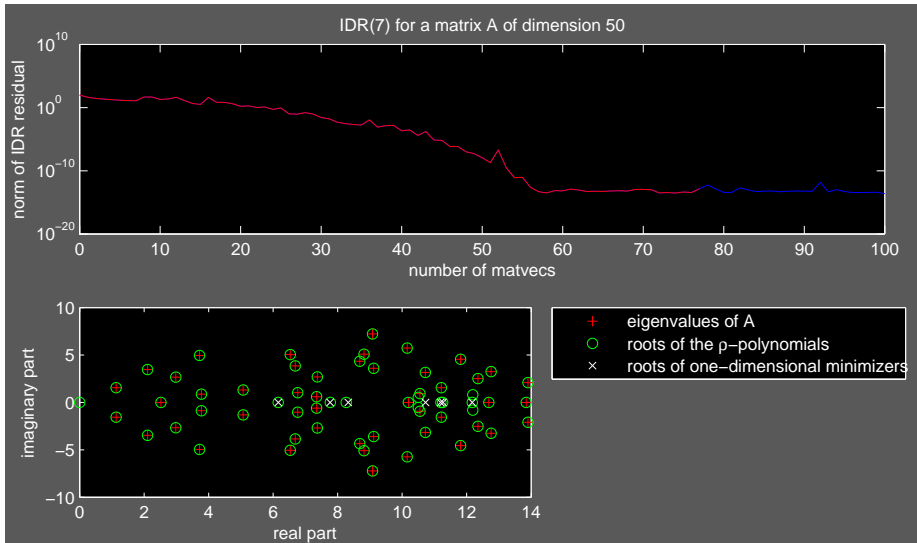
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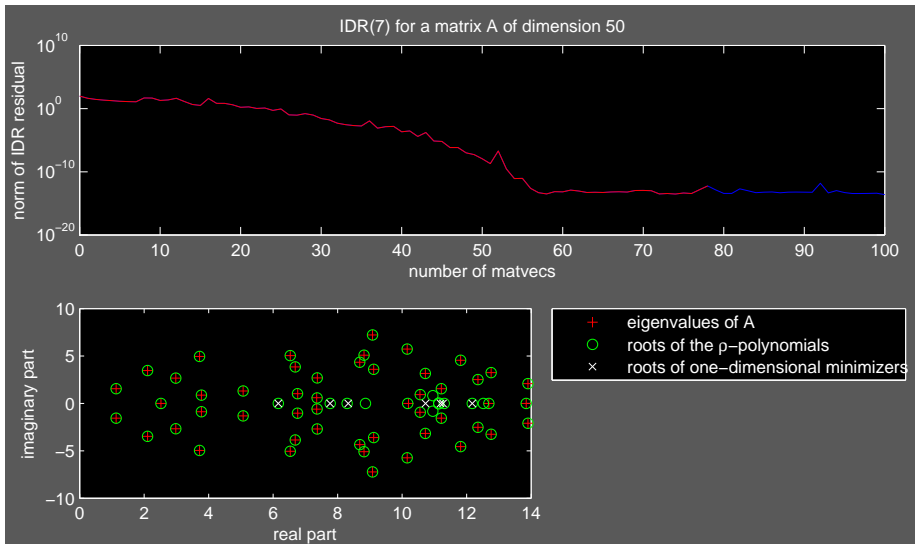
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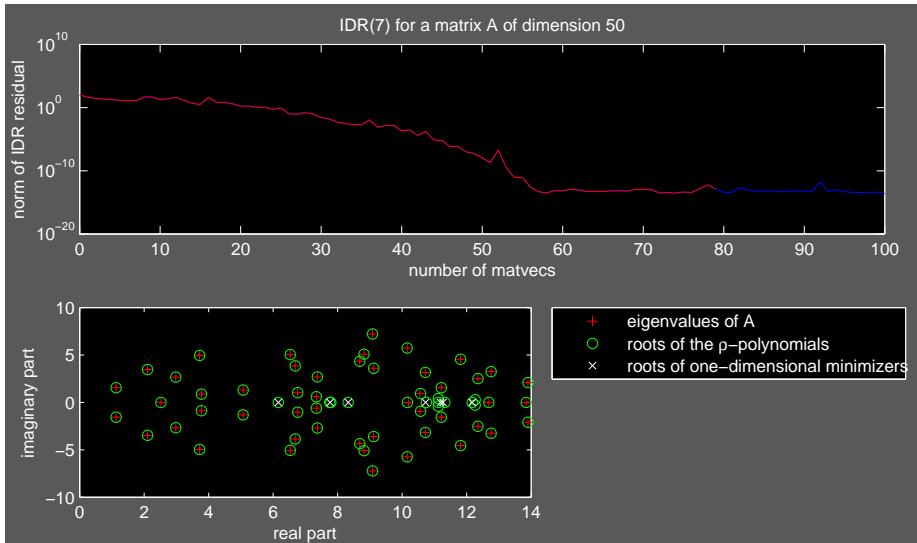
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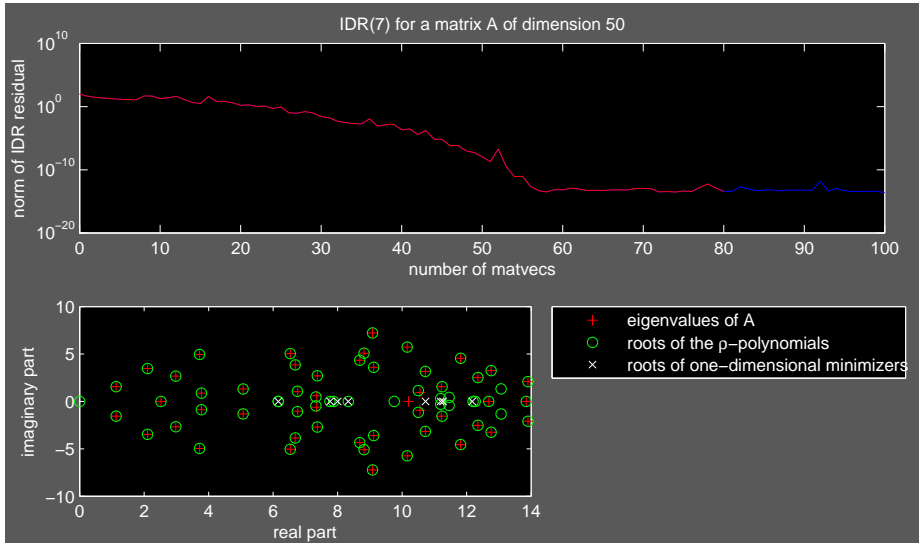
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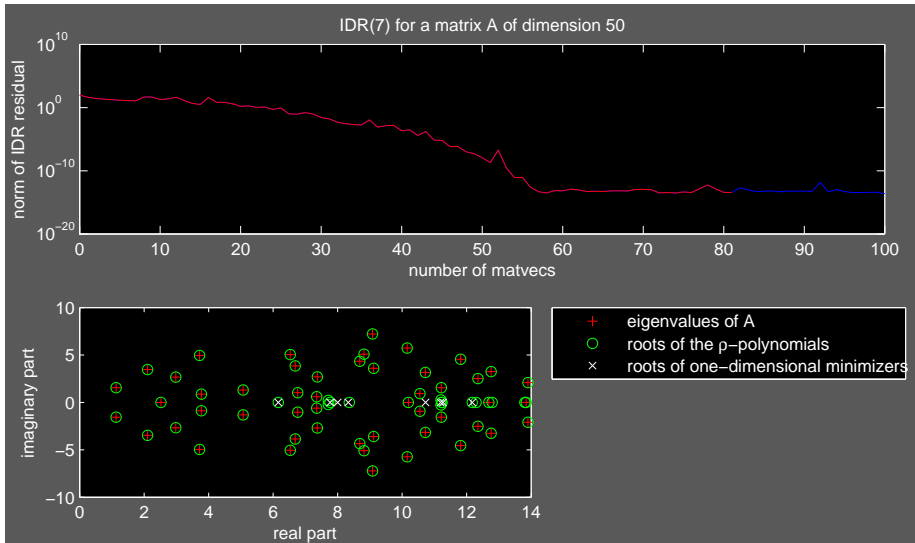
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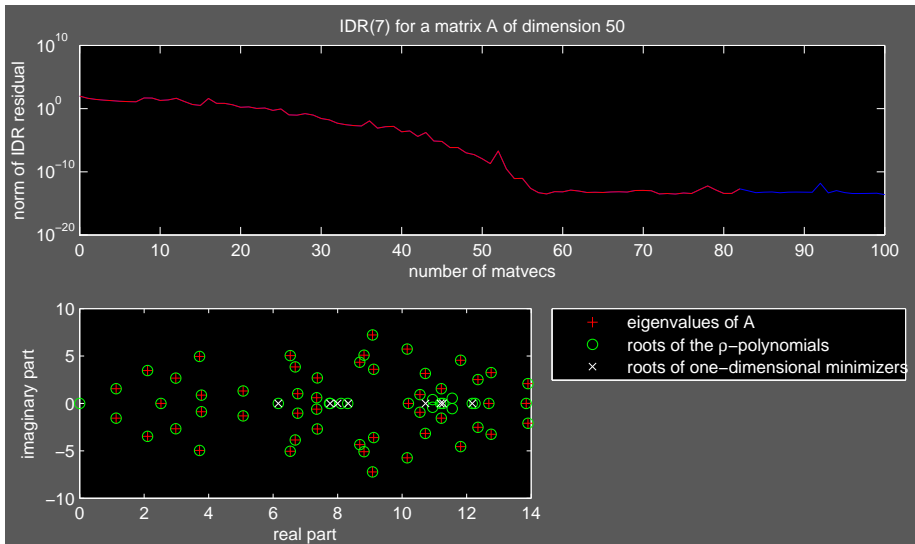
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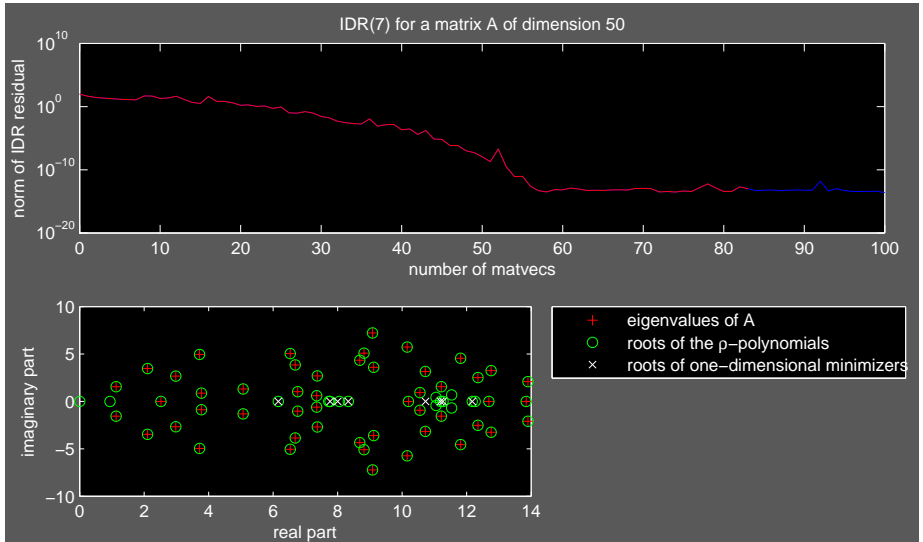
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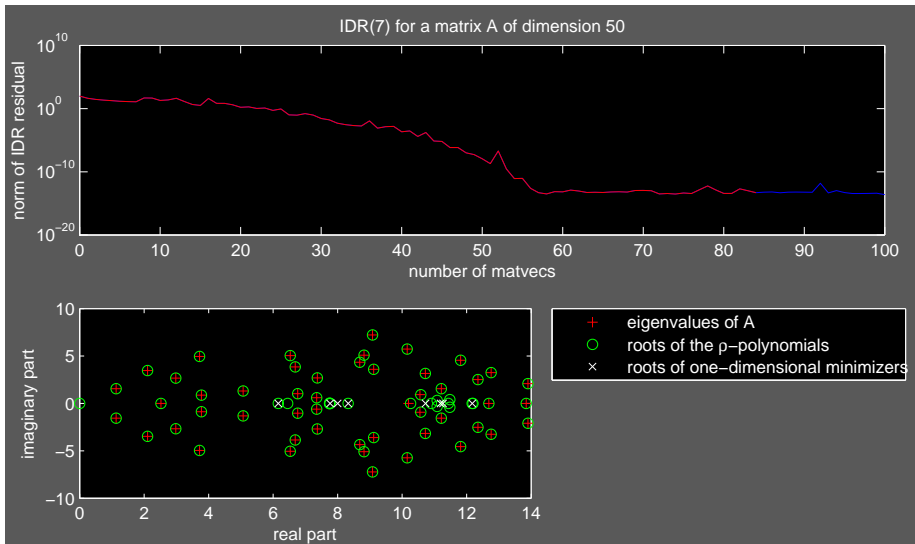
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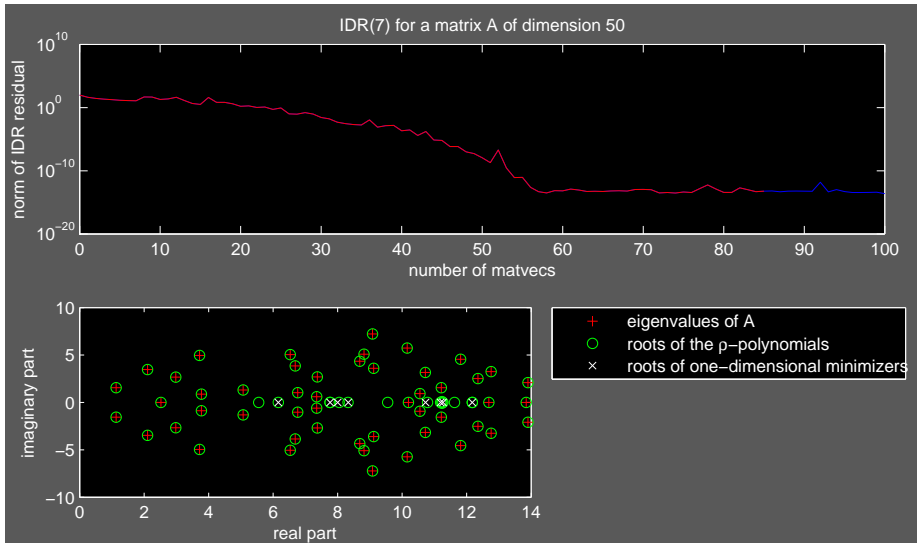
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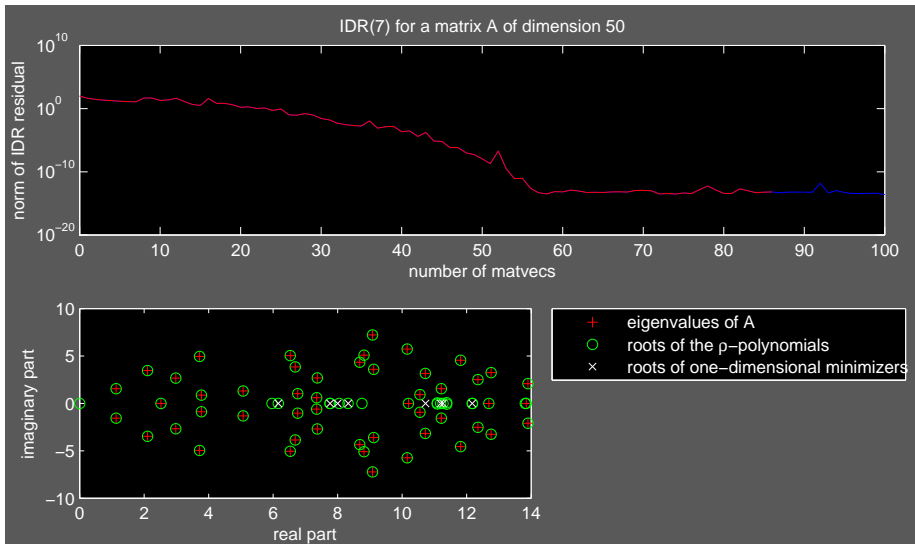
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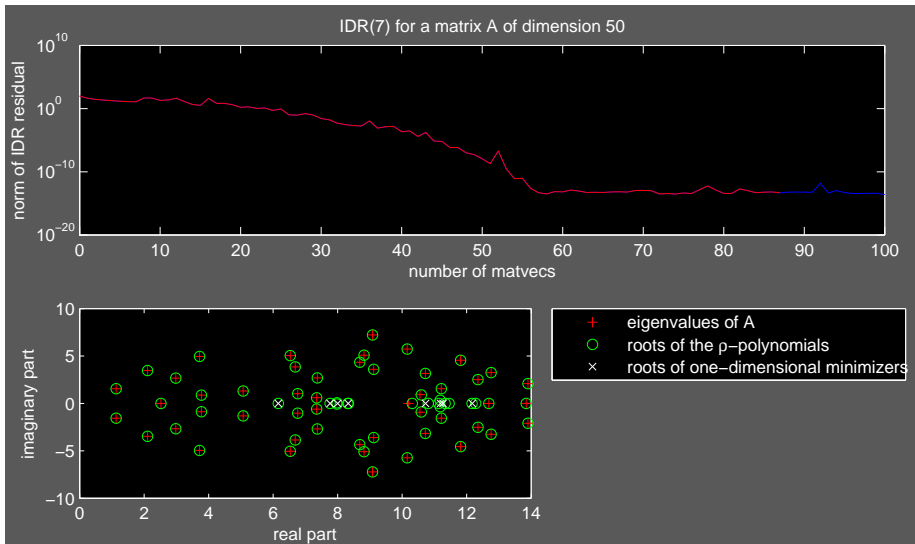
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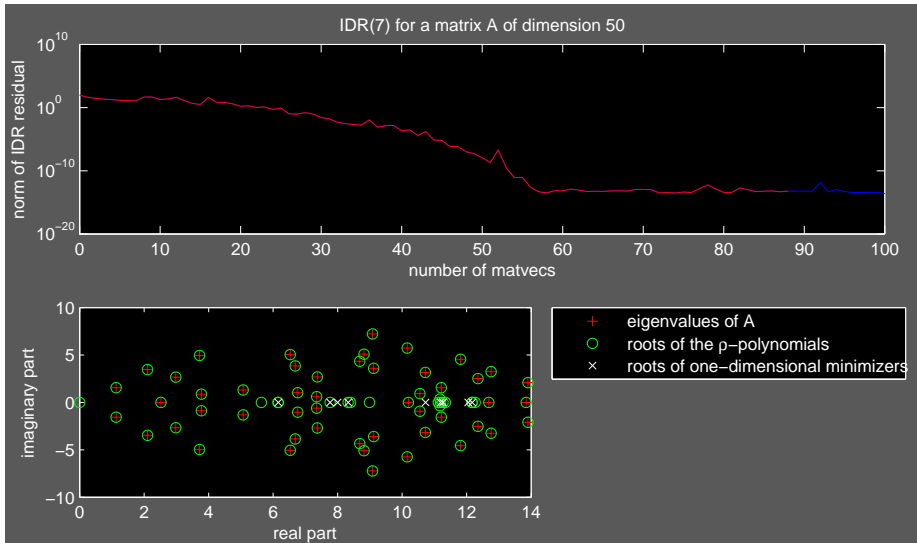
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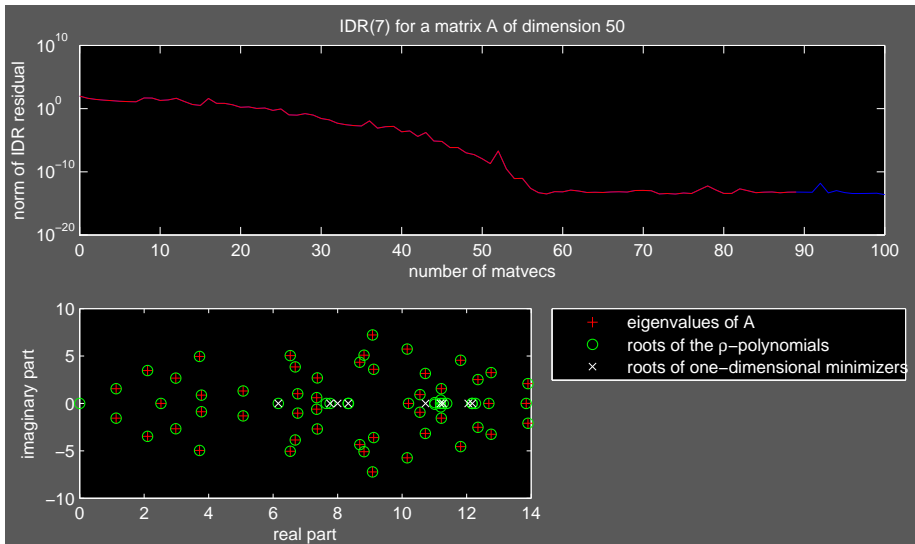
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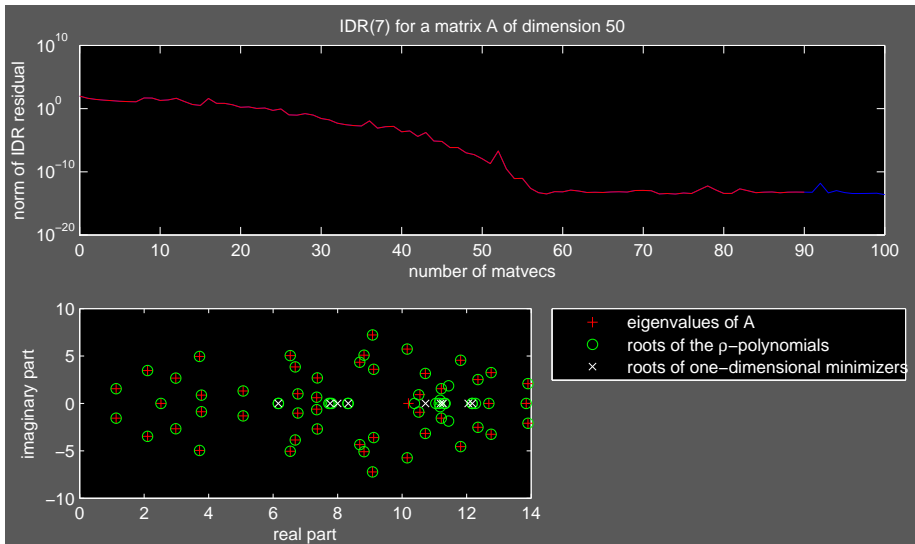
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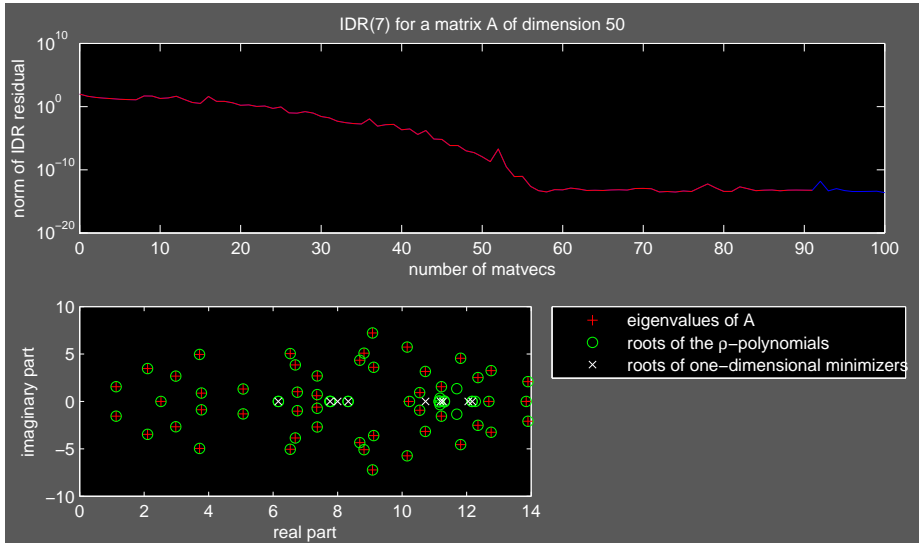
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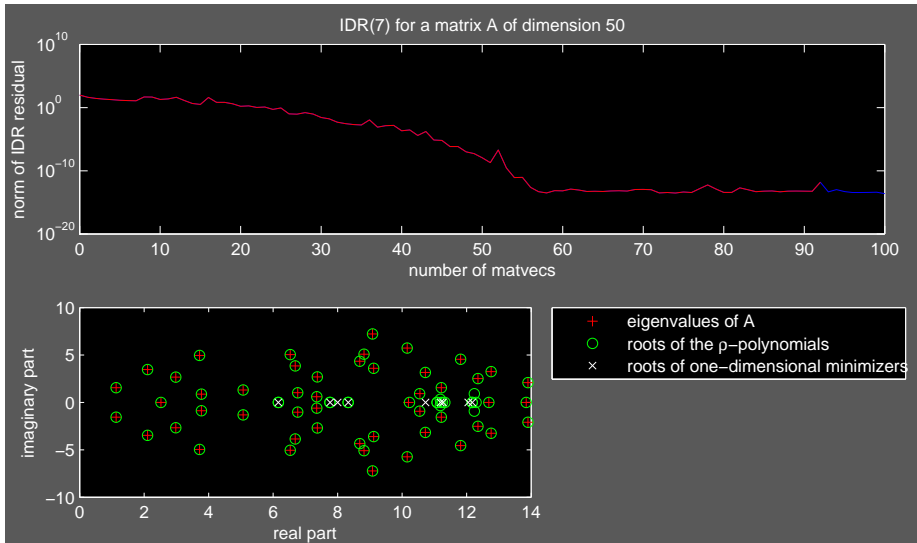
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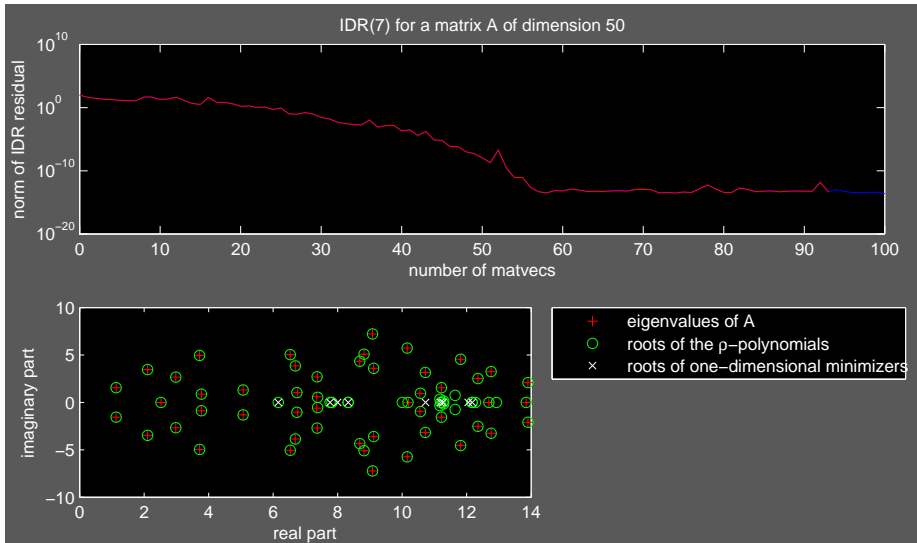
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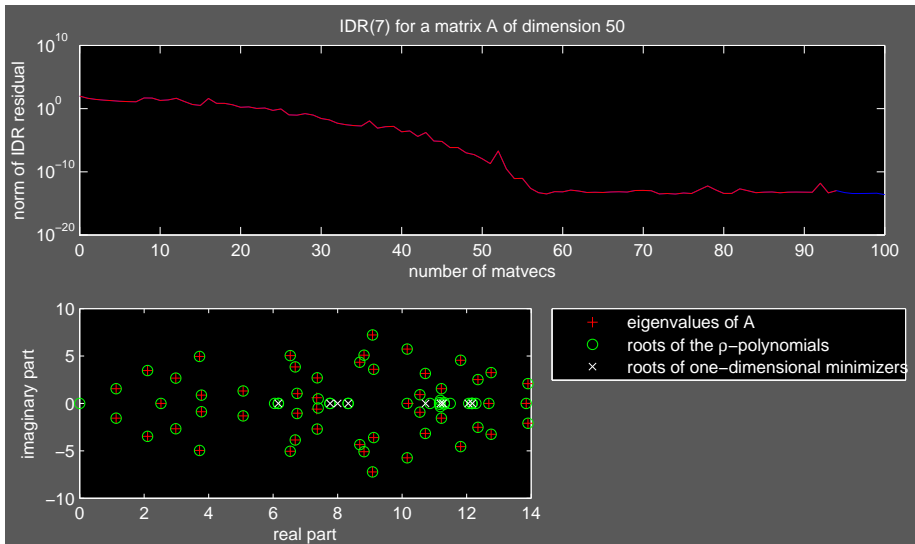
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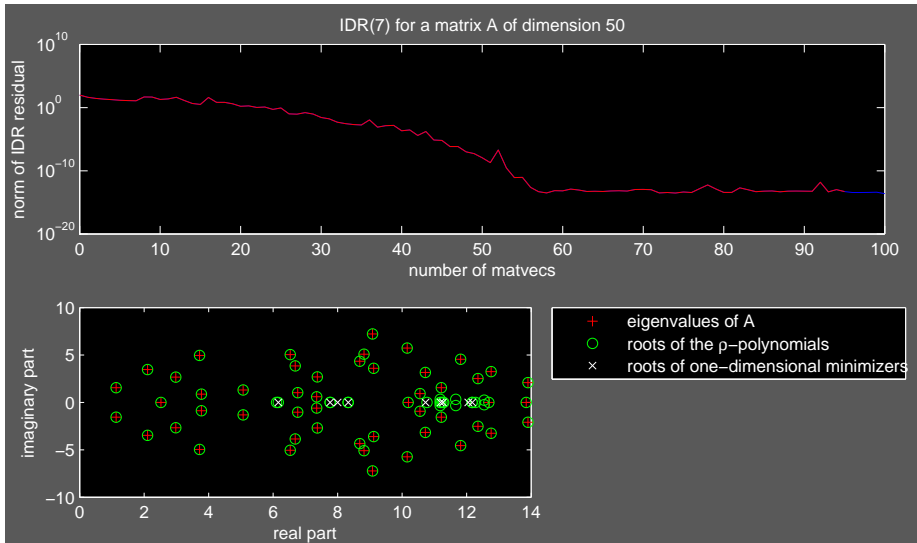
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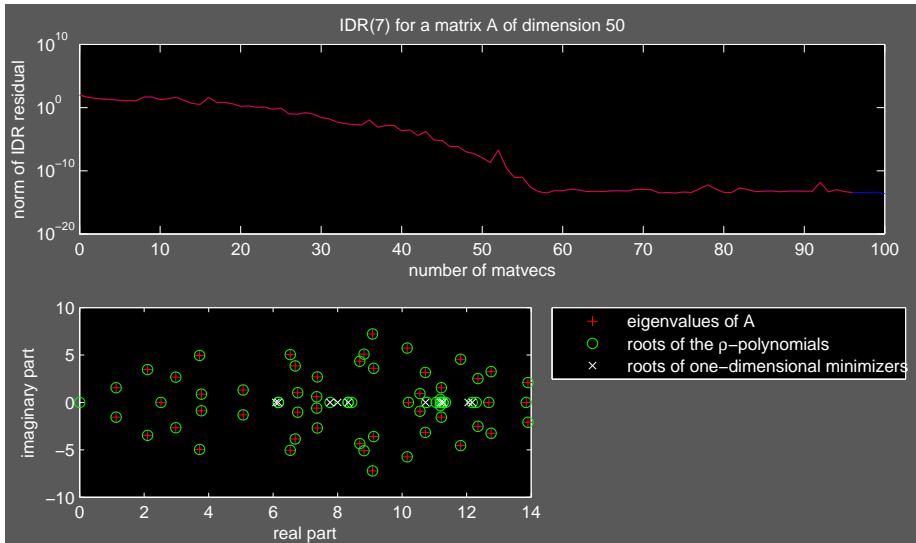
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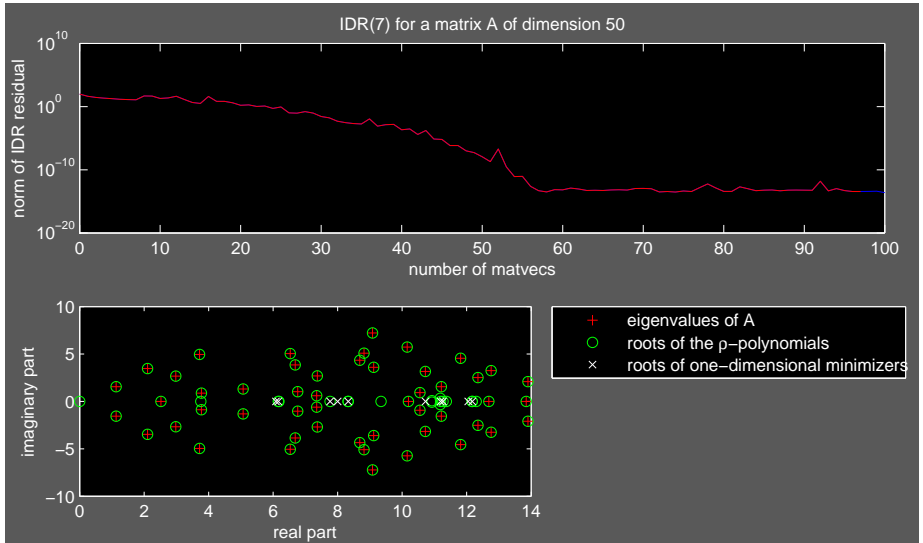
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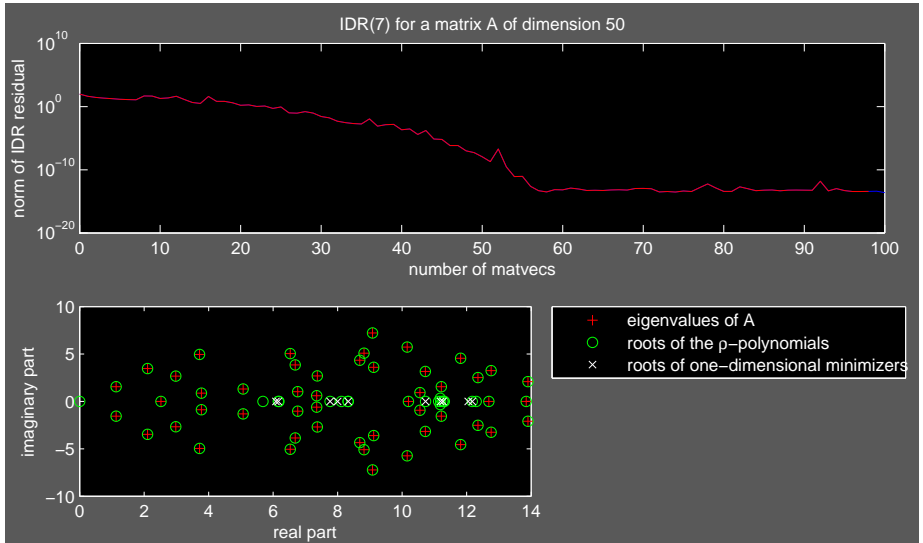
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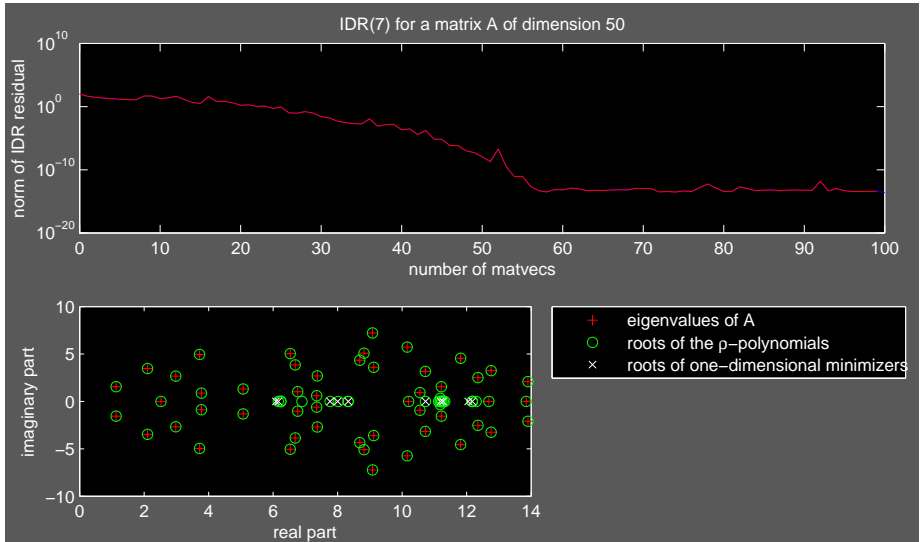
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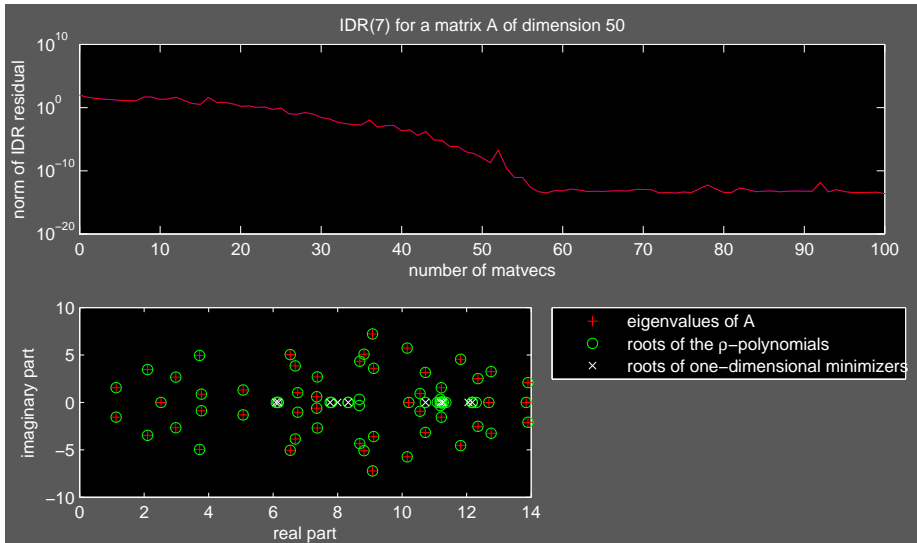
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IDR for eigenvalues

The expansion in the original IDR is based on ORTHORES, which is known to be unstable when zero is in the field of values. When we are only interested in eigenvalue approximations, we could scale differently and use an Arnoldi-based expansion in the inner sweeps.

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The choice of the ω_j could be adopted, this may have advantages for the computation of eigenvalues close to a given target or with large/small real part. The multiplier need not be or residual form, e.g., we could use $\alpha_j \mathbf{I} - \beta_j \mathbf{A}$ in place of $\mathbf{I} - \omega_j \mathbf{A}$, and even more general choices seem plausible.

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The new IDR(s)STAB(ℓ) variant by Sleijpen/van Gijzen based on coupling the ideas behind BICGSTAB(ℓ) with the IDR philosophy should also be useful for eigenvalue computations.

IDR for linear systems

As IDR is based on a clever way of computing a structured Hessenberg decomposition, we could refrain from the unstable ORTHORES-scaling and use a GMRES- or QMR-like approach, i.e., we could compute the solutions by updating the QR decomposition of the extended Hessenberg matrix of an Arnoldi-based IDR variant. This would at least smoothen the convergence curves ...

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The IDR(s)STAB(ℓ) variant by Sleijpen/van Gijzen should also be implemented based on a quasi-minimization by using the extended Hessenberg structure in computing the least-squares using Givens-QR.

IDRQMR for eigenvalues

The zeros of the residual polynomials of these QMR approaches are given by inverses of sections of the pseudoinverse of the extended Hessenberg matrices. These zeros are harmonic Ritz values and the Ritz vectors are frequently better approximations to “inner” eigenvectors.

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We could even adopt shifted harmonic Ritz, ρ -values, refined approaches similar to Jia’s and the QMREig approach based on Grassmannian optimization.

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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?

Herzlichen Glückwunsch zum 65. Geburtstag ...

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. . . und jetzt: „Guten Appetit!“