Abstract Perturbed Krylov Methods

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Outline

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Philosophical considerations

- A matrix equation
- The iterative point of view
- The polynomial point of view

The results on ...

- Ritz vectors
- QOR iterates
- QOR residuals

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The results on ...
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- QOR iterates
- QOR residuals

A "numerical" experiment
- Eigenvectors using Lanczos' method

A matrix-theoretical beginning

We start with the equation

$$\begin{aligned} AQ_k &= Q_{k+1}\underline{C}_k \\ &= Q_k C_k + q_{k+1} c_{k+1,k} e_k^T. \end{aligned} \tag{1}$$

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$\underline{C}_k = \begin{pmatrix} C_k \\ c_{k+1,k} e_k^T \end{pmatrix} \in \mathbb{C}^{(k+1,k)}$	is an extended Hessenberg matrix,
$F_k \in \mathbb{C}^{(n,k)}$	is a general perturbation.

The dependence on the iteration

We investigate this matrix equation iteratively:

$$\begin{aligned} AQ_k e_l + F_k e_l &= Q_{k+1} \underline{C}_k e_l \\ &= Q_k C_k e_l + q_{k+1} c_{k+1,k} \delta_{kl}, \qquad \forall l \leqslant k. \end{aligned} \tag{2}$$

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- Interpret perturbed Krylov methods as overlay of several polynomial methods.

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We study polynomials based on the computed C_k or $\underline{C}_k$ with certain useful properties.

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We restrict ourselves to $\mathcal{A}_k$, $\mathcal{L}_k[z^{-1}]$, $\mathcal{L}_k[1-\delta_{z0}]$ and $\mathcal{R}_k$.

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$$\mathcal{A}_k(\theta_j, C_k)e_1 = s_j, \qquad C_k s_j = \theta_j s_j$$

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- Generalization:

$$\mathcal{A}_{l+1:k}(\theta, z) \equiv \frac{\chi_{l+1:k}(\theta) - \chi_{l+1:k}(z)}{\theta - z}, \qquad l = 0, 1, \ldots, k.$$

Adjugate polynomials and Ritz vectors

Theorem (Ritz vectors)

Let $C_k S_\theta = S_\theta J_\theta$ (for a certain S_θ). Let the Ritz matrix be given by $Y_\theta \equiv Q_k S_\theta$. Then

$$\operatorname{vec}(Y_\theta) = \begin{pmatrix} \mathcal{A}_k(\theta, A) \\ \mathcal{A}'_k(\theta, A) \\ \vdots \\ \dfrac{\mathcal{A}_k^{(\alpha-1)}(\theta, A)}{(\alpha-1)!} \end{pmatrix} q_1 + \sum_{l=1}^{k} c_{1:l-1} \begin{pmatrix} \mathcal{A}_{l+1:k}(\theta, A) \\ \mathcal{A}'_{l+1:k}(\theta, A) \\ \vdots \\ \dfrac{\mathcal{A}_{l+1:k}^{(\alpha-1)}(\theta, A)}{(\alpha-1)!} \end{pmatrix} f_l, \qquad (3)$$

with derivation with respect to the shift θ.

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We might scale differently such that (here only for approximate eigenvectors)

$$y = \frac{\mathcal{A}_k(\theta, A)}{\prod_{\ell=1}^{k-1} c_{\ell+1,\ell}} q_1 + \sum_{l=1}^{k} \frac{\mathcal{A}_{l+1:k}(\theta, A)}{\prod_{\ell=l+1}^{k-1} c_{\ell+1,\ell}} \frac{f_l}{c_{l+1,l}}.$$

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Lagrange polynomials and QOR iterates

Theorem (QOR iterates)

Suppose all $C_{l+1:k}$ *are regular. Define* $z_k \equiv C_k^{-1} e_1 \|r_0\|$ *and* $x_k \equiv Q_k z_k$. *Then*

$$x_k = \mathcal{L}_k[z^{-1}](A) r_0 - \sum_{l=1}^{k} z_{lk} \, \mathcal{L}_{l+1:k}[z^{-1}](A) f_l. \qquad (4)$$

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Really sloppily speaking, in case of convergence,

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Proving convergence is the hard task.

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Two types of polynomials $\Rightarrow$ two expressions for the QOR residuals.

Residual polynomials and QOR residuals

Theorem (QOR residuals)

Suppose $q_1 = r_0/\|r_0\|$ *and let all* $C_{l+1:k}$ *be invertible. Let* x_k *denote the QOR iterate and* $r_k = r_0 - Ax_k$ *the corresponding residual.*
Then

$$\begin{aligned} r_k &= \mathcal{R}_k(A)r_0 + \sum_{l=1}^{k} z_{lk}\, \mathcal{L}^0_{l+1:k}[1-\delta_{z0}](A)f_l \\ &= \mathcal{R}_k(A)r_0 - \sum_{l=1}^{k} z_{lk}\, \mathcal{R}_{l+1:k}(A)f_l + F_k z_k. \end{aligned} \tag{5}$$

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First expression: related to perturbation amplification.

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First expression: related to perturbation amplification.

Second expression: related to the attainable accuracy.

An example: Lanczos’ method

We used the diagonal matrix

$$A = \texttt{diag([linspace(0,1,50),3])}$$

and the starting vector

$$e = \texttt{ones(51,1)}$$

in an implementation of Lanczos’ method in MATLAB on a PC conforming to ANSI/IEEE 754 with machine precision $\texttt{eps(1)} = 2^{-52} \approx 2.2204 \cdot 10^{-16}$.

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At step 10 the first Ritz value has converged (up to machine precision) to the eigenvalue 3, at step 27 the second one has converged.

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$$A = \texttt{diag([linspace(0,1,50),3])}$$

and the starting vector

$$e = \texttt{ones(51,1)}$$

in an implementation of Lanczos’ method in MATLAB on a PC conforming to ANSI/IEEE 754 with machine precision $\texttt{eps(1)} = 2^{-52} \approx 2.2204 \cdot 10^{-16}$.

At step 10 the first Ritz value has converged (up to machine precision) to the eigenvalue 3, at step 27 the second one has converged.

Eigenvalues and eigenvectors are computed using MRRR, i.e., LAPACK’s routine `DSTEGR`, since MATLAB’s `eig` (using LAPACK’s `DSYEV`, i.e., the QR algorithm implemented as `DSTEQR`) fails in delivering accurate eigenvectors.

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Additionally, we heavily used the symbolic toolbox, i.e., MAPLE.

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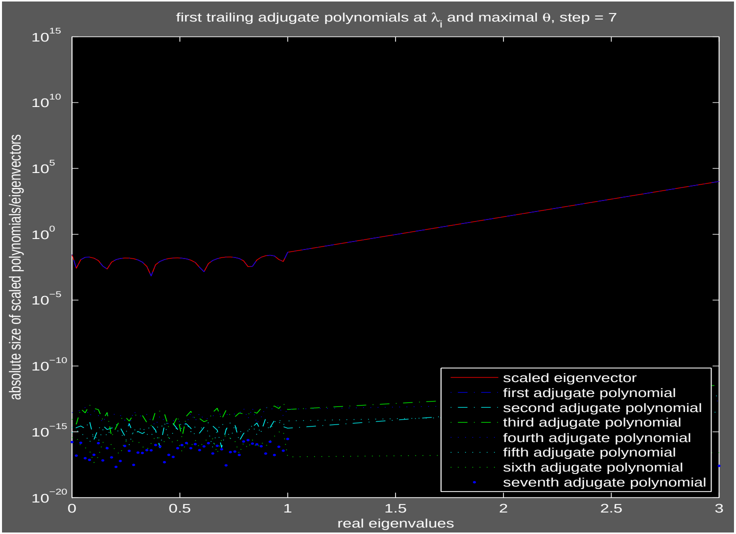

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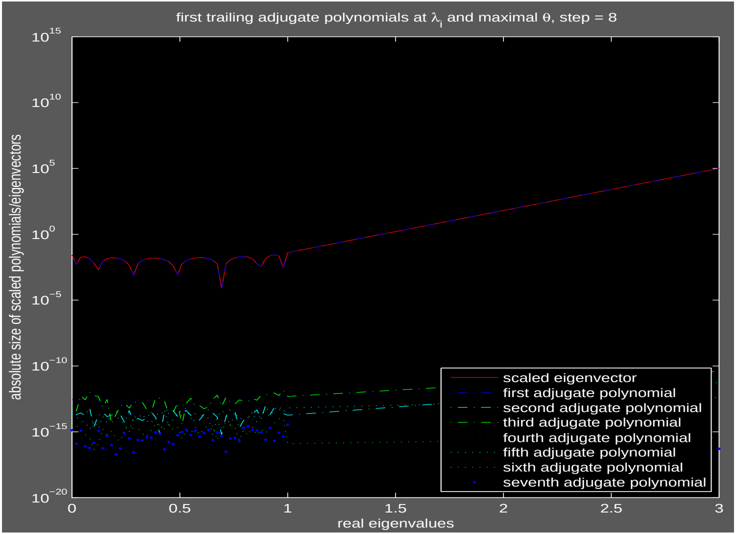

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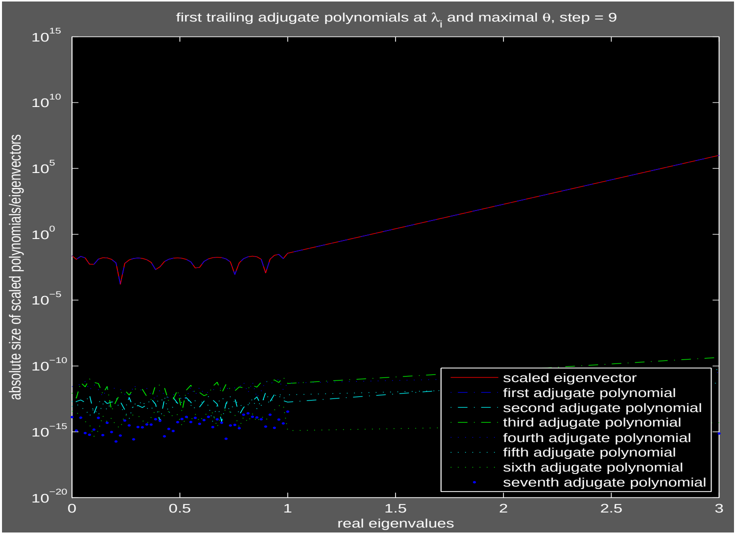

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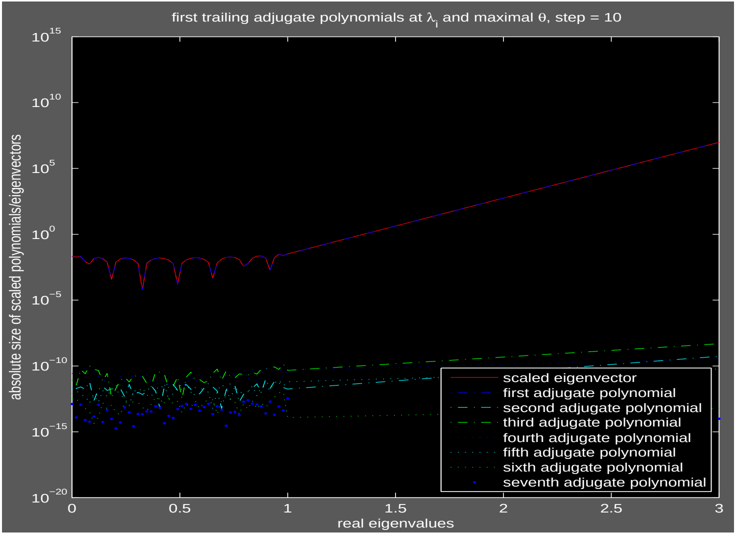

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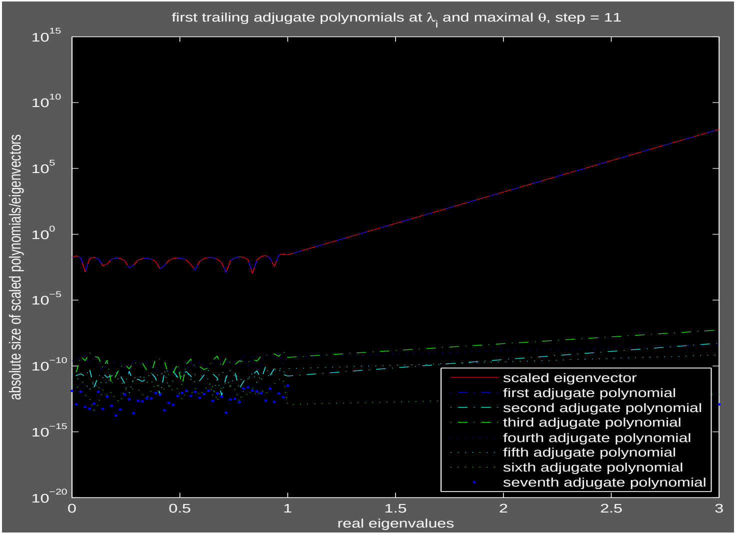

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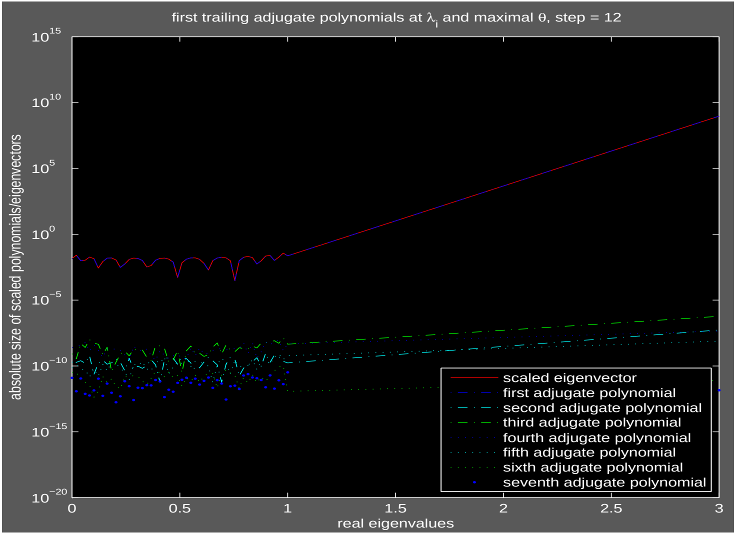

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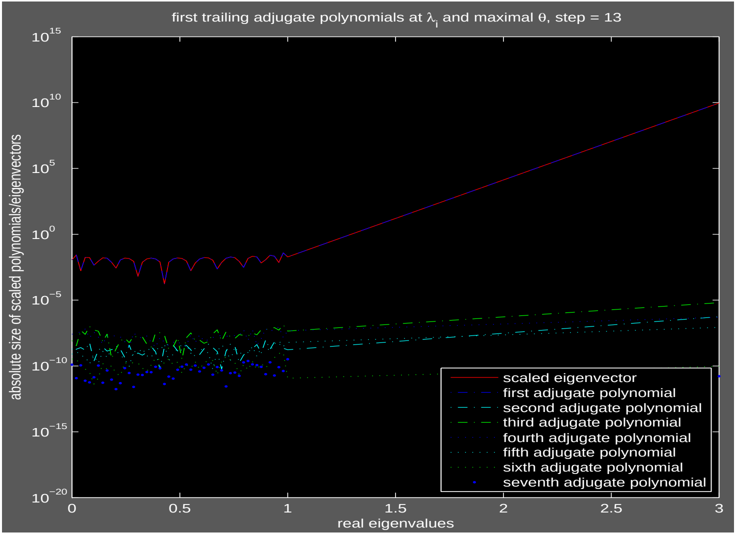

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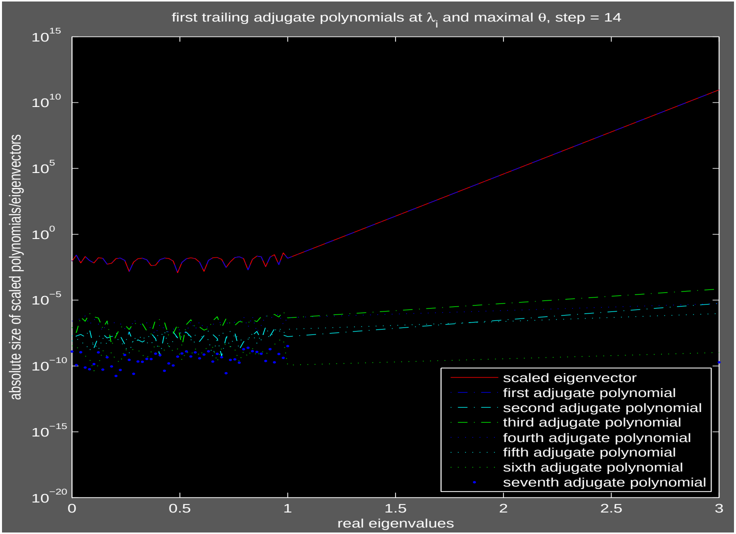

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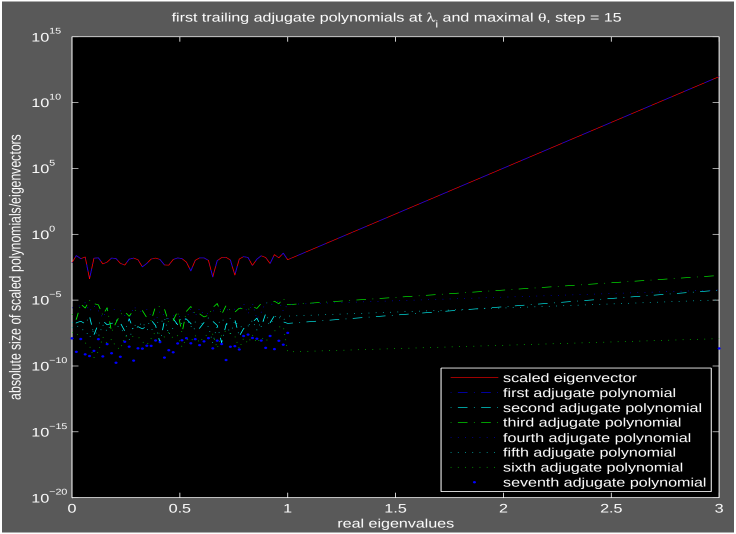

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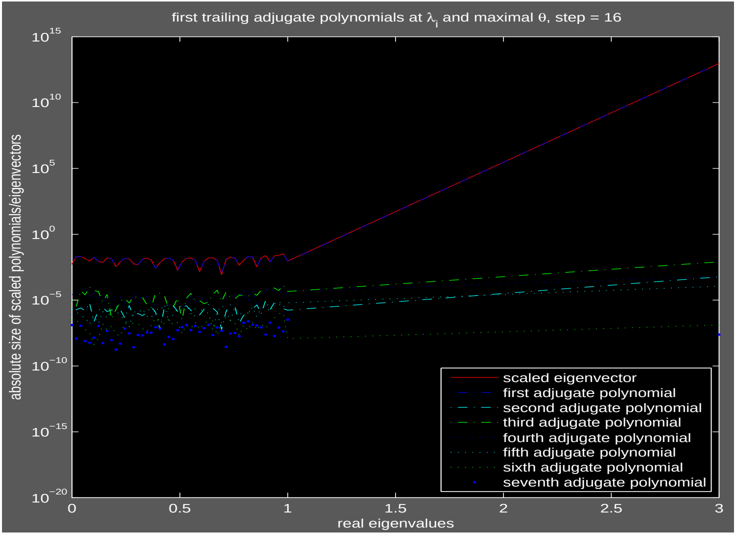

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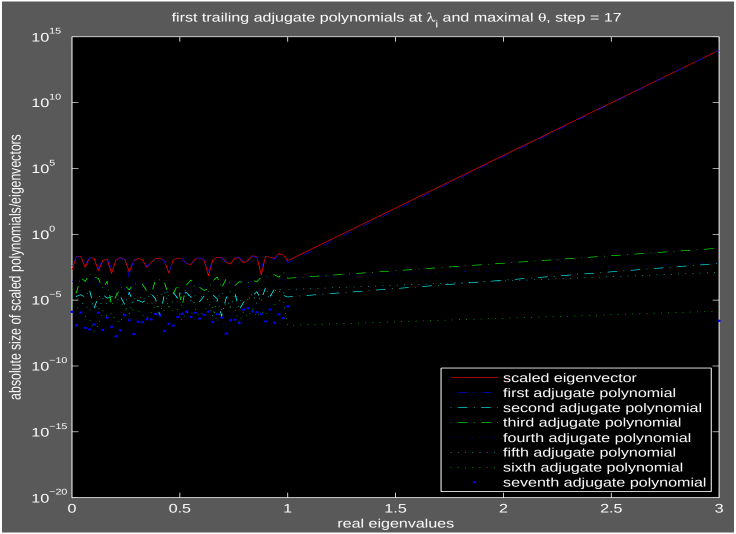

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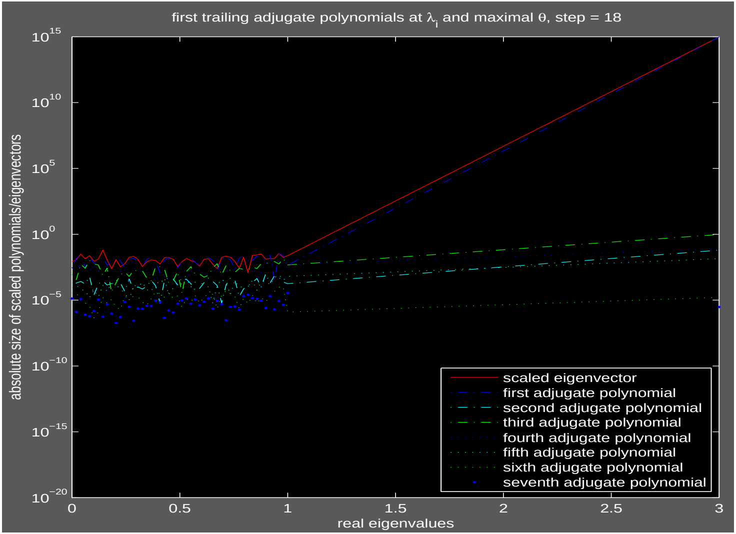

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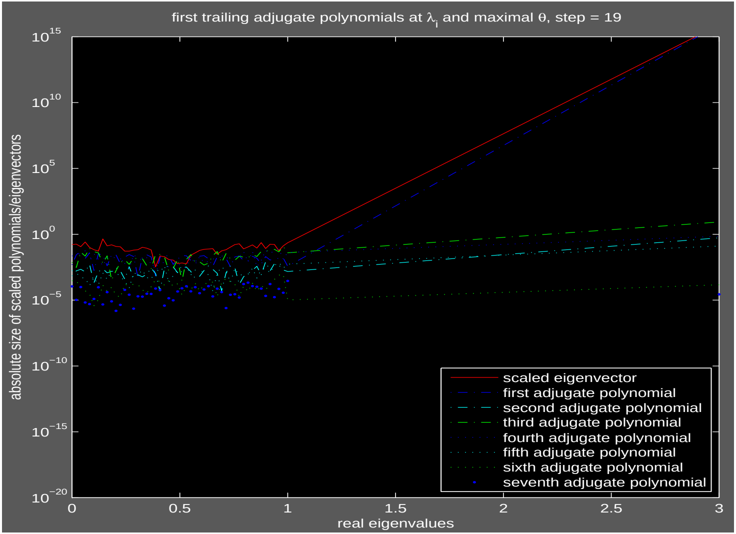

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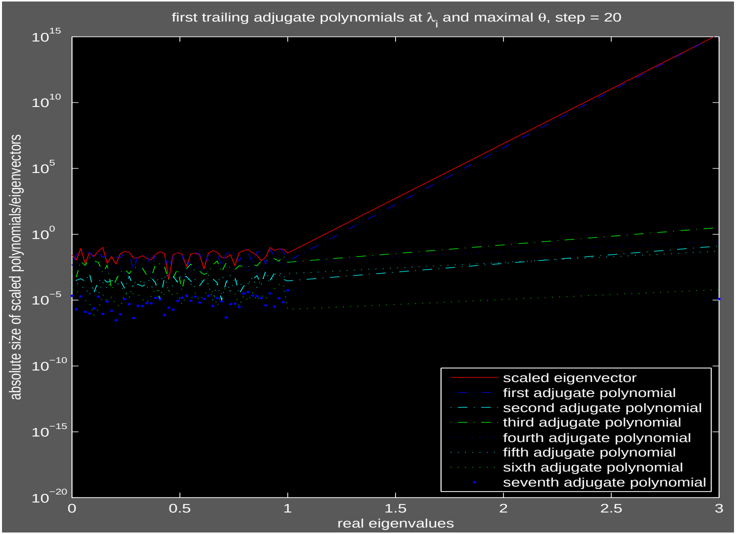

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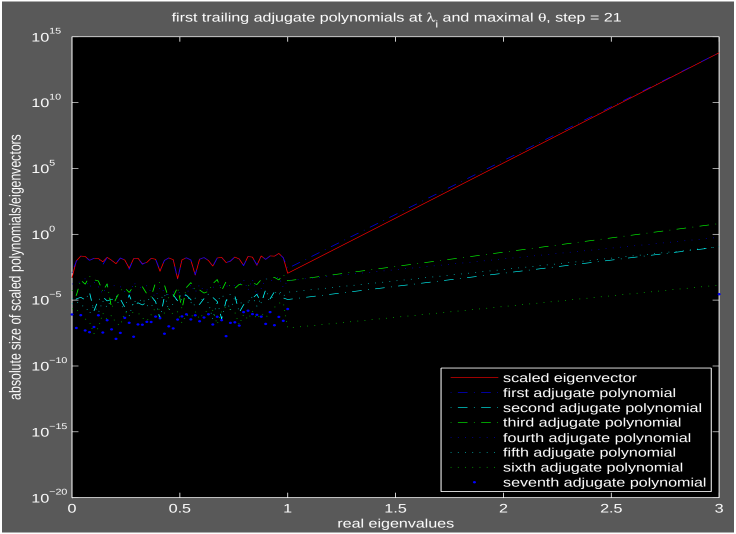

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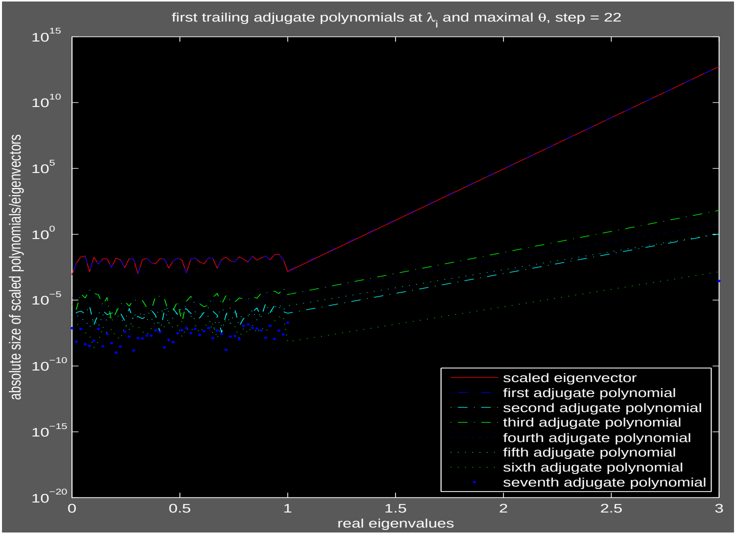

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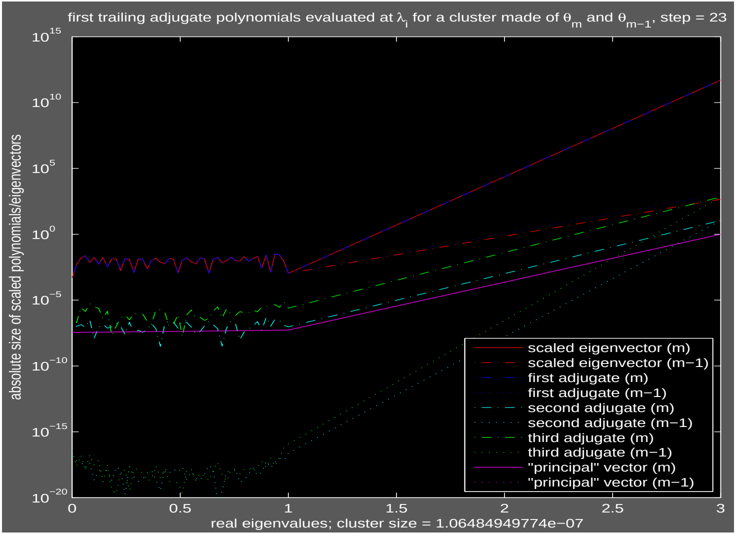

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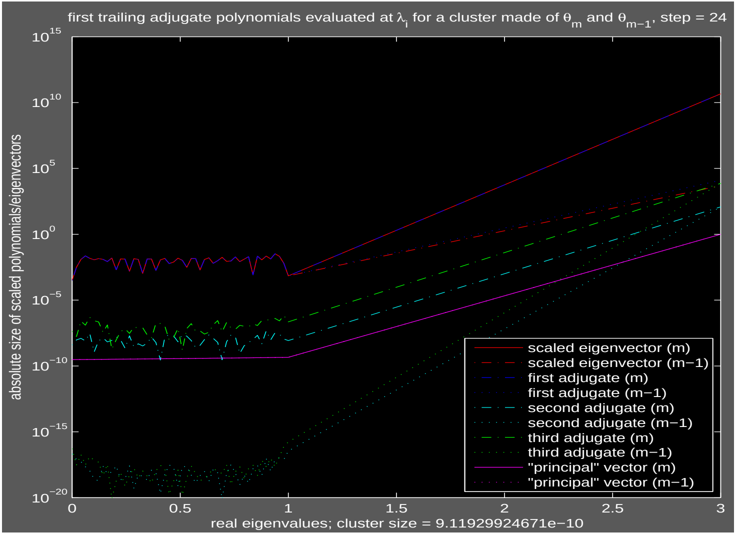

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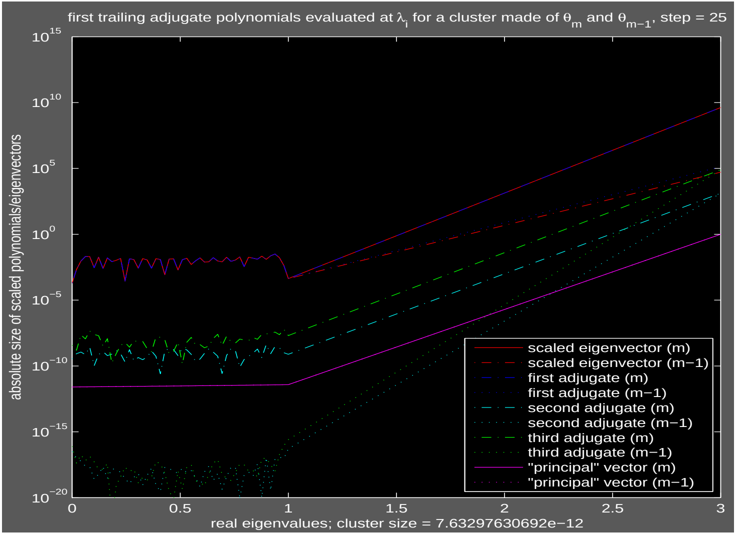

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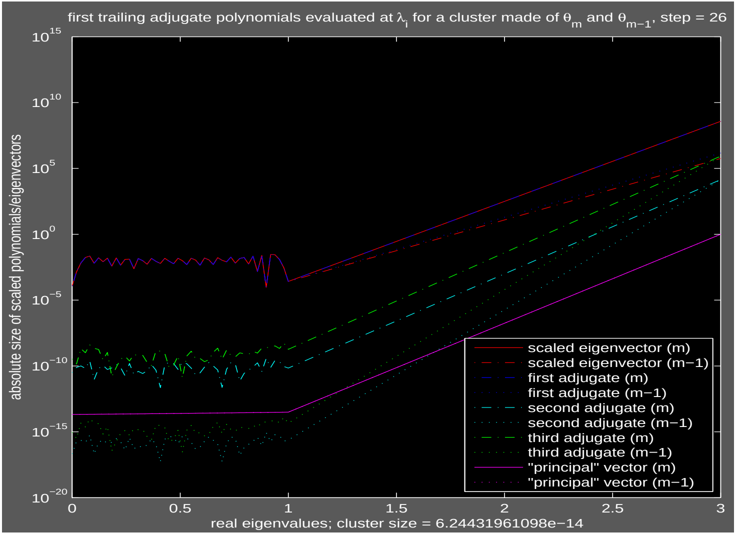

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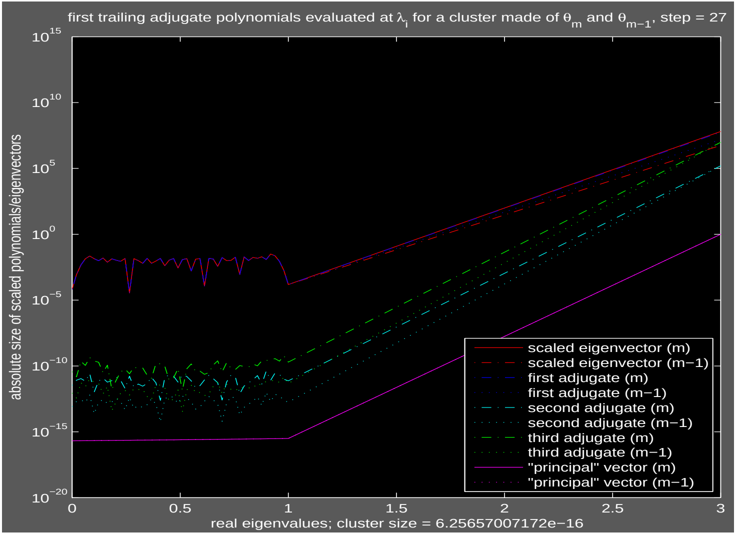

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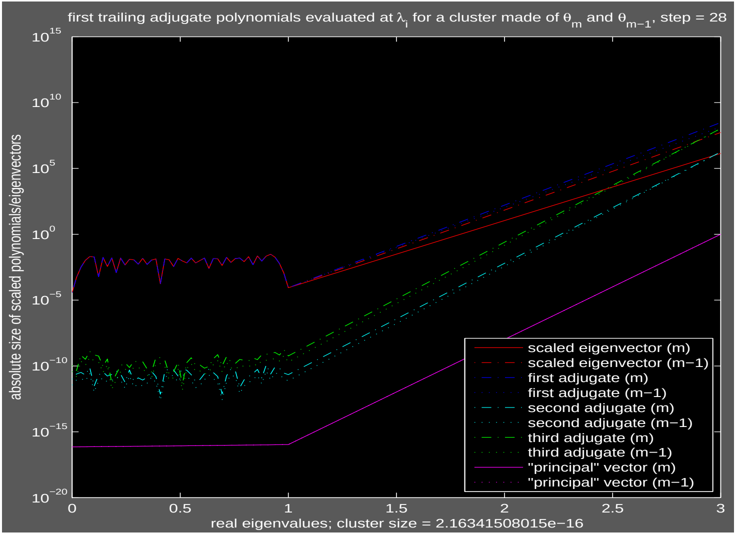

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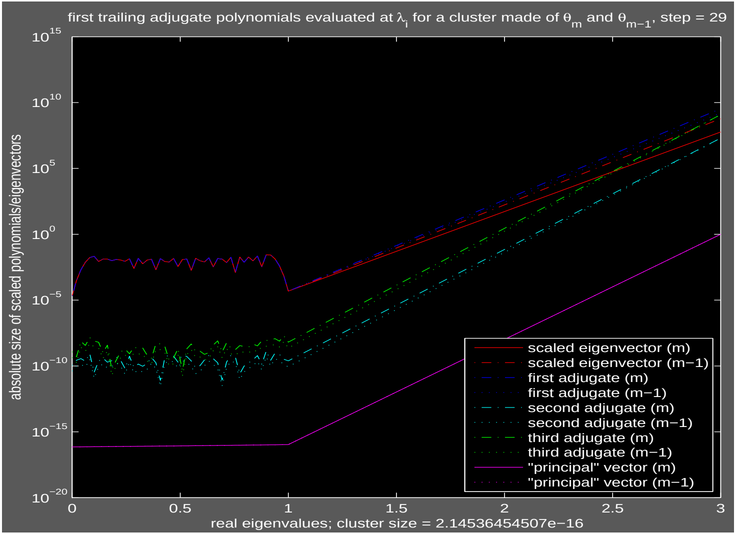

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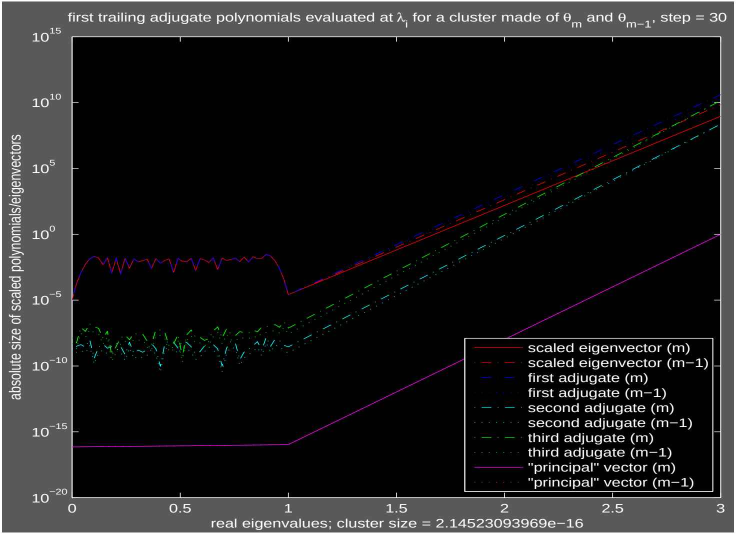

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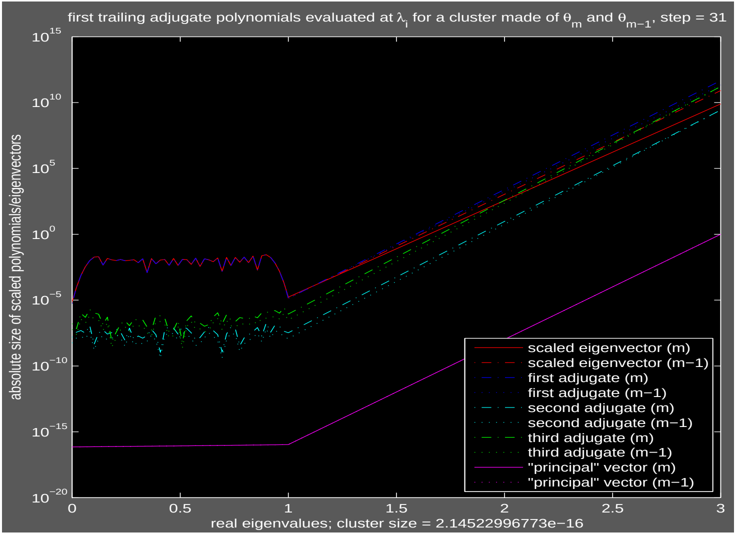

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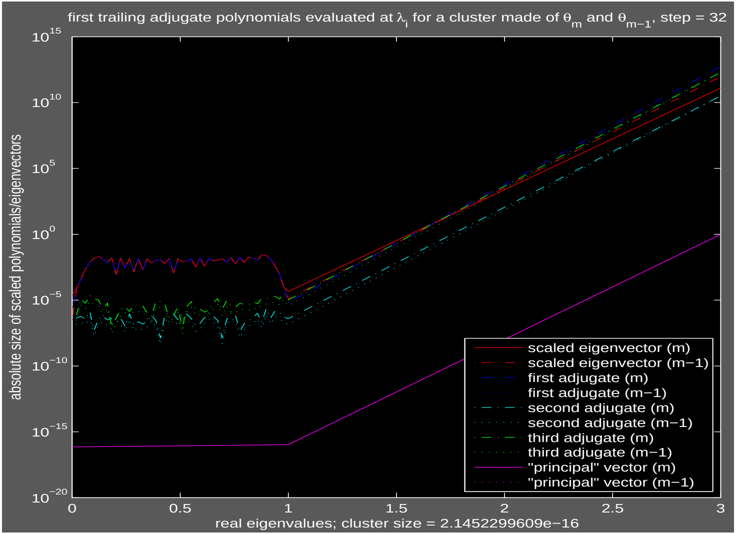

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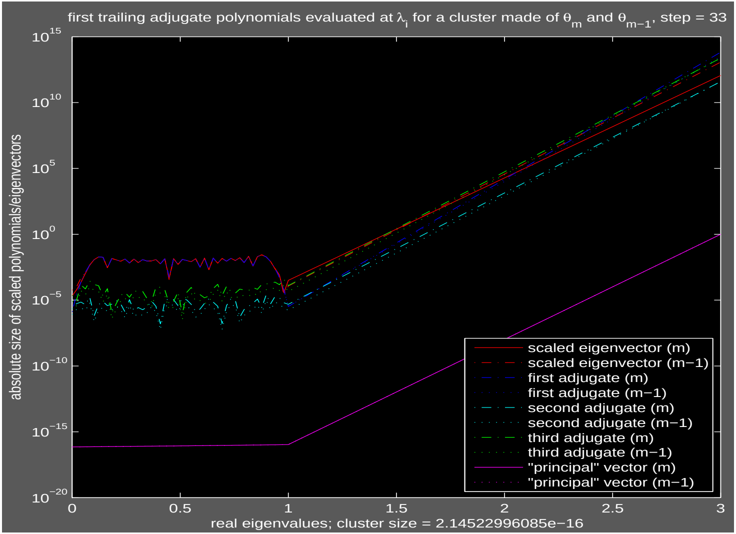

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