Fast Hessenberg QR Iteration for Companion Matrices

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Motivation: Polynomial root finding

A standard algorithm: QR iteration on a companion matrix

- Robust software exists
- It's normwise backward stable
- It's used in Matlab
- But it takes $O(n^3)$ time and $O(n^2)$ storage

Companion matrices

Given

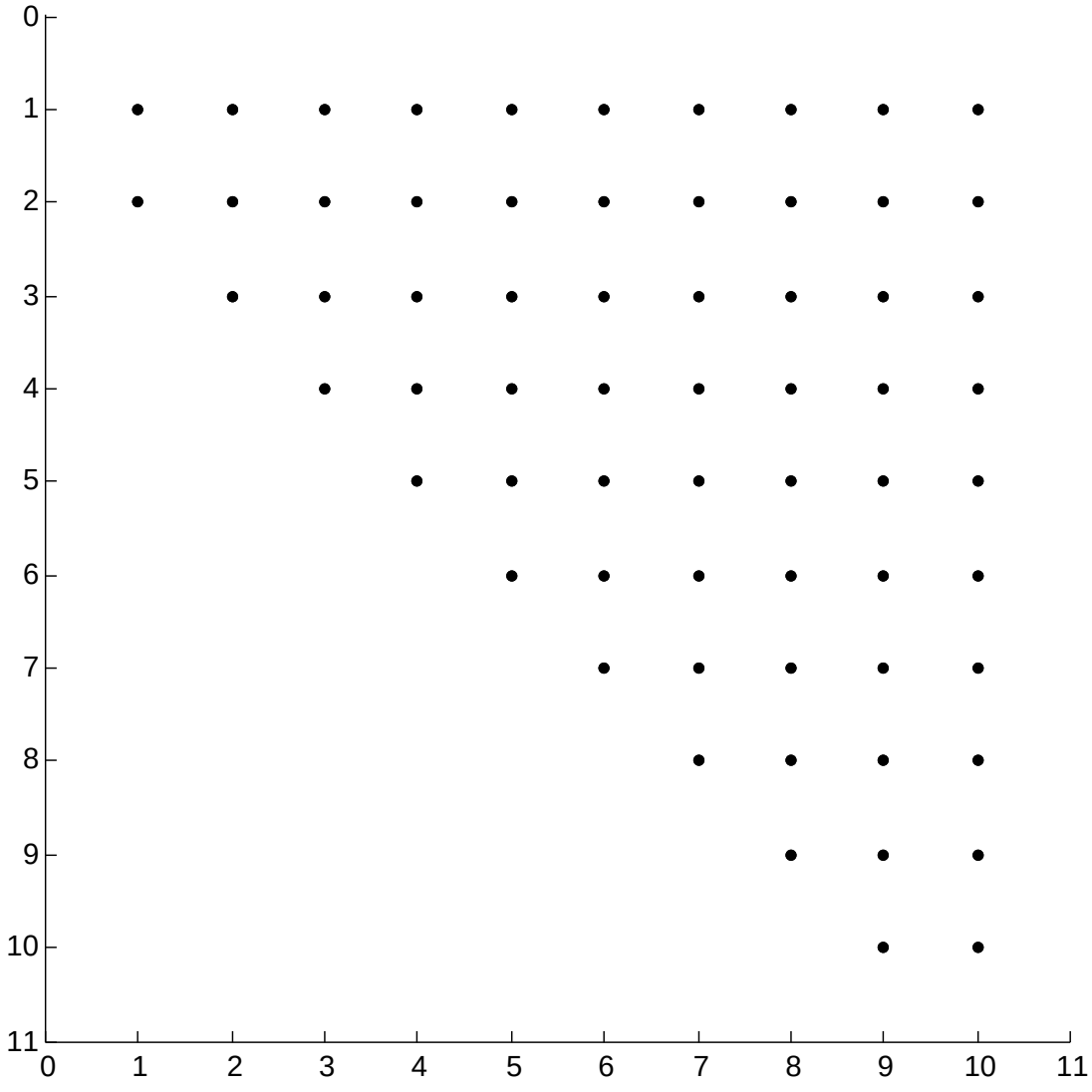
$$p(\lambda) = \lambda^n + a_{n-1}\lambda^{n-1} + \ldots + a_1\lambda + a_0$$

Define a companion matrix C:

$$C = \begin{bmatrix} -a_{n-1} & -a_{n-2} & -a_{n-3} & \ldots & -a_1 & -a_0 \\ 1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 1 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 1 & 0 \end{bmatrix}$$

For matrix polynomials, replace a_i by A_i and 1 by I.

Hessenberg QR iteration



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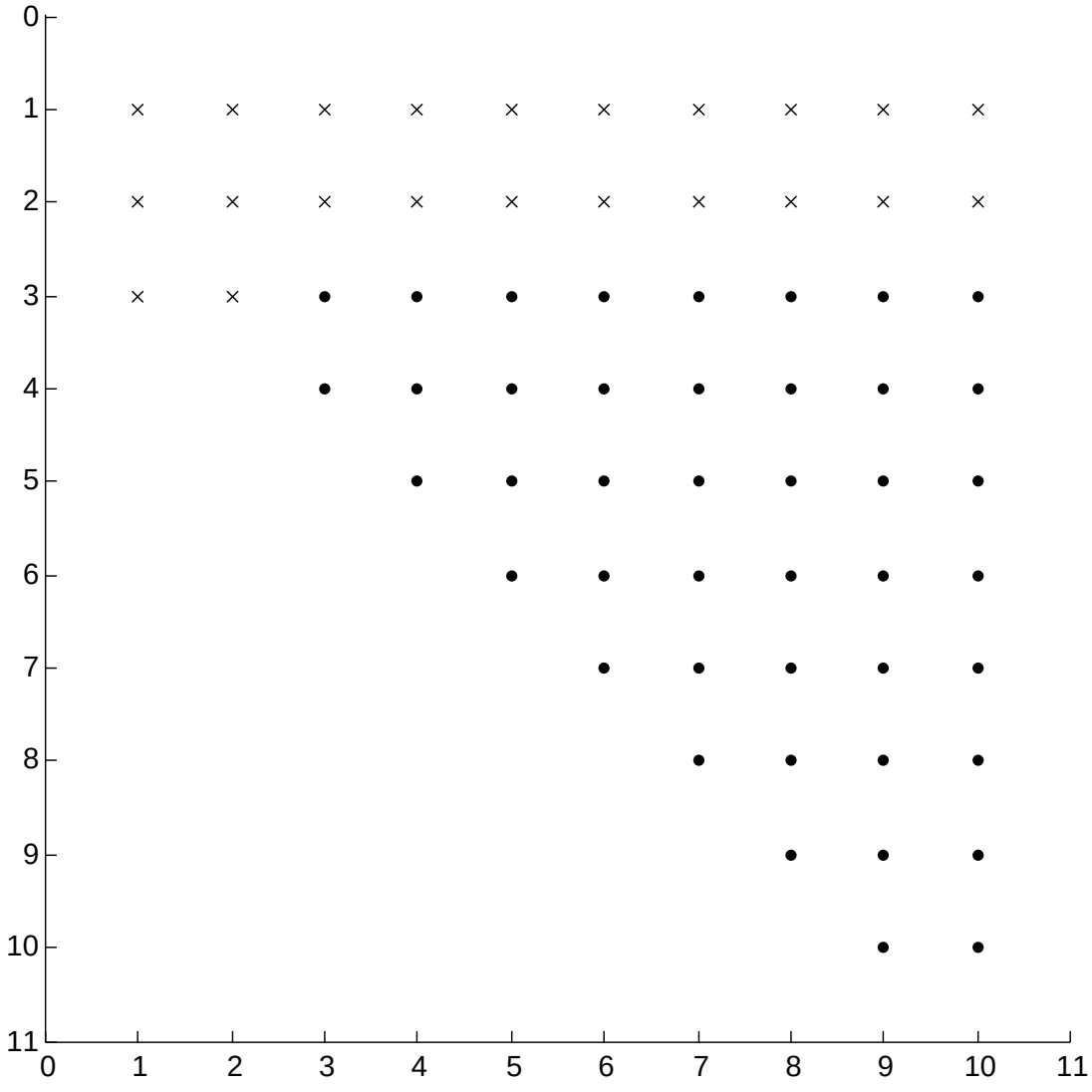

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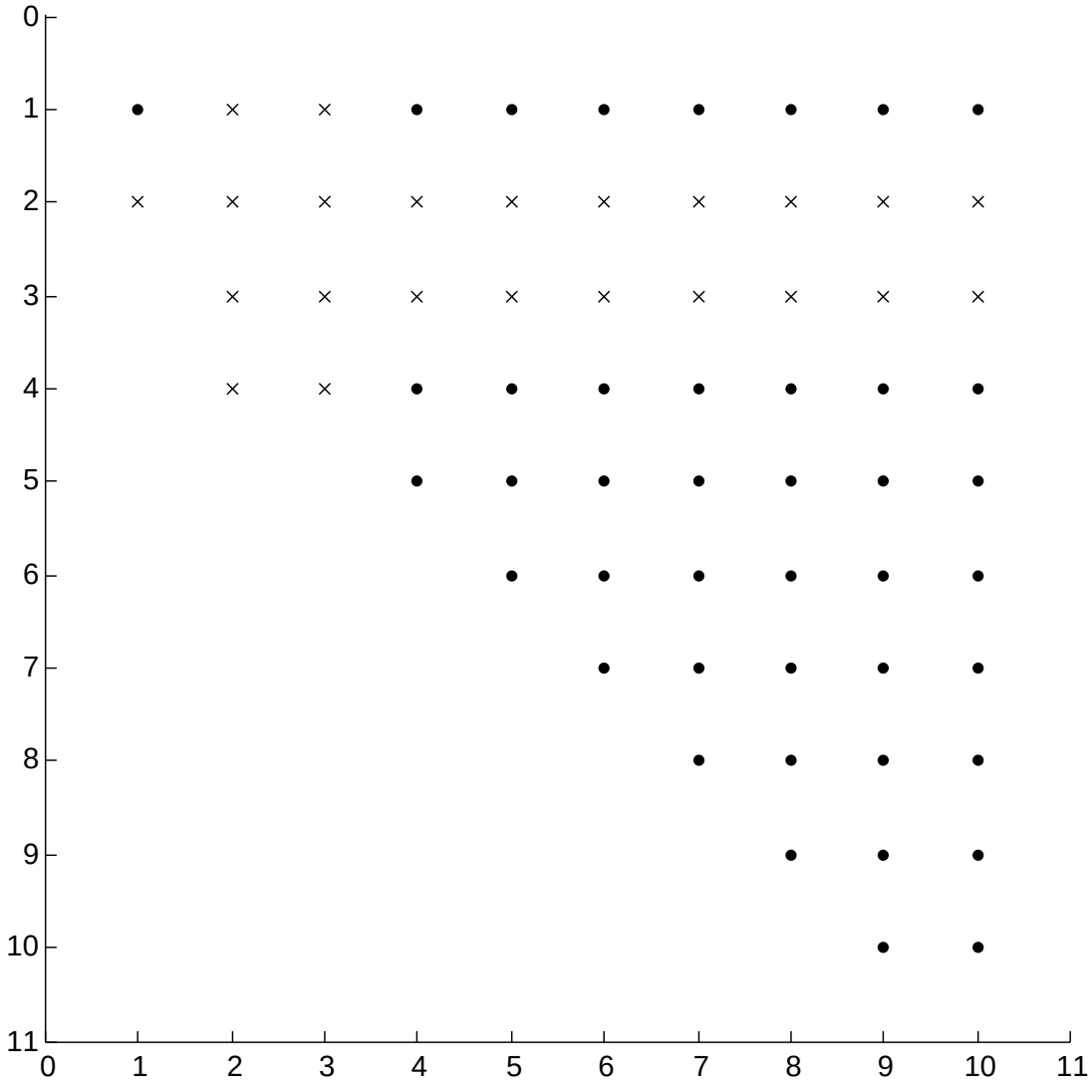

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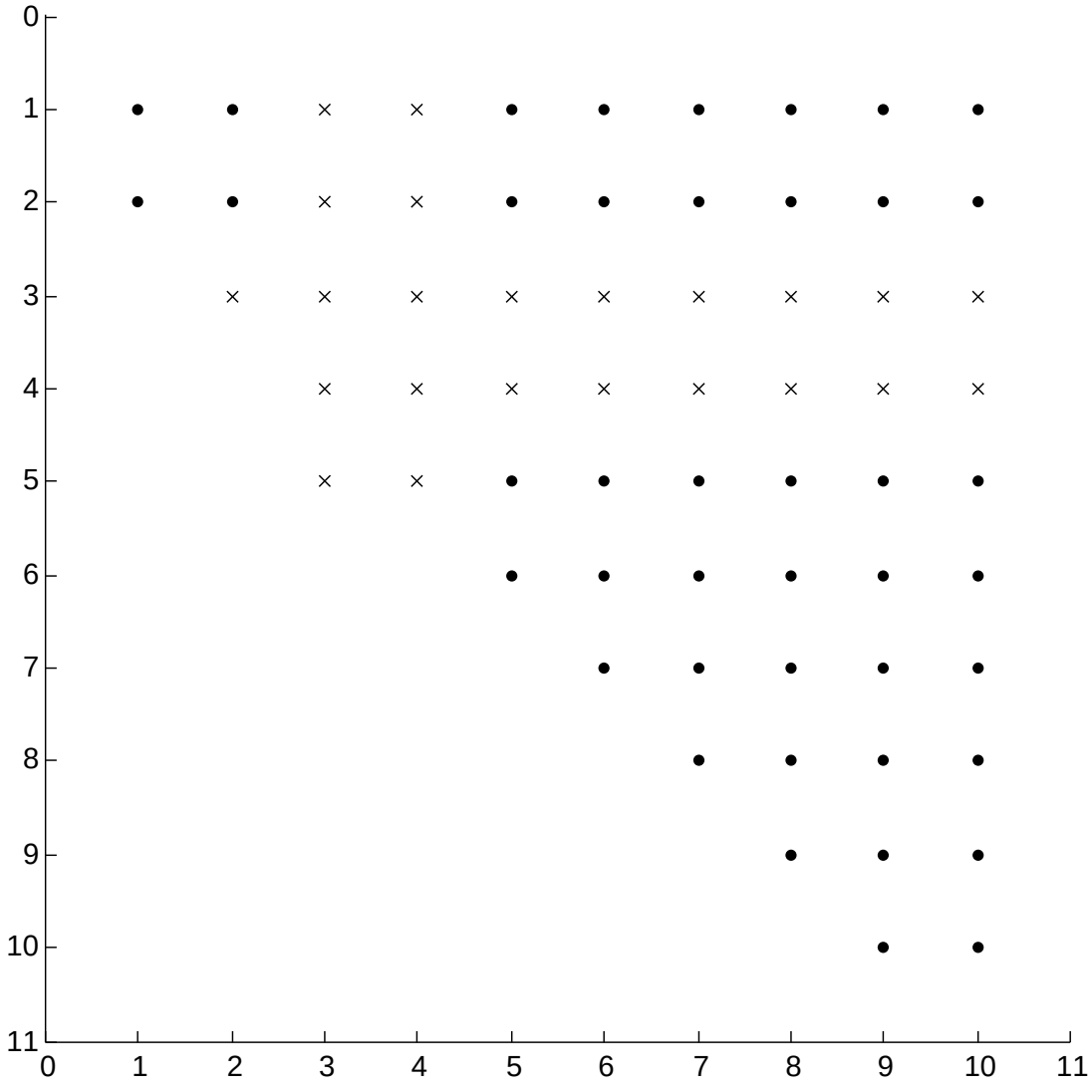

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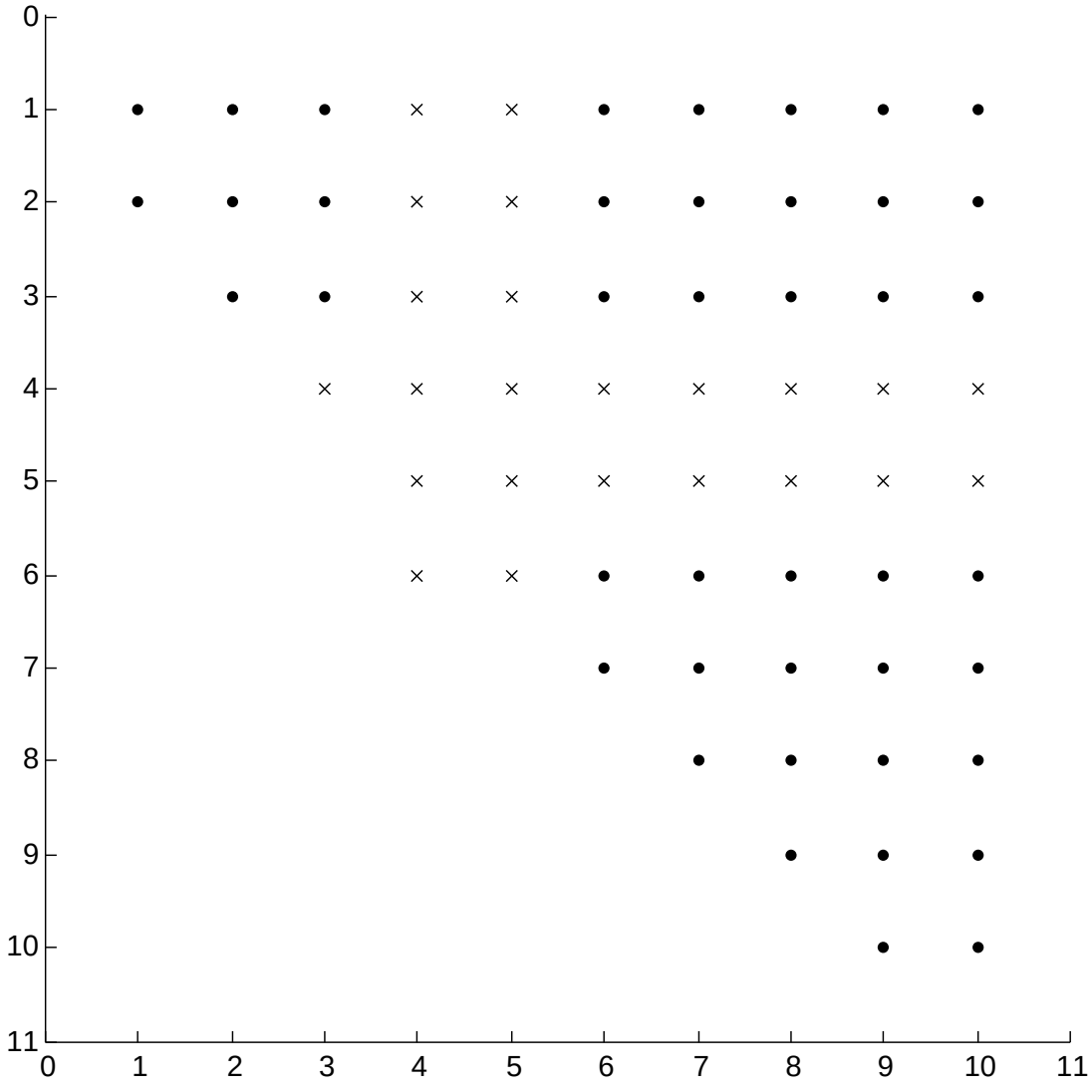

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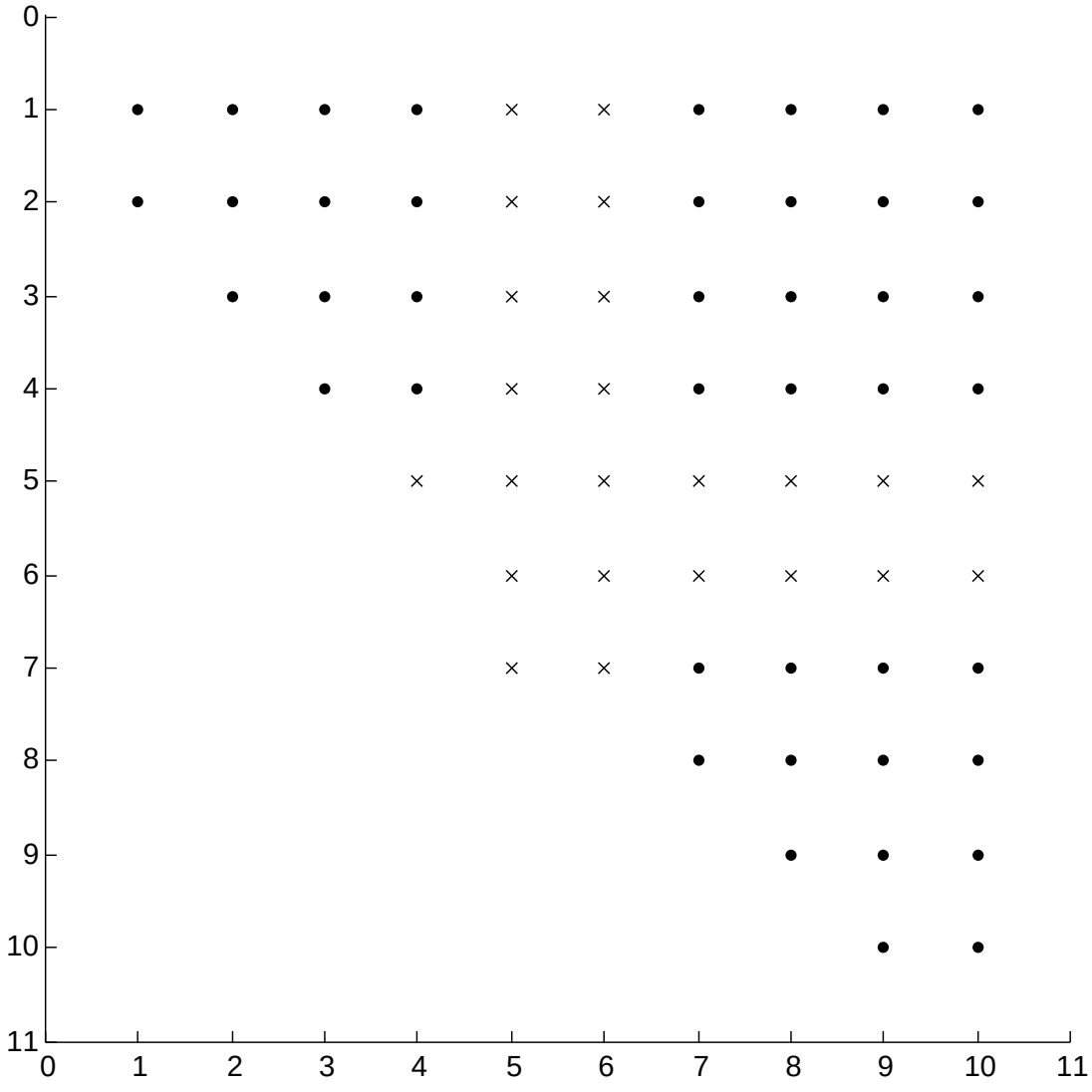

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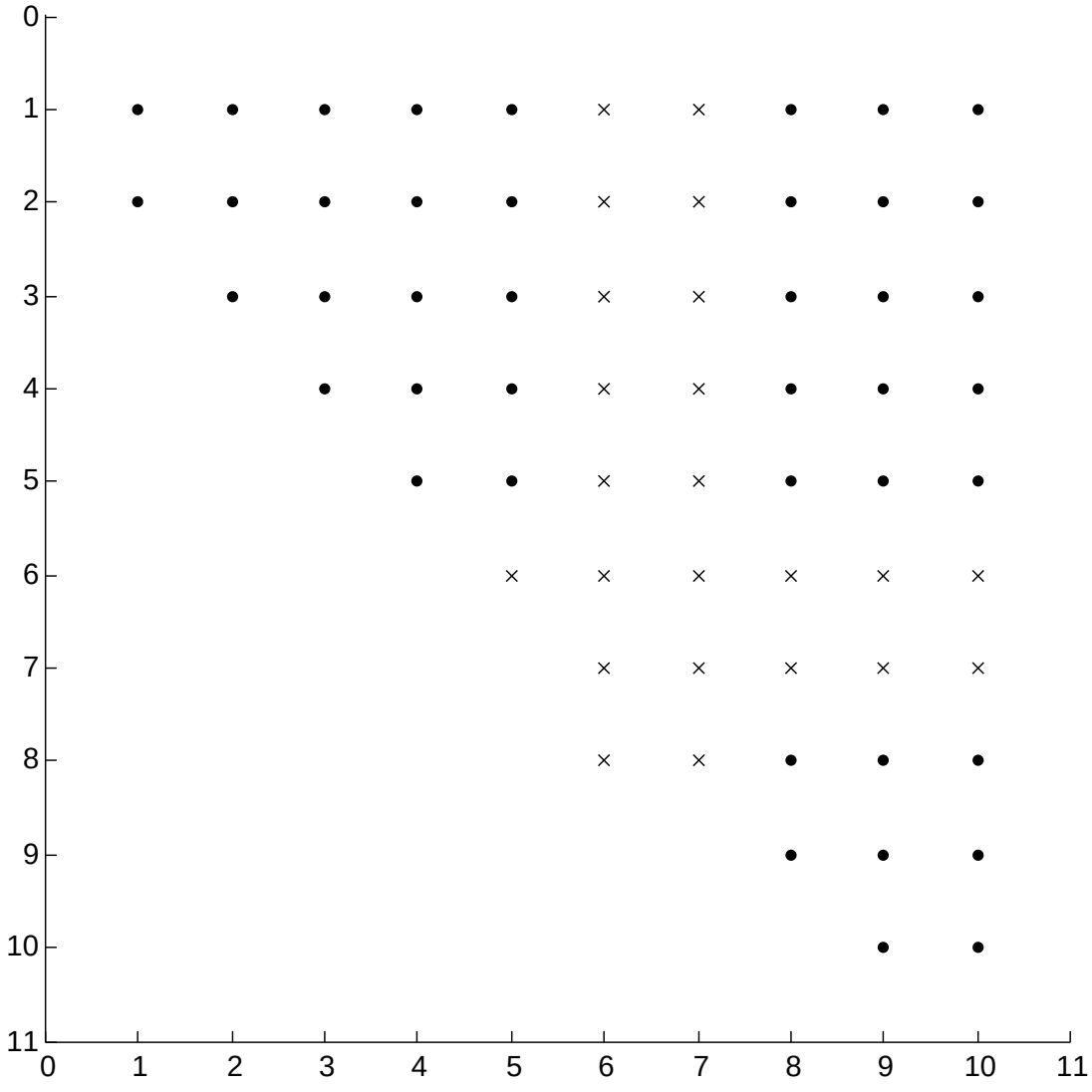

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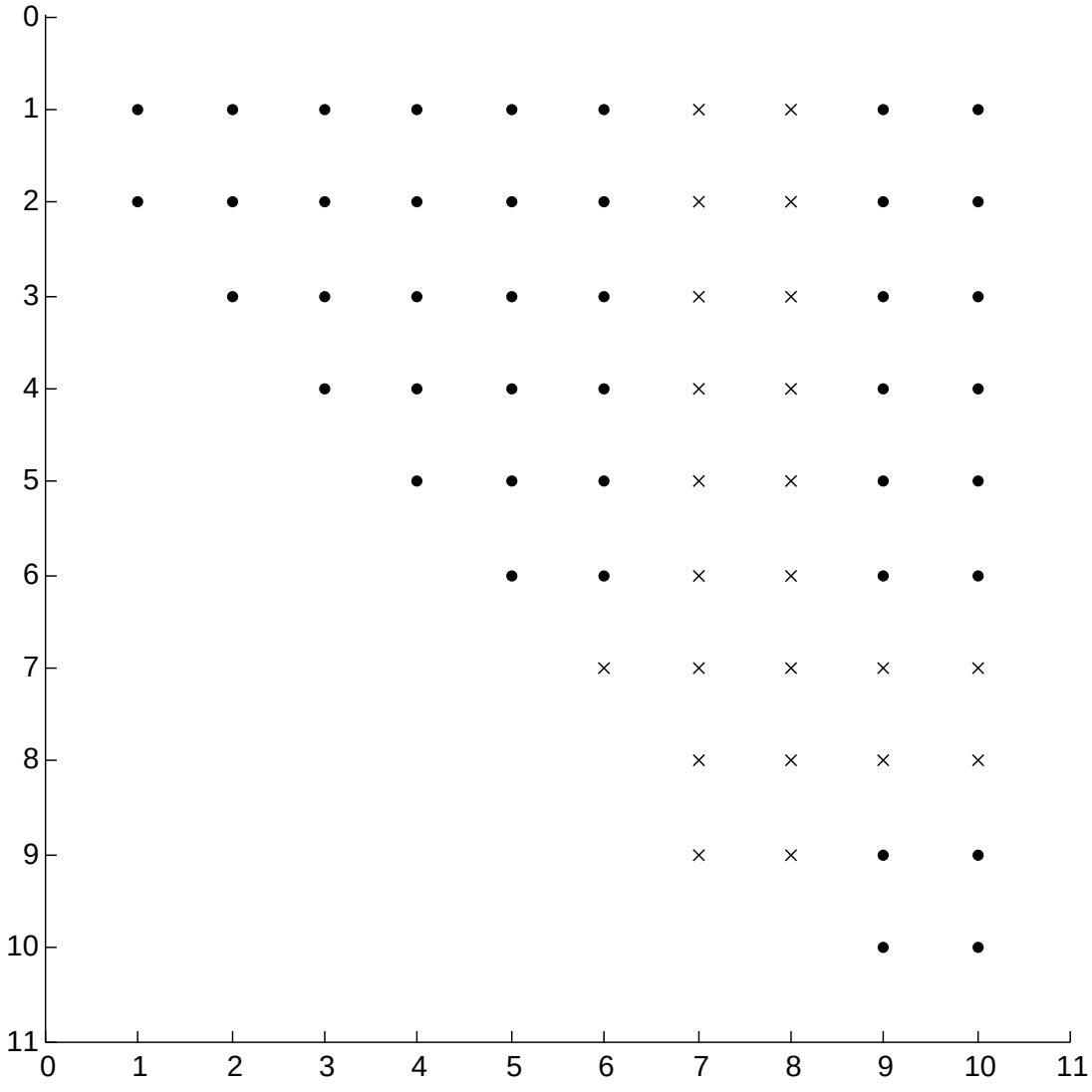

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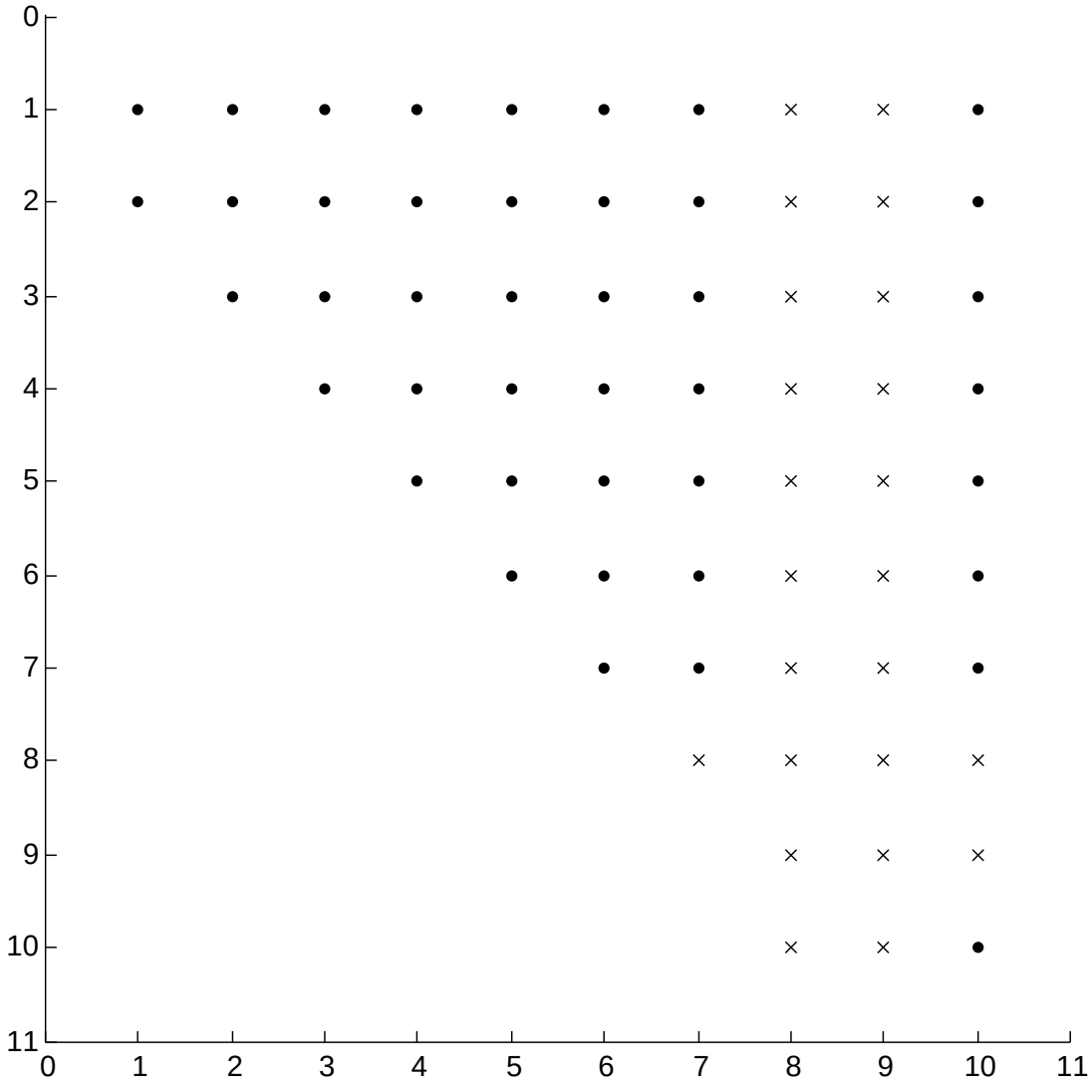

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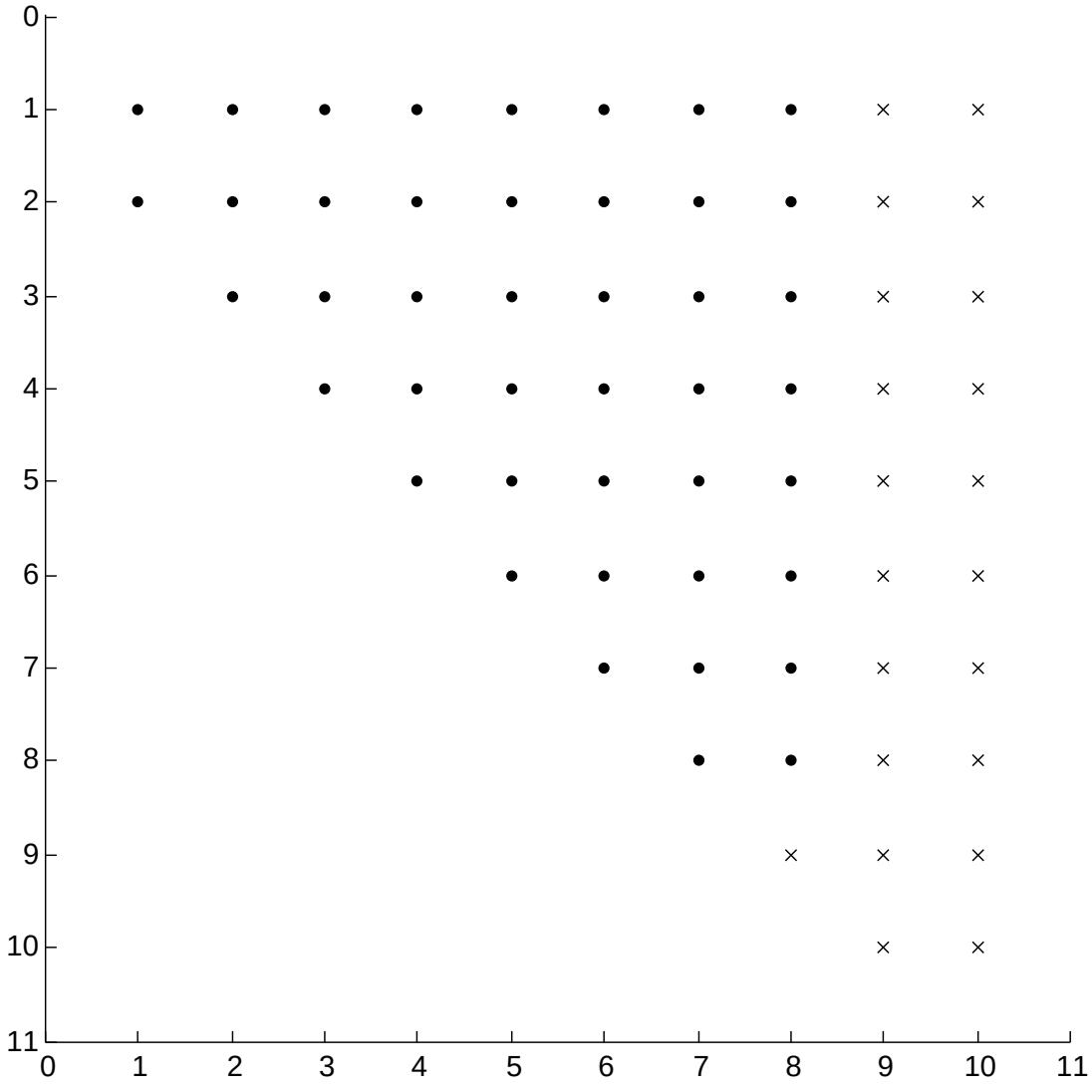

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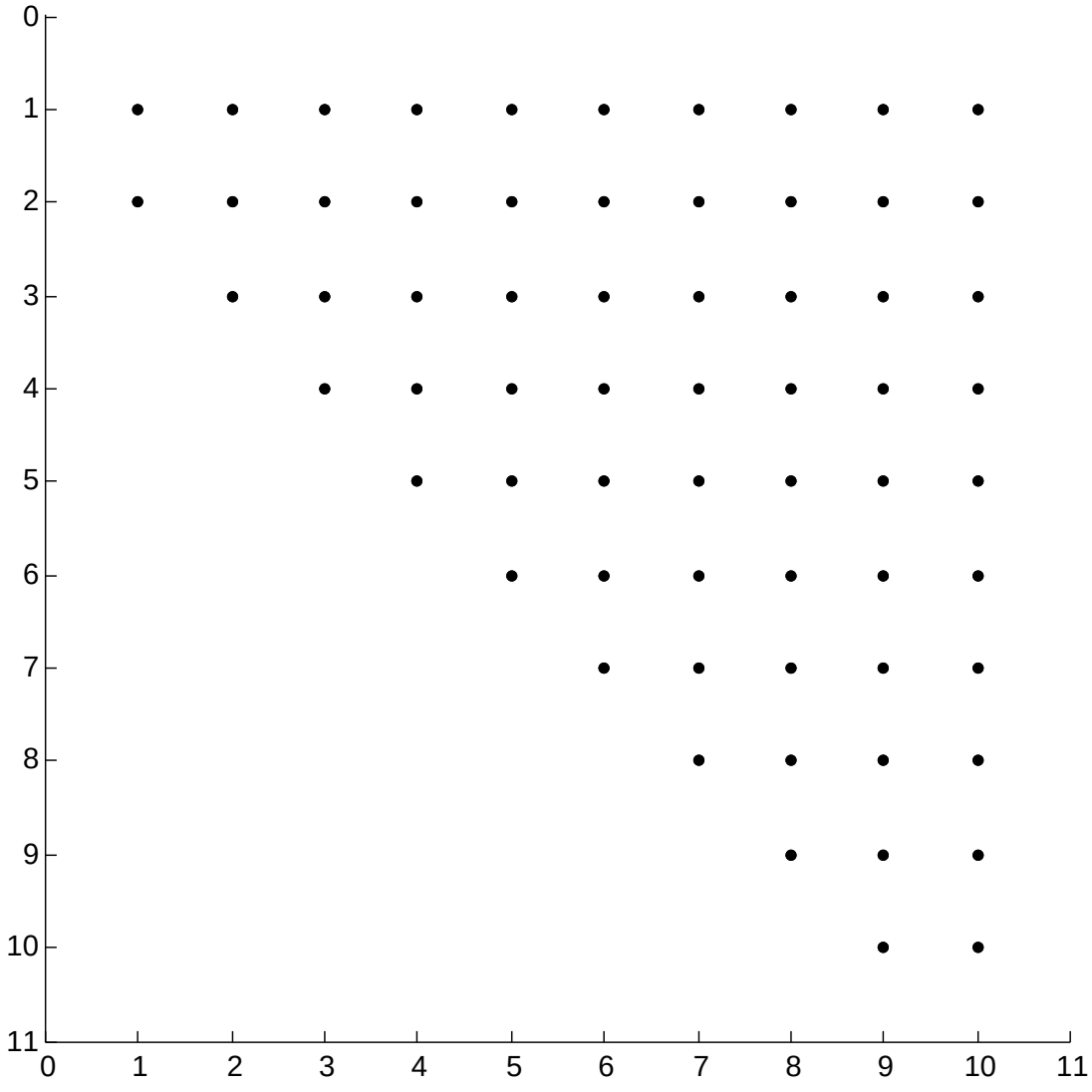

Accelerating QR

Have examples of how to do QR faster:

- Naive implementation $\Longrightarrow$ Hessenberg QR
- Tridiagonal QR (symmetric and skew problems)
- Unitary Hessenberg QR

Keys to fast QR:

- Find a structure preserved by the iteration
- Find a low-complexity representation for that structure

Rank symmetry

Call A *rank-symmetric* if rank$(A_{12}) =$ rank(A_{21}) for any 2-by-2 blocking of A with square A_{11} and A_{22}. Examples:

- Symmetric matrices
- Skew-symmetric matrices
- Orthogonal matrices (by the CS decomposition)
- J-orthogonal matrices (by hyperbolic CS decomposition)

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Examples of rank-symmetric + low rank:

- Companion matrices
- Problems which lose self-adjointness at boundary
- Linear oscillators with low-rank damping

Rank symmetric + low rank

Th: For A rank symmetric and L with rank k, both square block 2-by-2:

$$|\text{rank}(A_{12} + L_{12}) - \text{rank}(A_{21} + L_{21})| \leq 2k$$

Proof:

$\text{rank}(L_{ij}) \leq k$, so $|\text{rank}(A_{ij} + L_{ij}) - \text{rank}(A_{ij})| \leq k$.
Note $\text{rank}(A_{ij}) = \text{rank}(A_{ji})$ and apply triangle inequality.

Off-diagonal rank

Any matrix unitarily similar to C is orthogonal + rank 1. Therefore:

- Hessenberg forms similar to C have rank(super-diagonal block) ≤ 3.
- Real Schur forms similar to C have rank(super-diagonal block) ≤ 2.

(For polynomial matrices, make that $3d$ and $2d$).

SSS structure

Write Hessenberg matrices with low off-diagonal rank as narrow band matrix + SSS matrix.

$$H = B + \begin{bmatrix} 0 & U_1 V_2^T & U_1 W_2 V_3^T & U_1 W_2 W_3 V_4^T \\ 0 & 0 & U_2 V_3^T & U_2 W_3 V_4^T \\ 0 & 0 & 0 & U_3 V_4^T \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Write $H_{ij} = U_i W_{i+1} \dots W_{j-1} V_j$ for $i < j$ where $U_i \in \mathbb{R}^{m_b \times 2k+1}$, $V_i \in \mathbb{R}^{m_b \times 2k+1}$, and $W_i \in \mathbb{R}^{2k+1 \times 2k+1}$. Make the block size $m_b \geq 2k+1$.

Total storage cost: $O(nk)$.

SSS structure transformed

$$\begin{array}{cccc} B_{11} & U_1V_2^T & U_1W_2V_3^T & U_1W_2W_3V_4^T \\ B_{21} & B_{22} & U_2V_3^T & U_2W_3V_4^T \\ & B_{32} & B_{33} & U_3V_4^T \\ & & B_{43} & B_{44} \end{array}$$

- Start with an SSS representation

SSS structure transformed

$$
\begin{array}{cccc}
\mathbf{B_{11}} & \mathbf{U_1}V_2^T & \mathbf{U_1}W_2V_3^T & \mathbf{U_1}W_2W_3V_4^T \\
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$$

- Start with an SSS representation
- Bulge chase in B_{11}: changes B_{11} and U_1

SSS structure transformed

$$
\begin{array}{cccc}
\mathbf{B_{11}} & \mathbf{B_{12}} & \mathbf{\hat{U}_1} V_3^T & \mathbf{\hat{U}_1} W_3 V_4^T \\
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- Start with an SSS representation
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- *Merge* first two blocks and chase bulge across boundary

SSS structure transformed

$$\begin{array}{cccc} B_{11} & U_1 \mathbf{V_2}^T & U_1 W_2 V_3^T & U_1 W_2 W_3 V_4^T \\ B_{21} & \mathbf{B_{22}} & \mathbf{U_2} V_3^T & \mathbf{U_2} W_3 V_4^T \\ & B_{32} & B_{33} & U_3 V_4^T \\ & & B_{43} & B_{44} \end{array}$$

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- Continue until Hessenberg form is restored

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Row and column bases

Define C_j and G_j by the recurrences

$$C_1 = U_1 \text{ and } C_j = \begin{bmatrix} C_{j-1}W_j \\ U_j \end{bmatrix} \text{ for } j > 1$$

$$G_n = V_n \text{ and } G_j = \begin{bmatrix} V_v \\ G_{j+1}W_j^T \end{bmatrix} \text{ for } j < n.$$

C_j and G_j are row and column bases for the submatrix left of block column j and above block row j.

All C_j orthonormal: left proper form.
All G_j orthonormal: right proper form.

Splitting blocks

Start with C_{i-1} and G_{i+1} orthonormal.

$$\begin{bmatrix} H_{1,i} & \dots & H_{1,n} \\ \vdots & & \vdots \\ H_{i,i} & \dots & H_{i,n} \end{bmatrix} = \begin{bmatrix} C_{i-1} & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} V_i^T & W_i \\ H_{ii} & U_i \end{bmatrix} \begin{bmatrix} 0 & G_{i+1} \\ I & 0 \end{bmatrix}^T .$$

$$\begin{bmatrix} V_j^T & W_j \\ B_{jj} & U_j \end{bmatrix} \rightarrow \begin{bmatrix} V_j^{\alpha T} & W_j^{\alpha} V_j^{\beta T} & W_j^{\alpha} W_j^{\beta} \\ B_{jj}^{\alpha\alpha} & U_j^{\alpha} V_j^{\beta T} & U_j^{\alpha} W_j^{\beta} \\ B_{jj}^{\beta\alpha} & B_{jj}^{\beta\beta} & U_j^{\beta} \end{bmatrix}$$

Do pivoted QR or SVD decomposition to split U, V, W.

Choose $\begin{bmatrix} W_j^{\alpha} \\ U_j^{\alpha} \end{bmatrix}$ with orthonormal columns.

Balancing

Want to *balance* matrix to improve accuracy.
But general diagonal scaling destroys structure!

However: $|C|$ is a companion matrix with Perron vector:

$$x_i = \lambda^i$$

Let

$$D = \mathsf{diag}(x_i^{-1}) = \mathsf{diag}(\lambda^{-i}).$$

Then DCD^{-1}

- Is optimally balanced in the ∞-norm.
- Is $\lambda\times$ orthogonal + low rank
- Is scaling the polynomial indeterminate by λ.

Implementation

Modified DLAHQR (basic double-shift QR) to use the new data structure.

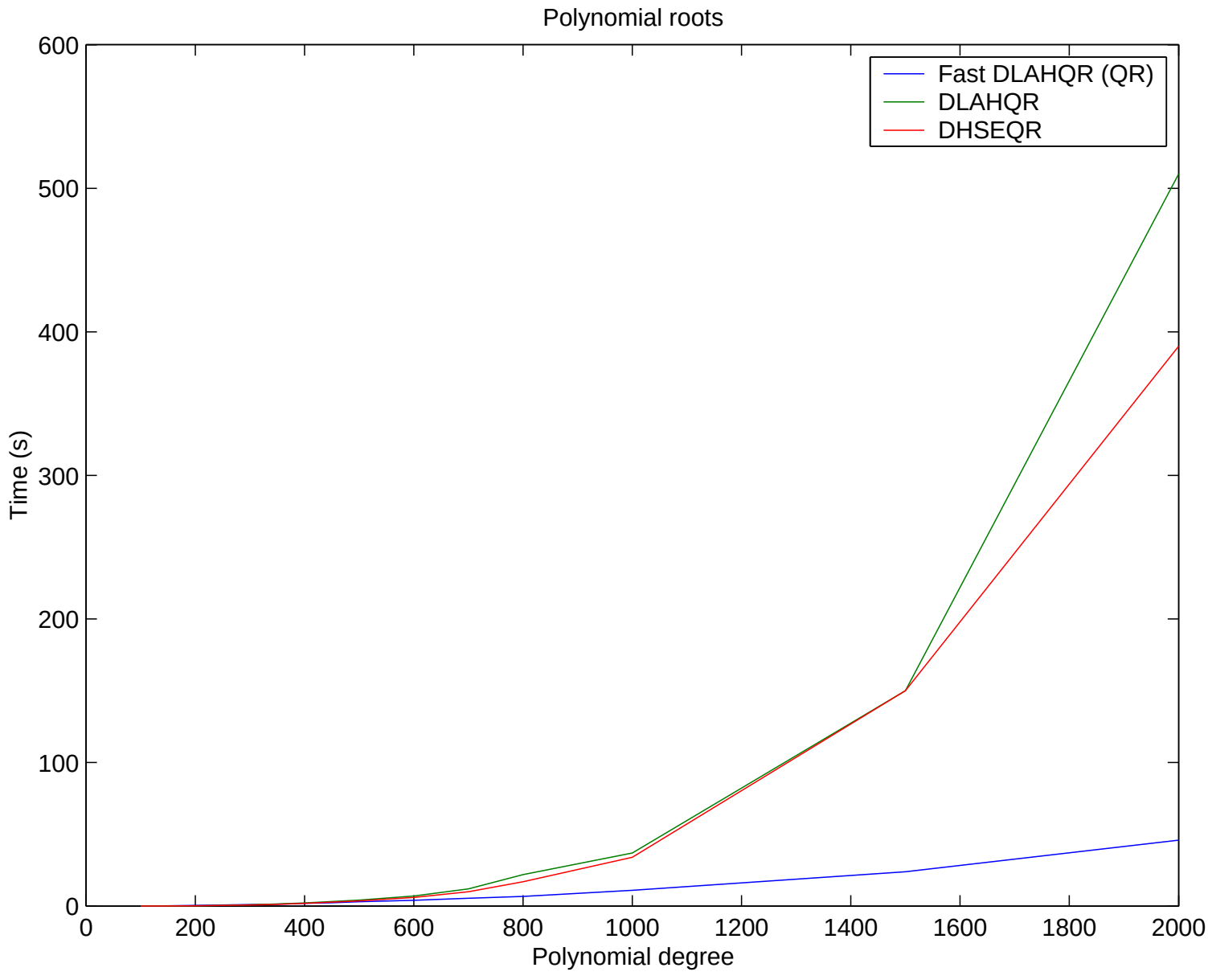
- Convert to right proper form.
- Choose shifts (logic from LAPACK).
- Bulge chase top to bottom / convert to left proper form.
- Check for convergence / deflate (logic from LAPACK).

Most of the code accesses data in the band part of the structure. This text is *identical* to the standard code – just change `LDA`.

Performance

- Compared against LAPACK DLAHQR and DHSEQR
- Compiled using g77/gcc with -O2 flag
- LAPACK with standard optimizations, ATLAS BLAS
- P4 processor at 1.5 GHz
- Polynomials of degree 100-2000.

Performance: QR-based



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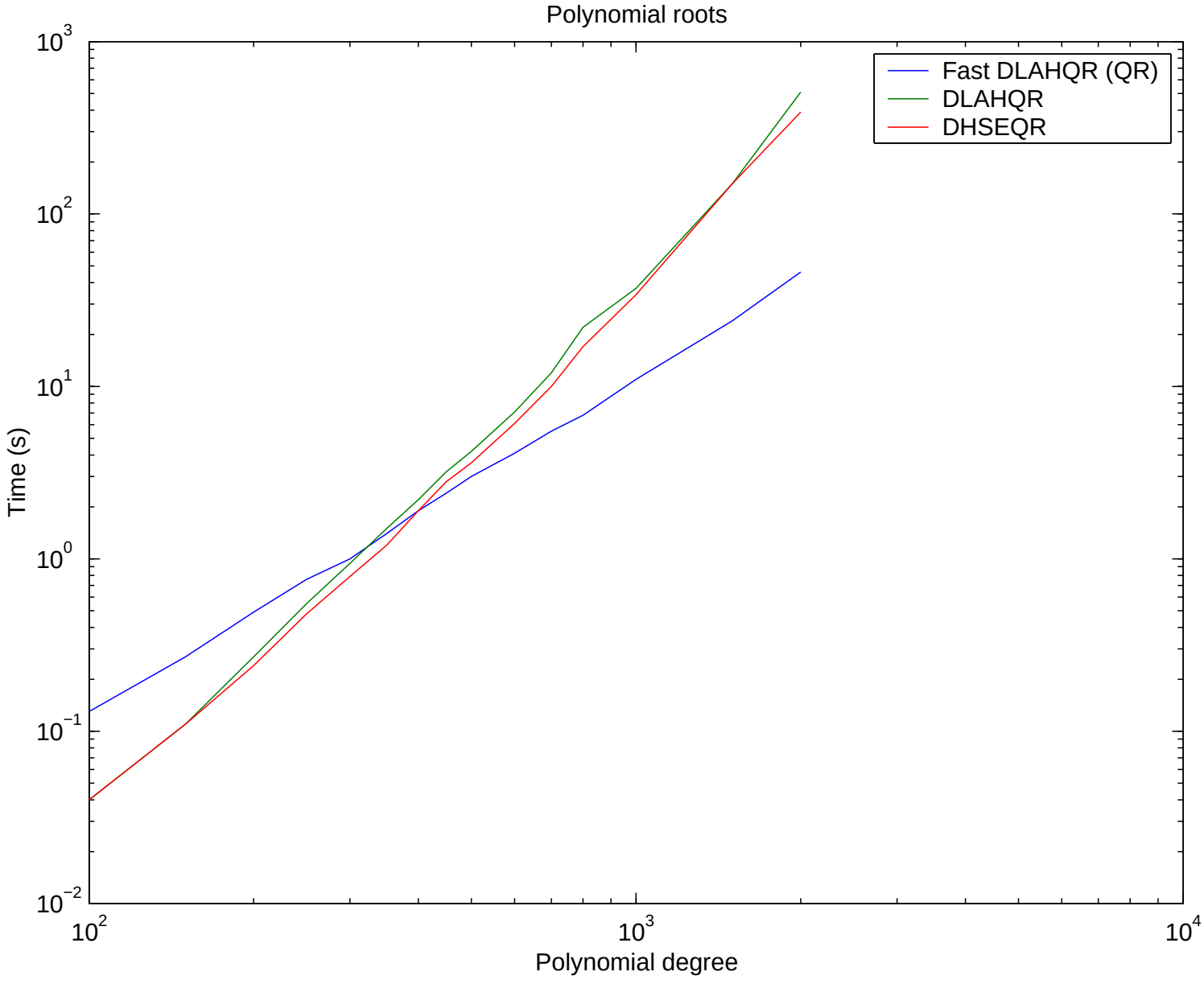
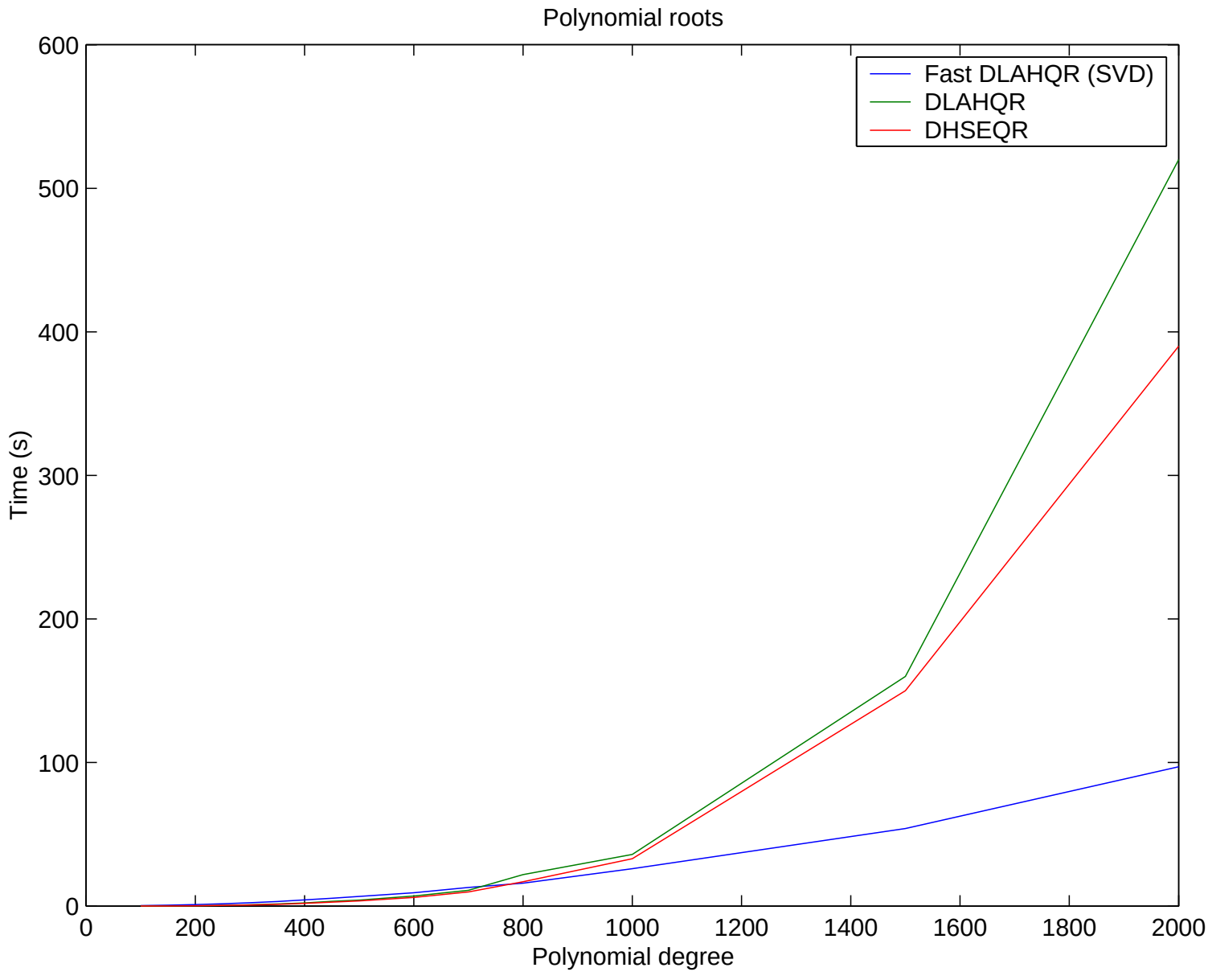


Performance: SVD-based



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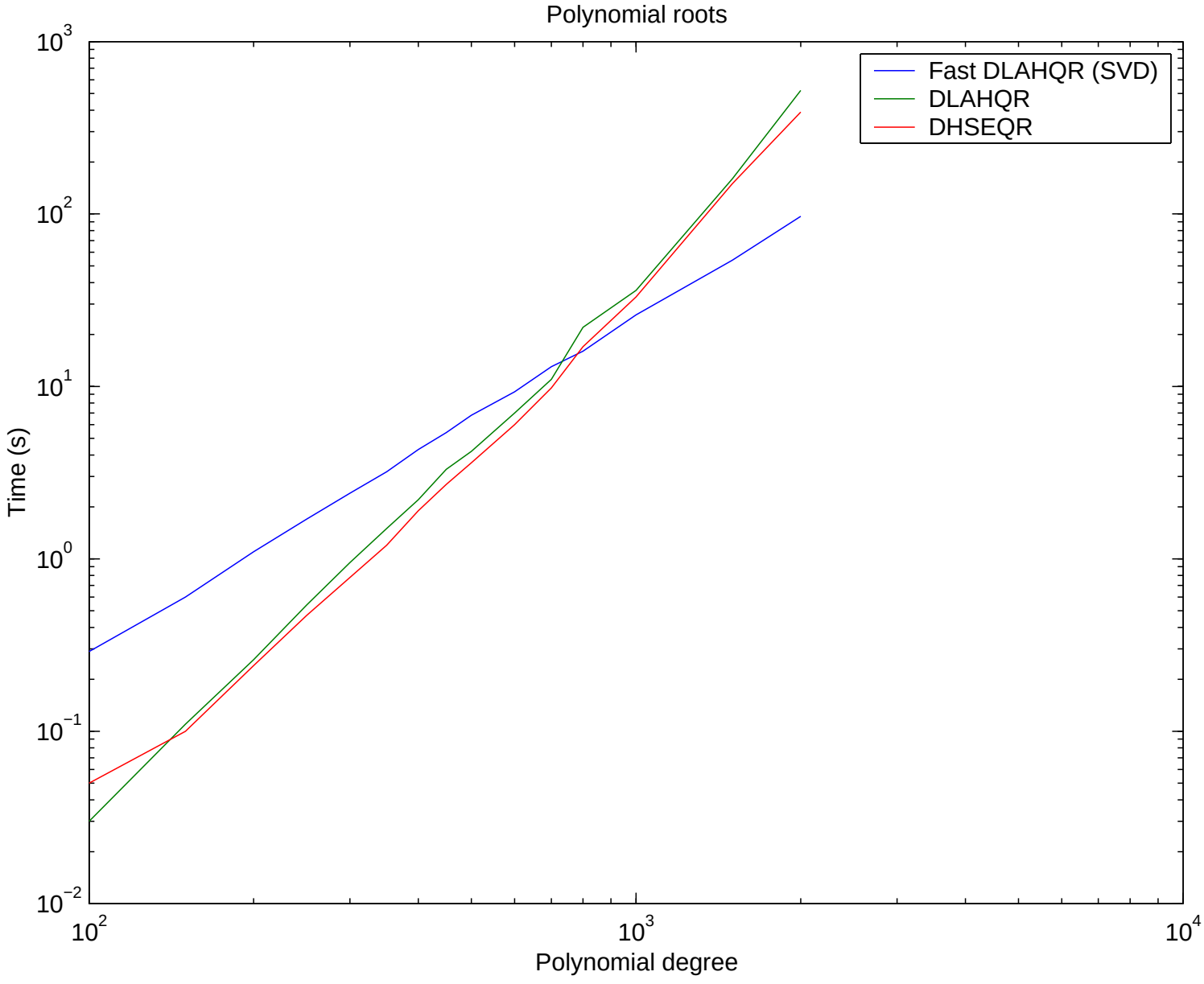

Conclusions

- Hessenberg({ symmetric, skew, unitary } + low rank) has low off-diagonal rank.
- Applies to (matrix) polynomial root finding, some damped vibration calculations.
- Can use low-rank structure for fast bulge-chasing.
- Can use-use most existing QR lore and code.
- Appears backward stable with SVD-based splitting.