A Fast Nonsymmetric Eigensolver for Structured Matrices

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Outline

- QR iteration
- Rank symmetry and nearly rank-symmetric matrices
- Examples of nearly rank-symmetric matrices
- A fast QR variant
- Stability and balancing
- Implementation and performance

QR iteration

Goal: Convert A to a quasi-upper-triangular matrix T by a sequence of orthogonal similarities.

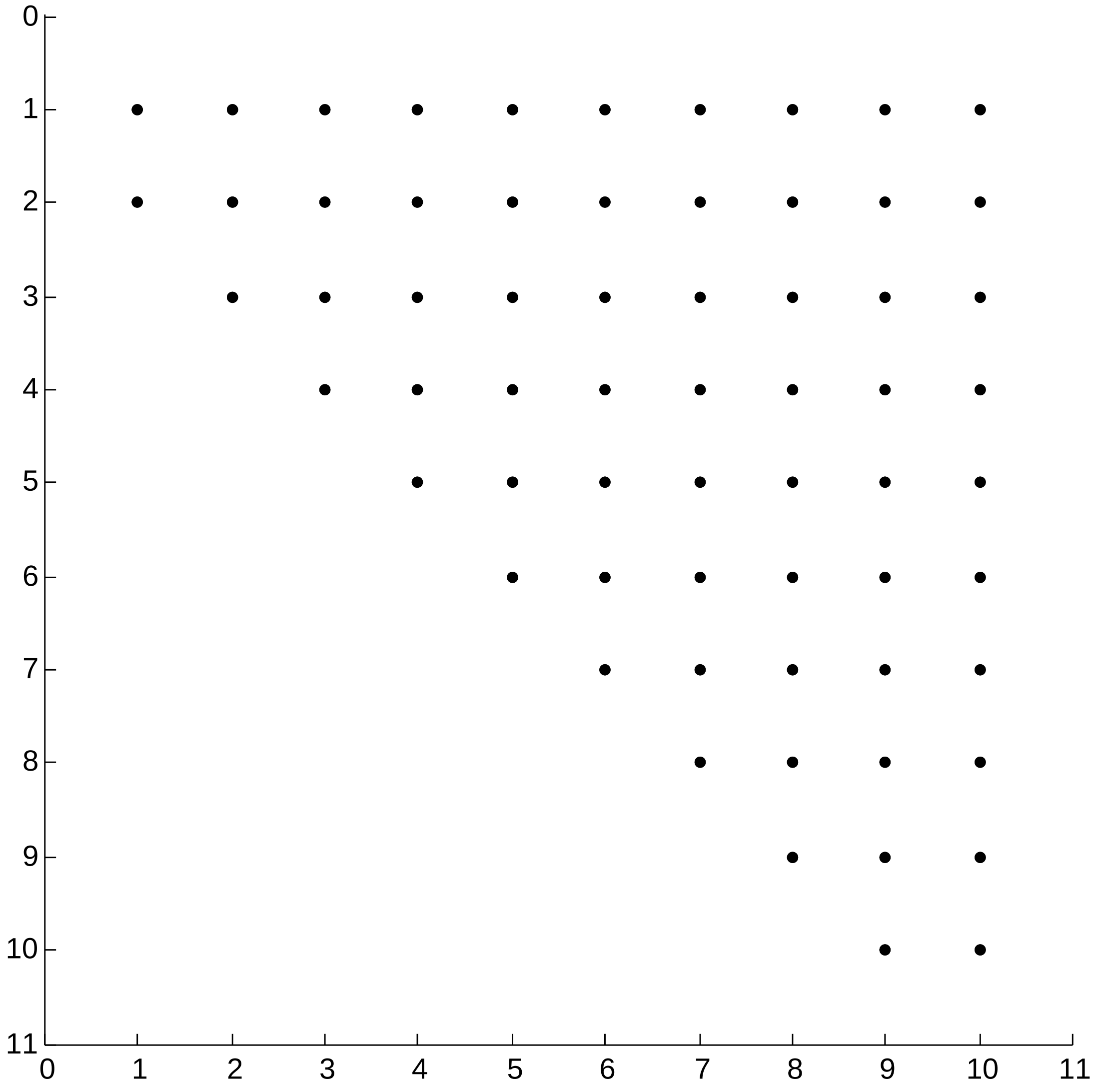
- Choose a shift σ_i
- $A_i - \sigma_i I = Q_i R_i$
- $A_{i+1} = R_i Q_i + \sigma_i I = Q_i^T A_i Q_i$

Cost per iteration: $O(n^3)$. Total cost is $O(n^4)$.

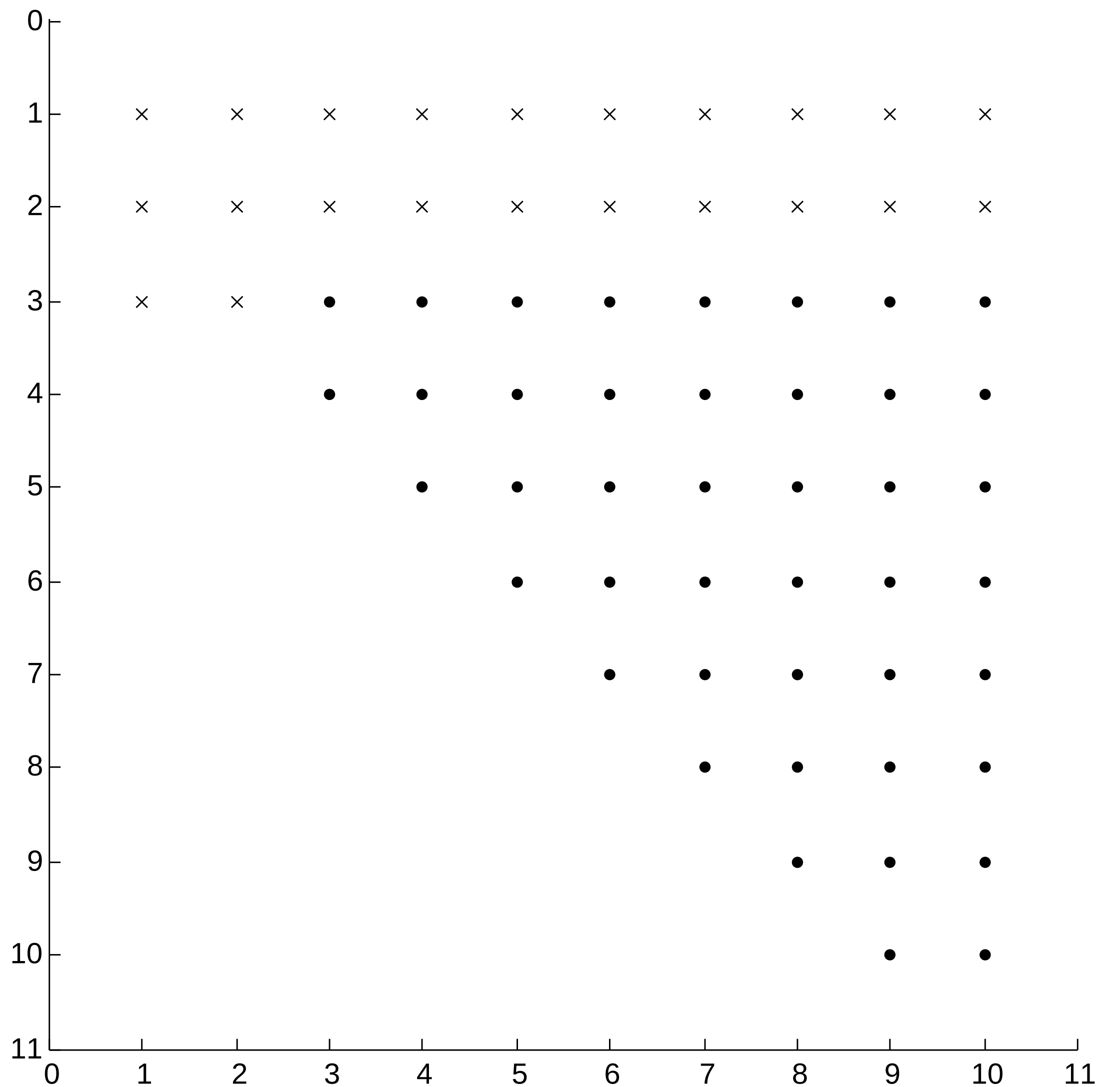
Hessenberg QR iteration

- Find an upper Hessenberg matrix $H = Q^T A Q$
- QR iteration preserves the Hessenberg structure
- Q is determined up to signs by first column
- Implicitly apply Q by *bulge-chasing*
- Cost per iteration is now $O(n^2)$.

Hessenberg QR iteration



Hessenberg QR iteration



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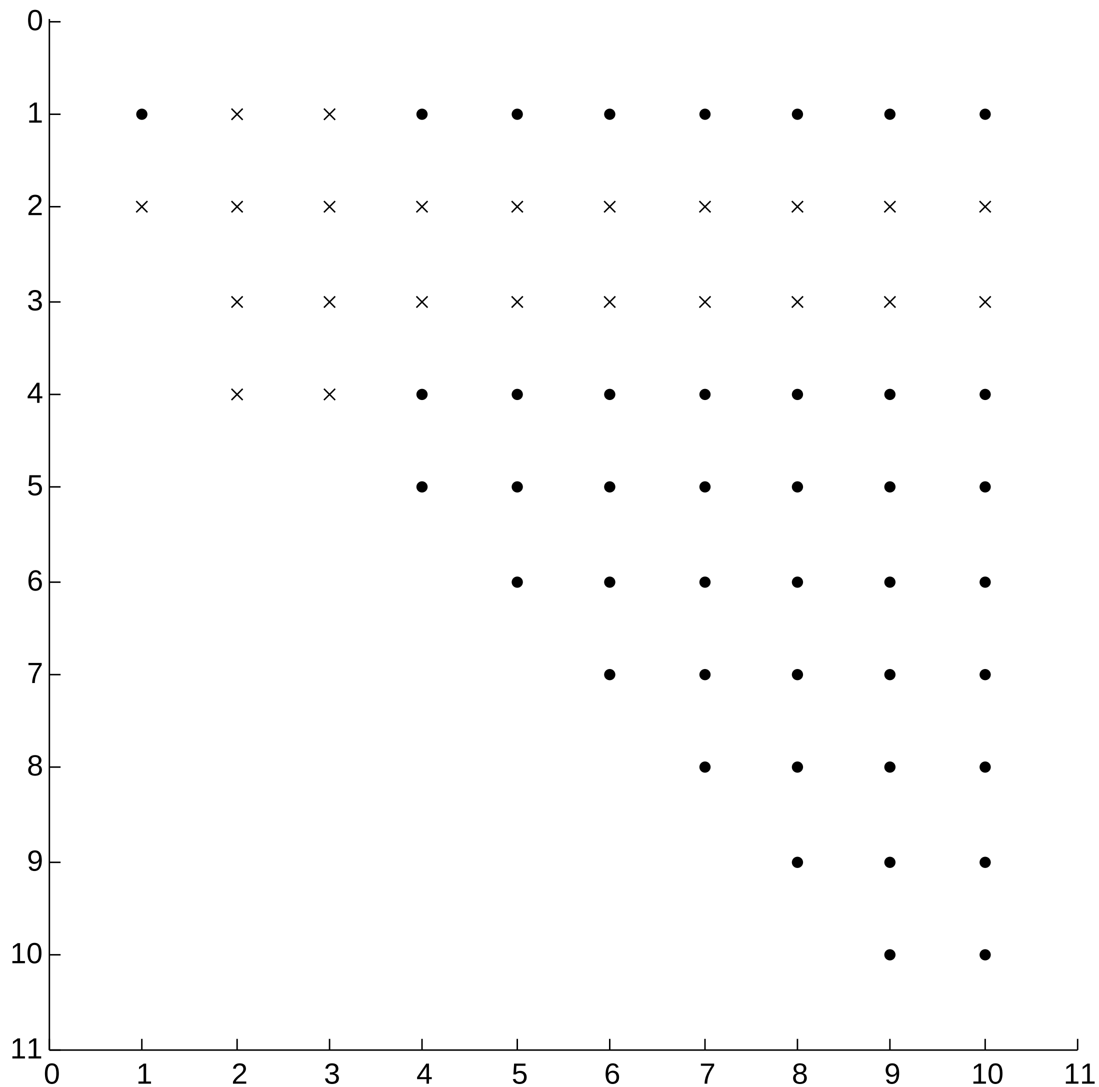

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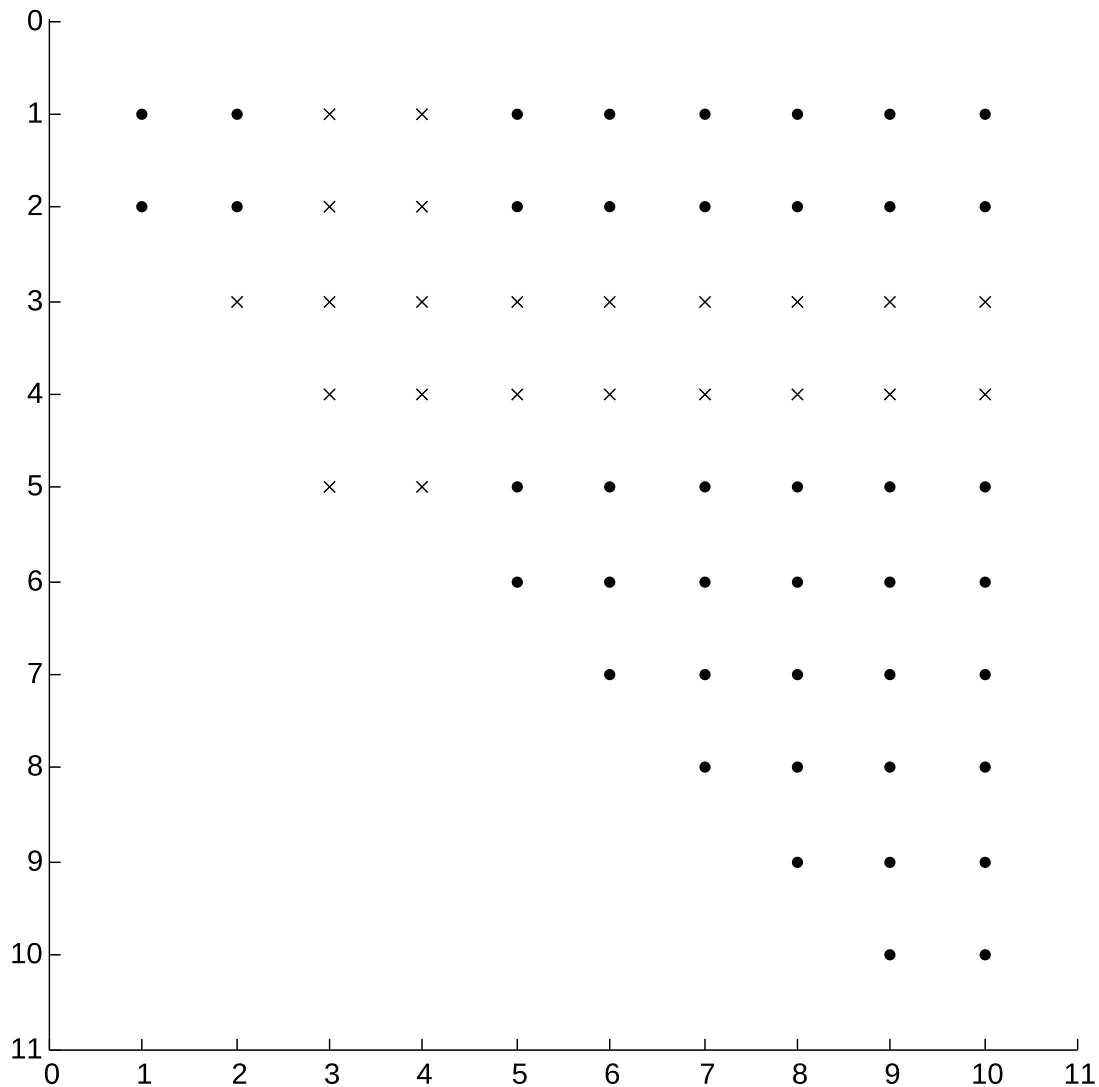
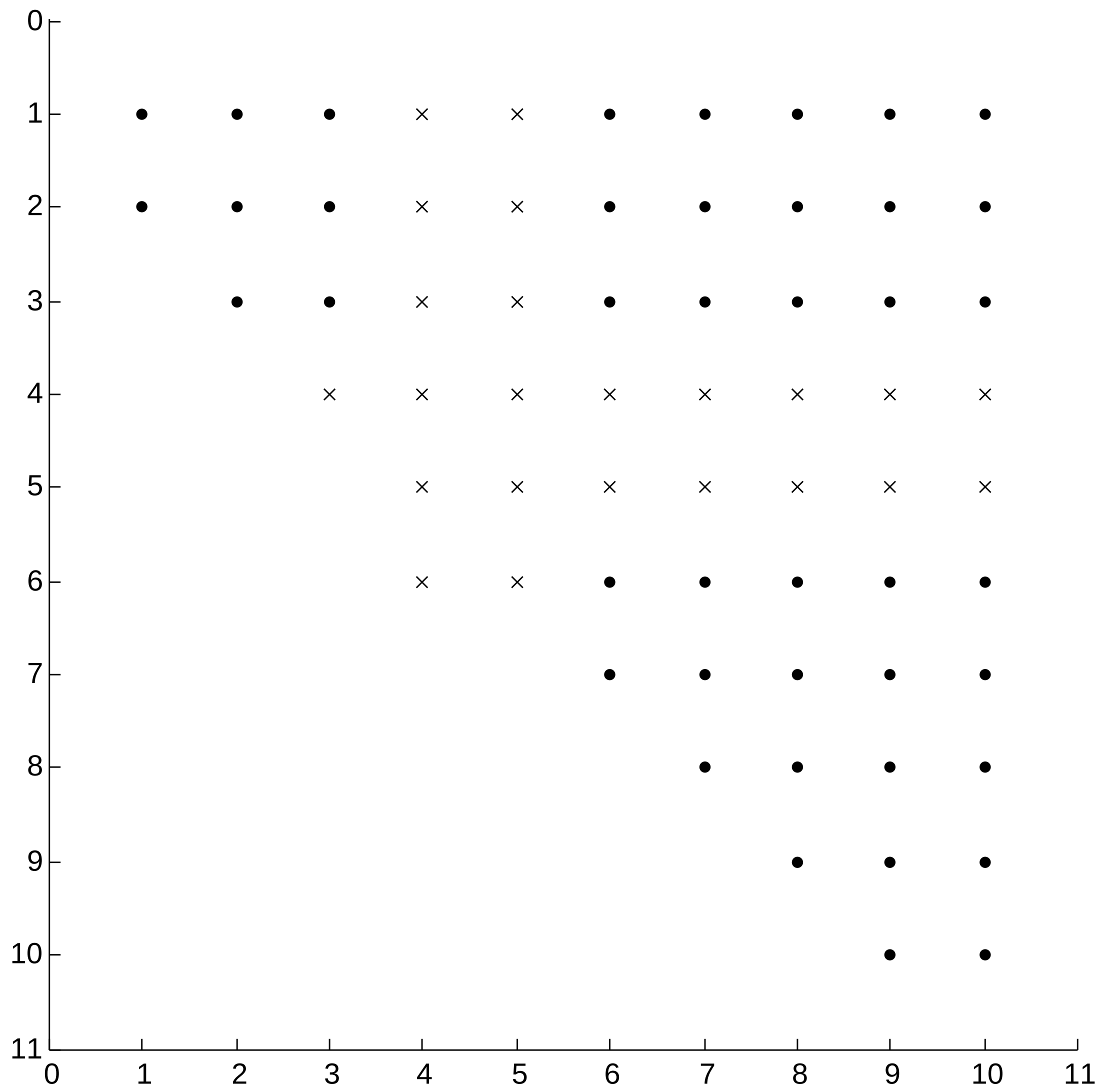
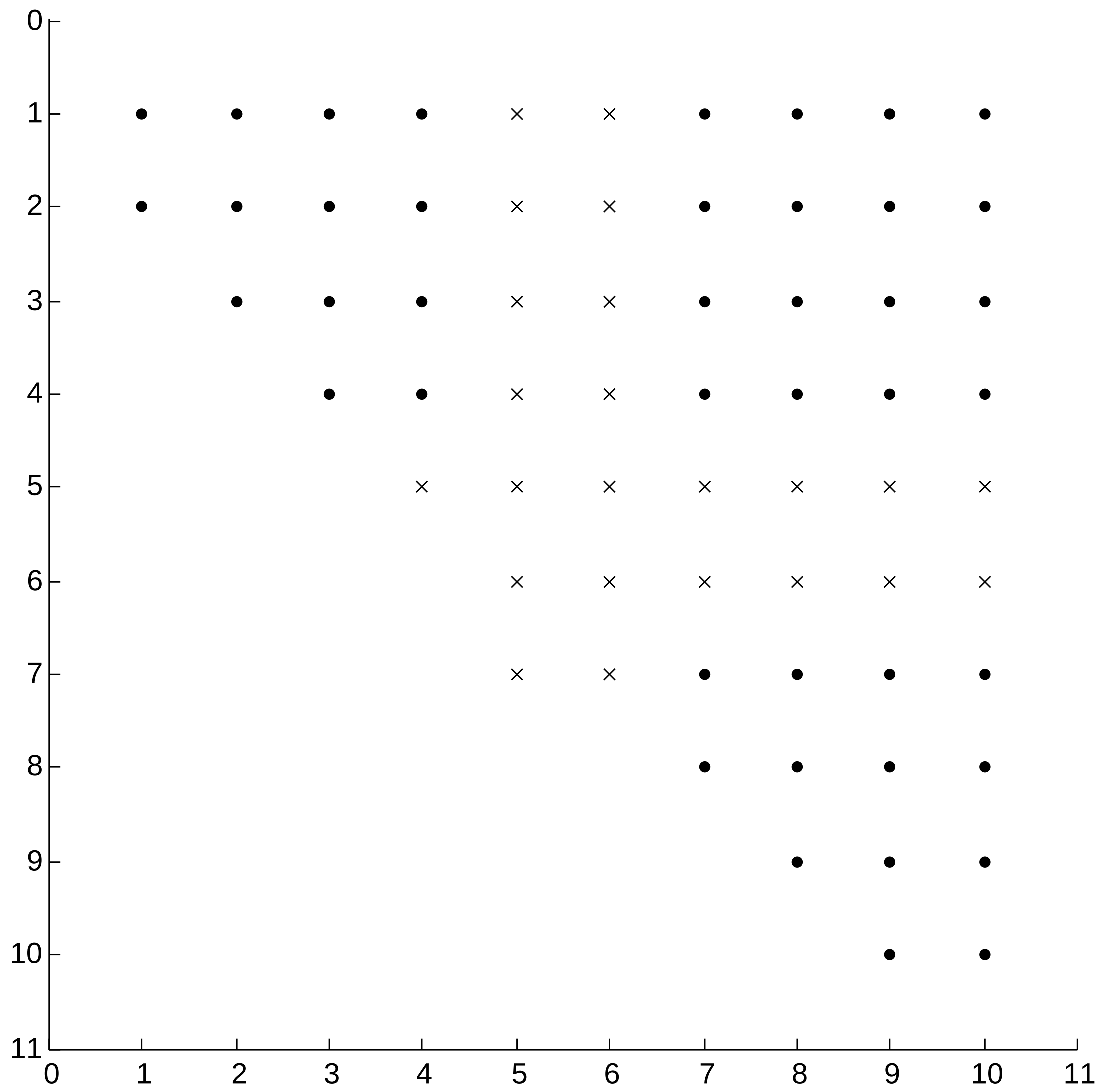


Hessenberg QR iteration



Hessenberg QR iteration



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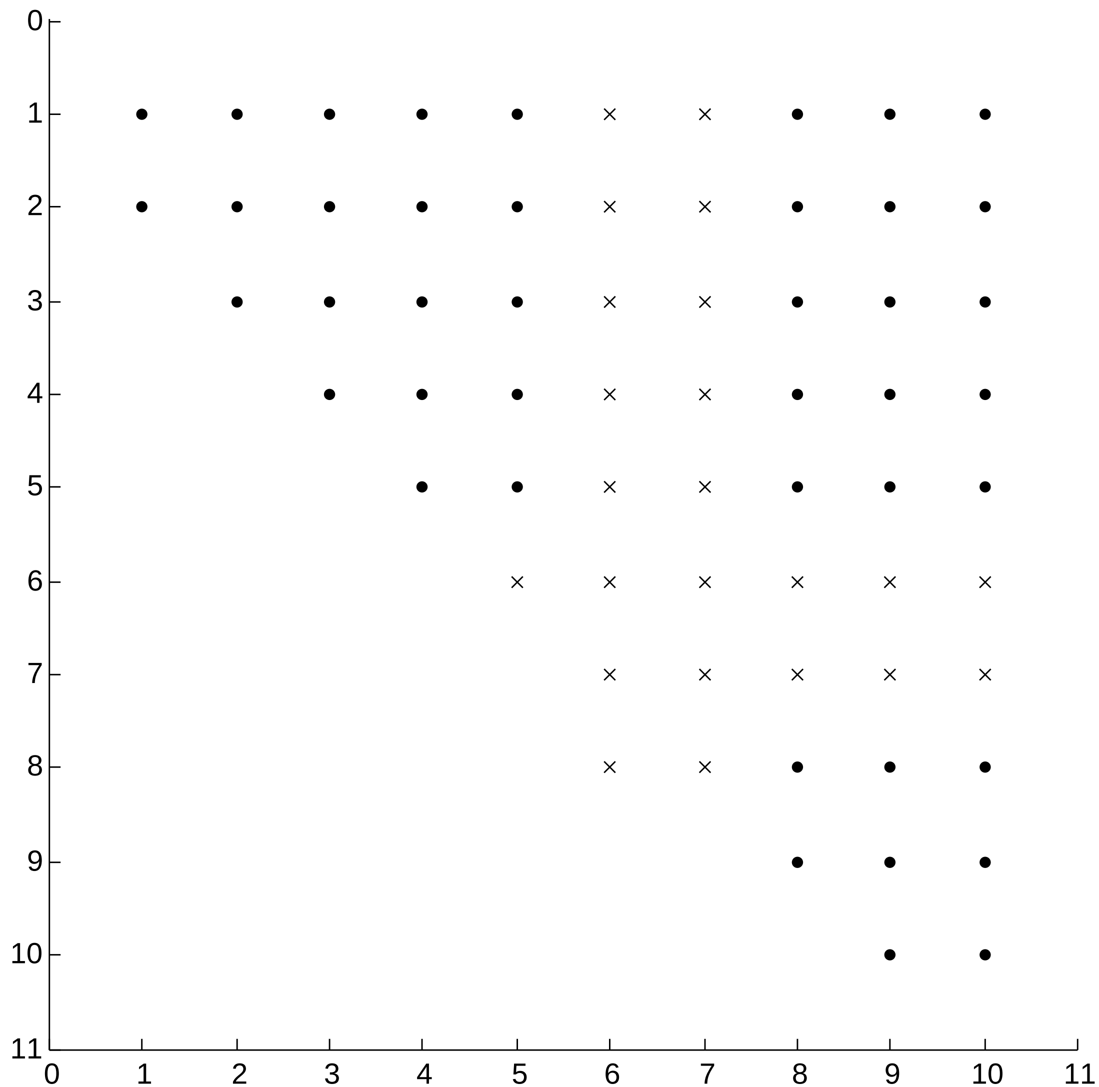

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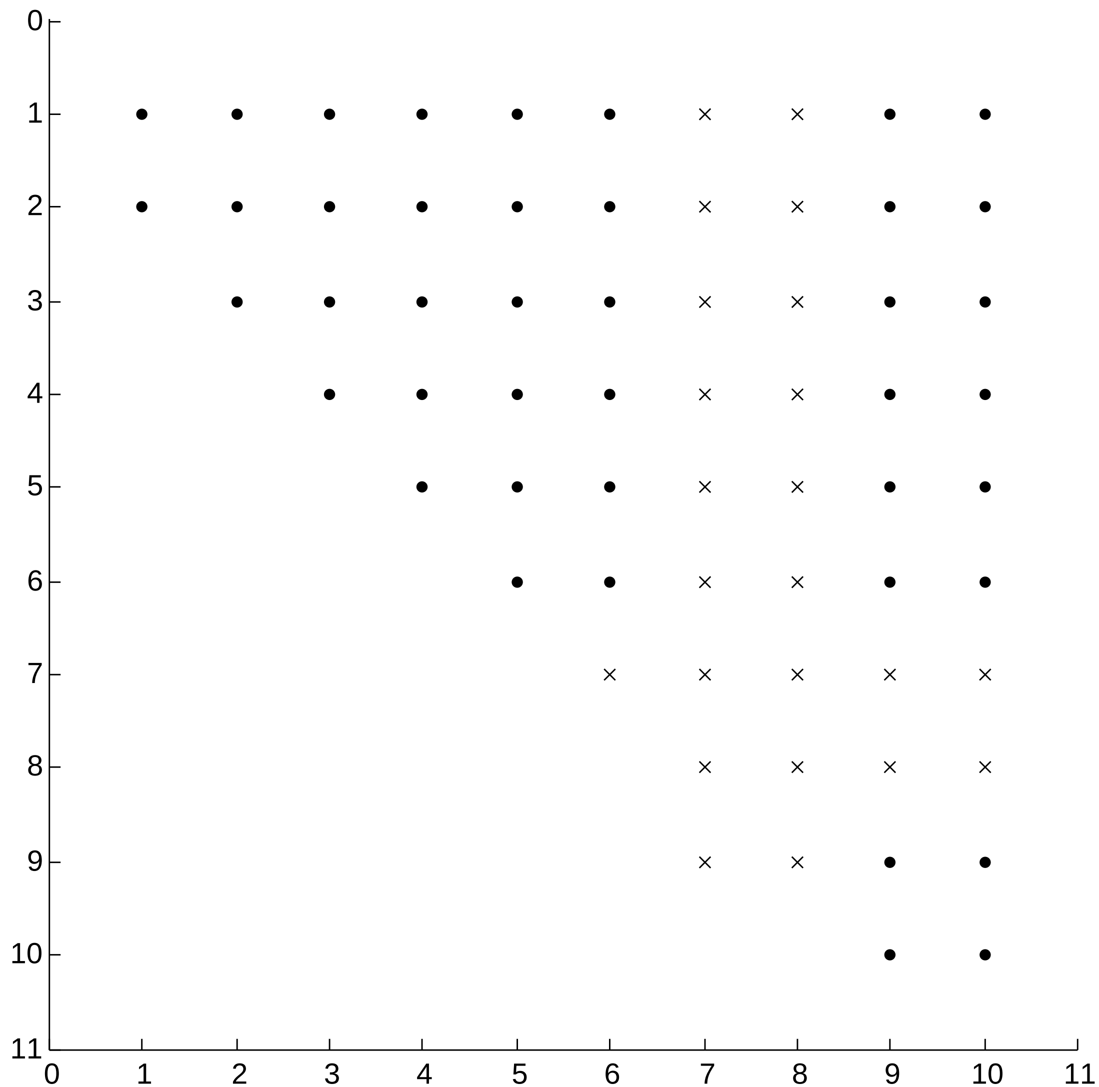
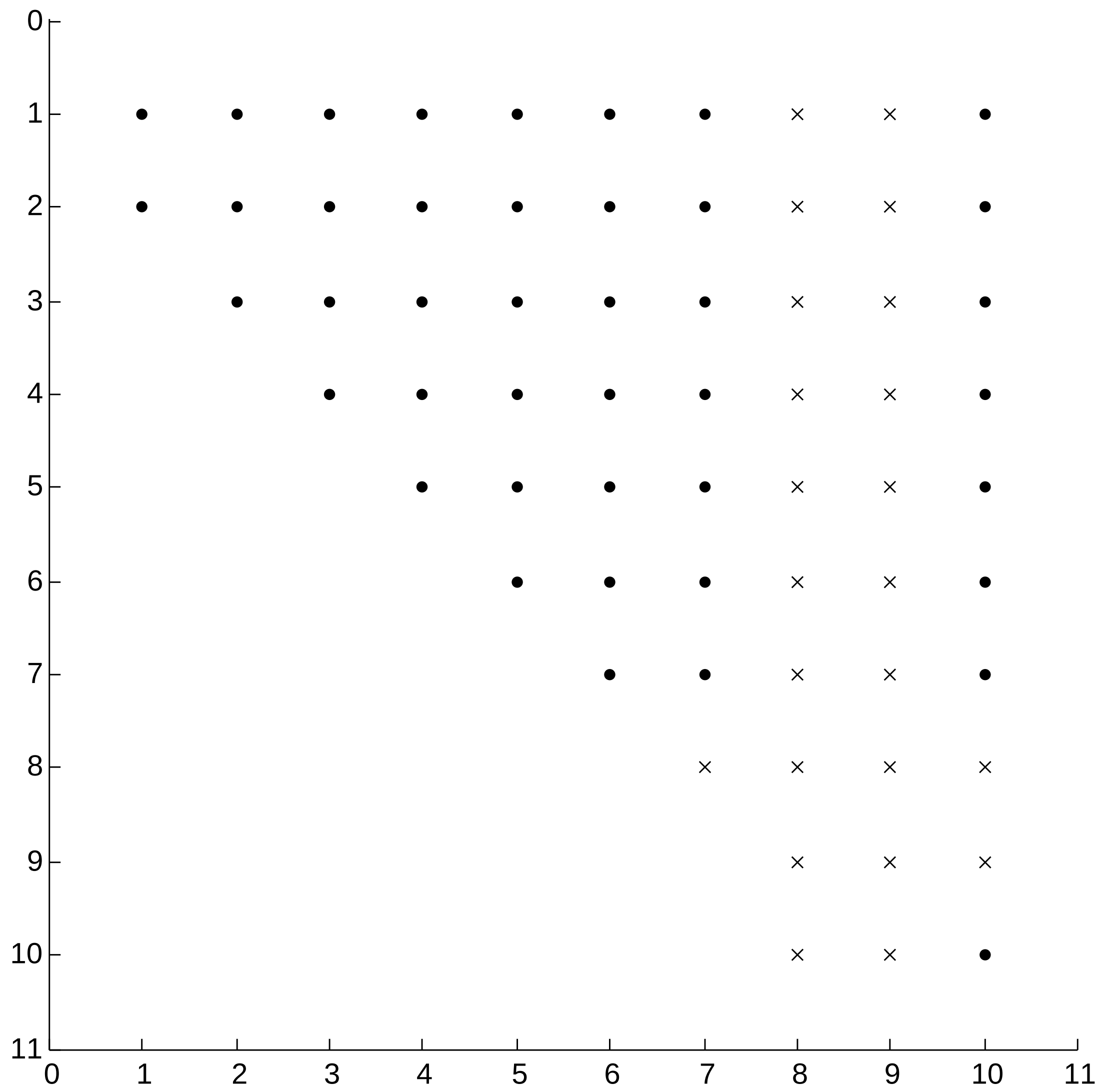
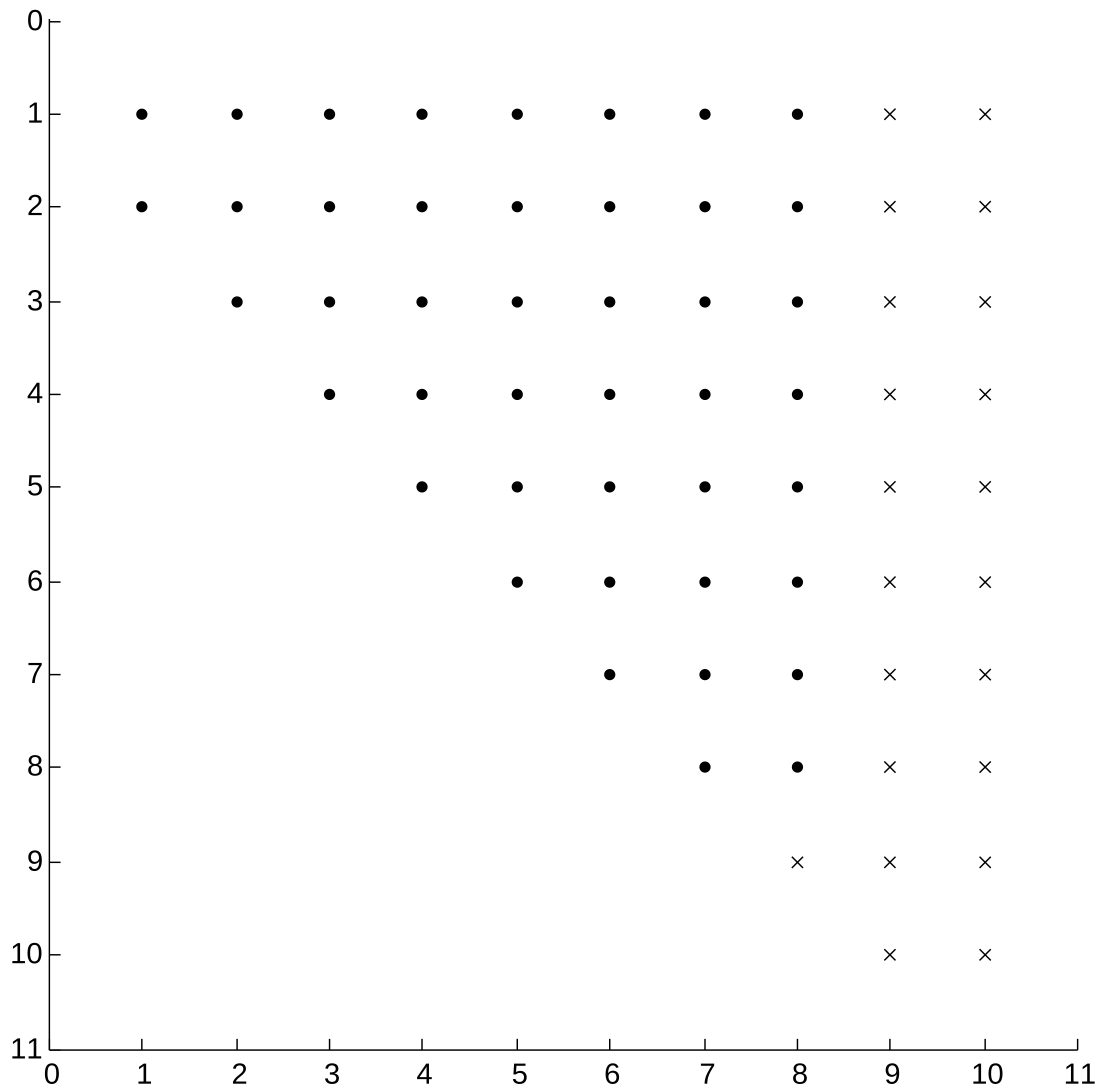


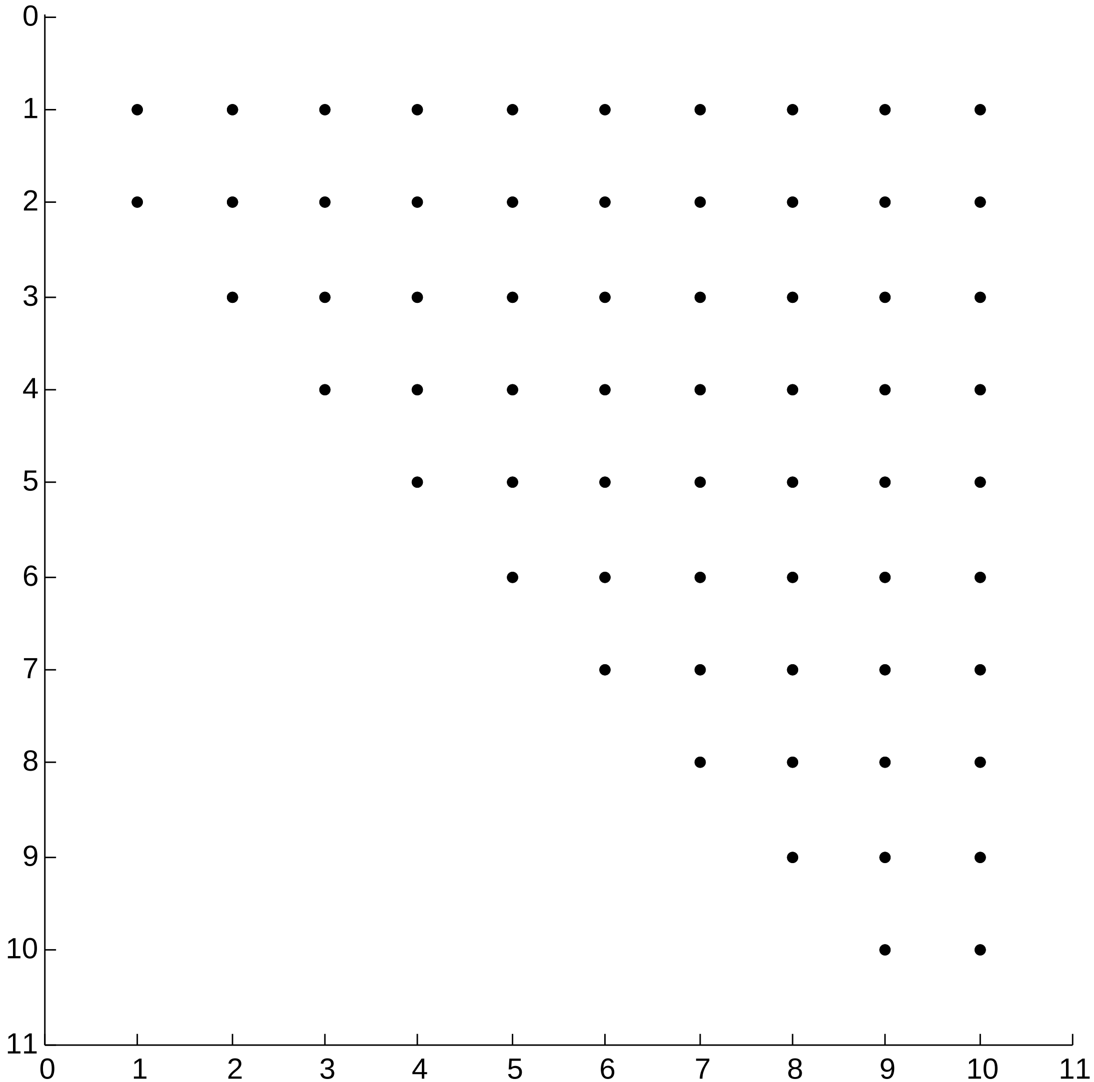
Hessenberg QR iteration



Hessenberg QR iteration



Hessenberg QR iteration



Even faster QR

Existing fast QR iterations:

- QR iteration preserves symmetry, orthogonality
- Symmetric tridiagonals: $O(n)$ parameters
- Unitary Hessenberg matrices: $O(n)$ parameters
- Use to do one QR iteration in $O(n)$ time

Even faster QR

New work:

- QR preserves symmetric or orthogonal + rank k
- Describe Hessenberg(symmetric or orthogonal + low rank k) with $O(nk)$ parameters.
- Use to do one QR iteration in $O(nk^2)$ time.

So who cares about matrices with this structure?

Example: 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

Use structure in QR iterates to get $O(n^2)$ time, $O(n)$ space.

Companion matrices

Given

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

Define a companion matrix C with $p(\lambda) = \det(C - \lambda I)$:

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

For matrix polynomials, replace a_i by A_i and 1 by I.
C is a permutation plus a rank one matrix.

Example: Damped oscillators

Differential equations for a damped linear oscillator:

$$Mu'' + Du' + Ku = 0$$

Scaled time-harmonic problem:

$$(\lambda^2 I + \lambda C + K)x = 0.$$

Let L be a Cholesky factor of K. Then

$$\begin{bmatrix} 0 & L \\ -L^T & -C \end{bmatrix} \begin{bmatrix} Lx \\ \lambda x \end{bmatrix} = \begin{bmatrix} Lx \\ \lambda x \end{bmatrix} \lambda$$

If damping comes from localized boundary conditions or effects in a small part of a domain, C can have low rank.

Rank symmetry

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

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

For symmetric, skew-symmetric, and orthogonal matrices, something stronger: the singular values of A_{12} and A_{21} are the same.

Rank symmetric + low rank

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:

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

Structure in Hessenberg form

Suppose $H = A + L$, where A is rank symmetric, L is rank k, and H is Hessenberg. Then

$$\text{rank}(H_{12}) \leq 2k + \text{rank}(H_{21}) \leq 2k + 1$$

If H is a Schur form, $H_{21} = 0$ and $\text{rank}(H_{12}) \leq 2k$.

If A is symmetric, skew-symmetric, or orthogonal, the structure is preserved under QR iteration. All the Hessenberg QR iterates will have low rank superdiagonal blocks.

SSS structure

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

$$H = B + \begin{bmatrix} 0 & U_1V_2^T & U_1W_2V_3^T & U_1W_2W_3V_4^T \\ 0 & 0 & U_2V_3^T & U_2W_3V_4^T \\ 0 & 0 & 0 & U_3V_4^T \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Write $H_{ij} = U_iW_{i+1}\ldots W_{j-1}V_j$ 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

$$\hat{H} = \begin{bmatrix} B_{11} & 0 & 0 & 0 \\ \hat{B}_{21} & \hat{B}_{22} & 0 & 0 \\ 0 & \hat{B}_{32} & B_{33} & 0 \\ 0 & 0 & B_{43} & B_{44} \end{bmatrix} + \begin{bmatrix} 0 & U_1 V_2^T & U_1 W_2 \hat{V}_3^T & U_1^T W_2 W_3 V_4^T \\ 0 & 0 & \hat{U}_2 \hat{V}_3^T & \hat{U}_2^T W_3 V_4^T \\ 0 & 0 & 0 & U_3 V_4^T \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Transform second row and column by reflection.
Only affects the band, U_2, and V_2.

What about transformations that cross block edges?
Merge blocks so it never happens – then split them.

Result: A bulge-chasing pass takes $O(nk^2)$ time vs $O(n^2)$

Splitting blocks

Define C_j and G_j by the recurrences

$$\begin{aligned} C_1 &= U_1 \text{ and } C_j = \begin{bmatrix} C_{j-1}W_j \\ U_j \end{bmatrix} \text{ for } j > 1 \\ G_n &= V_n \text{ and } G_j = \begin{bmatrix} V_v \\ G_{j+1}W_j^T \end{bmatrix} \text{ for } j < n. \end{aligned}$$

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

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

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

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.

Issue: Balancing

- Would like matrix to be *balanced* – scaled by diagonal similarity to reduce norm, improve accuracy
- General diagonal similarities destroy the structure!
- Rescaling a few rows and columns corresponds to making an additional low rank modification.
- For companion matrices, optimal balancing in infinity norm respects the structure.

Balancing

If C is a companion matrix, so is $|C|$. The Perron vector x of $|C|$ therefore has the form

$$x_i = c\lambda^i$$

Let

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

Then DCD^{-1} is optimally balanced in the ∞-norm. Corresponds to scaling the polynomial indeterminate by λ.

Issue: Normalization error

Write Hessenberg $H = A + L + E$ where

- $A_{12} = U_1 \Sigma V_2^T$ and $A_{21} = U_2 \Sigma V_1^T$
- rank$(L) = k$
- E is a perturbation

Then

$$H_{12} = (\widehat{H_{21}} - \widehat{L_{21}} + L_{12}) + (E_{12} - \widehat{E_{21}})$$

where

$$\begin{aligned} \widehat{H_{21}} &= (U_1 U_2^T) H_{21} (V_1 V_2^T) \\ \widehat{L_{21}} &= (U_1 U_2^T) L_{21} (V_1 V_2^T) \\ \widehat{E_{21}} &= (U_1 U_2^T) E_{21} (V_1 V_2^T) \end{aligned}$$

Normalization error

Can error grow during splitting?

- Only if we move away from (symmetric, skew, orthogonal) + low rank structure.
- Some growth with QR-based split (not with SVD).
- We can monitor error from splitting.
- Can we quickly perturb back to the right structure?
- Still thinking about this one.

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).

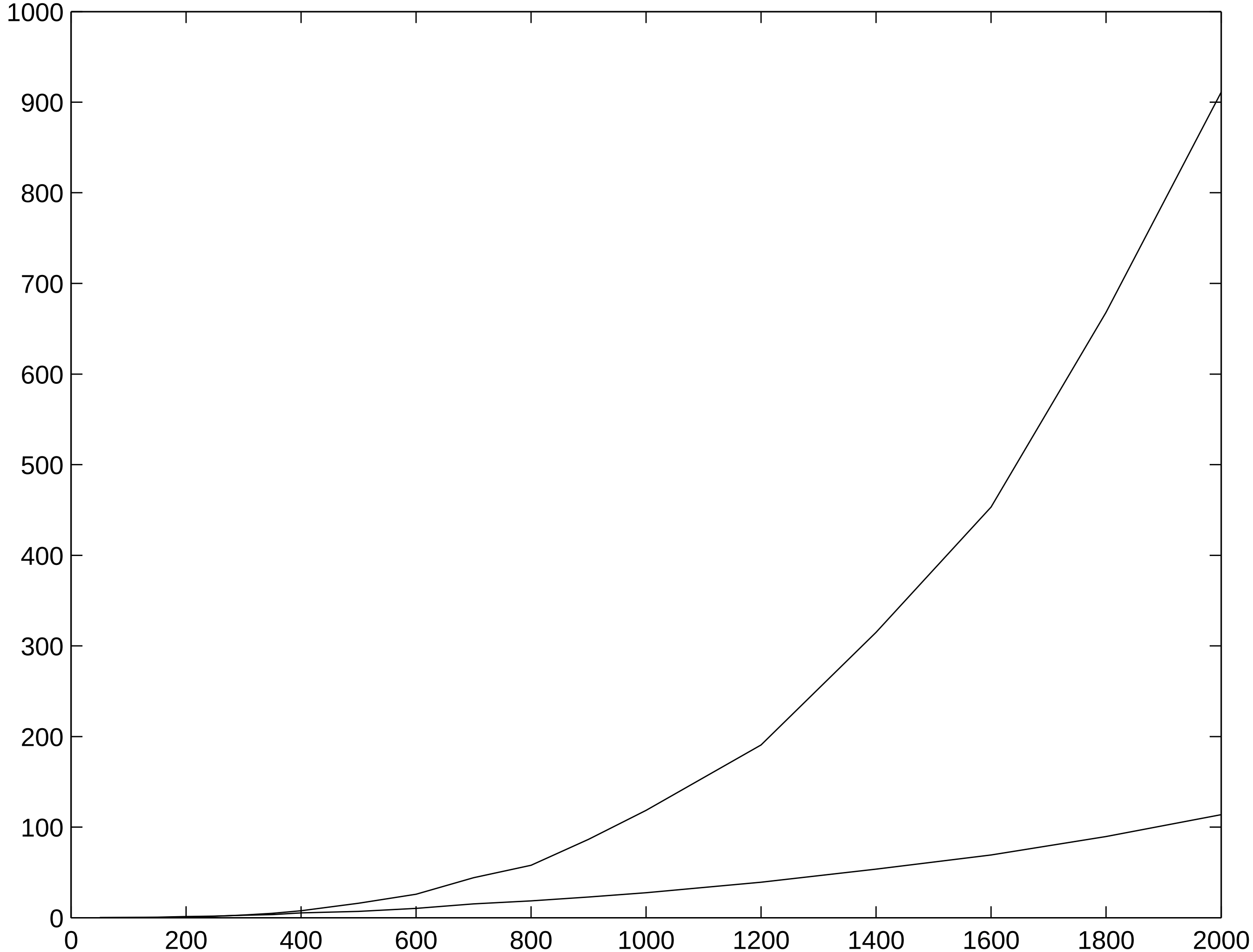
Most of the code accesses data in the band part of the structure. This text is *identical* to the standard code – just change `LDH`.

Performance

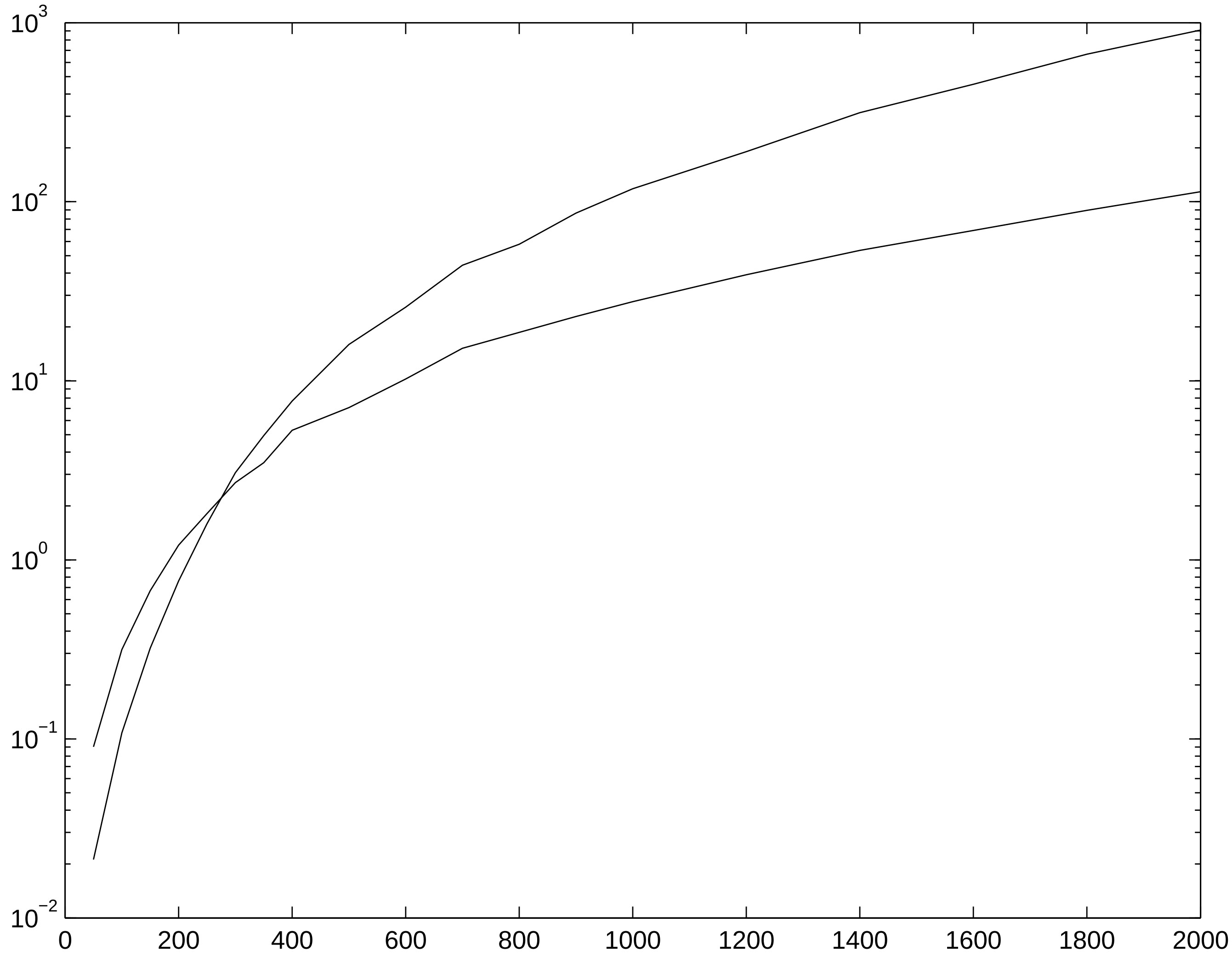
Update with most recent version

- Compared against LAPACK DLAHQR (not DHSEQR).
- Compiled using g77 without optimizations.
- LAPACK with standard optimizations, ATLAS BLAS
- Pentium 3 laptop at 700 MHz.
- Polynomials of degree 50-2000.
- For degree 10000, current code takes 41 minutes.

Performance



Performance



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.
- Have no direct fast method for Hessenberg reduction (though know how to do fast Arnoldi variant).
- Can balance companion matrices in ∞ norm, but general balancing destroys needed structure.
- Backward stable – except maybe for splitting step?