Exploiting BiStructured Computational Problems

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Outline

This is a talk about solving computational problems with methods **not preserving the special structure** of the underlying problem!

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1. Introduction
2. Simple (embarrassingly simple?) Examples
3. Cleaning up BiStructured problems
4. Less simple examples
5. Conclusions

Roughly speaking . . .

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Few have readily available, easily used numerical methods.

Computational Issues

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Specialized methods typically have . . .

- mathematical interest and elegance,
- reduced computational costs,
- improved numerical stability,
- and sometimes, the ability to solve otherwise intractable problems.

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- The structure of the problem may be unrecognized or ill-understood.
- A satisfactory structured algorithm may be unknown or may not exist.
- A satisfactory implementation may be unavailable, difficult or expensive. (. . . or eig is too easy to use.)

Questions

By not using structure preserving numerical methods, one gives up elegance and reduced computational cost.

- What about numerical stability?
- Is there an easy, inexpensive way to recover the accuracy of a structured numerical method from the computed results of an unstructured method?

$A \in \mathbf{R}^{n \times n}$

$$(A + E)x = \lambda x, \quad (\lambda, x) \in \mathbf{C} \times \mathbf{C}^n, \quad \textit{but}\ldots$$

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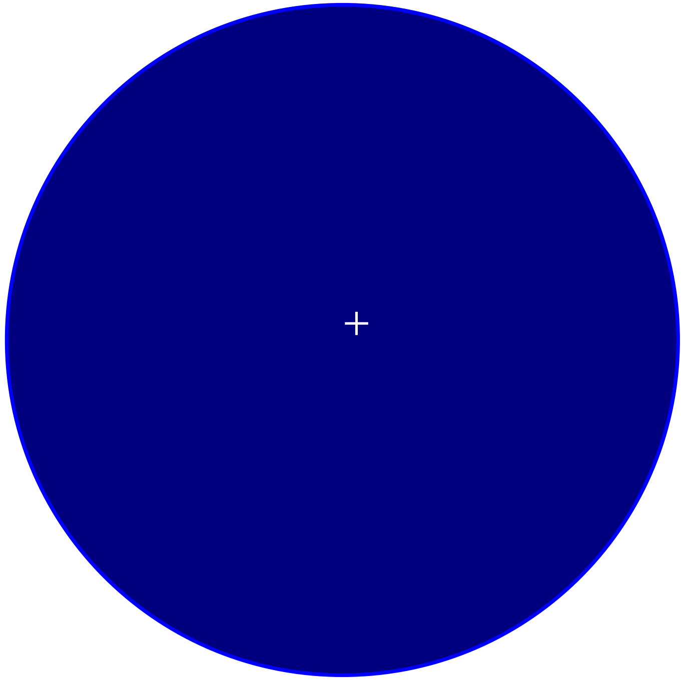
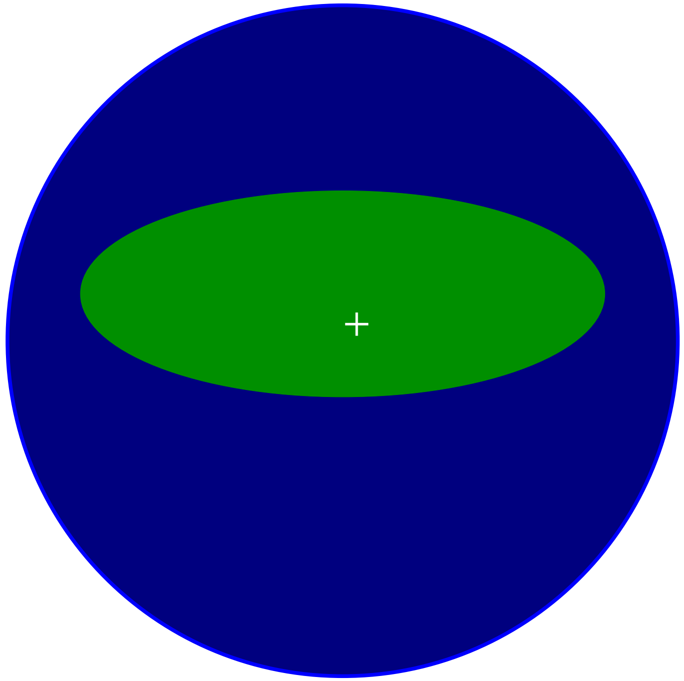
- $E \in \mathbf{R}^{n\times n}$, for real arithmetic algorithms,
- $E \in \mathbf{C}^{n\times n}$, for complex arithmetic algorithms.
- Are real arithmetic algorithms significantly more accurate?
- Can real-arithmetic-accuracy be recovered from a complex arithmetic computation?



$\underline{A \in \mathbf{R}^{n \times n}}$

$$\{\lambda(A+E) \mid E = E \in \mathbf{C}^{n\times n},\ \|E\| \le \varepsilon\}$$

ε-pseudospectral component containing an isolated, complex eigenvalue $\lambda = +$.



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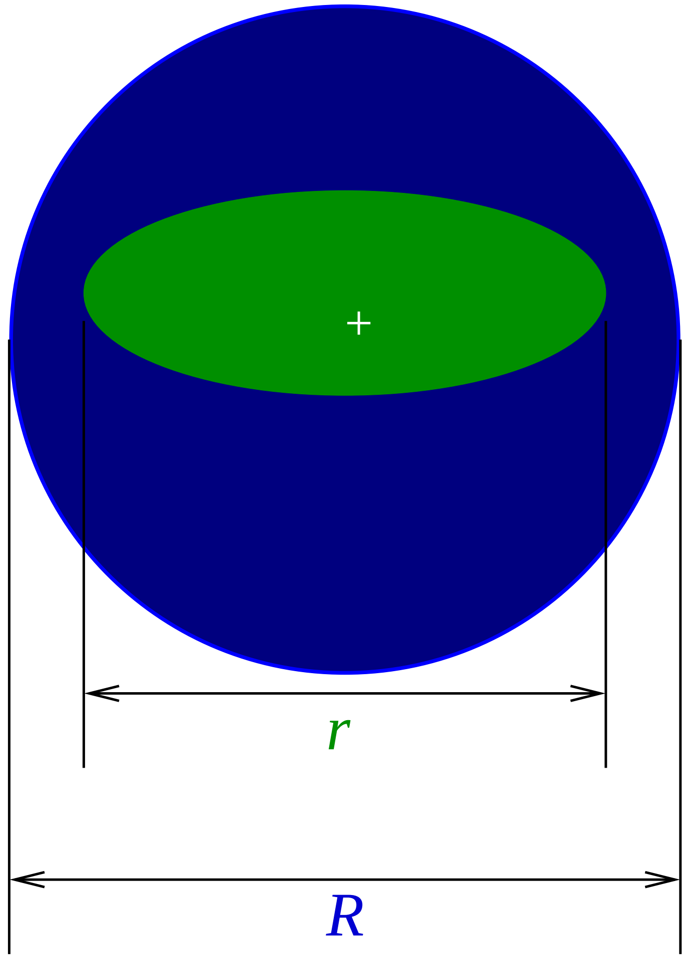
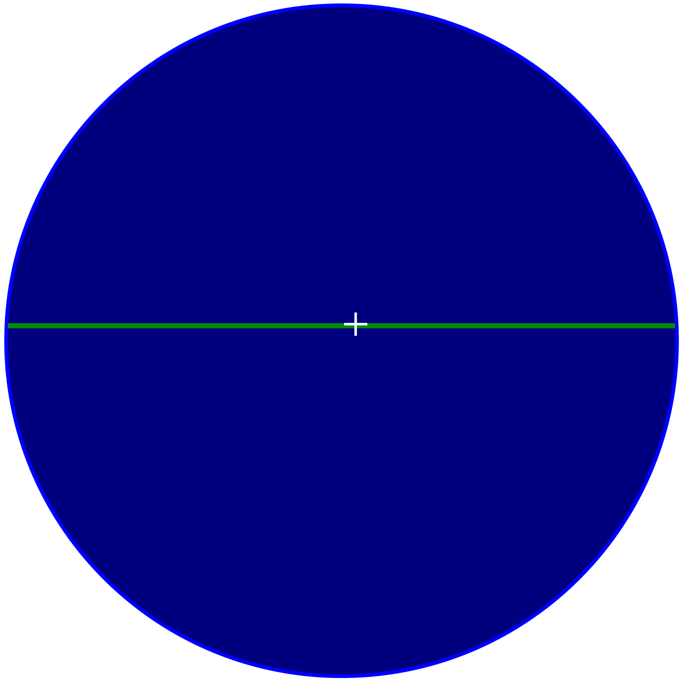
$$A \in \mathbf{R}^{n \times n}$$



$$r \leq R \leq \sqrt{2} r$$

B, Kressner (2004). See also Karow(2003)

$A \in \mathbf{R}^{n\times n}$



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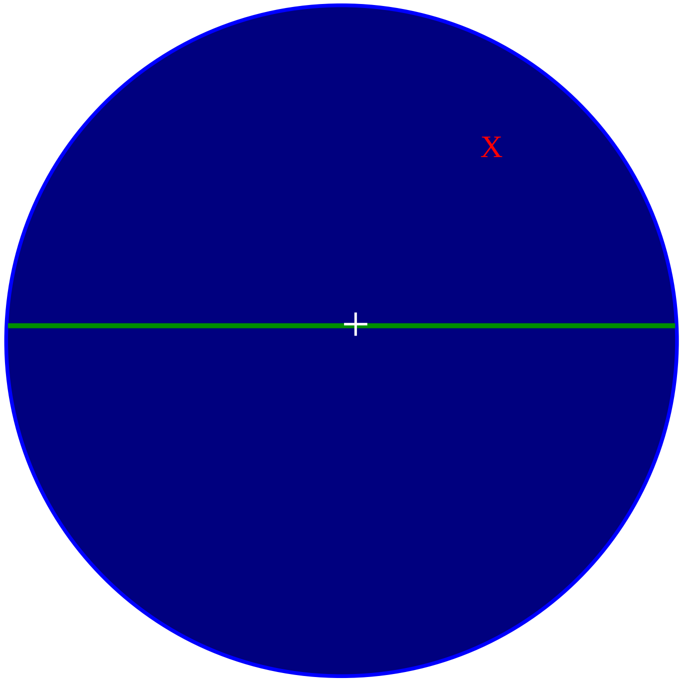
Are real arithmetic algorithms applied to real matrices significantly more accurate than complex arithmetic algorithms?

- No, worst case eigenvalue perturbations are within a factor of $\sqrt{2}$.

- Yes, perturbed eigenvalues must lie in a sometimes significantly smaller region.

$\underline{A \in \mathbf{R}^{n\times n}}$



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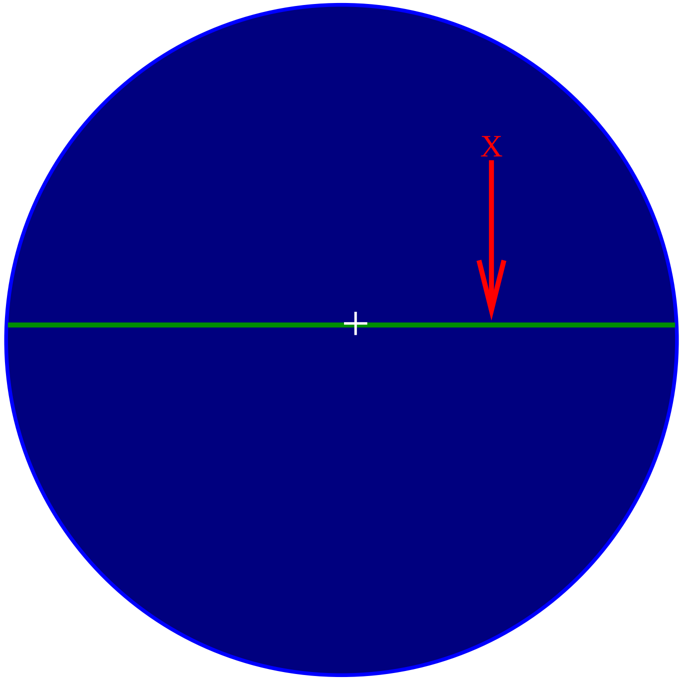

$A \in \mathbf{R}^{n \times n}$

Real arithmetic accuracy can be easily recovered for isolated, real eigenvalues: set the imaginary part of λ to zero.

$$A = A_R + iA_I \in \mathbf{C}^{n\times n}$$

A complex matrix is a structured real matrix.

$$A \in \mathbf{C}^{n\times n} \hookrightarrow \begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}.$$

These are related to quaternion matrices

$$A \in \mathbf{Q}^{n\times n} \hookrightarrow \begin{bmatrix} A_1 & -\bar{A}_2 \\ A_2 & \bar{A}_1 \end{bmatrix}. \qquad \begin{matrix} A_1 \in \mathbf{C}^{n\times n} \\ A_2 \in \mathbf{C}^{n\times n} \end{matrix}$$

quantum chemistry, for example.

$A = A_R + iA_I \in \mathbf{C}^{n \times n}$

Are structure preserving algorithms for

$$\begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}$$

significantly more accurate than others?

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

$$A \in \mathbf{C}^{n\times n} \hookrightarrow \begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}.$$

$$x \in \mathbf{C}^{n} \hookrightarrow \left(\begin{bmatrix} x \\ -ix \end{bmatrix}, \begin{bmatrix} \bar{x} \\ i\bar{x} \end{bmatrix} \right)$$

$$\lambda \in \mathbf{C} \hookrightarrow (\lambda, \bar{\lambda})$$

$$\lambda \in \mathbf{R} \hookrightarrow (\lambda, \lambda) \qquad \text{multiple}$$

$$(\lambda, \bar{\lambda}) \in \mathbf{C} \times \mathbf{C} \hookrightarrow (\lambda, \lambda),\ (\bar{\lambda}, \bar{\lambda}),\ \text{multiple}$$

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

The good news about

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The good news about

$$A \in \mathbf{C}^{n\times n} \hookrightarrow \begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}$$

is that the condition of the eigenvalues is unchanged by the embedding despite increased dimension and multiplicity. This is a consequence of Gerschgorin and special structure.

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The bad news about

$$A \in \mathbf{C}^{n\times n} \hookrightarrow \begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix} \cdots$$

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$$A \in \mathbf{C}^{n \times n} \hookrightarrow \begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix} \cdots$$

- Half the eigenvalue-vector pairs of the big matrix are extraneous. May need accurate eigenvectors to distinguish which are which.

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- Half the eigenvalue-vector pairs of the big matrix are extraneous. May need accurate eigenvectors to distinguish which are which.
- Well conditioned eigenvectors of A may embed into ill-conditioned eigenvectors.

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

MATLAB:

```
AA = [real(A) -imag(A); imag(A) real(A)];
[V, D] = eig(AA);
diag(D)
ans =
    0 + 25i
    0 - 25i
    0 + 25i
    0 - 25i
```

$A = A_R + iA_I \in \mathbf{C}^{n \times n}$

MATLAB:

```
V(:,[1 3])
ans =
  0.7065                    0.0168 - 0.0112i
  0.0292 - 0.0022i         -0.7068
 -0.0022 - 0.2259i         -0.0031 + 0.6739i
  0.0006 - 0.6701i         -0.0107 - 0.2140i
```

Not in $\begin{bmatrix} x \\ ix \end{bmatrix}$ or $\begin{bmatrix} x \\ -ix \end{bmatrix}$ form.

Which eigenvalues are extraneous?

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

Perturbing with $\|E\| < \varepsilon$, $\|F\| < \varepsilon$,

$$\begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix} + \begin{bmatrix} E_R & -E_I \\ E_I & E_R \end{bmatrix} + \begin{bmatrix} F_R & F_I \\ F_I & -F_R \end{bmatrix},$$

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perturbs a desired simple eigenvector to

$$\begin{bmatrix} x \\ -ix \end{bmatrix} + \begin{bmatrix} \hat{X} \\ -i\hat{X} \end{bmatrix} p + \begin{bmatrix} \bar{X} \\ i\bar{X} \end{bmatrix} q$$

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

$$\begin{bmatrix} x \\ -ix \end{bmatrix} + \begin{bmatrix} \hat{X} \\ -i\hat{X} \end{bmatrix} p + \begin{bmatrix} \bar{X} \\ i\bar{X} \end{bmatrix} q + O(\varepsilon^2)$$

$A = A_R + iA_I \in \mathbf{C}^{n \times n}$

$$\begin{bmatrix} x \\ -ix \end{bmatrix} + \begin{bmatrix} \hat{X} \\ -i\hat{X} \end{bmatrix} p + \begin{bmatrix} \bar{X} \\ i\bar{X} \end{bmatrix} q + O(\varepsilon^2)$$

where $p = T^{-1}(\mathcal{P}(E))$, where $\mathcal{P}$ is a projection and T is linear and nonsingular if the corresponding eigenvalue is a simple eigenvalue of A.

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

$$\begin{bmatrix} x \\ -ix \end{bmatrix} + \begin{bmatrix} \hat{X} \\ -i\hat{X} \end{bmatrix} p + \begin{bmatrix} \bar{X} \\ i\bar{X} \end{bmatrix} q + O(\varepsilon^2)$$

. . . and $q = S^{-1}(\mathcal{Q}(F))$, where $\mathcal{Q}$ is a projection and S is linear and nonsingular if the corresponding eigenvalue is a simple eigenvalue of $\begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}$.

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

- Possibly, $\begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}$ has multiple or nearly multiple eigenvalues when $A = A_R + iA_I$ does not, e.g., when A has a real eigenvalue or a complex conjugate pair.

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- Possibly, $\begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}$ has multiple or nearly multiple eigenvalues when $A = A_R + iA_I$ does not, e.g., when A has a real eigenvalue or a complex conjugate pair.
- Consequently, possibly, $\|q\|_2 \gg \|p\|_2$, i.e., an unstructured algorithm may be numerically unstable , but. . .

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

A simple *a posteriori* correction,

$$\begin{bmatrix} y \\ z \end{bmatrix} \in \mathbf{C}^n \times \mathbf{C}^n \longrightarrow \begin{bmatrix} y + iz \\ -i(y + iz) \end{bmatrix}$$

reduces F and q to second order perturbations.

$A = A_R + iA_I \in \mathbf{C}^{n\times n}$

MATLAB:

```
W=[V(1:2,:)+i*V(3:4,:)  ; -i*V(1:2,:)+V(3:4,:)];
W(:,[1 2])
ans =
   0.9324 - 0.0022i   0.4806 - 0.0022i
   0.6993 - 0.0016i  -0.6409 + 0.0029i
  -0.0022 - 0.9324i  -0.0022 - 0.4806i
  -0.0016 - 0.6993i   0.0029 + 0.6409i
eigval = diag(W'*AA*W)./diag(W'*W)
ans =
    0.0000 +25.0000i
    0.0000 -25.0000i
```

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Are structure preserving algorithms significantly more accurate than others?

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- Yes, the eigenvector conditioning under structured perturbations may be significantly smaller.

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Are structure preserving algorithms significantly more accurate than others?

- Yes, the eigenvector conditioning under structured perturbations may be significantly smaller.
- No, eigenvalue conditioning is unchanged. There is a simple *a posteriori* fix for eigenvectors.

Introduction to BiStructure

In the previous examples there are two structures. The data has a structure and the desired computed results also have a structure.

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- Compute a real eigenvalue of a real matrix: $A \in \mathbf{R}^{n \times n} \subset \mathbf{C}^{n \times n} \longrightarrow \lambda \in \mathbf{R}$.

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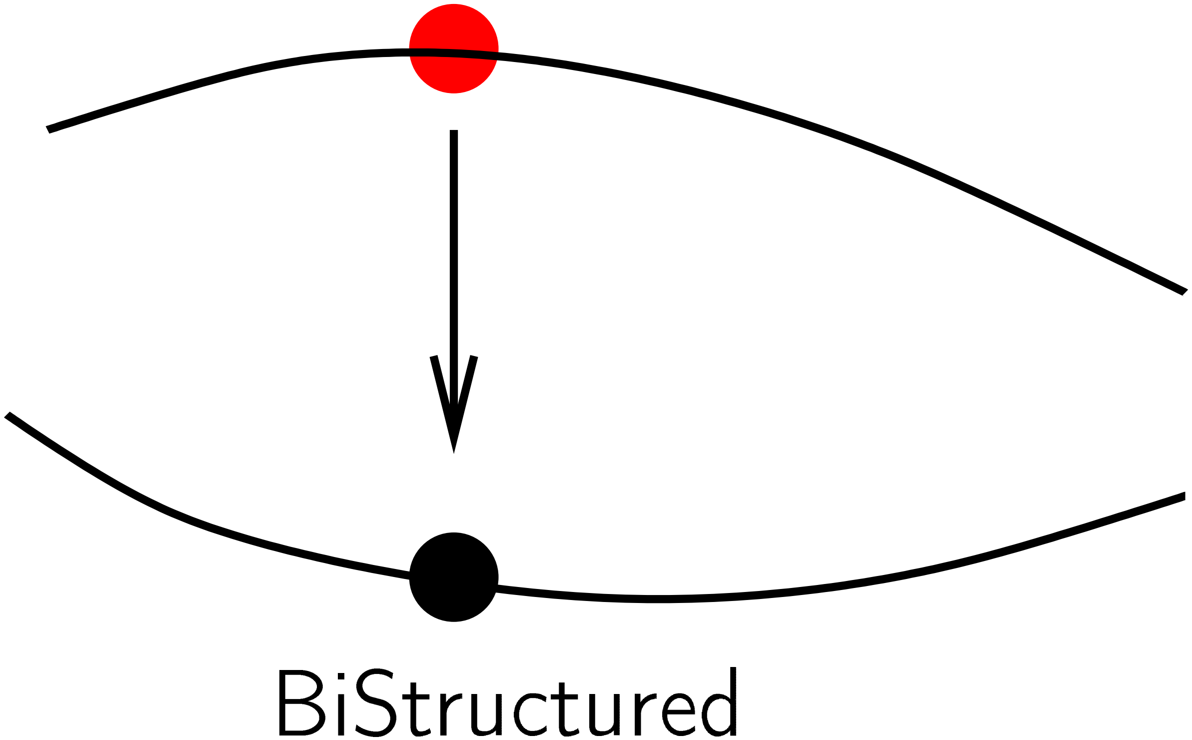
- Compute a real eigenvalue of a real matrix: $A \in \mathbf{R}^{n \times n} \subset \mathbf{C}^{n \times n} \rightarrow \lambda \in \mathbf{R}$.
- Compute eigenvalues and vectors of the structured matrix $\begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix}$:
$\left\{ \begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix} \right\} \rightarrow \lambda \in \mathbf{C}$ with $\begin{bmatrix} x \\ -ix \end{bmatrix} \in \mathbf{C}^{2n}$.

BiStructure Introduction



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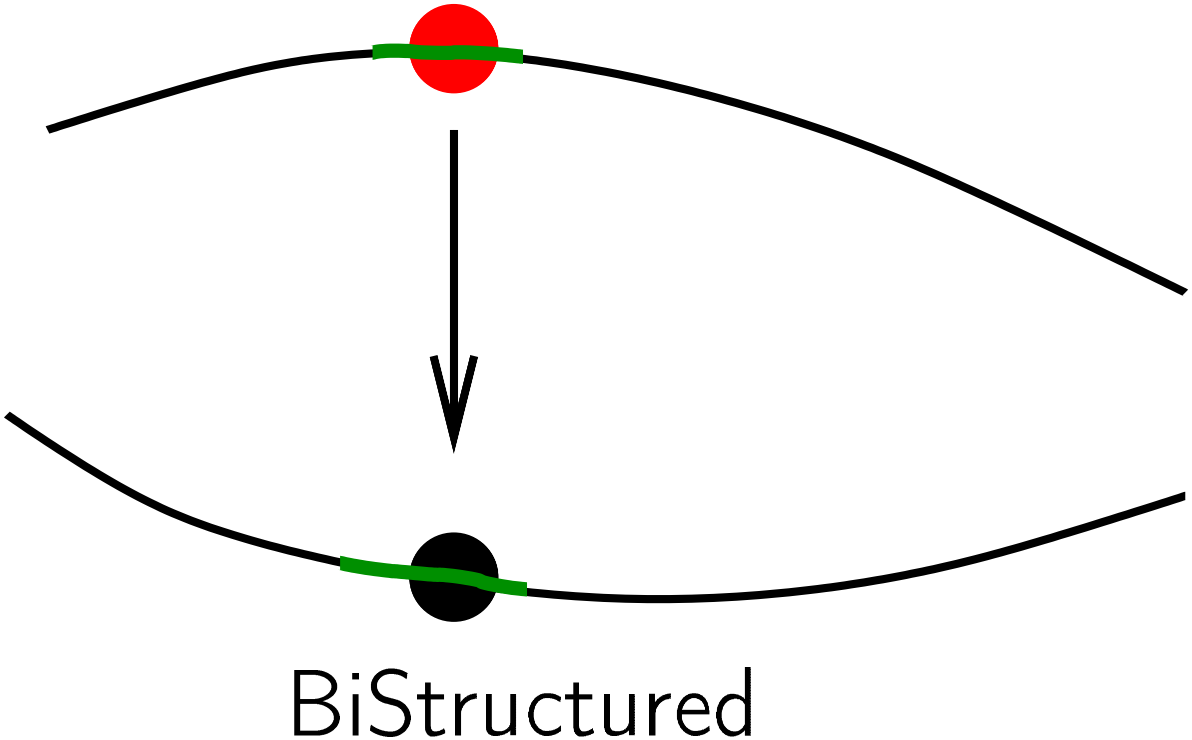

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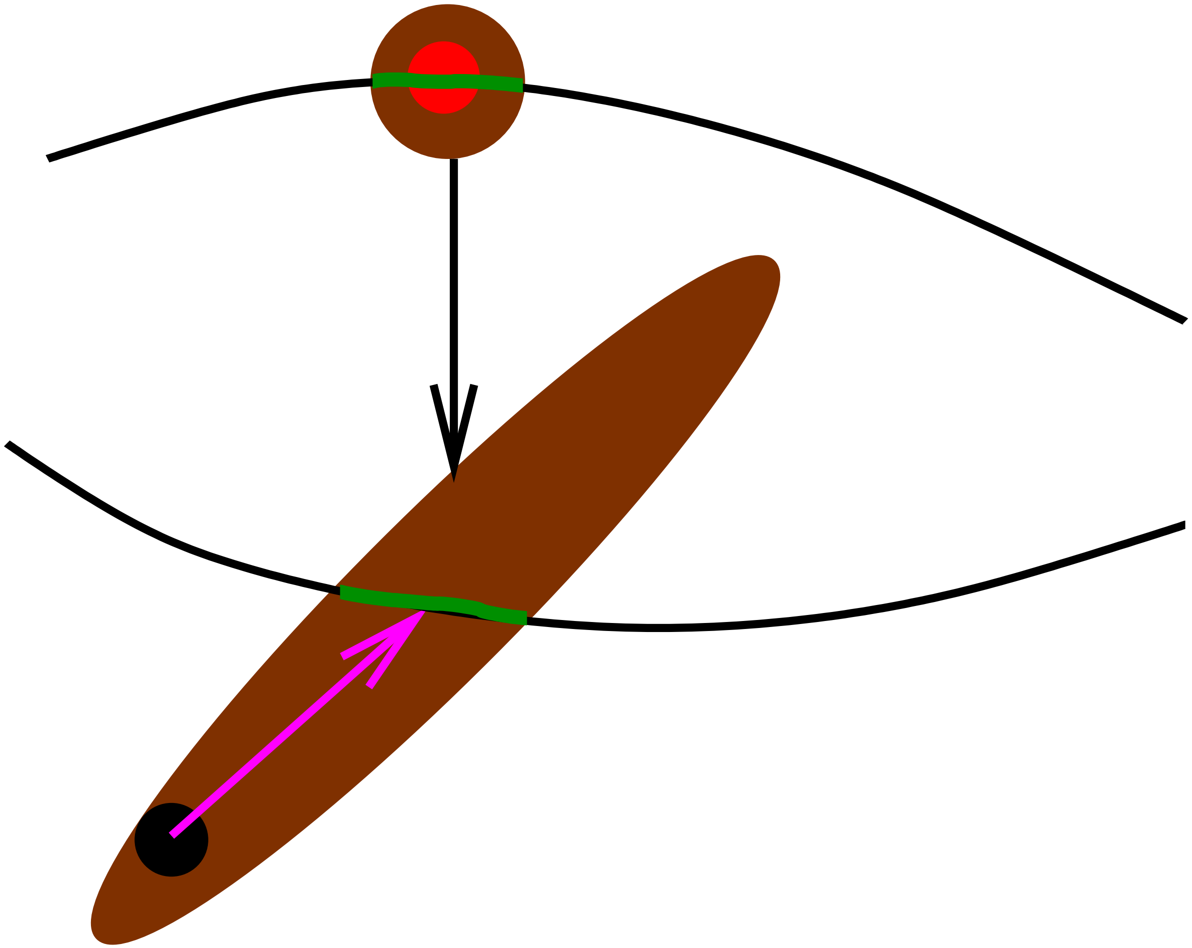
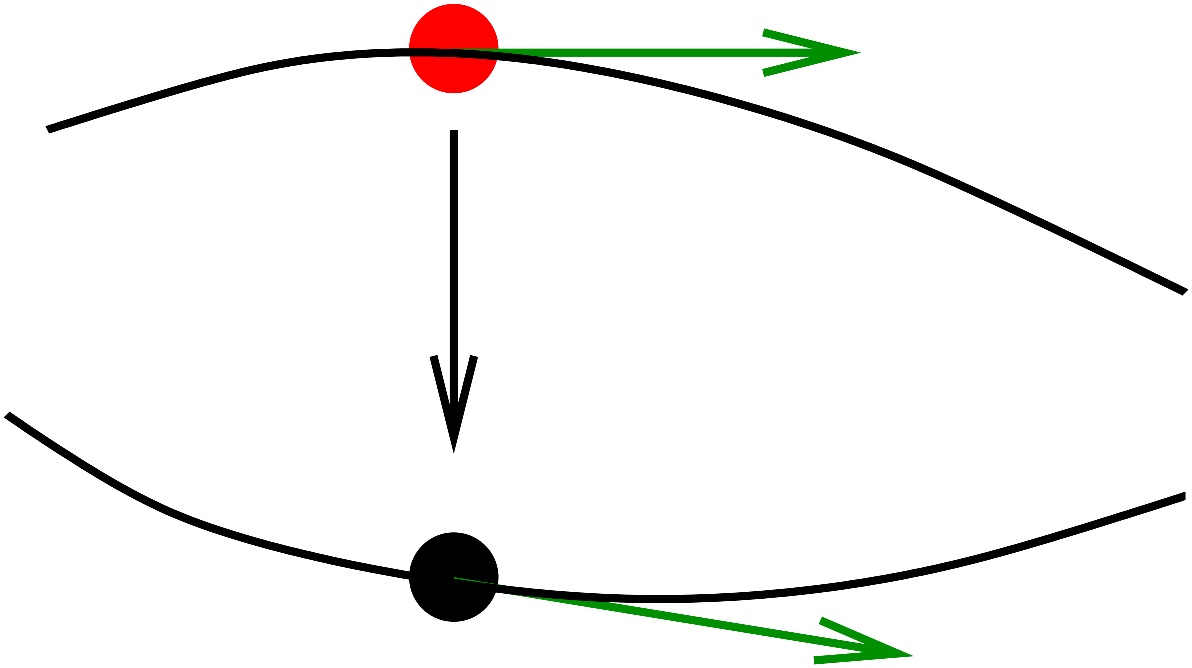


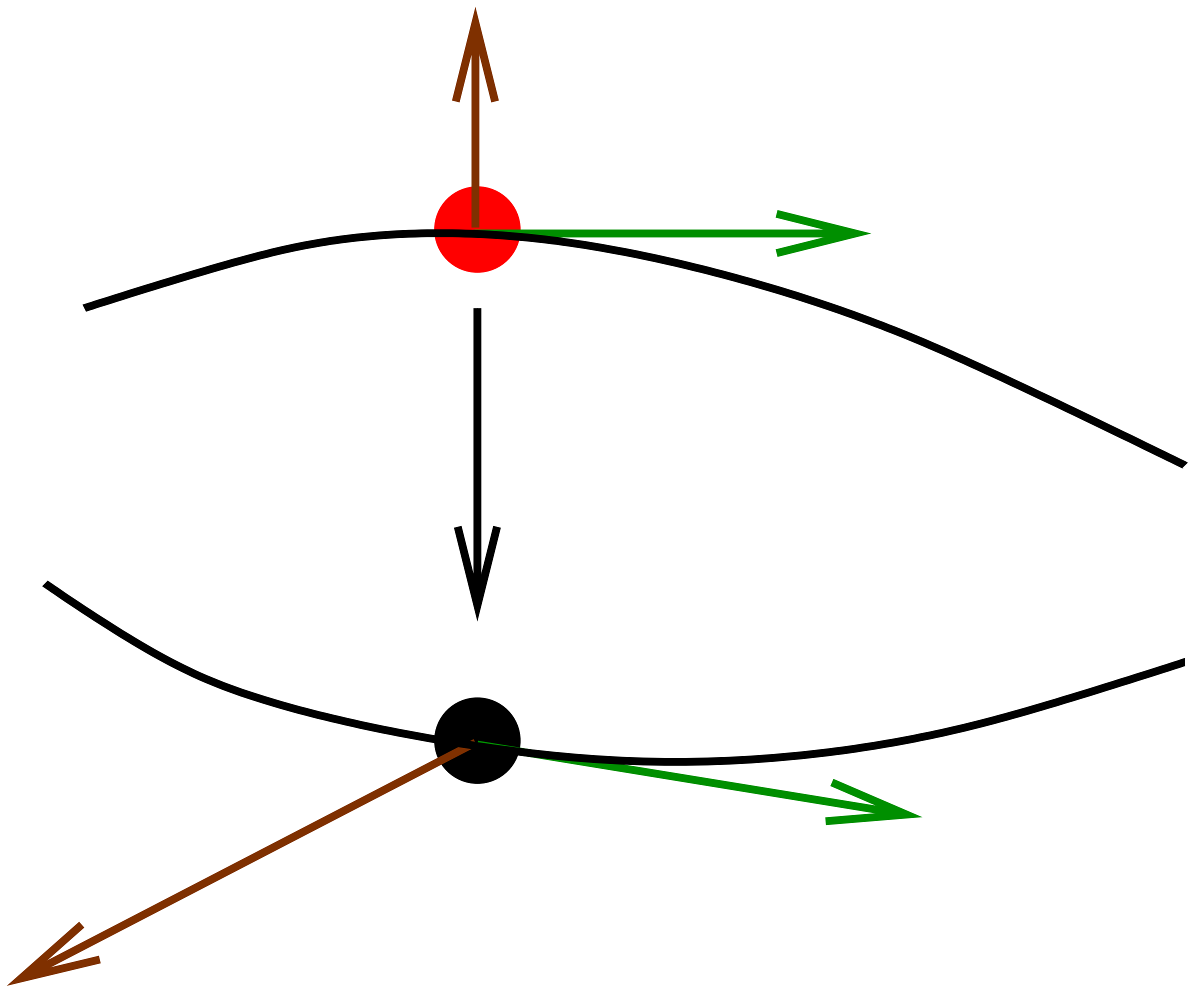
(Skew)-Projection Correction

BiStructure Introduction



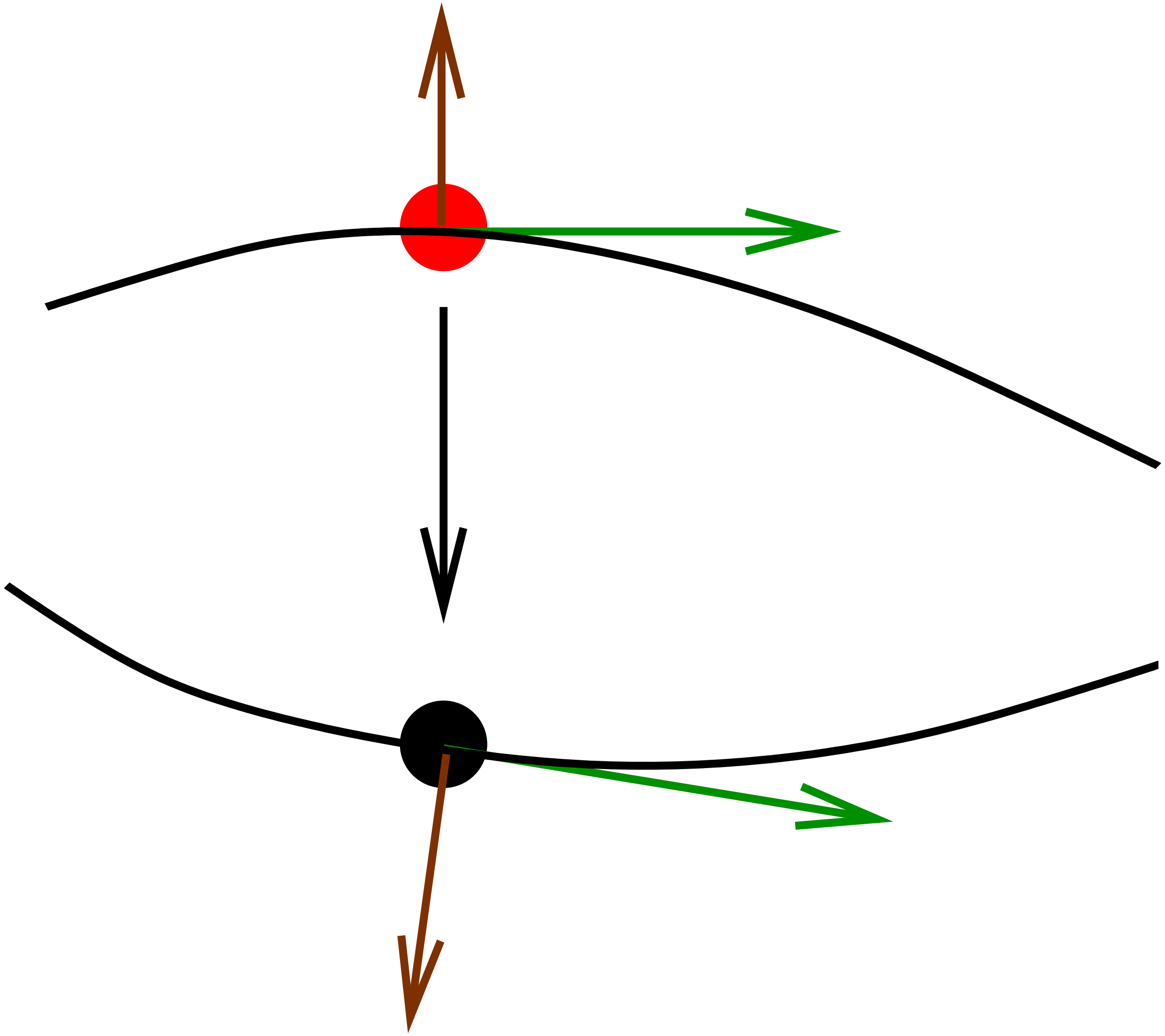
Tangent space $\longrightarrow$ tangent space

BiStructure Introduction



Not Orthogonaly Bistructured

BiStructure Introduction



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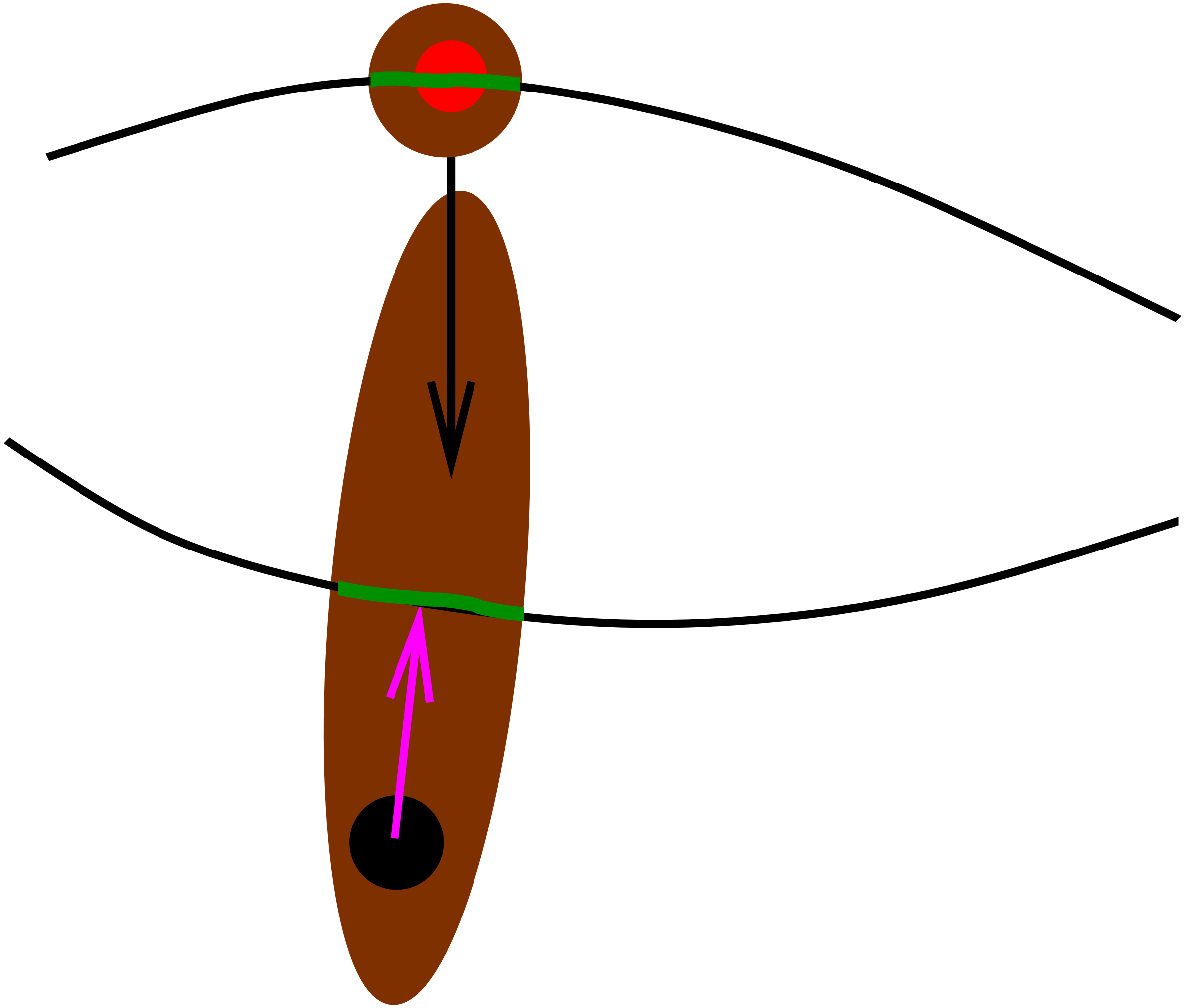
BiStructure Introduction



Orthogonaly Bistructured → Simple correction

Block Hamiltonian-Schur Form

- $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$
- $H \in \mathbf{R}^{2n\times 2n}$ is Hamiltonian if $(JH)^T = JH$, i.e.,

$$H = \begin{bmatrix} A & G \\ F & -A^T \end{bmatrix}, \quad F = F^T, \quad G = G^T.$$

- $H \in \mathbf{R}^{2n\times 2n}$ is skew-Hamiltonian if $(JH)^T = -JH$, i.e.,

$$H = \begin{bmatrix} A & G \\ F & A^T \end{bmatrix}, \quad F = -F^T, \quad G = -G^T.$$

- $S \in \mathbf{R}^{2n\times 2n}$ is Symplectic if $S^T JS = J$.
- $V \in \mathbf{R}^{2n\times n}$ is Lagranian if $V^T JV = 0$.

Block Hamiltonian-Schur Form

Given a Hamiltonian matrix H, calculate S and T such that

$$HS = ST = \begin{bmatrix} S_1 & -S_2 \\ S_2 & S_1 \end{bmatrix} \begin{bmatrix} T_1 & T_2 \\ 0 & -T_1^T \end{bmatrix}$$

where

- T is Hamiltonian
- S is symplectic and orthogonal
- $\sigma(T_1) \subset \mathbf{C}_-$, i.e., eigenvalues of T_1 have non-positive real part.

Block Hamiltonian-Schur Form

- Progress on a structure preserving algorithm for Hamiltonian-Schur Form by Ammar, Benner, Bunse-Gerstner, B, Chu, Faßbender, He, Golub, Laub, Mehrmann, Paige, Van Loan, Xu, . . .
- Note particularly work by Mehrmann and Chu 2005 or 2006.

Laub Trick

Laub trick: (Laub circa 1985)

1. Calculate unstructured Schur form

$$HQ = QR = \begin{bmatrix} Q_1 & Q_3 \\ Q_2 & Q_4 \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}.$$

   where $\sigma(R_{11}) \subset \mathbf{C}_-$.

2. $S = \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix}$

In exact arithmetic $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$ is Lagrangian and S is the symplectic-orthogonal factor of Hamiltonian-Schur Form.

Laub Trick

Problem:

Laub Trick

Problem: Not numericaly stable.

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As the stable invariant subspace span $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$ becomes ill-conditioned, rounding errors destroy Symplectic structure—just when the extra numerical stability of a structure preserving algorithm is most important.

Laub Trick

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As the stable invariant subspace span $\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$ becomes ill-conditioned, rounding errors destroy Symplectic structure—just when the extra numerical stability of a structure preserving algorithm is most important.

Gram-Schmidt-like Symplectic-reorthogonalization damages the invariant subspace.

A Bistructured Problem

Computational Problem:

$$F(H) = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$$

(So, $S = \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix}$ and $T = S^T H S$.)

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$$F(H) = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$$

(So, $S = \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix}$ and $T = S^T H S$.)

Domain

Structure: H Hamiltonian, i.e., $(JH)^T = JH$

Tangent space: $T_H = \{ M \mid (JM)^T = JM \}$

Normal space: $T_H^\perp = \{ M \mid (JM)^T = -JM \}$

A Bistructured Problem

Range

Structure: $$\left\{ Q \in \mathbf{R}^{2n\times n} \;\middle|\; \begin{matrix} Q^T J Q = 0 \\ Q^T Q = I \end{matrix} \right\}$$

Tangent space: $$T_Q = \left\{ \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix} \begin{bmatrix} Z \\ W \end{bmatrix} \;\middle|\; \begin{matrix} Z^T = - \\ W^T = \end{matrix} \right.$$

Normal space: $$T_Q^{\perp} = \left\{ \begin{bmatrix} Q_1 & -Q_2 \\ Q_2 & Q_1 \end{bmatrix} \begin{bmatrix} W \\ Z \end{bmatrix} \;\middle|\; \begin{matrix} Z^T = - \\ W^T = \end{matrix} \right.$$

A Bistructured Problem

$$F(H) \;=\; \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$$

$$DF(H) \;:\; T_H \longrightarrow T_Q$$

$$DF(H) \;:\; T_H^{\perp} \longrightarrow T_Q^{\perp}$$

Recover structured algorithm accuracy (to first order) by projecting computed solution back onto T_Q

Corrected Laub Trick

1. Calculate unstructured Schur form

$$HQ = QR = \begin{bmatrix} Q_1 & Q_3 \\ Q_2 & Q_4 \end{bmatrix} \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix}.$$

   where $\sigma(R_{11}) \subset \mathbf{C}_-$.

2. $Z = \frac{1}{2}\left(Q_1^T Q_2 - Q_2^T Q_1\right)$
3. $\begin{bmatrix} V_1 \\ V_2 \end{bmatrix} \rightarrow \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} + \begin{bmatrix} -Q_2 \\ Q_1 \end{bmatrix} Z$
4. $S = \begin{bmatrix} V_1 & -V_2 \\ V_2 & V_1 \end{bmatrix}$

(No need to correct orthogonality.)

$A \in \mathcal{M}$, $F(A) \in \mathcal{F}$

Rounding errors in a backward stable numerical method are equivalent to evaluating $F(A+E)$ for some small magnitude perturbation E.

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- Otherwise, possibly, $A + E \notin \mathcal{M}$.

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Rounding errors in a backward stable numerical method are equivalent to evaluating $F(A+E)$ for some small magnitude perturbation E.

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- Otherwise, possibly, $A + E \notin \mathcal{M}$.

To first order, perturbing A to $A + E$ gives

$$F(A+E) = F(A) + \boxed{D_A(E)} + O(\|E\|^2).$$

$A \in \mathcal{M}, \; F(A) \in \mathcal{F}$

For BiStructured problems, in appropriate orthonormal bases of $\mathcal{M}$ and $\mathcal{F}$,

$$D_A \;=\; \begin{bmatrix} D_{\mathcal{M}} & D_{\mathcal{N}} \\ 0 & D_{\mathcal{M}^\perp} \end{bmatrix}$$

$$\sim \;\; \begin{bmatrix} T_A \rightarrow T_{F(A)} & T_A^\perp \rightarrow T_{F(A)} \\ T_A \rightarrow T_{F(A)}^\perp & T_A^\perp \rightarrow T_{F(A)}^\perp \end{bmatrix}$$

(orthogonally BiStructured $\Longleftrightarrow D_{\mathcal{N}} = 0$)

Absolute Condition Numbers

$$\kappa_{\text{str}} = \|D_{\mathcal{M}}\|_2$$

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- If $\kappa_{\text{str}} \ll \kappa_{\text{abs}}$, then structured algorithms are probably more accurate.
- If D_A is well-scaled, then $\kappa_{\text{str}} \approx \kappa_{\text{abs}}$.

$A \in \mathcal{M}$, $F(A) \in \mathcal{F}$

$$F(A+E) = \begin{bmatrix} F_{\mathcal{F}} \\ F_{\mathcal{M}}^{\perp} \end{bmatrix} \sim \begin{bmatrix} \mathcal{F} \\ \mathcal{F}^{\perp} \end{bmatrix}$$

$$E = \begin{bmatrix} E_{\mathcal{M}} \\ E_{\mathcal{M}^{\perp}} \end{bmatrix} \sim \begin{bmatrix} T_A \\ T_{A^{\perp}} \end{bmatrix}$$

If $D_{\mathcal{M}^{\perp}} C = F_{\mathcal{M}^{\perp}} + O(||E||^2)$, then

$$\begin{bmatrix} F_{\mathcal{M}} - D_{\mathcal{N}} C \\ 0 \end{bmatrix} = F(A + E_{\mathcal{M}}) + O(||E||^2).$$

In orthogonaly BiStructured problems, $D_{\mathcal{N}} = 0$,

so correction is simple.

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- *a posteriori* fix: $\hat{X} \leftarrow (\tilde{X} + \tilde{X}^T)/2$

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- No, not always. It is not unusual that structured algorithm rounding errors may be as (nearly) great as unstructured algorithm errors, but. . .
- Orthogonally BiStructured problems admit an easy *a posteriori* correction to filter out unstructured errors (to first order).