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Scaling, Sensitivity and Stability in Numerical Solution of the Quadratic Eigenvalue Problem

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Joint work with Seamus Garvey, Steve Mackey and Françoise Tisseur

NLEVP Toolbox

with T. Betcke, V. Mehrmann, C. Schröder, F. Tisseur

Collection of Nonlinear Eigenvalue Problems:
$F(\lambda)x = 0$, where $F : \mathbb{C} \to \mathbb{C}^{m\times n}$.

- Provided as a MATLAB Toolbox.
- Problems from real-life applications + specially constructed problems.
- Available from
  http://www.mims.manchester.ac.uk/research/numerical-analysis/nlevp.html

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Further contributions are welcome.

Outline

1. QEP and Linearization Background
2. Conditioning of Linearizations
3. Scaling
4. Algorithm based on Linearization

Quadratic Eigenproblems

Consider

$$Q(\lambda) = \lambda^2 M + \lambda D + K, \qquad M, D, K \in \mathbb{C}^{n\times n}.$$

QEP: find scalars λ and nonzero $x, y \in \mathbb{C}^n$ satisfying $Q(\lambda)x = 0$ and $y^* Q(\lambda) = 0$.

- λ is an e'val, x, y are corresponding right and left e'vecs.
- $Q(\lambda)$ has $2n$ eigenvalues, solutions of $\det(Q(\lambda)) = 0$.

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- $Q(\lambda)$ has $2n$ eigenvalues, solutions of $\det(Q(\lambda)) = 0$.

When $\lambda = \infty$, consider **homogeneous form** of Q:

$$Q(\alpha, \beta) = \alpha^2 M + \alpha\beta D + \beta^2 K.$$

E'vals are pairs $(\alpha, \beta) \neq (0, 0)$ s.t. $\det Q(\alpha, \beta) = 0$.

Linearizations

$$L(\lambda) = \lambda X + Y, \qquad X, Y \in \mathbb{C}^{2n\times 2n}$$

is a **linearization** of $Q(\lambda) = \lambda^2 M + \lambda D + K$ if

$$E(\lambda)L(\lambda)F(\lambda) = \begin{bmatrix} Q(\lambda) & 0 \\ 0 & I_n \end{bmatrix} \qquad (*)$$

for some **unimodular** $E(\lambda)$ and $F(\lambda)$.

Example

For companion pencil $C_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & I_n \end{bmatrix} + \begin{bmatrix} D & K \\ -I_n & 0 \end{bmatrix}$,

$(*)$ holds with

$$E(\lambda) = \begin{bmatrix} I_n & \lambda M + D \\ 0 & -I_n \end{bmatrix}, \qquad F(\lambda) = \begin{bmatrix} \lambda I_n & I_n \\ I_n & 0 \end{bmatrix}.$$

Solution Process for QEP

- **Linearize** $Q(\lambda)$ into $L(\lambda) = \lambda X + Y$.
- Solve **generalized eigenproblem** $L(\lambda)z = 0$.
- **Recover** eigenvectors of Q from those of L.

Usual choice of linearization: companion linearization,

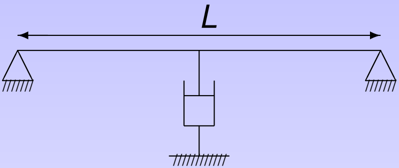
$$C_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D & K \\ -I & 0 \end{bmatrix}$$

for which right and left e'vecs have the form

$$z = \begin{bmatrix} \lambda x \\ x \end{bmatrix}, \qquad w = \begin{bmatrix} y \\ \bar{\lambda} K y \end{bmatrix},$$

x, y being right and left e'vecs of $Q(\lambda)$.

Beam Problem



Transverse displacement $u(x, t)$ governed by

$$\rho A \frac{\partial^2 u}{\partial t^2} + c(x)\frac{\partial u}{\partial t} + EI\frac{\partial^4 u}{\partial x^4} = 0.$$

Boundary conditions: $u(x, t) = u''(x, t) = 0$ at $x = 0, L$.

$u(x, t) = e^{\lambda t} v(x, \lambda)$ yields

e'val problem for the free vibrations:

$$\lambda^2 \rho A v(x, \lambda) + \lambda c(x) v(x, \lambda) + EI \frac{\partial^4}{\partial x^4} v(x, \lambda) = 0.$$

Discretized Beam Problem

Finite element method leads to

$$Q(\lambda) = \lambda^2 M + \lambda D + K$$

with **symmetric** $M, D, K \in \mathbb{R}^{n \times n}$.

Roots of $x^* Q(\lambda) x = 0$,

$$\lambda = \frac{-(x^* D x) \pm \sqrt{(x^* D x)^2 - 4(x^* M x)(x^* K x)}}{2(x^* M x)}.$$

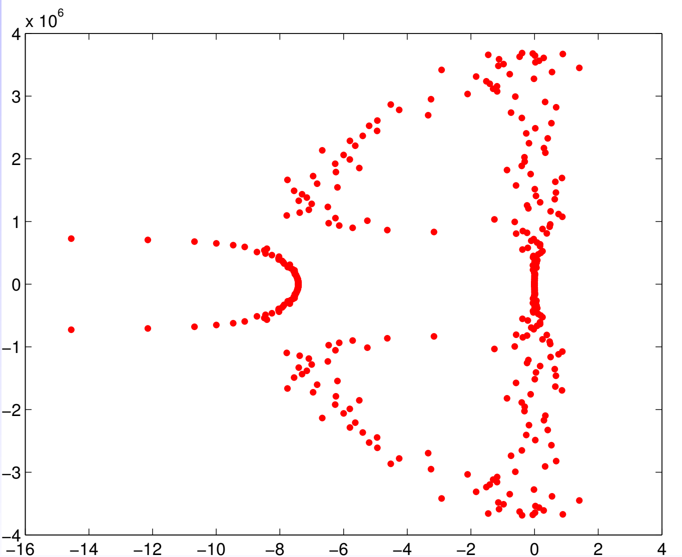
- $M > 0$, $K > 0$, $D \geq 0 \;\Rightarrow$ all ei'vals have $\mathrm{Re}(\lambda) \leq 0$.
- D is rank 1. Can show n pure imaginary ei'vals.

Eigenvalues of Q via First Companion C_1

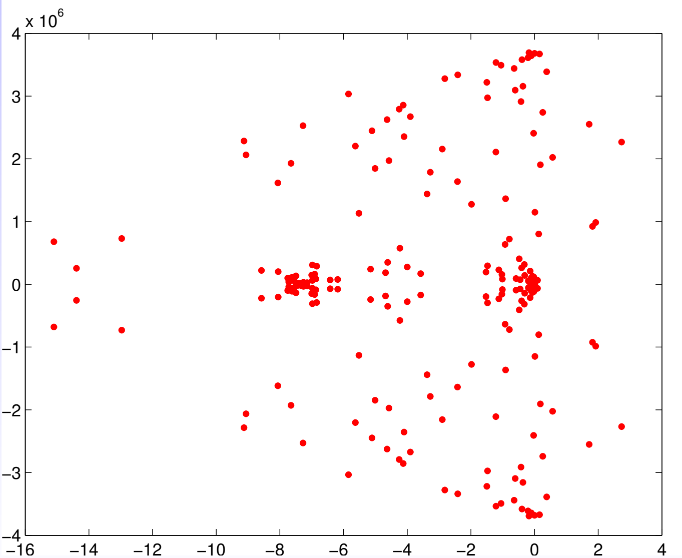
$$Q(\lambda) = \lambda^2 M + \lambda D + K, \quad C_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D & K \\ -I & 0 \end{bmatrix}.$$

```
nele = 100;
coeffs = nlevp('damped_beam',nele);
K = coeffs{1};
D = coeffs{2};
M = coeffs{3};
I = eye(2*nele); O = zeros(2*nele);
eval = eig([D K; -I O],-[M O; O I]);
plot(eval,'.r')
```

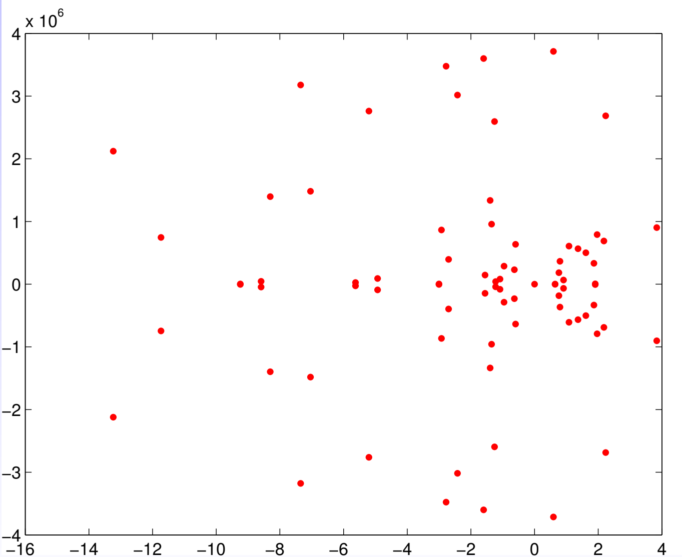
eig on Companion $C_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D & K \\ -I & 0 \end{bmatrix}$



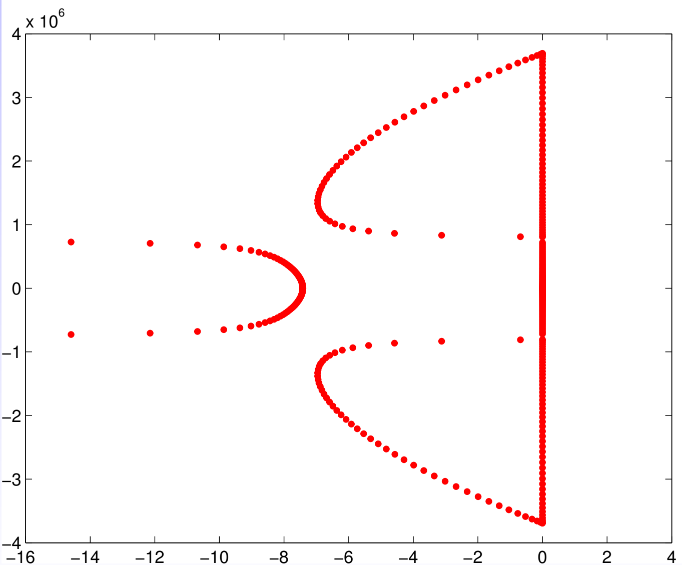
eig on Linearization $L_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & -K \end{bmatrix} + \begin{bmatrix} D & K \\ K & 0 \end{bmatrix}$



eig on Linearization $L_2(\lambda) = \lambda \begin{bmatrix} 0 & M \\ M & D \end{bmatrix} + \begin{bmatrix} -M & 0 \\ 0 & K \end{bmatrix}$



Spectrum of Beam Problem



Sensitivity and Stability of Linearizations

- **Condition number** measures sensitivity of the solution of a problem to perturbations in the data.
- **Backward error** measures how well the problem has been solved.

error in solution $\lesssim$ condition number $\times$ backward error.

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For a given $Q(\lambda)$, infinitely many linearizations exist:

- can have **widely varying eigenvalue condition numbers**,
- computed eigenpairs can have **widely varying backward errors**.

Desiderata for a Linearization

- Good conditioning.
- Backward stability.
- Suitable **eigenvector recovery** formulae.
- Preservation of structure, e.g. **symmetry**.
- Numerical preservation of key **qualitative** properties, including location and symmetries of spectrum.
- Preserve partial multiplicities of e'vals (strong linearization).

Vector Spaces $\mathbb{L}_1$, $\mathbb{L}_2$

Mackey, Mackey, Mehl & Mehrmann (2006) define

$$\mathbb{L}_1(Q) = \{\, L(\lambda) : L(\lambda)(\Lambda \otimes I_n) = v \otimes Q(\lambda),\ v \in \mathbb{C}^2 \,\},$$
$$\mathbb{L}_2(Q) = \{\, L(\lambda) : (\Lambda^T \otimes I_n)L(\lambda) = \widetilde{v}^T \otimes Q(\lambda),\ \widetilde{v} \in \mathbb{C}^2 \,\},$$

where $\Lambda := [\lambda, 1]^T$.

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where $\Lambda := [\lambda, 1]^T$.

$L(\lambda) = \lambda X + Y \in \mathbb{L}_1(Q)$ with $v \in \mathbb{C}^2$ iff

$$\begin{bmatrix} v_1 M & v_1 D & v_1 K \\ v_2 M & v_2 D & v_2 K \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} + Y_{11} & Y_{12} \\ X_{21} & X_{22} + Y_{21} & Y_{22} \end{bmatrix}.$$

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where $\Lambda := [\lambda, 1]^T$.

- Dimensions: $\mathbb{L}_1$, $\mathbb{L}_2$: $2n^2 + 2$.
- Almost all pencils in $\mathbb{L}_1$ and $\mathbb{L}_2$ are linearizations.

Eigenvector Recovery for $\mathbb{L}_1(Q)$

$$\mathbb{L}_1(Q) = \{\, L(\lambda) : L(\lambda)(\Lambda \otimes I_n) = v \otimes Q(\lambda),\ v \in \mathbb{C}^2 \,\} \quad \Lambda := [\lambda, 1]^T.$$

If $L \in \mathbb{L}_1(Q)$ with vector v then

- every right e'vec of L with finite e'val λ is of the form $\Lambda \otimes x$ for some right e'vec x of P, [M[4], 2006]
- if w is a left e'vec of L with e'val λ then $y = (v^* \otimes I_n)w$ is a left e'vec of P with e'val λ. [H, Li, Tisseur, 2007].

E'vecs of Q easily recovered from e'vecs of $L \in \mathbb{L}_1$.

Outline

Eigenvalue Condition Numbers $\kappa_Q(\lambda)$

$$Q(\lambda)x = 0, \quad y^*Q(\lambda) = 0.$$

$$\Delta Q(\lambda) = \lambda^2 \Delta M + \lambda \Delta D + \Delta K$$

For λ simple, nonzero and finite,

$$\kappa_Q(\lambda) = \lim_{\epsilon \to 0} \sup \left\{ \frac{|\Delta\lambda|}{\epsilon|\lambda|} : \big[(Q + \Delta Q)(\lambda + \Delta\lambda)\big](x + \Delta x) = 0, \right.$$
$$\left. \|\Delta M\|_2 \le \epsilon m,\ \|\Delta D\|_2 \le \epsilon d,\ \|\Delta K\|_2 \le \epsilon k \right\},$$

$$\kappa_Q(\lambda) = \frac{\big(|\lambda|^2 m + |\lambda| d + k\big)\|y\|_2\|x\|_2}{|\lambda||y^*(2\lambda M + D)x|}.$$

(Tisseur, 2000)

Eigenvalue Conditioning of Linearizations

For $L(\lambda) = \lambda X + Y$, $L(\lambda)z = 0$, $w^* L(\lambda) = 0$,

$$\kappa_L(\lambda) = \frac{(|\lambda| \|X\|_2 + \|Y\|_2)\|w\|_2 \|z\|_2}{|\lambda||w^* X z|}.$$

Define **growth factor** ϕ_L: $\kappa_L(\lambda) = \phi_L(\lambda) \cdot \kappa_Q(\lambda).$

Theorem (H, Mackey, Tisseur, 2006)

Let $L(\lambda) = \lambda X + Y \in \mathbb{B}(Q)$ with vector v. For λ simple, nonzero and finite,

$$\phi_L(\lambda; v) = \frac{|\lambda| \|X\|_2 + \|Y\|_2}{\lambda^2 m + \lambda d + k} \cdot \frac{\|\Lambda\|_2^2}{|\Lambda^T v|},$$

where $\Lambda = [\lambda,\ 1]^T$.

Sufficient conditions for $\kappa_Q \approx \kappa_L$

$$\rho = \max(m, d, k) / \min(m, k),$$

Linearization	Eigenvalue	Condition
C_1	No restriction	$m \approx d \approx k \approx 1$
L_1	$\lvert\lambda\rvert \gtrsim 1$	$\rho \approx 1$
	$\lvert\lambda\rvert \ll 1$	"not available"
L_2	$\lvert\lambda\rvert \gtrsim 1$	"not available"
	$\lvert\lambda\rvert \ll 1$	$\rho \approx 1$

$$C_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D & K \\ -I & 0 \end{bmatrix},$$

$$L_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & -K \end{bmatrix} + \begin{bmatrix} D & K \\ K & 0 \end{bmatrix}, \quad L_2(\lambda) = \lambda \begin{bmatrix} 0 & M \\ M & D \end{bmatrix} + \begin{bmatrix} -M & 0 \\ 0 & K \end{bmatrix}.$$

Beam Problem

$$\|M\|_2 = 6.7 \times 10^{-3}, \quad \|D\|_2 = 5, \quad \|K\|_2 = 1.7 \times 10^9.$$

Thus $\rho = 2.6 \times 10^{11}$ $\Rightarrow$ **beam problem is badly scaled**.

Approximations to growth factors $\phi_L(\lambda) = \kappa_L(\lambda)/\kappa_Q(\lambda)$:

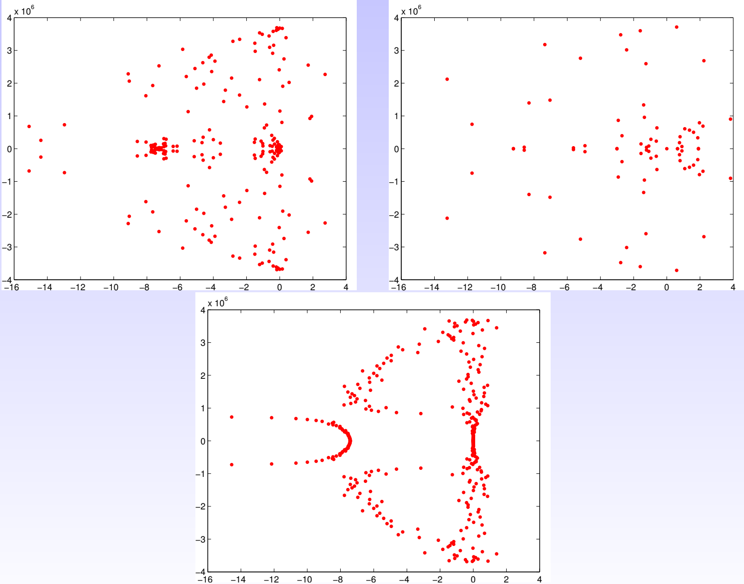
	$\phi_{C_1}(\lambda)$	$\phi_{L_1}(\lambda)$	$\phi_{L_2}(\lambda)$
$\lvert\lambda\rvert = 10^2$	1×10^2	1×10^4	1×10^4
$\lvert\lambda\rvert = 10^4$	1×10^4	1×10^8	1×10^8
$\lvert\lambda\rvert = 10^6$	2×10^5	2×10^{11}	2×10^{11}

For $|\lambda| = 10^6$, $\epsilon \approx 10^{-16}$,

$$|\Delta\lambda| \lesssim \epsilon|\lambda|\kappa_{L_i}(\lambda) = \epsilon|\lambda|\phi_{L_i}(\lambda)\kappa_Q(\lambda) = O(1), \ i = 1, 2.$$

E'vals on imaginary axis can be perturbed by distance $O(1)$ into the right half-plane.

Computed Spectrum of L_1, L_2 and C_1



Outline

Scaling $Q(\lambda) = \lambda^2 M + \lambda D + K$

Let $\lambda = \mu\gamma$ and convert

$$Q(\lambda) = \lambda^2 M + \lambda D + K \to \delta Q(\mu\gamma)$$
$$= \mu^2(\delta\gamma^2 M) + \mu(\delta\gamma D) + \delta K = \mu^2\widetilde{M} + \mu\widetilde{D} + \widetilde{K} =: \widetilde{Q}(\mu),$$

where $\gamma = \sqrt{\|K\|_2/\|M\|_2}, \quad \delta = 2/(\|K\|_2 + \|D\|_2\gamma)$.

- Fan, Lin and Van Dooren (2004).
- $2/3 \le \max(\|\widetilde{M}\|_2, \|\widetilde{D}\|_2, \|\widetilde{K}\|_2) \le 2$.
- Does not affect sparsity of M, D, K.
- Has no effect on κ_Q and η_Q.
- γ minimizes scaling factor ρ.

Effect of Scaling on Beam Problem

	Before scaling	After scaling
$\|M\|_2$	10^{-2}	1
$\|D\|_2$	1	10^{-3}
$\|K\|_2$	10^{9}	1
	$\rho = 10^{11}$	$\rho = 1$

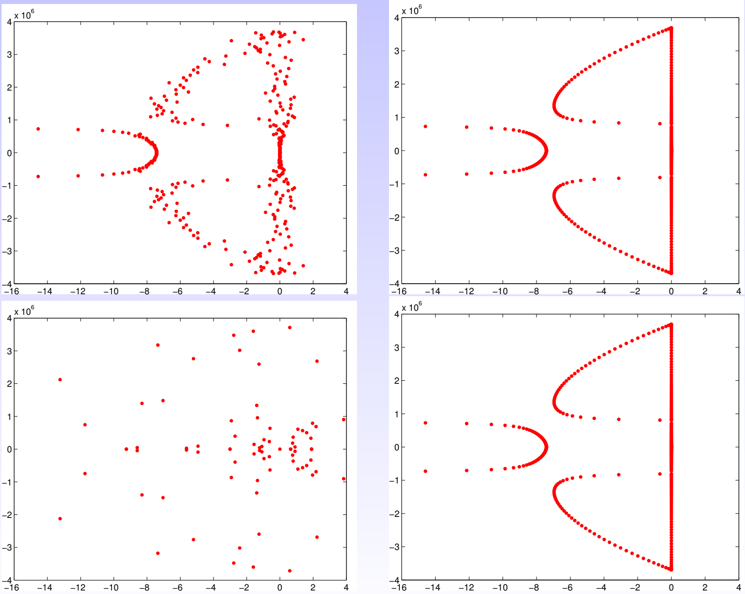
Our theory guarantees

- optimal conditioning and stability for the companion linearization,
- E'val bound

$$|\mu| \le \frac{1}{2}\tau\kappa_2(M)\Big(1 + \sqrt{1 + 4/(\tau^2\kappa_2(M))}\Big) = 7.25.$$

Can show this implies symm linearization L_2 optimal in terms of both conditioning and stability.

Spectrum of C_1, L_2 before/after Scaling



Outline

Meta-Algorithm for PEP

```
Balance, scale P (Fan, Lin & Van Dooren, 2004)
for one or more (scaled) linearizations L
    Deflate L
    Balance, scale L
    Apply QZ to L (maybe HZ if structured)
    Obtain relevant e'vals
    Recover left and right e'vecs
    Iteratively refine e'vecs
    Compute/estimate b'errs and condition numbers
    Detect nonregular problem
end
```

Balancing

- Ward (1981) for pencils.
- Lemonnier & Van Dooren (2006) for pencils.
- Betcke (2009) for polynomials.

Concluding Remarks

- ★ Analysis of conditioning & backward error for wide variety of linearizations.
- ★ E'vector recovery formulae *crucial*.
- ★ Scaling *crucial*.
- ★ Favour $L =$ companion form for general QEPs.
- ★ Results useful to develop a general QEP algorithm & code. New version of **`polyeig`** in preparation.

For papers and Eprints,
`http://www.ma.man.ac.uk/~higham`

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