

Heuristic methods for rank minimization with applications

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- - Karlstad University, Mechanical and Materials Engineering

Born in Kharkiv, Ukraine in 1986 •

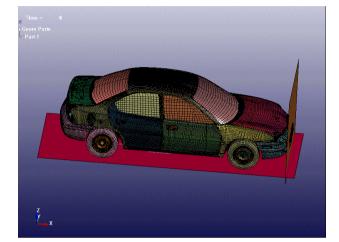
on dynamics Stuttgart (2015-2020)

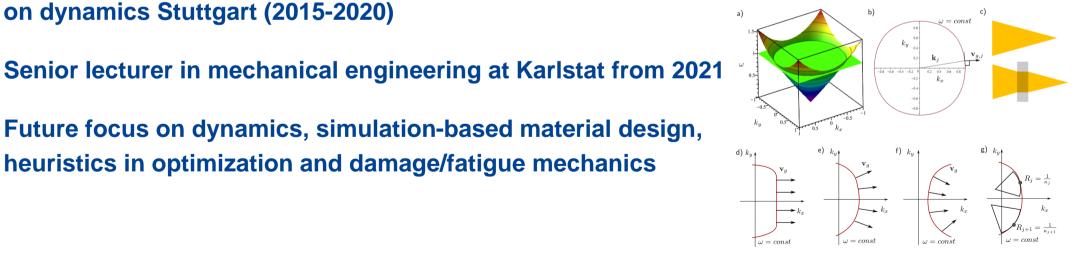
- Study of mechanical engineering at Kharkiv (2002-2007) and • computational mechanics at Stuttgart (2007-2009)
- Dr.-Ing. on finite element method with Manfred Bischoff in 2013 •

PostDoc with Kurt Maute at Colorado on 4D printing (2014) and

Future focus on dynamics, simulation-based material design,

heuristics in optimization and damage/fatigue mechanics







Outline



Origins of rank minimization formulations Minimal Euclidean embedding Matrix completion

Exact method for a special case

Rank minimization heuristics Trace and Log-Det

Applications of rank minimization formulations Numerical dispersion for finite difference stencils Minimization of numerical dispersion for FE stencils Dispersion design of periodic systems

Conclusions

Origins of rank minimization formulations

Minimal Euclidean embedding. Known information

Euclidean distance matrix

$$\mathbf{D} \in \mathbb{R}^{n \times n} \quad D_{ij} = |x_i - x_j|^2$$
$$x_i \in \mathbb{R}^r$$

Minimal possible *r* is called **embedding dimension**

Theorem by Schoenberg'1935: **D** is EDM with embedding dimension r iff

$$D_{ii} = 0$$

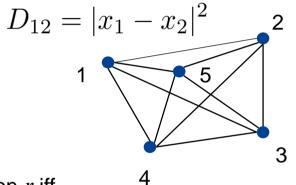
$$\mathbf{VDV} \prec 0 \quad \mathbf{V} = \operatorname{eye}(n) - \operatorname{ones}(n)/n$$

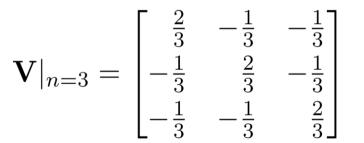
$$\operatorname{rank}(\mathbf{VDV}) \leq r$$

First two conditions are equivalent to distance properties

$$D_{ii} = 0 \quad D_{ij} = D_{ji} \ge 0 \quad D_{ik} + D_{ki} \ge D_{ij}$$







Example



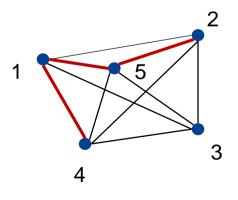
Minimal Euclidean embedding. Known information

Euclidean distance matrix with uncertainty in the measurement

$$n = 5 \quad \mathbf{D} \in \mathbb{R}^{n \times n}$$
$$\mathbf{D} = \begin{bmatrix} 0 & 18.86 & 15.89 & 57.72 \pm 10 & 78.61 \pm 10 \\ 18.86 & 0 & 15.21 & 15.46 & 112.77 \pm 10 \\ 15.89 & 15.21 & 0 & 48.61 & 45.48 \\ 57.72 \pm 10 & 15.46 & 48.61 & 0 & 182.93 \\ 78.61 \pm 10 & 112.77 \pm 10 & 45.48 & 182.93 & 0 \end{bmatrix}$$

Find the possible embedding dimension r by a problem

$$\min \operatorname{rank} (\mathbf{VDV})$$
$$D_{ii} = 0$$
$$-\mathbf{VDV} \succ 0 \quad \mathbf{V} = \operatorname{eye}(n) - \operatorname{ones}(n)/n$$
$$L_{ij} \le D_{ij} \le U_{ij}, \{ij\} \in Q$$



Example



Minimal Euclidean embedding. Solution

Euclidean distance matrix with uncertainty in the measurement

$$n = 5 \quad \mathbf{D} \in \mathbb{R}^{n \times n}$$
$$\mathbf{D} = \begin{bmatrix} 0 & 18.86 & 15.89 & 57.72 + x_1 & 78.61 + x_2 \\ 18.86 & 0 & 15.21 & 15.46 & 112.77 + x_3 \\ 15.89 & 15.21 & 0 & 48.61 & 45.48 \\ 57.72 + x_1 & 15.46 & 48.61 & 0 & 182.93 \\ 78.61 + x_2 & 112.77 + x_3 & 45.48 & 182.93 & 0 \end{bmatrix}$$
$$\mathbf{x}^* = \begin{bmatrix} 9.9947 & -9.9266 & -4.8421 \end{bmatrix}$$
$$\operatorname{rank} (\mathbf{VD}(\mathbf{x}^*)\mathbf{V}, tol = 10^{-6}) = 3$$
$$\operatorname{eig} (-\mathbf{VD}(\mathbf{x}^*)\mathbf{V}) = \begin{bmatrix} 202.0116 & 31.4276 & 1.2671 & 0.0000 & 0.0000 \end{bmatrix}$$

Origins of rank minimization formulations

Matrix completion

Partial information about a matrix

 $\mathbf{X} \in \mathbb{R}^{n imes m}$

$$\Phi : \mathbb{R}^{n \times m} \to \mathbb{R}^P \quad \Phi(\mathbf{X}) = (x_{ij})_{(ij) \in I} =: \mathbf{y}$$
$$P = \operatorname{round}(C(n+m)\log(n+m))$$

Low rank matrix completion

$$\begin{aligned} \mathbf{X}^* &= \arg \min \operatorname{rank} \left(\mathbf{X} \right) \\ \Phi(\mathbf{X}) &= \mathbf{y} \end{aligned}$$



Netflix prize (\$10⁶)

Predict preferences of users from few rating values

Columns (10⁶): ratings (100) of a user from 1 to 5 Rows (10⁵): films

	U1	U2	U3	
$\mathbf{X} =$	[*	3	*	Film 1
	5	*	2	Film 2
	4	5	*	Film 3
	*	2	5	Film 4

<u>Matrix Completion with Nuclear Norm Minimization (numerical-tours.com)</u> <u>Matrix Completion and the Netflix Prize - YouTube</u>

Exact method for a special case

Rank minimization problem with constraint on the norm difference

Problem definition

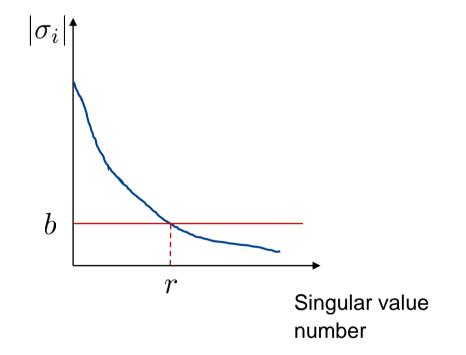
$$\mathbf{X}^* = rg \min \operatorname{rank} (\mathbf{X})$$

 $||\mathbf{X} - \mathbf{A}||_{2,F} \le b$

Solution

$$\begin{split} \mathbf{U}, \mathbf{\Sigma}, \mathbf{V}] &= \operatorname{svd}(\mathbf{A}) \\ \mathbf{\tilde{\Sigma}} &= \operatorname{diag}(f(\sigma_i)) \\ f(x) &= \begin{cases} x & |x| > b \\ 0 & |x| \le b \end{cases} \\ \mathbf{X}^* &= \mathbf{U}\mathbf{\tilde{\Sigma}}\mathbf{V}^T \end{split}$$

Thresholding of singular values





Requirements to RMP algorithms

- General, e.g. handle any symmetric positive semi-definite matrix and convex constraints $\mathbf{X}\in\mathcal{C}$
- No strict reqirements on initialization
- Numerically efficient, e.g., reduce to a quadratic programing problem
- Depend on few interpretable parameters
- Effective for practical problems

Herein, two heuristics from simple to more complex are presented.

Test example with square matrix *X* depending on parameters *a* and *b*

$$\mathbf{A} = \begin{bmatrix} \frac{5}{4} - 2b & \frac{1}{3} - a & \frac{1}{4} - 2b \\ \frac{1}{3} - a & \frac{1}{3} - a & \frac{1}{3} - a \\ \frac{1}{4} - 2b & \frac{1}{3} - a & \frac{1}{4} - 2b \end{bmatrix}$$
$$\mathbf{X} = \mathbf{A}\mathbf{A}^{\mathrm{T}}$$
Known rank-1 solution:
$$\mathbf{X}^{*} \left(a = \frac{1}{3}, b = \frac{1}{8} \right) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

 $0 \leq a \leq 1, 0 \leq b \leq 1$



Trace heuristics

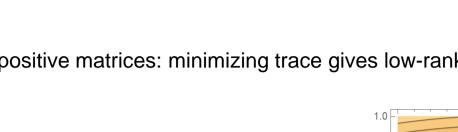
Observation for symmetric semi-positive matrices: minimizing trace gives low-rank solutions Smooth surrogate problem

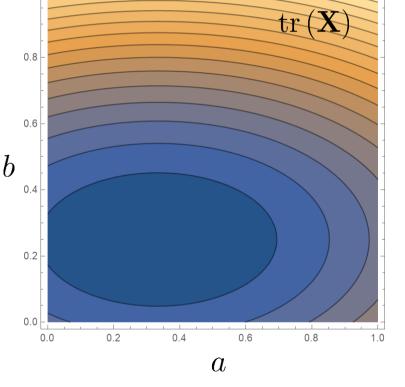
$$egin{aligned} \mathbf{X}^* &= rg\,\min \mathrm{trace}\,(\mathbf{X})\ \mathbf{X} \in \mathcal{C} \end{aligned}$$

Obtained rank-2 solution:

$$\mathbf{X}^* \left(a = \frac{1}{3}, b = \frac{1}{4} \right) = \begin{bmatrix} \frac{5}{8} & 0 & -\frac{1}{8} \\ 0 & 0 & 0 \\ -\frac{1}{8} & 0 & \frac{1}{8} \end{bmatrix}$$

MESBAHI, M., & PAPVASSILOUPOULOS, G. P. (1997, JUNE). SOLVING A CLASS OF RANK MINIMIZATION PROBLEMS VIA SEMI-DEFINITE PROGRAMS, WITH APPLICATIONS TO THE FIXED ORDER OUTPUT FEEDBACK SYNTHESIS. IN PROCEEDINGS OF THE 1997 AMERICAN CONTROL CONFERENCE (CAT. NO. 97CH36041) (VOL. 1, PP. 77-80). IEEE..







Log-det heuristics

Smooth surrogate problem

$$\begin{aligned} \mathbf{X}^* &= \arg \min \left(\log \det \left(\mathbf{X} + \delta \mathbf{I} \right) \right) \\ \mathbf{X} &\in \mathcal{C} \end{aligned}$$

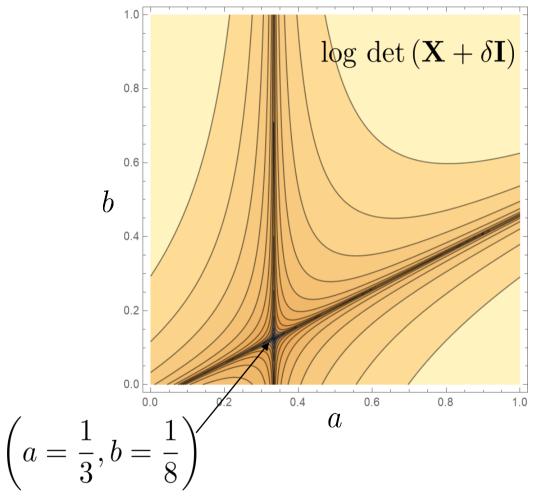
 $0 < \delta \ll 1$ $\;$ regularization parameter $\;$

Obtained rank-1 solution in 10 iterations:

$$\mathbf{X}^* (a = 0.3333331, b = 12503) = \begin{bmatrix} 0.998787 & 3 \cdot 10^{-6} & -0.00607 \\ 3 \cdot 10^{-6} & 3 \cdot 10^{-6} & -3 \cdot 10^{-6} \\ -0.00607 & 2 \cdot 10^{-11} & 7 \cdot 10^{-7} \end{bmatrix}$$

$$\delta = 10^{-6}$$





FAZEL, M., HAITHAM H., AND S.P. BOYD. "LOG-DET HEURISTIC FOR MATRIX RANK MINIMIZATION WITH APPLICATIONS TO HANKEL AND EUCLIDEAN DISTANCE MATRICES." AMERICAN CONTROL CONFERENCE, 2003. PROCEEDINGS OF THE 2003. Vol. 3. IEEE, 2003.

Log-det heuristics

Local approximation via Taylor expansion

weighted trace norm of increment, quadratic in parameters

$$\log \det(\mathbf{X} + \delta \mathbf{I}) \approx \log \det(\mathbf{X}_k + \delta \mathbf{I}) + \operatorname{trace} \left((\mathbf{X}_k + \delta \mathbf{I})^{-1} (\mathbf{X} - \mathbf{X}_k) \right)$$

 $\mathbf{W}_k = (\mathbf{X}_k + \delta \mathbf{I})^{-1}$ - weight for trace norm at k-th step

 $\log \det(\mathbf{X} + \delta \mathbf{I}) \approx \log \det(\mathbf{X}_k + \delta \mathbf{I}) + \operatorname{trace}(\mathbf{W}_k(\mathbf{X} - \mathbf{X}_k))$

Algorithm

- 1. Initialize matrix $\mathbf{X}_0 \in \mathcal{C}$, regularization $\delta > 0$ and tolerance $\epsilon > 0$
- 2. Repeat until $||\mathbf{X}_{k+1} \mathbf{X}_k||_2 > \epsilon$ otherwise goto end
- 3. Compute weighting $\mathbf{W}_k = (\mathbf{X}_k + \delta \mathbf{I})^{-1}$
- 4. Solve QP $\mathbf{X}_{k+1} = \operatorname{arg\,min}_{\mathbf{X} \in \mathcal{C}} \operatorname{trace} (\mathbf{W}_k(\mathbf{X} \mathbf{X}_k))$

5. goto 2.



Minimization of numerical dispersion for stencil of finite difference method Wave equation in 2D

$$\ddot{u} = c^2 \Delta u$$

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

Two discrete Laplacians

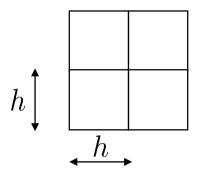
$$\Delta_h^1 = \frac{1}{h^2} \begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \Delta_h^2 = \frac{1}{2h^2} \begin{bmatrix} 1 & 0 & 1 \\ 0 & -4 & 0 \\ 1 & 0 & 1 \end{bmatrix}$$

A parametric family of stencils (9-point explicit)

$$\frac{u^{n+1} - 2u^n + u^{n-1}}{\Delta t^2} = c^2 ((1-\alpha)\Delta_h^1 + \alpha \Delta_h^2)u$$









 $\mathbf{\hat{k}} = [k_x, k_y]$

Minimization of numerical dispersion for stencil of finite difference method

Plane wave assumption for analytical solution and the dispersion relation

$$u = e^{-i(\omega t - k_x x - k_y y)}$$

$$\omega^2 = c^2 (k_x^2 + k_y^2)$$

$$c = \frac{\omega}{\sqrt{k_x^2 + k_y^2}}$$

Discrete dispersion relation for 9-point explicit stencil

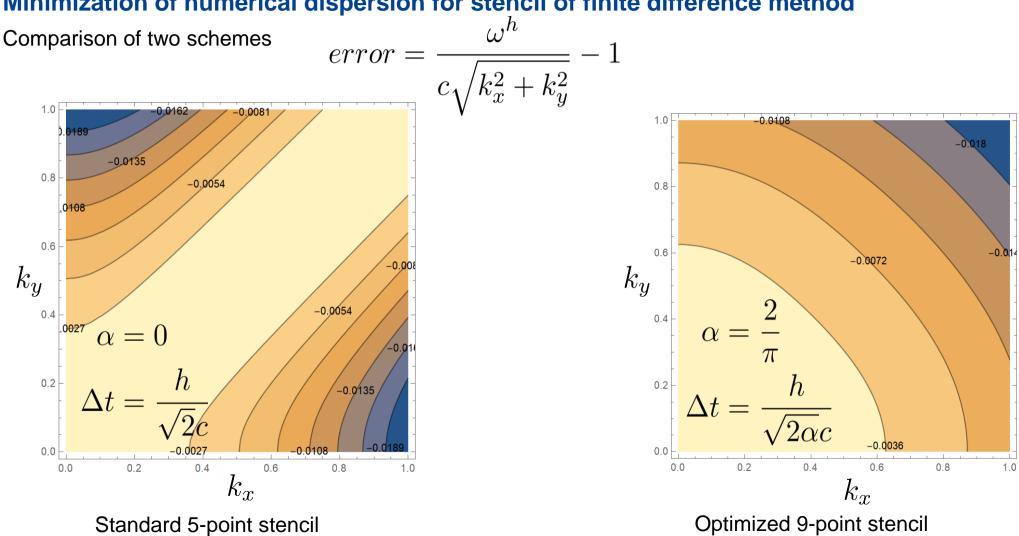
$$u = e^{-i(\omega^h \Delta t - k_x \Delta x - k_y \Delta y)}$$

$$1 - \cos\left(\omega^h \Delta t\right) = \frac{c^2 \Delta t^2}{h^2} \left[(1 - \alpha)(\cos(k_x h) + \cos(k_y h) - 2) + \alpha(\cos(k_x h)\cos(k_y h) - 1) \right]$$

Relative numerical dispersion error in phase speed

$$error = \frac{\omega^h}{c\sqrt{k_x^2 + k_y^2}} - 1$$





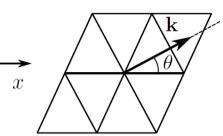
Minimization of numerical dispersion for stencil of finite difference method



Minimization of numerical dispersion for stencil of finite element method

Case of reciprocal mass matrices

$$\ddot{\mathbf{U}} = \mathbf{C}(\mathbf{F}^{\text{ext}} - \mathbf{K}\mathbf{U})$$



• equilibrium on representative patch level for plane wave ansatz $u(\mathbf{x},t) = \tilde{\mathbf{U}}e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$

$$\left(\mathbf{C}_{\mathrm{rep}}^{\circ}(\mathbf{k}, C_{2i})\mathbf{K}_{\mathrm{rep}}(\mathbf{k}) - \omega^{2}\mathbf{I}_{\mathrm{rep}}\right)\tilde{\mathbf{U}} = \mathbf{0}$$
 rank $\left(\mathbf{C}_{\mathrm{rep}}^{\circ}(\mathbf{k}, C_{2i})\mathbf{K}_{\mathrm{rep}}(\mathbf{k}) - \omega^{2}\mathbf{I}_{\mathrm{rep}}\right) < n_{\mathrm{rep}}$

 \mathbf{k}, ω - wavevector and angular frequency C_{2i} - customization parameters $\tilde{\mathbf{U}} \in \mathbb{C}^{n_{\mathrm{rep}}}$ - discrete amplitudes n_{rep} - size of representative patch

• heuristic objective

$$C_{2i} = \operatorname*{arg\,min}_{C_{2i}} \sum_{j} \operatorname{rank} \left(\mathbf{C}^{\circ}_{\operatorname{rep}}(\mathbf{k}_{j}, C_{2i}) \mathbf{K}_{\operatorname{rep}}(\mathbf{k}_{j}) - \omega_{j}^{2} \mathbf{I}_{\operatorname{rep}} \right)$$

TKACHUK, ANTON. "CUSTOMIZATION OF RECIPROCAL MASS MATRICES VIA LOG-DET HEURISTIC." INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING 121.4 (2020): 690-711..

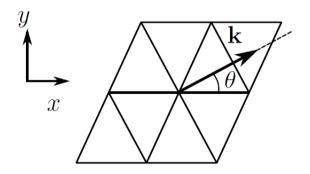


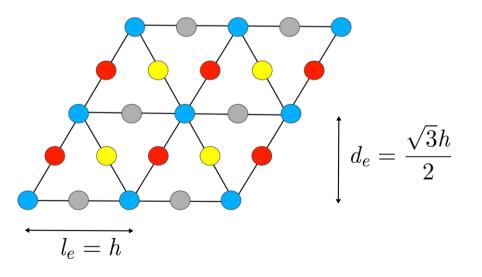
Minimization of numerical dispersion for stencil of finite element method

2D elastic-dynamics discretized with 6-node FE, hexagonal mesh

 $\left(\mathbf{C}_{\mathrm{rep}}^{\circ}(k, C_{21}, C_{22})\mathbf{K}_{\mathrm{rep}}(k) - \omega^{2}\mathbf{I}_{\mathrm{rep}}\right)\tilde{\mathbf{U}} = \mathbf{0}$

k, ω - wavevector and angular frequency C_{21}, C_{22} - customization parameters $\tilde{\mathbf{U}} = [\tilde{U}_{xc}, \tilde{U}_{yc}, \tilde{U}_{xm1}, \tilde{U}_{xm2}, \tilde{U}_{xm3}, \tilde{U}_{ym1}, \tilde{U}_{ym2}, \tilde{U}_{ym3}] \in \mathbb{C}^{n_{rep}}$ - 2 corner and 6 mid-node amplitudes $n_{rep} = 8$ - size of representative patch





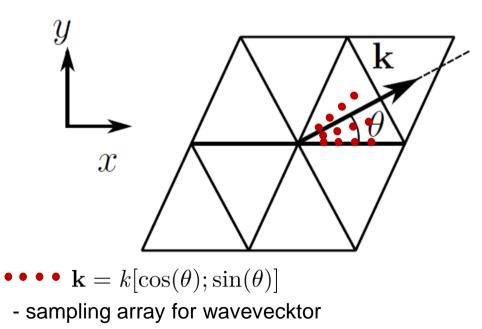
Applications to reciprocal mass matrix



Minimization of numerical dispersion for stencil of finite element method Reformulate for reduce the problem to Hermitian semi-positive definite

$$\tilde{\mathbf{A}}(\mathbf{k},\omega,C_{21},C_{22}) = \left(\mathbf{C}_{\mathrm{rep}}^{\circ}(\mathbf{k},C_{21},C_{22})\mathbf{K}_{\mathrm{rep}}(\mathbf{k}) - \omega^{2}\mathbf{I}_{\mathrm{rep}}\right)$$
$$\mathbf{X}(\mathbf{k},\omega,C_{21},C_{22}) = \tilde{\mathbf{A}}^{\mathrm{H}}\tilde{\mathbf{A}}$$

Surrogate problem



Two waves types (plane stress assumption)

- P-wave

$$\omega_{\rm P}^2 = \frac{E}{(1-\nu^2)\rho} \mathbf{k}^2$$

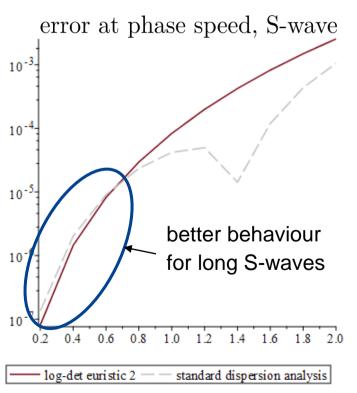
- S-wave

$$\omega_{\rm S}^2 = \frac{E}{2(1+\nu)\rho} \mathbf{k}^2$$



RMM example 3: 2D elastic-dynamics discretized with 6-node FE, hexagonal mesh Best results from log-det heuristics

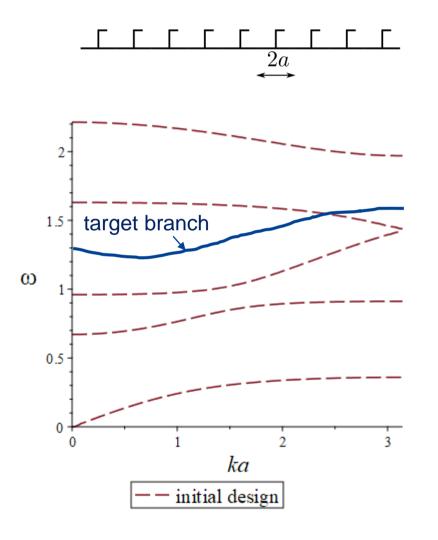
$n_k = 7 \quad k_j = [0.025; 0.05; 0.1; 0.2; 0.3; 0.4; 0.5] h$ $n_\theta = 5 \quad \theta_s = [0; \pi/30; \pi/15; \pi/10; \pi/6]$ $\omega_{j,s} = c_0 k_j \quad \delta = 3 \cdot 10^{-42}$

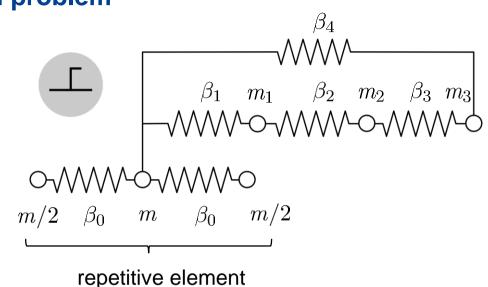


 $C_{21} = 0.35999923115819346922334586255,$ $C_{22} = 0.42181367522022318508140913666$ error at phase speed, P-wave 10-3 10-4 10⁻⁵-ت⁶-10 10 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 0.2 0.4 log-det euristic 2 standard dispersion analysis



Problem statement for a dispersion design problem



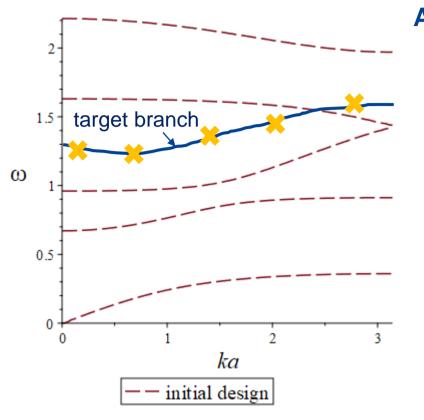


<u>*Given:*</u> a periodic system depending on a set of parameters s and a target branch with a dispersion relation $k = f(\omega)$. <u>*Find:*</u> a design whose dispersion relation matches the given dispersion relation best

Two desired features of algorithm

- performance function depends explicitly on the design parameters
- ordering of eigenfrequencies should be avoided

Dispersion design as matrix rank minimization problem



A possible formalization and relaxation

• equilibrium on representative patch level for plane wave ansatz

$$u(\mathbf{x},t) = \tilde{\mathbf{U}}e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)}$$
$$\left(\mathbf{K}_{\mathrm{rep}}(k,\mathbf{s}) - \omega^2 \mathbf{M}_{\mathrm{rep}}(\mathbf{s})\right)\tilde{\mathbf{U}} = \mathbf{0}$$

 $ilde{\mathbf{U}} \in \mathbb{C}^{n_{\mathrm{rep}}}$ - discrete amplitudes n_{rep} - size of representative patch

• require not full rank at discrete pairs (k_{j}, ω_{j})

rank
$$\left(\mathbf{K}_{\mathrm{rep}}(k_j, \mathbf{s}) - \omega_j^2 \mathbf{M}_{\mathrm{rep}}(\mathbf{s})\right) < n_{\mathrm{rep}}$$

· set up a heuristic objective function

$$J(\mathbf{s}) = \sum_{j} \operatorname{rank} \left(\mathbf{K}_{\operatorname{rep}}(k_j, \mathbf{s}) - \omega_j^2 \, \mathbf{M}_{\operatorname{rep}}(\mathbf{s}) \right)$$



Applications



Mass-spring system 1: targeting several points on two acoustic branches

 β_4 System topology m = 1 $\beta_0 = 1$ β_0 β_0 mmm⁻ repetitive element m_i - nodal masses *a* - distance between nodes - spring stiffness $n_{\rm rep} = 4$ - size of the representative patch β_i Admissible range of parameters Algorithm parameters $m_i \in [0.2,2] \quad \beta_{1,2,3} \in [0.3,4] \quad \beta_4 \in [0.005,4] \quad \delta = 3 \cdot 10^{-8}$

Initial design

$$m_1 = 1 \quad m_2 = 2 \quad m_3 = 1.2$$

$$\beta_1 = 1 \quad \beta_2 = 0.5 \quad \beta_3 = 0.6 \quad \beta_4 = 0.1$$

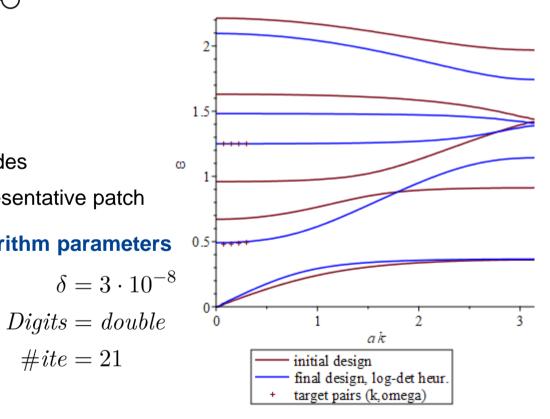
Target wave number-frequency pairs (8) $ak_1 = 0.075$ $\omega_1 = 0.4797$ $ak_2 = 0.150$ $\omega_2 = 0.4824$. . . 1.5 ω 0.5 ++++ Digits = double2 3 #ite = 21ak initial design + target pairs (k.omega)

Applications





$$\beta_1 = 0.49$$
 $\beta_2 = 0.3$ $\beta_3 = 0.41$ $\beta_4 = 0.005$



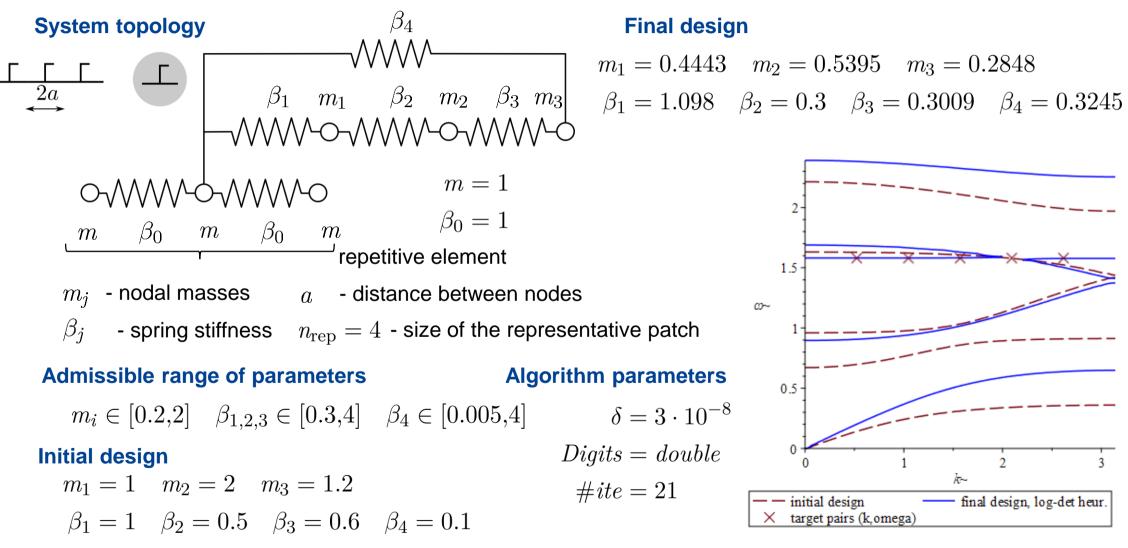
m = 1 $\beta_0 = 1$ $\beta_0 \quad m \quad \beta_0 \quad m$ m----' repetitive element m_i - nodal masses a - distance between nodes β_i - spring stiffness $n_{\rm rep} = 4$ - size of the representative patch Algorithm parameters Admissible range of parameters $m_i \in [0.2,2]$ $\beta_{1,2,3} \in [0.3,4]$ $\beta_4 \in [0.005,4]$ $\delta = 3 \cdot 10^{-8}$ **Initial design** $m_1 = 1$ $m_2 = 2$ $m_3 = 1.2$ #ite = 21

 $\beta_1 = 1$ $\beta_2 = 0.5$ $\beta_3 = 0.6$ $\beta_4 = 0.1$

Applications



Mass-spring system 1: targeting a constant optical branch



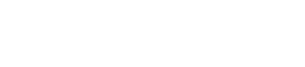
Conclusions

- Rank minimization formulation appear in several geometrical, data analysis and mechanical applications
- Sevaral tractable relaxation are known and usable
- · Instances of reciprocal mass matrices with reduced numerical dispersion are obtained via RMP
- Mechanical systems with prescribed dispersion are obtainable

Future work

- Larger systems and combination with reduced-ordering systems
- Dispersion customization for acoustic metamaterials
- Using other rank minimization heuristics

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Tack så mycket! Thank you! Vielen Dank!

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