International Symposium on Numerics and Scientific Computing Schloß Bruchsal, 22–24 October 2013

# Computing Eigenvalues of *H*(ackbusch) Matrices

Peter Benner Thomas Mach

Max Planck Institute for Dynamics of Complex Technical Systems Computational Methods in Systems and Control Theory

> KU Leuven Department of Computer Science



Hackbusch (*H*-)Matrices

LR Algorithr

Slicing Algorit

rithm

PINVIT

Conclusions

# Max Planck Mathematicians...

61st Annual Meeting of the Max Planck Society, Hannover, 2010



Courtesy of Joachim Heinze.

Max Planck Institute Magdeburg

Conclusions

# **Eigenvalue Problem**

### Definition

The pair  $(\lambda, v) \in \mathbb{R} \times \mathbb{R}^n$  is called an *eigenpair* of the symmetric matrix  $M = M^T \in \mathbb{R}^{n \times n}$ , if

 $Mv = v\lambda.$ 

# The set $\Lambda(M) = \{\lambda | \exists v : (\lambda, v) \text{ eigenpair of } M\}$ is the spectrum of M.

Similarity Transformation

 $\Lambda(M) = \Lambda(P^{-1}MP) \qquad \forall P \text{ invertible}$ 

Max Planck Institute Magdeburg

[Golub, Van der Vorst '00]

• Is *M* real or complex?

[Golub, Van der Vorst '00]

• Is M real or complex?  $M \in \mathbb{R}^{n \times n}$ 



Conclusions

# **Classification of Eigenvalue Problems**

- Is M real or complex?  $M \in \mathbb{R}^{n \times n}$
- Special properties (symmetric, Hermitian, skew-symmetric or unitary)?

- Is M real or complex?  $M \in \mathbb{R}^{n \times n}$
- Special properties (symmetric, Hermitian, skew-symmetric or unitary)?
   symmetric: M = M<sup>T</sup>

- Is M real or complex?  $M \in \mathbb{R}^{n \times n}$
- Special properties (symmetric, Hermitian, skew-symmetric or unitary)?
   symmetric: M = M<sup>T</sup>
- Further structure?

- Is M real or complex?  $M \in \mathbb{R}^{n \times n}$
- Special properties (symmetric, Hermitian, skew-symmetric or unitary)?
   symmetric: M = M<sup>T</sup>
- Further structure? Yep.

- Is M real or complex?  $M \in \mathbb{R}^{n \times n}$
- Special properties (symmetric, Hermitian, skew-symmetric or unitary)?
   symmetric: M = M<sup>T</sup>
- Further structure? Yep.  $M \in \mathcal{H}(T_{\mathfrak{I} \times \mathfrak{I}}, k) \Rightarrow \text{see next slide}$

- Is M real or complex?  $M \in \mathbb{R}^{n \times n}$
- Special properties (symmetric, Hermitian, skew-symmetric or unitary)?
   symmetric: M = M<sup>T</sup>
- Further structure? Yep.  $M \in \mathcal{H}(T_{\mathfrak{I} \times \mathfrak{I}}, k) \Rightarrow \text{see next slide}$
- Which eigenvalues required?

- Is M real or complex?  $M \in \mathbb{R}^{n \times n}$
- Special properties (symmetric, Hermitian, skew-symmetric or unitary)?
   symmetric: M = M<sup>T</sup>
- Further structure? Yep.
   M ∈ H(T<sub>J×J</sub>, k) ⇒ see next slide
- Which eigenvalues required? some (inner) or all eigenvalues



Some dense matrices, e.g. BEM or FEM, can be approximated by  $\mathcal{H}$ -matrices in a data-sparse manner.



rank-k-matrix: 
$$M_{a \times b} = AB^T$$
,  $A \in \mathbb{R}^{n \times k}$ ,  $B \in \mathbb{R}^{m \times k}$   $(k \ll n, m)$ ,

$\mathcal{H} extsf{-Matrices}$		[Hackbusc	н 1998] 🕜

### **Hierarchical Matrices**

 $\mathcal{H}(\mathcal{T}_{\mathbb{I}\times\mathbb{J}},k) = \left\{ M \in \mathbb{R}^{\mathbb{I}\times\mathbb{I}} | \operatorname{rank}(M_{a\times b}) \leq k \,\,\forall a \times b \,\, \text{admissible} \right\}$ 



- adaptive rank  $k(\varepsilon)$
- storage  $N_{St,\mathcal{H}}(T,k) = \mathcal{O}(n \log n \ k(\varepsilon))$
- complexity of approximate arithmetic

 $\begin{array}{ll} M_{\mathcal{H}} v & \mathcal{O}(n \log n \ k(\varepsilon)) \\ +_{\mathcal{H}}, -_{\mathcal{H}} & \mathcal{O}(n \log n \ k(\varepsilon)^2) \\ *_{\mathcal{H}}, \mathcal{H}LU(\cdot), (\cdot)_{\mathcal{H}}^{-1} & \mathcal{O}(n (\log n)^2 \ k(\varepsilon)^2) \end{array}$ 

$\mathcal{H} extsf{-Matrices}$		[Hackbusch	н 1998] 🧖

### **Hierarchical Matrices**

$$\mathcal{H}(\mathcal{T}_{\mathbb{J}\times\mathbb{J}},k) = \left\{ \left. M \in \mathbb{R}^{\mathbb{J}\times\mathbb{J}} \right| \operatorname{rank}\left( M_{a\times b} \right) \leq k \,\,\forall a \times b \,\, \text{admissible} \right\}$$



- adaptive rank  $k(\varepsilon)$
- storage  $N_{St,\mathcal{H}}(T,k) = \mathcal{O}(n \log n \ k(\varepsilon))$
- complexity of approximate arithmetic

$$\begin{array}{ll} M_{\mathcal{H}} v & \mathcal{O}(n \log n \ k(\varepsilon)) \\ +_{\mathcal{H}}, -_{\mathcal{H}} & \mathcal{O}(n \log n \ k(\varepsilon)^2) \\ *_{\mathcal{H}}, \mathcal{H}LU(\cdot), (\cdot)_{\mathcal{H}}^{-1} & \mathcal{O}(n (\log n)^2 \ k(\varepsilon)^2) \end{array}$$



Max Planck Institute Magdeburg

Hackbusch ( $\mathcal{H}$ -)Matrices LR Algorithm Slicing Algorithm PINVIT Conclusions Special Case:  $\mathcal{H}_{l}$ -Matrices [HACKBUSCH 1998]



Structure of a symmetric  $\mathcal{H}_3(k)$ -matrix.

Max Planck Institute Magdeburg



### $\mathcal{H}\text{lib}$

### $\mathcal{H}\mathsf{lib}$

#### Börm, Grasedyck, et al.]

We use the  $\mathcal{H}lib$  (www.hlib.org) for the  $\mathcal{H}$ -arithmetic operations and some examples out of the library for testing the eigenvalue algorithm.



Max Planck Institute Magdeburg

# **Eigenvalues of Symmetric** $\mathcal{H}$ -Matrices

$$M = M^T \in \mathcal{H}(T, k)$$
$$\Downarrow$$

$$\Lambda_{\mathcal{H}}(M) = \{\lambda_1, \ldots, \lambda_n\}$$
 in  $\mathcal{O}(n^2 (\log n)^{\alpha} k^{\beta})$ 

$$\{\lambda_i\} \in \Lambda_{\mathcal{H}}(M) \text{ in } \mathcal{O}(n(\log n)^{\alpha} k^{\beta})?$$

Max Planck Institute Magdeburg

# **Eigenvalues of Symmetric \mathcal{H}-Matrices**

$$M = M^T \in \mathcal{H}(T, k)$$
$$\Downarrow$$

$$\Lambda_{\mathcal{H}}(M) = \{\lambda_1, \ldots, \lambda_n\}$$
 in  $\mathcal{O}(n^2 (\log n)^{lpha} k^{eta})$ 

$$\{\lambda_i\} \in \Lambda_{\mathcal{H}}(M) \text{ in } \mathcal{O}(n(\log n)^{\alpha} k^{\beta})?$$

# dense: M + N, Mv in $\mathcal{O}(n^2)$ and $\Lambda(M)$ in $\mathcal{O}(n^3)$

Max Planck Institute Magdeburg

Hackbusch ( $\mathcal H$ -)Matrices

LR Algorithm

licing Algorithr

NVIT

Conclusions



### LR Cholesky Algorithm

# QR-like Algorithm

Max Planck Institute Magdeburg

Hackbusch (*H*-)Matrices

LR Algorithm

licing Algorithr

PIN

Conclusions



# LR Cholesky Algorithm

# LR Cholesky Algorithm

Max Planck Institute Magdeburg

### LR-Cholesky Transformation

for 
$$i = 1, \dots$$
 do  
 $\begin{vmatrix} L_i L_i^T = M_i \\ M_{i+1} = L_i^T L_i \end{vmatrix}$   
end

	LR Algorithm			
LR Cholesky	Algorithm	[Rutishauser	1958]	Ø

### LR-Cholesky Transformation

for 
$$i = 1, ...$$
 do  
 $\begin{vmatrix} L_i L_i^T = M_i \Rightarrow L_i = M_i L_i^{-T} \\ M_{i+1} = L_i^T L_i = L_i^T M_i L_i^{-T} \end{vmatrix}$   
end

$$\lim_{i\to\infty} M_i = \operatorname{diag} \left(\lambda_1, \lambda_2, \dots, \lambda_n\right) \in \mathcal{H}(\mathcal{T}, 0)$$

### LR-Cholesky Transformation

for 
$$i = 1, ...$$
 do  
 $\begin{vmatrix} L_i L_i^T = M_i - \mu_i \mathcal{I} \\ M_{i+1} = L_i^T L_i + \mu_i \mathcal{I} \end{vmatrix}$   
end

$$\lim_{\substack{i \to \infty \\ \forall i: }} M_i = \operatorname{diag} \left( \lambda_1, \lambda_2, \dots, \lambda_n \right) \in \mathcal{H}(\mathcal{T}, \mathbf{0})$$

### LR-Cholesky Transformation

for 
$$i = 1, \dots$$
 do  
 $\begin{vmatrix} L_i L_i^T = M_i - \mu_i \mathcal{I} \\ M_{i+1} = L_i^T L_i + \mu_i \mathcal{I} \end{vmatrix}$ 
end

$$\lim_{i \to \infty} M_i = \operatorname{diag} (\lambda_1, \lambda_2, \dots, \lambda_n) \in \mathcal{H}(\mathcal{T}, 0) \\ \forall i: M_i - \mu_i \mathcal{I} \text{ symmetric positive definite}$$

### H-LR-Cholesky Transformation

$$\begin{array}{l} \text{for } i=1,\ldots \text{ do} \\ \left| \begin{array}{c} \tilde{L}_i = \mathcal{H}\text{-Cholesky factorization}(\tilde{M}_i - \mu_i \mathcal{I}) \\ \tilde{M}_{i+1} = \tilde{L}_i^T *_{\mathcal{H}} \tilde{L}_i + \mu_i \mathcal{I} \end{array} \right| \\ \text{end} \end{array}$$

Max Planck Institute Magdeburg

### LR-Cholesky Transformation

for 
$$i = 1, ...$$
 do  
 $\begin{vmatrix} L_i L_i^T = M_i - \mu_i \mathcal{I} \\ M_{i+1} = L_i^T L_i + \mu_i \mathcal{I} \end{vmatrix}$   
end

$$\lim_{i \to \infty} M_i = \text{diag} \left( \lambda_1, \lambda_2, \dots, \lambda_n \right) \in \mathcal{H}(\mathcal{T}, 0) \\ \forall i: M_i - \mu_i \mathcal{I} \text{ symmetric positive definite}$$

### H-LR-Cholesky Transformation

# Example - $\mathcal{H}$ -Fill-In



Matrix FEM16 ( $\Delta_{2,h}$ , 16 inner discr. points).

Max Planck Institute Magdeburg



# Example - $\mathcal{H}$ -Fill-In





Matrix FEM16 ( $\Delta_{2,h}$ , 16 inner discr. points), after 1 step.

Max Planck Institute Magdeburg

### Example - $\mathcal{H}$ -Fill-In





Matrix FEM16 ( $\Delta_{2,h}$ , 16 inner discr. points), after 2 steps.

Max Planck Institute Magdeburg

# Example - $\mathcal{H}$ -Fill-In





Matrix FEM16 ( $\Delta_{2,h}$ , 16 inner discr. points), after 3 steps.

Max Planck Institute Magdeburg

## Example - $\mathcal{H}$ -Fill-In



Matrix FEM16 ( $\Delta_{2,h}$ , 16 inner discr. points), after 4 steps.

Max Planck Institute Magdeburg



Conclusions

# $\textbf{Example} \textbf{ - } \mathcal{H}\textbf{-}\textbf{Fill-In}$





Matrix FEM32 ( $\Delta_{2,h}$ , 32 inner discr. points).

Max Planck Institute Magdeburg

# $\textbf{Example} - \mathcal{H}\textbf{-Fill-In}$



Matrix FEM32 ( $\Delta_{2,h}$ , 32 inner discr. points), after 1 step.

Max Planck Institute Magdeburg



# Example - $\mathcal{H}$ -Fill-In



Matrix FEM32 ( $\Delta_{2,h}$ , 32 inner discr. points), after 50 steps.

Max Planck Institute Magdeburg

### **Computation Time**



# **Computation Time**


Hackbusch ( $\mathcal H$ -)Matrices

LR Algorithr

licing Algorith

n

#### Theorem

Adaption of [FASINO '05/PLESTENJAK, VAN BAREL, VAN CAMP '08]

$$M = \operatorname{diag}\left(d\right) + \sum_{i=1}^{r} \left(\operatorname{tril}\left(u_{i}v_{i}^{T}\right) + \operatorname{triu}\left(v_{i}u_{i}^{T}\right)\right)$$

icing Algorithr



Theorem

Adaption of [FASINO '05/PLESTENJAK, VAN BAREL, VAN CAMP '08]

$$M = \operatorname{diag} \left( d \right) + \sum_{i=1}^{r} \left( \operatorname{tril} \left( u_{i} v_{i}^{T} \right) + \operatorname{triu} \left( v_{i} u_{i}^{T} \right) \right)$$

#### Structure Preservation of dpss Matrices

Let M be a symmetric positive definite diagonal plus semiseparable matrix, with a decomposition as in the definition. The Cholesky factor L of  $M = LL^T$  can be written in the form

$$L = \operatorname{diag}\left(\widetilde{d}\right) + \sum_{i=1}^{r} \operatorname{tril}\left(u_{i}\widetilde{v}_{i}^{T}\right).$$

Multiplying the Cholesky factors in reverse order gives the next iterate  $N = L^T L$  of the LR Cholesky algorithm. The matrix N has the same form as M,

$$N = \operatorname{diag}\left(\hat{d}\right) + \sum_{i=1}^{r} \left(\operatorname{tril}\left(\hat{u}_{i}\tilde{v}_{i}^{T}\right) + \operatorname{triu}\left(\tilde{v}_{i}\hat{u}_{i}^{T}\right)\right).$$

Max Planck Institute Magdeburg

## **Proof Idea**



$$L_{1:p-1,1:p-1}L_{p,1:p-1}^{T} = M_{1:p-1,p} = \sum_{i} v_{i}u_{i}^{T}$$

$$\Rightarrow L_{1:p-1,1:p-1}\tilde{v}_{i}|_{1:p-1} = v_{i}|_{1:p-1} \text{ and } L_{p,1:p-1} = \sum_{i} u_{i}|_{p} \tilde{v}_{i}^{T}|_{1:p-1}$$

$$\tilde{d}_{p} + \sum_{i} u_{i}|_{p} \tilde{v}_{i}|_{p} = L_{pp} = \sqrt{M_{pp} - L_{p,1:p-1}L_{p,1:p-1}^{T}}$$

L is a dpss matrix.

Max Planck Institute Magdeburg

### **Proof Idea**

$$N = L^{T}L = \left(\operatorname{diag}\left(\tilde{d}\right) + \sum_{i} \operatorname{tril}\left(u_{i}\tilde{v}_{i}^{T}\right)\right)^{T}$$

$$\left(\operatorname{diag}\left(\tilde{d}\right) + \sum_{i} \operatorname{tril}\left(u_{i}\tilde{v}_{i}^{T}\right)\right)$$

$$\left(\tilde{u}^{i} = \left(Z + \operatorname{diag}\left(\tilde{d}\right)\right)u_{i}, \text{ with } Z_{\rho,:} = \sum_{j}\tilde{v}_{j}|_{p}\left[0 \cdots 0 \quad u_{j}|_{p} \quad u_{j}|_{p+1} \cdots \quad u_{j}|_{n}\right]$$

$$\operatorname{tril}\left(N, -1\right) = \sum_{i} \operatorname{tril}\left(\left(\operatorname{diag}(\tilde{d})u_{i} + Zu_{i}\right)\tilde{v}_{i}^{T}, -1\right)$$

$$= \sum_{i} \operatorname{tril}\left(\hat{u}_{i}\tilde{v}_{i}^{T}, -1\right)$$

N is a dpss matrix.

Max Planck Institute Magdeburg

# Structure of $\hat{u}$ and $\tilde{v}$

$$M = \operatorname{diag} (d) + \sum_{i=1}^{r} \operatorname{tril} (u_{i}v_{i}^{T}) + \dots$$

$$N = \operatorname{diag} (d) + \sum_{i=1}^{r} \operatorname{tril} (\hat{u}_{i}\tilde{v}_{i}^{T}) + \dots$$

$$v_{i} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix} \rightsquigarrow \tilde{v}_{i} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad u_{i} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{bmatrix} \implies \tilde{u}_{i} = \begin{bmatrix} * \\ \vdots \\ * \\ \vdots \\ * \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

## **Hierarchical Matrices**

#### **Hierarchical Matrices**

The structure of hierarchical matrices is not preserved under LR Cholesky transformations.

Max Planck Institute Magdeburg

 $\mathbf{tr}$ 

Slicing Algorithm

# $\textbf{Example - } \mathcal{H}\textbf{-}\textbf{Fill-In}$







icing Algorithm

# $\mathcal{H}_{\ell}\text{-Matrices}$



<i>F</i> <sub>1</sub>	$B_2 A_2^T$	$B_4 A_4^T$					
$A_2B_2^T$	F <sub>3</sub>			Bo 4T			
	рT	F <sub>5</sub>	$B_6 A_6^T$	$B_8A_8'$		A <sub>8</sub>	
	D <sub>4</sub>	$A_6 B_6^T$	F <sub>7</sub>				
	A DT			F9	$B_{10}A_{10}^{T}$	D AT	
				$A_{10}B_{10}^T$	F <sub>11</sub>	D12	A <sub>12</sub>
A808			$F_{13} B_{14}$		$B_{14}A_{14}^{T}$		
			$A_{12}B_{12}'$		$A_{14}B_{14}^T$	F <sub>15</sub>	

icing Algorithm





Max Planck Institute Magdeburg



licing Algorithm





<i>F</i> <sub>1</sub>							
I.	F <sub>3</sub>						
		F <sub>5</sub>					
		T	F7				
				F9			
				T	F <sub>11</sub>		
	1					F <sub>13</sub>	
						I.	F <sub>15</sub>

Max Planck Institute Magdeburg

icing Algorithm





$F_1$							
I	F <sub>3</sub>						
	-	F <sub>5</sub>					
	1	I	F <sub>7</sub>				
				F9			
		I		I	F <sub>11</sub>		
						F <sub>13</sub>	
						I	F <sub>15</sub>

licing Algorithm





<i>F</i> <sub>1</sub>							
п	F <sub>3</sub>						
		F <sub>5</sub>					
	1	П	F7				
				F9			
		I		П	F <sub>11</sub>		
		l				F <sub>13</sub>	
					I	П	F <sub>15</sub>

icing Algorithm

## $\mathcal{H}_{\ell}\text{-}Matrices$

F <sub>1</sub>							
Ξ	F <sub>3</sub>						
		F <sub>5</sub>					
I	I	Ш	F7				
				F9			
				ш	F <sub>11</sub>		
I			1	F <sub>13</sub>			
				I	ш	F <sub>15</sub>	



icing Algorithm





 $\Rightarrow$  rank bounded by  $\ell k$  instead of k

 $\Rightarrow$  total storage required by the low-rank parts of *M* is increased only from  $2nk\ell$  to  $2nk\frac{\ell(\ell-1)}{2}$ 

Max Planck Institute Magdeburg



Max Planck Institute Magdeburg

Hackbusch (*H*-)Matrices

LR Algorith

Slicing Algorithr

orithm

PINVIT

Conclusions



#### Slicing the Spectrum

# Slicing the Spectrum

Max Planck Institute Magdeburg

Bisectioning		[Parlett	· '80]







Max Planck Institute Magdeburg





















Max Planck Institute Magdeburg



$$\lambda_3 \in [-3.5, -2.75], \ \hat{\lambda}_3 = -3.125$$



Max Planck Institute Magdeburg

LR Algorithm

Slicing Algorithn

Conclusio



# **Evaluation of** $\nu(\mu)$

#### Sylvester's Law of Inertia

Each matrix M is congruent to a matrix

diag 
$$\left(-I_{\nu}, I_{\operatorname{rank}(M)-\nu}, \mathbf{0}_{n-\operatorname{rank}(M)}\right)$$
,

where  $\boldsymbol{\nu}$  is the number of negative eigenvalues. The triple

$$(\nu, \operatorname{rank}(M) - \nu, n - \operatorname{rank}(M))$$

is called the *inertia* of M.

$$M = LDL^{T} \qquad \Rightarrow \qquad \nu(M) = \nu(D)$$
$$M - \mu I = L_{\mu}D_{\mu}L_{\mu}^{T} \qquad \Rightarrow \qquad \nu(\mu) = \nu(M - \mu I) = \nu(D_{\mu})$$

Slicing Algorithm

n

C



Complexity

Flops per factorization (for  $\mathcal{H}_{\ell}$ -matrices):

$$\mathcal{O}\left(nk^{2}\left(\log n\right)^{4}\right)$$
.

Factorization per eigenvalue:

 $\mathcal{O}\left(\log(\left\|M\right\|_{2}/\epsilon)\right).$ 

Flops per eigenvalue:

$$\mathcal{O}\left(nk^{2}\left(\log n\right)^{4}\log\left\|M\right\|_{2}/\epsilon\right).$$

Slicing the whole spectrum:

$$\mathcal{O}\left(n^{2}k^{2}\left(\log n\right)^{4}\log(\left\|M\right\|_{2}/\epsilon)\right).$$

Max Planck Institute Magdeburg





Absolute error  $|\lambda_i - \hat{\lambda}_i|$  for the  $1024 \times 1024 \mathcal{H}_5(1)$ -matrix,  $\epsilon_{ev} = 10^{-8}$ .



Computation times for 10 eigenvalues of  $\mathcal{H}_{\ell}(1)$ -matrices ( $\ell = 8, \ldots, 15$ ).

Parallelization		Ø





Max Planck Institute Magdeburg

## **Parallelization Speedup**

#### OpenMP:

Name	п	t <sub>1 core</sub> in s	$t_{ m 1c}/t_{ m 2c}$	$t_{ m 1c}/t_{ m 4c}$	t <sub>8 core</sub>	$t_{1c}/t_{8c}$
H2 r1	128	0.33	1.83	3.30	0.06	5.50
H4 r1	512	9.44	1.94	3.67	1.43	6.60
H6 r1	2048	219.28	1.91	3.64	33.88	6.47
H8 r1	8 1 9 2	4 022.80	1.87	3.44	676.57	5.95
H10 r1	32768	49012.24	1.93	3.18	10 006.60	4.90

Slicing Algorithr

rithm

#### **Parallelization Speedup**

Open MPI:  $(\mathcal{H}_9(1) \in \mathbb{R}^{16\,384 \times 16\,384})$ 

No. of Processes	t in s	Speedup	Efficiency
1	16 564.58	1.00	1.00
2+1	8340.22	1.99	0.66
4+1	4044.13	4.10	0.82
6+1	2678.95	6.18	0.88
11 + 1	1 494.33	11.08	0.92
23+1	713.80	23.21	0.96
35+1	476.44	34.77	0.96
47+1	364.30	45.47	0.95
95+1	188.92	87.68	0.91
191+1	100.61	164.64	0.86
287+1	71.86	230.50	0.80
383+1	61.91	267.56	0.70



• Shifting affects the structure.

• The LDL<sup>T</sup> factorization is of almost linear complexity only for the original *H*-matrix and not necessarily for the shifted ones.

- For *H<sub>l</sub>*-matrices we use the exact LDL<sup>T</sup> factorization.
   For general *H*-matrices: The truncation introduces errors in the LDL<sup>T</sup> factorization the computed *D* may have another inertia
  - $\Rightarrow$  some eigenvalues may lie outside the computed interval
  - $\Rightarrow$  larger errors

Hackbusch (*H*-)Matrices

LR Algorithr

licing Algorith

Conclusions

#### **Preconditioned Inverse Iteration**

# Preconditioned Inverse Iteration for Hierarchical Matrices

Max Planck Institute Magdeburg

 ackbusch (H-)Matrices
 LR Algorithm
 Slicing Algorithm
 PINVIT
 Conclusions

 Preconditioned Inverse Iteration
 Image: Conclusion of the second second

[KNYAZEV, NEYMEYR, ET AL.]

#### Definition

The function

$$\mu(x) = \mu(x, M) = \frac{x^T M x}{x^T x}$$

is called the Rayleigh quotient.

 ackbusch (H-)Matrices
 LR Algorithm
 Slicing Algorithm
 PINVIT
 Conclusions

 Preconditioned Inverse Iteration
 Image: Conclusion of the second second

[KNYAZEV, NEYMEYR, ET AL.]

#### Definition

The function

$$\mu(x) = \mu(x, M) = \frac{x^T M x}{x^T x}$$

is called the Rayleigh quotient.

Minimize the Rayleigh quotient by a gradient method:

$$x_{i+1} := x_i - \alpha \nabla \mu(x_i), \quad \nabla \mu(x) = \frac{2}{x^T x} (Mx - x \mu(x)),$$

Max Planck Institute Magdeburg
ackbusch (H-)Matrices
LR Algorithm
Slicing Algorithm
PINVIT
Conclusions

Preconditioned Inverse Iteration
Image: Conclusion of the second second

[KNYAZEV, NEYMEYR, ET AL.]

#### Definition

The function

$$\mu(x) = \mu(x, M) = \frac{x^T M x}{x^T x}$$

is called the Rayleigh quotient.

Minimize the Rayleigh quotient by a gradient method:

$$x_{i+1} := x_i - \alpha \nabla \mu(x_i), \quad \nabla \mu(x) = \frac{2}{x^T x} (Mx - x \mu(x)),$$

+ preconditioning  $\Rightarrow$  update equation:

$$x_{i+1} := x_i - B^{-1} (Mx_i - x_i \mu(x_i)).$$

Max Planck Institute Magdeburg



[KNYAZEV, NEYMEYR 2009]

$$x_{i+1} := x_i - B^{-1} (M x_i - x_i \mu(x_i))$$

lf

- $M \in \mathbb{R}^{n \times n}$  symmetric positive definite and
- $B^{-1}$  approximates the inverse of M, such that

$$\left\|\mathcal{I}-B^{-1}M\right\|_{M}\leq c<1,$$

then Preconditioned INVerse ITeration (PINVIT) converges and the number of iterations is independent of *n*.



Slicing Algorithm

NVIT

Conclusions

**Algorithm and Complexity** 

The number of iterations is independent of matrix size *n*.

#### $\overline{\mathcal{H}}$ -PINVIT

Input:  $M \in \mathbb{R}^{n \times n}$ ,  $X_0 \in \mathbb{R}^{n \times d}$  ( $X_0^T X_0 = I$ , e.g. randomly chosen) Output:  $X_p \in \mathbb{R}^{n \times d}$ ,  $\mu \in \mathbb{R}^{d \times d}$ , with  $||MX_p - X_p\mu|| \le \epsilon$   $B^{-1} = (M)_{\mathcal{H}}^{-1}$  or  $B^{-1} = L_{\mathcal{H}}^{-T} L_{\mathcal{H}}^{-1}$   $R := MX_0 - X_0\mu$ ,  $\mu = X_0^T MX_0$ for  $(i := 1; ||R||_F > \epsilon; i + +)$  do  $|X_i := \text{Orthogonalize} (X_{i-1} - B^{-1}R)$   $R := MX_i - X_i\mu$ ,  $\mu = X_i^T MX_i$ end

Slicing Algorithm

INVIT

Conclusions

## **Algorithm and Complexity**

The number of iterations is independent of matrix size n.

#### $\overline{\mathcal{H}}$ -PINVIT

Input:  $M \in \mathbb{R}^{n \times n}$ ,  $X_0 \in \mathbb{R}^{n \times d}$   $(X_0^T X_0 = I$ , e.g. randomly chosen) Output:  $X_p \in \mathbb{R}^{n \times d}$ ,  $\mu \in \mathbb{R}^{d \times d}$ , with  $||MX_p - X_p\mu|| \le \epsilon$   $B^{-1} = (M)_{\mathcal{H}}^{-1}$  or  $B^{-1} = L_{\mathcal{H}}^{-T} L_{\mathcal{H}}^{-1}$   $\mathcal{O}(n(\log n)^2 k(c)^2)$   $R := MX_0 - X_0\mu$ ,  $\mu = X_0^T MX_0$ for  $(i := 1; ||R||_F > \epsilon; i + +)$  do  $|X_i := \text{Orthogonalize} (X_{i-1} - B^{-1}R)$   $\mathcal{O}(n(\log n) k(c)^2)$   $R := MX_i - X_i\mu$ ,  $\mu = X_i^T MX_i$   $\mathcal{O}(n(\log n) k(c))$ end

The complexity of the algorithm is determined by the  $\mathcal{H}$ -matrix inversion/Cholesky decomposition:  $\Rightarrow \mathcal{O}(n(\log n)^2 k(c)^2)$ .





#### **CPU** Time H-Cholesky PINVIT $10^{4}$ MATLAB eigs $\mathcal{H} ext{-}\mathsf{Cholesky}$ decomposition 10<sup>3</sup> CPU time in s 10<sup>2</sup> of memory 10<sup>1</sup> 10<sup>0</sup> out $10^{-1}$ $10^{-2}$ FEM3D16 4 096 FEM3D32 32 768 FEM3D128 2 079 152 262 144 512 64 FEM3D4 FEM3D8 FEM3D64

Slicing Algorithn

of memory

out

**CPU** Time H-Cholesky PINVIT  $10^{4}$ MATLAB eigs H-Cholesky decomposition 10<sup>3</sup> Slicing the Spectrum CPU time in s 10<sup>2</sup> 10<sup>1</sup> 10<sup>0</sup>  $10^{-1}$ Œ  $10^{-2}$ FEM3D16 4 096 FEM3D32 32 768 FEM3D64 262 144 512 64 FEM3D4 FEM3D8

Max Planck Institute Magdeburg

Folded Spectrum Method

[Wang, Zunger 1994]

$$M_{\sigma} = (M - \sigma \mathcal{I})^2$$

 $M_{\sigma}$  is s.p.d., if M is s.p.d. and  $\sigma \neq \lambda_i$ .





Folded Spectrum Method



[Wang, Zunger 1994]

$$M_{\sigma} = (M - \sigma \mathcal{I})^2$$

 $M_{\sigma}$  is s.p.d., if M is s.p.d. and  $\sigma \neq \lambda_i$ .

- The condition number of  $(M \sigma I)^2$  is large.
- $\Rightarrow$  The computation of  $M_{\sigma}^{-1}$  is more expensive.
- $\Rightarrow M_{\sigma}^{-1}$  has larger local ranks.
- $\Rightarrow M_{\sigma}^{-1}v$  is more expensive.

Folded Spectrum Method

[WANG, ZUNGER 1994]

$$M_{\sigma} = (M - \sigma \mathcal{I})^2$$

 $M_{\sigma}$  is s.p.d., if M is s.p.d. and  $\sigma \neq \lambda_i$ .

- The condition number of  $(M \sigma I)^2$  is large.
- $\Rightarrow$  The computation of  $M_{\sigma}^{-1}$  is more expensive.
- $\Rightarrow M_{\sigma}^{-1}$  has larger local ranks.
- $\Rightarrow M_{\sigma}^{-1}v$  is more expensive.
  - Multiple eigenvalues of  $M_{\sigma}$  may lead to incomplete subspace information.

$$\Rightarrow v^T M v / v^T v$$
 does not approximate  $\lambda$ .

Max Planck Institute Magdeburg



# Conclusions

Max Planck Institute Magdeburg





Peter Benner, Thomas Mach, Computing Eigenvalues of H(ackbusch) Matrices







LR Algorithr

licing Algorithm



- Three algorithms:
  - $\mathcal{H}$ -LR Cholesky algorithm: efficient only for  $\mathcal{H}_{\ell}$ -matrices, but expensive otherwise



- Three algorithms:
  - $\mathcal{H}$ -LR Cholesky algorithm: efficient only for  $\mathcal{H}_{\ell}$ -matrices, but expensive otherwise
  - Slicing the spectrum: efficient for  $\mathcal{H}_\ell\text{-matrices, good parallel performance}$



- Three algorithms:
  - $\mathcal{H}$ -LR Cholesky algorithm: efficient only for  $\mathcal{H}_{\ell}$ -matrices, but expensive otherwise
  - Slicing the spectrum: efficient for  $\mathcal{H}_\ell\text{-matrices, good parallel performance}$
  - *H*-**PINVIT**: efficient for the smallest eigenvalue(s) of positive definite *H*-matrices, computation of inner eigenvalues is possible. Subspace-accelerated variants, LOBPCG also investigated.



- Three algorithms:
  - $\mathcal{H}$ -LR Cholesky algorithm: efficient only for  $\mathcal{H}_{\ell}$ -matrices, but expensive otherwise
  - Slicing the spectrum: efficient for  $\mathcal{H}_\ell\text{-matrices, good parallel performance}$
  - *H*-**PINVIT**: efficient for the smallest eigenvalue(s) of positive definite *H*-matrices, computation of inner eigenvalues is possible. Subspace-accelerated variants, LOBPCG also investigated.
- $\bullet$  Other ideas ot compute eigenvalues of  $\mathcal H\text{-matrices:}$

#### J. Gördes

Eigenwertproblem von hierarchischen Matrizen mit lokalem Rang 1. Diplomarbeit, Mathematisch-Naturwissenschaftlichen Fakultät, CAU Kiel, May 2009.

#### W. Hackbusch and W. Kress.

A projection method for the computation of inner eigenvalues using high degree rational operators. COMPUTING 81:259–268, 2007.



S. Delvaux, K. Frederix, and M. Van Barel.

Transforming a hierarchical into a unitary-weight representation. ELECTR. TRANS. NUM. ANAL. 33:163–188, 2009.



- Three algorithms:
  - $\mathcal{H}\text{-}LR$  Cholesky algorithm: efficient only for  $\mathcal{H}_\ell\text{-}matrices,$  but expensive otherwise
  - Slicing the spectrum: efficient for  $\mathcal{H}_\ell\text{-matrices, good parallel performance}$
  - *H*-**PINVIT**: efficient for the smallest eigenvalue(s) of positive definite *H*-matrices, computation of inner eigenvalues is possible. Subspace-accelerated variants, LOBPCG also investigated.
- Probably similar conclusions for unsymmetric case.



- Three algorithms:
  - $\mathcal{H}\text{-}LR$  Cholesky algorithm: efficient only for  $\mathcal{H}_\ell\text{-}matrices,$  but expensive otherwise
  - Slicing the spectrum: efficient for  $\mathcal{H}_\ell\text{-matrices, good parallel performance}$
  - *H*-**PINVIT**: efficient for the smallest eigenvalue(s) of positive definite *H*-matrices, computation of inner eigenvalues is possible. Subspace-accelerated variants, LOBPCG also investigated.
- Probably similar conclusions for unsymmetric case.
- Possible improvements employing PDE theory?



- Three algorithms:
  - $\mathcal{H}$ -LR Cholesky algorithm: efficient only for  $\mathcal{H}_{\ell}$ -matrices, but expensive otherwise
  - Slicing the spectrum: efficient for  $\mathcal{H}_\ell\text{-matrices, good parallel performance}$
  - *H*-**PINVIT**: efficient for the smallest eigenvalue(s) of positive definite *H*-matrices, computation of inner eigenvalues is possible. Subspace-accelerated variants, LOBPCG also investigated.
- Probably similar conclusions for unsymmetric case.
- Possible improvements employing PDE theory?
- Concepts carry over to TT format, but so far not competitive with tensor-specific methods.

# Details to be found in...



#### Peter Benner and Thomas Mach. The LR Cholesky algorithm for symmetric hierarchical matrices. LINEAR ALGEBRA AND ITS APPLICATIONS 439(4):1150–1166, 2013.



Peter Benner and Thomas Mach.

Computing all or some eigenvalues of symmetric  $\mathcal{H}_{\ell}$ -matrices. SIAM JOURNAL ON SCIENTIFIC COMPUTING 34(1):A485–A496, 2012.



The preconditioned inverse iteration for hierarchical matrices. NUMERICAL LINEAR ALGEBRA WITH APPLICATIONS 20(1):150–166, 2013.



Peter Benner and Thomas Mach.

Locally optimal block preconditioned conjugate gradient method for hierarchical matrices.

PROCEEDINGS IN APPLIED MATHEMATICS AND MECHANICS 11:741-742, 2011.



Peter Benner and Thomas Mach. On the QR decomposition of *H*-matrices. COMPUTING 88(3–4):111–129, 2010.

# All about $\mathcal{H}$ ackbusch matrices to be found in...



Max Planck Institute Magdeburg

## All about $\mathcal{H}$ ackbusch matrices to be found in...



# HAPPY BIRTHDAYS!

Max Planck Institute Magdeburg