The Generalized Locally Toeplitz theory: introduction and applications

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Plan of the lecture

- Introduction: how to analyse the quality of a nonsymmetric Schur complement approximation?
- Generalized Locally Toeplitz theory: general description and properties
- Can we compute all eigenvalues of a large matrix exactly?
- ... or up to machine accuracy?
- What about eigenvectors?
- Conclusions and outlook
Introduction: Glacial isostatic adjustment (GIA)

Simplified 2D model of GIA (flat elastic Earth):

- Self-gravitation and density change is excluded.
- The Earth is modelled as incompressible.

\[-\nabla \cdot \sigma - \nabla (\mathbf{u} \cdot \nabla p_0) + (\nabla \cdot \mathbf{u}) \nabla p_0 = \mathbf{f}\]

\[\nabla \cdot \sigma = \nabla \cdot (2\mu \varepsilon(\mathbf{u})) + \lambda \nabla \cdot \mathbf{u}\]

\(\sigma\) – stress, \(\varepsilon\) – strain, \(\mathbf{u}\) – displacements
\(\mu, \lambda\) – material parameters.
The simplified problem

To enable fully incompressible models, i.e \( \lambda = \infty \)

\[-\nabla \cdot (2\mu \varepsilon(u)) - \nabla (u \cdot \nabla p_0) - \mu \nabla p = f \text{ in } \Omega\]

\[\mu \nabla \cdot u - \frac{\mu^2}{\lambda} p = 0 \text{ in } \Omega\]

- \( p_0 \) – pre-stress,
- \( p = \frac{\lambda}{\mu} \nabla \cdot u \) – kinematic pressure.

The geometry of the problem
FEM: weak form and discretization

\[ a(u_h, v_h) + b(v_h, p) = (v_h, g) + (v_h, \gamma) \]
\[ b(u_h, q_h) - \frac{\mu^2}{\lambda} m(p_h, q_h) = 0 \]

Discretize appropriately.

The algebraic systems of equations are large, sparse, nonsymmetric and indefinite with a saddle point structure,

\[ A = \begin{bmatrix} F & B^T \\ B & -M \end{bmatrix} \]

- The pivot block \( F \) is nonsymmetric.
- \( M \) is a scaled mass matrix.
Iterative solution of large scale linear systems: classical reasoning

\[ Au = f, \text{ Seek } P : P^{-1}Au = P^{-1}f \]

\[ A = \begin{bmatrix} F & B^T \\ B & -M \end{bmatrix} \]

A has a 2 × 2 block structure.
Classical task to solve large systems with matrices of saddle point form: preconditioned iterative solution method.
Iterative solution of large scale linear systems:

\[ A = \begin{bmatrix} F & B^T \\ B & -M \end{bmatrix}, \]  
preconditioned by \( P = \begin{bmatrix} \tilde{F} & 0 \\ B & -[S] \end{bmatrix} \)

- \( \tilde{F} \) approximates \( F \)
- \( S \) approximates the (negative) Schur complement matrix \( S_A = M + BF^{-1}B^T \)
- \([\cdot]\) means a (preconditioned, very efficient) inner solver.

From theory: very few (outer) iterations if
- \( \tilde{F} \) is solved accurately.
- \( S \) is a good approximation for \( S_A \).
How to approximate the Schur complement?

\[ S_A = M + BF^{-1}B^T \]

\[ F = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} \]
How to approximate the Schur complement?

\[ S_A = M + BF^{-1}B^T \]

\[ S \] – computed using the \textit{element-wise} approach: For any finite element pair of spaces, chosen to approximate \( u \) and \( p \), the system matrix \( A \) is

\[ A = \sum_{i=1}^{m} R_i^T A_i^{(e)} R_i, \quad \text{where} \quad A_i^{(e)} = \begin{bmatrix} F_i^{(e)} & (B_i^{(e)})^T \\ B_i^{(e)} & -M_i^{(e)} \end{bmatrix}, \]

\( R_i \) defines local-to-global mapping of the degrees of freedom

\( m \) is the number of the finite elements in the discretization mesh.
The Schur complement approximation, cont.

\[ S = \sum_{i=1}^{m} R_i^T S^{(e)}_i R_i, \quad \text{where} \quad S^{(e)}_i = M^{(e)}_i + B^{(e)}_i (F^{(e)}_i)^{-1} B^{(e)}_i)^T. \]

If \( A \) is a saddle point matrix with spd 11-block:

\[ 0 < \alpha S \leq S_A \leq \beta S \]

where \( \alpha = 1 \) and both bounds independent of \( h \).

However, how to analyse the case when \( S_A \) is nonsymmetric?!
The quality of the Schur complement approximation:

Numerical observation:

\[ \lambda(S^{-1}S_A) \]
The quality of the outer preconditioner

\[ \lambda(\mathcal{P}^{-1}A) \]
A nearly optimal performance

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<td></td>
<td></td>
<td>Iterations</td>
<td>Setup (s)</td>
<td>Solve (s)</td>
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**Table:** MPI performance and scalability results using Deal.ii and Trilinos-AMG; compressible and incompressible material
What to do?

When nothing goes right, go left!
Use the Generalized Locally Toeplitz theory.
Generalized Locally Toeplitz matrix sequences

Who are those?
Since many years, a scientific theory has been developed, namely, the so-called 'Generalized Locally Toeplitz' (GLT) sequences:

For certain classes of structured matrices, much richer than the classical Toeplitz matrices, GLT offers the possibility to associate an analytical function to (a sequence of) matrices, referred to as the symbol of the matrices.

Sampling the symbol gives an information about the spectrum of the corresponding matrix, i.e., a curve for spd matrices, on which all eigenvalues are located, except for possibly a finite number of outliers.
Recall: Toeplitz matrices I

\[ T = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots \\ a_1 & a_0 & a_{-1} & \cdots \\ a_2 & a_1 & a_0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}, \quad T_n = \begin{bmatrix} a_0 & a_{-1} & a_{-2} & \cdots & \cdots & a_{-n+1} \\ a_1 & a_0 & a_{-1} & \cdots & \vdots \\ a_2 & a_1 & a_0 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n-1} & \cdots & \cdots & a_1 & a_0 \end{bmatrix} \]
Recall: Toeplitz matrices II

Block-Toeplitz matrix / Multilevel Toeplitz matrix

\[
\begin{bmatrix}
A_0 & A_{-1} & A_{-2} & \cdots & \cdots & A_{-n+1} \\
A_1 & A_0 & A_{-1} & \ddots & \ddots & \vdots \\
A_2 & A_1 & A_0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \ddots & \ddots & A_{-1} & A_{-2} \\
\vdots & \ddots & \ddots & A_1 & A_0 & A_{-1} \\
A_{n-1} & \cdots & \cdots & A_2 & A_1 & A_0
\end{bmatrix}
\]
**Recall: Toeplitz matrices**

**Toeplitz matrix, generated by a function**

A Toeplitz matrix $T_m$ generated by $f(\theta)$ is a square matrix that has constant elements along each descending diagonal.

$$T_m(f) = \begin{bmatrix}
\hat{f}_0 & \hat{f}_{-1} & \hat{f}_{-2} & \cdots & \hat{f}_{1-m} \\
\hat{f}_1 & \hat{f}_0 & \hat{f}_{-1} & \cdots & \\
\hat{f}_2 & \hat{f}_1 & \hat{f}_0 & \cdots & \\
\vdots & \vdots & \vdots & \ddots & \\
\hat{f}_{m-1} & \hat{f}_2 & \hat{f}_1 & \hat{f}_0 & \\
\end{bmatrix}$$

where

$$\hat{f}_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta)e^{-ik\theta} d\theta, \quad k \in \mathbb{Z}.$$
**Formal definition of the symbol of a matrix**

**Definition [Symbol of Toeplitz sequences]**
Denote by \( f(x_1, \cdots, x_d) \) a \( d \)-variate complex-valued integrable function, defined over the domain \( Q^d = [-\pi, \pi]^d, \ d \geq 1 \).

Denote by \( \hat{f}_k \) the Fourier coefficients of \( f \),

\[
\hat{f}_k = \frac{1}{m\{Q^d\}} \int_{Q^d} f(s) e^{-i(k,s)} \, ds, \quad k = (k_1, \cdots, k_d) \in \mathbb{Z}^d, \quad i^2 = -1,
\]

where \((k, s) = \sum_{j=1}^d k_j s_j, \ n = (n_1, \cdots, n_d)\) and \(N(n) = n_1 \cdots n_d\).
Formal definition of the symbol of a matrix II

Using the properties of the Fourier coefficients, with each $f$ we can associate a sequence of Toeplitz matrices $\{T_n(f)\}$, where

$$
T_n(f) = \{\hat{f}_{k-\ell}\}^{n}_{k,\ell=0} e^T \in \mathbb{C}^{N(n),N(n)},
$$

$e = [1, 1, \cdots, 1] \in \mathbb{N}^d$.

The function $f$ is referred to as the generating function (or the symbol of) $T_n(f)$. 
GLT in practice: Symbol-to-Matrix

Given a function \( f \in L^1([−\pi, \pi]) \). It generates a Toeplitz matrix

\[
T_n(f) = \begin{bmatrix}
\hat{f}_0 & \hat{f}_{-1} & \cdots & \cdots & \hat{f}_{1-n} \\
\hat{f}_{1} & \ddots & \ddots & \ddots & \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\hat{f}_{n-1} & \ddots & \ddots & \ddots & \hat{f}_0
\end{bmatrix},
\]

where \( \hat{f} \) are the Fourier coefficients of \( f \).

\[ \{ T_n(f) \}_n \sim_{GLT, \sigma} f \]
Given a banded Toeplitz matrix

\[ T_n(f) = \begin{bmatrix}
\hat{f}_0 & \cdots & \hat{f}_{-m} \\
\vdots & \ddots & \vdots \\
\hat{f}_m & \cdots & \hat{f}_{-m} \\
\hat{f}_m & \cdots & \hat{f}_0
\end{bmatrix}. \]

Then

\[ f(\theta) = \hat{f}_0 + \sum_{k=1}^{m} \left( \hat{f}_k e^{ik\theta} + \hat{f}_{-k} e^{-ik\theta} \right). \]
GLT in practice: Matrix-to-Symbol

\[ T_n(f) = \begin{bmatrix} \hat{f}_0 & \cdots & \hat{f}_{-m} \\ \vdots & \ddots & \vdots \\ \hat{f}_m & \cdots & \hat{f}_0 \end{bmatrix}. \]

\[ f(\theta) = \hat{f}_0 + \sum_{k=1}^{m} \left( \hat{f}_k e^{i k \theta} + \hat{f}_{-k} e^{-i k \theta} \right) \]

If \( T_n(f) \) is real symmetric, then \( f \) is a real cosine trigonometric polynomial

\[ f(\theta) = \hat{f}_0 + 2 \sum_{k=1}^{m} \hat{f}_k \cos(k \theta) \]

\[ \{ T_n(f) \}_n \sim_{GLT, \lambda, \sigma} f \]
GLT in practice: 1D Laplace, 2nd order central differences

\[ u''(x) = b \]

\[ A_n u_n = \frac{1}{h^2} L_n u_n = \frac{1}{h^2} \begin{bmatrix} 2 & -1 \\ -1 & \ddots & \ddots \\ \ddots & \ddots & -1 \\ -1 & 2 \end{bmatrix} u_n = b_n. \]

\[ L_n = T_n(f) - \text{real symmetric}, \quad h = \frac{1}{n+1}. \] Thus,

\[ f(\theta) = \hat{f}_0 + 2 \sum_{k=1}^{m} \hat{f}_k \cos(k\theta) = 2 - 2\cos(\theta) \]
GLT in practice: 1D Laplace, 2nd order central differences

\[
A_n u_n = \frac{1}{h^2} L_n u_n = \frac{1}{h^2} \begin{bmatrix}
  2 & -1 & & \\
  -1 & \ddots & \ddots & \\
  & \ddots & \ddots & -1 \\
  & & -1 & 2 \\
\end{bmatrix} u_n = b_n.
\]

\[
f(\theta) = \hat{f}_0 + 2 \sum_{\omega=1}^{m} \hat{f}_\omega \cos(\omega \theta) = 2 - 2 \cos(\theta)
\]

In this case we know the exact eigenvalues of \( T_n(f) \),

\[
\lambda_j( T_n(f) ) = f(\theta_j, n), \ j = 1, 2, \ldots, n
\]

where \( \theta_{j, n} = j \pi h, \ h = 1/(n + 1) \).
Let $f$ be the symbol of $\{ T_n(f) \}_n$. An equidistant sampling of $f$ over $[-\pi, \pi]$ gives an approximation of the spectrum of $T_n(f)$ for $n$ large enough:

**$f$ real-valued:**

$$\lambda_j(T_n(f)) \approx f \left( -\pi + \frac{2\pi j}{n-1} \right), \ j = 0, \ldots, n-1$$

**$f$ complex-valued:**

$$\sigma_j(T_n(f)) \approx \left| f \left( -\pi + \frac{2\pi j}{n-1} \right) \right|, \ j = 0, \ldots, n-1$$
GLT: spectral analysis by means of the symbol

An equidistant sampling of $f$ over $[-\pi, \pi]$ ...

Q: How to sample?

- $f$ real-valued: \( \lambda_j(T_n(f)) \approx f\left(-\pi + \frac{2\pi j}{n+1}\right), \quad j = 0, \cdots, n-1 \)

- $f$ complex-valued: \( \sigma_j(T_n(f)) \approx \left|f\left(-\pi + \frac{2\pi j}{n+1}\right)\right|, \quad j = 0, \cdots, n-1 \)

For even functions use \( \frac{\pi j}{n+1} \).
Informal definition of a symbol for a generic matrix sequence

Assume:
- \( \{ A_n \}_n \) - matrix sequence, \( \text{dim}(A_n) = d_n \rightarrow \infty \)
- \( f : D \subset \mathbb{R}^d \rightarrow \mathbb{C} \), measurable, \( 0 < \text{measure}(D) < \infty \)

Then the eigenvalues of \( A_n \) are approximately a uniform sampling of \( f \) over \( D \).

\( f \) - spectral symbol of \( A_n \): \( \{ A_n \}_n \sim_{GLT, \lambda} (f, D) \)

The definition can be given in the singular value sense (replacing \( f \) by \( |f| \)): \( \{ A_n \}_n \sim_{GLT, \sigma} (f, D) \)
GLT building blocks

- \{ T_n(f) \}_n - Toeplitz sequence with
  - \( f : [-\pi, \pi] \to \mathbb{C}, f \in L^1([-\pi, \pi]) \)
  
  The symbol of \( T_n \) is \( f \).

- Let \( \{ D_n(a) \}_n \) be a diagonal sampling sequence with
  - \( D_n(a) = \text{diag}(a(j/n)), j = 1, \cdots, n \)
  - \( a(x) : [0,1] \to \mathbb{C} \), Riemann integrable function.
  
  The symbol of \( D_n \) is \( a \).

- \( \{ Z_n = R_n + E_n \}_n \) - low rank+small-norm sequence:
  - \( R_n : \lim_{n \to \infty} \frac{\text{rank}(R_n)}{d} = 0 \) (low rank)
  - \( E_n : \lim_{n \to \infty} \| E_n \| = 0 \) (small-norm)

  The symbol of \( Z_n \) is 0 (zero).
Consider $-u^{(iv)} = b$, discretized by 2nd order FD:

<table>
<thead>
<tr>
<th>Eq.</th>
<th>Symbol</th>
<th>Eig.val. relations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-u''$</td>
<td>$f(\theta) = 2 - 2\cos(\theta)$</td>
<td>${T_n(f)}_n \sim \lambda f$</td>
</tr>
<tr>
<td>$-u^{(iv)}$</td>
<td>$f^2(\theta) = 6 - 8\cos(\theta) + 2\cos(2\theta)$</td>
<td>${T_n(f^2)}_n \sim \lambda f^2$</td>
</tr>
</tbody>
</table>

But $T_n(f) T_n(f) \neq T_n(f^2)$
Elaborate on 'low-rank' and 'small-norm':

Indeed:

\[
\begin{bmatrix}
2 & -1 & 0 \\
-1 & 2 & -1 \\
0 & -1 & 2
\end{bmatrix}
\begin{bmatrix}
2 & -1 & 0 \\
-1 & 2 & -1 \\
0 & -1 & 2
\end{bmatrix}
= 
\begin{bmatrix}
5 & -4 & 1 \\
-4 & 6 & -4 \\
1 & -4 & 5
\end{bmatrix}
\]
Elaborate on 'low-rank' and 'small-norm':

\[ T_n(f^2) = \begin{bmatrix}
6 & -4 & 1 \\
-4 & \ddots & \ddots \\
1 & \ddots & \ddots & 1 \\
\vdots & \ddots & \ddots & 6 & -4 \\
1 & -4 & 6 \\
\end{bmatrix}
\]

\[ = \begin{bmatrix}
5 & -4 & 1 \\
-4 & \ddots & \ddots \\
1 & \ddots & \ddots & 1 \\
\vdots & \ddots & \ddots & 6 & -4 \\
1 & -4 & 6 \\
\end{bmatrix} + \begin{bmatrix}
1 & 0 & 0 \\
0 & \ddots & \ddots & 0 \\
\vdots & \ddots & \ddots & 0 \\
0 & 0 & 0 & 1 \\
\end{bmatrix} \]
Properties of the symbol I

Properties of the symbol - GLT overcoming substantial limitations:

**GLT1** Each GLT sequence has a symbol $f$. If the sequence is Hermitian then the symbol describes the eigenvalues. Otherwise the same formula holds true with the singular values in place of the eigenvalues and $|f| = (f^*f)^{1/2}$ in place of $f$.

**GLT2** The set of GLT sequences form a $\ast$-algebra (closed under linear combinations, conjugation, products, inversion (whenever the symbol vanishes, at most, in a set of zero Lebesgue measure)). Hence, the sequence obtained via algebraic operations on a finite set of input GLT sequences is still a GLT sequence and its symbol is obtained by the same algebraic manipulations on the corresponding symbols of the input GLT sequences.
Properties of the symbol II

Let $\{A_n\}_n \sim_{GLT} (f)$ and $\{B_n\}_n \sim_{GLT} (g)$. Then

- $\{A^*_n\}_n \sim_{GLT} (\overline{f})$
- $\{\alpha A_n + \beta B_n\}_n \sim_{GLT} (f + g)$ for all $\alpha, \beta \in \mathbb{C}$
- $\{A_n B_n\}_n \sim_{GLT} (fg)$
- If $f \neq 0$ a.e. then $\{A^\dagger_n\}_n \sim_{GLT} (f^{-1})$

**GLT3** If each $A_n$ is Hermitian, then $\{F(A_n)\}_n \sim_{GLT} (F(f))$ for any continuous function $F : \mathbb{C} \rightarrow \mathbb{C}$.

**GLT4** Every Toeplitz sequence generated by a $L^1$ function $f$ is a GLT sequence and its symbol is $f$, possessing the properties from item GLT1.
Properties of the symbol III

GLT5 The approximation of PDEs with non-constant coefficients, general domains, nonuniform meshes by local methods (FDM, FEM, IgA etc), under very mild assumptions leads also to GLT sequences.

GLT6 We encounter GLT structures for certain matrix sequences, related to preconditioners, based on approximations of PDEs by local methods. Moreover, the symbol includes information about the coefficients and the domain of the PDE, as well as information on the discretization schemes for the derivatives including the used meshes, which have to be described, at least asymptotically, as a map of a reference equispaced mesh (see Book, C. Garoni and S. Serra-Capizzano.)
GLT: some theoretical results

Theorem
For a real-valued continuous $f$, the eigenvalues of $T_n(f)$ for large $n$ are approximate evaluations of $f$, over a grid like $\{x_j^{(n)}\}$,

$$x_j^{(n)} = -\pi + \frac{2\pi j}{n}, \quad j = 1, \ldots, n.$$ 

Remark
When the generating function is either multivariate or matrix-valued, then the resulting matrices are either multilevel Toeplitz or block Toeplitz.
Assume
\[
\begin{cases}
-(\kappa_0 u')' + v' = g_1(x), \\
u' - \rho v = g_2(x),
\end{cases}
\]
\[\kappa_0 \in (0, 1]\]

Using linear FEM basis functions on a uniform mesh of stepsize $h$
leads to
\[A = \begin{bmatrix} K & B^T \\ B & -\rho M \end{bmatrix},\]
Toeplitz matrices II

Instructive example

\[ K = \kappa_0 \begin{bmatrix} 2 & -1 \\ -1 & 2 & -1 \\ & -1 & \ddots & \ddots \\ & & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}, \quad M = \frac{h^2}{6} \begin{bmatrix} 4 & 1 \\ 1 & 4 & 1 \\ & 1 & \ddots & \ddots \\ & & \ddots & \ddots & 1 \\ & & & 1 & 4 \end{bmatrix}, \]

\[ B = h \begin{bmatrix} 1 \\ -1 & 1 \\ & -1 & \ddots & \ddots \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots & -1 & 1 \end{bmatrix}. \]
Clearly, all the blocks have a Toeplitz character, thus, they have a generating symbol, found to be:

\[ K = \kappa_0 T_n(2 - 2 \cos(\theta)), \quad B = h T_n(1 - e^{i\theta}), \]
\[ B^T = h T_n(1 - e^{-i\theta}), \quad M = \frac{h^2}{3} T_n(2 + \cos(\theta)). \]

The negative Schur complement of \( A \) is defined as follows

\[ S = \rho M + B^T K^{-1} B \]

Note: that as \( \kappa_0 > 0 \), the matrix \( K \) is invertible.
We are in a position to construct the symbol of $S$, $f^S$.

First, $S$ expressed by Toeplitz matrices, reads as

$$
S = \frac{\rho}{3} T_n(2 + \cos(\theta)) + \frac{1}{\kappa_0} T_n(1 - e^{-i\theta}) T_n^{-1}(2 - 2\cos(\theta)) T_n(1 - e^{i\theta}).
$$

According to GLT3, the sequences $\{T_n(2 + \cos(\theta))\}$, $\{T_n(1 - e^{i\theta})\}$, $\{T_n(1 - e^{-i\theta})\}$ and $\{T_n(2 - 2\cos(\theta))\}$ are GLT sequences with symbols $2 + \cos(\theta)$, $1 - e^{i\theta}$, $1 - e^{-i\theta}$, $2 - 2\cos(\theta)$, respectively.

Furthermore, according to the structure of the $*$-algebra in GLT2, $\{S_n\}$ is a GLT sequence generated by the symbol

$$
f^S(\theta) = \frac{\rho}{3} (2 + \cos(\theta)) + \frac{1}{\kappa_0} (1 - e^{-i\theta}) \frac{1}{2 - 2\cos(\theta)} (1 - e^{i\theta})
$$

$$
= \frac{\rho}{3} (2 + \cos(\theta)) + \frac{1}{\kappa_0}.
$$
Since $S_n$ is Hermitian independently of its size, according to GLT1, we deduce that there holds that $\{S_n\} \sim \lambda f^S$, where $f^S$ is an even trigonometric polynomial.
Toeplitz matrices VI
Instructive example

(a) \( \kappa_0 = 0.4 \)

(b) \( \kappa_0 = 0.6 \)
Toeplitz matrices VII

Instructive example

(c) $\kappa_0 = 0.8$

(d) $\kappa_0 = 1$
Back to the GIA example: the quality of the approximate Schur complement $S$

\[
A = \begin{bmatrix}
K_{11} & K_{12} & B_1^T \\
K_{21} & K_{22} & B_2^T \\
B_1 & B_2 & -\rho M
\end{bmatrix}.
\]  

(1)

We note that the blocks $B_1$ and $B_2$ are rectangular, which in practice needs an additional care.
On square meshes, $M$ is block-three diagonal, and each block has a tridiagonal structure. The block-symbol of $M$, $f^M(\theta_1, \theta_2)$ is computed as follows,

$$f^M_{0b}(\theta) = 8(2 + \cos(\theta)), \quad f^M_{1b}(\theta) = f^M_{-1}(\theta) = 4 + 2\cos(\theta),$$

$$f^M(\theta_1, \theta_2) = f^M_{0b}(\theta_1) + f^M_{1b}(\theta_1)e^{i\theta_2} + f^M_{-1}(\theta_1)e^{-i\theta_2},$$

$$= 8(2 + \cos(\theta_1)) + 2(4 + 2\cos(\theta_1))\cos(\theta_2)$$

$$= 4(2 + \cos(\theta_1))(2 + \cos(\theta_2)),$$

where $\theta_1$ and $\theta_2$ are generic angles between 0 and $\pi$. 
The symbol of the mass matrix, cont.

**Figure:** Bilinear basis functions: The spectrum of $M$ and of $T(f^M)$
Remark: The spectrum of $M$ is uniformly a bit below the symbol $f^M$. This is explained as follows. As a result of the FEM assembly procedure, the Toeplitz matrix $T_n(f^M)$ can be seen as $T_n(f^M) = M + E$, where $E$ is a low rank nonnegative definite matrix, related to lesser contributions along the boundary of $\Omega$. The observed phenomenon is explained via a related interlacing theorem.
The symbol of an advection term

The symbol of the matrix, arising from the discretization of the term \((\nabla \cdot \mathbf{u}) \mathbf{c}\) with \(\mathbf{c} = [c_1, c_2]\).

\[
f^{A(2)} = -i 4 \begin{bmatrix} c_1 \sin(\theta_1)(2 + \cos(\theta_2)) & c_1 \sin(\theta_2)(2 + \cos(\theta_1)) \\ c_2 \sin(\theta_1)(2 + \cos(\theta_2)) & c_2 \sin(\theta_2)(2 + \cos(\theta_1)) \end{bmatrix}
\]
The symbol of the nonsymmetric Schur complement

\[ g_{S_A}(\theta_1, \theta_2) = f^M(\theta_1, \theta_2) + \frac{1}{2} \left( \sum_{m=0}^{1} G_{11} \left( \theta_1, \frac{\theta_2}{2} + m\pi \right) \right), \]

where \( G_{11} \) is the pivot block in \( G \), given by

\[
\begin{align*}
G(\theta_1, \theta_2) &= g_{\tilde{B}_1}(\theta_1, \theta_2)g^{-1}_{K_{11}}(\theta_1, \theta_2)g_{\tilde{B}_1}^T(\theta_1, \theta_2) + g_R(\theta_1, \theta_2)g^{-1}_{SK}(\theta_1, \theta_2)g_{B_1}^T(\theta_1, \theta_2), \\
g_R(\theta_1, \theta_2) &= g_{\tilde{B}_2}(\theta_1, \theta_2) - g_{\tilde{B}_1}(\theta_1, \theta_2)g^{-1}_{K_{11}}(\theta_1, \theta_2)g_{K_{12}}(\theta_1, \theta_2), \\
g_{SK}(\theta_1, \theta_2) &= g_{K_{22}}(\theta_1, \theta_2) - g_{K_{21}}(\theta_1, \theta_2)g^{-1}_{K_{11}}(\theta_1, \theta_2)g_{K_{12}}(\theta_1, \theta_2), \\
\end{align*}
\]

with \( 0 < \theta_1, \theta_2 \leq \pi \), \( g_{\tilde{B}_1} \) and \( g_{\tilde{B}_2} \) – conjugate transpose of \( g_{B_1}^T(1) \) and \( g_{B_1}^T(2) \).
The quality of the approx. Schur complement $S$

$eig(S), g_S(\theta_1, \theta_2)$
Eigenvalues of the true Schur complement matrix and the match with the sampling of its symbol $f^S$.

**Figure:** Q1isoQ1: The spectrum of $S$ and of $T(f^S)$, three refinements
So far, so good...

The symbol shows the general behaviour of the spectrum of a matrix from the GLT class. The exact eigenvalues are somewhere on the sampled symbol curve (in the simplest way) or surface, but where?!

The answer became more clear with the thesis of Sven-Erik Ekström Matrix-Less Methods for Computing Eigenvalues of Large Structured Matrices http://www.2pi.se/thesis.pdf

and several (actually, many) follow-up papers.
Is it possible to find the eigenvalues exactly without even constructing the matrix?

Observation: errors, \( f^2(\theta) = 6 - 8\cos(\theta) + 2\cos(2\theta) \)

\[
E_{j,n,0} = \lambda_j(T_n(f^2)) - f^2(\theta_{j,n}), \quad \theta_{j,n} = j\pi h, \quad h = 1/(n+1)
\]
Scaled Errors, \( f^2(\theta) = 6 - 8 \cos(\theta) + 2 \cos(2\theta) \)

\[
\frac{E_{j,n,0}}{h} = \frac{\lambda_j(T_n(f^2)) - f^2(\theta_{j,n})}{h}, \quad \theta_{j,n} = j\pi h, \quad h = 1/(n+1)
\]
Asymptotic Expansion for Banded Symmetric Toeplitz Matrices

Clearly, \[ \lambda_j(T_n(f)) = f(\theta_{j,n}) + E_{j,n,0}, \quad E_{j,n,0} = \mathcal{O}(h), \]
\[ \theta_{j,n} = j\pi h, \quad h = 1/(n + 1). \]

In a series of papers by Bogoya, Böttcher, Grudsky, Maximenko:

\[ \lambda_j(T_n(f)) = f(\theta_{j,n}) + E_{j,n,0} \]
\[ = f(\theta_{j,n}) + \sum_{k=1}^{\ell} c_k(\theta_{j,n}) h^k + E_{j,n,\ell} \]
\[ E_{j,n,0} = \mathcal{O}(h) \quad E_{j,n,\ell} = \mathcal{O}(h^{\ell+1}) \]
Asymptotic Expansion for Banded Symmetric Toeplitz Matrices

\[ \lambda_j(T_n(f)) = f(\theta_{j,n}) + E_{j,n,0} \]

\[ = f(\theta_{j,n}) + \sum_{k=1}^{\ell} c_k(\theta_{j,n}) h^k + E_{j,n,\ell} \]

Let us approximate those!
Asymptotic Expansion: Approximating \( c_k \)

\[
\lambda_j(T_n(f)) - f(\theta_j,n) = E_{j,n,0} = \sum_{k=1}^{\ell} c_k(\theta_j,n)h_1^k + E_{j,n,\ell}
\]

\[
\begin{align*}
E_{j_1,n_1,0} &= \sum_{k=1}^{\ell} c_k(\theta_{j_1,n_1})h_1^k + E_{j_1,n_1,\ell} \\
\vdots & \\
E_{j_i,n_i,0} &= \sum_{k=1}^{\ell} c_k(\theta_{j_i,n_i})h_i^k + E_{j_i,n_i,\ell} \\
\vdots & \\
E_{j_\ell,n_\ell,0} &= \sum_{k=1}^{\ell} c_k(\theta_{j_\ell,n_\ell})h_\ell^k + E_{j_\ell,n_\ell,\ell}
\end{align*}
\]
**Asymptotic Expansion: Approximating $c_k$**

Choose $\ell$ small grids

\[
\lambda_j(T_n(f)) - f(\theta_{j,n}) = E_{j,n,0} = \sum_{k=1}^{\ell} c_k(\theta_{j,n})h_1^k + E_{j,n,\ell}
\]

\[
j_1 = \{1, \ldots, n_1\}, \quad j_k = 2^{k-1}j_1
\]

\[
n_k = 2^{k-1}(n_1 + 1) - 1 \quad \Rightarrow \quad \theta_{j_i,n_i} = \theta_{j_1,n_1}, \ i = 1, \ldots, \ell
\]

*Figure from Sven-Erik Eksröm*
Asymptotic Expansion: Approximating $c_k$

Choose $\ell$ small grids

$$\lambda_j(T_n(f)) - f(\theta_j, n) = E_{j,n,0} = \sum_{k=1}^{\ell} c_k(\theta_j, n) h_1^k + E_{j,n,\ell}$$

\begin{align*}
  j_1 &= \{1, \ldots, n_1\} \quad j_k = 2^{k-1}j_1 \\
  n_k &= 2^{k-1}(n_1 + 1) - 1 \quad \Rightarrow \quad \theta_{j_i,n_i} = \theta_{j_1,n_1}, i = 1, \ldots, \ell
\end{align*}

\begin{align*}
  E_{j_1,n_1,0} &= \sum_{k=1}^{\ell} c_k(\theta_{j_1,n_1}) h_1^k + E_{j_1,n_1,\ell} \\
  \vdots \\
  E_{j_i,n_i,0} &= \sum_{k=1}^{\ell} c_k(\theta_{j_1,n_1}) h_i^k + E_{j_i,n_i,\ell} \\
  \vdots \\
  E_{j_\ell,n_\ell,0} &= \sum_{k=1}^{\ell} c_k(\theta_{j_1,n_1}) h_\ell^k + E_{j_\ell,n_\ell,\ell}
\end{align*}
Asymptotic Expansion: Drop errors $E_{j,n,\ell}$, introduce $\tilde{c}_k$

\[
E_{j_1,n_1,0} = \sum_{k=1}^{\ell} \tilde{c}_k(\theta_{j_1,n_1}) h_1^k \\
\vdots \\
E_{j_i,n_i,0} = \sum_{k=1}^{\ell} \tilde{c}_k(\theta_{j_1,n_1}) h_i^k \\
\vdots \\
E_{j_\ell,n_\ell,0} = \sum_{k=1}^{\ell} \tilde{c}_k(\theta_{j_1,n_1}) h_\ell^k
\]
Asymptotic Expansion

Construct Matrices $E$ and $V$

$$E = \begin{bmatrix} E_{j_1,n_1,0} \\ E_{j_2,n_2,0} \\ \vdots \\ E_{j_\ell,n_\ell,0} \end{bmatrix} \quad V = \begin{bmatrix} h_1 & h_1^2 & \ldots & h_1^\ell \\ h_2 & h_2^2 & \ldots & h_2^\ell \\ \vdots & \vdots & \ddots & \vdots \\ h_\ell & h_\ell^2 & \ldots & h_\ell^\ell \end{bmatrix} \quad \tilde{C} = \begin{bmatrix} \tilde{c}_1(\theta_{j_1,n_1}) \\ \tilde{c}_2(\theta_{j_1,n_1}) \\ \vdots \\ \tilde{c}_\ell(\theta_{j_1,n_1}) \end{bmatrix}$$

$$\tilde{C} = V^{-1}E$$
Asymptotic Expansion: Interpolating

\[ \tilde{c}_k(\theta_{j,n_1}) \rightarrow \tilde{c}_k(\theta_{j,n}) \]

We have \( \tilde{c}_k(\theta_{j,n_1}) \), \( \theta_{j,n_1} = \frac{j\pi}{n_1+1} \), \( j = 1, \ldots, n_1 \) We need an approximation of \( \lambda_j(T_n(f)) \), for some \( n \gg n_1 \),

\[ \tilde{\lambda}_j(T_n(f)) = f(\theta_{j,n}) + \sum_{k=1}^{\ell} \tilde{c}_k(\theta_{j,n}) h^k \]

\[ \theta_{j,n} = \frac{j\pi}{n + 1}, \quad j = 1, \ldots, n. \]
Asymptotic Expansion: Interpolating

\( \tilde{c}_k(\theta, n) \rightarrow \tilde{c}_k(\theta, n) \)

We have \( \tilde{c}_k(\theta, n_1) \), \( \theta, n_1 = \frac{j\pi}{n_1+1}, j = 1, \ldots, n_1 \) We need an approximation of \( \lambda_j(T_n(f)) \), for some \( n \gg n_1 \),

\[
\tilde{\lambda}_j(T_n(f)) = f(\theta, n) + \sum_{k=1}^{\ell} \tilde{c}_k(\theta, n) h^k
\]

\( \theta, n = \frac{j\pi}{n+1}, j = 1, \ldots, n. \)

We interpolate \( \tilde{c}_k(\theta_{j_1}, n_1) \) to \( \tilde{c}_k(\theta, n) \)!

Then \( \tilde{E}_{j,n,\ell} = \lambda_j(T_n(f)) - \tilde{\lambda}_j(T_n(f)) = O(h_1^\ell h). \)
Example, Approximate $\lambda_j(T_n(f))$, $\tilde{c}_k$

$f(\theta) = (2 - 2\cos(\theta))^2 = 6 - 8\cos(\theta) + \cos(2\theta)$

Figure from Sven-Erik Eksröm
Example, Approximate $\lambda_j(T_n(f))$, Errors

\[ f(\theta) = (2 - 2\cos(\theta))^2 = 6 - 8\cos(\theta) + \cos(2\theta) \]

\[ E_{j,n,0} = \lambda_j(T_n(f)) - f(\theta_j,n) \]
\[ \tilde{E}_{j,n,3} = E_{j,n,0} - \sum_{k=1}^{3} \tilde{c}_k(\theta_j,n)h^k \]

_Courtesy: Sven-Erik Eklöf_
Example, Approximate Preconditioned
\[ \lambda_j(T_n^{-1}(g)T_n(f)), \text{ Errors} \]

\[ f(\theta) = (2 - 2 \cos(\theta))^2 = 6 - 8 \cos(\theta) + 2 \cos(\theta) \]
\[ g(\theta) = 3 + 2 \cos(\theta) \]
\[ r(\theta) = f(\theta)/g(\theta) \]

\[ E_{j,n,0} = \lambda_j(T_n^{-1}(g)T_n(f)) - r(\theta_j,n) \]
\[ E_{j,n,3} = E_{j,n,0} - \sum_{k=1}^{3} \tilde{c}_k(\theta_j,n)h^k \]

*Figure from Sven-Erik Eksröm*
Recipe:

- Choose \( h \) (reasonably fine), \( h_1, h_2, \ldots, h_\ell \)
- Solve the system

\[
\begin{bmatrix}
  h_1 & h_1^2 & \cdots & h_1^\ell \\
  h_2 & h_2^2 & \cdots & h_2^\ell \\
  \vdots & \vdots & \ddots & \vdots \\
  h_\ell & h_\ell^2 & \cdots & h_\ell^\ell \\
\end{bmatrix}
\begin{bmatrix}
  \tilde{c}_1 \\
  \tilde{c}_2 \\
  \vdots \\
  \tilde{c}_\ell \\
\end{bmatrix}
= \begin{bmatrix}
  h_1 \\
  h_2 \\
  \vdots \\
  h_\ell \\
\end{bmatrix}.
\]

- Choose \( h_{\text{finest}} \) (resp. \( \theta_{\text{finest}} \)) and interpolate \( \tilde{c} \) to \( \theta_{\text{finest}} \)
- Sample the symbol with \( \theta_{\text{finest}} \) and add the correction.
Analytical expressions for $\mathbb{Q}_p$ Lagrange FEM, some IgA and DGM matrices.

Asymptotic expansion used on matrices arising from finite differences (FDM) and the isogeometric analysis (IgA).

Very fast and accurate computation of eigenvalues from Hermitian Toeplitz-like matrices (banded and blocks).

Can be applied on all (?) local PDE discretizations.

Highly accurate approximations of eigenvalues ($O(10^{-13})$ or more if high precision arithmetics).

For some matrices there exist also good approximations of the eigenvectors (work in progress).

The framework is (so far) applicable for structured matrices.
To summarize

The asymptotic expansion allows to approximate the whole spectrum of a large matrix $T_n(f)$ or $T_n^{-1}(g)T_n(f)$ knowing only the symbol $f$ (or the symbols $f$ and $g$), without the need to construct any matrices (matrix-less method).

Restrictions: GLT matrices and monotone symbols, also not yet for multivariate symbols.

Work in progress.
So far we can compute the eigenvalues

But what about the eigenvectors?!

Two cases:

- We know those too (easy). For example IgA $p = 1, 2$, some FDM.
- We know only an approximation of those (more difficult). What can we do?!

**Case A** Given the exact eigenvalues and approximations of the eigenvectors, compute the exact eigenvectors.

**Case B** Use the exact eigenvalues and the approximated eigenvectors in the deflated Krylov iterative methods. (ongoing work)

**Case C** Exploit an expansion for eigenvectors too (ongoing work)

A. Böttcher, J. M. Bogoya, S. M. Grudsky, E. Maximenko

*Asymptotic formulas for the eigenvalues and eigenvectors of Toeplitz matrices.* Sbornik Mathematics 208(11) (2018)
Conclusions

The feasibility to compute the exact eigenvalues (up to machine precision) and, possibly the eigenvectors, is of great potential. It gives answers/enables answering some questions that could not be satisfactorily accounted for till now, in particular, for large matrices:

- Compute the complete spectrum of large (structured) matrices in a cheap and accurate way.
- Determine all eigenvalues in a given interval.
- Use deflation techniques.
- Use methods, such as Chebyshev iteration, where accurate eigenvalue bounds are required.
Thank you for listening! Questions?
Recent references:

- Sven-Erik Ekström, Isabella Furci, Carlo Garoni, Stefano Serra-Capizzano, Hendrik Speleers, Carla Manni, *Are the eigenvalues of the B-spline isogeometric analysis approximation of $\Delta u = \lambda u$ known in almost closed form?*, NLA, 2018.