Groups and Symmetries in Numerical Linear Algebra
Part 2b
Mirrors and caleidoscopes

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"Chebyshev polynomials are everywhere dense in Numerical Analysis" (G. Forsythe?)

**Definition**

\[ T_k(x) = \cos(k\theta) \]
\[ U_k(x) = \frac{\sin((k + 1)\theta)}{\sin(\theta)} \]

where \( x = \cos(\theta) \).

**3-term recurrence**

\[ T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x) \]

\[ T_0(x) = 1 \]
\[ T_1(x) = x \]
\[ T_2(x) = 2x^2 - 1 \]
\[ T_3(x) = 4x^3 - 3x \]

\[ \ldots \]
Chebyshev 101 (classical theory)

Orthogonality - continuous and discrete

\[
\langle T_k, T_\ell \rangle_C = \int_{-1}^{1} \frac{T_k(x)T_\ell(x)}{\sqrt{1 - x^2}} \, dx
\]

\[
\langle T_k, T_\ell \rangle_E = \frac{1}{N} \sum_{x_j \in \{\ast\}} T_k(x_j)T_\ell(x_j)
\]

\[
\langle T_k, T_\ell \rangle_Z = \frac{1}{N} \sum_{x_j \in \{o\}} 'T_k(x_j)T_\ell(x_j)
\]
Chebyshev 101 (classical theory)

Chebyshev interpolation

\[ f(x) \approx \sum_{k=0}^{N} a(k) T_k(x), \text{ interpolating in extremal points } \{\star\} \]

\[ a(k) = \frac{\langle T_k, f \rangle_E}{\langle T_k, T_k \rangle_E}. \]

Note:

- \( \{f(x_j)\}_{x_j \in \{\star\}} \leftrightarrow \{a_k\}_{k=0}^{N} \) in \( \mathcal{O}(N \log N) \) flops via FCT.
- Lebesgue constant of Cheby-interpolation grows logarithmically

\[ L\{\star\} = \mathcal{O}(\log N). \]

- Exponentially fast convergence for analytic \( f(x) \).
Chebyshev interpolation

\[ f(x) \approx \sum_{k=0}^{N} a(k) T_k(x) \], interpolating in extremal points \(*\)

\[ a(k) = \frac{\langle T_k, f \rangle_E}{\langle T_k, T_k \rangle_E} \].

Clenshaw-Curtis quadrature

\[ \int_{-1}^{1} f(x) \, dx \approx \sum_{k=0}^{N} a(k) \int_{-1}^{1} T_k(x) \, dx. \]
Chebyshev 101 (classical theory)

Chebyshev interpolation

\[ f(x) \approx \sum_{k=0}^{N} a(k) T_k(x) \], interpolating in extremal points \{\ast\}

\[ a(k) = \frac{\langle T_k, f \rangle_E}{\langle T_k, T_k \rangle_E}. \]

Pseudospectral derivation

\[ f'(x)dx \approx \sum_{k=0}^{N} a(k) T'_k(x)dx = \sum_{k=0}^{N} b(k) T_k(x)dx. \]

\{a(k)\} \mapsto \{b(k)\} \text{ in } \mathcal{O}(N) \text{ flops by linear recursion.}
Example: Curve length

\[ L[f] = \int_{a}^{b} \| f'(t) \| \, dt \]

Pseudospectral derivation + Clenshaw-Curtis integration.
16 points on semicircle:

```plaintext
>>> ChebyL('semicircle',16)
ans = 3.141592653589623
error = 1.7 \cdot 10^{-13}
```
Example: Curve length

\[ L[f] = \int_{a}^{b} \| f'(t) \| dt \]

Archimedes: Inscribed 2N-gon:

- \( N = 16 \) points: error = 0.006
- \( N = 2 \cdot 10^6 \) points: error = \( 3.2 \cdot 10^{-13} \)
Spectral- and spectral element methods

Current practice ↑.

↑ We want this.
Triangular 'lego bricks' in spectral elements
MK 1989: "Symmetric FFTs, a general approach" (unpubl.)

Laplace–Dirichlet eigenfunctions by anti-symmetrization:

\[ \sigma : \text{mirror}, \quad \Delta \circ \sigma = \sigma \circ \Delta \]
\[ \Delta u = \lambda u \]
\[ u_a = \frac{1}{2} (u - u \circ \sigma) \]
\[ \Rightarrow \Delta u_a = \lambda u_a, \quad u_a = 0 \quad \text{on mirror} \]
Example: $A_2$–Kaleidoscope

**Weyl group $A_2$**

$$
\sigma_i = I - 2 \frac{\alpha_i \alpha_i^T}{\alpha_i^T \alpha_i}, \quad i = 1, 2
$$

$$
W = \langle \sigma_1, \sigma_2 \rangle
$$

**Laplacian eigenfunctions:**

$$
u(\theta) = \exp(ik\theta) \Rightarrow \Delta u = \lambda u
$$

$$
u_s = \frac{1}{|W|} \sum_{g \in W} u \circ g
$$

$$
\Delta \nu_s = \lambda \nu_s \quad \text{(Neumann)}
$$
Example: $A_2$–Kaleidoscope

Weyl group $A_2$

$$\sigma_i = I - 2 \frac{\alpha_i \alpha_i^T}{\alpha_i^T \alpha_i}, \quad i = 1, 2$$

$$W = \langle \sigma_1, \sigma_2 \rangle$$

Laplacian eigenfunctions:

$$u(\theta) = \exp(ik\theta) \Rightarrow \Delta u = \lambda u$$

$$u_a = \frac{1}{|W|} \sum_{g \in W} \det(g) u \circ g$$

$$\Delta u_a = \lambda u_a \quad \text{(Dirichlet)}$$
Example: $A_2$–Kaleidoscope

Properties of $u_a$ and $u_s$:

- Continuous and discrete orthogonality.
- Gaussian quadrature.
- Symmetric FFTs for interpolation, derivation, integration.
- Triangle based fast Poisson solvers.
- Sym. FFT have complicated data flow.
- Spectral convergence?
Weyl groups
How to define ’caleidoscopes’ on general periodic domains?

Definition

A root system is a subset of a euclidean space $\Phi = \{\alpha_i\} \subset E$ such that

1. $\Phi$ is finite, spans $E$ and does not contain 0.
2. If $\alpha \in \Phi$ then the only multiples of $\alpha$ in $\Phi$ are $\pm \alpha$.
3. If $\alpha \in \Phi$ then the reflection $\sigma_\alpha = I - 2 \frac{\alpha \alpha^T}{\alpha^T \alpha}$ leaves $\Phi$ invariant.
4. If $\alpha, \beta \in \Phi$ then $2 \frac{\alpha^T \beta}{\alpha^T \alpha} \in \mathbb{Z}$. 

Rootsystem A2

Hans Munthe-Kaas (Univ. of Bergen)
Caleidoscopes (the Affine Weyl group)

**Definition**

The group generated by the reflections $\mathcal{W} = \langle \sigma_{\alpha} | \alpha \in \Phi \rangle$ is called the **Weyl group**.

The set $\Lambda = \langle \theta \mapsto \theta + \alpha | \alpha \in \Phi \rangle$ is called the **Root lattice**.

The **affine Weyl group** $\mathcal{W}' = \Lambda \rtimes \mathcal{W}$ is the group generated by all these reflections and translations.
Classification of Root systems

(Cartan–Weyl–Coxeter–Dynkin)

Dynkin diagram:

- Nodes = generating mirrors.
- Edges indicate mirror-angles
  - no edge: 90°
  - one edge: 120°
  - two edges: 135°
  - three edges: 150°
- Arrow separates long and short roots.
Non-separable 2D cases: $A_2$, $B_2$ and $G_2$

Rootsystem $A_2$

- Blue dots: Roots.
- Blue arrows: Basis for root system.
- Red arrows: Fundamental dominant weights.
- Dotted lines: Mirrors in affine Weyl group.
- Yellow triangle: Fundamental domain of affine Weyl group.
- Red circles: Weights lattice.
- Black dots: Downscaled root lattice.
Root system $B_2$:

Blue dots: Roots.
Blue arrows: Basis for root system.
Red arrows: Fundamental dominant weights.
Dotted lines: Mirrors in affine Weyl group.
Yellow triangle: Fundamental domain of affine Weyl group.
Red circles: Weights lattice.
Black dots: Downscaled root lattice.
Root system $G_2$:

- Blue dots: Roots.
- Blue arrows: Basis for root system.
- Red arrows: Fundamental dominant weights.
- Dotted lines: Mirrors in affine Weyl group.
- Yellow triangle: Fundamental domain of affine Weyl group.
- Red circles: Weights lattice.
- Black dots: Downscaled root lattice.
Multivariate Chebyshev polynomials

Let $\Phi$ be $d$-dimensional root system, $W$ Weyl group and $\Lambda$ root lattice. Let $G = \mathbb{R}^d / \Lambda$ be the 'root-periodic' domain and $\hat{G} = \Lambda^\perp$ the reciprocal lattice (Fourier space).

**Definition**

Multivariate Chebyshev polynomials $T_k(x)$ are defined as follows for $\theta \in G$, $k \in \hat{G}$:

$$T_k(x) = \frac{1}{|W|} \sum_{g \in W} e^{i(gk)^T \theta}$$

$$x_j(\theta) = \frac{1}{|W|} \sum_{g \in W} e^{i(g\lambda_j)^T \theta}, \quad \lambda_j = (0, \ldots, 1, \ldots, 0)^T$$
Multivariate Chebyshev polynomials

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Example: 1-D case

$$\Phi = \{-\pi, \pi\}, \quad W = \{-1, 1\}$$

$$T_k(x) = \frac{1}{2} (e^{ik\theta} + e^{-ik\theta}) = \cos(k\theta)$$

$$x(\theta) = \frac{1}{2} (e^{i\theta} + e^{-i\theta}) = \cos(\theta).$$
Multivariate Chebyshev polynomials

**Definition**

\[ T_k(x) = \frac{1}{|W|} \sum_{g \in W} e^{i(gk)^T \theta}, \quad x_j(\theta) = \frac{1}{|W|} \sum_{g \in W} e^{i(g \lambda_j)^T \theta} \]

**Example: A₂ case**
Recurrence relations

\[ T_0 = 1, \quad T_{e_j} = x_j \]

\[ T_\ell T_k = \frac{1}{|W|} \sum_{g \in W} T_{k+g^T \ell}. \]

Classical \((A_1)\): \[ xT_k(x) = \frac{1}{2}(T_{k-1}(x) + T_{k+1}(x)) \]

Diagram:

- **Left Side:**
  - Node 1
  - Node 1
  - Node 1
  - Node 1
  \[ k \]

- **Right Side:**
  - Node 1
  - Node 1
  - Node 1
  \[ k-1 \]
  \[ k+1 \]
Recurrence relations

\[ T_0 = 1, \quad T_{e_j} = x_j \]

\[ T_\ell T_k = \frac{1}{|W|} \sum_{g \in W} T_{k+g^T \ell}. \]

A\textsubscript{2} recurrence:

\[ z = x_1, \quad \overline{z} = x_2 \]

\[ T_{-1,0} = \overline{z}, \quad T_{0,0} = 1, \quad T_{1,0} = z \]

\[ T_{n,0} = 3zT_{n-1,0} - 3\overline{z}T_{n-2,0} + T_{n-3,0} \]

\[ T_{n,m} = \frac{(3T_{n,0}T_{m,0} - T_{n-m,0})}{2}. \]
The example: $A_2$

Fundamental domain of affine Weyl group mapped to Deltoid by $\theta \mapsto x$:

\[
x_1 = \frac{1}{3} (\cos \theta_1 + \cos \theta_2 + \cos(\theta_1 - \theta_2)), \quad x_2 = \frac{1}{3} (\sin \theta_1 - \sin \theta_2 - \sin(\theta_1 - \theta_2)).
\]
Domains for $B_2$ and $G_2$ Chebyshev polynomials
A2 Chebyshev polynomials: 00r 10r 20r 30r | 10i 11r 21r 31r | 20i 21i 22r 32r
A2 Chebyshev polynomial $T_{52}$, real part:
Problem: Deltoid ≠ triangle

Possible solutions:

1. Straighten the deltoid to triangle.
2. Patch with overlap.
3. Work with (overdetermined) frame based on triangular trigonometric polynomials.
Straightening the deltoid

We have constructed a coordinate map which straightens the deltoid to a triangle. The map has analytically computable jacobian. It is well behaved away from the corners, but has corner singularities due to the cusps of the deltoid. Interpolation points are given analytically.
Lebesgue constant in triangular interpolation

Lebesgue constant: $L = \| I \|_\infty$, where $I$ is the (multivariate) interpolation operator in the given nodes. Slow growth of the Lebesgue constant is necessary for spectral convergence.

Define Lebesgue function:

$$\lambda(x) = \sum_{i \in I} |\ell_i(x)|,$$

where $\ell_i(x)$ is Lagrangian cardinal polynomial at node $i$, then $L = \|\lambda(x)\|_\infty$.

Bottom curve: Cheby-Lobatto points on Deltoid. All other curves: Interpolation points on triangle:

- Fekete points.
- Image of C–L points by straightening Deltoid to triangle.
- Hesthaven electrostatic points.
- Uniform meshpoints on triangle.
The root system $A_3$ (in 3D) is similar to the $A_2$ case:

- The Voronoi region of the root lattice is the *rhombic dodecahedron*.
- The fundamental domain of the affine Weyl group is a tetrahedron.
- Inside this tetrahedron sits a regular octahedron.
- Under the coordinate change $\theta \mapsto x$, the tetrahedron maps to a cusp-shaped domain, and the octahedron to a tetrahedron inside this.
- Restriction to faces: $A_3 \mapsto A_2$.
- Restriction to lines: $A_3 \mapsto A_1$. 
$A_3$ fundamental domains

Fundamental domain of affine Weyl group $A_3$
$A_3$ domain after change of variables
Numerical algorithms

We have analytical formulas and algorithms for

- Integrating $T_k(x)$ over whole $x$-domain (deltoid etc.).
- Integrating $T_k(x)$ over inscribed triangle ($A_2$ case) and tetrahedron ($A_3$ case).
- Computing $\nabla T_k(x)$ by recursion in Fourier domain.

All algorithms are FFT based, cost $O(N \log(N))$. Optimized symmetrized transforms exist.
Dirichlet problem on L-shaped domain, decomposed into triangles

solution N=48