Groups and Symmetries in Numerical Linear Algebra Part 1

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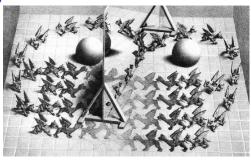
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Overview of my lectures





- How can we exploit symmetries in numerical linear algebra?
 - Symmetries and groups.
 - ► The generalized Fourier transform on groups w/ applications.
 - Abelian groups, lattice computations and kaleidoscopes (mirrors)
- Structured matrix problems related to Lie group theory:
 - $\,\blacktriangleright\,$ Approximation of the matrix exponential (Lie algebra \to Lie group)
 - Matrix factorizations, polar decompositions and Cartan decompositions with applications.

Circulant: $A_{i,j} = a(i-j \mod n)$.

$$a \in \mathbb{C}^{n}, \ A = \operatorname{circ}(a) = \begin{pmatrix} a(0) & a(n-1) & \cdots & a(1) \\ a(1) & a(0) & a(n-1) & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ & & a(1) & a(0) & a(n-1) \\ a(n-1) & \cdots & & a(1) & a(0) \end{pmatrix} \in \mathbb{C}^{n \times n}.$$

Convolution product (on discrete circle \mathbb{Z}_n):

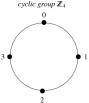
$$(a*x)(i) := \sum_{j=0}^{n-1} a(j)x(i-j \bmod n) = \sum_{j=0}^{n-1} a(i-j \bmod n)x(j)$$

Matrix \times vector: $\mathbf{A} \cdot \mathbf{x} = \mathbf{a} * \mathbf{x}$

Matrix \times matrix: $A \cdot B = \operatorname{circ}(a) \cdot \operatorname{circ}(b) = \operatorname{circ}(a * b)$



The domain $\mathbb{Z}_n = \{0, 1, 2, \dots, n-1\}$ with 'motion' $i, j \mapsto i + j$ and inverse $i \mapsto -i \pmod{n}$ forms a *group*.



Let
$$\mathbb{CZ}_n = \{x \colon \mathbb{Z}_n \to \mathbb{C}\} \simeq \mathbb{C}^n$$
. Define *shift* $S \colon \mathbb{CZ}_n \to \mathbb{CZ}_n$ as

$$(Sx)(j) = x(j-1).$$

Lemma

The following three conditions are equivalent:

- \bullet $A \in \text{Lin}(\mathbb{C}\mathbb{Z}_n, \mathbb{C}\mathbb{Z}_n)$ and AS = SA
- 2 $A \cdot x = a * x$ for some $a \in \mathbb{CZ}_n$
- **3** $A = \operatorname{circ}(a)$ for some $a \in \mathbb{C}\mathbb{Z}_n$.

Proof: exercise!



The Discrete Fourier Transform (DFT). Define $F: \mathbb{CZ}_n \to \mathbb{CZ}_n$ as

$$\mathbf{F}(x)(k) \equiv \widehat{x}(k) = \sum_{j \in \mathbb{Z}_n} e^{2\pi \mathbf{i} j k/n} x(j), \quad n \mathbf{F}^{-1} = \mathbf{F}^h.$$

The DFT diagonalizes convolutions,

$$\mathbf{F}(a * x)(k) = \widehat{a}(k)\widehat{x}(k) \Leftrightarrow \operatorname{circ}(a) = \mathbf{F}^{-1}\operatorname{diag}(\widehat{a})\mathbf{F}.$$

Why? F expresses a basis change to the *charaters* $\{\chi_k\}_{k\in\mathbb{Z}_n}\subset\mathbb{C}\mathbb{Z}_n$,

$$\chi_k(j) = e^{-2\pi i j k/n} \quad \Rightarrow \quad S\chi_k = \lambda_k \chi_k, \ \lambda_k = \chi_k(-1) = e^{2\pi i k/n},$$

Characters are eigenvectors of the shift S, equivalently

$$\chi_k \in \mathsf{Hom}(\mathbb{Z}_n, \mathbb{C}^{\times}) \quad \Leftrightarrow \quad \chi_k(j+\ell) = \chi_k(j)\chi_k(\ell),$$

where \mathbb{C}^{\times} is the multiplicative group of complex numbers with norm 1.

The FFT

 $x \leftrightarrow \hat{x}$ in $\mathcal{O}(n \log n)$ FLOPS via the *Fast Fourier Transform*.

Circulant computations costing $O(n \log n)$:

- Matrix mult. C = AB: $a, b \mapsto \widehat{a}, \widehat{b} \mapsto \widehat{c} = \widehat{a} \cdot \widehat{b} \mapsto C = \text{circ}(c)$.
- Linear solve: Ax = b: $a, b \mapsto \widehat{a}, \widehat{b} \mapsto \widehat{x} = \widehat{b}/\widehat{a} \mapsto x$.
- Eigenvalues: Eig(A) = \hat{a} .

Generalisations:

- Multidimensional versions.
- Non-circulant boundary conditions.
- Non-commutative groups.
- Smaller symmetry groups (non-transitive group actions).

Group = mathematical theory of symmetries

Definition

Group: set *G* with operation $a, b \mapsto ab \colon G \times G \to G$ such that:

- Associative: (ab)c = a(bc).
- ② Identity: $\exists 1 \in G$ such that a1 = 1a = a for all $a \in G$.
- **1** Inverse: $a \mapsto a^{-1}$ such that $aa^{-1} = 1$.

Common types of groups:

- Finite: $|G| < \infty$.
- Topological: $a, b \mapsto a^{-1}b$ is continuous.
 - compact or non-compact
 - discrete or continuous
- Lie: $a, b \mapsto a^{-1}b$ is smooth, differentiable.
- Abelian: ab = ba, where we often write $\{a + b, \mathbf{0}\}$ for $\{ab, \mathbf{1}\}$.

Group examples:













Abelian:

- $\{\mathbb{R}, +\}$ (non-compact, Lie)
- $\blacktriangleright \ \{\mathbb{Z},+\} \ (\text{non-compact, discrete})$
- ▶ ${\mathbb{Z}_n = \{0, 1, ..., n-1\}, +(\text{mod }n)\}}$ (finite, compact, discrete)

Finite, non-abelian:

► Dihedral groups, e.g. symmetries of snow-flake:

$$D_6 = \langle a, b \mid a^6 = b^2 = (ab)^2 = 1 \rangle$$

Symmetries of the five platonic solids: tetrahedron, cube,.....

Lie:

- General linear: $GL(n, \mathbb{R})$ (invertible real $n \times n$ matrices). GL(V): invertible linear operators on vector space V.
- ▶ Special linear: $SL(n) < GL(n, \mathbb{R})$ (det(A) = 1).
- ▶ Orthogonal: $O(n) < GL(n, \mathbb{R}), (A^T A = I)$
- ▶ Unitary: $U(n) < GL(n, \mathbb{C}), (A^h A = I)$
- Euclidean motion group: $E(3) = SO(3) \times \mathbb{R}^3$

Group action of group *G* on a set *X*

Left action: $\cdot: G \times X \to X$ such that for all $a, b \in G, x \in X$:

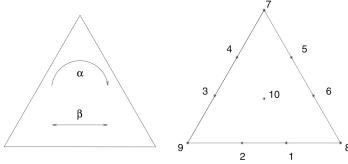
$$\mathbf{1} \cdot x = x$$
$$a \cdot (b \cdot x) = (ab) \cdot x$$

(Right: \cdot : $X \times G \rightarrow X$ s.t. $(x \cdot a) \cdot b = x \cdot (ab)$ and $x \cdot \mathbf{1} = x$.)

Properties of actions:

- Faithful (effective): $a \cdot x = x$ for all $x \in X$ implies a = 1.
- Free (fixpoint free): $a \cdot x = x$ for some $x \in X$ implies a = 1.
- Transitive: for all $x, y \in X$ there exists an $a \in G$ s.t. $a \cdot x = y$.
- Regular = free + transitive.
- A linear action on a vector space V is called a *representation*, i.e. $R: G \to GL(V)$ such that R(ab) = R(a)R(b).

Example: Symmetries of equilateral triangle in \mathbb{R}^2



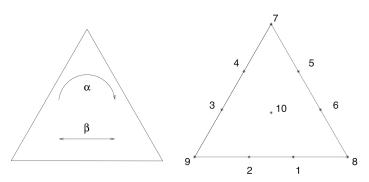
Dihedral group $D_3 = \langle \alpha, \beta \mid \alpha^3 = \beta^2 = (\alpha \beta)^2 = \mathbf{1} \rangle$. Representation of D_3 on \mathbb{R}^2 :

$$R(\alpha) = \begin{pmatrix} \cos(120^{\circ}) & -\sin(120^{\circ}) \\ \sin(120^{\circ}) & \cos(120^{\circ}) \end{pmatrix}, \quad R(\beta) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

The action restricted to the set $\mathcal{I}=\{1,2,3,4,5,6,7,8,9,10\}$ splits in three *orbits* $\{1,2,3,4,5,6\}$, $\{7,8,9\}$ and $\{10\}$.

Orbit representatives: $S = \{1, 7, 10\}$.

Example: Symmetries of equilateral triangle in \mathbb{R}^2



Problem:

Solve the PDE $\nabla^2 u = f$ on the triangle, with Dirichlet boundaries. Since $\nabla^2 \alpha = \alpha \nabla^2$ and $\nabla^2 \beta = \beta \nabla^2$, we may discretize $\nabla^2 \approx A$, such that the matrix A respects D_3 symmetries.

What does this mean?

Equivariant matrices

Let \mathcal{I} be a finite set, G a finite group and $i, g \mapsto ig$ a right action of G on \mathcal{I} . Let $V = \mathbb{C}^{\mathcal{I}}$ be the complex vector space with basis vectors in \mathcal{I} and $\mathbb{C}^{\mathcal{I} \times \mathcal{I}} = \text{Lin}(V, V)$ the matrices with indices in \mathcal{I} .

For $g \in G$ let $P(g) \in \mathbb{C}^{\mathcal{I} \times \mathcal{I}}$ denote the *permutation matrix* (P(g)x)(i) = x(ig). Since P(gh) = P(g)P(h), we call $g \mapsto P(g)$ the *permutation representation*.

Definition

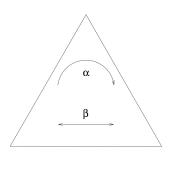
A is G-equivariant if AP(g) = P(g)A for all $g \in G$.

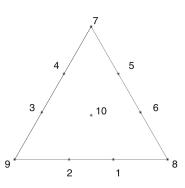
Lemma

A matrix $A \in \mathbb{C}^{\mathcal{I} \times \mathcal{I}}$ is G-equivariant if and only if

$$A_{ig,jg} = A_{i,j}$$
 for all $i, j \in \mathcal{I}$, $g \in G$.

Example (cont.)





$$(1,2,3,4,5,6,7,8,9,10)\alpha = (5,6,1,2,3,4,9,7,8,10)$$

 $(1,2,3,4,5,6,7,8,9,10)\beta = (2,1,6,5,4,3,7,9,8,10)$

A matrix $A \in \mathbb{C}^{10 \times 10}$ is D_6 equivariant if

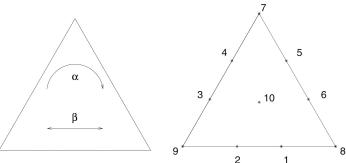
$$A_{i,j} = A_{i\alpha,j\alpha} = A_{i\beta,j\beta}$$
 for all $i,j \in \mathcal{I}$.



Equivariance and convolutions

We want to establish a correspondence equivariance \leftrightarrow convolution. Theory will be developed in three stages:

- **1** Regular action $i, g \mapsto ig$. There is just one orbit and $\mathcal{I} \simeq G$.
- **②** Free action $i, g \mapsto ig$. The set \mathcal{I} splits in several disjoint orbits. Each orbit can be identified with G.
- General (faithful) action. Get your hands dirty.



1. Regular action

Definition

The *group algebra* $\mathbb{C}G$ is the vector space $\mathbb{C}^{|G|}$ where each $g \in G$ is a basis vector, with the product * induced linearly from $g, h \mapsto gh$.

$$a * b = \left(\sum_{g \in G} a(g)g\right) * \left(\sum_{h \in G} b(h)h\right) = \sum_{g,h \in G} a(g)b(h)gh$$
$$= \sum_{g' \in G} \left(\sum_{h \in G} a(g'h^{-1})b(h)\right)g'.$$

The convolution product $*: \mathbb{C}G \times \mathbb{C}G \to \mathbb{C}G$

$$(a*b)(g) = \sum_{h \in G} a(gh^{-1})b(h) = \sum_{h \in G} a(h)b(h^{-1}g).$$

NOTE: a*(b*c)=(a*b)*c, $a*b \neq b*a$

1. Regular action

Pick $i \in \mathcal{I}$. Identify $ig \in \mathcal{I}$ with $g \in G$, $\mathcal{I} \simeq G$ and $\mathbb{C}^{\mathcal{I}} \simeq \mathbb{C}G$. For an equivariant $A \in \mathbb{C}^{G \times G}$ let $a \in \mathbb{C}G$ be defined as

$$a(g) := A_{g,1}$$
 (first column).

Note: $A_{g,h} = A_{gh^{-1},1} = a(gh^{-1})$, we recover A from its first column.

Lemma

For a regular action we have:

A equivariant
$$\Leftrightarrow$$
 $A \cdot x = a * x$ for all $x \in \mathbb{C}G$.

$$\frac{\text{Proof}}{\Rightarrow}: (Ax)(g) = \sum_{h \in G} A_{g,h} x(h) = \sum_{h \in G} a(gh^{-1}) x(h) = (a * x)(g).$$

\(\psi:\) Check that $P(g)x = x * g^{-1}$. If $Ax = a * x$ then

$$A(P(g)x) = a * (x * g^{-1}) = (a * x) * g^{-1} = P(g)Ax.$$



1. Regular action

G-equivariant matrices, regular action:

 $\mathsf{Matrix} \times \mathsf{matrix} : AB \quad \leftrightarrow \quad a * b$

 $\mathsf{Matrix} \times \mathsf{vector} : Ax \quad \leftrightarrow \quad a * x$

Permutation rep. : $P(g)A \leftrightarrow a * g^{-1}$

* - convolution in group algebra $\mathbb{C}G$.

How to exploit this 'hidden' structure? (patience please ... we first discuss more general actions)

2. Free action (non-transitive)

Group algebra: $\mathbb{C}G$: $G \to \mathbb{C}$. Block group algebra: $\mathbb{C}^{m \times \ell}G$: $G \to \mathbb{C}^{m \times \ell}$

$$a * b = \left(\sum_{g \in G} a(g)g\right) * \left(\sum_{h \in G} b(h)h\right) = \sum_{g,h \in G} a(g)b(h)gh$$
$$= \sum_{g' \in G} \left(\sum_{h \in G} a(g'h^{-1})b(h)\right)g'.$$

Block convolution product
$$*: \mathbb{C}^{m \times \ell} G \times \mathbb{C}^{\ell \times n} G \to \mathbb{C}^{m \times n} G$$

$$(a*b)(g) = \sum_{h \in G} a(gh^{-1})b(h) = \sum_{h \in G} a(h)b(h^{-1}g).$$



2. Free action (non-transitive)



 \mathcal{I} splits in m disjoint orbits, each orbit can be identified with G. Pick orbit representatives $\mathcal{S} \subset \mathcal{I}$, $|\mathcal{S}| = m$. The mapping

$$(i,g)\mapsto ig\colon \mathcal{S}\times G\to \mathcal{I},\quad \text{is } 1-1.$$

Let $n = |\mathcal{I}| = m|G|$. Define $\mu \colon \mathbb{C}^n \to \mathbb{C}^m G$ and $\nu \colon \mathbb{C}^{n \times n} \to \mathbb{C}^{m \times m} G$ as

$$\mu(x)_i(g) = x_{ig}$$
 $u(A)_{i,j}(g) = A_{ig,j} \quad \text{for all } i,j \in \mathcal{S}, g \in G.$

2. Free action (non-transitive)

Lemma

Let A, B be equivariant under free action on \mathcal{I} . Let $x \in \mathbb{C}^{|\mathcal{I}|}$. Then

$$\nu(AB) = \nu(A) * \nu(B)$$

$$\mu(AX) = \nu(A) * \mu(X),$$

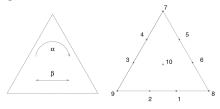
where * is the block convolution.

Proof.

$$\begin{split} \nu(AB)_{i,j}(g) &= (AB)_{ig,j} = \sum_{\ell \in \mathcal{S}, h \in G} A_{ig,\ell h} B_{\ell h,j} = \sum_{\ell \in \mathcal{S}, h \in G} A_{igh^{-1},\ell} B_{\ell h,j} \\ &= \sum_{h \in G} \sum_{\ell \in \mathcal{S}} \nu(A)_{i,\ell} (gh^{-1}) \nu(B)_{\ell,j}(h) = (\nu(A) * \nu(B))_{i,j}(g). \end{split}$$

Similar computation for matrix × vector.

3. General action



 \mathcal{I} splits in m orbits (ex. 3). Pick orbit representatives \mathcal{S} (ex. $\mathcal{S} = \{1,7,10\}$. For each $i \in \mathcal{S}$ let $G_i := \{g \in G : ig = g\}$ be the isotropy subgroups (ex. $G_1 = \{1\}$, $G_7 = \{1,\beta\}$, $G_{10} = G$). Orbit i has the structure of a homogeneous space, where the points are the right cosets $G_i \setminus G = \{G_i g\}_{g \in G}$ of the isotropy subgroups.

Idea:

We can think of each point in orbit i as being $|G_i|$ points merged into one. Doing this, we can still model equivariant matrix products as block convolutions in $\mathbb{C}^{m\times m}G$, restricted to a subspace taking a constant value on the isotropy subgropus. Detailes postponed or omitted!

The Genearlized Fourier Transform (GFT)

(Exploiting structure!)

Recall the convolution property of the classical (abelian) Fourier transform: $(\widehat{a*b})(k) = \widehat{a}(k)\widehat{b}(k)$. If $\widehat{a},\widehat{b} \in \mathbb{C}$, this cannot hold for our convolutions, since $a*b \neq b*a$. For matrix valued Fourier transforms, however, ...!

Let $R: G \to \mathbb{C}^{d_R \times d_R}$ be a complex representation of G, i.e. R(gh) = R(g)R(h) (matrix product). For $a \in \mathbb{C}^{m \times \ell}G$, $b \in \mathbb{C}^{\ell \times n}G$ define

$$\widehat{a}(R) := \sum_{g \in G} a(g) \otimes R(g), \quad \widehat{b}(R) := \sum_{g \in G} b(g) \otimes R(g).$$

Then

$$\widehat{(a*b)}(R) = \widehat{a}(R)\widehat{b}(R).$$

Proof: Exercise!



Irreducible representations

If $R: G \to \mathbb{C}^{d_R \times d_R}$ is a representation and $X \in \mathbb{C}^{d_R \times d_R}$ is invertible, then

$$\overline{R}(g) := XR(g)X^{-1}$$

is called an equivalent representation. A representation R which is equivalent to $\overline{R}=R_1\oplus R_2$ where $\overline{R}(g)$ simultaneously splits into a block-diagonal matrix for all $g\in G$ is called *reducible*, otherwise it is *irreducible*.

Frobenius theorem

Theorem

For any finite group G there exits a complete list $\mathcal R$ of non-equivalent irreducible representations such that

$$\sum_{R\in\mathcal{R}} d_R^2 = |G|.$$

For $a \in \mathbb{C}G$ define the GFT

$$\widehat{a}(R) = \sum_{g \in G} a(g)R(g).$$

then we may recover a by the inverse GFT (IGFT)

$$a(g) = \frac{1}{|G|} \sum_{R \in \mathcal{R}} d_R \operatorname{trace}(R(g^{-1})\widehat{a}(R)).$$

Example: D₃

 $D_3=\langle a,b\mid a^3=b^2=(ab)^2=\mathbf{1}\rangle$ has 6 elements. D_3 has a complete list of irreps $\mathcal{R}=\{R_1,R_2,R_3\}$, dimensions $d_1=d_2=1$, $d_3=2$, given as

$$\begin{split} R_1(g) &= 1 \quad \text{for all } g \in G \\ R_2(\alpha) &= 1, R_2(\beta) = -1 \\ R_3(\alpha) &= \left(\begin{array}{cc} \cos(120^o) & -\sin(120^o) \\ \sin(120^o) & \cos(120^o) \end{array} \right), \quad R_3(\beta) = \left(\begin{array}{cc} -1 & 0 \\ 0 & 1 \end{array} \right) \end{split}$$

Orthogonality of the GFT

For finite and compact groups we can prove that any representation is equivalent to a *unitary representation* $R: G \to U(V)$, thus we assume unitary or orthogonal representations. Inner products:

$$\mathbb{C}G$$
: $\langle a,b
angle = \sum_{g\in G} \overline{a(g)}b(g)$

$$\widehat{\mathbb{C}G} \colon \langle \widehat{a}, \widehat{b} \rangle = \sum_{R \in \mathcal{R}} \frac{d_R}{|G|} \operatorname{trace}(\widehat{a}(R)^h \widehat{b}(R)).$$

Lemma

For unitary \mathcal{R} , the GFT: $\mathbb{C}G \to \widehat{\mathbb{C}G}$ is unitary

$$\langle a,b\rangle = \langle \widehat{a},\widehat{b}\rangle.$$



Block GFT

Recall for $a \in \mathbb{C}^{m \times k} G$

$$\widehat{\mathsf{a}}(\mathsf{R}) := \sum_{g \in \mathsf{G}} \mathsf{a}(g) \otimes \mathsf{R}(g).$$

$$\mathsf{GFT}_b: \quad {}^\smallfrown \colon \mathbb{C}^{m \times k} G \equiv \mathbb{C}^{m,k} \otimes G \to \widehat{\mathbb{C}^{m,k}} \equiv \mathbb{C}^{m \times k} \otimes \mathbb{C} \widehat{G}$$

Everything is componentwise computations in the block:

$$\mathsf{GFT}_b = I \otimes \mathsf{GFT}_s \colon \mathbb{C}^{m \times k} \otimes \mathbb{C}G \to \mathbb{C}^{m \times k} \otimes \widehat{\mathbb{C}G}$$

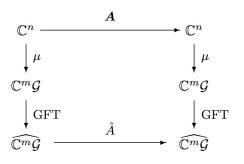
$$\mathsf{IGFT}_b = I \otimes \mathsf{IGFT}_s \colon \mathbb{C}^{m \times k} \otimes \widehat{\mathbb{C}G} \to \mathbb{C}^{m \times k} \otimes \mathbb{C}G$$

Computing GFT_b and $IGFT_b$:

Just do everything componentwise in the block.



The GFT block-diagonalizes any equivariant *A*, independently of the data in *A*!



 \widehat{A} is *block diagonal* with blocks of size $md_R \times md_R$, where m is the number of orbits and d_R the dimension of the irreducible representations.

Example: Solve Ax = b, equivariant A

- Compute \widehat{A} and \widehat{b} by GFT_b.
- ② For each $R \in \mathcal{R}$, solve $\widehat{A}(R)\widehat{x}(R) = \widehat{b}(R)$ for \widehat{x}
- **3** Compute $x = \mu^{-1} \circ \mathsf{IGFT}_{b}(\widehat{x})$

CAVEAT: For general group actions (non-free), we have that \widehat{A} is singular (even for regular A), but \widehat{A} is regular on a subspace of vectors being constant on the right 'cosets' of the isotroy subgroups. Some care must be taken!

The GFT is used similarly for computing eigenvalues and matrix exponentials, and matrix \times vector computations.

Computational savings?

• $\mathcal{O}(n^3)$ computations:

$$W_{\text{direct}}/W_{\text{fspace}} = \left(\sum_{R \in \mathcal{R}} d_R^2\right)^3 / \sum_{R \in \mathcal{R}} d_R^3.$$

• $\mathcal{O}(n^2)$ computations:

$$W_{\text{direct}}/W_{\text{fspace}} = \left(\sum_{R \in \mathcal{R}} d_R^2\right)^2 / \sum_{R \in \mathcal{R}} d_R^2.$$

Example: symmetries of platonic solids











Domain	G	$ \mathcal{G} $	$\{d_R\}_{R\in\mathcal{R}}$	$W_{ m direct}/\mathcal{O}(n^2)$	${\cal O}(n^3)$
triangle tetrahedron	\mathcal{D}_3 \mathcal{S}_4	6 24	$\{1, 1, 2\}$ $\{1, 1, 2, 3, 3\}$	3.6 9	21.6 216
cube	$\mathcal{S}_4 imes \mathcal{C}_2$	48	$\{1,1,1,1,2,2,3,3,3,3,3\}$	18	864
icosahedron	$\mathcal{A}_5 imes \mathcal{C}_2$	120	$\{1, 1, 3, 3, 3, 3, 4, 4, 5, 5\}$	29.5	3541

Icosahedral symmetries with reflections: $G = C_2 \times A_5$





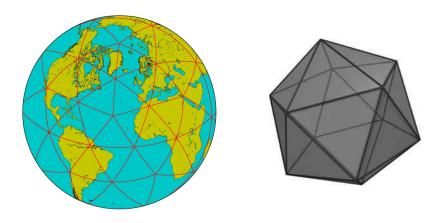
Cost of matrix exponential (Icoashedral symmetries): |G| = 120, direct computation $120^3 = 1728000$ operations. Block diagonalization by GFT:

$$1^3 + 1^3 + 3^3 + 3^3 + 3^3 + 3^3 + 4^3 + 4^3 + 5^3 + 5^3 = 488$$

⇒ factor 3500 reduction in cost!

Application: PDEs and Domain symmetries

Ex.: Heat equation on sphere $u_t = \nabla^2 u$.



Compute $\exp(tA)$ where $A \approx \nabla^2$ on sphere. Exploit icosahedral symmetries.

More on matrix exponentials in the sequel!