Exploiting symmetry in complex network analysis

Rubén J. Sánchez García

1Mathematical Sciences, University of Southampton, University Road, Southampton SO17 1BJ, United Kingdom
2R.Sanchez-Garcia@soton.ac.uk

ABSTRACT

Virtually all network analyses involve structural measures or metrics between pairs of vertices, or of the vertices themselves. The large amount of redundancy present in real-world complex networks is inherited by such measures, and this has practical consequences which have not yet been explored in full generality, nor systematically exploited by network practitioners. Here we present a complete theory for the study of symmetry in empirical networks and their effects on arbitrary network measures, and show how this can be exploited in practice in a number of ways, from redundancy compression, to computational reduction. We also uncover the spectral signatures of symmetry for an arbitrary network measure such as the graph Laplacian. Computing and decomposing network symmetries is very efficient in practice, and we test real-world examples up to several million nodes. We illustrate our methods with some popular network measures. Our results are widely applicable, and place previous work on network symmetry in a common framework.

Network models of real-world complex systems have been extremely successful at revealing structural and dynamical properties of these systems. The success of this approach is due to its simplicity, versatility, and surprising universality, with common properties and principles shared by many disparate systems and computational reduction, algorithms achieving remarkable space (up to 74%) and time (up to 89%) savings in our test networks (Table 1, Figs. 3, 4). We generalise the spectral decomposition in to arbitrary network measures, uncovering the spectral signatures of symmetry and thus predicting and explaining most of the discrete part of the spectrum of a network measure, such as the graph Laplacian (Fig. 5). Moreover, symmetry can be exploited to compute the full spectrum of a network in a fraction (typically 30-70%) of the time (Fig. 4). We show that computing network symmetries and motifs is very efficient in practice, testing real-world examples up to several million nodes (Table 1). Our theoretical framework generalise and helps understand other network symmetry results thereafter.

Results

Symmetry in complex networks

The notion of network symmetry is captured by the mathematical concept of graph automorphism. This is a permutation of the vertices (nodes) preserving adjacency (Fig. 1), and can be expressed in matrix form using the adjacency matrix of the network. If a network (mathematically, a finite simple graph) has vertices, labelled 1 to , its adjacency matrix is an matrix with if there is an edge between nodes and , and zero otherwise. A graph automorphism is then a permutation, or relabelling, of the vertices such that is an edge only if is an edge, or, equivalently, for all . In matrix terms, this can be written as

where is the permutation matrix corresponding to , that is, the matrix with entry 1 if and 0 otherwise. The automorphisms of a graph form a mathematical structure called a group, the automorphism group of . In principle, any (finite) group is the automorphism group of some graph , but, in practice, real-world networks exhibit very specific types of symmetries generated at some small subgraphs called symmetric motifs. We can partition the vertex set into the asymmetric core of fixed points (an automorphism moves a vertex if and fixes it otherwise), and the vertex sets of the symmetric motifs,

where

\[
\text{(1)}
\]

\[
\text{(2)}
\]
as shown in Fig. 1 for a toy example.

Real-world networks typically exhibit a core of fixed points, and a large number of relatively small symmetric motifs, where all the network symmetry is generated, and hence the size of the automorphism group is often extremely large, in stark contrast to random graphs, typically asymmetric. However, each symmetry is the product (composition) of automorphisms permuting a very small number of vertices within a symmetric motif (Fig. 1).

Each symmetric motif can be further subdivided into orbits of structurally equivalent nodes (shown by colour in Fig. 1). As vertices in the same orbit are structurally indistinguishable, orbits contribute to network redundancy and thus to the robustness of the underlying system.

Empirically, most symmetric motifs of real-world networks are made of orbits of the same size with the geometric factor realising every possible permutation of the vertices in each orbit, while fixing vertices outside the motif (Fig. 1). Such motifs are called basic symmetric motifs (BSMs), and have a very constrained structure (e.g. each orbit has to be either an empty or a complete graph). Non-basic symmetric motifs (typically branched trees) are called complex; they are rare (Table 1), and can be studied on a case-by-case basis.

The definition of network automorphism (1) carries to an arbitrary $n \times n$ real matrix $A = (a_{ij})$. Such matrix can be seen as the adjacency matrix of a network with $n$ vertices labelled 1 to $n$, and an edge (link) from node $i$ to node $j$ with weight $a_{ij}$ if $a_{ij} \neq 0$, and no such edge if $a_{ij} = 0$. This means that an automorphism does not only preserve edges, but also their weights and directions. This may not be a realistic assumption for real-world weighted networks, where the weights often come from observational or experimental data, but it applies to the matrix representing a network structural measure, as we explain next.

**Structural network measures**

A (pairwise) structural network measure is a function $F(i, j)$ on pairs of vertices which depends on the network structure alone, and not, for example, on node or edge labels, or other meta-data. Most network measures are structural, including graph metrics (e.g. shortest path, resistance), and matrices algebraically derived from the adjacency matrix (e.g. communicability, Laplacian matrix). (We identify matrices $M$ with pairwise measures via $F(i, j) = |M|_{ij}$.) Crucially, structural measures are independent of the ordering or labelling of the vertices and hence satisfy, for any automorphism $\sigma \in \text{Aut}(\mathcal{G})$,

$$F(\sigma(i), \sigma(j)) = F(i, j) \quad \text{for all } i, j \in V. \quad (3)$$

(One can take this as the mathematical definition of structural measure.) In contrast, functions depending, explicitly or implicitly, on some vertex ordering or labelling, are not structural, for example the shortest path length through a given node, or a measure involving a ‘source’, ‘target’, or any other node or edge meta-data. Our results can still be adapted to the presence of node or edge labels, or weights, by restricting to automorphisms preserving the additional structure. For simplicity, here we discuss the unlabelled case only.

We can encode a structural measure $F$ as a network with adjacency matrix $[F(A)]_{ij} = F(i, j)$, and write (3) in matrix form as

$$F(A) P = P F(A), \quad (4)$$

where $P$ is the permutation matrix corresponding to $\sigma$. That is, a network representation of $F$, $F(\mathcal{G})$, inherits all the symmetries of $\mathcal{G}$, and hence has the same decomposition into symmetric motifs (2), and orbits. The BSMs in $F(\mathcal{G})$ occur on the same vertices $M_i$ although they are now all-to-all weighted subgraphs in general (Fig. 1 inset). Nevertheless, they have a very constrained structure: the intra and inter orbit connectivity depends on two parameters only (Fig. 2).

The results in this article apply to arbitrary structural measures, although the two most common cases in practice are the following. We call $F$ full if $F(i, j) \neq 0$ for most $i, j \in V$ (e.g. a graph metric), and sparse if $F(i, j) = 0$ if $a_{ij} = 0$, for most $i, j \in V$ (e.g. the graph Laplacian). The graph representation of $F(\mathcal{G})$ is an all-to-all weighted graph if $F$ is full, and has a sparsity similar to $\mathcal{G}$ if $F$ is sparse.

From now on, we will assume that $\mathcal{G}$ is undirected and $F$ is symmetric, $F(i, j) = F(j, i)$, which may not be the case even if $\mathcal{G}$ is undirected (e.g. the transition probability of a random walker $F(i, j) = \frac{a_{ij}}{\deg(i)}$), and discuss directed networks and asymmetric measures in the Supporting Information.
Figure 2. Structure of a BSM for an arbitrary network measure \( F \). (a) Every orbit in a BSM is an \((\alpha, \beta)\)-uniform graph \( k_{\alpha,\beta} \), the graph with \( n \) vertices and adjacency matrix \( A = (a_{ij}) \) with \( a_{ij} = \alpha = F(i,j) \) if \( i \neq j \) and \( a_{ii} = \beta = F(i,i) \). (b) The connectivity between two orbits \( \Delta_1 \) and \( \Delta_2 \) in the same BSM (after a suitable relabelling \( \Delta_1 = \{v_1, \ldots, v_n\}, \Delta_2 = \{w_1, \ldots, w_n\} \)) is given by \( \gamma = F(v_i, w_j) \) for \( i \neq j \), and \( \delta = F(v_i, w_i) \), the \((\delta, \gamma)\)-uniform join of the two orbits. (c) In the quotient, the BSM orbit becomes a single vertex with a self-loop weighted by \( (n-1)\alpha + \beta \), and the two orbits are joined by an edge weighted by \( (n-1)\gamma + \delta \). Note that, by annotating each orbit in the quotient by \( n \) and \( \alpha \) (or \( \beta \)), and each intra-motif edge by \( \gamma \) (or \( \delta \)), we can recover each BSM from the quotient.

Redundancy in network measures
The formal procedure to quantify and eliminate structural redundancies in a network is via the quotient network. This is the graph with one vertex per orbit or fixed point (see Fig. 1, bottom) and edges representing orbits connectivity (see Methods for full details). The quotients of real-world networks are often significantly smaller (in vertex and edge size) than the parent networks\(^{10,18}\) (Table 1), and this reduction quantifies the structural redundancy present in a network model.

We can use the quotient network to eliminate the symmetry-induced redundancies inherited by an arbitrary network measure \( F \), which present themselves as repeated values by Eq. (3). The amount of symmetry-induced redundancy inherited by a network measure can be remarkable: In our test networks, we found up to 70% of redundancy due to symmetry alone (Fig. 3).

A simple algorithm (Methods) eliminates these redundancies and achieves exact recovery for external edges (between vertices in different symmetric motifs) and average recovery for internal edges (between vertices in the same symmetric motif). Note that the vast majority of edges in the network representation of a network measure are external (at least 99.999% for a full measure in our test networks, see \( \text{int}_f \) in Table 1). Nonetheless, we can achieve lossless compression (external and internal edge recovery) by annotating (cf. Fig. 2) the basic quotient, which leaves non-basic motifs unchanged, and retains most of the symmetry in a typical real-world network (Methods, Fig. 3).

Computational reduction
Network symmetries can also reduce the computational time of evaluating an arbitrary network measure \( F \). By Equation (3), we only need to evaluate \( F \) on orbits, resulting in a computational reduction ratio of between \( \bar{m}_2 \) and \( \bar{n}_2 \) (Table 1) for sparse, respectively full, network measures. Of course, this assumes that the computation on each pair of vertices \( F(i,j) \) is independent of one another, which is often not the case. Moreover, the calculation of \( F(i,j) \) is still performed on the whole network \( G \).

A more substantial computational reduction can be obtained by evaluating \( F \) on the (often much smaller) quotient network instead. We call \( F \) quotient recoverable if it can be applied to the quotient network \( Q \), and \( F(G) \) can be recovered from \( F(Q) \), for all networks \( G \). Note that this may involve, beyond evaluating \( F(Q) \), an independent (hence parallelizable) computation on each symmetric motif (typically a very small graph). We illustrate quotient recoverability on several popular network measures in the Applications section. By evaluating \( F \) in the quotient network, we can obtain very substantial computational time savings (Fig. 4), depending on the amount of symmetry present and the computational complexity of \( F \).

Spectral signatures of symmetry
The spectrum of a network (its adjacency matrix) relates to a multitude of structural and dynamical properties\(^1\). The presence of symmetries is reflected in the spectrum of the network\(^2\), and indeed in the spectrum of any network measure. Symmetries give rise to high-multiplicity eigenvalues (shown as ‘peaks’ in the spectral density) and, in fact, we can explain...
Table 1. Symmetry in some real-world networks. For each test network, we show the number of vertices ($n$), edges ($m$), number of generators (gen) of the automorphism group (sizes, $10^{153}$ to $10^{197,552}$, not shown), computing times of generators ($t_1$) and geometric decomposition ($t_2$), in seconds, number of symmetric motifs ($sm$) and proportion of BSMs (bsm), proportion of vertices moved by an automorphism (mv), proportion of vertices ($\tilde{n}$) and edges ($\tilde{m}$) in the quotient, proportion of external edges in the sparse case (exts, in percentage), and of internal edges in the full case (intf, closest power of 10), full compression ratio ($c_{full}$, closest power of 10), and spectral computational reduction ($sp = \tilde{n}$), all for the largest connected component. Datasets available at [source], except HumanDisease, Yeast, and HumanPPI. Computations on a desktop computer (3.2 GHz Intel Core i5 processor, 16 GB 1.6 GHz DDR3 memory). All networks are symmetric, although the amount of symmetry (as measured by $mv$ or $\tilde{n}$) ranges from several networks with 50% quotient reduction, to CaliforniaRoads with only 4% of vertices participating in any symmetry. However, the effect of compression and computational reduction multiplies as e.g. $c_{full} = \tilde{n}$ and $sp = \tilde{n}$, achieving significant results for most of our test networks.

| Name            | $n$ | $m$ | gen | $t_1$ | $t_2$ | $sm$ | bsm | mv | $\tilde{n}$ | $\tilde{m}$ | exts | intf | $c_{full}$ | sp       |
|-----------------|-----|-----|-----|-------|-------|------|-----|----|-------------|-------------|------|------|------------|---------|
| HumanDisease    | 1,419 | 2,738 | 713 | 0.00  | 0.16  | 272  | 96.0 | 71.0 | 48.3        | 83.8        | 83.3 | 10^{-3} | 27.2      | 11.3    |
| Yeast           | 1,647 | 2,736 | 380 | 0.00  | 0.01  | 149  | 99.3 | 33.3 | 76.3        | 83.5        | 63.5 | 10^{-3} | 58.4      | 44.4    |
| OpenFlights     | 3,397 | 19,230 | 732 | 0.00  | 0.11  | 321  | 93.5 | 32.4 | 77.3        | 94.4        | 93.9 | 10^{-3} | 63.5      | 46.2    |
| USPowerGrid     | 4,941 | 6,594 | 414 | 0.00  | 0.09  | 302  | 97.4 | 61.7 | 90.2        | 91.3        | 97.6 | 10^{-4} | 83.9      | 73.3    |
| HumanPPI        | 9,270 | 36,918 | 972 | 0.00  | 0.12  | 318  | 99.9 | 54.3 | 55.0        | 78.2        | 99.9 | 10^{-5} | 30.3      | 16.7    |
| Astro-Ph        | 17,903 | 196,972 | 3,232 | 0.01 | 0.21  | 1,682 | 99.4 | 81.9 | 80.4        | 95.5        | 94.6 | 10^{-4} | 74.0      | 54.9    |
| InternetAS      | 34,761 | 107,720 | 15,587 | 0.03 | 0.29  | 3,189 | 99.9 | 54.3 | 55.0        | 78.2        | 99.9 | 10^{-5} | 30.3      | 16.7    |
| WordNet         | 145,145 | 656,230 | 52,152 | 0.18 | 0.62  | 28,456 | 92.0 | 60.0 | 58.0        | 89.9        | 95.4 | 10^{-5} | 49.3      | 21.6    |
| Amazon          | 334,863 | 925,872 | 32,098 | 0.20 | 0.39  | 23,302 | 99.8 | 16.8 | 90.2        | 91.3        | 97.6 | 10^{-6} | 81.6      | 73.6    |
| Actors          | 374,511 | 15,014,839 | 182,803 | 0.95 | 1.38  | 36,703 | 99.9 | 58.6 | 51.2        | 66.4        | 90.4 | 10^{-5} | 26.2      | 13.4    |
| InternetAS-skitter | 1,694,616 | 11,094,209 | 319,738 | 1.71 | 4.17  | 84,675 | 99.1 | 19.7 | 85.4        | 92.8        | 99.9 | 10^{-6} | 73.5      | 62.3    |
| CaliforniaRoads | 1,957,027 | 2,760,388 | 36,430 | 0.47 | 0.16  | 35,210 | 98.8 | 4.0  | 97.9        | 98.4        | 99.7 | 10^{-7} | 96.3      | 93.9    |
| LiveJournal     | 5,189,808 | 48,687,945 | 410,575 | 8.02 | 3.59  | 245,211 | 99.9 | 12.7 | 92.1        | 96.5        | 99.7 | 10^{-7} | 84.8      | 78.0    |

Figure 4. Quotient computational reduction.
Computational time reduction of several structural measures in some of our test networks (Table 1) obtained by performing the calculation in the quotient network versus the original network. The computations are: spectral decomposition of the adjacency matrix ($\text{spectral}$), exponential matrix $\exp(A)$ ($\text{commun}$), pseudoinverse of the Laplacian matrix ($\text{laplacian}$), shortest path distance ($\text{distance}$), closeness centrality ($\text{closeness}$), betweenness centrality ($\text{btwness}$) and eigenvector centrality ($\text{eigc}$), using MATLAB R2017a built-in functions. For $\text{spectral}$, we also show (left column) the reduction including the (sequential) symmetric motif calculation. In each case, median computational reduction over at least 10 iterations shown.

and predict most of the discrete part of the spectrum of an arbitrary network measure on a typical real-world network (cf. Fig. 5).

First, we can show (Methods) that the eigenvalues and eigenvectors of a network are those of the quotient network together with those arising from individual symmetric motifs. Formally, we can find an eigenbasis of the form $\{Sv_1, \ldots, Sv_m, \tilde{w}_1, \ldots, \tilde{w}_{m-s} \}$, where $\{v_1, \ldots, v_m\}$ is any eigenbasis of the quotient network, $Sv_i$ is the vector $v_i$ lifted to the parent network by repeating entries on each orbit, each $w_j$ is an eigenvector of a symmetric motif $M$. $\tilde{w}_j$ is the vector $w_j$ localised on $M$, that is, zero outside $M$, and the eigenvalues of $v_i$ and $Sv_i$, respectively $w_j$ and $\tilde{w}_j$, are the same.

Furthermore, each symmetric motif $M$ contributes the same (called redundant) eigenpairs to any network containing $M$ as a symmetric motif. Since most symmetric motifs in real-world networks are basic, and they have a very constrained structure (Fig. 2), we can in fact determine the redundant spectrum of BSMs with up to a few orbits, that is, we can predict where the most significant ‘peaks’ in the spectral density of an arbitrary network function will occur. These values are shown on Table 2 and can be obtained, for each BSM, simply by solving a quadratic equation. For example, for the graph Laplacian, we predict high-multiplicity eigenvalues at the positive integers due to the symmetry, and this is confirmed in our test networks (Fig. 5), with symmetry explaining between 89% and 97% of the discrete spectrum.

Moreover, decoupling the contribution of symmetry to the spectrum leads to an eigendecomposition algorithm that exploits the presence of symmetries: The spectrum and eigenba-
Redundant spectra of BSMs with one or two

Table 2. (red), given as relative probability of eigenvalue count, with

if it only depends on the network structure and,

\begin{align*}
K_n^{α, β} & \overset{γ, δ}{\rightarrow} K_n^{α_2, β_2} \\
-α + β & n - 1 \quad e_i \\
-b - κ_1 c & n - 1 \quad (κ_1 e_i, e_j) \\
-b - κ_2 c & n - 1 \quad (κ_2 e_i, e_j)
\end{align*}

Table 2. Redundant spectra of BSMs with one or two

orbits. We write \( e_i \) for the vector with non-zero entries 1 at

position 1, and -1 at position \( i \) (2 ≤ \( i \) ≤ \( n \)), \( κ_1 \) and \( κ_2 \) for the two

solutions of the quadratic equation \( cκ^2 + (-α + β)κ - c = 0 \) where

\( a = α - β, \quad b = α - β \) and \( c = γ - δ \), and \( |v|w \) represents

concatenation of vectors. For unweighted graphs without loops, this

formula recovers the redundant eigenvalues predicted in [11].

Figure 5. Spectral signatures of network symmetry.

Laplacian spectrum of six test networks (blue) and of their quotient

(red), given as relative probability of eigenvalue count, with

multiplicity, in bins of size 0.1. Only the most significant part of the

spectrum is shown. Most of the ‘peaks’ observed in the spectral

density occur at positive integers, as predicted. (Inset) Percentage of

density in Table 1. The network (adjacency) eigendecomposition

\( \tilde{Q} = U f \) in Table 1. For the network (adjacency) eigendecomposition

and the quotient compression ratio reported in [18], here \( c_{\text{sparce}} = \tilde{n}_Q \) in Table 1. The network (adjacency) eigendecomposition

can be significantly sped up by exploiting symmetries (Fig. 4).

Communicability

Communicability is a very general choice of structural measure,

consisting on any analytical function \( f(x) = \sum a_n x^n \) applied to the adjacency matrix,

\[ f(A) = \sum_{n=0}^{m} a_n A^n, \]

and it is a natural measure of network connectivity, since

the matrix power \( A^k \) counts walks of length \( k \) [30]. Its network

representation, the graph \( f(\mathcal{G}) \) with adjacency matrix \( f(A) \), inherits all the symmetries of \( \mathcal{G} \) and thus it has the same sym-

metric motifs and orbits. The BSMs are uniform joins of

orbits (Fig. 1).

Therefore, satisfies

\[ G(i) = G(\sigma(i)) \]

for each automorphism \( \sigma \in \text{Aut}(\mathcal{G}) \), that is, it is constant on

orbits (Fig. 1).

Applications

We illustrate our methods on several popular pairwise and

vertex-based network measures. These are example applica-

tions: Our methods are general and similar results should

apply to any network measure.

Adjacency matrix

The methods in this paper can be applied to the network

itself, that is, to its adjacency matrix seen as a sparse network

measure. We recover the structural and spectral results in [10, 11],

and the quotient compression ratio reported in [18], here \( c_{\text{sparce}} = \tilde{n}_Q \) in Table 1. The network (adjacency) eigendecomposition

can be significantly sped up by exploiting symmetries (Fig. 4).

Communicability

Communicability is a very general choice of structural measure,

consisting on any analytical function \( f(x) = \sum a_n x^n \) applied to the adjacency matrix,

\[ f(A) = \sum_{n=0}^{m} a_n A^n, \]

and it is a natural measure of network connectivity, since

the matrix power \( A^k \) counts walks of length \( k \) [30]. Its network

representation, the graph \( f(\mathcal{G}) \) with adjacency matrix \( f(A) \), inherits all the symmetries of \( \mathcal{G} \) and thus it has the same sym-

metric motifs and orbits. The BSMs are uniform joins of

orbits, and each orbit is a uniform graph (Fig. 2) characterised

by the communicability of a vertex to itself (a natural measure

of centrality) [25], and the communicability between distinct ver-

tices. As a full network measure, the compression ratio \( c_{\text{full}} \) applies (Table 1), indicating the fraction of storage needed by

using the quotient to eliminate redundancies (Fig. 3). More-

over, we can recover the communicability of a network from

its quotient (Methods), or by using the spectral decomposi-

tion algorithm on the adjacency matrix (\( A = UDU^T \) implies \( f(A) = U f(D) U^T \)) reducing the computation, typically cubic on

the number of vertices, by \( sp = \tilde{n}_Q^3 \) (Table 1, Fig. 4).
Shortest path distance
This is the simplest metric on a (connected) network, namely the length of a shortest path between vertices. As a full structural measure, the compression rate $c_{\text{full}}$ (Table 1) applies. Moreover, automorphisms $\sigma$ preserve the shortest path metric, $d(i, j) = d(\sigma(i), \sigma(j))$, and indeed shortest paths themselves. As shortest paths cannot contain intra-orbit edges, we can compute shortest distances from the quotient,

$$d^\theta(\alpha, \beta) = d^\theta(i, j), \quad \alpha \in V_i, \beta \in V_j,$$

whenever $V_i$ and $V_j$ are orbits in different symmetric motifs. This accounts for all but the (small) intra-motif distances and reduces the computation as shown in Fig. 4. (See Methods for full details.)

Laplacian matrix
The Laplacian matrix of a network $L = D - A$, where $D$ is the diagonal matrix of vertex degrees, is a sparse network measure and therefore inherits all the symmetries of the network. The symmetric motifs are identical to the subgraphs in the network except edges are now weighted by $-1$, and self-loops by vertex degrees in the network, and hence they depend on how the motif is embedded in the network.

Quotient compression and computational reduction are less useful in this case, however the spectral results are more interesting. Spectral decomposition and eigenvalue localisation apply, and we can compute redundant Laplacian eigenvalues directly from Table 2, for instance positive integers for BSMs with one orbit (Methods). This explains and predicts most of the ‘peaks’ (high multiplicity eigenvalues) in the Laplacian spectral density, confirmed on our test networks (Fig. 5).

Commute distance and matrix inversion
The commute distance is the expected time for a random walker to travel between two vertices and back. In contrast to the shortest path distance, it is a global metric which takes into account all possible paths between two vertices. The commute distance is equal up to a constant (the volume of the network) to the resistance metric $\frac{1}{2}r_{ij}$, which can be expressed in terms of $L^2 = (I + L)$, the pseudoinverse (or Moore-Penrose inverse) of the Laplacian, as $r(i, j) = I_{ji} + I_{ij} - 2I_{ij}$.

The commute (or resistance) distance is a (full) structural measure, and all our structural and spectral results apply. Crucially, we can use eigendecomposition algorithm to obtain $L = UD^TU^T$ (and hence $L^2 = UD^2U^T$, and $r$) from the quotient and symmetric motifs, resulting in significant computational gains (Fig. 4). More generally, if $M_F$ is the matrix representation of a network measure, its pseudoinverse $M_F^\dagger$ is also a network measure, and the comments above apply. Note that $M_F^\dagger$ is generally a full measure even if $M_F$ is sparse.

Closeness centrality
This is the average shortest path distance to every node in the graph. It is preserved by symmetries and hence constant on each orbit, as it is in fact the average of a pairwise structural measure, the shortest path distance. Moreover, closeness centrality can be recovered up to a very small error from the quotient, or exactly from an annotated quotient (Methods), substantially reducing the computation (Fig. 4).

Betweenness centrality
This is the sum of proportions of shortest paths between pairs of vertices containing a given vertex. Using symmetries in this case is more subtle, as shortest paths through a given vertex are only preserved by symmetries fixing that vertex. However, betweenness can be computed from shortest path distances and number of shortest paths, both pairwise structural measures, reducing the computation of a naive $O(n^3)$ time, $O(n^2)$ space implementation by $\tilde{n}^2$ and $\tilde{n}^3$. It would be interesting to adapt a faster algorithm such as $3^3$ to exploit symmetries, but this is beyond our scope.

Eigenvector centrality
Eigenvector centrality is obtained from a Perron-Frobenius eigenvector (i.e. of the largest eigenvalue) of the adjacency matrix of a connected graph. This eigenvector equals the Perron-Frobenius eigenvector of the quotient network with constant values on orbits (Methods), and hence the computation (quadratic time by power iteration) can be reduced by $\tilde{n}^2$ (see Fig. 4).

Discussion
We have presented a general theory to describe and quantify real-world network symmetry and its effects on arbitrary network measures, and explained how this can be exploited in practice in a number of ways.

We show that the amount of network symmetry is amplified in a network measure but can be easily manipulated using the quotient network. We can for instance eliminate the symmetry-induced redundancies, or use them to simplify the calculation by avoiding unnecessary computations. Symmetry has also a profound effect on the spectrum, explaining the characteristic ‘peaks’ observed in the spectral densities of empirical networks, and occurring at values we are able to predict.

We describe how to effectively compute and manipulate the network symmetry of a (possibly very large) empirical network and, for the large but sparse graphs typically found in applications, we show that the symmetry computation is extremely fast, making it an inexpensive pre-processing step.

Our framework is very general and apply to any pairwise or vertex-based network measure beyond the ones we discuss as examples. We emphasise practical and algorithmic aspects throughout, present the results in an accessible way with minimal references to the abstract material in graph and group theory which often obscures its relevance in applications, and provide pseudocode (Methods) and full implementations for rapid dissemination.

Since network models are ubiquitous in the Applied Sciences, and typically contain a large degree of structural redundancy, our results are not only significant, but widely applicable, and relevant to any network practitioner.
Methods
We include minimal details for reproducibility but encourage the reader to consult an extended version in the Supporting Information (SI).

Geometric decomposition
We write $\text{Aut}(\mathcal{G})$ for the automorphism group of an (unweighted, undirected, possibly very large) network $\mathcal{G} = (V, E)$ (see the SI for a discussion of directed and weighted networks). The symmetry results depend on the so-called geometric decomposition[10] of $\text{Aut}(\mathcal{G})$. Each automorphism (symmetry) $\sigma \in \text{Aut}(\mathcal{G})$ is a permutation of the vertices and its support is the set of vertices moved by $\sigma$,

$$\text{supp}(\sigma) = \{i \in V \text{ such that } \sigma(i) \neq i\}. \tag{8}$$

Two automorphisms $\sigma$ and $\tau$ are support-disjoint if the intersection of their supports is empty, $\text{supp}(\sigma) \cap \text{supp}(\tau) = \emptyset$. The orbit of a vertex $i$ is the set of vertices to which $i$ can be moved to by an automorphism, that is,

$$\{\sigma(i) \text{ such that } \sigma \in \text{Aut}(\mathcal{G})\}. \tag{9}$$

A symmetric motif is made of one or more orbits of structurally equivalent vertices. If all the orbits have the same size $k$ and every permutation of the vertices in each orbit is a network automorphism, we call the symmetric motif basic (or BSM) of type $k$. If it is not basic, we call it complex or of type 0.

Network symmetry computation
First, we compute a list of generators of the automorphism group from an edge list (we use saucy3[33]). Then, we partition the set of generators $X$ into support-disjoint classes $X = X_1 \cup \ldots \cup X_m$, that is, $\sigma$ and $\tau$ are support-disjoint whenever $\sigma \in X_i$, $\tau \in X_j$ and $i \neq j$. To find the finest such partition, we use a bipartite graph representation of vertices $V$ and generators $X$. Namely, let $\mathcal{G}$ be the graph with vertex set $V \cup X$ and edges between $i$ and $\sigma$ whenever $i \in \text{supp}(\sigma)$. Then $X_1, \ldots, X_m$ are the connected components of $\mathcal{G}$ (as vertex sets intersected with $X$). Each $X_i$ corresponds to the vertex set $M_i$ of a symmetric motif $\mathcal{M}_i$, as $M_i = \bigcup_{\sigma \in X_i} \text{supp}(\sigma)$. Finally, we use GAP[36] to compute the orbits and type of each symmetric motif (Alg. 1). Full implementations of all the procedures outlined above are available at a public repository[34].

**Algorithm 1:** Orbits and type of a symmetric motif.

```
Input: X a set of permutations of a symmetric motif
Output: O1,...,Ok orbits, and type m, of the symmetric motif
H ← Group(X)
{O1,...,Ok} ← Orbits(H)
m ← min(size(O1),...,size(Ok))
if m = max(size(O1),...,size(Ok)) then
  for i ← 1 to k do
    if not IsNaturalSymmetricGroup(Act(H,Oi)) then
      m ← 0
    break
  end
else
  m ← 0
end
m = m

Structure of a BSM
Consider the network representation $F(\mathcal{G})$ of a (pairwise) structural network measure $F$ applied to a network $\mathcal{G}$. The structure of the BSMs in $F(\mathcal{G})$, depicted in Fig. 2, is formally described below.

**Theorem 1.** Let $M$ be the vertex set of a BSM of a network $\mathcal{G}$, and $F$ a structural network measure. Then the graph induced by $M$ in $F(\mathcal{G})$ is a BSM of $F(\mathcal{G})$, and satisfies:

(i) for each orbit $\Delta = \{v_1, \ldots, v_\ell\}$, there are constants $\alpha$ and $\beta$ such that the orbit internal connectivity is given by $\alpha = F(v_i, v_j)$ for all $i \neq j$ and $\beta = F(v_i, v_i)$ for all $i$;

(ii) for every pair of orbits $\Delta_1$ and $\Delta_2$, there is a labelling $\Delta_1 = \{v_1, \ldots, v_\ell\}$, $\Delta_2 = \{w_1, \ldots, w_\ell\}$ and constants $\gamma_1$, $\gamma_2$, $\delta_1$, $\delta_2$ such that $\gamma_1 = F(v_i, w_j)$, $\gamma_2 = F(w_j, v_i)$, $\delta_1 = F(v_i, v_i)$, and $\delta_2 = F(w_j, w_j)$ for all $i \neq j$.

The proof is a generalisation of the argument on [37, p.48] to weighted directed graphs with symmetries, and can be found in the SI. If $\mathcal{G}$ is undirected and $F$ is symmetric, then $\gamma_1 = \gamma_2$ and $\delta_1 = \delta_2$ and each orbit is a $(\alpha, \beta)$-uniform graph $K_{\alpha, \beta}$ and each pair of orbits form a $(\gamma, \delta)$-uniform join (Fig. 2). Formally, a $(\alpha, \beta)$-uniform graph, $K_{\alpha, \beta}$ is the graph with adjacency matrix

$$A_{\alpha, \beta} = \alpha C_n + \beta I_n \tag{10}$$

where $C_n$ is the adjacency matrix of a complete graph (0 diagonal and 1 off-diagonal entries), and $I_n$ the identity matrix. A $(\gamma, \delta)$-uniform join of two uniform graphs $K_{\alpha_1, \beta_1}$ and $K_{\alpha_2, \beta_2}$ is the graph with adjacency matrix, possibly after a suitable reordering of the vertices,

$$A = \left( \frac{A_{\alpha_1, \beta_1}}{A_{\alpha_2, \beta_2}} \frac{A_{\gamma_1}}{A_{\gamma_2}} \right) \tag{11}$$

where the submatrices are given as per (10).

Quotient network
If $A$ is the $n \times n$ adjacency matrix of a graph $\mathcal{G}$, the quotient network with respect to a partition of the vertex set $V = V_1 \cup \ldots \cup V_m$ is the graph $\mathcal{Q}$ with $m \times m$ adjacency matrix the quotient matrix $Q(A) = (q_{ij})$ defined by

$$q_{ij} = \frac{1}{|V_i|} \sum_{j \in V_i} a_{ij} \tag{12}$$

the average connectivity from a vertex in $V_i$ to vertices in $V_j$. There is an explicit matrix equation for the quotient. Consider the $n \times m$ characteristic matrix $\mathcal{S}$ of the partition, that is, $[\mathcal{S}]_{ik} = 1$ if $i \in V_k$, and zero otherwise, and the diagonal matrix $\Lambda = \text{diag}(n_1, \ldots, n_m)$, where $n_k = |V_k|$. Then

$$Q(A) = \Lambda^{-1} \mathcal{S}^T \mathcal{A} \mathcal{S} \tag{13}$$

The quotient network is a directed and weighted network in general. If we remove weights, directions and self-loops, we have the quotient skeleton as in Fig. 1. In the context of quotient networks, we call $\mathcal{G}$ the parent network of $\mathcal{Q}$. From now on, we will only refer to the quotient with respect to the partition of the vertex set into orbits. This quotient removes all the symmetries from the network: if $\sigma(i) = j$, then $i$ and $j$ are in the same orbit and hence represented by the same vertex in the quotient network, which is then fixed by $\sigma$. We can, therefore, infer and quantify properties arising from redundancy alone by comparing a network with its quotient.

Average compression
We can eliminate the symmetry-induced redundancy (Alg. 2) and recover (Alg. 3) all but the internal symmetric motif connectivity, which is replaced by the average connectivity, as the next result guarantees (proof in the SI).

**Theorem 2.** Let $A = (a_{ij})$ be the $n \times n$ adjacency matrix of a (possibly directed and weighted) network with vertex set $V$. Let $S$ be the $n \times n$ characteristic matrix of the partition of $V$ into orbits of the automorphism group of the network, and $\Lambda$ the diagonal matrix of column sums of $S$. Define $B = S^T A S$ and $A_{\text{avg}} = R B R^T = (\bar{a}_{ij})$ where $R = S \Lambda^{-1}$. Then,

(i) if $i, j \in V$ belong to different symmetric motifs, $\bar{a}_{ij} = a_{ij}$,

(ii) if $i, j \in V$ belong to orbits $i \in \Delta_1$ and $j \in \Delta_2$ in the same symmetric motif,

$$\bar{a}_{ij} = \frac{1}{|\Delta_1|} \frac{1}{|\Delta_2|} \sum_{v \in \Delta_1} a_{iv} \tag{14}$$

Lossless compression
Pseudocode for lossless compression and recovery based on the basic quotient are shown below (Algorithms 4 and 5), and MATLAB implementations for BSMs up to two orbits are available at a public repository[34].
**Input:** adjacency matrix $A$, characteristic matrix $S$
**Output:** quotient matrix $B$

$B \leftarrow S^{-1}AS$

**Algorithm 2:** Average symmetry compression.

**Input:** quotient matrix $B$, characteristic matrix $S$
**Output:** adjacency matrix $A_{sym}$

$A_{sym} \leftarrow \text{diag}(\text{sum}(S))$

$R \leftarrow SA^{-1}$

$A_{sym} \leftarrow RBR^T$

**Algorithm 3:** Average symmetry decompression.

**Input:** adjacency matrix $A$, characteristic matrix for the basic quotient $S$, list of BSM motifs
**Output:** quotient matrix $B$, annotation structure $a$

$B \leftarrow S^{-1}AS$

extract orbits from $S$

foreach orb in orbits do

$\beta \leftarrow A_{sym}(\text{rep}, \text{rep})$

store $\beta$ in annotation structure $a$

end

$k_{max} \leftarrow \min(\text{size}(\text{motifs}))$, maximal number of orbits in a motif

for $k \leftarrow 2 \text{ to } k_{max}$ do

extract $k$-BSM (list of BSMs with $k$ orbits) from motifs

foreach pairs of distinct orbits $V_1, V_2$ in bsm do

compute $\delta$ and permutation of $V_2$ perm such that $A(k, \text{perm}(k)) = \delta$ for all $k \in V_1$

store orbit numbers (with respect to $S$), $\delta$ and perm in annotation structure $a$

end

end

**Algorithm 4:** Lossless symmetry compression.

**Spectral decomposition**

If $B$ is the quotient matrix of the adjacency matrix $A$ with respect to the orbit partition, and $S$ is the characteristic matrix of the partition, then $AS = SB$. This immediately implies that if $(\lambda, v)$ is an $B$-eigenpair, then $(\lambda, Sv)$ is an $A$-eigenpair. In particular, $A$ has an eigenbasis of the form $\{Sv_1, \ldots, Sv_n, w_1, \ldots, w_{n-m}\}$, where $\{v_1, \ldots, v_n\}$ is any eigenbasis of $B$. Moreover, the eigenvectors $w_1, \ldots, w_{n-m}$ can be chosen localised to symmetric motifs, by the result below. (For proofs and more details, see the SI)

We call an eigenvector $w$ (and its eigenvalue $\lambda$) redundant if the sum of the entries of $w$ on each orbit is zero.

**Theorem 3.** Let $\mathcal{M}$ be a symmetric motif of a (possibly weighted) undirected graph $G$. If $(\lambda, w)$ is a redundant eigenpair of $\mathcal{M}$, then $(\lambda, w)$ is a eigenpair of $G$, where $\mathcal{M}$ is equal to $w$ (on the vertices of) $\mathcal{M}$, and zero elsewhere.

**Reducant spectrum of BSMs**

We give more details of the computation of the redundant spectrum of BSMs up to two orbits (Table 2), with full proofs deferred to the SI. A BSM with one orbit is an $(\alpha, \beta)$-uniform graph $K_n^{\alpha, \beta}$ with adjacency matrix $A_n^{\alpha, \beta} = (a_{ij})$ given by $a_{ij} = \alpha$ and $a_{ii} = \beta$ for all $i \neq j$. Then $K_n^{\alpha, \beta}$ has eigenvalues $(n-1)(\alpha + \beta)$ (non-redundant), with multiplicity 1, and $-\alpha + \beta$ (redundant), with multiplicity $n-1$. The corresponding eigenvectors are $1$, the constant vector 1 (non-redundant), and $e_i$, the vectors with non-zero entries 1 at position $i$, and 0 at position $i$, $2 \leq i \leq n$ (redundant). For unweighted graphs without loops ($\beta = 0$, $\alpha \in \{0, 1\}$), we recover the redundant eigenvalues 0 and $-1$ predicted in $11$. A BSM with two orbits is a uniform join of the form $K_{\alpha_1, \beta_1} \phi_{\alpha_2, \beta_2}$ and its redundant spectrum is given below.

**Theorem 4.** The eigenvalues of a BSM with two orbits $K_{\alpha_1, \beta_1} \phi_{\alpha_2, \beta_2}$ are

$$
\lambda_1 = -b - cK_1 = \frac{-(a + b) + \sqrt{(a - b)^2 + 4(ac + 2b^2)}}{2} \quad (15)
$$

$$
\lambda_2 = -b - cK_2 = \frac{-(a + b) - \sqrt{(a - b)^2 + 4(ac + 2b^2)}}{2} \quad (16)
$$

where $K_1$ and $K_2$ are the two solutions of the quadratic equation $cK^2 + (b - a)K - c = 0$, $a = \alpha_1 - \beta_1$, $b = \alpha_2 - \beta_2$, and $c = \gamma - \delta \neq 0$.

For unweighted graphs without loops, we recover the redundant eigenvalues predicted in $11$, that is, $-2, -\varphi, -1, 0, \varphi - 1$ and 1, where $\varphi = \frac{1 + \sqrt{5}}{2}$, the golden ratio.

**Eigendecomposition algorithm**

We can compute the eigendecomposition of a weighted undirected network with symmetries (that is, a diagonalisation of its symmetric adjacency matrix $A = UDU^T$), such as $F(\mathcal{M})$, from the quotient and the symmetric motifs. Algorithm 6 computes the eigendecomposition of the quotient matrix, then, for each motif, the redundant eigenvectors. A MATLAB implementation is available at $34$.

In Alg. 6, we first compute the spectral decomposition $e_\mathcal{M}$ of the symmetric quotient $B_{\mathcal{M}} = \Lambda^{-1/2}S\Lambda^{-1/2}A_{\mathcal{M}}$ where $\Lambda$ is the diagonal matrix of the orbit sizes (which can be obtained as the column sums of $S$). This matrix is symmetric and has the same eigenvalues as the left quotient. Moreover, if $B_{\mathcal{M}} = U_{\mathcal{M}}D_{\mathcal{M}}U_{\mathcal{M}}^{-1}$ then the left quotient eigenvectors are the columns of $\Lambda U_{\mathcal{M}}$. These become, in turn, eigenvectors of $A$ by repeating their values on each orbit, we can be obtained mathematically by left multiplying by the characteristic matrix $S$. Then, for each motif, we compute the redundant eigenvectors using a null space matrix (see below), storing eigenvalues and localised (zero outside the motif) eigenvectors.

Only redundant eigenvectors of a symmetric motif (that is, those which add up to zero on each orbit) become eigenvectors of $A$ by extending them as zero outside the symmetric motif (Theorem 3). Therefore, we need to construct redundant eigenvectors from the output of $e_\mathcal{M}$ on each motif (the spectral decomposition of the corresponding submatrix). If $U_{\mathcal{M}} = (v_1 | \ldots | v_k)$ are $\lambda$-eigenvectors of a symmetric motif with characteristic matrix of the orbit partition $S_{\mathcal{M}}$, we need to find linear combinations such that

$$
S_{\mathcal{M}}(\alpha_1 v_1 + \ldots + \alpha_k v_k) = 0 \iff S_{\mathcal{M}}U_{\mathcal{M}} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_k \end{pmatrix} = 0 \quad (17)
$$
We define the which implies exact recovery for external edges, and average recovery for \( f \) where
\[
B_{\text{sym}} = \left(A^{-1/2} S^T A S A^{-1/2}\right).
\]

\[U_q, D_q, U_y \leftarrow \text{eig}(B_{\text{sym}}) \text{ so that } B_{\text{sym}} = U_q D_q U_y^{-1}
\]

\[
U_y \leftarrow \text{null}(S_m U_q),
\]

\[
D \leftarrow \text{diag}(\text{null}(S_m U_q)),
\]

for each motif do
\[
\begin{align*}
A_{nm} & \leftarrow A(\text{motif}, \text{motif}) \\
S_m & \leftarrow S(\text{motif}, \text{orbits}) \\
[U_{nm}, D_{nm}] & \leftarrow \text{eig}((A_{nm}))
\end{align*}
\]

\[
\text{end}
\]

\[\text{for } \lambda \in \text{unique}((\text{diag}(D_{nm}))) \text{ do}
\]

\[
\begin{align*}
U_\lambda & \leftarrow \lambda-\text{eigenvectors from } A_{nm} \\
Z & \leftarrow \text{null}((S_m U_\lambda)/\lambda) \\
d & \leftarrow \text{null}(Z)
\end{align*}
\]

\[
\text{if } d > 0 \text{ then} \quad \text{store } U_\lambda Z \text{ in } U \\
\text{store } \lambda \text{ in } D \text{ with multiplicity } d
\]

\[\text{end}
\]

\[\text{end}
\]

\[\text{Algorithm 6: Eigendecomposition algorithm.}
\]

Therefore, if the matrix \( Z \neq 0 \) represents the null space of \( S_m U_\lambda \), that is, \( S_m U_\lambda Z = 0 \) and \( Z^T Z = 0 \), then the columns of \( U_\lambda Z \) are precisely the redundant eigenvectors. This is implemented in Alg. 6 within the innermost for loop.

**Vertex measures**

As a vertex measure \( G \) is constant on orbits, we only need to store one value per orbit. Let \( S \) be the characteristic matrix of the partition of the vertex set into orbits, and \( A \) the diagonal matrix of orbit sizes (column sums of \( S \)). If \( G \) is represented by a vector \( v = G(i) \) of length \( n_G \), we can store one value per orbit by taking \( w = \Lambda^{-1/2} S^T v \), a vector of length \( n_G \). We recover \( v = S^T w \), as the next result guarantees.

**Theorem 5.** If \( v \) is a vector of length \( n_G \) that is constant on orbits, then
\[
SA^{-1/2} S^Tv = v.
\]

**Communicability**

Let \( f \) be a real analytic function within radius of convergence \( R \) around 0,
\[
f(x) = \sum_{k=0}^\infty a_k x^k \quad |x| < R.
\]

We define the \( f \)-communicability matrix of a network with adjacency matrix \( A \) as
\[
f(A) = \sum_{k=0}^\infty a_k A^k \quad \text{if } \|A\| < R,
\]

where \( \| \cdot \| \) is a given matrix norm, and the power series convergence is with respect to that norm. We represent communicability as a network \( f(A) \) with adjacency matrix \( A(A) \). If we write \( Q(A) \) for the quotient of a matrix \( A \), communicability satisfies
\[
f(Q(A)) = f(Q(A)),
\]

which implies exact recovery for external edges, and average recovery for internal edges. (This holds for any network measure with this property.) For exact recovery, we can use the spectrum eigendecomposition, as \( A = UDU^T \) implies \( f(A) = Uf(D)U^T \).

The \( f \)-communicability network has eigenvalues \( f(\lambda) \), where \( \lambda \) is an eigenvalue of the original network, and same eigenvectors \( A \nu = \lambda \nu \) implies \( f(A)\nu = f(\lambda)\nu \). In particular, for undirected, unweighted networks, we predict high-multiplicity eigenvalues due to symmetry at \( f(-2), f(-\phi), f(-1), f(0), f(\phi - 1) \) and \( f(1) \).

**Shortest path distance**

Let \( A = (a_{ij}) \) be the adjacency matrix of an unweighted network \( G \). A path of length \( n \) is a sequence \((v_1, v_2, \ldots, v_{n+1})\) of distinct vertices, except possibly \( v_1 = v_{n+1} \), such that \( v_i \) is connected to \( v_{i+1} \) for all \( 1 \leq i \leq n - 1 \). The shortest path distance \( d^G(u, v) \) is the length of the shortest (minimal length) path from \( u \) to \( v \). A path \( p \) is a shortest path if it is of minimal length between its endpoints. The following result contains the claims in the Results section.

**Theorem 6.** Let \( A = (a_{ij}) \) be as above. Then
\[ (i) \text{ if } (v_1, v_2, \ldots, v_n) \text{ is a shortest path from } v_1 \text{ to } v_n \text{ and } \sigma \in \text{Aut}(G) \text{, then } (\sigma(v_1), \sigma(v_2), \ldots, \sigma(v_n)) \text{ is a shortest path from } \sigma(v_1) \text{ to } \sigma(v_n); \]
\[ (ii) \text{ if } (v_1, v_2, \ldots, v_n) \text{ is a shortest path from } v_1 \text{ to } v_n \text{ and } v_1 \text{ and } v_{n+1} \text{ belong to different symmetric motifs, then } v_i \text{ and } v_{i+1} \text{ belong to different orbits, for all } 1 \leq i \leq n - 1; \]
\[ (iii) \text{ if } u \text{ and } v \text{ belong to orbits } \Delta \text{, respectively } \Delta', \text{ in different symmetric motifs, then the distance from } u \text{ to } v \text{ in } G \text{ equals the distance from } \Delta \text{ to } \Delta' \text{ in the skeleton quotient } Q. \]

These statements mean that (i) automorphisms preserve shortest paths and their lengths; (ii) shortest paths do not contain intra-orbit edges; and (iii) we can compute the shortest path distance between points in different symmetric motifs from the quotient.

**Laplacian matrix**

The Laplacian matrix of a network \( G \) is a sparse network measure. Its network representation is the graph \( G' \) with adjacency matrix \( L = D - A \). The symmetric motifs in \( G' \) are identical to those in \( G \), except that all edges are weighted by \(-1\), and all vertices have self-loops weighted by their degrees in \( G \). (Note that the motif structure depends on the how it is embedded in the network.) Define the external degree of a vertex as the number of adjacent vertices outside the motif it belongs to.

**Theorem 7.** Let \( M \) be the vertex set of a symmetric motif \( \mathcal{M} \) in a graph \( \mathcal{G} \). Then \( M \) induces a symmetric motif in the Laplacian network \( G' \) with adjacency matrix
\[
L_{\mathcal{M}} = (d_1 I_m \oplus \ldots \oplus d_n I_m),
\]

where \( L_{\mathcal{M}} \) is the ordinary Laplacian matrix of \( \mathcal{M} \) considered as a graph on its own, and \( d_1, \ldots, d_n \) are the external degrees of the \( k \) orbits of \( \mathcal{M} \) of sizes \( m_1, \ldots, m_k \). (Here \( I_m \) is the identity matrix of size \( n \) and we use \( \oplus \) to construct a block diagonal matrix.)

For a motif \( \mathcal{M} \) with one orbit, the matrix \( (21) \) is the Laplacian of the motif translated by a multiple of the identity. In particular, the redundant eigenvalues of a BSM with one orbit are the redundant Laplacian eigenvalues of an empty or complete graph of size \( n \) plus the external degree \( d \), that is, \( d \), respectively \( d + n \). Therefore, we expect high-multiplicity eigenvalues due to symmetry in the Laplacian spectral density at (small) positive integers, which indeed agrees what we observed in our test networks (Fig.5). Additionally, the spectral decomposition applies, so Alg. 6 provides an efficient way of computing the Laplacian eigendecomposition with an expected \( sp = h^3 \_d \) (Table 1) computational time reduction.

**Closeness centrality**

The closeness centrality of a node \( i \) in a graph \( G \), \( cc^G(i) \), is the average shortest path length to every node in the graph. As symmetries preserve distances, they also preserve closeness centrality, and therefore it is constant on orbits, as expected. Moreover, closeness centrality can be recovered from the quotient (shortest paths does not contain intra-orbit edges between vertices in different symmetric motifs by Theorem 6(ii)), as
\[
cc^G(i) = \sum_{j \neq i} n_j d_{ij}^{-2} (V_k, V_l) + \frac{n_i d_i}{n_k}
\]

if \( i \) belongs to the orbit \( V_k \) and \( d_i \) is the average intra-motif distance, that is, the average distances of a vertex in \( V_k \) to every vertex in \( \mathcal{M} \), the motif containing \( V_k \). By annotating each orbit by \( d_i \), we can recover betweenness centrality exactly. Alternatively, as \( d_i \ll n \) (note that \( d_i \ll m \) if \( \mathcal{M} \) has \( m \) orbits), we can approximate \( cc^G(i) \) by the first summand, or simply by the quotient centrality \( cc^G(V_k) \).

9/22
Eigenvector centrality

Since the Perron-Frobenius eigenvalue is simple, it cannot be a redundant eigenvalue. Hence it is a quotient eigenvalue and, as those are a subset of the parent eigenvalues, it must still be the largest (hence the Perron-Frobenius) eigenvalue of the quotient. Its eigenvector can then be lifted to the parent network by repeating entries on orbits. All in all, if \((\lambda, \nu)\) is the Perron-Frobenius eigenpair of the quotient, then \((\lambda, S\nu)\) is the Perron-Frobenius eigenpair of the parent network. In practice, we use the symmetric quotient \(B_{\text{sym}} = \Lambda^{-1/2} S^T A S A^{-1/2}\) for numerical reasons (Alg. 7), obtaining the computational time reductions reported in Fig. 4. If \(A\) is not symmetric (but irreducible), Algorithm 7 gives the right Perron-Frobenius eigenpair of \(A\), and replacing \(B_{\text{sym}}\) by \(\Lambda^{-1/2} S^T A S A^{-1/2}\) and \(Rw\) by its transpose, we obtain the left Perron-Frobenius eigenpair of \(A\).

**Algorithm 7:** Eigenvector centrality from the quotient network.

**Input:** adjacency matrix \(A\), characteristic matrix \(S\)

**Output:** (right) Perron-Frobenius eigenpair \((\lambda, \nu)\) of \(A\)

\[
\begin{align*}
A & \leftarrow \text{diag}(\text{sum}(S)) \\
R & \leftarrow \Lambda^{-1/2} \\
B_{\text{sym}} & \leftarrow R^T A R \\
(\lambda, w) & \leftarrow \text{eig}(B_{\text{sym}}, 1) \text{ eigenpair of the largest eigenvalue} \\
\nu & \leftarrow Rw
\end{align*}
\]

Acknowledgements

Special thanks to Ben MacArthur for support and advice during the writing of this article. The Newton Institute in Cambridge supported the author during this article. The Newton Institute in Cambridge supported the author during the writing of this article. The Newton Institute in Cambridge supported the author during the writing of this article. The Newton Institute in Cambridge supported the author during the writing of this article. The Newton Institute in Cambridge supported the author during the writing of this article. The Newton Institute in Cambridge supported the author during the writing of this article. The Newton Institute in Cambridge supported the author during the writing of this article.

References

1. Newman, M. Networks: An Introduction. *Oxf. Univ. Press.* (2010).
2. Watts, D. & Strogatz, S. Collective dynamics of small-world networks. *Nature* **393**, 440–442 (1998).
3. Barabási, A.-L. & Albert, R. Emergence of scaling in random networks. *Science* **286**, 509–512 (1999).
4. Milo, R. *et al.* Network motifs: simple building blocks of complex networks. *Science* **298**, 824–827 (2002).
5. Tononi, G., Sporns, O. & Edelman, G. M. Measures of degeneracy and redundancy in biological networks. *Proc Natl Acad Sci USA* **96**, 3257–3262 (1999).
6. Albert, R. & Barabási, A.-L. Statistical mechanics of complex networks. *Rev Mod Phys* **74**, 47 (2002).
7. Chung, F., Lu, L., Dewey, T. G. & Galas, D. J. Duplication models for biological networks. *J Comput Biol* **10**, 677–687 (2003).
8. Xiao, Y., Xiong, M., Wang, W. & Wang, H. Emergence of symmetry in complex networks. *Phys Rev E* **77**, 061108 (2008).
9. Nishikawa, T. & Motter, A. E. Network-complement transitions, symmetries, and cluster synchronization. *Chaos* **26**, 094818 (2016).
10. MacArthur, B. D., Sánchez-García, R. J. & Anderson, J. W. Symmetry in complex networks. *Discrete Appl Math* **156**, 3525–3531 (2008).
11. MacArthur, B. D. & Sánchez-García, R. J. Spectral characteristics of network redundancy. *Phys Rev E* **80**, 026117 (2009).
12. Nicosia, V., Valencia, M., Chavez, M., Díaz-Guilera, A. & Latora, V. Remote synchronization reveals network symmetries and functional modules. *Phys Rev Lett* **110**, 174102 (2013).
13. Pecora, L. M., Sorrentino, F., Hagerstrom, A. M., Murphy, T. E. & Roy, R. Cluster synchronization and isolated desynchronization in complex networks with symmetries. *Nat Commun* **5**, 4079 (2014).
14. Sorrentino, F., Pecora, L. M., Hagerstrom, A. M., Murphy, T. E. & Roy, R. Complete characterization of the stability of cluster synchronization in complex dynamical networks. *Sci Adv* **2**, e1501737 (2016).
15. Schaub, M. T. *et al.* Graph partitions and cluster synchronization in networks of oscillators. *Chaos: An Interdiscip. J. Nonlinear Sci.* **26**, 094821 (2016).
16. Pecora, L. M., Sorrentino, F., Hagerstrom, A. M., Murphy, T. E. & Roy, R. Discovering, constructing, and analyzing synchronous clusters of oscillators in a complex network using symmetries. In *Advances in Dynamics, Patterns, Cognition*, 145–160 (Springer, 2017).
17. Siddique, A. B., Pecora, L., Hart, J. D. & Sorrentino, F. Symmetry- and input-cluster synchronization in networks. *Phys. Rev. E* **97**, 042217 (2018).
18. Xiao, Y., MacArthur, B. D., Wang, H., Xiong, M. & Wang, W. Network quotients: Structural skeletons of complex systems. *Phys Rev E* **78**, 046102 (2008).
19. Xiao, Y., Wu, W., Pei, J., Wang, W. & He, Z. Efficiently indexing shortest paths by exploiting symmetry in graphs. In *Proceedings of the 12th International Conference on Extending Database Technology: Advances in Database Technology*, 493–504 (ACM, 2009).
20. Wang, J., Huang, Y., Wu, F.-X. & Pan, Y. Symmetry compression method for discovering network motifs. *IEEE/ACM Trans Comput Biol Bioinf* **9**, 1776–1789 (2012).
21. Karalus, S. & Krug, J. Symmetry-based coarse-graining of evolved dynamical networks. *Europhys Lett* **111**, 38003 (2015).
22. Nyberg, A., Gross, T. & Bassler, K. E. Mesoscopic structures and the laplacian spectra of random geometric graphs. *J Complex Networks* **3**, 543–551 (2015).
23. Do, A.-L., Höfener, J. & Gross, T. Engineering mesoscale structures with distinct dynamical implications. *New J Phys* **14**, 115022 (2012).
24. Biggs, N. *Algebraic graph theory* (Cambridge University Press, 1993).
25. Estrada, E. & Rodriguez-Velazquez, J. A. Subgraph centrality in complex networks. *Phys Rev E* **71**, 056103 (2005).
26. Internet topology network dataset – KONECT. http://konect.uni-koblenz.de/networks/ (2018).
27. A Network Graph for Human Diseases. http://exploring-data.com/info/human-disease-network/ (2018).
28. Yeast Interactome Project. http://interactome.dfci.harvard.edu/S_cerevisiae/ (2018).
29. Human Protein Reference Database, *Release9_062910*. http://www.hprd.org/ (2018).
30. Estrada, E. & Hatano, N. Communicability in complex networks. *Phys Rev E* **77**, 036111 (2008).
31. Lovász, L. Random Walks on Graphs: A Survey (1993).
32. Klein, D. J. & Randić, M. Resistance distance. *J Math Chem* **12**, 81–95 (1993).
33. Brandes, U. A faster algorithm for betweenness centrality. *J Math Sociol* **25**, 163–177 (2001).
34. Bitbucket repository. https://bitbucket.org/rubenjsanchezgarcia/networksymmetry/ (2018).
35. saucy 3.0. http://vlscad.eecs.umich.edu/SAUCY/ (2012).
36. The GAP Group. GAP – Groups, Algorithms, and Programming, Version 4.8.7 (2017).
37. Liebeck, M. W. Graphs whose full automorphism group is a symmetric group. *J Aust Math Soc* **44**, 46–63 (1988).
38. Horn, R. A. & Johnson, C. R. *Matrix analysis* (Cambridge University Press, 1990).
39. Godsil, C. & Royle, G. *Algebraic graph theory* (Springer, 2013).
40. Cvetkovic, D. M., Rowlinson, P. & Simic, S. *An introduction to the theory of graph spectra* (Cambridge University Press, 2010).
41. Brouwer, A. E. & Haemers, W. H. *Spectra of graphs* (Springer, 2011).
We have kept the content as self-contained as possible, by including details on Piperno, A. Search space contraction in canonical labeling of graphs. Congr Numer 30, 45–87 (1981).

Gal, E. et al. Rich cell-type-specific network topology in neocortical microrcuitry. Nat Neurosci 20, 1004 (2017).

McKay, B. D. & Piperno, A. Practical graph isomorphism. II. J Symb Comput 60, 94–112 (2014).

Piperno, A. Search space contraction in canonical labeling of graphs. arXiv preprint arXiv:0804.4881 (2008).

Junttila, T. & Kaski, P. Engineering an efficient canonical labeling tool for large and sparse graphs. In 2007 Proceedings of the Ninth Workshop on Algorithm Engineering and Experiments, 135–149 (SIAM, 2007).

Darga, P. T., Sakallah, K. A. & Markov, I. L. Faster symmetry discovery using sparsity of symmetries. In Design Automation Conference, 2008 (45th ACM/IEEE), 149–154 (IEEE, 2008).

de la Peña, J. A., Gutman, I. & Rada, J. Estimating the estrada index. Linear Algebra Appl 427, 70–76 (2007).

Higham, N. J. & Al-Mohy, A. H. Computing matrix functions. Acta Numer 19, 159 (2010).

Supporting Information

This Supporting Information provides additional details, including full mathematical proofs, of the statements in the Main Text (Results and Methods). It is organised into sections of the same headings as in the Main Text, to which they correspond. We assume the terminology and notation in the Main Text.

Related Work

We have kept the content as self-contained as possible, by including details on material relatively well known in the graph theoretic literature, but perhaps not so for an applied audience. The automorphism group of a graph is well studied in algebraic and spectral graph theory, and the concepts of equitable partitions, characteristic matrix and quotient graph can be found in e.g. 30, 39, 40, including the relation between quotient and parent eigenvalues, and the main ingredients of the spectral decomposition for binary graphs [40, Remark 3.9.6]. More recently, Francis et al. [32, 42] have developed a general theory of equitable decompositions for automorphism compatible matrices. The geometric decomposition and symmetric motifs were originally defined in 10, and the redundant spectrum and spectral decomposition in 11, in both cases for binary adjacency matrices only.

Following the seminal work of MacArthur et al. 30, 11, symmetry has been used in empirical networks, for instance to study the quotient as a coarse graining tool real-world networks 20, detect symmetric motifs via symmetry compression 20, and reduce shortest path query computations 19. The redundant Laplacian spectrum has been explored for regular degree 21 and random geometric graphs 22, and the dynamical implications of eigenvector localisation analysed 23. A key motivation of this article has been to develop the most general common framework for these (and other) results.

SI Symmetry in Complex Networks

On Labels and Symmetries

A network is a combinatorial object which encodes pairwise relations (edges or links) between objects (vertices or nodes). It is therefore independent of the ordering, or labelling, of the vertices. An ordering is needed to refer to, and work with, a network. We can choose an ordering simply by enumerating the vertices 1 to \( n = |V| \). Such ordering is needed, for example, to define the adjacency matrix. Note that a different ordering results in a (possibly) different adjacency matrix of the same network. We always assume a chosen, and thereafter fixed, labelling 1 to \( n = |V| \) of the vertices.

On the other hand, a symmetry, or automorphism, of a network is a permutation of the vertices preserving adjacency. It can also be thought of as a vertex relabelling, but one that results on the same adjacency matrix. (This is expressed mathematically by the condition \( AP = PA \), Eq. (1) in the Main Text.) Therefore, to find symmetries, we first fix an initial labelling of the vertices (and in particular an adjacency matrix), so we can unequivocally refer to the vertices, and then look for further relabelling preserving the adjacency matrix.

However, as a relabelling, a symmetry or automorphism \( \sigma \) produces the same graph, and, necessarily, vertices \( i \) and \( \sigma(i) \), or edges \( \{i,j\} \) and \( \{\sigma(i),\sigma(j)\} \), are indistinguishable from one another and therefore structurally equivalent. In particular, for a vertex, respectively pairwise, network measure depending on structure alone, we have \( G(i) = G(\sigma(i)) \), respectively \( F(i,j) = F(\sigma(i),\sigma(j)) \), for all \( \sigma \in \Aut(\mathcal{G}) \), and for all \( i,j \in V \), that is, Eqs. (5) and (3) in the Main Text.

Geometric Decomposition

We now explain the geometric decomposition introduced in Methods, in more detail, following MacArthur et al. 30. We start with some preliminary notions. Each automorphism \( \sigma \in \Aut(\mathcal{G}) \) is a permutation of the vertices of the graph, and automorphisms can be composed by applying one permutation after the other, forming a mathematical structure called a group 41. The support of the permutation \( \sigma \) is the set of vertices moved by \( \sigma \),

\[
\text{supp}(\sigma) = \{ i \in V \text{ such that } \sigma(i) \neq i \}.
\]

Two automorphisms \( \sigma \) and \( \tau \) are support-disjoint if the intersection of their supports is empty, \( \text{supp}(\sigma) \cap \text{supp}(\tau) = \emptyset \). In particular, \( \sigma \) and \( \tau \) commute, that is, the order in which they are applied does not affect the result, mathematically \( \sigma \tau = \tau \sigma \). Similarly, two arbitrary subsets of automorphisms \( S, T \subset \Aut(\mathcal{G}) \) are support-disjoint if \( \sigma \in S \) and \( \tau \) are support-disjoint for every pair \( \sigma \in S \text{ and } \tau \in T \).

The geometric decomposition is obtained by partitioning a set of generators \( \mathcal{G} = \{ \sigma_1, \ldots, \sigma_k \} \subset \Aut(\mathcal{G}) \) (that is, every automorphism \( \sigma \in \Aut(\mathcal{G}) \) is the product, or composition, of elements in \( \mathcal{G} \)), which the additional property of being essential (explained below), into pairwise support-disjoint subsets

\[
\mathcal{G} = \{ \sigma_1 \} \cup \cdots \cup \sigma_k
\]

(How to obtain in practice an essential set of generators, and the support-disjoint partition, is explained in the Network Symmetry Computation section below). Let us call \( M_i \) the set of vertices moved by generators in \( \mathcal{G}_i \), that is,

\[
M_i = \{ i \in V \text{ such that } \sigma(i) \neq i \text{ for some } \sigma \in \mathcal{G}_i \} = \bigcup_{\sigma \in \mathcal{G}_i} \text{supp}(\sigma),
\]

and \( \mathcal{M} \) the subgraph induced by \( M_i \) (that is, the graph with vertex set \( M_i \) and all edges in \( \mathcal{G} \) between vertices in \( M_i \)). Further, define \( H_i = \{ X_i \} \), the subgroup generated by \( X_i \) (that is, all the permutations obtained by composing elements in \( X_i \) and call it a geometric factor. The support-disjoint decomposition of \( X \), (24), gives a direct product decomposition of \( \Aut(\mathcal{G}) \) into geometric factors

\[
\Aut(\mathcal{G}) = H_1 \times \cdots \times H_k,
\]

called the geometric decomposition of \( \Aut(\mathcal{G}) \). In other words, every automorphism \( \sigma \in \Aut(\mathcal{G}) \) can be uniquely decomposed as a product (composition)

\[
\sigma = \tau_1 \tau_2 \cdots \tau_k \text{, } \quad \tau_i \in H_i = \{ X_i \},
\]

of permutations \( \tau_i \) of vertices of \( M_i \) only. Hence understanding the symmetries of each subgraph \( \mathcal{M}_i \), we recover all automorphisms of \( \mathcal{G} \). (Of course not every automorphism of \( \mathcal{M}_i \), considered as a graph on its own, is an automorphism of \( \mathcal{G} \), as it also depends on how \( \mathcal{M}_i \) is embedded in \( \mathcal{G} \).) The subgraphs \( \mathcal{M}_i \) are called symmetric motifs since they generate all the network symmetry. In real-world networks, symmetric motifs are typically small, however, as the network automorphisms consists on all possible combinations of these localised symmetries, their presence explains the large size, in absolute terms, of \( \Aut(\mathcal{G}) \) observed empirically (SI Table 3).

Proposition 1. The support-disjoint decomposition (24) implies the direct product decomposition (26).

11/22
We then have a partition of the vertex set

\[ M_0 = \{ i \in V \text{ such that } \sigma(i) = i \text{ for all } \sigma \in \text{Aut}(\mathcal{G}) \}. \]  

(28)

We have then a partition of the vertex set

\[ V = M_0 \cup M_1 \cup \ldots \cup M_k. \]  

(29)

That is, each network can be partitioned into an asymmetric core (the subgraph, typically connected, induced by the fixed vertices \( M_0 \)) and the symmetric motifs. The asymmetric core is related, but not equal, to the quotient (as a vertex set, the quotient equals the asymmetric core plus one vertex per orbit, see the Quotient Network section below).

Every symmetric motif can be further decomposed into one or more orbits of structurally equivalent vertices. The orbit of a vertex \( i \) is the set of vertices to which \( i \) can be moved by an automorphism, that is,

\[ \{ \sigma(i) \mid \sigma \in \text{Aut}(\mathcal{G}) \}. \]  

(30)

Every vertex belongs to an orbit (made of just the vertex itself if it is fixed) and if a symmetric motif contains a vertex in an orbit, then it must contain all the vertices in the orbit.

**Proposition 2.** If vertices \( i \) and \( j \) belong to the same orbit, then they also belong to the same symmetric motif.

**Proof.** We can assume \( i \neq j \). As they belong to the same orbit, there is an automorphism \( \sigma \) with \( \sigma(i) = j \). Write \( \sigma \) as a product of generators \( \sigma = x_1 \ldots x_l, x_l \in X \) and argue by induction on \( l \geq 1 \). If \( l = 1 \), then \( x_1(i) = j \) and \( i \neq j \) hence \( j \in \text{supp}(x_1) \). In addition, \( j \in \text{supp}(x_1) \): otherwise \( x_1(j) = j \) implies \( j = x_1^{-1}(j) = i \), a contradiction. As \( i, j \in \text{supp}(x_1) \), they are in the same symmetry motif, by (25). Suppose now \( l > 1 \) and the induction hypothesis. Write \( k = x_2 \ldots x_l(i) \) so that \( j = x_k(i) \). Assume \( j \neq k \) (otherwise remove \( x_1 \) so that \( j = x_2 \ldots x_l(i) \)). By the induction hypothesis, \( k \) and \( j \) belong to the same symmetric motif, and, by the same argument as in the case \( l = 1 \), \( j \neq k \) also belong to the same symmetric motif.

This proposition, implicit in\(^{10}\), proves that the vertices in each symmetric motif can be partitioned into orbits.

\[ M_i = V^{(1)}_i \cup \ldots \cup V^{(m_i)}_i. \]  

(31)

Note that any set of generators can be partitioned into support-disjoint subsets (24), and this gives the direct product decomposition (26) when \( H_i = \langle X_i \rangle \). However, this decomposition is not unique (a geometric factor could be further decomposed) and depends on the choice of generators (for example, adding a generator \( x_1 x_2 \) to \( X \), where \( x_1 \in X_1 \) and \( x_2 \in X_2 \) would force \( X' = X \cup X_2 \) and \( H'_2 = H_2 \times H_2 \), a coarser geometric decomposition). By requiring \( X \) to be essential (see below), the geometric decomposition (26) is unique (up to permutation of the factors \( H_i \)), and the finest possible (each \( H_i \) cannot be further decomposed into a direct product of non-trivial support-disjoint subgroups), see Proposition 2.1 in\(^{10}\). In particular, the geometric decomposition and symmetric motifs are well-defined.

A set of generators \( X \) is essential if \( (1) \) it does not contain the identity \( 1 \) (trivial permutation); \( (2) \) \( x \neq \emptyset \in X \) with \( x \) and \( h \) support-disjoint implies \( g = 1 \) or \( h = 1 \); and \( (3) \) if \( X \subset X \) generates \( H \times H \), \( H \) support-disjoint (as sets), then \( X' = X \cup X \) (necessarily support-disjoint) with \( X \) generating \( H \). Graph automorphism algorithms such as NAUTY produce essential sets of generators (Theorem 2.34 in\(^{35}\) and so does SAUCY, at least in practice (see the Network Symmetry Computation section below). Having said this, all the results in the Main Text are independent of whether the geometric decomposition is indeed the finest possible or not, and hence, any decomposition into a (possibly large) number of small symmetric motifs can be used to exploit network symmetry as explained in this article.

In real-world networks, symmetry is localised at small subgraphs (the symmetric motifs) and thus generated by low degree vertices. The universality of power-law degree distributions\(^{1} \) guarantees the abundance of such low degree vertices and justifies the large (in absolute terms) automorphism groups observed in real-world networks. Indeed, the authors in\(^{23} \) show how a Barabasi-Albert model reproduces the characteristic symmetry found in real-world networks. On the other hand, without a power-law degree distribution, we can find real-world networks with trivial automorphism group, such as the Blue Brain connectome\(^{46} \), which has hardly any low degree vertices (neurons). Even with a power-degree distribution, we found networks with relatively low symmetry, such as CaliforniaRoads, where only 4% of all the vertices participate in any symmetry (Table 1 in the Main Text).

**Basic Symmetric Motifs**

In theory, any finite group can be the automorphism group of a graph\(^{24} \). In real-world networks, however, \( \text{Aut}(\mathcal{G}) \) is the direct (occasionally, semidirect) product of symmetric groups\(^{10,10} \). Moreover, most symmetric motifs are made of orbits of the same size with the geometric factor realising every possible permutation of the vertices in each orbit. Formally, a symmetric motif \( \mathcal{M} \) is called basic if it consists of one or more orbits of \( n \) vertices, and the symmetric factor \( H \) is the symmetric group \( S_n \) realising all the \( n! \) permutations of each orbit. (We then call \( \mathcal{M} \) a basic symmetric motif of type \( n \).) Most (over 90%) of symmetric motifs in our test networks are basic (Table 1 in the Main Text), similar to the results in\(^{10} \).

Basic symmetric motifs (BSMs) have a very constrained structure:

- every orbit is a complete or an empty graph;
- each pair of orbits in the same symmetric motif can only be connected in one of four possible ways (each vertex in one orbit connected to either all, none, one, or \( n - 1 \) vertices in the other orbit);
- every vertex not in the symmetric motif joins either all or none of the vertices in an orbit, for each orbit.

(For a proof, see\(^{11} \), or the more general Theorem 9 below.) It is easy to show (or see Theorem 9) that the third property holds for any symmetric motif, basic or not. Also note that for a BSM with only two orbits, the ‘all-to-all’ or ‘none-to-none’ connectivity need not be considered, since in that case the orbits can be classified as two separate BSMs of one orbit each.

Non-basic symmetric motifs are called complex; they are rare in real-world networks and can be studied on a case-by-case basis. Typical complex symmetric motifs are branched trees (\( M_T \) in Fig. 1), among others\(^{10} \).

**Weighted and Directed Networks**

The adjacency matrix of a network can encode arbitrary weights and directions, as explained in the Main Text, making a general \( n \times n \) real matrix \( A \) the adjacency matrix of some (weighted, directed) network. The definition of automorphism group, geometric decomposition, geometric factor, symmetric motif and orbit, and their properties, as they are defined only in terms of \( A \), carry verbatim to arbitrarily weighted and directed networks. In this setting, a symmetry (automorphism), respects not only adjacency, but weights and directions. In particular, the automorphism group is smaller than (a subgroup of) the automorphism group of the underlying undirected, unweighted network. By introducing edge weights or directions, some symmetries will disappear, removing (and occasionally subdividing) geometric factors, symmetric motifs and orbits.

**Theorem 8.** Let \( A_w = (w_{ij}) \) be the adjacency matrix of an arbitrarily weighted and directed network \( \mathcal{G}_w \), and \( A = (a_{ij}) \) the adjacency matrix of the underlying undirected and unweighted network \( \mathcal{G} \), that is, \( a_{ij} = \text{sgn}(w_{ij} + |w_{ji}|) \). Consider the geometric decomposition

\[ \text{Aut}(\mathcal{G}) = H_1 \times \ldots \times H_m, \]

\[ \text{Aut}(\mathcal{G}_w) = H'_1 \times \ldots \times H'_m, \]

with symmetric motifs with vertex sets \( M_1, \ldots, M_M \), respectively \( M'_1, \ldots, M'_m \).

Then for every \( 1 \leq i \leq m' \) there is a unique \( 1 \leq j \leq m \) such that \( H'_j \leq H_i \) and, consequently, \( M'_j \leq M_i \). In other words, the geometric decomposition of \( \mathcal{G}_w \) is a refinement of that of \( \mathcal{G} \). Similarly, each vertex orbit in \( \mathcal{G}_w \) is a subset of a vertex orbit in \( \mathcal{G} \).
Table 3. Symmetry in some real-world networks (continued).

In addition to the summary statistics shown in Table 1 in the Main Text, here we report the size of the automorphism group to the closest power of 10 (aut), the number of BSMS with one, two, or more than two orbits (bsm1, bsm2, bsm3+), the average number of orbits per motif (opm) and vertices per orbit (vpo), and the proportion of vertices $g_{\text{basic}}^0$ and edges $g_{\text{basic}}^1$ in the basic quotient.

![Table 3. Symmetry in some real-world networks (continued).](image)

**Proof.** First, we show that if $\sigma$, $\tau$ are support-disjoint permutations, then $\sigma \cdot \tau$ is a support-disjoint permutation. Define $\sigma$ and $\tau$ such that

$$\sigma(i) = \sigma(j) \quad \text{and} \quad \tau(i) = \tau(j)$$

then $\sigma \cdot \tau(i) = \sigma((\tau(i)) = \sigma((\tau(j)) = \sigma(j)$ and $\tau((\sigma(j)) = \tau(j)$. Since $\sigma$ and $\tau$ are support-disjoint, $\sigma \cdot \tau$ is also support-disjoint.

**Theorem 9.** Let $M$ be the vertex set of a BSM of a network $G$ (that is, a symmetric motif made of one or more orbits of size $n$ with geometric factor the symmetric group $S_n$, realising all the permutation in each orbit), and $F$ a structural network measure. Then the graph induced by $M$ in $\overline{G}(\vartheta)$ is a BSM of $F(G)$, and satisfies:

(i) for each orbit $\Delta = \{v_1, \ldots, v_k\}$, there are constants $\alpha$ and $\beta$ such that the orbit internal connectivity is given by $F(v_1, v_1) = \alpha F(v_1, v_1)$ for all $i \neq j$ and $F(v_1, v_1) = \beta F(v_1, v_1)$ for all $i$; 

(ii) for every pair of orbits $\Delta_1$ and $\Delta_2$, there is a labelling $\lambda = \{v_1, \ldots, v_k\}$, $\Delta_1 = \{v_1, \ldots, v_k\}$ and constants $\gamma_1, \gamma_2, \delta_1, \delta_2$ such that $\gamma_i = F(v_i, v_i)$, $\gamma_j = F(v_j, v_j)$, $\delta_1 = F(v_1, v_2)$, $\delta_2 = F(v_1, v_2)$, $\delta_i = F(v_i, v_1)$ for all $i$; 

(iii) every vertex $v$ not in the BSM is joined uniformly to all the vertices in each orbit $\{v_1, \ldots, v_k\}$ in the BSM, that is, $F(v_1, v_1) = F(v_1, v_1)$ and $F(v_1, v_1) = F(v_1, v_1)$ for all $i$.

Moreover, property (iii) holds in general for any symmetric motif.

Note that, if $\vartheta$ is undirected and $F$ is symmetric, $\gamma_i = \gamma_j$ and $\delta_1 = \delta_2$, and, in the terminology of the Main Text, each orbit is a $(\alpha, \beta)$-uniform graph $G_{\text{BSM}}$, and each pair of orbits form a $(\gamma, \delta)$-uniform join, explaining Fig. 2 (a-b) in the Main Text. Also note that, for unweighted, undirected graphs without loops, we recover the statements in the previous section: every orbit is an empty or complete graph ($\beta = 0$, $\alpha = 0$), and every pair of orbits are joined in one of the four possible ways ($\gamma, \delta = 0, 1$).

**Proof of Theorem.** As $G(\vartheta)$ inherits all the symmetries of $G$, $M$ has the same orbit decomposition and the geometric factor is $S_n$ acting in the same way, hence $M$ induces a BSM in $F(G)$ too. For the internal connectivity, note that every permutation of the vertices $v_i$ is realisable. Thus, given arbitrary $1 \leq i, j, k, l \leq n$, we can find $\sigma \in \text{Aut}(\vartheta)$ such that $\sigma(v_i) = v_j$ and, if $i \neq j$ and $i \neq k$, additionally satisfies $\sigma(v_k) = v_j$. This gives

$$F(v_i, v_j) = F(\sigma(v_k), \sigma(v_j)) = F(v_j, v_j),$$

as $F$ is a structural network measure. The other case, $i = j$ and $k = l$, gives

$$F(v_i, v_j) = F(\sigma(v_k), \sigma(v_j)) = F(v_j, v_j).$$

For the orbit connectivity result (ii), we generalise the argument in [37, p.48] to weighted directed graphs with symmetries, particularly $F(G)$. We assume some basic knowledge and terminology about group actions and symmetric groups $S_n$. Given two orbits $\Delta_1 = \{v_1, \ldots, v_k\}$ and $\Delta_2 = \{w_1, \ldots, w_k\}$ and $1 \leq i \leq n$, define

$$\Gamma_i = \{w_j \in \Delta_2 | F(v_i, w_j) \neq 0\},$$

the vertices in $\Delta_2$ joined to $v_i$ in $F(G)$. If a finite group $G$ acts on a set $X$, the stabiliser of a point $G_i = \{g \in G | gx = x\}$ is a subgroup of $G$ of index $[G : \{g \in G | gx = x\}] = n$ equals to the size of the orbit of $x$. Hence the stabilisers $G_i$ or $G_{\alpha_i}$ are subgroups of $S_n$ of index $n$, for all $i, j$. The group $S_n$ has a unique, up
and similarly SI Redundancy in Network Measures (diagonal entries), and the Main Text, every orbit is a fact, the set \( w \) is the 1-v-orbit, which gives the connectivity result, as follows. Fix \( 1 \leq i \leq n \). For \( 1 \leq j, k \leq n \) different from \( i \), the vertices \( w_1 \) and \( w_2 \) are in the same \( G_i \)-orbit so there is \( \sigma \in G_i \) with \( w_1 = w_2 \) and, therefore, 

\[
F(v_1, w_1) = F(\sigma v_1, \sigma w_1) = F(v_1, w_1).
\]

The argument is general, so we have shown \( a_j = F(v_1, w_j) \) is constant for all \( j \neq i \). It is enough to show \( a_i = a_i \) for all \( i \). Fix \( j \neq i \), then 

\[
a_i = F(v_1, w_j) = F(\sigma v_1, \sigma w_j) = F(v_1, \sigma^{-1} \sigma v_1) = a_j
\]

as long as \( \sigma^{-1} \sigma v_1 \neq w_1 \), which cannot happen as otherwise \( \sigma^{-1} \sigma \in G_i = G_i \) implies \( \sigma^{-1} \sigma v_1 = v_1 \) or \( v_1 = \sigma v_1 = v_1 \), a contradiction. Hence we have shown \( F(v_1, w_j) \) is a constant, call it \( \gamma_i \), for all \( j \neq i \). In addition, 

\[
F(v_1, w_i) = F(\sigma v_1, \sigma v_i) = F(v_1, v_i)
\]

is also a constant, call it \( \delta_i \), for all \( i \). The cases \( \gamma_i = F(v_1, v_i) \) and \( \delta_i = F(v_i, v_1) \) are identical, reversing the roles of \( \Delta_1 \) and \( \Delta_2 \).

Property (iii) holds for any symmetric motif, not necessarily basic, as follows. By the definition of orbit, for each pair \( i, j \) we can find an automorphism \( \sigma \) in the geometric factor such that \( \sigma(v) = v_1 \). Since \( v \) is not in the support of that geometric factor, it is fixed by \( \sigma \), that is, \( \sigma(v) = v \). Therefore 

\[
F(v, v_i) = F(\sigma(v), \sigma(v)) = F(v, v_i),
\]

and similarly \( F(v, v_j) = F(v, v_j) \).

Consequently, every orbit in a BSM is characterised by three parameters: its size \( n \), the connectivity between any pair of distinct vertices \( \alpha \) and the connectivity of a vertex with itself \( \beta \). In the terminology and notation of the Main Text, every orbit is a \((\alpha, \beta)\)-uniform graph, \( K_\alpha^\beta \), the graph with adjacency matrix 

\[
A_{\alpha, \beta} = \alpha C_0 + \beta I_0.
\]

(32)

where \( C_0 \) is the adjacency matrix of a complete graph (0 diagonal and 1 off-diagonal entries), and \( I_0 \) is the identity matrix. For example, a \((1,0)\)-uniform graph is a complete graph, and a \((0,0)\)-uniform graph is an empty graph.

Similarly, every pair of orbits in the same BSM forms a \( (\gamma_1, \gamma_2, \gamma_3, \gamma_4) \)-uniform join of two uniform graphs \( K_{\alpha_1}^{\beta_1} \) and \( K_{\alpha_2}^{\beta_2} \), that is, the graph with adjacency matrix, possibly after a suitable reordering of the vertices, 

\[
A = \begin{pmatrix}
A_{\alpha_1, \beta_1} & A_{\gamma_2, \gamma_3} \\
A_{\gamma_4, \gamma_1} & A_{\alpha_2, \beta_2}
\end{pmatrix},
\]

(33)

where the submatrices are given as per (32).

This constrained structure will be important when we discuss the quotient network, and the spectral signatures of symmetry.

### SI Redundancy in Network Measures

#### Quotient Network

If \( A \) is the \( n \times n \) adjacency matrix of a graph \( G \), the quotient network with respect to a partition of the vertex set \( V = V_1 \cup \ldots \cup V_n \) is the graph \( G \) with \( m \times m \) adjacency matrix the quotient matrix \( Q(A) = (h_{ij}) \) defined by 

\[
h_{ij} = \frac{1}{|V_i|} \sum_{k \in V_i} a_{kj},
\]

(34)

the average connectivity from a vertex in \( V_i \) to vertices in \( V_j \). That is, the quotient amalgamates the vertices of each \( V_k \) into a single vertex, and have edges representing average connectivity.

There is an explicit matrix equation for the quotient. Consider the \( n \times m \) characteristic matrix \( S \) of the partition, that is, \( S \{ i \} = 1 \) if \( i \in V_i \), and zero otherwise, and the diagonal matrix \( A = \text{diag}(n_1, \ldots, n_k) \), where \( n_k = |V_k| \). Then

\[
Q(A) = A^{-1} S A S^{-1}
\]

(35)

They are other ways of taking the average in (34), such as \( 1/n_i \) or \( 1/(\sqrt{n_i} \sqrt{m}) \) instead of \( 1/m_i \) (34), giving slightly different, but spuriously equivalent, quotient matrices \( S A S^{-1} \) respectively \( A^{-1} S A S^{-1} \). We refer to our choice as the left quotient (matrix or network), and the other two as the right respectively symmetric quotient, writing \( Q_1(A) \) or \( Q_2(A) \) when necessary. (Note that \( Q_1(A) = Q_2(A)^T \) if \( A \) is symmetric.) Occasionally, it will be convenient to ignore weights and directions: we call unweighted quotient to the underlying unweighted, undirected quotient network, and, if we also remove self-loops (so that two orbits are connected if they are distinct and at least one vertex of one orbit is connected to a vertex of the other orbit) this is the quotient skeleton in Fig. 1 (the s-skeleton in [38]). Finally, in the context of quotient networks, we call the parent network of \( G \).}

Note that the (left) quotient \( G \) is a directed and weighted network even if the parent network \( G \) is not: \( b_{ij} = b_{ji} = \{0, 1\} \) in general. However, \( Q_1(A) \) is spectrally equivalent to the symmetric matrix \( Q_2(A) \), hence in particular has real eigenvalues if \( G \) is undirected (SI Spectral Signatures of Symmetry).

A natural quotient in the context of symmetries is given by the partition of vertices into orbits, Eqs. (29) and (31). Note that this partition is finer than the one associated to the geometric decomposition, as each symmetric motif consists of one or more orbits, and that each fixed point in \( V_0 \) (the asymmetric core) becomes its own orbit, that is, it is not identified with any other vertex in the quotient. From now on, we will implicitly refer to this quotient unless stated otherwise. Occasionally, we will consider the quotient with respect to a subgroup of \( \text{Aut}(G) \) (cf. Theorem 8), or only certain symmetric motifs (e.g. basic quotient, explained below).

A crucial property of the quotient with respect to orbits is that it removes all the symmetries from the network: if \( \sigma(j) = i \), then \( i \) and \( j \) are in the same orbit and hence represented by the same vertex in the quotient network, which is then fixed by \( \sigma \). (Although new symmetries might appear in the quotient, these are rare and would not be symmetries of the parent network, and hence of no interest to us.) We can, consequently, infer and quantify properties arising from redundancy alone by comparing a network with its quotient. This is the approach taken in [38] for spectral properties, which we will generalise to undirected, arbitrarily weighted, networks with symmetries, such as the network representation of a network measure (SI Spectral Signatures of Symmetry).

As we explain in the the Main Text, we can also exploit the quotient in the context of network structural measures for compression (storage savings), and for computational reduction (time and memory savings).

#### Quotient Compression and Recovery

The network representation of a structural network measure \( F(\mathcal{G}) \) inherits all the symmetries of \( \mathcal{G} \), which present themselves as redundancies, namely as repeated values. For instance, for each symmetric motif \( \mathcal{M} \), the values \( F(u, v) \) are constant, for each \( u \) not in \( \mathcal{M} \) and each \( v \) in the same orbit of \( \mathcal{M} \). If the network has \( n \) vertices, this means \( (n-k)! \approx n! \) repeated values for each orbit of size \( k \) in a symmetric motif of size \( k \) (typically \( k \) and \( l \) are very small). The internal connectivity of a symmetric motif can also be efficiently encoded, for instance each orbit in a BSM can be recovered from three values, its size \( n \) and constants \( \alpha \) and \( \beta \), and the connectivity between pairs of orbits in the same BSM from two or four values (undirected/directed case), and a permutation of the second orbit (Theorem 9). All this can be exploited in a compression algorithm that eliminates redundancies induced by symmetries in an arbitrary network structural measure, as we explain next. We first observe that this is most useful for full measures, since for sparse structural measures, the values \( F(u, v) \) above are mostly 0 and hence a sparse representation of \( F(\mathcal{G}) \) will account for most of the aforementioned redundancies.
### Average Compression and Recovery

If we are not interested in the internal symmetric motif connectivity, or it can be recovered easily by other means (e.g. locally one motif at a time), a simple algorithm (Algorithm 8) compresses and recovers all but the internal symmetric motif connectivity, which is replaced by the average connectivity, as the next result (Theorem 2 in Methods) shows.

**Theorem 10.** Let $A = (a_{ij})$ be the $n \times n$ adjacency matrix of a (possibly directed and weighted) network with vertex set $V$. Let $S$ be the $n \times m$ characteristic matrix of the partition of $V$ into orbits of the automorphism group of the network, and $Λ$ the diagonal matrix of column sums of $S$. Define $B = S^T AS$ and $\Lambda_{\text{avg}} = RBR^T = (\hat{a}_{ij})$ where $R = SΛ^{-1}$. Then,

1. if $i,j \in V$ belong to different symmetric motifs, $\hat{a}_{ij} = a_{ij}$.
2. if $i,j \in V$ belong to orbits $i \in \Delta_i$ and $j \in \Delta_j$ in the same symmetric motif,

$$\hat{a}_{ij} = \frac{1}{|\Delta_i|} \frac{1}{|\Delta_j|} \sum_{\alpha \in \Delta_i} \sum_{\beta \in \Delta_j} a_{\alpha \beta}.$$  

(36)

Before proving this statement, we make a few observations. The column sums of $S$ equal the sizes of the vertex partition sets, that is, the matrix $Λ$ in the statement is the same as in the definition of quotient matrix, (35), and can be obtained easily from $S$. The matrix $S$ is very sparse and can be stored very efficiently, as it has at most $n$ non-zero elements (each row has a unique non-zero entry). Case (i) covers the vast majority of vertex pairs (external edges) for a network measure (see $ext_1$ and $int_1$ in Table 1 in the Main Text). In (ii), the case $\Delta_i = \Delta_j$ is allowed. The matrix $B = S^T AS$ is symmetric with integer entries if $A$ is too, hence generally easier to store than $Q_i(A) = Λ^{-1}S^T Λ S$. However, the theorem still holds for the left, right, and symmetric quotient, as

$$\Lambda_{\text{avg}} = SA^{-1/2} AS^{-1/2} = S Q_i(A) Λ^{-1} S^T = S Q_i(A) S^T$$

(37)

$$= S A^{-1/2} Q_i(A) S^{-1/2}.$$  

(38)

**Proof of Theorem.** Let $V = \Delta_1 \cup \ldots \cup \Delta_n$ be the partition into orbits, and write $n_k := |\Delta_k|$. Clearly, the row sums of $S$ equals $n_1, \ldots, n_n$. Writing $[M]_{ij}$ for the $(i,j)$-entry of a matrix $M$, matrix multiplication gives

$$[R]_{ik} = \sum_{\alpha \in \Delta_i} S_{\alpha k} = \sum_{\alpha \in \Delta_i} S_{\alpha k} = \frac{1}{n_k} \sum_{\alpha \in \Delta_i} a_{\alpha k},$$

if $i \in \Delta_k$, otherwise.

Similarly, assuming $i \in \Delta_i$ and $j \in \Delta_j$, we have

$$\hat{a}_{ij} = \sum_{\alpha \beta} [R]_{\alpha i} [B]_{\beta j} = \frac{1}{n_k n_l} \sum_{\alpha \beta} [S]_{\alpha i} [S]_{\beta j} = \frac{1}{n_k n_l} \sum_{\alpha \beta} a_{\alpha \beta}.$$  

This expression reduces to $a_{ij}$ if the orbits belong to different symmetric motifs, since in this case all the summands in $\sum_{\alpha \in \Delta_i, \beta \in \Delta_j} a_{\alpha \beta}$ are equal to one another. Indeed, given $i_1, i_2 \in \Delta_i$, and $j_1, j_2 \in \Delta_j$, we can find, by the definition of orbit and symmetric motif, automorphisms $\sigma$ and $\tau$ such that $\sigma(i_1) = i_2$ while fixing $j_1$, and $\tau(j_1) = j_2$ while fixing $i_1$. This gives

$$\hat{a}_{i_1 j_1} = a_{\sigma(i_1) \tau(j_1)} = a_{\sigma(i_2) \tau(j_2)} = a_{i_2 j_2}.$$  

A similar proof to case (1) above shows that, if $Q_i(A) = (b_{ij})$ is the left quotient, then

$$a_{ij} = \frac{1}{n_l} b_{ij} = \frac{1}{n_l} - b_{ij},$$

where vertex $i$, respectively $j$, belongs to an orbit of size $n_i$, respectively $n_j$. As in the proof, each summand in $\sum_{\alpha \in \Delta_i, \beta \in \Delta_j} a_{\alpha \beta}$ is constant and, therefore,

$$b_{ij} = \frac{1}{|\Delta_i|} \sum_{\alpha \in \Delta_i} a_{\alpha \beta} = \frac{1}{|\Delta_i|} [\Delta_i]_{\Delta_i} [\Delta_i]_{\alpha} = [\Delta_i]_{\alpha},$$

which gives the first equality. The second equality follows from observing that, although $Q_i(A) = (b_{ij})$ is non-symmetric, $b_{ij} = \frac{1}{2} b_{ij}$ for all $k, l$.

As in the Main Text, we quantify the redundancy in an arbitrary sparse, respectively full, network measure using

$$c_{\text{spare}} = \frac{c_{\text{basic}}}{m_G} = \bar{m}_G \text{ and } c_{\text{full}} = \frac{c_{\text{basic}}}{n_G} = \bar{n}_G.$$  

These are therefore the compression ratios obtained by using the quotient to represent a sparse, respectively full, network measure on $\mathcal{G}$. The values of $c_{\text{spare}} = \bar{m}_G$ and $c_{\text{full}} = \bar{n}_G$ for our test networks are given in Table 1 in the Main Text.

In summary, we have a simple compression/decomposition procedure (Algorithms 8 and 9 below, or 2 and 3 in Methods) that eliminates the symmetry-induced redundancies in a network measure, and achieves exact recovery for external edges (the vast majority of edges, or vertex pairs), and average recovery for internal edges.

**Algorithm 8:** Average symmetry compression.

**Algorithm 9:** Average symmetry decomposition.

### Lossless Compression and Recovery

We can achieve lossless compression if we recover the exact internal motif connectivity as well. This can be done by exploiting the structure of BSMs, which account for most of the symmetry in real-world networks. If the motif is basic, we can preserve the exact parent network connectivity in an annotated quotient, as follows. Each orbit in a BSM is a uniform graph $K^\beta_{a, b}$ which appears in the quotient as a single vertex with a self-loop weighted by $(n - 1)\alpha + \beta$ (Fig. 2(c, top)). Hence if we annotate this vertex in the quotient by not only $n$ but also $\alpha$, or $\beta$, we can recover the internal connectivity. Similarly, the connectivity between two orbits in the same symmetric motif is given by two parameters $\gamma, \delta$ (undirected case) and appears in the quotient as an edge weighted $(n - 1)\gamma + \delta$ (Fig. 2(c, bottom) in Main Text) and thus can also be recovered from a quotient with edges annotated by $\gamma, or \delta$.

There is no general formula for an arbitrary non-basic symmetric motif, and for those we can either record their internal connectivity separately, or, alternatively, leave them unchanged in the quotient, by taking a partial quotient, the basic quotient, written $2\Lambda_{\text{basic}}$ with respect to the partition of the vertex set into orbits in BSMs only (vertices in non-basic symmetric motifs become fixed points and become part of the asymmetric core). The annotated (as above) basic quotient achieves most of the symmetry reduction in a typical empirical network $(\bar{h}_{G^\text{BSM}} \approx \bar{h}_{G}, \bar{n}_{G^\text{BSM}} \approx \bar{n}_{G}, \text{see SI Table 3})$ while retaining all the parent network connectivity. However, to maintain the same vertex labelling as in the parent network, we also need to record, for each pairs of orbits in the same symmetric motif, the corresponding permutation of the second orbit (Theorem 9(ii)), as otherwise we lose vertex identity on each orbit.

Similarly to average compression, we introduce compression ratios for lossless compression with respect to the basic quotient

$$c_{\text{spare}} = \frac{m_{G \text{ basic}}}{m_G} = \bar{m}_{G \text{ basic}} \text{ and } c_{\text{full}} = \frac{n_{G \text{ basic}}}{n_G} = \bar{n}_{G \text{ basic}}^2,$$  

(39)

and note that typically $c_{\text{spare}} \approx c_{\text{spare}}$ and $c_{\text{full}} = c_{\text{full}}$ for a real-world network (SI Table 3).

Algorithms for lossless compression and recovery with vertex identity based on the basic quotient are described below (Algorithms 10 and 11), and MATLAB implementations for BSMs up to two orbits are available at 34. The results reported in Fig. 3 in the Main Text are with respect to these implementations, and the actual compression ratios reported include the size of the annotation data for lossless compression with vertex identity (a very small fraction of the size of the quotient in practice, adding at most 0.02% to the basic compression ratio in all our test cases).
SI Computational Reduction

Network symmetries can also be used to reduce the computational time of a network measure $F$. Recall that a sparse, respectively full, network measure consists on at most $m_d$, respectively $n^2$, non-zero values $F(i,j)$. Since $F(i, j) = F(\sigma(i), \sigma(j))$ for each $\sigma \in \text{Aut}(\mathcal{G})$, we essentially need to evaluate $F$ on $m_d$, respectively $n^2$, orbit representatives only. This amounts to a computational reduction ratio between $c_{\text{sparse}}$ and $c_{\text{full}}$. Of course, this assumes that the calculation on each pair of vertices is independent of one another, which is often not the case. Moreover, the calculation on each pair $F(i,j)$ is still performed on the whole network $\mathcal{G}$. Next we investigate whether we could perform the calculation on the quotient instead, which would lead to greater computational gains by evaluating $F$ on a smaller graph.

We call a network measure $F$ partially quotient recoverable if it can be applied to a quotient network and all the external edges of $F(\mathcal{G})$ can be recovered from $F(\mathcal{G})$, for all networks $\mathcal{G}$. (Here $\mathcal{D}$ is a quotient of $\mathcal{G}$, possibly basic or annotated.) Since the quotient averages the network connectivity, we can often recover the average values of $F$ between orbits as well. We call $F$ average quotient recoverable if, in addition to external edges, the average intra-motif edges can be recovered from $F(\mathcal{G})$. A typical situation is when $F(\mathcal{D})$ equals the quotient representation of $F$, $Q(F(\mathcal{G}))$, that is, in symbols,

\[ F(\mathcal{D}) = Q(F(\mathcal{G})). \tag{40} \]

(Recall that we can recover the external edges, and the average internal edges, of $F(\mathcal{G})$ from $Q(F(\mathcal{G}))$, for any version of the quotient, by Theorem 10 and (37)). We will show that communicability is average quotient recoverable (see the Communicability section below), and shortest path distance is partially, but not average, quotient recoverable (see the Shortest Path Distance below). Not every measure can be (partially) recovered from the quotient, for example by reconstructing each motif at a time (see Shortest Path Distance). When quotient recoverability holds, there is a substantial computational reduction by evaluating $F$ on a smaller graph. For instance, if $F$ has time complexity $O(f(n,m))$, then we can evaluate $F$ on $\mathcal{D}$ on a fraction $f(\delta, \delta)$ of the time.

SI Spectral Signatures of Symmetry

Preliminaries

Symmetry naturally produces high-multiplicity eigenvalues: if $v$ is an eigenvector of the adjacency matrix $A$ of a (possibly weighted, directed) network $\mathcal{G}$ with eigenvalue $\lambda$, so is $Pv$,

\[ APv = P \lambda v, \tag{41} \]

for any $P$ permutation matrix representing an automorphism of $\mathcal{G}$, and $v$ and $Pv$ will generally be linearly independent. In 13, the authors formalise and quantify the effects of network symmetry on the spectrum and eigenvectors of real-world networks, predicting the observed "peaks" in spectral density and showing that symmetry explains most of their multiplicity. Here we explain how the spectral results in 13 generalise to weighted networks with symmetries, such as the network representation $F(\mathcal{G})$ of a structural network measure $F$.

Let $A = (a_{ij})$ be the $n \times n$ adjacency matrix of an arbitrarily weighted and directed network, $B = (b_{ij})$ its $m \times m$ (left) quotient matrix with respect to the orbit partition $V_1 \cup \ldots \cup V_m$, and $S$ the $n \times m$ characteristic matrix of the partition. A vector $v \in \mathbb{R}^n$, respectively $w \in \mathbb{R}^m$, can be seen as a vector on (the vertices of) the parent, respectively quotient, network. Then $Sw$ is the vector $w$ lifted to the parent network by repeating the entries on each $V_i$. Similarly, $S^T v$ (where $S^T$ is the matrix transpose) is the vector $v$ projected to the quotient by adding all its entries on each $V_i$. Note that $Sw \neq 0$ if $w \neq 0$. We call the vector $v$ orthogonal to the partition if its projection $S^T v$ is zero, that is, the sum of the entries of $v$ on each orbit is zero.

The partition into orbits satisfy important regularity conditions. A partition of the vertex set $V = V_1 \cup \ldots \cup V_m$ is left equitable if

\[ \sum_{j \in V_i} a_{ij} = \sum_{j \in V_k} a_{ij} \quad \text{for all } i, j = 1, \ldots, m, \tag{42} \]

is the, if the connectivity from a node in $V_i$ to all nodes in $V_j$ is independent of the chosen node in $V_i$. Similarly, the partition is right equitable if

\[ \sum_{i \in V_j} a_{ij} = \sum_{i \in V_k} a_{ij} \quad \text{for all } j, k = 1, \ldots, m. \tag{43} \]
Clearly, if $A$ is symmetric, being left and right equitable are equivalent properties. Next we show matrix characterisations of left and right equitability, and that the partition into orbits is both left and right equitable.

**Proposition 3.** Let $V = V_1 \cup \cdots \cup V_m$ be a partition of the vertex set of a graph with adjacency matrix $A = (a_{ij})$, and let $S$ be the characteristic matrix of the partition. Write $Q_i(A)$, respectively $Q(A)$ for the left, respectively right, quotient with respect to the partition.

(i) The partition is left equitable partition if and only if $AS = SQ_i(A)$.

(ii) The partition is right equitable partition if and only if $A^T S = SQ(A)^T$.

(iii) The partition into the automorphism group $V = \Delta_1 \cup \cdots \cup \Delta_m$ is left and right equitable.

**Proof.** (i) Fix $1 \leq i \leq n$ and $1 \leq k \leq m$, and suppose $i \in V_k$. Then
\[ [AS]_{ik} = \sum_{j \in V_k} a_{ij}, \]
and, using the left equitable condition,
\[ [SQ_i(A)]_{ik} = [Q_i(A)]_{ik} = \frac{1}{|V_i|} \sum_{j \in V_i} a_{ij} = \frac{1}{|V_i|} |V_i| \sum_{j \in V_k} a_{ij} = \sum_{j \in V_k} a_{ij}. \]
For the converse, note that $[AS]_{ik}$ does not depend on $i$ but on the orbit of $i$. Namely, given $i_1, i_2 \in V_k$,
\[ \sum_{j \in V_k} a_{ij_1} = [AS]_{i_1k} = [Q_i(A)]_{i_1k} = [AS]_{i_2k} = \sum_{j \in V_k} a_{ij_2}. \]
(ii) Similarly, with $i, k$ and $i$ as above,
\[ [A^T S]_{ik} = \sum_{j \in V_i} a_{ji}, \]
and, using the right equitable condition,
\[ [SQ(A)^T]_{ik} = [Q(A)]_{ik} = \frac{1}{|V_i|} \sum_{j \in V_i} a_{ji} = \frac{1}{|V_i|} |V_i| \sum_{j \in V_i} a_{ji} = \sum_{j \in V_i} a_{ji}. \]
For the converse, let $j_1, j_2 \in V_k$ then
\[ \sum_{i \in V_k} a_{ij_1} = [A^T S]_{j_1k} = [Q(A)]_{j_1k} = [A^T S]_{j_2k} = \sum_{i \in V_k} a_{ij_2}. \]
(iii) Given $i_1$ and $i_2$ in the same orbit $\Delta_i$, choose an automorphism $\sigma$ such that $\sigma(i_1) = i_2$. Then, since automorphisms respects the adjacency matrix,
\[ \sum_{j \in V_k} a_{\sigma(i_1)j} = \sum_{j \in V_k} a_{\sigma(i_2)j} = \sum_{j \in V_k} a_{\sigma(i_2)j} \]
where the last equality follows from the fact that an element in a group permutes orbits, in this case, $\{ j : i \in \Delta_i \} = \{ \sigma(j) : j \in \Delta_i \}$. Hence the partition into orbits is left equitable. A similar argument shows that it is right equitable as well.

Note (iii) holds for any subset of orbits or any subgroup of the automorphism group (in particular, for the basic quotient).

**Spectral Decomposition Theorem**

The key spectral property of the quotient into orbits of the automorphism group (or any subgroup) is that its eigenvalues are a subset of the eigenvalues of the parent network. Namely, if $v$ is a right (respectively left) eigenvector of $Q_i(A)$ (respectively $Q(A)$) with eigenvalue $\lambda$, then $Sv$ (respectively $vS^T$) is a right (respectively left) eigenvector of $A$ with the same eigenvalue. (These two statement are obviously equivalent if $A$ is symmetric.) This follows immediately from the matrix characterisation of eigenvalue above:

\[ Q_i(A)v = \lambda v \implies A(Sv) = SQ_i(A)v = \lambda Sv \]
\[ vQ(A) = \lambda \implies A^T (S^T v) = SQ(A)^T v = S(vQ(A))^T = \lambda S^T v \]
\[ = \lambda S^T v \iff (vS^T)A = \lambda vS^T. \]
(Recall that $Sv \neq 0$ if $v \neq 0$.) All in all, the spectrum of the quotient is a subset of the spectrum of the graph, with eigenvectors lifted from the quotient by repeating entries on orbits. Moreover, we can complete an eigenbasis with eigenvectors orthogonal to the partition (adding up to zero on each orbit), at least in the symmetric case.

**Theorem 11.** Suppose $A$ is an $n \times n$ real symmetric matrix and $B$ the $m \times m$ (left) quotient matrix with respect to an equitable partition $V_1 \cup \cdots \cup V_m$ of the set $\{ 1, 2, \ldots, n \}$. Let $S$ be the characteristic matrix of the partition. Then $A$ has an eigenbasis of the form
\[ \{ Sv_1, \ldots, Sv_m, w_1, \ldots, w_{m-1} \}, \]
where $\{ v_1, \ldots, v_m \}$ is any eigenbasis of $B$, and $S^T w_i = 0$ for all $i$.

**Proof.** Recall that $Sv \neq 0$ if $v \neq 0$ ($S$ lifts the vector $v$ from the quotient by repeating entries on each orbit) so the linear map
\[ \mathbb{R}^n \to \mathbb{R}^m, v \mapsto Sv \]
has trivial kernel and hence it is an isomorphism onto its image. In particular, $\mathbb{R}^m = \mathbb{R}^m \mapsto \mathbb{R}^m \mathbb{R}^m$, and $S^T w_i = 0$ holds for redundant eigenvectors of $B$.

The statement and proof above holds for arbitrary matrices $A$ by replacing ‘eigenbasis’ by ‘maximal linearly independent set’ and removing the condition $S^T w_i = 0$. It would be interesting to know whether the condition $S^T w_i = 0$ holds for motif eigenvectors in the directed case as well (the proof above is no longer valid).

We call $\{ Sv_1, \ldots, Sv_m \}$ quotient eigenvectors of $B$: they arise from a quotient eigenbasis by repeating values on each orbit; and we call $\{ w_1, \ldots, w_{m-1} \}$ redundant eigenvectors of $B$: they arise from the symmetries in the network (and they ‘disappear’ in the quotient), and add up to zero on each orbit ($S^T w_i = 0$). Similarly, we use the terminology quotient and redundant eigenvalues for their associated spectrum.

Further to the spectral decomposition theorem, we can give an even more precise description of the redundant spectrum: it is made of the contributions from the spectrum of each individual symmetric motif, as we explain next.

**Redundant Spectrum of Symmetric Motifs**

As stated in the Main Text (Theorem 3 in Methods), the redundant spectrum of a graph $\mathcal{M}$ is a subset of the spectrum of any (undirected) network $\mathcal{G}$ containing $\mathcal{M}$ as a symmetric motif. This essentially follows from the condition $S^T w = 0$ for redundant eigenvectors of $\mathcal{M}$.

**Theorem 12.** Let $\mathcal{M}$ be a symmetric motif of a (possibly weighted) undirected graph $\mathcal{G}$. If $(\lambda, w)$ is a redundant eigenpair of $\mathcal{M}$ then $(\lambda, w)$ is a eigenpair of $\mathcal{G}$, where $\tilde{w}$ is equal to $w$ on (the vertices of) $\mathcal{M}$, and zero elsewhere.

**Proof.** Since $(\lambda, v)$ is an $\mathcal{M}$-eigenpair,
\[ \sum_{j \in V(\mathcal{M})} [A_{\mathcal{M}}]_{ij} w_j = \lambda w_i \quad \forall i \in V(\mathcal{M}), \]
where $A_{\mathcal{M}}$ is the adjacency matrix of $\mathcal{M}$. We can decompose $\mathcal{M}$ into orbits, $V(\mathcal{M}) = V_1 \cup \cdots \cup V_m$, and, by the spectral decomposition theorem above applied to $\mathcal{M}$, $w$ is orthogonal to each orbit, that is,
\[ \sum_{j \in V_i} w_j = 0 \quad \forall 1 \leq i \leq m. \]
We need to show that $(\lambda, \tilde{w})$ is a $\mathcal{G}$-eigenpair. Let us write $A$ for the adjacency matrix of $\mathcal{G}$ (recall $\mathcal{M}$ is a subgraph so $A$ restricts to $A_{\mathcal{M}}$ on $\mathcal{M}$). We need to show $Aw = \tilde{w}$. Given $i \in V(\mathcal{G})$, we have two cases. First, if $i \in V(\mathcal{M})$,
\[ \sum_{j \in V(\mathcal{M})} [A_{\mathcal{M}}]_{ij} \tilde{w}_j = \sum_{j \in V(\mathcal{M})} [A_{\mathcal{M}}]_{ij} w_j + \sum_{j \in V(\mathcal{G}) \setminus V(\mathcal{M})} [A_{\mathcal{M}}]_{ij} \tilde{w}_j \]
\[ = \sum_{j \in V(\mathcal{M})} [A_{\mathcal{M}}]_{ij} w_j = \lambda \tilde{w}_i. \]
since $\tilde{w}$ equals $w$ on $\mathcal{M}$, and is zero outside $\mathcal{M}$. The second case, when $i \in V(\mathcal{G}) \setminus (V(\mathcal{M}))$, gives
$$\sum_{j \in V(\mathcal{G})} [A_{ij}]\tilde{w}_j = \sum_{j \in V(\mathcal{M})} [A_{ij}]w_j,$$
as before, and then we use the decomposition of $\mathcal{M}$ into orbits,
$$\sum_{j \in V(\mathcal{M})} [A_{ij}]w_j = \sum_{k=1}^{m} \sum_{j \in V_k} [A_{ij}]w_j = \sum_{k=1}^{m} \alpha_k \sum_{j \in V_k} w_j.$$
Here we have assumed that the vertex $i$, outside the motif, connects uniformly to each orbit (see Main Text), that is, $A_{ij} = A_{ij}$ for all $j \in j_2 \in V_k$, and we call this quantity $\alpha_k$. Finally, recall that $w$ is orthogonal to each orbit, to conclude
$$\sum_{j \in V(\mathcal{M})} [A_{ij}]w_j = \sum_{k=1}^{m} \alpha_k \sum_{j \in V_k} w_j = 0 \Leftrightarrow \tilde{w} = 0.$$

Therefore, the redundant spectrum of $\mathcal{G}$ is the union of the redundant eigenvalues of the symmetric motifs, together with their redundant eigenvectors localised on them. Since most symmetric motifs in real-world networks are basic, most symmetric motifs in the representation of a network measure will be basic too. Given their constrained structure, one can in fact determine the redundant spectrum of BSMS with up to few orbits, for arbitrary undirected networks with symmetry. This is what we do next.

**Redundant Spectrum of a 1-orbit BSM**

A BSM with one orbit is an $\alpha, \beta$-uniform graph $K_{n,\beta}^\alpha$ with adjacency matrix $A_{\alpha,\beta} = (a_{ij})$ given by $a_{ij} = \alpha$ and $a_{ij} = \beta$ for all $i \neq j$. Then $K_{n,\beta}^\alpha$ has eigenvalues $(n-1)(\alpha + \beta)$ (non-redundant), with multiplicity 1, and $\alpha + \beta$ (redundant), with multiplicity $n-1$. The corresponding eigenvectors are $1$, the constant vector 1 (non-redundant), and $e_i$, the vectors with non-zero entries at position 1 and $-1$ at position $i$, $2 \leq i \leq n$ (redundant). This can be shown directly by computing $A_{\alpha,\beta}^2 = \alpha A_{\alpha,\beta}$ and $A_{\alpha,\beta}^\alpha e_i$, and noting that $1$, $e_2$, $\ldots$, $e_n$ are linearly independent (although not orthogonal) and thus form an eigenbasis. Indeed, $A_{\alpha,\beta}^2 = \alpha A_{\alpha,\beta}$ is the vector of column sums of the matrix $A_{\alpha,\beta}$, which are constant $(n-1)(\alpha + \beta)$, and $A_{\alpha,\beta}^\alpha e_i$ is the constant 0 vector, except possibly at position 1, which equals $\alpha - \beta$, and $e_i$ which equals $\alpha + \beta$.

Note that, for unweighted graphs without loops ($\beta = 0$, $\alpha \in \{0,1\}$), we recover the redundant eigenvalues of 0 and $1$ predicted in.

**Redundant Spectrum of a 2-orbit BSM**

A BSM with two orbits is a uniform join of the form
$$K_{n,\beta_1}^\alpha \Join K_{n,\beta_2}^\alpha \Rightarrow K_{n,\beta_1,\beta_2}^\alpha \beta,$$

Define $a = \alpha_1 - \beta_1$, $b = \alpha_2 - \beta_2$, $c = \gamma - \delta$, and note that $c \neq 0$: otherwise $\gamma = \delta$ and we can freely permute one orbit while fixing the other, that is, this would not be a BSM with two orbits but rather two BSMs with one orbit each. As above, let $e_i$ be the vector with non-zero entries at position 1 and $-1$ at position $i$, for any $2 \leq i \leq n$.

**Lemma 1.** The following set of vectors is linearly independent
\[
\{(\kappa_1 e_i | e_i), (\kappa_2 e_i | e_i) | 2 \leq i \leq n\}
\]
for all $\kappa_1 \neq \kappa_2 \in \mathbb{R}$.

**Proof.** Define the $(n-1) \times n$ matrix
$$B_n = \begin{bmatrix} 1 & -1 \end{bmatrix}_{n-1}$$
where 1 is a constant 1 column vector, and $\mathbb{I}_{n-1}$ the identity matrix of size $n-1$. The set of vectors in the statement can be arranged in block matrix form as
$$\begin{pmatrix} \kappa_1 B_n & \kappa_2 B_n \end{pmatrix}.$$
This matrix has a minor of order 2 $(n-1)$,
$$\det(-\kappa_1 \mathbb{I}_{n-1} - \kappa_2 \mathbb{I}_{n-1}) = \det(-\kappa_1 \mathbb{I}_{n-1} - \kappa_2 \mathbb{I}_{n-1}).$$
Using that $\det(A B) = AD - BC$ whenever $A, B, C, D$ are square blocks of the same size and $C$ commutes with $B^D$, this minor equals
$$\det(-\kappa_1 \mathbb{I}_{n-1} - \kappa_2 \mathbb{I}_{n-1}) = (-1)^{n-1}(\kappa_1 + \kappa_2)^{n-1} \neq 0 \iff \kappa_1 \neq \kappa_2.$$

Next we derive conditions for a vector $v_j = (\kappa_j e_i | e_i)$ to be an eigenvector of the uniform join (47), that is, $Av_j = \lambda \cdot v_j$, for some $\lambda \in \mathbb{R}$, where $A$ is the (symmetric) adjacency matrix of the uniform join,
$$A = \begin{pmatrix} \alpha_1 \beta_1 & \alpha_1 \beta_2 & \alpha_2 \beta_1 \alpha_2 \beta_2 \end{pmatrix}.$$  (48)

The $j$th entry of the vector $Av_j$ is
\[
\kappa_1\beta_1 - \kappa_1\alpha_1 + \gamma - \delta = -(\kappa_1\alpha_1 - c)
\]
and
\[
\kappa_2\beta_2 - \kappa_2\alpha_2 - \kappa_1\beta_1 + \gamma - \delta = -(\kappa_2\beta_1 + \kappa_1\alpha_1 - c).
\]

The two equations on the right-hand side are satisfied if and only if $\lambda = -\kappa_1\alpha_1 - \kappa_2\beta_2$ and $\lambda$ is a solution of the quadratic equation
$$cK_2 + (b-a)\kappa - c = 0,$$

which has two distinct real solutions
$$\frac{a-b}{2\kappa} \pm \sqrt{(a-b)^2 + 4c^2}$$
since $c \neq 0$, as explained above. Together with the lemma, we have shown the following (Theorem 4 in Methods).

**Theorem 3.** The redundant spectrum of a symmetric motif with two orbits
$$A^\alpha_{\alpha-1,\beta_1} \Join A^\beta_{\alpha,\beta} \Rightarrow (\kappa_1 e_i | e_i),$$

where $\kappa_1, \kappa_2$ are the solutions of the quadratic equation
$$c^2 + (b-a)\kappa - c = 0,$$

each with multiplicity $n-1$, and eigenvectors $(\kappa_1 e_i | e_i)$ and $(\kappa_2 e_i | e_i)$ respectively, where $\kappa_1$ and $\kappa_2$ are the solutions of the quadratic equation
$$c^2 + (b-a)\kappa - c = 0,$$

each with multiplicity $n-1$, and eigenvectors $(\kappa_1 e_i | e_i)$ and $(\kappa_2 e_i | e_i)$ respectively, where $\kappa_1$ and $\kappa_2$ are the solutions of the quadratic equation
$$c^2 + (b-a)\kappa - c = 0,$$

each with multiplicity $n-1$, and eigenvectors $(\kappa_1 e_i | e_i)$ and $(\kappa_2 e_i | e_i)$ respectively, where $\kappa_1$ and $\kappa_2$ are the solutions of the quadratic equation
$$c^2 + (b-a)\kappa - c = 0,$$

each with multiplicity $n-1$, and eigenvectors $(\kappa_1 e_i | e_i)$ and $(\kappa_2 e_i | e_i)$ respectively, where $\kappa_1$ and $\kappa_2$ are the solutions of the quadratic equation
$$c^2 + (b-a)\kappa - c = 0.$$
Eigendecomposition Algorithm

We can use the spectral decomposition theorem above to compute the spectrum and eigenbasis of a weighted undirected network with symmetries (equivalently, a diagonalisation of the symmetric adjacency matrix $A = UDU^T$, such as $F(\mathcal{G})$, from those of the quotient, and the redundant ones of the symmetric motifs. The algorithm (Algorithm 12 below, or 4 in Methods) computes the spectral decomposition (eigendecomposition) of the quotient matrix, then, for each motif, the redundant eigenpairs.

**Input:** adjacency matrix $A$, characteristic matrix $S$, list of motifs

**Output:** spectral decomposition $A = UDQ$

initialise $U$, $D$ to zero matrices

$A \leftarrow \text{diag}(\sum(S))$

$B_{\text{sym}} \leftarrow A^{-1/2} S A^{-1/2}$

$[U \_D] \leftarrow \text{eig}(B_{\text{sym}})$ so that $B_{\text{sym}} = U \_D D U^T$

$U \_q \leftarrow U \_D q$

$D \leftarrow (D_q \begin{bmatrix} 0 \\ 0 \end{bmatrix})$

foreach motif do

$A_{\text{motif}} \leftarrow A(\text{motif}, \text{motif})$

compute orbits from motif and $S$

$S_{\text{motif}} \leftarrow S(\text{motif, orbits})$

$[U_{\text{motif}} D_{\text{motif}}] \leftarrow \text{eig}(A_{\text{motif}})$

for $\lambda \in \text{unique}(\text{diag}(D_{\text{motif}}))$ do

$U_{\lambda} \leftarrow \lambda$-eigenvectors from $U_{\text{motif}}$

$Z \leftarrow \text{null}(S_{\text{motif}} U_{\lambda})$

$d \leftarrow \text{eig}(Z)$

if $d > 0$ then

store $U_{\lambda} Z$ in $U$

store $\lambda$ in $D$ with multiplicity $d$

end

end

Algorithm 12: Eigendecomposition algorithm.

In more detail, we first compute the spectral decomposition $\text{eig}$ of the symmetric quotient $B_{\text{sym}} = A^{-1/2} S A^{-1/2}$ where $A$ is the diagonal matrix of the orbit sizes (which can be obtained as the column sums of $S$). This matrix is symmetric and has the same eigenvalues as the left quotient. Moreover, if $B_{\text{sym}} = U \_D D U^T$ then the left quotient eigenvalues are the columns of $U \_D$. These become, in turn, eigenvectors of $A$ by repeating their values on each orbit, we can be obtained mathematically by left multiplying by the characteristic matrix $S$. Then, for each motif, we compute the redundant eigenpairs using a null space matrix (see below), storing eigenvalues and localised (zero outside the motif) eigenvectors.

Only redundant eigenvectors of a symmetric motif (that is, those which add up to zero on each orbit) become eigenvectors of $A$ by extending them as zero outside the symmetric motif (Theorem 12). Therefore, we need to construct redundant eigenvectors from the output of $\text{eig}$ on each motif (the spectral decomposition of the corresponding submatrix). If $U_{\lambda} = \{v_1, \ldots, v_n\}$ are $\lambda$-eigenvectors of a symmetric motif with characteristic matrix of the orbit partition $S_{\text{motif}}$, we need to find linear combinations such that

$$S_{\text{motif}}^T (\alpha_1 v_1 + \ldots + \alpha_n v_n) = 0$$

Therefore, the matrix $Z \neq 0$ represents the null space of $S_{\text{motif}}^T U_{\lambda}$, that is, $S_{\text{motif}}^T U = 0$ and $Z^T Z = 0$, then the columns of $U_{\lambda} Z$ are precisely the redundant eigenvectors. This is implemented in Algorithm 12 within the innermost for loop.

SI Vertex Measures

The network representation we have exploited so far does not apply directly to a vertex measure $G$, unless $G$ is defined via a pairwise network measure (this is often the case). We still have, however, symmetry-induced compression, and computational reducibility, as mentioned in the Main Text and detailed below.

As a vertex measure $G$ is constant on orbits, we only need to store one value per orbit. Let $S$ be the characteristic matrix of the partition of the vertex set into orbits, and $A$ the diagonal matrix of orbit sizes (column sums of $S$). If $G$ is represented by a vector $\nu = (G(i))$ of length $n_S$, we can compress it by storing only one value per orbit, formally $W = \Lambda^{-1/2} \nu$, a vector of length $n_W$. We recover $\nu = S \_W$, as the next result guarantees (Theorem 7 in Methods).

**Theorem 14.** If $\nu$ is a vector of length $n_S$ constant on orbits, then $S \_W = \nu$.

**Proof.** First, note that $S \_W = \Lambda$ (this holds for any partition of the vertex set),

$$\begin{bmatrix} | S_{\alpha} | S_{\beta} \end{bmatrix} = \begin{bmatrix} 0 & | V_{\alpha} | \end{bmatrix}$$

when $\alpha \neq \beta$. We still have, however, symmetry-induced compression, and computational reducibility, as mentioned in the Main Text and detailed below.

In terms of computational reduction, we only need to evaluate $G$ once per orbit, achieving an $\tilde{O}$ time reduction, assuming $G$ is evaluated at vertices independently, which is often not the case. More interesting is the case when $G$ can be recovered from its value at the quotient network. We call $G$ quotient recoverable if $G(\mathcal{G})$ can be obtained from $G(\mathcal{G})$, where $\mathcal{G}$ is a (possibly annotated, or basic) quotient of $\mathcal{G}$, for all networks $\mathcal{G}$. Not every vertex measure is quotient recoverable, but when one is, it can lead to a significant computational time reduction (Fig. 4 in the Main Text).

SI Applications

Network Symmetry Computation

The results in the Main Text depend on an effective computation, storage and manipulation of the symmetries on an (unweighted, undirected, possibly very large) network $\mathcal{G}$. Here we present our approach, based in the geometric decomposition of the automorphism group of the graph. Full implementations of the algorithms outlined below are available at https://github.com/saucy. (For weighted or directed network, see concluding remarks in this section.)

We obtain the geometric decomposition in three steps. First, we use a graph automorphism algorithm to compute generators. Secondly, we partition the generators into disjoint-support classes (each class corresponds to a symmetric motif). Thirdly, we compute symmetric motif orbits and types from the generators and their disjoint-support partition. Below we explain each step in more detail.

We use saucy 3.5 to compute a list of generators of the automorphism group from an edge list. Other open-source software tools are available, such as nauty4.3, traces5, or bliss57. Although saucy does not compute a canonical labelling (relevant to the graph isomorphism problem but not to the geometric decomposition), it is extremely fast for large but sparse networks58 such as the ones representing real-world systems. In practice, we found a list of generators in less than two seconds for all our test networks, except our largest example LiveJournal, in just over eight seconds (Table 1 in the Main Text). Due to the similarities with nauty, it would be interesting to know whether the set of generators produced by saucy is also essential, which would guarantee that the geometric decomposition below is optimal; this seems to be the case in practice for all our test networks.

The next step is to partition the set of generators $X$ into support-disjoint classes $X = \{X_1, \ldots, X_k\}$. For that, we use a bipartite graph representation of vertices $V$ and generators $X$. Let $\mathcal{G}$ be the graph with vertex set $\cup X$ and undirected edges $\{i, \sigma\}$ whenever $i \in \text{supp}(\sigma)$. Clearly, the finest partition into support-disjoint classes of generators correspond to the connected components of $\mathcal{G}$ (as vertex sets intersected with $X$). Using for instance Tarjan’s algorithm, we can find an efficient procedure to find the support-disjoint decomposition in linear time. In practice, this step took less than five seconds for each of our test networks. Each class in the support-disjoint partition above corresponds to (the vertex set of) a symmetric motif, by Eqs. 24 and 25.
The last step consists of computing the orbits and type of each symmetric motif. This was done in GAP\cite{GAP}, but any computer algebra system that can manipulate permutation groups can be used. We applied Algorithm 13 (Algorithm 1 in Methods) to each \( X_i \) in the support-disjoint decomposition above (this can be done in parallel). The pseudocode in Algorithm 13 assumes a computer algebra system that can compute the group generated by a set of permutations, its orbits, and whether the induced action on an orbit is a natural symmetric group (that is, a group acting as the symmetric group on its moved points). If that is the case, and all orbits are of the same size \( m \), it is a basic symmetric motif of type \( m \), that is, the corresponding geometric factor is \( S_m \). If this is not the case, it is a complex symmetric motif and we set \( m = 0 \). Algorithm 13 outputs a list of orbits, and the integer \( m \). Note that the second part of the algorithm (the outermost if-then-else loop) is only necessary if we need the orbit types, for example in order to later compute the basic quotient. In terms of computational time, our GAP non-parallel implementation computes about 2,000 generators per second in our small and medium networks, which suggests at most 205 seconds for our largest network (and divided by the number of processors available in a parallel implementation). Unfortunately, the generator-per-second rate decreases (up to 10 generators per second for the largest network) due to the internal representation of permutation groups in GAP.

\section{Communicability}

Communicability is a measure of network connectivity between pairs of vertices which takes into account all possible walks from one vertex to the other by using the powers of the adjacency matrix \( A \). Namely, if we choose coefficients \( a_k \) such as the matrix series

\[ \sum_{k=0}^{\infty} a_k A^k \]  

converges, then the \((i,j)\)-entry of this limit matrix is a weighted sum of all the walks from \( i \) to \( j \), and thus can be used as a network connectivity measure. We normally expect coefficients \( a_k \) such that we obtain positive values for the communicability, and which give less weight to longer walks. An standard choice is the factorial coefficients \( a_k = \frac{1}{k!} \), which guarantees convergence for any matrix \( A \) and, in fact,

\[ e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!}, \]  

the exponential matrix of \( A \). The diagonal entry \([e^A]_{ii}\) is called the subgraph centrality of vertex \( i \)\cite{BaumannBridges}, and its sum over all the vertices the Estrada index of the network\cite{Estrada}. In general, one can define communicability for an arbitrary real analytic function (such as \( f(x) = e^x \)) within its radius of convergence \( R \) around 0,

\[ f(x) = \sum_{k=0}^{\infty} a_k e^{kx} \]  

Given such a function \( f \), we define the \( f \)-communicability matrix of a network with adjacency matrix \( A \) as

\[ f(A) = \sum_{k=0}^{\infty} a_k A^k \]  

where \( \| \cdot \| \) is a given matrix norm, and the power series convergence is with respect to that norm. (For a detailed treatment of matrix norms and convergence see\cite{HornJohnson}.) From now on we will implicitly assume all calculations to be within the convergence radius of \( f \), possibly by normalising the matrix \( A \). The \( f \)-communicability from vertex \( i \) to vertex \( j \) is thus the \((i,j)\)-entry of the communicability matrix \( f(A) \). For consistent terminology, we will call the \( f \)-communicability of a vertex with itself its \( f \)-centrality, inherently a network centrality measure. (We consider other centrality measures, including subgraph centrality, and the effect of symmetry on them, below.) Note that matrix functions \( f(A) \) can be defined in more generality\cite{ben2007}), however the power series definition is the one with an obvious graph theoretic interpretation.

\section{Structural Properties}

We represent communicability as a network on the same set of nodes. Namely, we define the \( f \)-communicability graph of \( G \), written \( f(G) \), as the graph with adjacency matrix \( f(A) \), which we call the communicability matrix. This is a weighted, complete (and possibly directed, if \( A \) is not symmetric) graph with loops. For every \( i \neq j \), there is an edge from vertex \( i \) to vertex \( j \) weighted by the communicability from \( i \) to \( j \), and a self-loop at every vertex weighted by its \( f \)-centrality. The \( f \)-communicability network, although dense, inherits all the symmetries of \( G \) and hence \( f(G) \) has the same geometric decomposition, symmetric motifs, and orbits. For real-world networks, most symmetric motifs will be basic and, as induced graphs, the basic symmetric motifs are uniform joins of orbits, and each orbit is a uniform graph hence characterised by two parameters, the subgraph centrality of each vertex, and the communicability between different vertices, within the orbit. In particular, this explains what we observed in our toy example, Fig. 1 in the Main Text. In terms of post-processing compression, as a full network measures, average symmetry compression with ratio \( \frac{e_{full}}{e_{full}} \) and lossless symmetry compression with ratio \( \frac{e_{full}}{e_{full}} \) apply, accounting for the symmetry-induced redundancy present on \( f(G) \), or \( f(A) \).

\section{Quotient Recoverability}

Communicability satisfies average quotient recoverability, as it ‘commutes’ with the quotient, that is, the communicability of the quotient is the quotient of the communicability, in symbols,

\[ f(Q(A)) = Q(f(A)). \]  

(57)

This is (40) for communicability, and implies exact recovery for external edges, and average recovery for internal edges. To prove (57), let \( B = Q(A) \)

\[\begin{align*}
\text{Input:} & \quad X \text{ a set of permutations of a symmetric motif} \\
\text{Output:} & \quad O_1, \ldots, O_k \text{ orbits, and type } m, \text{ of the symmetric motif} \\
& \quad H \leftarrow \text{Group}(X) \\
& \quad \{O_1, \ldots, O_k\} \leftarrow \text{Orbits}(H) \\
& \quad m \leftarrow \min(\text{size}(O_1), \ldots, \text{size}(O_k)) \\
& \quad \text{if } m = \max(\text{size}(O_1), \ldots, \text{size}(O_k)) \text{ then} \\
& \quad \quad \text{for } i \leftarrow 1 \text{ to } k \text{ do} \\
& \quad \quad \quad \text{if not IsNaturalSymmetricGroup(}\text{Action}(H, O_i)\text{) then} \\
& \quad \quad \quad \quad m \leftarrow 0 \\
& \quad \quad \quad \text{break} \\
& \quad \quad \text{end} \\
& \quad \quad \text{end} \\
& \quad \quad \text{else} \\
& \quad \quad \quad m \leftarrow 0 \\
& \quad \quad \text{end} \\
\end{align*}\]

Algorithm 13: Orbits and type of a symmetric motif.
be the (left) quotient matrix with respect to the partition into orbits. Since the partition is equitable, we have $AS = SB$, and hence $A' = SB'$. Now, using the matrix definition of the quotient, we have

$$Q(f(A)) = A^{-1}S\left(\sum_{n=0}^{\infty} a_n A^n\right) = \sum_{n=0}^{\infty} a_n (A^{-1}S A^n S) = \sum_{n=0}^{\infty} a_n (A^{-1}S B^n) = \sum_{n=0} a_n f(B),$$

since $A^{-1}S$ is the identity matrix.

Exhaustive recovery for vertices within the same symmetric motif cannot be done in general, as the internal connectivity, replaced by the average connectivity, is lost in the quotient. However, as mentioned in the Main Text, we can use the spectral decomposition algorithm to reduce the computation of the communicability, as $A = UD(U^T)$ clearly implies $f(A) = U f(D) U^T$. The computational time reduction of this approach is displayed in Figure 4 in the Main Text, for the exponential function.

**Spectral Properties**

The $f$-communicability network has eigenvalues $f(\lambda)$, where $\lambda$ is an eigenvalue of the original network, and same eigenvalues: $Av = \lambda v$ implies $f(A)v = f(\lambda)v$ (equivalently, $A = UD(U^T)$ implies $f(A) = U f(D) U^T$). In particular, its redundant spectrum consists of the function $f$ applied to the redundant spectrum of $G$, together with the redundant eigenvalues localised on the symmetric motifs. In particular, for undirected, unweighted networks,

$$RSpec^{\text{conn}}_1 = \{ f(\lambda) | \lambda \in RSpec_1 \} = \{ f(0), f(-1) \},$$

and

$$RSpec^{\text{conn}}_2 = \{ f(\lambda) | \lambda \in RSpec_2 \} = \{ f(-2), f(-\varphi), f(-1), f(0), f(-\varphi - 1), f(1) \},$$

account for most of the discrete part of the spectrum of the matrix $f(A)$, for the adjacency matrix $A$ of a typical real-world network.

**Shortest Path Distance**

Let $A = (a_{ij})$ be the adjacency matrix of an unweighted, but possibly directed, network $G$. A path of length $n$ is a sequence $(v_1, v_2, \ldots, v_{n+1})$ of distinct vertices, except possibly $v_1 = v_{n+1}$, such that $v_i$ is connected to $v_{i+1}$, for all $1 \leq i \leq n - 1$. The shortest path distance $d^G(u, v)$ is the length of the shortest (minimal length) path from $u$ to $v$. (Technically, it is only a distance, or metric, if $G$ is undirected.) If $p = (v_1, v_2, \ldots, v_n)$ is a path and $\sigma \in Aut(G)$, we define $\sigma(p) = (\sigma(v_1), \sigma(v_2), \ldots, \sigma(v_n))$ also a path since $\sigma$ is a bijection. A subpath of $p$ is a path of the form $(v_{i-1}, v_i, v_{i+1}, \ldots, v_j)$ for some $1 \leq k \leq f \leq n$. A path $p$ is a shortest path if it is of minimal length between its endpoints. The following result contains the claims in the Main Text (Theorem 6 in Results).

**Theorem 15.** Let $A = (a_{ij})$ be as above. Then

(i) if $(v_1, v_2, \ldots, v_n)$ is a shortest path from $v_1$ to $v_n$ and $\sigma \in Aut(G)$, then $(\sigma(v_1), \sigma(v_2), \ldots, \sigma(v_n))$ is a shortest path from $\sigma(v_1)$ to $\sigma(v_n)$;

(ii) if $(v_1, \ldots, v_n)$ is a shortest path from $v_1$ to $v_n$, and $v_1$ and $v_n$ belong to different symmetric motifs, then $v_1$ and $v_{m+1}$ belong to different orbits, for all $1 \leq i \leq n - 1$;

(iii) if $u$ and $v$ belong to orbits $U$, respectively $V$, in different symmetric motifs, then the distance from $u$ to $v$ in $G$ equals the distance from $U$ to $V$ in the unweighted (or quotient) network $\mathcal{G}$.

These statements mean that (i) automorphisms preserve shortest paths and their lengths; (ii) shortest paths do not contain intra-orbit edges; and (iii) shortest path distance is a partially quotient recoverable structural measure.

**Proof of Theorem.** (i) Since automorphisms are bijections and preserve adjacency, $(\sigma(v_1), \sigma(v_2), \ldots, \sigma(v_n))$ is a path from $\sigma(u)$ to $\sigma(v)$ of the same length. If there were a shorter path $|\sigma(u)| = w_1, w_2, \ldots, \sigma(v) = w_m$, $m < n$, the same argument applied to $\sigma^{-1}$ gives a shorter path $|a(u) = \sigma^{-1}(w_1), \sigma^{-1}(w_2), \ldots, \sigma^{-1}(w_m))$ from $u$ to $v$, a contradiction.

(ii) Any subpath of a minimal length path is also of minimal length between its endpoints. Arguing by contradiction, there exists a subpath $p = (w_1, \ldots, w_k)$ (or $p = (w_{n-k}, w_{n-k+1}, \ldots, w_n)$), such that $w_1$ and $w_k$ belong to the same orbit, and $w_a$ belongs to a different symmetric motif. Hence, we can find $\sigma \in Aut(G)$ with $\sigma(w_2) = w_1$ and fixing $w_k$. This implies $\sigma(w_1) = (\sigma(w_1), \sigma(w_2), \ldots, \sigma(w_n)) = w_1$, a shortest path by (i), of length $n - 1$. The subpath $(w_1, \sigma(w_3), \ldots, w_n)$ has length $n - 2$, contradicting $p$ being a minimal length path from $w_1$ to $w_k$. (The case $p = (w_n, w_{n-1}, \ldots, w_1)$ is analogous.)

(iii) Let $(\sigma = (v_1, v_2, \ldots, v_{n+1})$ be a shortest path from $u$ to $v$, so that $d^G(u, v) = n$. Let $V_0$ be the orbit containing $v_j$, for all $1 \leq i \leq k \leq n$ such that $q = (U = V_1, V_2, \ldots, V_{n+1} = V)$ is a path in $\mathcal{G}$ and $d^G(U, V) \leq n$. By contradiction, assume there is a shorter path in $\mathcal{G}$ from $U$ to $V$, that is, $(U = W_1, W_2, \ldots, W_{n+1} = V)$ with $m < n$. We can construct a path in $\mathcal{G}$ from $u$ to $v$ of length $m$ (a contradiction), as follows. For each 1 $\leq i \leq m$, $W_i$ is connected to $W_{i+1}$ in $\mathcal{G}$, hence there is a vertex in $W_i$ connected to at least one vertex in $W_{i+1}$. Since vertices in an orbit are structurally equivalent, any vertex in $W_i$ is then connected to at least one vertex in $W_{i+1}$. As vertices in an orbit are structurally equivalent, any vertex in $W_i$ is then connected to $\sigma(v_i)$ in $W_{i+1}$. This allows us to construct a path in $\mathcal{G}$ from $u$ to $v$ of length $m < n$, a contradiction. □

Distances between points within the same motif cannot in general be directly recovered from the quotient, not even for BSMs. (Consider for instance the double star, motif $M_2$, Figure 1 in the Main Text. The distance from the top red to the bottom blue vertex is three, while in the quotient it is one.) In general, therefore, the shortest path distance is partial but not average, quotient recoverable. Intra-motif distances, if needed, could still be recovered one motif at a time. (If we are only interested in large distances, computing them in the quotient suffices as one can show that $d(i, j) \leq 2k$ for $i, j$ vertices in a symmetric motif with $k$ orbits.)

Note that these results can be exploited for other graph-theoretic notions defined in terms of distance, for example eccentricity (and thus radius or diameter), which only depends on maximal distances and thus can be computed directly in the quotient (see section Eccentricity below). In terms of post-calculation compression, the quotient compression ratio $cR$ of applies, accounting for the amount of structural redundancy due solely to symmetries. The spectral results, although perhaps less relevant, still apply for $d^G$, the graph encoding pairwise shortest path distances. The adjacency matrix $d^G = (d^G(i, j))$ is nonzero outside the diagonal, hence $d^G$ is a full-all to-all weighted network without self-loops and integer weights, and so is each symmetric motif. Using the formula in Theorem 13, we can compute values of the most significant part of the discrete spectrum (redundant eigenvalues) of $d^G$.

$$RSpec^{\text{conn}}_1 = \{ -2, -1 \},$$

and

$$RSpec^{\text{conn}}_2 = \{-3 \pm 2, -1 \pm 2\sqrt{3}, -3 \pm 2\sqrt{3}\}.$$
where $L_\mathcal{M}$ is the ordinary Laplacian matrix of $\mathcal{M}$ considered as a graph on its own, and $d_1, \ldots, d_k$ are the external degrees of the $k$ orbits of $\mathcal{M}$ of sizes $m_1, \ldots, m_k$. (Here $I_\mathcal{N}$ is the identity matrix of size $n$ and we use $\oplus$ to construct a block diagonal matrix.)

(The proof of this theorem should be clear from the comments above.) Note that, for a motif with one orbit, this is the Laplacian of the motif translated by a multiple of the identity. In particular, the redundant eigenvalues of a BSM with one orbit are the redundant (high multiplicity) Laplacian eigenvalues of an empty or complete graph of size $n$ plus the external degree $d$, that is, $d + n$. In particular,

$$\text{RSpec}_\mathcal{M}^1 = \mathbb{Z}^+$,$$

and we expect ‘peaks’ in the Laplacian spectral density at (small) positive integers, which indeed agrees what we observed in our test networks (Fig. 5 in the Main Text). Using the formula in Theorem 13, we could compute the redundant spectrum for 2-orbit BSMs, and for other versions of the Laplacian (e.g. normalised, vertex weighted), but we believe this is out of the scope of the present article.

Observe that spectral decomposition applies, since $L$ inherits all the symmetries of $A$, so Algorithm 12 provides an efficient way of computing the Laplacian eigendecomposition with an expected $sp = \tilde{n}^2_2$ (see Table 1 in the Main Text) computational time reduction.

Degree Centrality

The degree of a node (in- or out-degree if the network is directed) is a natural measure of vertex centrality. As expected, the degree is preserved by any automorphism $\sigma$, which can also be checked directly,

$$d_i = \sum_{j \in V} a_{ij} = \sum_{j \in V} a_{\sigma(i)\sigma(j)} = \sum_{j \in V} a_{\sigma(i)j} = d_{\sigma(i)},$$

as automorphisms permute orbits (so $j \in V$ and $\sigma(j) \in V$ are the same elements but in a different order). In particular, the degree is constant on orbits.

We can recover the degree centrality from the quotient, as the out-degree of the left quotient (or the in-degree of the right quotient), as follows. (This is for illustration purposes rather than a worthwhile computational gain in using the quotient for degree calculations.) Let $B = (b_{ij})$ be the adjacency matrix of the left quotient, and $V = V_1 \cup \ldots \cup V_m$ the partition of the vertex set into orbits. If $i \in V_a$, then

$$d_{a}^\text{out} = \sum_{j \in V} a_{ij} = \sum_{j \in V_b} a_{ij} + \ldots + \sum_{j \in V_m} a_{ij} = \frac{1}{n_1} \sum_{j \in V_b} a_{ij} + \ldots + \frac{1}{n_m} \sum_{j \in V_m} a_{ij} = b_{1i} + \ldots + b_{mi} = d_{a}^\text{out}.$$

Eccentricity

Although not discussed in the Main Text, the reciprocal of the eccentricity is a natural centrality measure. The eccentricity of a vertex is the maximal (shortest path) distance to any vertex in the network. As shortest path distance is partially quotient recoverable, and eccentricity depends on large distances only, so in practice we can ignore intra-motif distances and therefore recover eccentricity directly from the (unweighted, or skeleton) quotient as

$$\text{ecc}_{a}^\mathcal{M}(i) = \text{ecc}_{a}^\mathcal{M}(\sigma) \quad \text{if} \quad i \in V_a.$$

In particular, the diameter (maximal eccentricity) and radius (minimal eccentricity) of a network coincides with that of the (unweighted, or skeleton) quotient.

Closeness Centrality

The closeness centrality of a node $i$ in a graph $\mathcal{M}$, $cc_{a}^\mathcal{M}(i)$, is the average shortest path length to every node in the graph. As symmetries preserve distance, they also preserve closeness centrality, explicitly,

$$cc(a) = \frac{1}{n_\mathcal{M}} \sum_{i \in V} d(i, j) = \frac{1}{n_\mathcal{M}} \sum_{i \in V} d(\sigma(i), \sigma(j))$$

and centrality is constant on each orbit, as expected. Moreover, closeness centrality can be recovered from the quotient (shortest paths do not contain intra-orbit edges, except between vertices in the same symmetric motif, see Theorem 15), as

$$cc_{a}^\mathcal{M}(i) = \sum_{j \in V} \frac{d_{a}^\text{out}}{n_\mathcal{M}} d_{a}(V_i, V_j) + \frac{n_i}{n_\mathcal{M}} d_{k}$$

if $i$ belongs to the orbit $V_i$ and $d_{k}$ is the average intra-motif distance, that is, the average distances of a vertex in $V_i$ to any vertex in $\mathcal{M}$, the motif containing $V_i$. By annotating each orbit by $d_{k}$, we can recover betweenness centrality exactly. Alternatively, as $d_{k} \ll n$ (note that $d_{k} \leq m$ if $\mathcal{M}$ has $m$ orbits), we can approximate $cc_{a}^\mathcal{M}(i)$ by the first summand, or simply by the quotient centrality $cc_{a}^\mathcal{M}(\sigma)$, in most practical situations.

Eigenvalue Centrality

Since the Perron-Frobenius eigenvalue is always simple, it cannot be a redundant eigenvalue. Hence it is a quotient eigenvalue, and, as those are a subset of the parent eigenvalues, it must still be the largest (hence the Perron-Frobenius) eigenvalue of the quotient. Its eigenvector can then be lifted to the parent network, by repeating entries on orbits. That is, if $(\lambda, v)$ is the Perron-Frobenius eigenpair of the (left) quotient, then $(\lambda, S_v)$ is the Perron-Frobenius eigenpair of the parent network (44). In practice, we use the symmetric quotient $B_{\mathcal{M}} = A_{\mathcal{M}}^{\mathcal{M}}/\mathcal{A}_{\mathcal{M}}$ for numerical reasons (Algorithm 14), obtaining significant reductions in computational times (Fig. 4 in the Main Text). If $A$ is not symmetric (but irreducible), Algorithm 14 (Alg. 7 in Methods) gives the right Perron-Frobenius eigenpair of $A$, and replacing $B_{\mathcal{M}}$ by $A_{\mathcal{M}}$ is the same geometric decomposition, orbits, and symmetric motifs (as vertex sets) — see the Weighted and Directed Networks subsection in SI Symmetry in Complex Networks.

### FURTHER ACKNOWLEDGEMENTS

Thanks to Yair Moreno and Emanuele Cozzo, whose ‘simple’ question inadvertently prompted this lengthy answer more than a year later, and to Gareth Jones for reminding the author that $S_5$ has two conjugacy classes of subgroups of index 6. Special thanks to my wife Kate for her unwavering support.