Symmetries of independent statistical observables for ultrametric populations

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When $N=2^G$, random data X_i, $i=1,\ldots,N$ show ultrametric covariations, represented by a binary tree, decorrelated observables are defined by a covariance matrix diagonalization. Eigenvalue degeneracies lead one to regroup such observables into eigenprojectors. Symmetries of such projectors are discussed. Such symmetries and degeneracies influence the robustness of the corresponding measurements under random permutations of data.

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I. REMINDER OF PREVIOUS RESULTS

Ultrametric correlations are of interest [1,2], in genetics for instance. It is useful to define observables whose correlations are disentangled. In a previous paper [3], we linearly rearranged correlated variables X_i, $i=1,\ldots,2^G$ into independent ones, by diagonalizing the covariation matrix $\mathcal{C}$, with elements $C_{ij}=\langle X_i X_j\rangle-\langle X_i\rangle\langle X_j\rangle$. Here, $\langle\ \rangle$ denotes the probabilistic average with respect to the probability governing such variables X_i. These were assumed to derive from a binary ultrametric tree with G generations. The rearranged observables read $\mathcal{O}_\tau=\Sigma_{i\in I}X_i-\Sigma_{j\in J}X_j$, where τ designates suitable partitions $I\cup J$ of the X's subscripts into two equal subsets. The spectrum of $\mathcal{C}$ is so highly degenerate [4] that it seems necessary to define independent observables related to eigenprojectors rather than eigenvectors. The present report studies symmetry properties of such eigenprojector observables (EPO's). We try to understand their significance, and also appraise their robustness if, as a not uncommon perturbation of experimental data, some mislabeling occurs for the leaves of the tree.

For the sake of definiteness, we often illustrate this report with the case $G=3$ and sometimes use notations $s,t,\ldots,z$ instead of $X_1,X_2,\ldots,X_8$. Generalizations to any G are most often obvious. The covariance matrix under study and its eigenprojectors read, respectively,

$$\mathcal{C}_3=\begin{bmatrix} 1 & c_1 & c_2 & c_2 & c_3 & c_3 & c_3 & c_3\\ c_1 & 1 & c_2 & c_2 & c_3 & c_3 & c_3 & c_3\\ c_2 & c_2 & 1 & c_1 & c_3 & c_3 & c_3 & c_3\\ c_2 & c_2 & c_1 & 1 & c_3 & c_3 & c_3 & c_3\\ c_3 & c_3 & c_3 & c_3 & 1 & c_1 & c_2 & c_2\\ c_3 & c_3 & c_3 & c_3 & c_1 & 1 & c_2 & c_2\\ c_3 & c_3 & c_3 & c_3 & c_2 & c_2 & 1 & c_1\\ c_3 & c_3 & c_3 & c_3 & c_2 & c_2 & c_1 & 1 \end{bmatrix},\quad \mathcal{Q}_1=\frac{1}{2}\begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0\\ -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0\\ 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0\\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1\\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix},$$

$$\mathcal{Q}_2=\frac{1}{4}\begin{bmatrix} \mathbf{1} & \overline{\mathbf{1}} & \mathbf{0} & \mathbf{0}\\ \overline{\mathbf{1}} & \mathbf{1} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{1} & \overline{\mathbf{1}}\\ \mathbf{0} & \mathbf{0} & \overline{\mathbf{1}} & \mathbf{1} \end{bmatrix},\quad \mathcal{Q}=\frac{1}{8}\begin{bmatrix} \mathbf{1} & \overline{\mathbf{1}}\\ \overline{\mathbf{1}} & \mathbf{1} \end{bmatrix}. \tag{1}$$

Here 1, $\overline{\mathbf{1}}$, and $\mathbf{0}$ are suitable 2×2 or 4×4 blocks of ones, "minus ones," and zeroes. For the sake of simplicity [3], the subtraction $-\langle X_i\rangle\langle X_j\rangle$ can be omitted. The numbers c_k are positive and smaller than 1. A normalization is implemented, $c_0\equiv\langle X_i^2\rangle=1$. The ranks of projectors $\mathcal{Q}_1$, $\mathcal{Q}_2$, and $\mathcal{Q}_3$ are, respectively, 4, 2, and 1. The corresponding eigenvalues are $E_1=1-c_1$, $E_2=1+c_1-2c_2$, and $E_3=1+c_1+2c_2-4c_3$. Generalizations for $G\geqslant4$ are obvious. With G generations in a binary tree and for any positive integer $k\leqslant G$, there exists an eigenvalue $E_k=1+\Sigma_{n=1}^{k-1}2^{n-1}c_n-2^{k-1}c_k$, with degeneracy 2^{G-k}. Figure 1 shows the "$G=3$" tree. Degrees u and v, e.g., have parentage 1, because of their nearest common

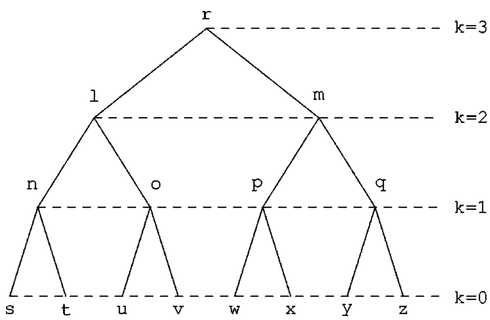

FIG. 1. Binary tree with three generations.

ancestor, o. In turn, e.g., degrees x and z have parentage 2 because of ancestor m. Ultrametricity is implemented because, whenever X_i and X_j have parentage k, then C_{ij} depends on k only, $C_{ij}=c_k$.

II. OBSERVABLES AND THEIR SYMMETRIES

Consider the row vector $V\equiv[X_1,X_2,\ldots,X_N]$ and its transposed V^T, with a normalization $\Sigma_{i=1}^{N}X_i^2=N$. The matrix elements $\Lambda_k\equiv V\mathcal{Q}_k V^T$ are the observables of interest in this paper. They are normalized by the sum rule $\Sigma_{k=0}^{G}\Lambda_k=N$. The projector $\mathcal{Q}^{E_0}$ upon the symmetric eigenvector $[1,1,\ldots,1]$ is irrelevant here. For $G=3$, the useful observables read [see Eqs. (1)],

$$\Lambda_1=\frac{(s-t)^2+(u-v)^2+(w-x)^2+(y-z)^2}{2}, \tag{2a}$$

$$\Lambda_2=\frac{(s+t-u-v)^2+(w+x-y-z)^2}{4}, \tag{2b}$$

$$\Lambda_3=\frac{(s+t+u+v-w-x-y-z)^2}{8}. \tag{2c}$$

An interpretation is in order. Consider at level k the binary graph with G generations. The leaf and root levels are labeled by $k=0$ and $k=G$, respectively. At any level k, one counts 2^{G-k} vertices. The same number 2^{G-k} holds for the ''ingoing'' branches coming from the root direction into these vertices. Twice as many, namely 2^{G-k+1}, ''outgoing'' branches emerge from such vertices toward the leaf direction. Each such outgoing branch ultimately generates 2^{k-1} leaves, hence the $2^{G-k+1}\times 2^{k-1}=2^G$ total number N of degrees of freedom X_i. It is clear that Λ_k is a sum, over the vertices at level k, of ''square contrasts'' between the two outgoing branches at each vertex. More precisely, replace each label i of a variable X_i with a combined label $\{\alpha,\beta,\gamma\}$, where $\alpha=1,\ldots,2^{G-k}$ denotes the vertex at level k, then $\beta=1,2$ tells which of the two emerging branches is involved, and finally $\gamma=1,\ldots,2^{k-1}$ labels the leaves ultimately related to that emerging branch. Then the observables read

$$\Lambda_k=2^{-k}\sum_{\alpha=1}^{2^{G-k}}\left(\sum_{\gamma=1}^{2^{k-1}}X_{\alpha 1\gamma}-\sum_{\gamma=1}^{2^{k-1}}X_{\alpha 2\gamma}\right)^2. \tag{3}$$

Consider the two branches emerging from each vertex at level k, defining two ''subfamilies'' at level 0 (leaf level). Sum the degrees of freedom inside each subfamily. Square the ''subfamily contrast,'' namely, the difference between the two sums. Finally, sum such squares over all the pairs of such subfamilies derived from level k. This makes Λ_k. The preexisting normalizations make it unnecessary to renormalize Λ_k into ''subfamily internal averages'' and ''averages upon subfamily pairs'' by additional denominators such as 2^{k-1}, the population of each subfamily, and 2^{G-k}, the number of subfamily pairs.

Should Λ_k strongly jump at a level K, one might suspect that genetic diversification occurs at this level.

Each Λ_k exhibits three kinds of symmetries. First, it is a symmetric function of the ingoing branches, see the index α in Eq. (2). This ''ingoing permutation group'' makes $(2^{G-k})!$ symmetries. Then Λ_k is a symmetric function of those leaves related to each outgoing branch, see the index γ in Eq. (3). Each outgoing branch provides a symmetry group of $(2^{k-1})!$ permutations for leaves. Hence, because of 2^{G-k+1} outgoing branches, we find $[(2^{k-1})!]^{(2^{G-k+1})}$ ''outgoing symmetries.'' Finally, Λ_k is even under the exchange of the two branches emerging from each vertex. Hence $2^{(2^{G-k})}$ ''parities.'' The number of distinct permutations under which Λ_k is invariant reads

$$\mathcal{S}(k)=(2^{G-k})![(2^{k-1})!]^{(2^{G-k+1})}2^{(2^{G-k})}. \tag{4}$$

Special values are $\mathcal{S}(1)=2^{(2^{G-1})}(2^{G-1})!$ and $\mathcal{S}(G)=2[(2^{G-1})!]^2$. A general asymptotic estimate is

$$\ln\mathcal{S}(k)\simeq\left(\frac{1+G-k}{2}-2^G+2^{G-k}+2^{G-k}G+2^G k\right)\times\ln 2+\left(\frac{1}{2}+2^{G-k}\right)\ln\pi-2^G-2^{G-k}. \tag{5}$$

When k increases from 1 to G for a given G, the number $\mathcal{S}(k)$ first decreases, reaches a minimum for $k\simeq\log_2 G$, and then increases. Indeed, from Eq. (5),

$$\frac{d\ln[\mathcal{S}(k)]}{dk}\simeq 2^{G-k}\ln 2(2^k-G\ln 2-\ln\pi-\ln 2+1-2^{-G+k-1}). \tag{6}$$

It is reasonable to consider that simultaneously $G\gg 1$, $k\gg 1$, $(G-k)\gg 1$. At leading orders in all of these, the derivative Eq. (6), vanishes when $k\simeq\log_2(G\ln 2)\simeq\log_2 G$. This is confirmed by Fig. 2, where of $\ln[\ln\mathcal{S}(k)]$ for

$G=8$ and $G=16$ is plotted (in arbitrary units). The use of $\ln[\ln\mathcal{S}]$ is due to the strong dependence of $\mathcal{S}$ in terms of k and to the sharpness of the minima.

To summarize this section, the number of symmetries of the EPO's strongly depends on the level label k. This differs from the number of symmetries for those eigenvector observables (EVO's) discussed in Ref. [3]. Indeed, the EVO's read $\mathcal{O}_\tau=\Sigma_{i\in I}X_i-\Sigma_{j\in J}X_j$, where τ designates suitable partitions $I\cup J$ of the subscripts into two equal subsets. Hence,

$\forall\tau$, the number of permutations that leave a given $\mathcal{O}_\tau$ invariant is just $[(N/2)!]^2=\mathcal{S}(G)/2$, the same for all EVO's for a given G. We found in Ref. [3] that the most robust EVO's likely correspond to $k\simeq\log_2 G$. This may seem paradoxical, because this value of k generates a minimum number of symmetries for the EPO's. The next Sections tell how EPO robustness can be defined and lift the paradox.

III. CONSEQUENCES OF LABELING CONFUSION

Consider a random permutation of the labels i of the experimental data X_i. Let P be the $N\times N$ matrix representing the permutation (zeroes everywhere, except for one ''1'' in each row and each column). The projectors $\mathcal{Q}_k$ become $P\mathcal{Q}_kP^{-1}$. If P does not belong to the symmetry group of Λ_k, the diagonalization property, $(\mathcal{C}-E_k)P\mathcal{Q}_kP^{-1}=0$, does not hold. Are such perturbed operators still close enough to eigenprojectors of $\mathcal{C}$ and can they define reliable observables $VP\mathcal{Q}_kP^{-1}V^T$, keeping in mind that P is a random unknown? This problem of robustness, investigated in [3] for EVO's $\mathcal{O}_\tau$, will now be discussed for EPO's Λ_k.

We define as the most robust that eigenprojector that minimizes the average, over all permutations, of the ''quadratic error,'' namely, the squared Hermitian norm of $(\mathcal{C}-E_k)P\mathcal{Q}_kP^{-1}$. More precisely, since $\mathcal{Q}_k^2=\mathcal{Q}_k$, $(P\mathcal{Q}_kP^{-1})^2=P\mathcal{Q}_kP^{-1}$ and, $\forall P,\mathrm{Tr}\,P\mathcal{Q}_kP^{-1}=2^{G-k}$, we minimize, in terms of k, the quantity

$$\mathcal{G}=(N!)^{-1}\sum_P \mathrm{Tr}\{[(\mathcal{C}-E_k)P\mathcal{Q}_kP^{-1}][P\mathcal{Q}_kP^{-1}(\mathcal{C}-E_k)]\}$$

$$=2^{G-k}E_k^2+(N!)^{-1}\sum_P [(\mathrm{Tr}\,\mathcal{C}^2P\mathcal{Q}_kP^{-1})$$

$$-2E_k(\mathrm{Tr}\,\mathcal{C}P\mathcal{Q}_kP^{-1})]. \tag{7}$$

Upon examining the above equations, we notice the occurrence of several ''permutation averaged'' operators of the form

$$\overline{\mathcal{A}}\equiv(N!)^{-1}\sum_P P\mathcal{A}P^{-1}=(N!)^{-1}\sum_P P^{-1}\mathcal{A}P. \tag{8}$$

These are easily evaluated, according to the following obvious two rules, (i) all the diagonal elements of $\overline{\mathcal{A}}$ are equal to the average of the diagonal elements of $\mathcal{A}$, and, (ii) all the off-diagonal elements of $\overline{\mathcal{A}}$ are equal to the average of the off-diagonal elements of $\mathcal{A}$. If $G=3$, e.g., we find that $\overline{C_3}$ has its diagonal equal to 1, and that all its off-diagonal elements read $\mathbf{c}=(c_1+2c_2+4c_3)/7$. We also find, for $\overline{\mathcal{C}_3^2}$ the diagonal elements $\mathbf{d}=1+c_1^2+2c_2^2+4c_3^2$, and the off-diagonal ones, $\mathbf{e}=2(c_1+2c_2+4c_3+2c_1c_2+c_2^2+4c_1c_{c3}+8c_2c_3+6c_3^2)/7$. Simultaneously we obtain,

$$2^{-2}\overline{Q}_1=2^{-1}\overline{Q}=\overline{Q}_3=\frac{1}{7}\mathcal{I}-\frac{1}{56}\mathbf{1}, \tag{9}$$

$\mathcal{I}$ is the unit matrix and $\mathbf{1}$ is an 8×8 block of ones.

To generalize for $G>3$, the rules governing $\mathbf{c}$ and $\mathbf{d}$ are transparent. We just state how one finds $\mathbf{e}$. It is the average of all the off-diagonal elements of $\mathcal{C}^2$. Since $\mathcal{C}^2$ is ultrametric like $\mathcal{C}$, all its rows and columns differ only by the order of the very same elements that they contain, with the very same multiplicities. Now, trivially, $\Sigma_j(\mathcal{C}^2)_{ij}=\Sigma_{jk}\mathcal{C}_{ik}\mathcal{C}_{kj}$, and the sum upon j generates a constant $\sigma=\Sigma_j\mathcal{C}_{kj}=1+c_1+2c_2+4c_3+\cdots$, which does not depend on k. Hence $\Sigma_j(\mathcal{C}^2)_{ij}=\sigma^2$. There remains to subtract the diagonal element $\mathbf{d}=1+c_1^2+2c_2^2+\cdots$, and finally the average off-diagonal element reads $\mathbf{e}=(N-1)^{-1}[(1+\Sigma_{n=1}^G2^{n-1}c_n)^2-1-\Sigma_{n=1}^G2^{n-1}c_n^2]$.

The equality between $\overline{\mathcal{R}_1}=\overline{\mathcal{Q}_1/4}$, $\overline{\mathcal{R}_2}=\overline{\mathcal{Q}_2/2}$, and $\overline{\mathcal{R}_3}=\overline{\mathcal{Q}_3}$ is not surprising. Indeed, after the renormalization by 2^{k-G}, the global factor is the same—2^{-G}. More important, the block structure of such ''projectors'' $\mathcal{R}_k$ and the equal numbers of $+1$ and -1 matrix elements, beside zeroes, makes $1/(1-N)$ the net average of the off-diagonal elements, since diagonal elements are just $+1$. The same reasoning holds for any G. Hence the k dependence of $\mathcal{G}$ reads

$$\mathcal{G}=2^{G-k}(E_k^2-2E_k\,\mathrm{Tr}\,\mathcal{C}\overline{\mathcal{R}_k}+\mathrm{Tr}\,\mathcal{C}^2\;\overline{\mathcal{R}_k})$$

$$=2^{G-k}(E_k^2-2E_k\,\mathrm{Tr}\,\overline{\mathcal{C}}\mathcal{R}_k+\mathrm{Tr}\,\overline{\mathcal{C}^2}\mathcal{R}_k), \tag{10}$$

where there is no dependence upon the subscript k of $\overline{\mathcal{R}_k}\equiv2^{k-G}\;\overline{\mathcal{Q}_k}$. For $G=3$, we obtain $\mathrm{Tr}\,\mathcal{C}\overline{\mathcal{R}}=1-\mathbf{c}=(7-c_1-2c_2-4c_3)/7$ and $\mathrm{Tr}\,\mathcal{C}^2\overline{\mathcal{R}}=\mathbf{d}-\mathbf{e}=(7-2c_1-4c_2-8c_3+7c_1^2-4c_1c_2+12c_2^2-8c_1c_3-16c_2c_3+16c_3^2)/7$.

More generally, all matrices $\overline{\mathcal{A}}$, being invariant under the permutation group, depend on two parameters $\mathbf{u}$ and $\mathbf{v}$ only, their diagonal and off-diagonal elements, respectively. Any diagonal element of any product $\overline{\mathcal{A}}\mathcal{R}_k$ contains on one hand $\mathbf{u}$, weighted by the diagonal element N^{-1} of $\mathcal{R}_k$, and on the other hand $\mathbf{v}$, weighted by all the off-diagonal zeroes, $+N^{-1}$ and $-N^{-1}$ in a column of $\mathcal{R}_k$. The net balance of such off-diagonal weights is $-N^{-1}$. Hence, the diagonal element of the product boils down to $N^{-1}(\mathbf{u}-\mathbf{v})$. Finally, the trace operation gives the general result $\mathrm{Tr}\,\overline{\mathcal{A}}\mathcal{R}_k=\mathbf{u}-\mathbf{v}$.

To summarize this section, criterion $\mathcal{G}$, Eqs. (10), is available for the robustness of EPO's. While ultrametricity is sufficient to define eigenvectors and eigenprojectors, the easy calculation of $\mathcal{G}$, however, demands an explicit model for the elements c_k of $\mathcal{C}$, which govern the eigenvalues. This is the subject of the next section.

IV. ILLUSTRATIVE NUMERICAL EXAMPLE

We use the model described earlier [5]. The covariances are parametrized by one parameter δ only, $c_k=\delta^k$. The parameter δ is a positive number, slightly smaller than one, and represents a ''survival'' probability along any segment of the ''genetic'' (ultrametric) graph. If $\delta=1-\varepsilon$, the parameter ε indicates a small mutation probability for each generation. The formula for $\mathcal{G}$ then becomes

$$2^{k-G}\mathcal{G}=\left[1+\delta\frac{(2\delta)^{k-1}-1}{2\delta-1}-2^{k-1}\delta^k\right]^2$$

$$-2\left[1+\delta\frac{(2\delta)^{k-1}-1}{2\delta-1}-2^{k-1}\delta^k\right]$$

$$\times\left[1-\delta\frac{(2\delta)^G-1}{(2^G-1)(2\delta-1)}\right]$$

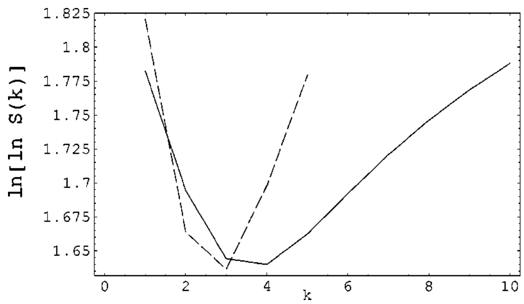

FIG. 2. $\ln[\ln \mathcal{S}(k)]$ as a function of k for $G=8$, dashed line, and $G=16$, solid line. Notice the minima for $k=\log_2 G$. Scales arbitrarily adjusted to locate these minima at similar levels.

$$+1+\delta^2\,\frac{(2\,\delta^2)^G-1}{2\,\delta^2-1}-(2^G-1)^{-1}$$
$$\times\left\{\left[1+\delta\frac{(2\,\delta)^G-1}{2\,\delta-1}\right]^2-1-\delta^2\,\frac{(2\,\delta^2)^G-1}{2\,\delta^2-1}\right\}. \qquad (11)$$

A slightly tedious operation gives the expansion,

$$\frac{\partial \mathcal{G}}{\partial k}=(2^{G+k}-2^{2G+1-k})\varepsilon^2\ln 2+\mathcal{O}(\varepsilon^3), \qquad (12)$$

The minimum for $k\simeq(G+1)/2$ is confirmed by Fig. 3, showing several cases, $G=8{,}16{,}20$ with $\delta=0.99{,}0.95$. Similar conclusions hold for values of ε in the few percent range. Despite the logarithmic scale used in Fig. 3, it is reasonable to claim that the shown minima are not very sharp. Hence a reasonably broad band of values of k makes robust enough quite a few EPO's around the optimal value $k\simeq(G+1)/2$. Naturally, the conclusion is valid for the present model only, but it is likely to have a wider range. A further discussion of the validity of ultrametricty for realistic data is also in order, anyhow. To the interested reader we suggest Ref. [6].

V. DISCUSSION AND CONCLUSION

In the situation of G generations with ''binary ultrametricity'' for genetic data, the results of Ref. [3] and the present work can be summarized and discussed as follows.

(i) One can Fourier analyze experimental data $X_i, i=1,\ldots,2^G$ into ''eigenvector components'' $\mathcal{O}_\tau, \tau=1,\ldots,2^G-1$ or ''eigenprojector intensities'' $\Lambda_k, k=1,\ldots,G$. Both sets of observables list decorrelated informations about contrasts between the subfamilies described by the levels of the genetic graph. Both sets are useful to detect contrasts that might hint at genetic diversification.

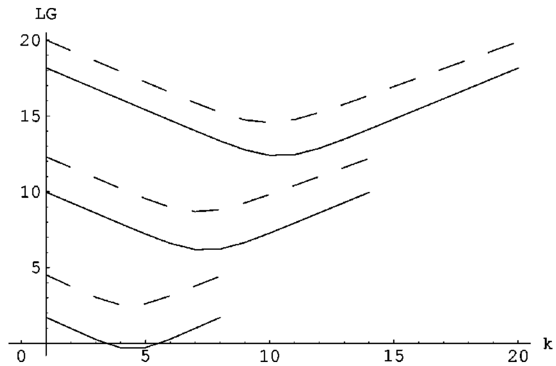

FIG. 3. $\mathrm{LG}\equiv\ln\mathcal{G}$ as a function of k for $G=20$ (upper pair), $G=14$ (middle), and $G=8$ (lower pair). Solid lines, $\delta=0.99$, dashed lines, $\delta=0.95$. Notice the minima for $k\simeq(G+1)/2$.

(ii) All $\mathcal{O}_\tau$'s show the same number of symmetries, hence a similar robustness if one suspects that few data X_i carry erroneous labels i. Conversely, Λ_k's with $k\simeq\log_2 G$ have a minimum number of symmetries, hence are likely to be slightly perturbed.

(iii) If many labels i are suspect, robustness can be estimated from criterions averaging over all permutations. In both this paper and Ref. [3], we used criterions answering the question ''How do $\mathcal{O}_\tau$ and Λ_k differ from eigenobservables with eigenvalue E_k?'' This is a significant question, because E_k and the level in the graph are in a one-to-one correspondence. Our criterions take into account several factors, such as the whole set of E_k's with their hierarchy, their multiplicities, and the numbers of symmetries of the observables under label reshuffling.

(iv) In that case, of completely random permutations, and in the more specific model where $c_n=\delta^n$, two distinct compromises occur between the factors influencing such robustness criterions. For $\mathcal{O}_\tau$, the large degeneracy 2^{G-k} favors low values $k\simeq\log_2 G$, because random permutations might still convert an eigenvector into a mixture of eigenvectors with the same E_k. The high degeneracy compensates for the fact that E_k lies at the lower end of the spectrum. For Λ_k, which by its very definition (degeneracy already collected) shows no degeneracy, values $k\simeq G/2$ bring both a bigger symmetry group and an eigenvalue well embedded in the spectrum.

In practice, the reasonably flat minima shown in Fig. 3 make it reasonable to first use the EPO analysis. Jumps in the Λ_k sequence might trigger some attention. The situation for robustness can be appraised, depending on whether the likely number of wrong labels for the leaves of the graph is small or large. After such considerations, an EVO analysis can make a useful complement.

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