Higher-Order Neural Networks, Polyà Polynomials, and Fermi Cluster Diagrams

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Abstract

The problem of controlling higher-order interactions in neural networks is addressed with techniques commonly applied in the cluster analysis of quantum many-particle systems. For multi-neuron synaptic weights chosen according to a straightforward extension of the standard Hebbian learning rule, we show that higher-order contributions to the stimulus felt by a given neuron can be readily evaluated via Polyà’s combinatoric group-theoretical approach or equivalently by exploiting a precise formal analogy with fermion diagramatics.

PACS numbers: 07.05.Mh, 02.20.-a, 05.30.Fk, 07.05.Pj
In attempting to unravel the mechanisms of information processing and attendant adaptive behavior in neurobiological systems, considerable attention is currently being directed to non-linear processing in dendritic trees and to the computational power that can be gained from multiplicative or higher-order interactions between neurons [1,2]. This focus is supported by a large body of theoretical work demonstrating enhanced performance in artificial neural networks involving such higher-order or multi-neuron interactions, as applied to a variety of information-processing tasks, most notably memory storage and recall [3–13]. Introduction of higher-order couplings is accompanied, however, by the threat of a combinatoric explosion that may strongly inhibit analysis, evaluation, and optimization. In this note we expose some simple techniques based on group-theoretic symmetry arguments that serve, in some cases, to reduce the severity of these problems and give access to the advantages of higher-order networks for problem domains involving complex correlations. Our study is guided by interesting parallels with the diagrammatic analysis of fermion clusters in many-body physics.

We consider the following simple but standard model of a higher-order neural network. The network consists of \( N \) binary-output hard-threshold units (model neurons) \( i \) whose state variables \( \sigma_i \) take the value +1 if the unit is active (“firing”) and −1 if the unit is inactive (“not firing”). Model neuron \( i \) receives inputs from exactly \( K_i \) other units of the network, with self interactions excluded so that \( 1 \leq K_i \leq N - 1 \). A given neuron updates its state on a discrete time grid according to the deterministic threshold rule

\[
\sigma_i(t + 1) = \text{sgn} [h_i(t)] , \quad i = 1, \ldots, N . \quad (1)
\]

Here \( h_i(t) \) is the net stimulus felt by the neuron at time \( t \), coming from internal and external inputs but reduced by a threshold parameter. For our purposes it is immaterial whether sequential or parallel updating is imposed. The general higher-order synaptic structure of the network model is expressed in the assumed form
\[ h_i(t) = c_{i0}(t) + \sum_{j_1} c_{ij_1}(t) \sigma_{j_1} + + \sum_{j_1j_2} c_{ij_1j_2}(t) \sigma_{j_1}(t) \sigma_{j_2}(t) + \cdots + \]
\[ + \sum_{j_1 < j_2 < \cdots < j_{K_i}} c_{ij_1j_2 \cdots j_{K_i}}(t) \sigma_{j_1}(t) \sigma_{j_2}(t) \cdots \sigma_{j_{K_i}}(t) \]
\[ = C_0(t) + C_1(t) + C_2(t) + \cdots + C_{K_i}(t), \quad (2) \]

where the sums include only those \( K_i \) neurons from which neuron \( i \) receives inputs. The first term represents any external input to neuron \( i \) (reduced by its threshold), while the second term is the usual one representing binary interactions, a simple linear sum of states of input neurons weighted by synaptic strengths \( c_{ij_1} \). The higher-order terms in the expansion, for \( n \geq 2 \), represent “multiplicative” interactions in that they are linear combinations of the products of two or more input-neuron states. One also speaks of a “sum-of-products” form for such interactions.

We observe that the general \( n \)th-order contribution,
\[ C_n = \sum_{j_1 < j_2 < \cdots < j_n} c_{ij_1j_2 \cdots j_n} \sigma_{j_1} \sigma_{j_2} \cdots \sigma_{j_n}, \quad (3) \]
representing the irreducible interaction of \( n \) neurons with neuron \( i \), introduces \( \binom{K_i}{n} \) = \( K_i! / n!(K_i - n)! \) weight parameters. Accordingly, specification of the net stimulus \( (2) \) requires \( 2^{K_i} \) parameters. The exponential explosion of parameters with increasing connectivity \( K_i \) has deterred widespread application of higher-order networks, in spite of their theoretical advantages.

Indeed, complete optimization of a network of a network having all possible combinations of higher-order terms is patently impractical for sizable values of \( K_i \) typically needed in real-world applications. However, a restricted optimization problem has been attacked by retaining only a strongly reduced pattern-specific connectivity \[14,15\], while otherwise implementing the extended Hebbian learning rule to be introduced below. A similar strategy based on a connection-pruning scheme adapted to the pattern domain has been employed to tame the combinatoric explosion of parameters in higher-order probabilistic perceptrons \[16\].

Of course, if the entire array of coefficients \( c_{ij_1j_2 \cdots j_n} \) is specified at the outset, the explosive
combinatoric optimization problem becomes moot. In this note we shall focus on the fully
connected network in an important special case of “one-shot” learning in which it is feasible
and straightforward to evaluate the general term $C_n$ of the series (2). In fact, by exploiting
standard group-theoretic results, we are actually able to sum this series in the limit of
asymptotically large connectivity ($K_i \to \infty$, implying an infinitely large network).

We consider the familiar task of storage and recall of $p$ random patterns $S^\mu =
\{S_1^\mu, S_2^\mu, \ldots, S_N^\mu\}$ in the firing activities of the neuronal units, where again $S_j \in \{-1,1\}$. As is well known [4,7,8], such patterns can be faithfully sto-
red as fixed points of the dynamics (1) of the network model to a capacity $p = O(N^K)$ (with $K = \min_i K_i$), if the
weight parameters of the stimulus expression (2) are chosen according to an extension of the
classical Hebbian learning rule to the presence of interactions of all orders up to $K_i$:

$$c_{ij_1j_2\ldots j_n} = \sum_{\mu=1}^p S_i^\mu S_{j_1}^\mu S_{j_2}^\mu \cdots S_{j_n}^\mu, \quad n = 1, \ldots, K_i. \quad (4)$$

The efficacy of memory storage is commonly analyzed in terms of the overlaps

$$m^\mu(t) = \sum_j S_j^\mu \sigma_j(t) \quad (5)$$

of the current network configuration $\{\sigma_1(t), \sigma_2(t), \cdots, \sigma_N(t)\}$ with a given pattern $S^\mu$. When a relative-entropy cost function is adopted [17], this specification can be shown to be optimal
among the class of simple local learning rules (where “local” implies that changes of synaptic
strength depend only on the states of the neurons interacting at the given synapse).

The generic term (3) in the stimulus expansion (2) is evaluated as follows. We first
examine the modified $n$th-order contribution

$$\overline{c}_n = \sum_{j_1\ldots j_n} c_{ij_1\ldots j_n} \sigma_{j_1}(t)\cdots \sigma_{j_n}(t) \quad (6)$$

to the net stimulus, which consists of $K_i^n$ terms. This auxiliary quantity contains redundant
terms of two kinds: (i) “diagonal” terms in which two or more of the indices $j_1, \ldots, j_n$
coincide and (ii) “symmetrical” terms differing only through a permutation of distinct labels
$j_1, \ldots, j_n$, which may be combined into a single term by redefining the weight parameter
c_{j_1 \cdots j_n} as the sum of the weight parameters with permuted indices. The former terms are redundant because they already appear in lower-order contributions of the expansion (2). The latter terms lead to overcounting by a factor \( n! \).

Inserting the learning rule (4) into Eq. (6) and interchanging the order of the summations, we may write

\[
C_n = \sum_{j_1 \cdots j_n} c_{ij_1 \cdots j_n} \sigma_{j_1} \cdots \sigma_{j_n} = \sum_{j_1 \cdots j_n} \sum_{\mu=1}^{p} S_i^{\mu} S_{j_1}^{\mu} \cdots S_{j_n}^{\mu} \sigma_{j_1} \cdots \sigma_{j_n}
\]

\[
= \sum_{\mu=1}^{p} S_i^{\mu} \left( \sum_{j_1} S_{j_1}^{\mu} \sigma_{j_1} \right) \cdots \left( \sum_{j_n} S_{j_n}^{\mu} \sigma_{j_n} \right) = \sum_{\mu=1}^{p} S_i^{\mu} \left[ \sum_{j} S_{j}^{\mu} \sigma_{j} \right]^n .
\]

The desired \( n \)th-order contribution \( C_n \) and its modified counterpart \( \overline{C}_n \) are evidently related by

\[
C_n = \sum_{j_1 < \cdots < j_n} c_{ij_1 \cdots j_n} \sigma_{j_1} \cdots \sigma_{j_n} = \frac{1}{n!} \overline{C}_n \det(\delta_{j_\alpha j_\beta}) .
\]

The \( n \times n \) determinant in (4.3) eliminates all “diagonal” terms with two or more indices coincident, while the statistical factor \( n! \) compensates for the overcounting of symmetrical terms.

It is next convenient to define “generalized” overlaps

\[
m_{\alpha}^{\mu}(t) = \sum_{j} [S_j^{\mu} \sigma_j(t)]^\alpha
\]

of the current network configuration with one of the prescribed patterns, \( \alpha \) being a positive integer. Since \( S_j^2 = \sigma_j^2 = 1 \), the quantity \( m_{\alpha}^{\mu}(T) \) reduces to \( K_i \) for \( \alpha \) even and to \( m_{\mu}(t) \) for \( \alpha \) odd. Appealing to direct evaluation of the right-hand side of Eq. (3) or Eq. (8) for \( n = 1 - 4 \), we establish the pattern of behavior for the higher orders:

\[
C_1 = \sum_{\mu=1}^{p} S_i^{\mu} [m_1^{\mu}] ,
\]

\[
C_2 = \sum_{\mu=1}^{p} S_i^{\mu} \frac{1}{2!} [(m_1^{\mu})^2 - m_2^{\mu}] ,
\]

\[
C_3 = \sum_{\mu=1}^{p} S_i^{\mu} \frac{1}{3!} [(m_1^{\mu})^3 - 3m_1^{\mu}m_2^{\mu} + 2m_3^{\mu}] ,
\]

\[
\]
and
\[ C_4 = \sum_{\mu=1}^p S_4^\mu \frac{1}{4!} [(m_1^\mu)^4 - 6(m_1^\mu)^2 m_2^\mu + 8m_1^\mu m_3^\mu + 3(m_2^\mu)^2 - 6m_4^\mu]. \] (13)

It is seen that the generic term \( C_n \) is built as a sum over all patterns of individual terms of the form
\[ S_4^\mu \frac{1}{4!} \gamma(\alpha_1, \ldots, \alpha_n) \prod_{l=1}^n (m_l^\mu)^{\alpha_l}, \] (14)

where \( \gamma(\alpha_1, \ldots, \alpha_n) \) is a statistical weight factor and the generalized overlaps \( m_l^\mu \) enter with positive integral powers satisfying the partitioning condition
\[ \sum_{l=1}^n l\alpha_l = n. \] (15)

The statistical factor is found to obey the sum rules
\[ \sum_{\alpha} \gamma(\alpha_1, \ldots, \alpha_n) = 0 \quad \text{and} \quad \sum_{\alpha} |\gamma(\alpha_1, \ldots, \alpha_n)| = n!, \] (16)

and can be constructed as
\[ \gamma(\alpha_1, \ldots, \alpha_n) = n!/[\prod_{l=1}^n (-1)^{\alpha_l+1} (l^{\alpha_l}!)\alpha_l!]. \] (17)

Thus, for arbitrary \( n \), the contribution \( C_n \) can be written explicitly as
\[ C_n = \sum_{\mu=1}^p S_4^\mu \mathcal{P}_n(m_1^\mu, \ldots, m_n^\mu) \] (18)

where
\[ \mathcal{P}_n(m_1, \ldots, m_n) = \frac{1}{n!} \sum_{\alpha} \prod_{l=1}^n \gamma(\alpha_1, \ldots, \alpha_n) m_l^{\alpha_l}. \] (19)

The sum over \( \alpha \) in definition (19) extends only over those \( n \)-dimensional vectors \( \alpha = (\alpha_1, \ldots, \alpha_n) \) whose components satisfy the constraint (15). The quantity \( \mathcal{P}_n(m_1, \ldots, m_n) \) is identified as a generalized Polyà polynomial [18] of the symmetric group \( S_n \), with the signs \((-1)^{\alpha_l+1}\) of the corresponding cyclic permutations incorporated.

For given \( n \), the total number of solutions \( P(n) \) of condition (15) can be determined by induction from the recurrence relation [21].
\[ P(n) = \frac{1}{n} \sum_{q=1}^{n} \rho(q) P(n-q), \quad (20) \]

in which the divisor function \( \rho(l) \) is the sum of the first powers of the divisors of \( q \). For large \( n \), \( P(n) \) behaves asymptotically as

\[ P(n) = \frac{1}{4n\sqrt{3}} e^{\pi \sqrt{\frac{2}{3}} n}. \quad (21) \]

Finally, the generating function of the Polyà polynomials may be employed to calculate the sum of all individual \( n \)-order contributions, i.e. the net internal stimulus \( h_i(t) \) of Eq. (2), in limit of large connectivity \( K_i \), which is equivalent to the thermodynamic limit. One finds

\[ \sum_{n=0}^{\infty} C_n = \sum_{\mu=1}^{\rho} S_\mu^l \exp \left[ \sum_{l=1}^{\infty} \frac{(-1)^{l+1}}{l} m_i^l \right] \quad (K_i \to \infty). \quad (22) \]

While this is a beautiful formal result, practical neural network applications often work with a single fixed order or with a few low orders adapted to the complexity of the problem (see, e.g. Ref. [22]).

Combinatoric group-theoretical considerations reveal an interesting one-to-one correspondence between the \( n \)th-order contribution \( C_n \) to the stimulus sum (2) and the sum of planar \( n \)-particle cluster diagrams for noninteracting particles obeying Fermi statistics. (Substitution of a permanent for the determinant in expression (8) would produce a one-to-one correspondence with the sum of Bose \( n \)-body cluster diagrams.) Each fermion cluster diagram is uniquely defined by an \( n \)-dimensional vector \((\alpha_1, ..., \alpha_n)\) satisfying relation (15) and specifying a partitioning of the \( n \)-particle cluster into sub-clusters correlated by exchange, namely into \( \alpha_1 \) 1-cycles, \( \alpha_2 \) 2-cycles, ... and \( \alpha_n \) \( n \)-cycles. The statistical weight factor \( \gamma(\alpha_1, ..., \alpha_n) \) is the number of ways in which \( n \) particles can be assigned to \( \alpha_l \) exchange clusters of size \( l \), with \( l \) running from 1 to \( n \). Figure 1 shows all possible cluster diagrams up to order \( n = 7 \). Each contribution diagram consists of \( n \) filled dots and the associated exchange lines. Reflecting the Fermi (or Bose) symmetry of the wave function, the exchange lines only occur in closed loops: the particles belonging to a given exchange cluster appear as nodes in a continuous circuit of lines that represents a transposition or
cyclic permutation. Cluster diagrams of this type (though with additional lines representing dynamical correlations) are used in the description of non-interacting fermions or bosons in the correlated wave-function and correlated density-matrix formalisms \[19,20\].

A large number of computer experiments \[23\] have established the following behavior of higher-order networks when applied to problems in pattern recognition. When the patterns to be recognized are structured rather than random, the network dynamics usually converges to the pattern with closest \textit{structural} similarity to the initial pattern, rather than to (or to a state very near) the pattern having largest overlap with the initial state. This behavior contrasts with that of first-order networks having only binary synapses \[24\]: relative to these conventional systems, higher-order networks demonstrate a greatly enhanced capability for structural discrimination of arbitrarily complex patterns. Moreover, when functioning in the regime of dilute pattern storage (i.e., far from saturation, thus \(p \sim N << N^K, K \geq 2\)), the basins of attraction of the memorized patterns are dramatically enlarged. Finally, it is to be emphasized that in the model we have considered, the combinatoric explosion of weight coefficients is obviated, since the network only needs to know the overlaps of the present state with all the patterns to be embedded.

This paper is a contribution to the ZiF Research Year on the Sciences of Complexity: From Mathematics to Complexity to a Sustainable World. The research was supported in part by the U.S. National Science Foundation under Grant No. PHY-9900713.
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Figure Caption

Fig. 1. All possible fermion cluster diagrams for $n = 2, 3, ..., 7$, in the absence of dynamical correlations.
