Symmetric neural networks

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1 General case for y = Ax

$$\boxed{\text{original}} \quad y_j = \sum_i a_{ij} x_i. \tag{1}$$

Equivariance implies:

swapped
$$y_j(\sigma(x_j x_k)x) = y_k$$
 original
$$\sum_{i \neq j,k} a_{ij}x_i + a_{kj}x_j + a_{jj}x_k = \sum_{i \neq j,k} a_{ik}x_i + a_{jk}x_j + a_{kk}x_k.$$
 (2)

Comparing coefficients yields:

In other words, the matrix A is of the form:

$$A = \alpha I + \beta 11^T. \tag{4}$$

2 Case for $y_k = A_k x \cdot x$

The general form of a "quadratic" vector function is:

$$y = (Ax) \cdot x + Bx + C. \tag{5}$$

We just focus on the quadratic term $(Ax) \cdot x$:

$$\boxed{\text{original}} \quad y_k = \sum_{i} \left[\sum_{i} a_{ij}^k x_i \right] x_j. \tag{6}$$

Note that the matrix A is "3D" and has $N \times N \times N$ entries.

Equivariance implies:

$$\sum_{j \neq h, k} \sum_{i \neq h, k} a_{ij}^k x_i x_j + a_{hh}^k x_k^2 + a_{kh}^k x_h x_k + a_{hk}^k x_k x_h + a_{kk}^k x_h^2 = \sum_{j \neq h, k} \sum_{i \neq h, k} a_{ij}^h x_i x_j + a_{hh}^h x_h^2 + a_{hh}^h x_h x_h + a_{hk}^h x_h x_k + a_{hk}^h x_h^2$$

which yields:

$$a_{ij}^{h} = a_{ij}^{k} \qquad \forall h, k, (i \neq h, k, j \neq h, k)$$

$$a_{hh}^{h} = a_{kk}^{k} \qquad \forall h, k$$

$$a_{hh}^{k} = a_{kk}^{h} \qquad \forall h, k$$

$$a_{kh}^{k} + a_{hk}^{k} = a_{kh}^{h} + a_{hk}^{h} \qquad \forall h, k.$$

$$(8)$$

With output space "folded in half"

Now suppose the output is only 1/2 the dimension of the input. Define a new form of equivariance such that the input permutation would act on the output as "folded in half".

In other words, equivariance is changed to:

swapped
$$y_k \cdot \sigma(x_k | x_h) = y_h \text{ or } y_{h-N/2} \text{ original}$$
 (9)

where τ is σ acting on y as double its length and identifying $y_i = y_{i+N/2}$.

3.1 Linear case

Just notice that the dimension of y is halved:

$$\boxed{\text{original}} \quad y_j = \sum_i a_{ij} x_i. \tag{10}$$

"Folded" equivariance implies:

$$\begin{bmatrix}
swapped \\
y_j(\sigma(x_j x_k)x) &= y_k \\
\sum_{i \neq j,k} a_{ij}x_i + a_{kj}x_j + a_{jj}x_k &= \sum_{i \neq j,k} a_{ik}x_i + a_{jk}x_j + a_{kk}x_k
\end{bmatrix} (11)$$

with the restriction $j \in \{1, ..., N/2\}$, and $k \in \{1, ..., N\}$.

The constraints obtained are same as before, except that index ranges are different:

These constraints give rise to a matrix of this form (for the 6×2 case, numbers represent different colors):

$$5 1 1 2 3 4
1 5 1 2 3 4
1 1 5 2 3 4$$
(12)

This pattern is obtained from my Python code.

3.2 Quadratic case