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■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... We can now analyze and characterize the combinatorial nature and complexity of the "classification results" table from page 9 (1/12/2023) – and the "classification cases" table from the same page. The "cases" (C) that arise in the specific example associated with these two tables – considering "words" of length 3 consisting of the letters '0', '1', '2' and '3' – can be explained via COMPOSITIONS (of the integer 3) and MULTINOMIAL COEFFICIENS. The multinomial coefficient $\binom{M}{m_1,\ldots,m_k}$ is defined as $\frac{M!}{m_1!\cdot\ldots\cdot m_k!}$.

(N=3)	case C	n_3	n_2	n_1	n_0	P^x
(3)	here: $\binom{4}{1}=4$	0	0	0	3	1
		0	0	3	0	1
		0	3	0	0	1
		3	0	0	0	1
(1,2)	here: $\binom{4}{2}=6$	0	0	1	2	3
		0	1	0	2	3
		1	0	0	2	3
		0	1	2	0	3
		1	0	2	0	3
		1	2	0	0	3
(2,1)	here: $\binom{4}{2}=6$	0	0	2	1	3
		0	2	0	1	3
		2	0	0	1	3
		0	2	1	0	3
		2	0	1	0	3
		2	1	0	0	3
(1,1,1)	here: $\binom{4}{3}=4$	0	1	1	1	6
		1	0	1	1	6
		1	1	0	1	6
		1	1	1	0	6

Compositions of N=3.

$\Rightarrow$ Total no. of cases: $4\cdot 1 + 2\cdot 6\cdot 3 + 4\cdot 6 = 64 = (\text{noLetters})^N = 4^3$

In our setting, it defines the number of possible, different "words" consisting of N letters from the set {'0', '1', '2', '3'} – where '0' appears n_0 times, ... and '3' appears n_3 times. Thus, $N = n_0 + n_1 + n_2 + n_3$. The left table organizes the cases based on the $2^{N-1} = 2^2 = 4$ compositions of N: (3), (1,2), (2,1) and (1,1,1). The sub-cases for the 4 compositions consist of $\binom{4}{1}$, $\binom{4}{2}$, $\binom{4}{2}$ and $\binom{4}{3}$ combinatorial possibilities, as indicated in the table.

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OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

- *Laplacian eigenfunctions and neural networks:...*

× The table on the previous page includes the (not-normalized) probability values of **P** — for the four compositions of the "word" length $N = 3$. The P-values are given by the following multinomial coefficients:

$$\binom{3}{0,0,0,3} = \binom{3}{0,0,3,0} = \binom{3}{0,3,0,0} = \binom{3}{3,0,0,0} = \frac{3!}{0!0!0!3!} = 1$$

$$\binom{3}{0,0,1,2} = \ldots = \binom{3}{1,2,0,0} = \binom{3}{0,0,2,1} = \ldots = \binom{3}{2,1,0,0} = \frac{3!}{0!0!1!2!} = 3$$

$$\binom{3}{0,1,1,1} = \binom{3}{1,0,1,1} = \binom{3}{1,1,0,1} = \binom{3}{1,1,1,0} = \frac{3!}{0!1!1!1!} = 6$$

composition for N=4		n_3	n_2	n_1	n_0	$P^{\times}$
(4)	4	0	0	0	4	1
		...				
		4	0	0	0	1
(1,3)	6	0	0	1	3	4
		...				
		1	3	0	0	4
(3,1)	6	0	0	3	1	4
		...				
		3	1	0	0	4
(2,2)	6	0	0	2	2	6
		...				
		2	2	0	0	6
(1,1,2)	4	0	1	1	2	12
		...				
		1	1	2	0	12
(1,2,1)	4	0	1	2	1	12
		...				
		1	2	1	0	12
(2,1,1)	4	0	2	1	1	12
		...				
		2	1	1	0	12
(1,1,1,1)	1	1	1	1	1	24

Compositions of $N=4$ and cases.

⇒ Total number of cases:

$$4\cdot1 + 2\cdot6\cdot4 + 6\cdot6 + 3\cdot4\cdot12 + 24$$
$$= 4 + 48 + 36 + 144 + 24$$
$$= \underline{256} = 4^4 = (\text{noLetters})^N$$

The left table shows all combinatorial cases and sub-cases for "words" of length $N = 4$. The number of compositions of 4 is $2^{4-1} = 8$. The P-values are these multinomial coefficients:

$$\binom{4}{0,0,0,4} = \ldots = \frac{4!}{0!0!0!4!} = 1$$

$$\binom{4}{0,0,1,3} = \ldots = \frac{4!}{0!0!1!3!} = 4$$

$$\binom{4}{0,0,2,2} = \ldots = \frac{4!}{0!0!2!2!} = 6$$

$$\binom{4}{0,1,1,2} = \ldots = \frac{4!}{0!1!1!2!} = 12$$

$$\binom{4}{1,1,1,1} = \frac{4!}{1!1!1!1!} = 24$$

■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... To better understand how this combinatorial progression evolves for $N > 4$, we sketch the possibilities for $N = 5$. **The** $2^{N-1} = 2^{5-1} = 2^4 = 16$ compositions of 5 are:

(5), (1,4), (4,1), (2,3), (3,2), (1,1,3), (1,3,1), (3,1,1),

(1,1,1,2), (1,1,2,1), (1,2,1,1), (2,1,1,1),

(1,2,2), (2,1,2), (2,2,1), (1,1,1,1,1).

composition (N=5)		n_3	n_2	n_1	n_0	P^x
(5)	4	0	0	0	5	1
		...				
		5	0	0	0	1
2 {(1,4) & (4,1)}	6	0	0	1	4	5
		...				
		1	4	0	0	5
2 {(2,3) & (3,2)}	6	0	0	2	3	10
		...				
		2	3	0	0	10
3 {(1,1,3) & (1,3,1) & (3,1,1)}	4	0	1	1	3	20
		...				
		1	1	3	0	20
3 {(1,2,2) & (2,1,2) & (2,2,1)}	4	0	1	2	2	30
		...				
		1	2	2	0	30
(1,1,1,2)	1	1	1	1	2	60
(1,1,2,1)	1	1	1	2	1	60
(1,2,1,1)	1	1	2	1	1	60
(2,1,1,1)	1	2	1	1	1	60
(1,1,1,1,1)? NOT USED: only n_0, n_1, n_2, n_3!						

Compositions of $N=5$ and cases.

⇒ Total number of cases:

$4\cdot 1 + 2\cdot 6\cdot 5 + 2\cdot 6\cdot 10$

$+ 3\cdot 4\cdot 20 + 3\cdot 4\cdot 30 + 60 + 60 + 60 + 60$

$= 4 + 60 + 120 + 240 + 360 + 240$

$= \mathbf{1024} = 4^5 = (\text{noLetters})^N$

In this case, the relevant multinomial coefficients defining the P-values are:

$$\binom{5}{0,0,0,0,5} = \frac{120}{120} = 1$$

$$\binom{5}{0,0,0,1,4} = \frac{120}{24} = 5$$

$$\binom{5}{0,0,0,2,3} = \frac{120}{12} = 10$$

$$\binom{5}{0,0,1,1,3} = \frac{120}{6} = 20$$

$$\binom{5}{0,0,1,2,2} = \frac{120}{4} = 30$$

$$\binom{5}{0,1,1,1,2} = \frac{120}{2} = 60$$

Given a number N, it is interesting that the numbers of terms in N's compositions are given by binomial co-efficients.

...

OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks: ... We consider the cases $N=3$, $N=4$ and $N=4$ to show the relationship between the numbers of terms in compositions of N and binomial coefficients:

$N=3$	$\binom{2}{k}$	$N=4$	$\binom{3}{k}$	$N=5$	$\binom{4}{k}$
3	1	4	1	5	1
12 21	2	13 31 22	3	14 41 23 32	4
111	1	112 121 211	3	113 131 311 122 212 221	6
		1111	1	1112 1121 1211 2111	4
				11111	1

Compositions are written simply as abcd... instead of (a,b,c,d,...).

The table shows that the number of terms in a composition of N satisfies the law

$$\binom{N-1}{k-1} = p_k^N,$$

$k = 1, \ldots, N$, where k is the number of non-zero terms and p_k^N is the number of possibilities to express N as a k-term composition.

1) OUR APPLICATION CONCERNS A MULTI-CLASS CLASSIFICATION PROBLEM. Thus, one must ultimately generalize this detailed combinatorial analysis of from the binary to the multi-class setting.

2) The combinatorial insight gained from this detailed analysis of "classification result words" should ultimately guide, for example, the CHOICES OF WEIGHTS USED IN THE PERFORMANCE FUNCTION for the various classification result types, i.e., TN, TP_{cl}, FN_{cl}, FP_{cl} and $MC_{cl1,cl2}$.

...

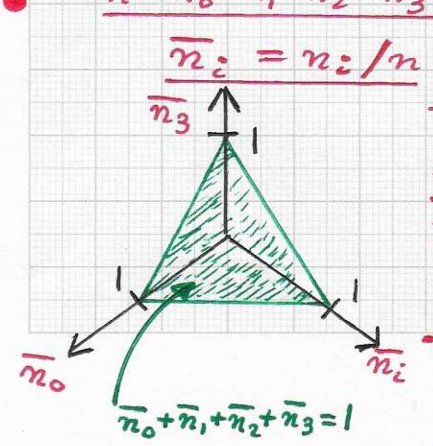
■ OBJECT AND MATERIAL EIGENFUNCTIONS – Cont'd.

• Laplacian eigenfunctions and neural networks:... First, we turn our attention to problem 2) described on the previous page, i.e., associating and using weights for certain classification result outcomes. We describe this problem and a possible solution approach for the binary classification setting. For example, the classification of ten materials analyzed and classified by the system might have the following associated result type tuple:

$$(TN, FN, TN, TP, TN, FP, TP, FP, TN, TP)$$
$$\hat{=} \; (\text{'3'}, \text{'0'}, \text{'3'}, \text{'2'}, \text{'3'}, \text{'1'}, \text{'2'}, \text{'1'}, \text{'3'}, \text{'2'})$$

(These result types are obtained during the performance evaluation phase of the system – where the ground truth classes of all system-classified materials are known.) We use n_0, n_1, n_2 and n_3 to denote the numbers of '0', '1', '2' and '3' result outcomes in the result tuple. Here, we have the values $n_0 = 1$, $n_1 = 2$, $n_2 = 3$ and $n_3 = 4$. Further, we can define $n = n_0 + n_1 + n_2 + n_3 = 10$ and use it to "normalize", i.e.,

$$\overline{n_i} = n_i / n \Rightarrow \overline{n_0} = 1/10,\ \overline{n_1} = 2/10,\ \overline{n_2} = 3/10,\ \overline{n_3} = 4/10.$$



The left figure shows the hyper-plane $\sum_{i=0}^{3} \overline{n_i} = 1$, where $\overline{n_i} \geq 0$. A "USER" CAN DEFINE THE PERFORMANCE VALUE p FOR A SET OF $\overline{n_i}$ VALUES, I.E.,

$$\boxed{w_0 \overline{n_0} + w_1 \overline{n_1} + w_2 \overline{n_2} + w_3 \overline{n_3} = p} \Rightarrow \boxed{\sum_{i=0}^{3} w_i \overline{n_i}^{\,j} = p_j}.$$

$j = 1 \ldots J$ ...

COMPUTE $\{w_i\}$ VIA LIN. SYSTEM.