

Multi-index Permutations

Given a multi-index $\alpha = (\alpha_1, \dots, \alpha_n)$ with $\dim(\alpha_i) = d_i$ an arbitrary positive integer, how does one compute $\sigma(\alpha) = (\alpha_{\sigma(1)}, \dots, \alpha_{\sigma(n)})$ for any $\sigma \in S_n$? We are interested in this question so that we can permute multi-indices in matrices as needed to sort grouped physical indices and bond indices as needed without restricting our algorithms to strict formats.

To begin, $\text{id}(\alpha) = \alpha \Rightarrow (1, 2, \dots, \overset{n}{\underset{j=1}{\text{d}_j}}),$ so we might ask how do we recreate this sequence from the $\alpha_i.$

When $d_i=2$ it is easier to visualize
in binary: $\alpha_i = (0, 1)$, but in the
whole multi-index, this turns into
 $\alpha'_1 \Rightarrow (0, 1, 0, 1, \dots, 0, 1, 0, 1)$
 $\alpha'_2 \Rightarrow (0, 0, 1, 1, \dots, 0, 0, 1, 1)$
 \vdots
 $\alpha'_n \Rightarrow (0, 0, 0, 0, \dots, 1, 1, 1, 1)$

Where we obtained this from $I_k = \text{diag}(I_k)$

$$\alpha'_i = I_{d_n} \otimes \cdots \otimes I_{d_{i+1}} \otimes \alpha_i \otimes I_{d_i} \otimes \cdots \otimes I_{d_1}$$

But we wont recover α by adding
the α_i . It turns out that

$$\alpha = \sum_{i=1}^n \left(\prod_{j=1}^{i-1} d_j \right) \alpha'_i \quad \because \text{each term}$$

is weighted by the dimension of
the multi-index that precedes it.

To do a permutation, we want
to keep the weights: $w_i = \prod_{j=1}^{i-1} d_j$

but modify the structure of the tensor product. The short story is

$$\sigma(\alpha) = \sum_{i=1}^n w_i \beta'_i \quad \text{where}$$

$$\beta'_i = I_{d_{\sigma(i)}} \otimes \cdots \otimes I_{d_{\sigma(i)}} \otimes \alpha_{\sigma(i)} \otimes I_{d_{\sigma(i-1)}} \otimes \cdots \otimes I_{d_{\sigma(1)}}$$

which distributes the index in its location. The fact we keep the weights from before makes this permutation work, otherwise

$$\sum_{i=1}^n w_{\sigma(i)} \beta'_i = \sum_{i=1}^n w_{\tilde{\sigma}'(i)} \alpha'_{\tilde{\sigma}'(i)} = \sum_{j=1}^n w_j \alpha'_j = \alpha$$

by noting the bijectivity of permutations and making use of the dummy indices.

That's pretty much it. Implementing this requires a convention of $i, \sigma(i)$ or $\tilde{\sigma}'(j), j$ for $j=\sigma(i)$. Combinatorics isn't obvious.