Step 1: Creating a .json file containing information of each element

The following information is one-hot encoded (ODE) for the first 100 elements of periodic table as a long contiguous vector and stored in a common **atom_init.json file**. This will be accessed to represent each atom in the crystal structure during the process of convolution.

Property	Unit	Range	No. of categories
Group number	-	1-18	18
Period number	-	1-9	9
Electronegativity	-	0.5-4.0	10
Covalent radius	pm	25-250	10
Valence electrons	-	1-12	12
First ionization energy	eV	1.3-3.3	10
Electron affinity	eV	-3-3.7	10
Block	-	s, p, d, f	4
Atomic volume	cm^3/mol	1.5-4.3	10

Step 2: Preparing the atomic feature, neighboring atom feature and distance matrices

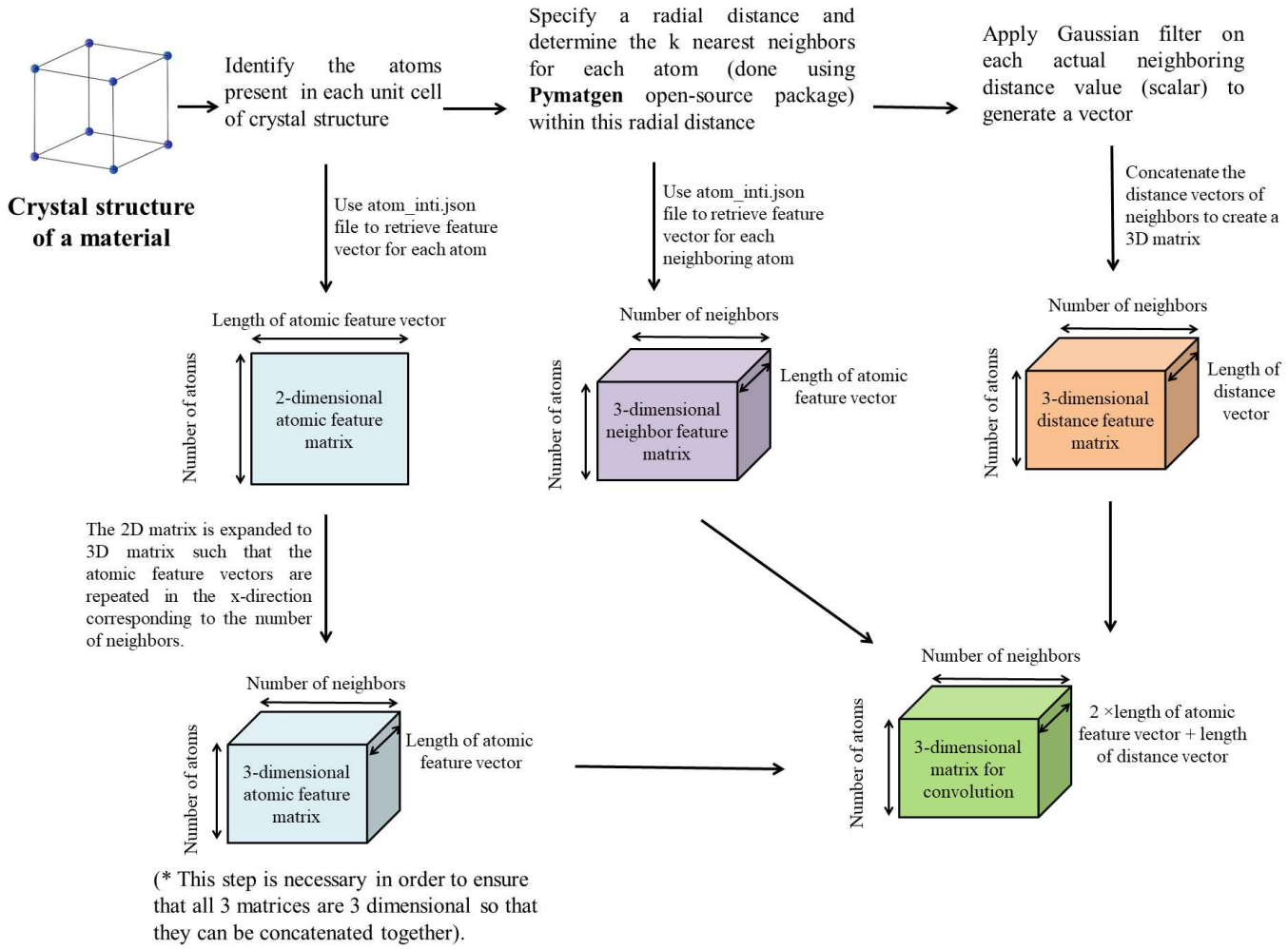

Figure 3.3: Illustration of feature extraction from crystal structure

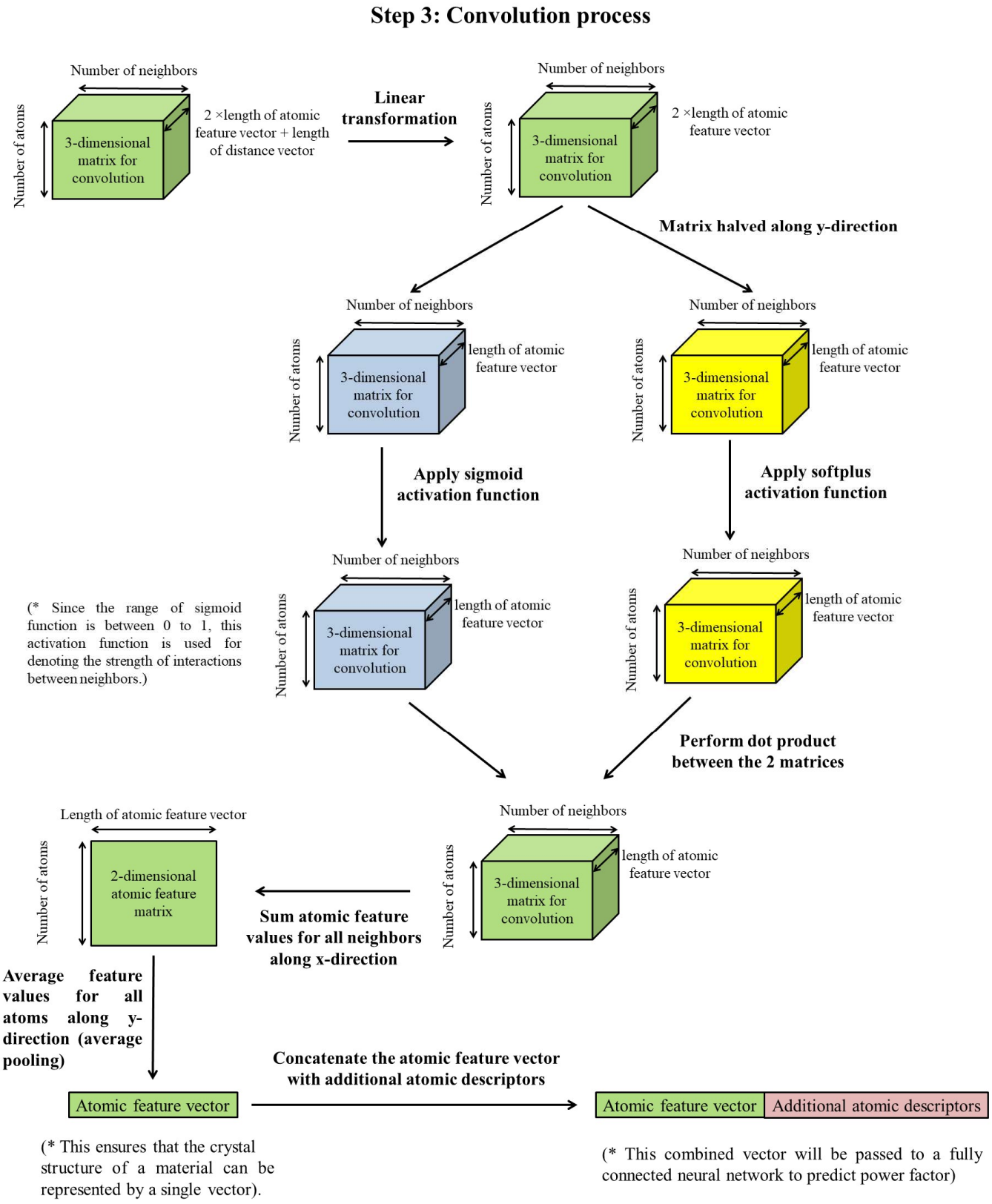

Figure 3.4: Illustration of convolution process