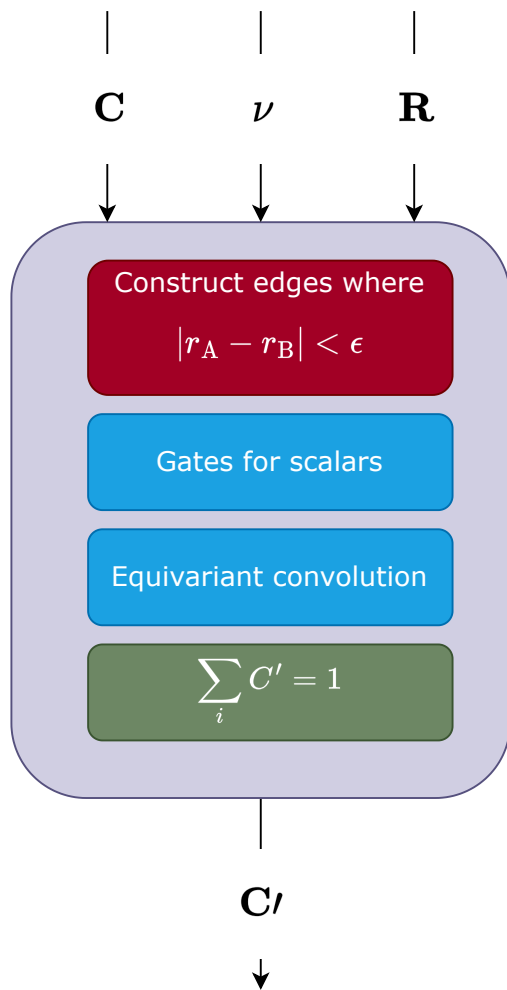a)

Constrained Network Block

$\mathbf{C}$ ν $\mathbf{R}$

Construct edges where
$$|r_{\mathrm{A}} - r_{\mathrm{B}}| < \epsilon$$

Gates for scalars

Equivariant convolution

$$\sum_i C' = 1$$

$\mathbf{C}\prime$

b)

$\mathbf{C}_{\mathrm{reactant}}$ ν $\mathbf{R}_{\mathrm{reactant}}$ $\mathbf{C}_{\mathrm{product}}$ ν $\mathbf{R}_{\mathrm{product}}$

Constrained Network Block   Constrained Network Block

$\mathbf{C}'_{\mathrm{reactant}}$ $\mathbf{C}'_{\mathrm{product}}$

Weighted average
$$X_{\mathrm{transition-state}} = (1-p)X_{\mathrm{reactant}} + pX_{\mathrm{product}}$$
$\longleftarrow p$

$\mathbf{C}'_{\mathrm{transition-state}}$ $\mathbf{R}'_{\mathrm{transition-state}}$ ν

Constrained Network Block

$\mathbf{C}_{\mathrm{transition-state}}$

Element-wise subtraction and mean   **Coefficients of the transition state**

Activation barrier