

Diagram for calculating the cost function Z_2

Concentrations of species in grid box j , denoted as $\mathbf{n}_j = \{ n_{i,j}, i \text{ is for species} \}$

Convert to $\mathbf{y}_j = \{ y_{i,j} \}$, where $y_{i,j}=1$ if the block is fast or $y_{i,j}=0$ if the block is slow. A fast block means at least one species in the block is fast.

If \mathbf{y}_j can be represented by the M chemical regimes

The number of fast species is calculated as $\sum_i y_{i,j}$

If \mathbf{y}_j cannot be represented by the M chemical regimes

For each of the M chemical regimes, check if \mathbf{y}_j can be represented by this chemical regime after moving some blocks from slow to fast. If it can, calculate the number of moves needed. We refer to $y_{i,j}^*$ as the indicators adjusted by these changes.

Identify the chemical regime that needs the least number of moves, and the number of fast species is calculated as $\sum_i y_{i,j}^*$