

Descriptors generation for mixture A-B

Compound A

$$\{D_1^A, D_2^A, \dots, D_n^A\}$$

+

Compound B

$$\{D_1^B, D_2^B, \dots, D_n^B\}$$

Unweighted descriptors

$$\{(D_i^A + D_i^B)/2\} \quad \text{OR} \quad \{D_i^A + D_i^B, |D_i^A - D_i^B|\}$$

Mixture A-B (one mixture -> one descriptor vector)

Each mixture has only one property value.

D_i^A - the i^{th} descriptor of compound A

$$X_A + X_B = 1$$

Weighted descriptors

Mixture A-B (one mixture -> several descriptor vectors)

The property of one mixture depends on the composition of its pure composants.

$$\{X_A * D_i^A + X_B * D_i^B\} \quad \text{OR} \quad \{X_A * D_i^A + X_B * D_i^B, |X_A * D_i^A - X_B * D_i^B|\}$$