

## Note on binding of an association property to semantic properties

D. Gueorguiev 11/25/21

Let us consider two properties -  $P_i$  and  $P_j$  connected through association property (or link)  $A_{i,j}$ .

$$P_i \text{---} A_{i,j} \text{---} P_j$$

The properties  $P_i$  and  $P_j$  are represented by their property signatures  $\mathbf{p}_i$  and  $\mathbf{p}_j$ . The association link  $A_{i,j}$  is represented with its association matrix  $\mathbf{a}_{i,j}$  and semantic significance vector  $\mathbf{w}_{i,j}$ .

The association matrix has the following structure:

$$\mathbf{a}_{i,j} = \begin{bmatrix} \mathbf{r}_1 & \mathbf{r}^1 \\ \mathbf{0} & \mathbf{0} \\ \mathbf{r}_2 & \mathbf{r}^2 \\ \mathbf{0} & \mathbf{0} \\ \vdots & \vdots \\ \mathbf{0} & \mathbf{0} \\ \mathbf{r}_k & \mathbf{r}^l \end{bmatrix}$$

Here  $\mathbf{r}_i, i = 1..k$  denote regions of interest in the property signature of the property on the left of  $A_{i,j}$  -  $P_i$ . Similarly,  $\mathbf{r}^j, j = 1..l$  denote regions of interest in the property signature of the property on the right of  $A_{i,j}$  -  $P_j$ . Let us assume that there is a universal law which allows us to calculate the binding force between  $P_i$  and  $P_j$  given with their signature vectors  $\mathbf{p}_i$  and  $\mathbf{p}_j$ . Let us assume a general form for this law:

$$F^b(P_i, P_j) = f(\mathbf{p}_i, \mathbf{p}_j)$$

Obviously, the binding force between the properties depends only on the presence of specific regions of the property signatures, namely  $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k$  and  $\mathbf{r}^1, \mathbf{r}^2, \dots, \mathbf{r}^l$ . Thus, it will be true:

$$f(\mathbf{p}_i, \mathbf{p}_j) = f([\mathbf{r}_1, \mathbf{0}, \mathbf{r}_2, \mathbf{0} \dots \mathbf{0}, \mathbf{r}_k], [\mathbf{r}^1, \mathbf{0}, \mathbf{r}^2, \mathbf{0}, \dots, \mathbf{0}, \mathbf{r}^l])$$

~~Further removal of a non-zero subregion from any of the regions  $\mathbf{r}_i, i = 1..k$  and  $\mathbf{r}^j, j = 1..l$  will lead to decrease of the binding force to a value lower than  $f(\mathbf{p}_i, \mathbf{p}_j)$ . We will assume that the positions and length of the zero regions is unique i.e. there is no other set with the same number of zeros which will lead to the same value of the binding force.~~

Then the binding force  $f(\mathbf{p}_i, \mathbf{p}_j)$  between the two properties will be equal to the sum of all regional attraction forces minus the sum of all regional repulsion forces

Those non-zero regions  $\mathbf{r}_i, i = 1..k$  and  $\mathbf{r}^j, j = 1..l$  will be denoted as the **active regions** of the association link between the two properties.

The binding force can be calculated for any pair of active regions in the following manner:

We keep a registry of active region pairs for which we know the binding force value (which could be positive or negative). Let us denote those "registered" region pairs with hat over the symbol denoting the region. Then we have:

$$(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j) \rightarrow \hat{f}_{i,j} \text{ for all } (\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j) \in \mathfrak{R}, \hat{f}_{i,j} \in \mathfrak{F}$$

Here with  $\mathfrak{R}$  we denote the set of all registered region pairs and with  $\mathfrak{F}$  the set of all registered binding force values. So the region registry is represented by the map  $R: \mathfrak{R} \rightarrow \mathfrak{F}$ . If an active region pair  $(\mathbf{r}_1, \mathbf{r}_2)$  is not found in the registry we are going to extrapolate its binding force by finding the set of the closest matching pairs in the registry and find the value of  $f(\mathbf{r}_1, \mathbf{r}_2)$  by using some learned function. This function can be as simple as assigning some default value determined by looking into certain interesting characteristics of the new pair of regions. The total binding force  $f(\mathbf{p}_i, \mathbf{p}_j)$  between the two properties will be given as the sum of the attraction forces minus the repulsion forces between the *relevant region pairs*  $(\mathbf{r}_a, \mathbf{r}_b)$ :

$$f(\mathbf{p}_i, \mathbf{p}_j) = \sum_{a,b} f^+(\mathbf{r}_a, \mathbf{r}_b) - \sum_{c,d} f^-(\mathbf{r}_c, \mathbf{r}_d)$$

~~Let us denote by  $f_{\max} > 0$  the pair of regions from  $\mathbf{p}_i$  and  $\mathbf{p}_j$  which generates the maximum binding force by absolute value; that is:  $f_{\max} = \max_{a,b} |f(\mathbf{r}_a, \mathbf{r}_b)| > 0$ . Here we are assuming that there is a pair of regions in  $\mathbf{p}_i$  and  $\mathbf{p}_j$  which generate non-zero binding force.~~

~~**Definition:** relevant region pair  $(\mathbf{r}_a, \mathbf{r}_b)$  is such pair for which  $|f(\mathbf{r}_a, \mathbf{r}_b)| \geq \frac{f_{\max}}{L}$  where  $L > 0$  is appropriately chosen large integer.~~

Let us sort the pairs of regions from  $\mathbf{p}_i$  and  $\mathbf{p}_j$  by the absolute value of the binding force.

**Definition:** relevant region pair  $(\mathbf{r}_a, \mathbf{r}_b)$  is such pair which has absolute binding force value **not in** the  $\ell$ -th quantile for some  $\ell > 0$ . In other words, all region pairs which are in the  $\ell$ -th quantile are irrelevant.

## Introduction of a new property

Let us consider the particle  $V_1$  and introduce a new property  $P_{11}$  under  $P_0$ .

