Supplementary Material for "Continuous Scatterplot Operators for Bivariate Analysis and Study of Electronic Transitions"

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Abstract

This document presents additional statistics and experimental results supporting the paper "Continuous Scatterplot Operators for Bivariate Analysis and Study of Electronic Transitions". It includes a detailed description of the method used to compute the donor strength Δ and the corresponding error estimate. Individual tables listing the computed quantities and corresponding errors for the case studies discussed in the paper are also included in this document.

1 Donor Strength Computation

The CSPs presented in the paper are computed using TTK. As discussed in the paper, the accuracy of the CSP and quantification depends on the image resolution. Generating a high resolution CSP is computationally intensive. Due to these issues, we compute the donor strength using a 2D discrete histogram based implementation. All histograms are reported on a 1000×1000 grid whose x-axis represents ϕ_h and y-axis represents ϕ_p. A vertex from the spatial domain is mapped to the appropriate bin in the histogram, its function value is rounded to the midpoint of the bin, and its contribution to the donor strength depends on the bin value. Aggregating the value associated with all the bins results in the overall donor strength for the domain segment under consideration.

For example, if t vertices map to a bin with bivariate field ranging from $(\phi_{h_{min}}, \phi_{p_{min}})$ to $(\phi_{h_{max}}, \phi_{p_{max}})$ then the contribution from this bin towards donor strength is

$$\Delta_{bin} = t \cdot \left[\left(\frac{\phi_{h_{min}} + \phi_{h_{max}}}{2} \right)^2 - \left(\frac{\phi_{p_{min}} + \phi_{p_{max}}}{2} \right)^2 \right].$$

We aggregate contributions from all bins of the histogram to compute donor strength,

$$\Delta = \sum_{bin=1}^{M} \Delta_{bin}.$$

M is the total number of bins and depends on the grid resolution. For a bin ranging from $(\phi_{h_{min}}, \phi_{p_{min}})$ to $(\phi_{h_{max}}, \phi_{p_{max}})$

$$bin\_size_h = \phi_{h_{max}} - \phi_{h_{min}}$$

represents the hole_NTO step size for each bin. Since every vertex in a bin is mapped to the nearest mid point, the maximum error possible due to this approximation is $bin\_size_h/2$. Similarly, the maximum error along the y-axis is $bin\_size_p/2$. For a particular bin, the donor strength including the maximum possible error can be computed as

$$\Delta_{bin} = t \cdot \left[\left(\frac{\phi_{h_{min}} + \phi_{h_{max}}}{2} \pm \frac{bin\_size_h}{2} \right)^2 - \left(\frac{\phi_{p_{min}} + \phi_{p_{max}}}{2} \pm \frac{bin\_size_p}{2} \right)^2 \right]$$

As the resolution $X_h \times Y_p$ approaches ∞, bin_size_h and bin_size_p approach 0 making the overall error equal 0. Table 1 lists the donor strengths together with corresponding errors for the Thiophene-Quinoxaline case study. Table 2 shows the donor strength for the ligand based case study of copper complexes and Table 3 for the different excitation based case study of copper complexes.

	0°	60°	90°	120°	180°	Relaxed (35.3°)
Thiophene	0.440 ± 0.006	0.026 ± 0.003	-0.006 ± 0.002	0.227 ± 0.004	0.429 ± 0.005	0.480 ± 0.006
Quinoxaline	-0.440 ± 0.010	-0.026 ± 0.017	0.006 ± 0.017	-0.227 ± 0.013	-0.429 ± 0.009	-0.480 ± 0.012

TABLE 1: Δ values with maximum possible computation error for different dihedral angle based molecular conformations of Thiophene-Quinoxaline.

	Cu-PHE-PHE	Cu-PHE-PHEOME	Cu-PHE-XANT
Cu	0.681 $\pm$ 0.007	0.634 $\pm$ 0.005	0.328 $\pm$ 0.003
PHE	-0.289 $\pm$ 0.030	-0.811 $\pm$ 0.032	-0.876 $\pm$ 0.020
Ligand	-0.391 $\pm$ 0.032	0.177 $\pm$ 0.017	0.547 $\pm$ 0.024

TABLE 2: Δ values with maximum possible computation error for different ligand based molecular conformations of copper complexes.

	Cu-PHE-PHEOME		Cu-PHE-XANT	
	State 9	State 10	State 3	State 10
Cu	0.933 $\pm$ 0.006	0.033 $\pm$ 0.001	0.335 $\pm$ 0.003	0.031 $\pm$ 0.001
PHE	-0.943 $\pm$ 0.026	-0.025 $\pm$ 0.012	-0.906 $\pm$ 0.021	-0.022 $\pm$ 0.003
Ligand	0.010 $\pm$ 0.009	-0.008 $\pm$ 0.003	0.571 $\pm$ 0.025	-0.009 $\pm$ 0.026

TABLE 3: Δ values with maximum possible computation error for different states of two copper complexes.