Multipartite correlations

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1. Theory of multipartite correlations – Outline

- framework for the classification of multipartite correlations
- measures for the quantification of multipartite correlations
- algorithm for multipartite correlation clustering

2. Setting the stage

- state vector: $|\psi\rangle \in \mathcal{H}$ (normalized)
- pure state: $\pi = |\psi\rangle\langle\psi| \in \mathcal{P}$
- mixed state (of an ensemble): $\varrho = \sum_j p_j \pi_j \in \mathcal{D} = \mathrm{Conv}\,\mathcal{P}$
- mixedness: e.g. von Neumann entropy $S(\varrho) = -\operatorname{tr}\varrho\ln\varrho$
- distinguishability: e.g. relative entropy $D(\varrho\|\sigma) = \operatorname{tr}\varrho(\ln\varrho - \ln\sigma)$

3. Structure of multiorbital correlations [1, 2, 3, 4, 5]

Level 0: subsystems

- system: $L = [n] = \{1, 2, \dots, n\}$
- subsystem: $X \in 2^L$, then $\mathcal{H}_X$, $\mathcal{P}_X$, $\mathcal{D}_X$ — Boolean lattice structure: $P_0 = 2^L$

Level I: partitions

- partitions of the system: $\xi = \{X_1, X_2, \dots, X_{|\xi|}\} \equiv X_1|X_2|\dots|X_{|\xi|} \in \Pi(L)$
- refinement: $\upsilon \preceq \xi$ def.: $\forall Y \in \upsilon, \exists X \in \xi : Y \subseteq X$ — lattice structure: $P_\mathrm{I} = \Pi(L)$
- ξ-uncorrelated states: $\varrho = \otimes_{X\in\xi}\varrho_X \in \mathcal{D}_{\xi-\mathrm{uncorr}}$, then $\upsilon \preceq \xi \Leftrightarrow \mathcal{D}_{\upsilon-\mathrm{uncorr}} \subseteq \mathcal{D}_{\xi-\mathrm{uncorr}}$
- ξ-correlation (ξ-mutual information):

$$C_\xi(\varrho) = \min_{\sigma\in\mathcal{D}_{\xi-\mathrm{uncorr}}} D(\varrho\|\sigma) = \sum_{X\in\xi} S(\varrho_X) - S(\varrho)$$

- multipartite monotonicity: $\upsilon \preceq \xi \Leftrightarrow C_\upsilon \geq C_\xi$

Level II: multiple partitions

- down-sets of partitions: $\boldsymbol{\xi} = \{\xi_1, \xi_2, \dots, \xi_{|\boldsymbol{\xi}|}\} \subseteq P_\mathrm{I}$ (closed downwards w.r.t. $\preceq$)
- partial order: $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi}$ def.: $\boldsymbol{\upsilon} \subseteq \boldsymbol{\xi}$, — lattice structure, $P_\mathrm{II} = \mathcal{O}_\downarrow(P_\mathrm{I}) \setminus \{\emptyset\}$
- $\boldsymbol{\xi}$-uncorrelated states: $\mathcal{D}_{\boldsymbol{\xi}-\mathrm{uncorr}} = \cup_{\xi\in\boldsymbol{\xi}}\mathcal{D}_{\xi-\mathrm{uncorr}}$, then $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi} \Leftrightarrow \mathcal{D}_{\boldsymbol{\upsilon}-\mathrm{uncorr}} \subseteq \mathcal{D}_{\boldsymbol{\xi}-\mathrm{uncorr}}$
- $\boldsymbol{\xi}$-correlation:

$$C_{\boldsymbol{\xi}}(\varrho) = \min_{\sigma\in\mathcal{D}_{\boldsymbol{\xi}-\mathrm{uncorr}}} D(\varrho\|\sigma) = \min_{\xi\in\boldsymbol{\xi}} C_\xi(\varrho)$$

- multipartite monotonicity: $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi} \Leftrightarrow C_{\boldsymbol{\upsilon}} \geq C_{\boldsymbol{\xi}}$
- spec.: k-partitionability and k'-poducibility (chains)

$$\boldsymbol{\mu}_k = \{\mu \in P_\mathrm{I} \mid |\mu| \geq k\}, \qquad \boldsymbol{\nu}_{k'} = \{\nu \in P_\mathrm{I} \mid \forall N \in \nu : |N| \leq k'\}$$

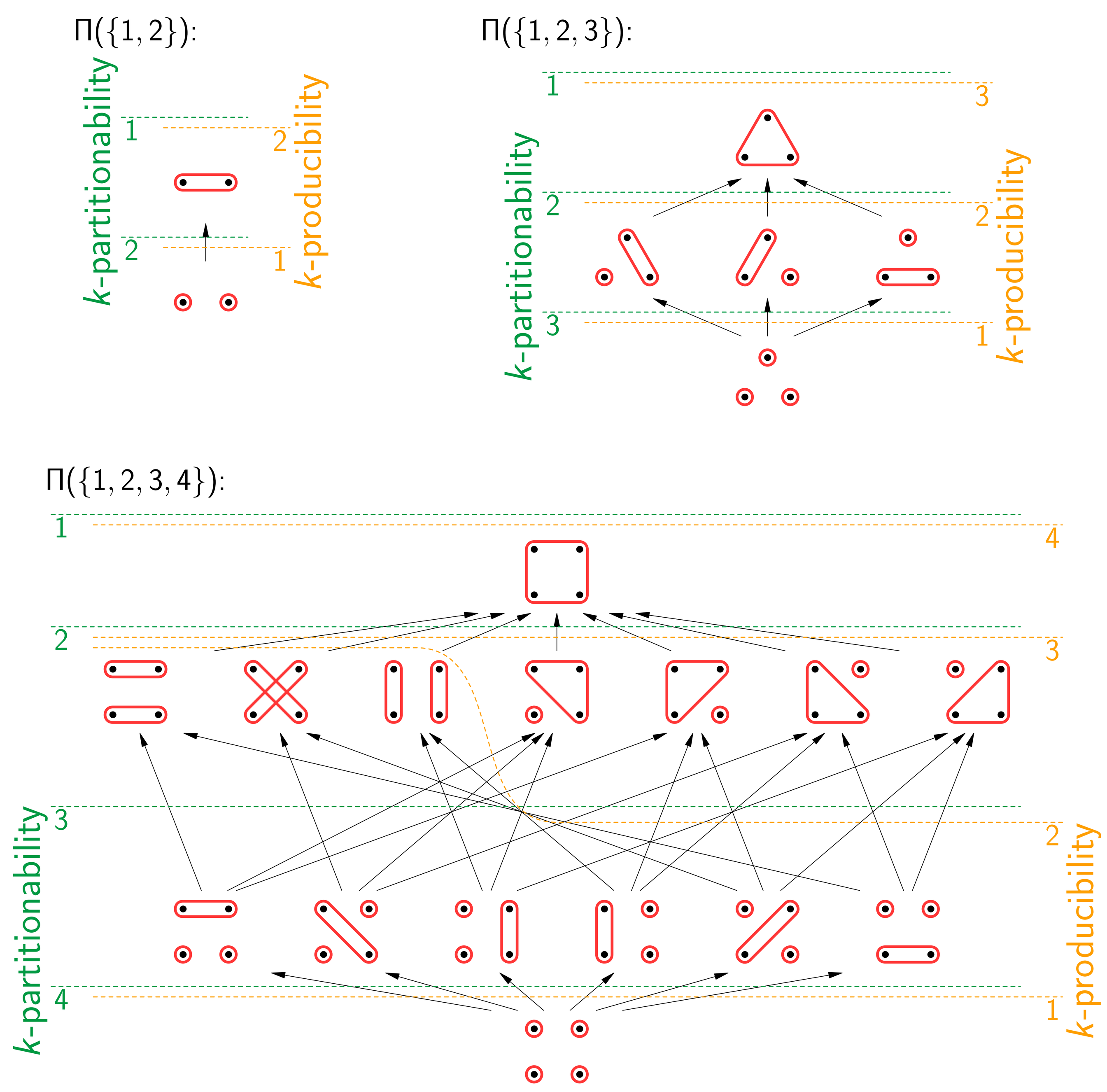
k-partitionability-correlation and k'-poducibility correlation:

$$C_{k\text{-part}}(\varrho_L) = C_{\boldsymbol{\mu}_k}(\varrho_L) = \min_{|\mu|\geq k} C_\mu(\varrho_L), \qquad C_{k'\text{-prod}}(\varrho_L) = C_{\boldsymbol{\nu}_{k'}}(\varrho_L) = \min_{\forall N\in\nu:|N|\leq k'} C_\nu(\varrho_L)$$

Level III: classes, see [2]

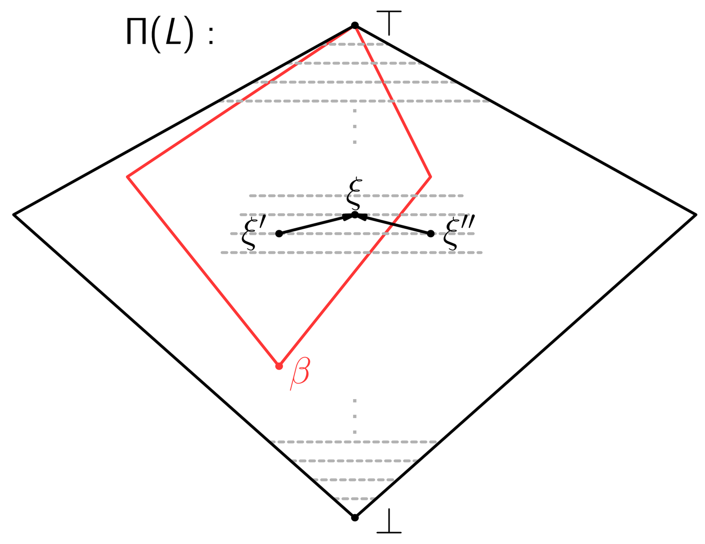
- intersections of $\mathcal{D}_{\boldsymbol{\xi}-\mathrm{sep}} = \mathrm{Conv}\,\mathcal{D}_{\boldsymbol{\xi}-\mathrm{uncorr}}$ — lattice structure: $P_\mathrm{III} = \mathcal{O}_\uparrow(P_\mathrm{II}) \setminus \{\emptyset\}$

4. Illustrations [1, 2]

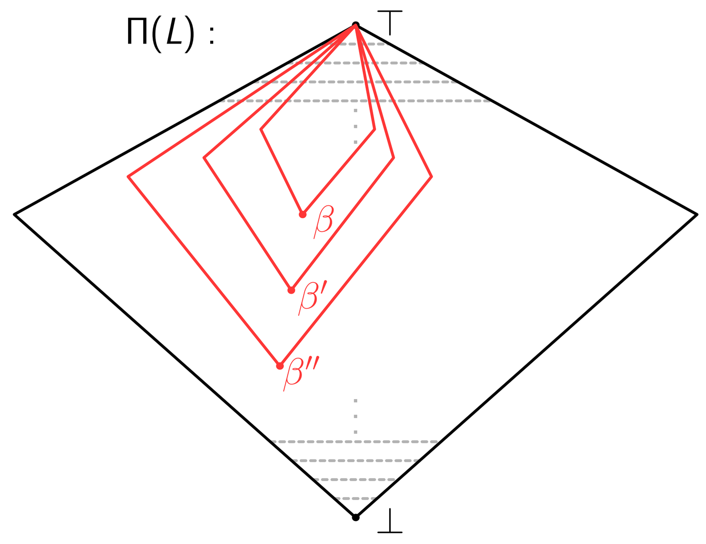


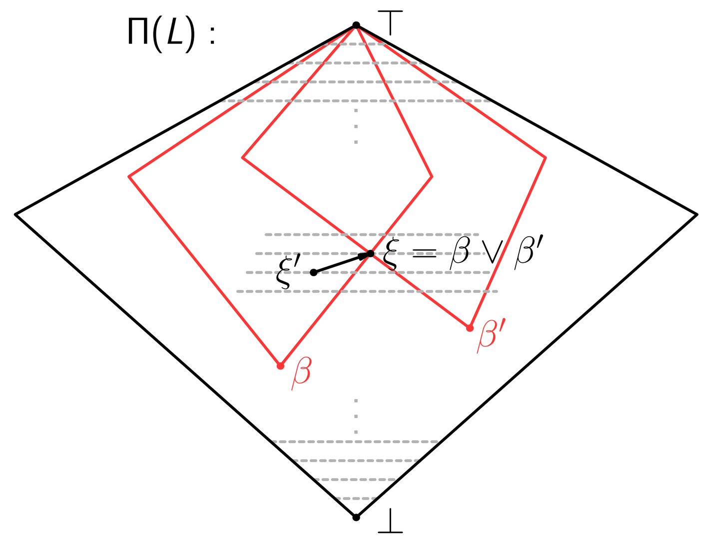
5. Multipartite correlation clustering [1]

- bipartite correlation clustering: $\gamma = G_1|G_2|\dots|G_{|\gamma|} \in \Pi(L)$
  connectivity clustering of the graph of vertices L and edges $C_{i|j} \geq T_\mathrm{b} > 0$
- multipartite correlation clustering: $\beta = B_1|B_2|\dots|B_{|\beta|} \in \Pi(L)$, for which
  (i) the subsystems described by the parts $B \in \beta$ are weakly correlated with one another,
  (ii) the elementary subsystems $i \in B$ inside a part $B \in \beta$ are strongly correlated with one another.

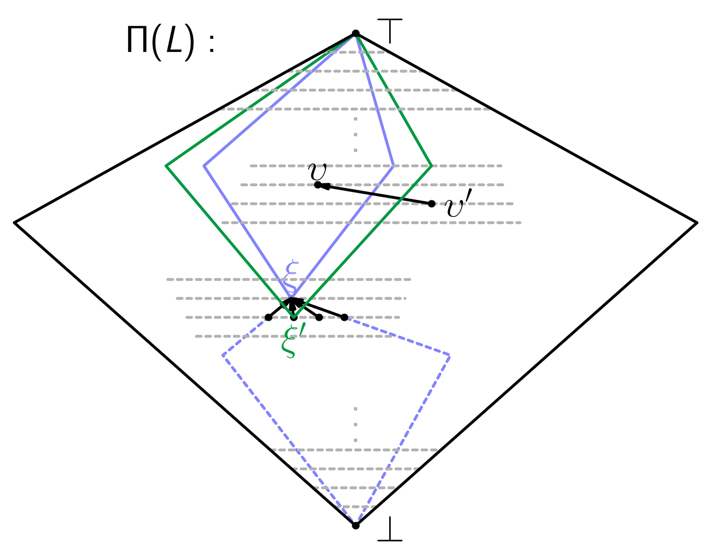


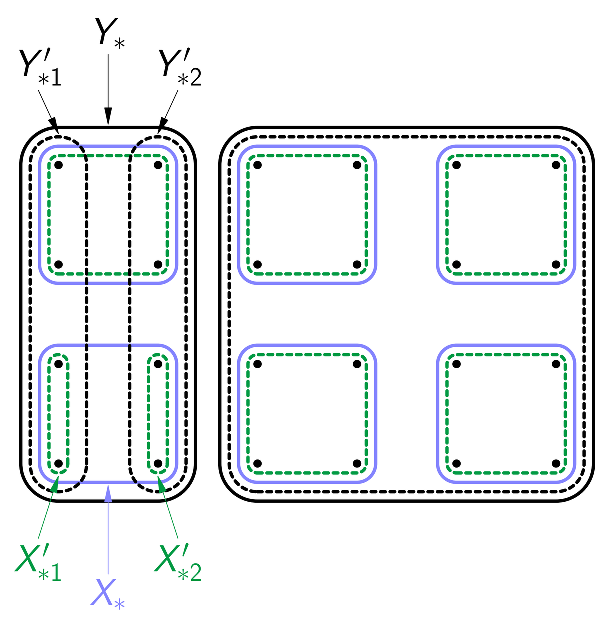
- covering (being neighbours): $\xi' \prec\!\!\cdot\; \xi$ def.:
  $\xi' \setminus \xi = \{X'_{*1}, X'_{*2}\} \in \Pi(X_*)$,
  $\xi \setminus \xi' = \{X_*\} \in \Pi(X_*)$
- derivative: $C_{\xi'}(\varrho_L) - C_\xi(\varrho_L) = C_{\xi'\setminus\xi}(\varrho_{X_*})$
- reformulation: $\exists T_\mathrm{m} > 0$, such that
  $\forall \xi, \xi' \in \Pi(L)$ such that $\xi' \prec\!\!\cdot\; \xi$, and $\beta \preceq \xi$,
  then $\beta \preceq \xi' \;\Leftrightarrow\; C_{\xi'}(\varrho_L) - C_\xi(\varrho_L) \leq T_\mathrm{m}$
- there might not exist such clustering
- there may exist compatible clusterings, but there exist no contradictory ones:





- finding β: successive refinement from $\top$ to $\bot$ (taking the smallest step):
  $\forall \upsilon, \upsilon' \in \Pi(L)$ such that $\upsilon' \prec\!\!\cdot\; \upsilon$, and $\forall \xi \in \Pi(L)$ such that $\xi \preceq \upsilon$ but $\xi \npreceq \upsilon'$,
  then $\min_{\xi'\prec\cdot\xi} C_{\xi'}(\varrho_L) - C_\xi(\varrho_L) \leq C_{\upsilon'}(\varrho_L) - C_\upsilon(\varrho_L)$





- hint: $T_\mathrm{b} \leq C_{\xi'}(\varrho_L) - C_\xi(\varrho_L)$ for $G \in \gamma$ (bipartite correlation clustering)
  if ξ does not dissect G while ξ' does, so don't dissect G
- hidden correlation: $\gamma \prec \beta$

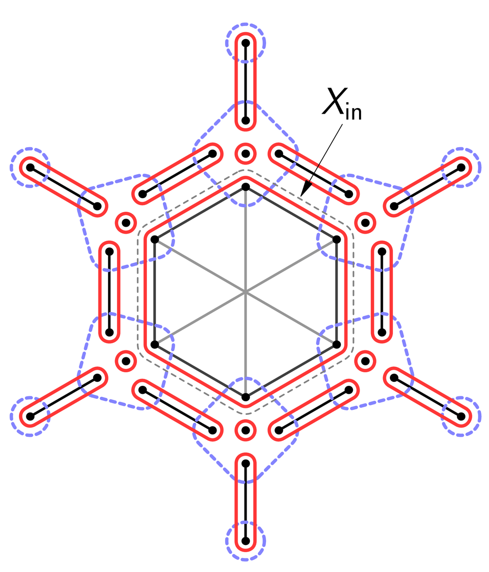
6. Examples [1]

"atoms": $\alpha = A_1|A_2|\dots|A_{|\alpha|}$, "bonds": $\beta = B_1|B_2|\dots|B_{|\beta|}$

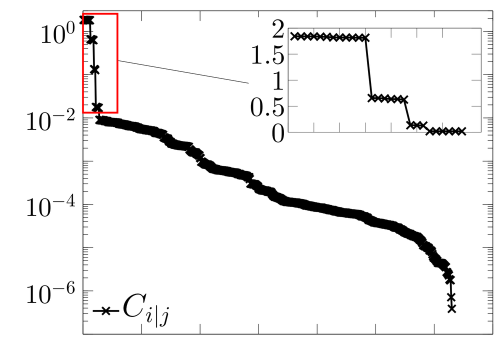
$$\sum_{A\in\alpha} C_{\perp,A}(\varrho_A) + C_\alpha(\varrho_M) = \sum_{B\in\beta} C_{\perp,B}(\varrho_B) + C_\beta(\varrho_M) = C_\perp(\varrho_M)$$

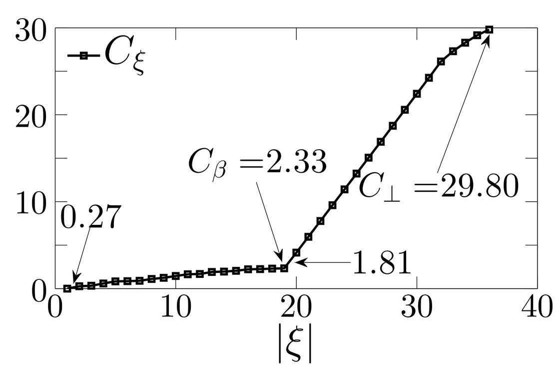
(values are in units ln 4)

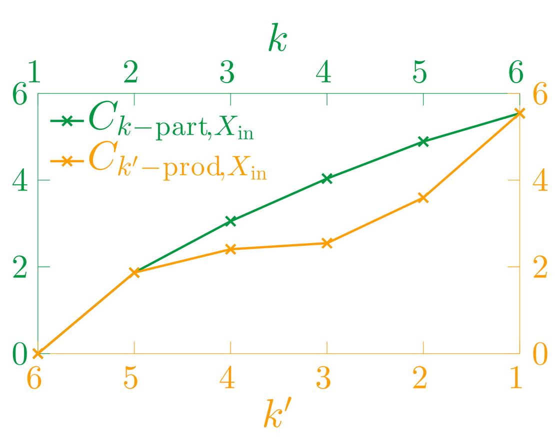
C_6H_6 (benzene):

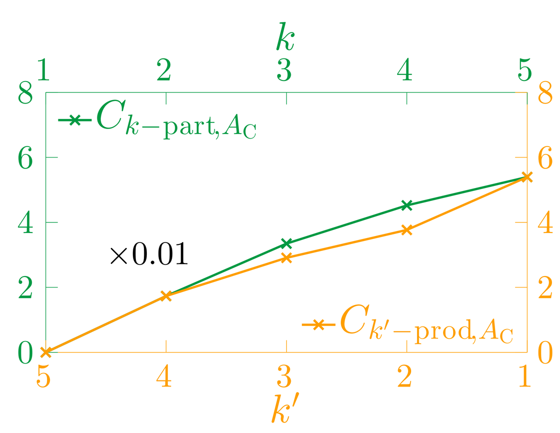


$C_\alpha = 29.52$, $C_\beta = 2.33$

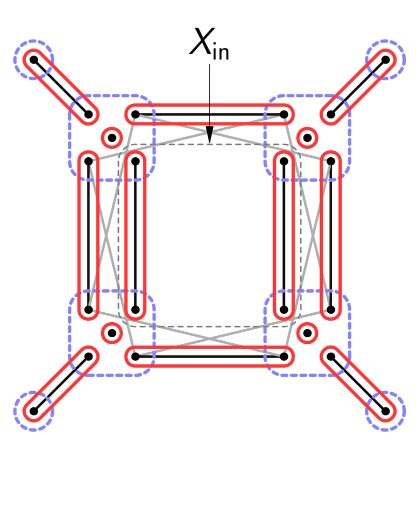




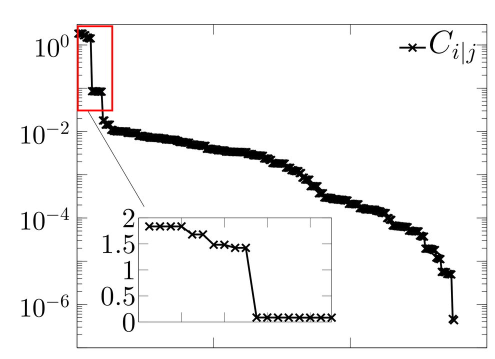


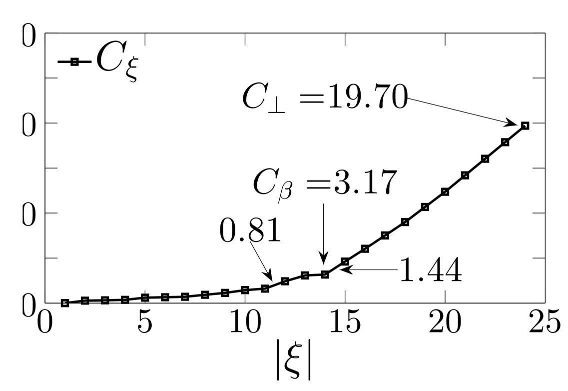


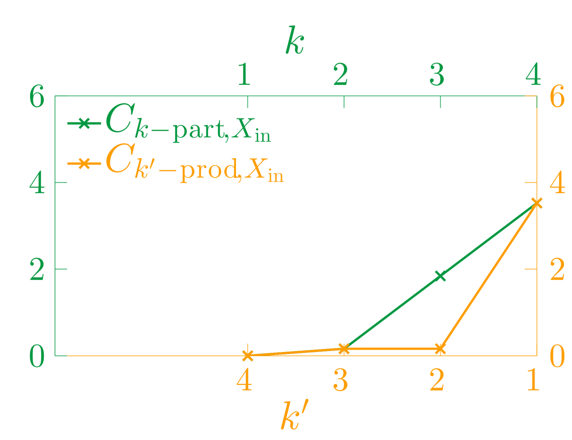
C_4H_4 (cyclobutadiene):

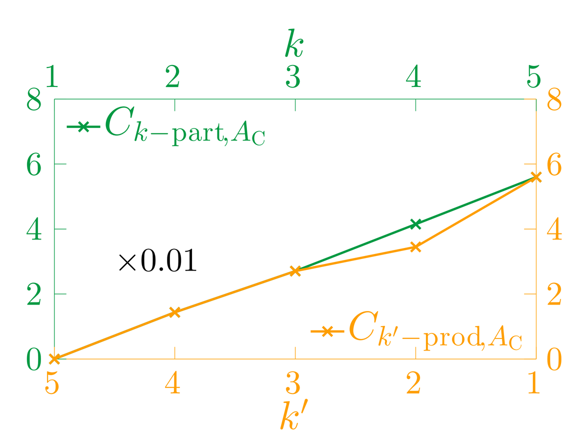


$C_\alpha = 19.48$, $C_\beta = 3.17$









7. Acknowledgement

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8. Bibliography

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