Multipartite entanglement and multipartite correlation
Entanglement in strongly correlated systems 2019, Benasque

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Introduction

Correlations in quantum systems

- can be only classical
- or can contain also quantum part (steering, discord, entanglement)
- entropic quantities: observable-independent

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- w.r.t. possible splittings of the system (Level II.)
- disjoint classification of these (Level III.)
- and these properties of different subsystems of the whole system

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Application: electronic structure of molecules

- localized orbitals
- clustering: strong correlation inside the chemical bonds
  weak correlation among the chemical bonds

Quantum states

States of discrete finite quantum systems

- *state vector:* $|\psi\rangle \in \mathcal{H}$ (normalized) superposition
- *pure state:* $\pi = |\psi\rangle\langle\psi| \in \mathcal{P}$
  we are uncertain about the outcomes of the measurement,
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- $\mathcal{D}$ is convex, moreover, $\mathcal{P} = \text{Extr}\,\mathcal{D}$

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Mixedness and distinguishability

Measure of mixedness:

- von Neumann entropy: $S(\varrho) = -\operatorname{Tr} \varrho \ln \varrho$
  - concave, nonnegative, vanishes iff ϱ pure
- Schur-concavity: *entropy = mixedness*
- increasing in bistochastic quantum channels
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Measure of distinguishability:

- (Umegaki's) quantum relative entropy: $D(\varrho \| \sigma) = \operatorname{Tr} \varrho (\ln \varrho - \ln \sigma)$
- jointly convex, nonnegative, vanishes iff $\varrho = \omega$
- quantum Stein's lemma: *relative entropy = distinguishability*
  (rate of decaying of the probability of error
  in hypothesis testing, Hiai & Petz)

- decreasing in quantum channels

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Notions of correlation:

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- the state is *uncorrelated* iff $\text{CORR}(A, B) = 0$ for all A, B,
  iff $\langle AB \rangle = \langle A \rangle \langle B \rangle$ for all A, B, iff $\varrho = \varrho_1 \otimes \varrho_2$, iff $\Gamma = 0$

Bipartite correlation and entanglement

Pure states

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- state of subsystem (e.g., $\mathrm{Tr}_2 \pi \in \mathcal{D}_1$) not necessarily pure

- π is entangled if (and only if) $\mathrm{Tr}_2 \pi$ and $\mathrm{Tr}_1 \pi$ are mixed
  In this case, *"the best possible knowledge of the whole does not involve the best possible knowledge of its parts."* (Schrödinger)

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- *separable:* there exists separable decomposition:

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- classically correlated sources produce states of this kind (Werner)
  preparable by Local Operations and Classical Communication (LOCC)
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  else *entangled* $(\mathcal{D} \setminus \mathcal{D}_{\mathsf{sep}})$
- the decomposition is not unique
- deciding separability is difficult

Bipartite correlation and entanglement – measures

- correlation "of the state itself": $\Gamma := \varrho - \varrho_1 \otimes \varrho_2$
  then $\text{COV}(\varrho; A, B) = \langle AB \rangle - \langle A \rangle \langle B \rangle = \text{Tr}\,\Gamma A \otimes B = \langle \Gamma | A \otimes B \rangle_{\text{HS}}$
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- correlation might not be seen well from COV, but for all A, B,

$$\frac{1}{2}\,\text{COV}(\varrho; \hat{A}, \hat{B})^2 \le C(\varrho), \qquad \hat{A} = A/\|A\|_\infty, \hat{B} = B/\|B\|_\infty$$

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- *correlation* (mutual information):

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- faithful: $C(\varrho) = 0 \Leftrightarrow \varrho \in \mathcal{D}_{\text{unc}}$, $E(\varrho) = 0 \Leftrightarrow \varrho \in \mathcal{D}_{\text{sep}}$
- $E(\varrho)$ is hard to calculate

Multipartite correlation and entanglement – structure

Level 0.: subsystems

Boolean lattice structure: $P_0 = 2^L$

- whole system: $L = \{1, 2, \ldots, n\}$
- subsystem: $X \subseteq L$, then $\mathcal{H}_X$, $\mathcal{P}_X$, $\mathcal{D}_X$

Szalay, Barcza, Szilvási, Veis, Legeza, SciRep **7**, 2237 (2017)
Szalay, PRA **92**, 042329 (2015)   Seevinck, Uffink, PRA **78**, 032101 (2008)
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lattice structure: $P_I = \Pi(L)$

- partition: $\xi = \{X_1, X_2, \ldots, X_{|\xi|}\} \in \Pi(L)$
- refinement (partial order): $\upsilon \preceq \xi$ def.: $\forall Y \in \upsilon, \exists X \in \xi : Y \subseteq X$

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- ξ-uncorrelated states: $\mathcal{D}_{\xi\text{-unc}} = \left\{ \bigotimes_{X \in \xi} \varrho_X \right\}$
  LO-closed $\upsilon \preceq \xi \Leftrightarrow \mathcal{D}_{\upsilon\text{-unc}} \subseteq \mathcal{D}_{\xi\text{-unc}}$
- ξ-separable states: $\mathcal{D}_{\xi\text{-sep}} = \text{Conv}\,\mathcal{D}_{\xi\text{-unc}}$
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- faithful: $C_\xi(\varrho) = 0 \Leftrightarrow \varrho \in \mathcal{D}_{\xi\text{-unc}}$, $E_\xi(\varrho) = 0 \Leftrightarrow \varrho \in \mathcal{D}_{\xi\text{-sep}}$

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Multipartite correlation and entanglement – measures

- ξ-correlation (ξ-mutual information):

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

  LO-monotone (proper correlation measure)

- ξ-entanglement (of formation):

$$E_\xi(\pi) = C_\xi|_\mathcal{P}(\pi), \qquad E_\xi(\varrho) = \min\left\{\sum_i p_i E_\xi(\pi_i) \;\Big|\; \sum_i p_i \pi_i = \varrho\right\}$$

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- faithful: $C_\xi(\varrho) = 0 \Leftrightarrow \varrho \in \mathcal{D}_{\xi\text{-unc}}$, $E_\xi(\varrho) = 0 \Leftrightarrow \varrho \in \mathcal{D}_{\xi\text{-sep}}$
- multipartite monotone: $\upsilon \preceq \xi \Leftrightarrow C_\upsilon \geq C_\xi, E_\upsilon \geq E_\xi$

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Multipartite correlation and entanglement – structure

Level II.: multiple partitions   lattice structure: $P_{\text{II}} = \mathcal{O}_{\downarrow}(P_{\text{I}}) \setminus \{\emptyset\}$

- partition ideal: $\boldsymbol{\xi} = \{\xi_1, \xi_2, \ldots, \xi_{|\boldsymbol{\xi}|}\} \subseteq P_{\text{I}}$, closed downwards w.r.t. $\preceq$
- partial order: $\boldsymbol{v} \preceq \boldsymbol{\xi}$ def.: $\boldsymbol{v} \subseteq \boldsymbol{\xi}$

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Multipartite correlation and entanglement – structure

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- partial order: $\boldsymbol{\upsilon} \preceq \boldsymbol{\xi}$ def.: $\boldsymbol{\upsilon} \subseteq \boldsymbol{\xi}$
  $n = 3$:

Multipartite correlation and entanglement – structure

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- $\boldsymbol{\xi}$-*uncorrelated states*: $\mathcal{D}_{\boldsymbol{\xi}\text{-unc}} = \cup_{\xi \in \boldsymbol{\xi}} \mathcal{D}_{\xi\text{-unc}}$
  LO-closed $\boldsymbol{v} \preceq \boldsymbol{\xi} \Leftrightarrow \mathcal{D}_{\boldsymbol{v}\text{-unc}} \subseteq \mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$

- $\boldsymbol{\xi}$-*separable states*: $\mathcal{D}_{\boldsymbol{\xi}\text{-sep}} = \text{Conv}\, \mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$
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Multipartite correlation and entanglement – structure

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- spec.: k-partitionable and k'-producible (chains)
  $$\boldsymbol{\mu}_k = \big\{ \mu \in P_I \mid |\mu| \geq k \big\}, \qquad \boldsymbol{\nu}_{k'} = \big\{ \nu \in P_I \mid \forall N \in \nu : |N| \leq k' \big\}$$

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$n = 2$:

Multipartite correlation and entanglement – structure

- spec.: k-partitionable and k'-producible (chains)

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

$n = 3$:

Multipartite correlation and entanglement – structure

- spec.: k-partitionable and k'-producible (chains)

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

$n = 4$:

Multipartite correlation and entanglement – structure

Level II.: multiple partitions   lattice structure: $P_{II} = \mathcal{O}_{\downarrow}(P_I) \setminus \{\emptyset\}$

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- with these:
  k-partitionably and *k'-producibly uncorrelated*
  k-partitionably and *k'-producibly separable* states

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Multipartite correlation and entanglement – measures

- ξ-correlation:

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

LO-monotone (proper correlation measure)

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Multipartite correlation and entanglement – measures

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  k-partitionability and k'-producibility correlation
  k-partitionability and k'-producibility entanglement

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Example: Electron system of molecules

- elementary subsystems: localized atomic orbitals (Pipek-Mezey)
- "atomic split": $\alpha = \{A_1, A_2, \ldots, A_{|\alpha|}\}$ (blue)
- "bond split": $\beta = \{B_1, B_2, \ldots, B_{|\beta|}\}$ (red)

Example: Electron system of molecules

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- "bond split": $\beta = \{B_1, B_2, \ldots, B_{|\beta|}\}$ (red)

benzene (C_6H_6): $C_\alpha = 29.52$, $C_\beta = 2.33$
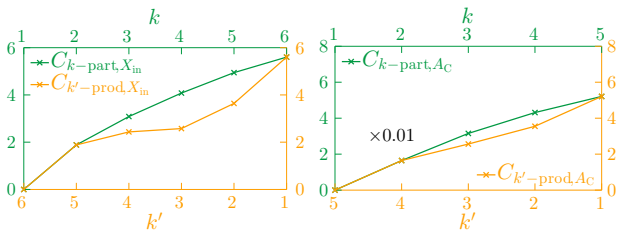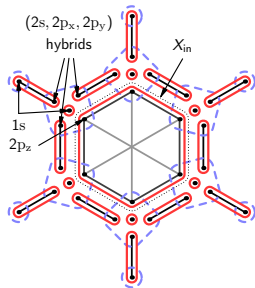
(in units $\ln 4$)

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Example: Electron system of molecules

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- "bond split": $\beta = \{B_1, B_2, \ldots, B_{|\beta|}\}$ (red)

cyclobutadiene (C_4H_4): $C_\alpha = 19.48$, $C_\beta = 3.17$
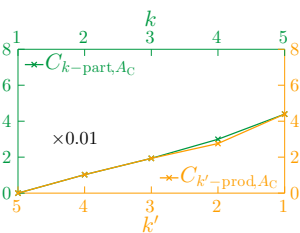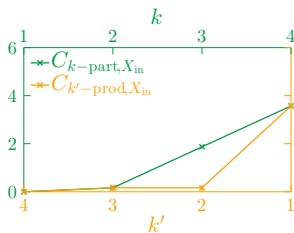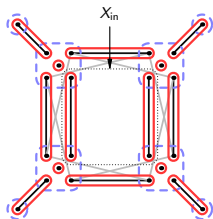
(in units $\ln 4$)

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Level III: Entanglement classes   lattice structure: $P_{\text{III}} = \mathcal{O}_{\uparrow}(P_{\text{II}}) \setminus \{\emptyset\}$

- ideal filter: $\underline{\boldsymbol{\xi}} = \{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \ldots, \boldsymbol{\xi}_{|\underline{\boldsymbol{\xi}}|}\} \subseteq P_{\text{II}}$ (closed upwards w.r.t. $\preceq$)
- partial order: $\underline{\boldsymbol{\upsilon}} \preceq \underline{\boldsymbol{\xi}}$ def.: $\underline{\boldsymbol{\upsilon}} \subseteq \underline{\boldsymbol{\xi}}$

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Level III: Entanglen

- ideal filter: $\underline{\xi}$ =
- partial order: $\underline{\varrho}$

P_{I}

$P_{\mathrm{II}} = \mathcal{O}_{\downarrow}(P_{\mathrm{I}}) \setminus \{\emptyset\}$

$P_{\mathrm{III}} = \mathcal{O}_{\uparrow}(P_{\mathrm{II}}) \setminus \{\emptyset\}$

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Entanglement classes

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- partial separability classes: intersections of $\mathcal{D}_{\underline{\boldsymbol{\xi}}\text{-sep}}$

$$\mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-sep}} := \bigcap_{\boldsymbol{\xi} \notin \underline{\boldsymbol{\xi}}} \overline{\mathcal{D}_{\underline{\boldsymbol{\xi}}\text{-sep}}} \cap \bigcap_{\boldsymbol{\xi} \in \underline{\boldsymbol{\xi}}} \mathcal{D}_{\underline{\boldsymbol{\xi}}\text{-sep}}$$

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Entanglement classes

Level III: Entanglen

- ideal filter: $\underline{\boldsymbol{\xi}}$ =
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- partial separab

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P_I

$P_{II} = \mathcal{O}_\downarrow(P_I) \setminus \{\emptyset\}$

$P_{III} = \mathcal{O}_\uparrow(P_{II}) \setminus \{\emptyset\}$

Entanglement classes

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- LOCC convertibility:
  if $\exists \varrho \in \mathcal{C}_{\underline{\boldsymbol{v}}}$, $\exists \Lambda$ LOCC map s.t. $\Lambda(\varrho) \in \mathcal{C}_{\underline{\boldsymbol{\xi}}}$ then $\underline{\boldsymbol{v}} \preceq \underline{\boldsymbol{\xi}}$

Level III: Entanglen

- ideal filter: $\underline{\xi}$ =
- partial order: ϱ
- partial separab

- LOCC converti
  if $\exists \varrho \in \mathcal{C}_{\underline{v}}$, $\exists \Lambda$

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P_I

$P_{II} = \mathcal{O}_\downarrow(P_I) \setminus \{\emptyset\}$

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Correlation classes

- partial separability classes: intersections of $\mathcal{D}_{\boldsymbol{\xi}\text{-sep}}$

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Correlation classes

Level III: Corr./Ent. classes   lattice structure: $P_{\mathrm{III}} = \mathcal{O}_\uparrow(P_{\mathrm{II}}) \setminus \{\emptyset\}$

- partial correlation classes: intersections of $\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$

$$\mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-unc}} := \bigcap_{\boldsymbol{\xi} \notin \underline{\boldsymbol{\xi}}} \overline{\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}} \cap \bigcap_{\boldsymbol{\xi} \in \underline{\boldsymbol{\xi}}} \mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$$

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Correlation classes

Level III: Corr./Ent. classes   lattice structure: $P_{\text{III}} = \mathcal{O}_\uparrow(P_{\text{II}}) \setminus \{\emptyset\}$

- partial correlation classes: intersections of $\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}$

$$\mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-unc}} := \bigcap_{\boldsymbol{\xi} \notin \underline{\boldsymbol{\xi}}} \overline{\mathcal{D}_{\boldsymbol{\xi}\text{-unc}}} \cap \bigcap_{\boldsymbol{\xi} \in \underline{\boldsymbol{\xi}}} \mathcal{D}_{\boldsymbol{\xi}\text{-unc}} \neq \emptyset \qquad \text{iff } \underline{\boldsymbol{\xi}} = \uparrow \{\boldsymbol{\xi}\} \text{ (proven)}$$

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- LO convertibility:
  if $\exists \varrho \in \mathcal{C}_{\underline{\boldsymbol{v}}\text{-unc}}$, $\exists \Lambda$ LO map s.t. $\Lambda(\varrho) \in \mathcal{C}_{\underline{\boldsymbol{\xi}}\text{-unc}}$ then $\underline{\boldsymbol{v}} \preceq \underline{\boldsymbol{\xi}}$
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Szalay, JPhysA **51**, 485302 (2018)
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Correlation-based clustering – Overview

Bipartite correlation clustering (for treshold T_b): split $\gamma = C_1|C_2|\ldots|C_{|\gamma|}$, the connectivity clustering of the graph $\left(L, \{(i,j)\}_{T_b \leq c_{i|j}}\right)$,

Szalay, Barcza, Szilvási, Veis, Legeza, SciRep **7**, 2237 (2017)

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Multipartite correlation clustering:
give a split $\beta = B_1|B_2|\ldots|B_{|\beta|}$, *if exists*, for which

- the subsystems $B \in \beta$ are weakly correlated with one another C_β low
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Problems

- hidden correlation: $\gamma \prec \beta$
- hard to find β, too many possibilities to check
- meaning/definition of "C_β low" and "$C_{k\text{-part},B}, C_{k\text{-prod},B}$ high"

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We have a method to handle these.

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- multipartite monotonity: $v \preceq \xi \Leftrightarrow C_v \geq C_\xi$
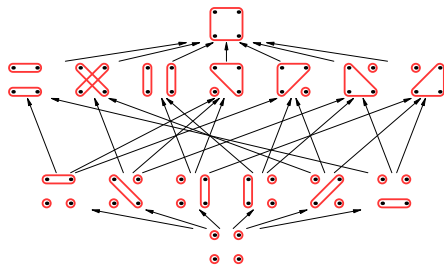
Correlation-based clustering – Definition

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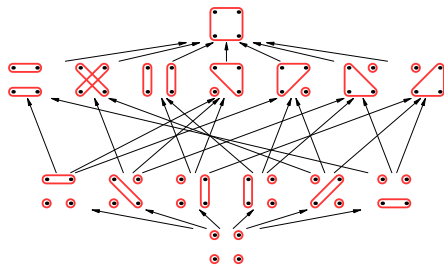
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- reformulation: $\exists T_m > 0$, such that
  $\forall \xi, \xi' \in \Pi(L)$ such that $\xi' \prec \xi$, and $\beta \preceq \xi$, then
  $\beta \preceq \xi' \Leftrightarrow C_{\xi'}(\varrho_L) - C_\xi(\varrho_L) \leq T_m$
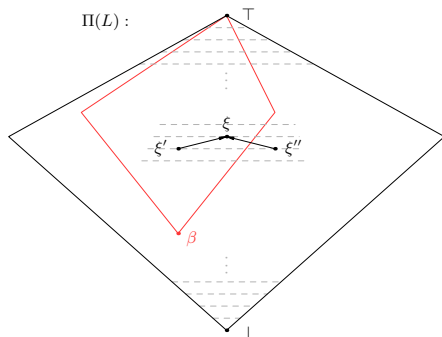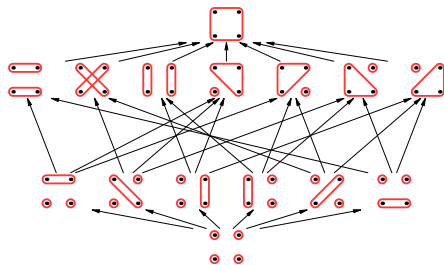
Correlation-based clustering – Properties

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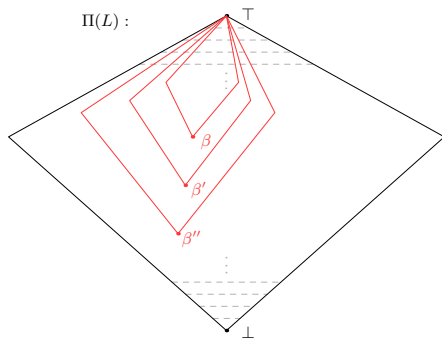
Correlation-based clustering – Properties

- there might not exist such clustering
- there may exist compatible clusterings (of different T_ms),

  but there exist no contradictory ones:
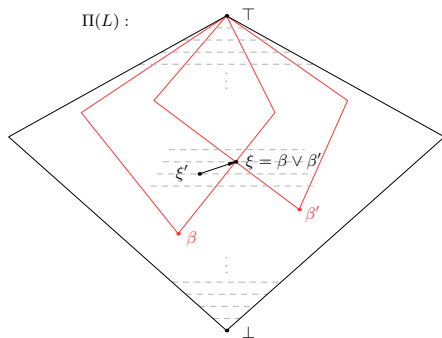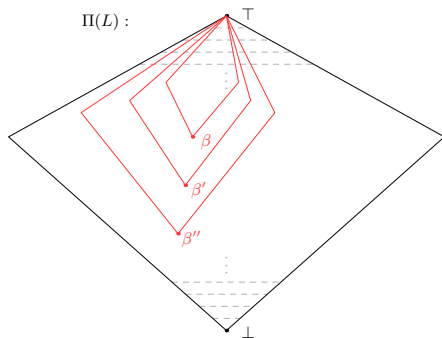
- successive refinement from $\top$ to $\bot$ (taking the smallest step):
  $\forall v, v' \in \Pi(L)$ s.t. $v' \prec v$, and $\forall \xi \in \Pi(L)$ s.t. $\xi \preceq v$ but $\xi \not\preceq v'$,
  then $\min_{\xi' \prec \xi} C_{\xi'}(\varrho_L) - C_{\xi}(\varrho_L) \leq C_{v'}(\varrho_L) - C_v(\varrho_L)$

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- hint: does not dissect $G \in \gamma$ (bipart. corr. clustering), since
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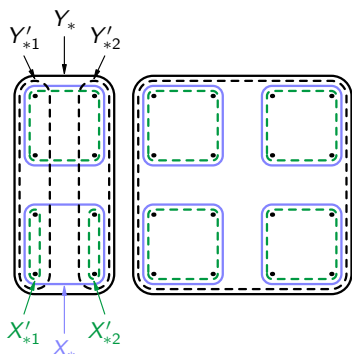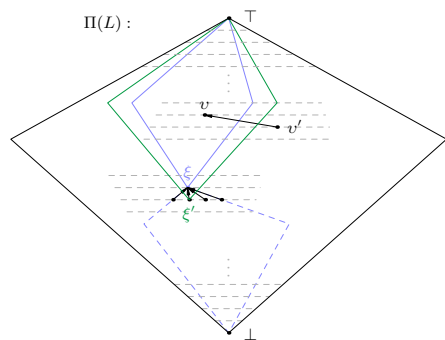
Correlation-based clustering – Finding β

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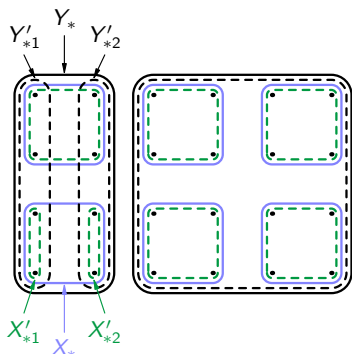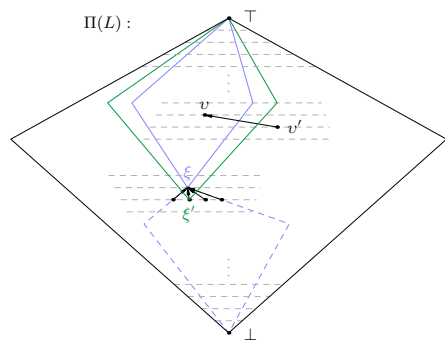
Example: Electron system of molecules

benzene (C_6H_6)
$C_\alpha = 29.52$
$C_\beta = 2.33$
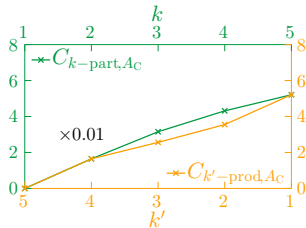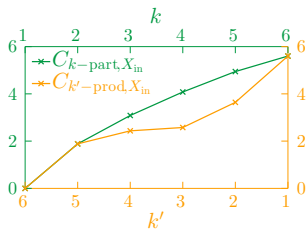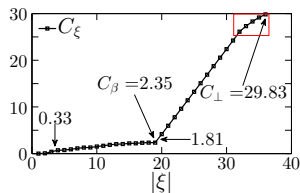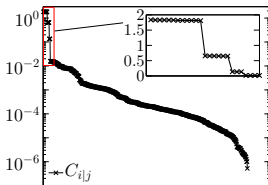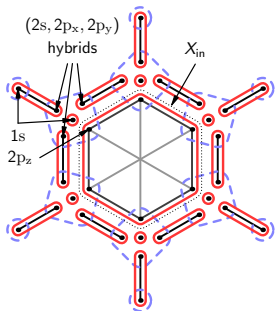
(in units $\ln 4$)

Example: Electron system of molecules

cyclobutadiene (C_4H_4)
$C_\alpha = 19.48$
$C_\beta = 3.17$

(in units ln 4)
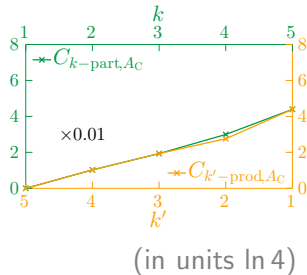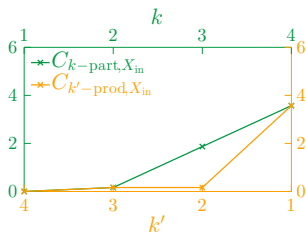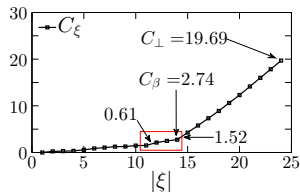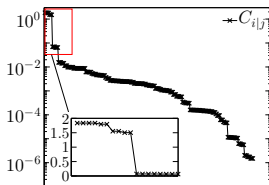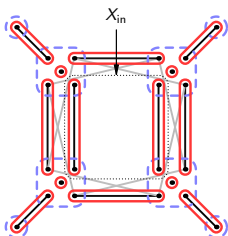
Example: Electron system of molecules

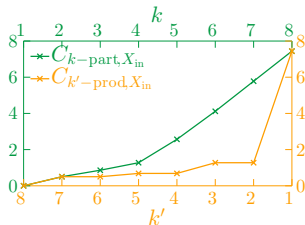ethane (C_2H_6)

$C_\alpha = 13.84$

$C_\beta = 0.90$
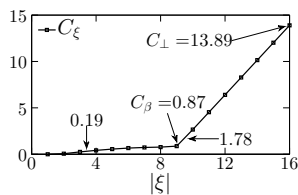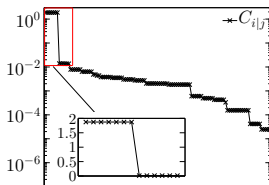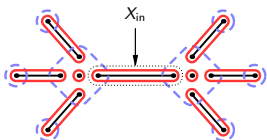
$$C_{\text{2-part},X_{\text{in}}} = C_{\text{1-prod},X_{\text{in}}}$$
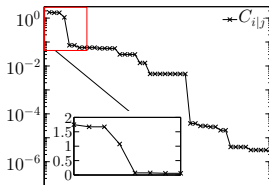$$= C_{\perp,X_{\text{in}}} = 1.796$$
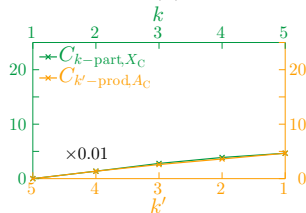
(in units $\ln 4$)

Example: Electron system of molecules

ethylene (C_2H_4)

$C_\alpha = 11.76$

$C_\beta = 1.00$
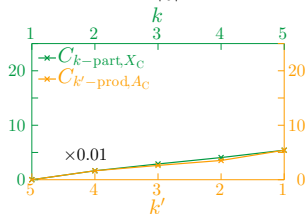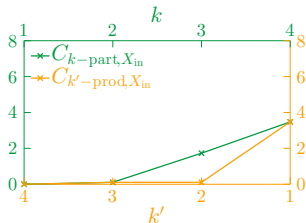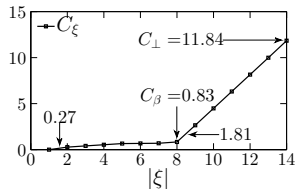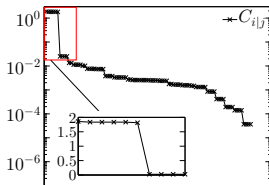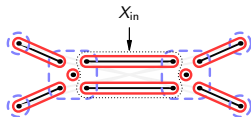
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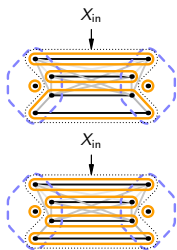acetylene (C_2H_2)
$C_\alpha = 9.74$
$C_\beta = 0.45, 1.30$
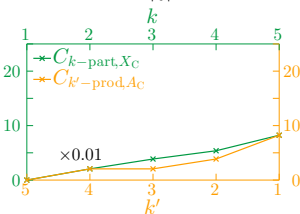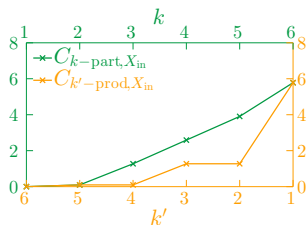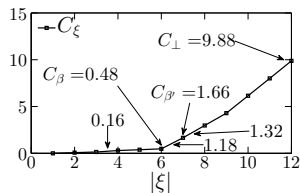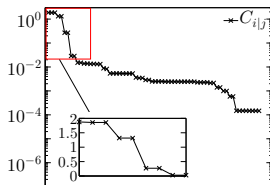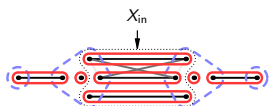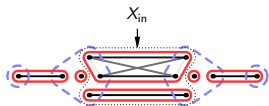
(in units $\ln 4$)

Example: Electron system of molecules

dicarbon (C_2H_0)
$C_\alpha = 7.06$
$C_\beta = 0.89, 1.51$
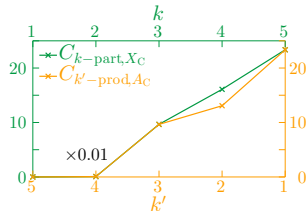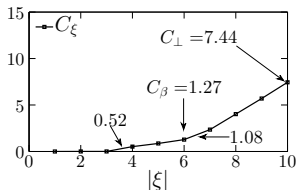
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Notions of correlations:

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Chemical bonds are where the electrons can freely move among atoms,
this is reflected in the correlation of occupations of localized orbitals.

Thank you for your attention!

Szalay, JPhysA **51**, 485302 (2018)

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