Cluster expansions for hard-core systems. II. Overview (end) and convergence criteria

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The setup

Ingredients

- *Countable* family $\mathcal{P}$ of objects: polymers, animals, ...
- *Incompatibility* constraint: $\gamma \nsim \gamma'$ (with $\gamma \nsim \gamma$)
- *Activities* $\boldsymbol{z} = \{z_\gamma\}_{\gamma \in \mathcal{P}} \in \mathbb{C}^{\mathcal{P}}$.

The basic ("finite-volume") measures

For each *finite* family $\mathcal{P}_\Lambda \subset \mathcal{P}$

$$\mathrm{W}_\Lambda\big(\{\gamma_1, \gamma_2, \ldots, \gamma_n\}\big) \;=\; \frac{1}{\Xi_\Lambda(\boldsymbol{z})}\, z_{\gamma_1} z_{\gamma_2} \cdots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}}$$

$$\Xi_\Lambda(\boldsymbol{z}) = 1 + \sum_{n \geq 1} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n) \in \mathcal{P}_\Lambda^n} z_{\gamma_1} z_{\gamma_2} \ldots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}}$$

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Graph-theoretical framework

Incompatibility graph $\mathcal{G} = (\mathcal{P}, \mathcal{E})$

- Incompatible = neighboring ($\gamma \nsim \gamma' \equiv \gamma \leftrightarrow \gamma'$)
- Polymer system = hard-core gas in a complicated lattice
- $\mathcal{N}^*_{\gamma_0} = \{\gamma \in \mathcal{P} : \gamma \nsim \gamma_0\}$; $\mathcal{N}_{\gamma_0} = \mathcal{N}^*_{\gamma_0} \setminus \{\gamma_0\}$
- *Independent vertices* = non-neighboring vertices
- *Independent sets* = sets formed by independent vertices

Thus,

$$\Xi_\Lambda(z) = \sum_{\substack{\Gamma \subset \mathcal{P}_\Lambda \\ \text{independent}}} z^\Gamma \qquad \text{with} \quad z^\Gamma = \prod_{\gamma \in \Gamma} z_\gamma$$

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Ratios of partition functions

- Correlations:

$$\mathrm{Prob}_\Lambda\big(\{\gamma_1,\ldots,\gamma_k \text{ are present}\}\big) \;=\; z_{\gamma_1}\cdots z_{\gamma_k}\,\frac{\Xi_{\Lambda\setminus\{\gamma_1,\ldots,\gamma_k\}^*}}{\Xi_\Lambda}$$

- Characteristic functions: If $S_\Lambda(\gamma_1,\ldots,\gamma_n)=\sum_{i=1}^n \alpha(\gamma_i)$

$$E_\Lambda\big(\mathrm{e}^{\xi\,S_\Lambda}\big) \;=\; \frac{\Xi_\Lambda(\boldsymbol{z}^\xi)}{\Xi_\Lambda(\boldsymbol{z})} \quad \text{with} \quad z^\xi_\gamma = z_\gamma\,\mathrm{e}^{\xi\alpha(\gamma)}$$

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$$f(\beta,\boldsymbol{h}) \;=\; \lim_{\Lambda\to\mathbb{L}} \frac{1}{|\Lambda|}\log Z^\sigma_\Lambda$$

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Previous example: Single-call loss networks

- $\mathcal{P}$ = finite connected families of links of $\mathbb{Z}^d$ —the *calls*
- z_γ = Poissonian rate for the call γ
- Compatibility = use of disjoint links (no intersection)
- Basic measures are invariant for the finite-region process
- Thermodynamic limit: infinite-volume process

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Using the *contour representation*:

- Polymers = contours (connected closed surfaces)
- Compatibility = no intersection
- $z_\gamma = \exp\{-2\beta J\ |\gamma|\}$

Then

$$W_\Lambda(\omega \mid +) = \frac{1}{\Xi_\Lambda} \prod_{\gamma \in \Gamma(\omega)} z_\gamma$$

with

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Previous example: LTE for Ising ferromagnets

Write

$$H_\Lambda(\omega) \;=\; -\sum_{B\in\mathcal{B}_\Lambda} J_B\big(\omega^B - 1\big) - \sum_{B\in\mathcal{B}_\Lambda} J_B$$

- *Contour* = connected component of (excited) bonds
- $z_\gamma \;=\; \exp\{-2\beta \sum_{B\in\gamma} J_B\}$
- $\gamma \sim \gamma'$ iff $\underline{\gamma} \cap \underline{\gamma}' = \emptyset$ (disjoint bases); $\underline{\gamma} = \cup\{B : B \in \gamma\}$

Then $Z_\Lambda = |\mathcal{S}_\Lambda|\; \Xi^{\rm LT}_\Lambda$ with

$$\mathcal{S}_\Lambda \;=\; \big\{\chi : \chi^B = 1 \text{ for all } B \in \mathcal{B}_\Lambda\big\}$$

(symmetry group) and

$$\Xi^{\rm LT}_\Lambda(\boldsymbol{z}) = 1 + \sum_{n\ge1} \frac{1}{n!} \sum_{(\gamma_1,\dots,\gamma_n)\in\mathcal{C}^n_\Lambda} z_{\gamma_1} z_{\gamma_2}\cdots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j\sim\gamma_k\}}$$

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Geometrical polymer models

Original polymer models of Gruber and Kunz:

- $\mathcal{P}$ = family of finite subsets of some set $\mathbb{V}$
- $\gamma \sim \gamma' \iff \gamma \cap \gamma' = \emptyset$

Usually

- $\mathbb{V}$ = vertex set of a graph (lattice, dual lattice)
- Polymers defined by connectivity properties
- Compatibility determined by graph distances

Warning: Do not confuse with the incompatibility graph

A little more general: decorated geometrical polymers

$$\gamma = (\underline{\gamma}, D_\gamma) \quad , \quad \underline{\gamma} = \text{"base"} \subset\subset \mathbb{V} \; , \; D_\gamma = \text{ "decoration"}$$

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Cluster expansions

Write the polynomials (in $(z_\gamma)_{\gamma\in\mathcal{P}}$)

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as *formal* exponentials of a *formal* series

$$\Xi_\Lambda(\boldsymbol{z}) \stackrel{\mathrm{F}}{=} \exp\Bigl\{\sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\dots,\gamma_n)\in\mathcal{P}_\Lambda^n} \phi^T(\gamma_1,\dots,\gamma_n)\, z_{\gamma_1} \dots z_{\gamma_n}\Bigr\}$$

- The series between curly brackets is the *cluster expansion*
- $\phi^T(\gamma_1,\dots,\gamma_n)$: *Ursell* or *truncated* functions (symmetric)
- *Clusters*: Families $\{\gamma_1,\dots,\gamma_n\}$ s.t. $\phi^T(\gamma_1,\dots,\gamma_n) \neq 0$
- Clusters are *connected* w.r.t. "$\not\sim$"

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Classical cluster-expansion strategy

Find a Λ-*independent* polydisc where cluster expansions converge *absolutely*

That is, find $\rho_\gamma > 0$ independent of Λ such that cluster expansions converge absolutely in the region

$$\mathcal{R} \;=\; \Big\{\boldsymbol{z} : |z_\gamma| \le \rho_\gamma \,,\, \gamma \in \mathcal{P}\Big\}$$

To this, find $\boldsymbol{\rho} > 0$ such that

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converges. Within this region

- No Ξ_Λ has a zero
- Explicit series expressions for free energy and correlations
- Explicit δ-mixing
- Central limit theorem

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Associated polymer models

Associated polymer model = same partition ratios

More precisely,

$$Z_\Lambda^{\text{model}}(\text{param.}) \;=\; \text{const}_\Lambda \, \Xi_\Lambda^{\text{polymer}}(\boldsymbol{z})$$

$(\text{const}_\Lambda \sim a^{|\Lambda|})$.

Useful observation: Distributivity property

If S finite set and $(\varphi_a)_{a\in S}$, $(\psi_a)_{a\in S}$ complex-valued:

$$\prod_{a\in S}[\psi_a + \varphi_a] \;=\; \sum_{A\subset S}\prod_{a\in A}\varphi_a \prod_{a\in S\setminus A}\psi_a$$

$[\prod_\emptyset \equiv 1]$

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Models at high temperature

$$\exp\Big\{-\beta \sum_{A\in\mathcal{B}_\Lambda} \phi_A(\omega)\Big\} = \prod_{A\in\mathcal{B}_\Lambda} \Big[1+\big(\mathrm{e}^{-\beta\,\phi_A(\omega)}-1\big)\Big]$$

$$= \sum_{\boldsymbol{B}\subset\mathcal{B}_\Lambda} \prod_{A\in\boldsymbol{B}} \big(\mathrm{e}^{-\beta\,\phi_A(\omega)}-1\big)$$

Separating $\boldsymbol{B}$ into connected (w.r.t. overlapping) components,

$$Z_\Lambda =$$

$$\sum_{n\geq 0} \frac{1}{n!} \sum_{\substack{(\boldsymbol{B}_1,\ldots,\boldsymbol{B}_n)\subset\boldsymbol{B}_\Lambda^n \\ \boldsymbol{B}_i \text{ conn.}}} \prod_{i=1}^{n} \int_{\underline{\boldsymbol{B}_i}} \prod_{A\in\boldsymbol{B}_i} \big(\mathrm{e}^{-\beta\,\phi_A(\omega)}-1\big) \bigotimes_{x\in\cup\underline{\boldsymbol{B}_i}} \mu_E(d\omega_x)$$

$$\times \prod_{i<j} \mathbb{1}_{\{\underline{\boldsymbol{B}_i}\cap\underline{\boldsymbol{B}_j}=\emptyset\}}$$

$[\underline{\boldsymbol{B}} = \text{support of } \boldsymbol{B} = \cup\{B : B\in\boldsymbol{B}\}]$

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$$= \sum_{\boldsymbol{B}\subset\mathcal{B}_\Lambda} \prod_{A\in\boldsymbol{B}} (\mathrm{e}^{-\beta\,\phi_A(\omega)} - 1)$$

Separating $\boldsymbol{B}$ into connected (w.r.t. overlapping) components,

$$Z_\Lambda =$$

$$\sum_{n\geq 0}\frac{1}{n!} \sum_{\substack{(\boldsymbol{B}_1,\ldots,\boldsymbol{B}_n)\subset\boldsymbol{B}_\Lambda^n \\ \boldsymbol{B}_i \text{ conn.}}} \prod_{i=1}^{n}\int_{\underline{\boldsymbol{B}_i}} \prod_{A\in\boldsymbol{B}_i} (\mathrm{e}^{-\beta\,\phi_A(\omega)} - 1) \bigotimes_{x\in\cup\underline{\boldsymbol{B}_i}} \mu_E(d\omega_x)$$

$$\times \prod_{i<j} \mathbb{1}_{\{\underline{\boldsymbol{B}_i}\cap\underline{\boldsymbol{B}_j}=\emptyset\}}$$

[$\underline{\boldsymbol{B}}$ = support of $\boldsymbol{B} = \cup\{B : B\in\boldsymbol{B}\}$]

High-temperature expansion

Hence

$$Z_\Lambda \;=\; \Xi_\Lambda^{\mathrm{HT}}$$

for the polymer system with

- $\mathcal{P} = \{\text{connected finite subsets of bonds}\}$
- $\boldsymbol{B} \sim \boldsymbol{B}'$ iff $\underline{\boldsymbol{B}} \cap \underline{\boldsymbol{B}'} = \emptyset$
- $$z_{\boldsymbol{B}} = \int_{\underline{\boldsymbol{B}}} \prod_{A \in \boldsymbol{B}} (\mathrm{e}^{-\beta\,\phi_A(\omega)} - 1) \bigotimes_{x \in \underline{\boldsymbol{B}}} \mu_E(d\omega_x)$$

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HTE for Ising ferromagnets

Obtained by exploiting in

$$Z_\Lambda \;=\; \sum_{\omega_\Lambda} \prod_{B\in\mathcal{B}_\Lambda} \mathrm{e}^{-\beta J_B \omega^B}$$

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$$\mathrm{e}^{-\beta J_B \omega^B} \;=\; \cosh(\beta J_B) + \omega^B \sinh(\beta J_B)$$

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Group of cycles

But

$$\prod_{B\in\boldsymbol{B}} \omega^B \;=\; \omega^{\sum_{B\in\boldsymbol{B}}}$$

with $\sum$ =symmetric difference, and

$$\sum_{\omega_\Lambda} \omega^B \;=\; \begin{cases} 2^{|\Lambda|} & \text{if } B=\emptyset \\ 0 & \text{otherwise} \end{cases}$$

Hence

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Ferromagnetic HT polymer model

The maximally *connected* elements of $\mathcal{K}_\Lambda$ are the *cycles*

($\mathcal{K}_\Lambda$ is a group for "$\sum$", generated by the cycles)

Factorizing the contribution of cycles,

$$Z_\Lambda = 2^{|\Lambda|}\Big[\prod_{B\in\mathcal{B}_\Lambda}\cosh(\beta J_B)\Big]\Xi_\Lambda^{\mathrm{IHT}}$$

for the polymer system with

- Polymers $\mathcal{P} = \{\text{ cycles}\}$
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LTE vs HTE for Ising ferromagnets

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HT–LT duality

Let us absorb β into the couplings J_B

$\left(\Lambda^*, \mathcal{B}^*_\Lambda, (J^*_B)_{B\in\mathcal{B}^*_\Lambda}\right)$ is the *HT–LT dual* of $\left(\Lambda, \mathcal{B}_\Lambda, (J_B)_{B\in\mathcal{B}_\Lambda}\right)$ if there exists a surjective map $D : \mathcal{B}_\Lambda \to \mathcal{B}^*_\Lambda$ such that

(i) The map

$$\begin{aligned} \overline{D} : \mathcal{P}(\mathcal{B}_\Lambda) &\longrightarrow \mathcal{P}(\mathcal{B}^*_\Lambda) \\ \overline{D}(\boldsymbol{B}) &= \cup_{B\in\boldsymbol{B}} D(B) \end{aligned}$$

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$$\mathrm{e}^{-2J^*_{B^*}} = \prod_{B\in D^{-1}(B^*)} \tanh(J_B)$$

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Dual systems

For HT–LT duals

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Hence:

convergent C.E. for $Z^*_{\Lambda^*}\iff$ convergent C.E. for Z_Λ

That is,

analyticity of $f^*\iff$ analyticity of f

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Construction of HT–LT duals

- Consider a family $\{\boldsymbol{B}_1, \ldots, \boldsymbol{B}_k\}$ of generators of $\mathcal{K}_\Lambda$
- Associate to each $\boldsymbol{B}_i$ a site $x_i^* \in \Lambda^*$
- Define

$$D(B) \;=\; \{x_i^* : \boldsymbol{B}_i \ni B\}$$

In particular

- Regular 2-d Ising is self-dual
- Ising with four body has as dual the usual Ising

Comments

- *Strong duality*: $\mathcal{K}_\Lambda = \mathcal{C}_\Lambda^*$
- Similarly there are LT–HT, HT–HT and LT–LT duals

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Potts model

$\mathbb{L}$ any (eg. $\mathbb{Z}^d$), $E = \{1, \ldots, q\}$, $\mathcal{F}$ =discrete, μ_E =counting

$$\phi_B(\omega) = \begin{cases} -J_{x\,y}\left(\delta_{\omega_x\omega_y} - 1\right) & \text{if } B = \{x,y\} \text{ n.n.} \\ 0 & \text{otherwise} \end{cases}$$

- $\phi_{\{x,y\}} = J$ if $\omega_x \neq \omega_y$, 0 otherwise
- If $q = 2$, Potts=Ising

$$Z_\Lambda^{\text{Potts}}(\beta, q) = \sum_{\omega_\Lambda} \prod_{\{x,y\}\subset\Lambda} \mathrm{e}^{\beta J_{x\,y}(\delta_{\omega_x\omega_y}-1)}$$

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The FK trick

Crucial observation:

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\begin{aligned}
e^{\beta J_{x\,y}(\delta_{\omega_x \omega_y}-1)} &= \delta_{\omega_x \omega_y} + e^{-\beta J_{x\,y}}(1-\delta_{\omega_x \omega_y}) \\
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with $p_{x\,y} = 1 - e^{-\beta J_{x\,y}}$. Hence

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($\mathcal{B}$ = bonds)

The FK expansion

As

$$\sum_{\omega_\Lambda} \prod_{\{x,y\}\in \boldsymbol{B}} \delta_{\omega_x \omega_y} \;=\; q^{C(\boldsymbol{B})}$$

with $C(\boldsymbol{B}) = \#$ connected components of $\boldsymbol{B}$,

$$Z_\Lambda^{\mathrm{Potts}}(\beta, q) \;=\; \sum_{\boldsymbol{B}\subset\mathcal{B}} q^{C(\boldsymbol{B})} \prod_{\{x,y\}\in\boldsymbol{B}} p_{x\,y} \prod_{\{x,y\}\notin\boldsymbol{B}} (1-p_{x\,y})$$

- $q = 1$: regular (independent) bond percolation in $\mathbb{Z}^d$
- $q > 1$: dependent percolation due to $q^{C(\boldsymbol{B})}$

FK model

$$
\begin{aligned}
Z_\Lambda^{\text{Potts}}(\beta, q) &= \Bigg[\prod_{\{x,y\}\in\mathcal{B}} (1 - p_{x\,y})\Bigg] \sum_{\boldsymbol{B}\subset\mathcal{B}} q^{C(\boldsymbol{B})} \prod_{\{x,y\}\in\boldsymbol{B}} \frac{p_{x\,y}}{1 - p_{x\,y}} \\
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with

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Z_\Lambda^{\text{FK}}(q, \boldsymbol{v}) = \sum_{\boldsymbol{B}\subset\mathcal{B}} q^{C(\boldsymbol{B})} \prod_{\{x,y\}\in\boldsymbol{B}} v_{x\,y}
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FK polymer model

(Also called *random-cluster model*)

Reorder the sum:

- Each $\boldsymbol{B}$ defines a graph $G = (V_{\boldsymbol{B}}, \boldsymbol{B})$
- Let $G_i = (V_i, \boldsymbol{B}_i)$, $i = 1, \ldots, k$ connected components
  - The vertex sets are disjoints: $V_i \cap V_j = \emptyset$ if $i \neq j$
  - The sets of bonds $\boldsymbol{B}_i$ are such that each G_i is connected

Furthermore

$$\begin{aligned} C(\boldsymbol{B}) &= k + \#\text{ isolated points} \\ &= k + |\Lambda| - \sum |V_i| \\ &= |\Lambda| - \sum (|V_i| - 1) \end{aligned}$$

FK polymer model

(Also called *random-cluster model*)

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High-q expansion

Then

$$\frac{Z_\Lambda^{\mathrm{FK}}(q,\boldsymbol{v})}{q^{|\Lambda|}} = \sum_{k\geq 0}\frac{1}{k!}\sum_{\substack{(V_1,\dots,V_k)\in\Lambda^k\\ \text{disjoints}}}\prod_{i=1}^{k}\Biggl[q^{-(|V_i|-1)}\sum_{\substack{\boldsymbol{B}_i\subset\mathcal{B}_{V_i}\\ (V_i,\boldsymbol{B}_i)\text{ conn.}}}\prod_{\{x,y\}\in\boldsymbol{B}_i} v_{x\,y}\Biggr]$$

$$= \Xi_\Lambda^{\mathrm{FK}}(\boldsymbol{z})$$

FK geometrical polymer system: $\mathcal{P} = \{V \subset\subset \mathbb{L}\}$,

$$z_V = q^{-(|V|-1)}\sum_{\substack{B\subset\mathcal{B}_V\\ (V,\boldsymbol{B})\text{ connected}}}\prod_{\{x,y\}\in\boldsymbol{B}} v_{x\,y}$$

decreases as $q\to\infty$ (or as $\beta\to 0$)

Corresponding cluster expansion = *high-q (high-T) expansion*

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Chromatic polynomials

Given a graph $G = \big(V(G), E(G)\big)$:

$$P_G(q) \;=\; \#\text{ ways of properly coloring } G \text{ with } q \text{ colors}$$

"properly" = adjacents vertices have different colors

If $\omega : V(G) \to \{1, \ldots, q\}$ denote colorings

$$P_G(q) \;=\; \sum_{\omega} \prod_{\{x,y\} \in E(G)} \left[1 - \delta_{\omega_x\, \omega_y}\right]$$

Introduced by Birkhoff (1912) to determine

$$\chi_G \;=\; \min\big\{q : P_G(q) > 0\big\}$$

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Tutte polynomial

Slight generalization: $(-1) \to v_{x\,y}$

$$P_G(q, \boldsymbol{v}) \;=\; \sum_{\omega} \prod_{\{x,y\}\in E(G)} \Big[1 + v_{x\,y}\,\delta_{\omega_x\,\omega_y}\Big]$$

- Dichromatic polynomial
- Dichromate
- Whitney rank function
- Tutte polynomial

For us

$$P_G(q, \boldsymbol{v}) \;=\; Z_\Lambda^{\mathrm{FK}}(q, \boldsymbol{v}) \;=\; q^{|\Lambda|}\,\Xi_\Lambda^{\mathrm{FK}}(\boldsymbol{z})$$

This identity proves that $P_G(q, \boldsymbol{v})$ is a polynomial in q

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Chromatic numbers and cluster expansions

If $J_{x\,y} < 0$ (antiferromagnetic Potts model)

$$v_{x\,y} = \mathrm{e}^{\beta J_{x\,y}} - 1 \xrightarrow[\beta\to\infty]{} -1$$

Hence

$$P_G(q) \;=\; Z_\Lambda^{\mathrm{FK}}(q,-1) \;=\; q^{|\Lambda|}\,\Xi_\Lambda^{\mathrm{FK}}(\boldsymbol{z}^-)$$

with

$$z_V^- \;=\; q^{-(|V|-1)} \sum_{\substack{\mathbf{B}\subset\mathcal{B}_{\mathbf{V}} \\ (\mathbf{V},\boldsymbol{B})\text{ conn.}}} (-1)^{|\boldsymbol{B}|}$$

Region free the zeros of $P_G(q) \to$ bound on χ_G

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Inhomogeneous Markov chains

Let $(X_n)_{n\geq 0}$ be a Markov chain, $X_n : \Omega \to E$, characterized by

$$\begin{aligned} p_n(x_{n-1}, x_n) &= \mathbb{P}(X_n = x_n \mid X_{n-1} = x_{n-1}) \\ p_0(x) &= \mathbb{P}(X_0 = x) \end{aligned}$$

Denote

$$p_{[0,n]}(x_0^n) = p_0(x_0)\, p_1(x_0, x_1) \cdots p_n(x_{n-1}, x_n)$$

Consider $\alpha : E \to \mathbb{R}$,

$$S_n(x_0^n) = \sum_{i=0}^{n} \alpha(x_i)$$

and the characteristic function

$$\phi_n(\xi) = \sum_{x_0^n} p_{[0,n]}(x_0^n)\, \mathrm{e}^{\xi S_n(x_0^n)}$$

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Polymer representation (Dobrushin)

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\begin{aligned}
\mathrm{e}^{\xi S_n(x_0^n)} &= \prod_{i=0}^{n}\Big[1+\big(\mathrm{e}^{\xi\,\alpha(x_i)}-1\big)\Big] \\
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Hence

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$$p_{[b,a]} \;=\; \left[p_{[a,b]} - p_a\right] + p_a$$

with $p_a(x_a) = \mathbb{P}(X_a = x_a)$. Result:

$$\phi_n(z) \;=\; \Xi_{[0,n]}$$

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$$\mathcal{P} \;=\; \Big\{(\underline{a},\underline{b}) = (a_1, b_1, a_2, b_2, \ldots, a_k, b_k) : 0 \le a_i \le b_i \le n \;,\; b_i < a_{i+1}\Big\}$$

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Small if $p_{[b,a]} - p_a$ and $|\xi|$ small. Relaxation $\to$ CLT

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Generalization: Continuous polymer systems

More generally,

$$\frac{1}{n!}\sum_{(\gamma_1,\ldots,\gamma_n)\in\mathcal{P}_\Lambda^n} \longrightarrow \frac{1}{n!}\int_{\mathcal{P}_\Lambda^n} d\gamma_1\cdots d\gamma_n$$

where $d\gamma_1\cdots d\gamma_n$ is an appropriate product measure That is, we consider measures on $\sum_n \mathcal{P}^n$ with projections on $\mathcal{P}^n$

$$\frac{1}{\Xi}\,\frac{1}{n!}\,z_{\gamma_1}z_{\gamma_2}\cdots z_{\gamma_n}\prod_{j<k}\mathbb{1}_{\{\gamma_j\sim\gamma_k\}}\,d\gamma_1\cdots d\gamma_n$$

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Correlations and cluster expansions

The correlation functions are probability densities —with respect to $d\gamma_1 \cdots d\gamma_n$— of finding polymers $\gamma_1, \ldots, \gamma_n$:

$$\rho(\gamma_1, \ldots, \gamma_n) \;=\; z_{\gamma_1} \ldots z_{\gamma_n} \, \frac{\Xi_{\mathcal{P}\setminus\{\gamma_1,\ldots,\gamma_k\}^*}}{\Xi}$$

The cluster expansion is the formal series such that

$$\Xi \;\stackrel{\mathrm{F}}{=}\; \exp\Bigl\{\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathcal{P}^n} \phi^T(\gamma_1, \ldots, \gamma_n) \, z_{\gamma_1} \ldots z_{\gamma_n} \, d\gamma_1 \cdots d\gamma_n\Bigr\}$$

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Example: Classical continuous gas

Basic setting

- Particles moving in a continuous space $\mathbb{S}$ (e.g. $\mathbb{S} = \mathbb{R}^d$)
- Initially particles in a box $\Lambda \subset\subset \mathbb{S}$, eventually $\Lambda \to \mathbb{S}$
- Particles are distinguishable, but interest focuses on which points are occupied and not by whom

Hence:

- Configuration: momenta and positions of particles in a box
- There is a $1/n!$ factor averaging permutations among sites

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Ingredients of a continuous systems

- *Energy* of n particules of momenta p_i and positions x_i:

$$H(p_1,\ldots,p_n,x_1,\ldots,x_n) \;=\; \sum_{i=1}^{n} \frac{p_i^2}{2m} + U(x_1,\ldots,x_n)$$

  where U is the *configurational Hamiltonian*

$$U(x_1,\ldots,x_n) \;=\; \sum_{A\subset\{1,\ldots,n\}} \phi_{|A|}\big((x_i)_{i\in A}\big)$$

- *Gibbs chemical potential* μ (acts as a “field”)

Grand canonical ensemble

Measures on $\sum_n \big[(\mathbb{R}^d)^n \times \Lambda^n\big]$ (with $\Lambda \subset\subset \mathbb{S}$), s.t. projected on $(\mathbb{R}^d)^n \times \Lambda^n$:

$$\frac{1}{\widetilde{Z}_\Lambda} \frac{e^{\beta\mu n}}{n!} \prod_{i=1}^n \Big[\exp\Big(-\beta \frac{p_i^2}{2m}\Big) dp_i\Big] \exp\Big[-\beta\, U(x_1,\ldots,x_n)\Big] dx_1 \cdots dx_n$$

with

$$\begin{aligned}\widetilde{Z}_\Lambda &= \sum_{n\geq 0} \frac{e^{\beta\mu n}}{n!} \prod_{i=1}^n \Big[\int_{\mathbb{R}^d} \exp\Big(-\beta \frac{p_i^2}{2m}\Big) dp_i\Big] \\ &\qquad \times \int_{\Lambda^n} \exp\Big[-\beta\, U(x_1,\ldots,x_n)\Big] dx_1 \cdots dx_n\end{aligned}$$

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$$\begin{aligned}\widetilde{Z}_\Lambda &= \sum_{n\ge 0}\frac{\mathrm{e}^{\beta\mu n}}{n!}\prod_{i=1}^{n}\Big[\int_{\mathbb{R}^d}\exp\Big(-\beta\frac{p_i^2}{2m}\Big)dp_i\Big] \\ &\qquad\times\int_{\Lambda^n}\exp\Big[-\beta\,U(x_1,\ldots,x_n)\Big]dx_1\cdots dx_n\end{aligned}$$

Configurational ensemble

If no questions on momenta,

$$\int_{\mathbb{R}^d} \exp\Big(-\beta\frac{p_i^2}{2m}\Big)dp_i \;=\; \Big(\frac{2\pi m}{\beta}\Big)^{d/2}$$

and ensemble reduces to a measure on $\sum_n \Lambda^n$ with projections

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Gas of hard spheres

Points = centers of spheres of diameter R:

$$\phi_n(x_1,\ldots,x_n) \;=\; \begin{cases} \infty & \text{if } n=2 \text{ and } |x_1-x_2|\le R \\ 0 & \text{otherwise} \end{cases}$$

This gives a continuous polymer system with

- Polymers = centers of spheres in Λ:

$$\mathcal{P} \;=\; \mathcal{P}_\Lambda \;=\; \{x\in\Lambda : \operatorname{dist}(x,\mathbb{S}\setminus\Lambda) > R/2\}$$

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Cluster expansions - Classical strategy

Recall: Write

$$\Xi_\Lambda(\boldsymbol{z}) = 1 + \sum_{n\geq 1} \frac{1}{n!} \sum_{(\gamma_1,\dots,\gamma_n)\in\mathcal{P}_\Lambda^n} z_{\gamma_1} z_{\gamma_2} \dots z_{\gamma_n} \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}}$$

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The series between curly brackets is the *cluster expansion*

Need somme formal-series algebraic handling

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Multiplicity functions

In general, we are dealing with series of the form

$$F(\boldsymbol{z}) = \sum_{n\geq 0} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\in\mathcal{P}^n} a(\gamma_1,\ldots,\gamma_n)\, z_{\gamma_1}\cdots z_{\gamma_n}$$

Let us not assume anything about the coefficients other than

$a(\gamma_1,\ldots,\gamma_n)$ is symmetric under permutations of $(\gamma_1,\ldots,\gamma_n)$

Therefore, $a(\gamma_1,\ldots,\gamma_n)$ is a fcn. of the *multiplicty function*:

$$\boldsymbol{M} : \mathcal{P}^{(\mathbb{N})} \longrightarrow \mathbb{N}^{(\mathcal{P})}$$

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Exponential generating functions

Let $a(\boldsymbol{\alpha}) \;=\; a(\gamma_1, \ldots, \gamma_n)$ if $\boldsymbol{M}(\gamma_1, \ldots, \gamma_n) = \boldsymbol{\alpha}$. Then

$$F(\boldsymbol{z}) \;=\; \sum_{n \geq 0} \frac{1}{n!} \sum_{\boldsymbol{\alpha}:|\boldsymbol{\alpha}|=n} a(\boldsymbol{\alpha})\, N_{\boldsymbol{\alpha}}\, \boldsymbol{z}^{\boldsymbol{\alpha}}$$

where $|\boldsymbol{\alpha}| = \sum_\gamma \alpha_\gamma$ and

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Multivariate exponential generating function

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Multivariate exponential generating function

The truncated coefficients

The problem

Given functions $a(\boldsymbol{\alpha})$, find functions $a^{\mathrm{T}}(\boldsymbol{\alpha})$ s.t.

$$\sum_{\boldsymbol{\alpha}} \frac{a(\boldsymbol{\alpha})}{\boldsymbol{\alpha}!}\, \boldsymbol{z}^{\boldsymbol{\alpha}} \;=\; \exp\Bigl\{\sum_{\boldsymbol{\beta}} \frac{a^{\mathrm{T}}(\boldsymbol{\beta})}{\boldsymbol{\beta}!}\, \boldsymbol{z}^{\boldsymbol{\beta}}\Bigr\}$$

Then, $a^{\mathrm{T}}(\gamma_1,\ldots,\gamma_n) = a^{\mathrm{T}}\bigl(\boldsymbol{M}(\gamma_1,\ldots,\gamma_n)\bigr)$

The key relation

Equating coefficients of $\boldsymbol{z}^{\boldsymbol{\alpha}}$

$$\frac{a(\boldsymbol{\alpha})}{\boldsymbol{\alpha}!} = \sum_{k\ge 1} \frac{1}{k!} \sum_{\substack{(\boldsymbol{\beta}_1,\ldots,\boldsymbol{\beta}_k)\\ :\sum \boldsymbol{\beta}_i=\boldsymbol{\alpha}}} \prod_{i=1}^{k} \frac{a^{\mathrm{T}}(\boldsymbol{\beta}_i)}{\boldsymbol{\beta}_i!} \qquad (1)$$

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Algebraic facts

Key observation 1:

Previous expression *uniquely* determines a^{T}:

$$\begin{array}{lrcl}
|\boldsymbol{\alpha}| = 1 & a(\gamma) & = & a^{\mathrm{T}}(\gamma) \\
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|\boldsymbol{\alpha}| = n & & \ldots & \text{(induction)}
\end{array}$$

Key observation 2:

Better to go back to n-tuples

$$a(\gamma_1, \ldots, \gamma_n) = \boldsymbol{\alpha}! \sum_{k \geq 1} \frac{1}{k!} \sum_{\substack{(\boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_k) \\ : \sum \boldsymbol{\beta}_i = \boldsymbol{\alpha}}} \prod_{i=1}^{k} \frac{a^{\mathrm{T}}(\gamma_{I_i})}{\boldsymbol{\beta}_i!}$$

$\{I_1, \ldots, I_k\}$ partition of $\{1, \ldots, n\}$ (subseqs.) s.t. $\boldsymbol{\beta}_i = M(\gamma_{I_i})$

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Number of partitions

Q: How many partitions $\{I_1, \ldots, I_k\}$ satisfy $\boldsymbol{\beta}_i = \boldsymbol{M}(\gamma_{I_i})$?

Preliminary example: $\alpha_{\gamma_0} = n$ and $\alpha_\gamma = 0$ for $\gamma \neq \gamma_0$

Then $\left(\boldsymbol{\beta}_i\right)_{\gamma_0} = m_i$ and $\left(\boldsymbol{\beta}_i\right)_\gamma = 0$ for $\gamma \neq \gamma_0$ and

$$\#\left\{\text{partitions } \{I_1, \ldots, I_k\} \text{ with } |I_i| = m_i\right\} = \binom{n}{m_1 \cdots m_k}$$

More generally: $\alpha_{\gamma_1} = n_1, \ldots, \alpha_{\gamma_\ell} = n_\ell$, otherwise $\alpha_\gamma = 0$

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Defining relation

Bottom line: If a and a^{T} are perm.-sym. and satisfy:

$$a(\gamma_1, \ldots, \gamma_n) \;=\; \sum_k \sum_{\substack{\{I_1,\ldots,I_k\} \\ \text{part. of } \{1,\ldots,n\}}} a^{\mathrm{T}}(\gamma_{I_1}) \cdots a^{\mathrm{T}}(\gamma_{I_k})$$

Then, as formal power series,

$$1 + \sum_{n\geq 1} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)} a(\gamma_1, \ldots, \gamma_n)\, z_{\gamma_1} \cdots z_{\gamma_n}$$

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Most popular case

$$a(\gamma_1,\ldots,\gamma_n) \;=\; \prod_{\{i,j\}} \varphi(\gamma_i,\gamma_j)$$

$[\varphi(\gamma_i,\gamma_j) = \mathrm{e}^{-\beta\, U(\gamma_1,\gamma_j)}$; $\beta \to \infty$ for "hard-core"$]$. Writing

$$\varphi(\gamma_i,\gamma_j) \;=\; 1 + \Big(\varphi(\gamma_i,\gamma_j) - 1\Big) \;=\; 1 + \psi(\gamma_i,\gamma_j)$$

We have

$$\begin{aligned} a(\gamma_1,\ldots,\gamma_n) \;&=\; \prod_{\{i,j\}} \Big[1 + \psi(\gamma_i,\gamma_j)\Big] \\ &=\; \sum_{C\subset G_n} \prod_{e\in G} \psi(\gamma_e) \end{aligned}$$

- G_n =complete graph with vertices $\{1,\ldots,n\}$
- Sum over (not necessarily spanning) subgraphs of G_n
- $E(G)$ = edge set of G

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Connected graphs and partitions

Decomposing each G into connected components,

$$a(\gamma_1,\ldots,\gamma_n) \;=\; \sum_{k=1}^{n} \sum_{\substack{\{G_1,\ldots,G_k\} \\ \text{conn. part. of } G_n}} \prod_{i=1}^{k} \Big[\prod_{e\in E(G)} \psi(\gamma_e) \Big]$$

[G_i can be a single vertex, $\prod_\emptyset \equiv 1$]

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THE formula

Conclusion: If

$$a(\gamma_1, \ldots, \gamma_n) \;=\; \prod_{\{i,j\}} \varphi(\gamma_i, \gamma_j)$$

then

$$a^{\mathrm{T}}(\gamma_1, \ldots, \gamma_n) \;=\; \sum_{\substack{G \subset G_n \\ \text{conn. span.}}} \; \prod_{e \in E(G)} \psi(\gamma_e)$$

with

$$\psi(\gamma_i, \gamma_j) \;=\; \varphi(\gamma_i, \gamma_j) - 1$$

Truncated functions for hard core

For hard core:

$$\psi(\gamma_i, \gamma_j) \;=\; \mathbb{1}_{\{\gamma_i \sim \gamma_j\}} - 1 \;=\; \begin{cases} -1 & \text{if } \gamma_i \nsim \gamma_j \\ 0 & \text{if } \gamma_i \sim \gamma_j \end{cases}$$

Hence: For each n-tuple $(\gamma_1, \ldots, \gamma_n)$ construct the graph

$\mathcal{G}_{(\gamma_1,\ldots,\gamma_n)}$ with $V(\mathcal{G}) = \{1, \ldots, n\}$ and $E(\mathcal{G}) = \{\{i.j\} : \gamma_i \nsim \gamma_j\}$

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$$\phi^T(\gamma_1, \ldots, \gamma_n) \;=\; \begin{cases} 1 & n = 1 \\ \displaystyle\sum_{\substack{G \subset \mathcal{G}_{(\gamma_1,\ldots,\gamma_n)} \\ G \text{ conn. spann.}}} (-1)^{|E(G)|} & n \geq 2\,,\ \mathcal{G} \text{ conn.} \\ 0 & n \geq 2\,,\ \mathcal{G} \text{ not c.} \end{cases}$$

This formula involves a huge number of cancellations

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Penrose identity

Penrose realized that these cancellations can be optimally handled through what is now known as the property of *partitionability* of the family of connected spanning subgraphs

Theorem

For any connected graph $\mathcal{G} = (\mathbb{V}, \mathbb{E})$ there exists a family of spanning trees —the Penrose trees $\mathcal{T}_{\mathcal{G}}^{\text{Penr}}$— such that

$$\sum_{G \subset \mathcal{G}} (-1)^{|E(G)|} = (-1)^{|\mathbb{V}|-1} \left| \mathcal{T}_{\mathcal{G}}^{\text{Penr}} \right|$$

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Partitionability of subgraphs

Let

- $\mathbb{G} = (\mathbb{U}, \mathbb{E})$ a finite connected graph
- $\mathcal{C}_{\mathbb{G}} = \{$connected spanning subgraphs of $\mathbb{G}\}$
- $\mathcal{T}_{\mathbb{G}} = \{$trees belonging to $\mathcal{C}_{\mathbb{G}}\}$

Partial-order $\mathcal{C}_{\mathbb{G}}$ by bond inclusion:

$$G \leq \widetilde{G} \iff E(G) \subset E(\widetilde{G})$$

If $G \leq \widetilde{G}$, let

$$[G, \widetilde{G}] = \{\widehat{G} \in \mathcal{C}_{\mathbb{G}} : G \leq \widehat{G} \leq \widetilde{G}\}$$

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Partition schemes

A *partition scheme* for $\mathcal{C}_{\mathbb{G}}$ is a map

$$\begin{array}{rcl} R : \mathcal{T}_{\mathbb{G}} & \longrightarrow & \mathcal{C}_{\mathbb{G}} \\ \tau & \longmapsto & R(\tau) \end{array}$$

such that

(i) $E\big(R(\tau)\big) \supset E(\tau)$, and

(ii) $\mathcal{C}_{\mathbb{G}}$ is the disjoint union of the sets $[\tau, R(\tau)]$, $\tau \in \mathcal{T}_{\mathbb{G}}$.

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Penrose scheme

- Fix an enumeration $v_0, v_1, \ldots, v_n$ for the vertices of $\mathbb{G}$
- For each $\tau \in \mathcal{T}_{\mathbb{G}}$ let $d(i)$ = tree distance of v_i to v_0
- $R_{\text{Pen}}(\tau)$ is obtained adding to τ $\{v_i, v_j\} \in \mathbb{E} \setminus E(\tau)$ s.t.

  (p1) $d(i) = d(j)$ (edges between vertices of the same generation), or

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Penrose identity

For a partition scheme R, let

$$\mathcal{T}_R \;:=\; \Big\{\tau \in \mathcal{T}_{\mathbb{G}} \;\Big|\; R(\tau) = \tau\Big\}$$

(set of R-*trees*).

Proposition

$$\sum_{G \in \mathcal{C}_{\mathbb{G}}} (-1)^{|E(G)|} \;=\; (-1)^{|\mathbb{V}|-1} \big|\mathcal{T}_R\big|$$

for any partition scheme R

Proof of Penrose identity

For any numbers x_e, $e \in \mathbb{E}$,

$$\sum_{G \in \mathcal{C}_{\mathbb{G}}} \prod_{e \in E(G)} x_e = \sum_{\tau \in \mathcal{T}_{\mathbb{G}}} \prod_{e \in E(\tau)} x_e \sum_{\mathcal{F} \subset E(R(\tau)) \setminus E(\tau)} \prod_{e \in \mathcal{F}} x_e$$

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- If $x_e = -1$, the last factor kills the contributions of any tree τ with $E(R(\tau)) \setminus E(\tau) \neq \emptyset$
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Comments

- Hard-core condition is crucial. If only soft repulsion,

$$|1 + x_e| \leq 1$$

and we get the weaker *tree-graph bound*

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- The smaller the number of triangle diagrams, the larger the number of Penrose trees. Hence:

$$\begin{aligned} \mathcal{R}(\mathcal{G}) &\supset \mathcal{R}(\text{tree with larger degrees}) \\ &\supset \mathcal{R}(\text{homogeneous tree with max. degree}) \end{aligned}$$

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