Cluster expansions for hard-core systems. I. Overview

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The setup

Goal: To study systems of objects constrained only by a "non-overlapping" condition

Countable family $\mathcal{P}$ of objects: polymers, animals, ..., characterized by

- An *incompatibility* constraint:

$$\begin{matrix} \gamma \nsim \gamma' \\ \gamma \sim \gamma' \end{matrix} \qquad \text{if } \gamma, \gamma' \in \mathcal{P} \qquad \begin{matrix} \text{incompatible} \\ \text{compatible} \end{matrix}$$

  For simplicity: each polymer incompatible with itself ($\gamma \nsim \gamma$, $\forall \gamma \in \mathcal{P}$)

- A family of *activities* $\boldsymbol{z} = \{z_\gamma\}_{\gamma \in \mathcal{P}} \in \mathbb{C}^{\mathcal{P}}$.

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The basic ("finite-volume") measures

Defined, for each *finite* family $\mathcal{P}_\Lambda \subset \mathcal{P}$, by weights

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

for $n \geq 1$ $\gamma_1, \gamma_2, \ldots, \gamma_n \in \mathcal{P}_\Lambda$, and $\mathrm{W}_\Lambda(\emptyset) = 1/\Xi_\Lambda$, where

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

- Λ = some label, often finite subset of a countable set
- As compatible polymers are necessarily different,

$$\frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\in\mathcal{P}_\Lambda^n} [\bullet] \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}} \;=\; \sum_{\{\gamma_1,\ldots,\gamma_n\}\subset\mathcal{P}_\Lambda} [\bullet] \prod_{j<k} \mathbb{1}_{\{\gamma_j \sim \gamma_k\}}$$

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The questions:

- Existence of the limit $\mathcal{P}_\Lambda \to \mathcal{P}$ ("thermodynamic limit")
- Properties of the resulting measure (mixing properties, dependency on parameters,...)
- Asymptotic behavior of Ξ_Λ

Motivation

Immediate:

- *Physics:* Grand-canonical ensemble of polymer gas with activities z_γ and hard-core interaction
- *Statistics:* Invariant measure of point processes with not-overlapping grains and birth rates z_γ

Less immediate:

- Statistical mechanical models at high and low temperatures are mapped into such systems
- More generally: most perturbative arguments in physics involve maps of this type (choice of the "right" variables)
- Zeros of the partition functions Ξ_Λ relate to phase transitions (sphere packing, chromatic polynomials,. . .)

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Graph-theoretical framework

Equivalently, consider the *incompatibility graph* $\mathcal{G} = (\mathcal{P}, \mathcal{E})$

Unoriented graph with:

- Vertices = polymers
- Edges = incompatible pairs

$$\gamma \nsim \gamma' \quad \text{iff} \quad \{\gamma, \gamma'\} \in \mathcal{E} \quad \text{or} \quad \gamma \leftrightarrow \gamma' \tag{1}$$

  (contrast!)
- $\mathcal{E}$ is arbitrary; vertices can be of infinite degree (polymers incompatible with infinitely many other polymers)

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Polymers as lattice gases

In this graph-theoretical framework:

- Incompatible polymers = neighboring vertices
- Polymer system = hard-core gas in a complicated lattice
- *Neighborhood of* γ_0:

$$\mathcal{N}^*_{\gamma_0} = \{\gamma \in \mathcal{P} : \gamma \nsim \gamma_0\}$$
$$\mathcal{N}_{\gamma_0} = \mathcal{N}^*_{\gamma_0} \setminus \{\gamma_0\}$$

- *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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Example: Single-call loss networks

Definition

- $\mathcal{P}$ = finite subsets of $\mathbb{Z}^d$ —the *calls*
- A call γ is attempted with Poissonian rates z_γ
- Call succeeds if it does not intercept existing calls
- Once established, calls have an exp(1) life span

Remarks

- Basic measures are invariant for the finite-region process ($\gamma \not\sim \gamma' \iff \gamma \cap \gamma' \neq \emptyset$)
- Thermodynamic limit: infinite-volume process
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Statistical mechanical lattice models

Their ingredients are:

- *Lattice* $\mathbb{L}$ countable set of sites (e.g. $\mathbb{Z}^d$)
- *Single-site space* $(E, \mathcal{F}, \mu_E)$ with natural measure structure (e.g. counting measure if E countable, Borel if $E \subset \mathbb{R}^d$)
- *Configuration space* $\Omega = E^{\mathbb{L}}$, with product measure
- *Interaction* $\Phi = \{\phi_B : B \subset\subset \mathbb{L}\}$ where $\phi_B = \phi_B(\omega_B)$
  - *Bonds* are sets B such that $\phi_B \neq 0$
  - *Exclusions:*
    - $\Phi_B(\omega_B) = \infty$ (physicist)
    - $\Omega_{\text{all}} \subset \Omega$ (math-phys)

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Statistical mechanical measures

Their finite-volume versions are defined by

- *Hamiltonians:* For $\Lambda \subset\subset \mathbb{L}$, and boundary condition σ

$$H_\Lambda(\omega \mid \sigma) = \sum_{B \subset \Lambda} \phi_B(\omega_\Lambda \sigma)$$

- Boltzmann Probability densities (weights)

$$W_\Lambda(\omega \mid \sigma) \;=\; \frac{\exp\{-\beta H_\Lambda(\omega \mid \sigma)\}}{Z_\Lambda^\sigma}$$

$(\omega, \sigma \in \Omega_{\rm all})$ with

$$Z_\Lambda^\sigma \;=\; \int_{\Omega_{\rm all}} \exp\{-\beta H_\Lambda(\omega \mid \sigma)\} \bigotimes_{x \in \Lambda} \mu_E(d\omega_x)$$

$(\beta =$ inverse temperature$)$

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Example zero: Hard-core lattice gases

$\mathbb{L}$ =vertices of a graph (eg. $\mathbb{Z}^d$), $E = \{0,1\}$
($\mathcal{F}$ =discrete, μ_E =counting)

$$\phi_B(\omega) = \begin{cases} -u\,\omega_x & \text{if } B = \{x\} \\ \infty & \text{if } B = \{x,y\} \text{ n.n.} \\ 0 & \text{otherwise} \end{cases}$$

Let

$$\Gamma(\omega) = \{x : \omega_x = 1\}$$

Then, for $\Lambda \subset\subset \mathbb{L}$,

$$W_\Lambda(\omega \mid 0) = \frac{1}{Z^0_\Lambda} \prod_{x \in \Gamma(\omega_\Lambda)} e^{\beta u} \prod_{x,y \in \Gamma(\omega_\Lambda)} \mathbb{1}_{\{x \not\leftrightarrow y\}}$$

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Lattice gas = polymer model

This is a polymer model with

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$$H_\Lambda(\omega \mid +) \;=\; 2J\,F_\Lambda(\omega) - J N_\Lambda\;;$$

$$\begin{aligned} F_\Lambda(\omega) \;&=\; \#\{B \text{ frustrated} : B \cap \Lambda \neq \emptyset\} \\ N_\Lambda \;&=\; \#\{B : B \cap \Lambda \neq \emptyset\} \end{aligned}$$

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Contour representation

- Place a plaquette (segment) orthogonally at the midpoint of each frustrated bond
- These plaquettes form a family of disjoint closed connected surfaces (curves)
- Each such closed surface is a *contour*. Denote

$$\mathcal{C}_\Lambda = \{\text{contours } \gamma : \gamma \subset \Lambda\}$$

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Contour polymer model

$$\exp\Big\{-2\beta J\, F_\Lambda(\omega)\Big\} = \exp\Big\{-\sum_{\gamma\in\Gamma(\omega)} 2\beta J\, |\gamma|\Big\} = \prod_{\gamma\in\Gamma(\omega)} z_\gamma$$

with $z_\gamma = \exp\{-2\beta J\, |\gamma|\}$. Hence

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Contour polymer model

$$\exp\{-2\beta J\, F_\Lambda(\omega)\} = \exp\Big\{-\sum_{\gamma\in\Gamma(\omega)} 2\beta J\,|\gamma|\Big\} = \prod_{\gamma\in\Gamma(\omega)} z_\gamma$$

with $z_\gamma = \exp\{-2\beta J\,|\gamma|\}$. Hence

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Generalization: LTE for Ising ferromagnets

$\mathbb{L}$ =any, $E = \{-1, 1\}$, interactions

$$\phi_B(\omega) \;=\; -J_B\,\omega^B \quad , \text{with } J_B \geq 0$$

Without loss, free boundary conditions:

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

with

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[for $H_\Lambda(\cdot \mid +)$ use $\mathcal{B}_\Lambda^+$, etc]

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Generalized contours

Write

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

- A bond B is *excited* or *frustrated* if $\omega^B = -1$
- $\Gamma(\omega_\Lambda)$ = set of frustrated bonds in Λ
- A *contour* is a maximal connected component of Γ (connexion = intersection)
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Contours and probability weights

$$W_\Lambda(\omega) = \frac{\prod_{\gamma \in \Gamma(\omega_\Lambda)} e^{-\beta E(\gamma)}}{\widetilde{Z}_\Lambda}$$

where $E(\gamma) = \sum_{B \in \gamma} 2J_B$ and

$$\widetilde{Z}_\Lambda = \sum_{\sigma_\Lambda} \prod_{\gamma \in \Gamma(\sigma_\Lambda)} e^{-\beta E(\gamma)} = \sum_{\Gamma \in \mathcal{C}_\Lambda} N_\Gamma \prod_{\gamma \in \Gamma} e^{-\beta E(\gamma)}$$

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We compute N_Γ with a little help from group theory

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Geometrical polymer models

Polymers of previous examples (loss networks, Peierls contours) are points of a set

These are the original polymer models of Gruber and Kunz

Formally, geometrical polymer models are defined by:

- A set $\mathbb{V}$ (eg. possible calls, surfaces)
- A family $\mathcal{P}$ of finite subsets of $\mathbb{V}$ (eg. connected)
- Activity values $(z_\gamma)_{\gamma \in \mathcal{P}}$
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General geometrical polymers

Vertex-set polymers

$\mathbb{V}$ = vertex set of a graph (lattice, dual lattice)

- Polymers are defined through connectivity properties (graph-connected)
- Compatibility determined by graph distances (overlapping, being neighbors or sufficiently close)

WARNING! Second-level graph. On top: incompatibility graph

Decorated geometrical polymers

$\gamma = (\underline{\gamma}, D_\gamma)$ where

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Ratios of partition functions

Partition functions play a central role. Three reasons:

- Correlations are ratios of partition functions
- So are characteristic and moment-generating functions
- (Complex) zeros of partition functions related to phase transitions, coloring problems, etc

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Polymer correlation functions

Let

- Prob_Λ the basic measure in $\mathcal{P}_\Lambda$
- $\gamma_1, \ldots, \gamma_k$ mutually compatible polymers in $\mathcal{P}_\Lambda$

Then

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

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Statistical mechanical correlations

Likewise, for the stat-mech models, let

- $\mathrm{Prob}_\Lambda(\,\cdot \mid \sigma)$ be the measure in Λ with b.c. σ
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Characteristic/moment-generating functions

Let $\alpha : \mathcal{P} \to \mathbb{R}$ and

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for $\{\gamma_1, \ldots, \gamma_n\} \subset \mathcal{P}_\Lambda$. Hence $E_\Lambda\big(\mathrm{e}^{\xi\, S_\Lambda}\big)$ equals

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Complex ξ are of interest!

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Zeros and phase transitions

For (translation-invariant) stat-mech models

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

exists and is independent of the boundary condition σ

- Spin systems: $-f/\beta$ =free-energy density
- Gas models: f/β = pressure

Key information: smoothness as function of β and $\boldsymbol{h}$

Loss of analyticity = phase transition (of some sort)

Sufficient conditions for analyticity of f:

- Zeros of Z_Λ Λ-uniformly away from $(\beta, \boldsymbol{h})$
- Λ-independent radius of analyticity of $\frac{1}{|\Lambda|} \log Z_\Lambda$

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Alternative lines of attack

Physicist:

Control Ξ through expansion techniques $\longrightarrow$ cluster expansions

- Genesis/reincarnations: Mayer, virial, high-temperature, low-density, ... expansions
- Not everybody's cup of tea
- Involves algebraic and graph theoretical considerations
- Less natural for purely probabilistic studies (analyticity?)

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Models with exclusions = invariant measures of point processes

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- Weaker results (no analyticity!) but wider applicability
- Can use probabilistic techniques (coupling!)
- Leads to (perfect) simulation algorithms

Alternative lines of attack

Physicist:

Control Ξ through expansion techniques $\longrightarrow$ cluster expansions

- Genesis/reincarnations: Mayer, virial, high-temperature, low-density, . . . expansions
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Cluster expansions

The idea is to write the polynomials in $(z_\gamma)_{\gamma\in\mathcal{P}}$

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

as *formal* exponentials of another *formal* series

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

The series between curly brackets is the *cluster expansion*

WATCH OUT!: No consistency requirement, thus

$$\frac{1}{n!} \sum_{(\gamma_1,\dots,\gamma_n)\in\mathcal{P}_\Lambda^n} \neq \sum_{\{\gamma_1,\dots,\gamma_n\}\subset\mathcal{P}_\Lambda}$$

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Clusters and truncated functions

- $\phi^T(\gamma_1, \ldots, \gamma_n)$: *Ursell* or *truncated* functions (symmetric)
- *Clusters*: Families $\{\gamma_1, \ldots, \gamma_n\}$ s.t. $\phi^T(\gamma_1, \ldots, \gamma_n) \neq 0$
- The formula of ϕ^T will be given later. Highlights:
  - Clusters are *connected* w.r.t. "$\not\sim$"
  - $$\phi^T(\gamma) = 1 \quad , \quad \phi^T(\gamma, \gamma') = \begin{cases} -1 & \text{if } \gamma \not\sim \gamma' \\ 0 & \text{otherwise} \end{cases}$$

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Telescoping, ratios of partitions = product of one-contour ratios

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Classical cluster-expansion strategy

Find convergence conditions for the series

$$\Pi_{\gamma_0}(\boldsymbol{\rho}) \;:=\; 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\in\mathcal{P}^n} \left|\phi^T(\gamma_0,\gamma_1,\ldots,\gamma_n)\right| \, \rho_{\gamma_1}\ldots\rho_{\gamma_n}$$

for $\rho_\gamma > 0$. Then,

Cluster expansions converge *absolutely* for $|z_\gamma| \leq \rho_\gamma$ *uniformly in* Λ (complex valued allowed!)

This determines a region of analyticity $\mathcal{R}$ *common for all* Λ

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Consequences

- Zeros of all Ξ_Λ outside $\mathcal{R}$ (no phase transitions!)
- Within $\mathcal{R}$
  - Explicit series expressions for free energy and correlations
  - Explicit δ-mixing:

$$\left|\frac{\mathrm{Prob}(\{\gamma_0\,,\,\gamma_x\})}{\mathrm{Prob}(\{\gamma_0\})\,\mathrm{Prob}(\{\gamma_x\})} - 1\right| = \left|\mathrm{e}^{F[d(\gamma_0,\gamma_x)]} - 1\right|$$

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Free-energy expansion

Within $\mathcal{R}$

$$\log \Xi_\Lambda = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\in\mathcal{P}_\Lambda^n} \phi_n^T(\gamma_1,\ldots,\gamma_n)\, z_{\gamma_1}\ldots z_{\gamma_n}$$

$$= \sum_{\gamma\in\mathcal{P}_\Lambda} z_\gamma - \frac{1}{2} \sum_{\substack{(\gamma,\gamma')\in\mathcal{P}_\Lambda^2\\ \gamma\not\sim\gamma'}} z_\gamma\, z_{\gamma'} + O(|z|^3)$$

Each term is $O(|\Lambda|)$

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Free-energy-density (pressure) expansion

Within $\mathcal{R}$: For the translation-invariant geometrical model

$$f \;=\; \lim_{\Lambda} \frac{1}{|\Lambda|} \log \Xi_{\Lambda}$$

exists and is analytic on parameters (no phase transitions!)

$$\begin{aligned} f \;&=\; \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{(\gamma_1,\ldots,\gamma_n)\,:\,0\in\cup\gamma_i} \phi_n^T(\gamma_1,\ldots,\gamma_n)\, z_{\gamma_1}\ldots z_{\gamma_n} \\ &=\; \sum_{\gamma\ni 0} z_\gamma - \frac{1}{2} \sum_{\substack{\gamma\nsim\gamma' \\ 0\in\gamma\cup\gamma'}} z_\gamma\, z_{\gamma'} + O(|\boldsymbol{z}|^3) \end{aligned}$$

Correlations

$$\mathrm{Prob}_\Lambda\big(\{\gamma_0\}\big) \;=\; z_{\gamma_0}\,\frac{\Xi_{\Lambda\setminus\{\gamma_0\}^*}}{\Xi_\Lambda} \;=\; z_{\gamma_0}\,\frac{\exp\Big\{\sum_{\substack{\mathcal{C}\subset\mathcal{P}_\Lambda\\ \mathcal{C}\nsim\gamma_0}} W^T(\mathcal{C})\Big\}}{\exp\Big\{\sum_{\mathcal{C}\subset\mathcal{P}_\Lambda} W^T(\mathcal{C})\Big\}}$$

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Mixing properties

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\mathrm{Prob}_\Lambda(\{\gamma_0\} \mid \{\gamma_x\}) &= \frac{\mathrm{Prob}_\Lambda(\{\gamma_0\,,\,\gamma_x\})}{\mathrm{Prob}_\Lambda(\{\gamma_x\})} \\
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Central Limit Theorem

Lemma (Dobrushin)

Let (S_n) *be a sequence of random variables such that*

(i) $\mathbb{E}(S_n^2) < \infty$

(ii) $\mathrm{Var}(S_n) \geq c\,n$

(iii) $\exists\, R > 0$ *such that*

$$\left|\log\left|\mathbb{E}(\mathrm{e}^{\xi S_n})\right|\right| \;\leq\; \widetilde{c}\,n \qquad \textit{if } |\xi| < R$$

Then

$$\frac{S_n - \mathbb{E}(S_n)}{\sqrt{\mathrm{Var}(S_n)}} \xrightarrow{\text{Law}} \mathcal{N}(0,1)$$

Inductive strategy (Kotecký-Preiss, Dobrushin)

Find conditions on $\mathbf{z}$ defining a region $\mathcal{R}$ such that

$$\Xi_{\Lambda\setminus\{\gamma_0\}^*} \neq 0 \text{ in } \mathcal{R} \quad \Longrightarrow \quad \Xi_\Lambda \neq 0 \text{ in } \mathcal{R}$$

for all Λ, $\gamma_0 \notin \Lambda$

- Expansion neither needed nor obtained (*no-cluster-expansion* method)
- A posteriori: expansion converges in $\mathcal{R} \longrightarrow$ above concl.

Questions raised

- Why the alternative approach lead to better results?
- Can it be interpreted in terms of the classical approach?

Answer: Classical theory revisited

Inductive strategy (Kotecký-Preiss, Dobrushin)

Find conditions on $\mathbf{z}$ defining a region $\mathcal{R}$ such that

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for all Λ, $\gamma_0 \notin \Lambda$

- Expansion neither needed nor obtained (*no-cluster-expansion* method)
- A posteriori: expansion converges in $\mathcal{R}$ $\longrightarrow$ above concl.

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Associated polymer models

A model has an associated polymer model if partition ratios are the same

Equivalently,

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

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

Useful observation

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

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

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