Convergence of cluster expansions: Kirkwood-Salzburg versus Kotecky-Preiss-Dobrushin

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Roman's 60th birthday, November 2009

The basic 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:

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

  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

Example zero: Hard-core lattice gases

Measures on configurations $\omega \in \mathbb{L}^E$ with

- $\mathbb{L}$ =vertices of a graph (eg. $\mathbb{Z}^d$),
- $E = \{0,1\}$ (“1”=occupied)

For each $\Lambda \subset\subset \mathbb{L}$, let

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

Then,

- No occupied neighbors are allowed
- Allowed configurations have weights $\sim \exp(\mu\beta\,|\Gamma|)$ (μ=Gibbs chemical potential, β=inverse temperature)

That is,

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

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Lattice gas = polymer model

This is a polymer model with

- $\mathcal{P} = \{\text{vertices of } \mathbb{L}\}$
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Ising model at low temperatures

Measures on configurations $\omega \in \mathbb{Z}^{d^{\{-1,1\}}}$. For each $\Lambda \subset\subset \mathbb{L}$,

$$W_\Lambda(\omega \mid \omega) \;=\; \frac{\exp\{\beta J \sum_{\{x,y\} n.n.} \omega_x\omega_y\}}{\sum_{\sigma_\Lambda} \exp\{\exp\{\beta J \sum_{\{x,y\} n.n.} \sigma_x\sigma_y\}}$$

Write $-J\,\omega_x\omega_y = -J\,(\omega_x\omega_y - 1) - J$ Call a bond $B = \{x, y\}$ *excited* or *frustrated* if $\omega_x\omega_y = -1$: and

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

As N_Λ is independent of ω

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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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$$\begin{aligned}\exp\Bigl\{-2\beta J\, F_\Lambda(\omega)\Bigr\} &= \exp\Bigl\{-\sum_{\gamma\in\Gamma(\omega)} 2\beta J\, |\gamma|\Bigr\}\\ &= \prod_{\gamma\in\Gamma(\omega)} z_\gamma\end{aligned}$$

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

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Geometrical polymer models

Previous examples: polymers formed by points of a set

These are the original polymer models of Gruber and Kunz

Formally, a geometrical polymer model is defined by:

- A set $\mathbb{V}$ (sites)
- A family $\mathcal{P}$ of finite subsets of $\mathbb{V}$ (grains, connected sets)
- Activity values $(z_\gamma)_{\gamma\in\mathcal{P}}$
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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

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

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Basic principles of KS and KP-D approaches

Shared features:

- The basic objects of study are the partition ratios

$$\Phi_\Lambda(X) \;=\; \frac{\Xi_{\Lambda\setminus X}}{\Xi_\Lambda}$$

for $\Lambda, X \subset\subset \mathbb{V}$.

- Analysis starts from the *addition identity*

$$\Xi_{\Delta\cup\{x\}} \;=\; \Xi_\Delta + \sum_{\substack{\gamma\ni x\\ \gamma\subset\Lambda\cup\{x\}}} z_\gamma\, \Xi_{\Delta\setminus\gamma} \qquad (1)$$

for $\Delta \subset\subset \mathbb{V}$ and $\gamma \notin \Delta$

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Gruber-Kunz criterion *alla* Dobrushin

Strategy: Find a complex polydisc of the form

$$\mathcal{D}_{\boldsymbol{\rho}} \;=\; \Big\{\boldsymbol{z} : |z_\gamma| \le \rho_\gamma, \gamma \in \mathcal{P}\Big\} \qquad (\rho_\gamma > 0)$$

where the ratios $\Phi_\Lambda(X)$ are analytic *uniformly in* Λ, X.

Then use

- either Vitalli theorem plus convergence results for $z_\gamma > 0$,
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Main result

Theorem

Assume there exist $a > 0$ *and* $\rho_\gamma > 0$ *such that*

$$\sum_{\gamma \ni x} \rho_\gamma \, \mathrm{e}^{a|\gamma|} \;\leq\; \mathrm{e}^{a} - 1 \tag{2}$$

for all $x \in \mathbb{V}$*. Then, if* $|z_\gamma| \leq \rho_\gamma$

$$\left| \log \left| \frac{\Xi_\Lambda}{\Xi_{\Lambda \setminus \{x\}}} \right| \right| \;\leq\; a \tag{3}$$

Comments

- Gruber-Kunz = (2) but with "<"
- Note that if $\Lambda' \subset \Lambda$, telescoping,

$$\left| \log \left| \frac{\Xi_\Lambda}{\Xi_{\Lambda'}} \right| \right| \;\leq\; a \,|\Lambda \setminus \Lambda'| \;<\; \infty \tag{4}$$

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Comparison with other popular versions

- *Kotecký-Preiss:*

$$\sum_{\gamma\ni x}\rho_\gamma\,\mathrm{e}^{a|\gamma|}\ \le\ a$$

- *Dobrushin:*

$$\prod_{\gamma\ni x}\Big[1+\rho_\gamma\,\mathrm{e}^{a|\gamma|}\Big]\ \le\ \mathrm{e}^{a}$$

- *Gruber-Kunz:*

$$\sum_{\gamma\ni x}\rho_\gamma\,\mathrm{e}^{a|\gamma|}\ \le\ \mathrm{e}^{a}-1$$

Proof of the main result

By induction on $|\Lambda|$. Start with

$$\left|\frac{\Xi_\Lambda}{\Xi_{\Lambda\setminus\{x\}}}\right| \leq 1 + \sum_{\substack{\gamma\ni x \\ \gamma\subset\Lambda\cup\{x\}}} \rho_\gamma \left|\frac{\Xi_{\Lambda\setminus\gamma}}{\Xi_{\Lambda\setminus\{x\}}}\right|$$

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Then use logarithmic inequalities. □

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$$\Phi_\Lambda : \{X \subset \Lambda\} \longrightarrow \mathbb{C}$$

involving a Λ-*independent* operator K.

- Search for solutions in a suitable Banach space
- Solutions = fixed points
- K contraction yields
  - Convergence as $\Lambda \to \mathbb{V}$
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Kirkwood-Salzburg approach

Strategy: Set up systems of linear equations for the functions

$$\Phi_\Lambda : \{X \subset \Lambda\} \longrightarrow \mathbb{C}$$

involving a Λ-*independent* operator K.

- Search for solutions in a suitable Banach space
- Solutions = fixed points
- K contraction yields
  - Convergence as $\Lambda \to \mathbb{V}$
  - Analyticity of ratios and its limits

Derivation of the equations

- For each $X \subset\subset \mathbb{V}$ choose some (first) $x \in X$
- Write addition identity as *deletion identity*, with $\Lambda \to \Lambda \setminus X$

$$\Xi_{\Lambda\setminus X} \;=\; \Xi_{\Lambda\setminus(X\setminus\{x\})} - \sum_{S\subset\Lambda\setminus X} z_{\{x\}\cup S}\, \Xi_{\Lambda\setminus(X\,\mathrm{sup}\,S)}$$

- Dividing by Ξ_Λ

$$\Phi_\Lambda(X) \;=\; \Phi_\Lambda(X\setminus\{x\}) - \sum_{S\subset\Lambda\setminus X} z_{\{x\}\cup S}\, \Phi_\Lambda(X\cup S)$$

- The identity $\Phi_\Lambda(\emptyset) = 1$ is considered as inhomogenity
- The condition $X \subset \Lambda$ is introduced as a factor

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Kirkwood-Salzburg equations

The equations are:

$$\Phi_\Lambda \; = \; \chi_\Lambda \alpha + \chi_\Lambda K_{\boldsymbol{z}} \Phi_\Lambda$$

with

$$\chi_\Lambda(X) \; = \; \begin{cases} 1 & \text{if } X \subset \Lambda \\ 0 & \text{otherwise} \end{cases} \quad , \quad \alpha(X) \; = \; \begin{cases} 1 & \text{if } |X| = 1 \\ 0 & \text{otherwise} \end{cases}$$

and $K_{\boldsymbol{z}}$ the operator on $\mathbb{C}^{\{\text{non}-\text{empty fin parts of } \mathbb{V}\}}$

$$(K_{\boldsymbol{z}} f)(X) \; = \; 1\!\!1_{\{|X| \geq 2\}} \, f(X \setminus \{x\}) - \sum_{S \subset\subset \mathbb{V} \setminus X} z_{\{x\} \cup S} \, f(X \cup S)$$

Standard treatment

Aiming at factorized weights, introduce norms

$$\|f\|_\xi \;=\; \sup_{X\subset\subset\mathbb{V}} \frac{|f(X)|}{\xi^{|X|}}$$

for $\xi > 0$. Then

$$|(K_{\boldsymbol{z}}f)(X)| \;\le\; \xi^{|X|-1}\,\|f\|_\xi + \sum_{S\subset\subset\mathbb{V}\setminus X} \left|z_{\{x\}\cup S}\right| \xi^{|X|+|S|}\,\|f\|_\xi$$

and

$$\|K_{\boldsymbol{z}}\|_\xi \;\le\; \frac{1}{\xi}\Big[1+\sup_{x\in\mathbb{V}}\sum_{\gamma\ni x}|z_\gamma|\,\xi^{|\gamma|}\Big]$$

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Gruber-Kunz condition

If for some $\rho_\gamma > 0$

$$\frac{1}{\xi}\Big[1+\sup_{x\in\mathbb{V}}\sum_{\gamma\ni x}\rho_\gamma\,\xi^{|\gamma|}\Big] \;<\; 1 \tag{5}$$

then, for $|z_\gamma| \le \rho_\gamma$, the operators $1-\xi_\Lambda K_{\boldsymbol{z}}$ are invertible and

$$\Phi_\Lambda \;=\; \big[1-\xi_\Lambda K_{\boldsymbol{z}}\big]^{-1}\chi_\Lambda\alpha \tag{6}$$

is the only solution of the Λ-KS-equation.

Furthermore, as (5) is Λ-independent,

- The ratios converge

$$\Phi_\Lambda(X) \xrightarrow[\Lambda\to\mathbb{V}]{} \big([1-K_{\boldsymbol{z}}]^{-1}\alpha\big)(X)$$

- The ratios, and their limits have analytic dependence on $\boldsymbol{z}$

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Comparison with the inductive result

Choosing $\xi = \mathrm{e}^a$, GK-condition (5) becomes

$$\sum_{\gamma \ni x} \rho_\gamma \, \mathrm{e}^{a|\gamma|} \; < \; \mathrm{e}^a - 1$$

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Alternative strategy

Find another way of making sense of the formula

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As

$$(K_{\boldsymbol{z}} f)(X) = \mathbb{1}_{\{|X|\geq 2\}}\, f(X\setminus\{x\}) - \sum_{S\subset\subset \mathbb{V}\setminus X} z_{\{x\}\cup S}\, f(X\cup S)$$

The series (7) is term-by-term dominated by

$$\Phi_{\boldsymbol{\rho}} = \sum_{n\geq 0} K_{-\boldsymbol{\rho}}^n\, \alpha$$

as long as $|z_\gamma| \leq \rho_\gamma$.

(As in cluster expansions: singularities at negative fugacities)

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Kotecky-Preiss-like bound

Find functions $\xi(X)$ such that

$$\big(\alpha + K_{-\boldsymbol{\rho}}\,\xi\big)(X) \;\le\; \xi(X) \tag{8}$$

Recursively this implies that

$$\sum_{n=0}^{N} K_{-\boldsymbol{\rho}}^{n}\,\alpha \;\le\; \xi$$

and hence $\Phi_{\boldsymbol{\rho}}$ converges.

Reciprocally, if $\Phi_{\boldsymbol{\rho}}$ is finite, (8) holds with $\xi = \Phi_{\boldsymbol{\rho}}$

Conclusion:

(8) is necessary and sufficient for the convergence of $\Phi_{\boldsymbol{\rho}}$

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Why factorization

If X_1 and X_2 are disjoint,

$$\Phi_\Lambda(X_1 \cup X_2) \;=\; \frac{\Xi_{\Lambda\setminus(X_1\cup X_2)}}{\Xi_{\Lambda\setminus X_2}}\,\frac{\Xi_{\Lambda\setminus X_2}}{\Xi_\Lambda} \;=\; \Phi_{\Lambda\setminus X_2}(X_1)\,\Phi_\Lambda(X_2)\;.$$

In the limit $\Lambda \to \mathbb{V}$ we should obtain

$$\Phi(X_1 \cup X_2) \;=\; \Phi(X_1)\,\Phi(X_2)\;.$$

It is natural, to look for factorized majorizing functions.

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GK alla Dobrushin recovered

Postulating

$$\xi(X) \;=\; \xi^{|X|} \qquad (\xi > 0)$$

(8) holds for all X iff it holds for a single-site:

$$\big(\alpha + K_{-\boldsymbol{\rho}}\,\xi\big)(\{x\}) \;\leq\; \xi(\{x\}) \;=\; \xi$$

Writing $\xi = \mathrm{e}^{a}$, this condition is

$$1 + \sum_{\gamma \ni x} \rho_\gamma \,\mathrm{e}^{a|\gamma|} \;\leq\; \mathrm{e}^{a}$$

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Final meditations

We have shown:

1. The strong GK bound can be obtained alla Dobrushin
2. Dobrushin arguments seem stronger than KS
3. With an iterative argument ($\sim$FP2007): KS$\equiv$Dobrushin

Some concluding meditations:

- Sometimes it pays to be more elementary
- Improvements? Can we go beyond factorization?
  - Stronger, non-factorized convergence result in FP 2007
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