Combinatorics and bounds in Mayer’s theory of cluster and virial expansions

Warwick Statistical Mechanics Seminar

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1. Virial Expansion Bounds
2. Combinatorial Species of Structure - an Overview
3. Graphical Involution
4. Multispecies Expansions
Cluster and Virial Expansion History

- Generalise ideal gas law $PV = NkT$ with power series expansion (1901 - Kamerlingh-Onnes)
- Mayer (40) - understood cluster and virial coefficients as (weighted) connected and two-connected graphs respectively
- The work of Groeneveld [62, 63] found upper and lower bounds on the radius of convergence of both expansions and are tight for positive potentials and the cluster expansion
- Further bounds made by Lebowitz and Penrose [64] Ruelle [63, 64, 69]
- Useful thermodynamic inequalities and bounds on expansions were made by Lieb, Lebowitz, Penrose and Percus [1960s]
- These depend on the Kirkwood-Salsburg equations
- The Subset Polymer Gas of Gruber Kunz [71]
Abstract Polymer Gas representation introduced by Kotecký-Preiss [86] and further developed by Dobrushin and Fernández-Procacci [07] provides a general setting for cluster expansions and their convergence, avoiding the expansion itself - it can be understood as part of a tree fixed-point equation - Faris [08]

Connections made between the Dobrushin Criterion and the approach of Gruber and Kunz

Further applications and improvements on this abstract polymer model may be found in Poghosyan and Ueltschi [09]

Much work was also done on graph-tree inequalities by Battle, Brydges and Federbush [80s] and there are recent articles on using such inequalities by Abdesselam and Rivasseau [94]

Improving cluster expansion bounds improves virial expansion bounds

Recent work by Pulvirenti and Tsagkarogiannis [11] and Morais and Procacci [13] focuses on using Canonical Ensemble methods - these involved using inductive approaches to cluster expansions from Bovier and Zahradnik [00]
Brief History of Combinatorial Species of Structure

- 1981 André Joyal - original paper on Combinatorial Species of Structure - giving a rigorous definition for labelled objects
- Importance is relating generating function with combinatorial structures
- Bergeron Labelle Leroux *Combinatorial Species and Tree-like Structures* - Useful Algebraic Identities (through combinatorics)
- Flajolet and Sedgewick - *Analytic Combinatorics*
- Leroux (04) and Faris (08, 10) - links to Statistical Mechanics
- Combinatorial Species - understand bounds better - quick way to recognise virial expansion
Overview

1. Virial Expansion Bounds

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We have the Canonical Ensemble partition function:

$$Z_n := \sum_{(p_i, q_i) \in \mathbb{R}^n \times V^n} \exp (-\beta H_n(\{p_i, q_i\}))$$

$\beta$ is inverse temperature; $H_n$ is the $n$-particle Hamiltonian; $q_i$ are generalised coordinates and $p_i$ are the conjugate momenta.

The Grand Canonical Partition Function:

$$\Xi(z) := \sum_{n=0}^{\infty} \frac{z^n}{n!} Z_n$$

where $z = e^{\beta \mu}$ is the fugacity parameter and $\mu$ is the chemical potential.
The Cluster Expansion and Virial Expansion

- The Grand Canonical Partition function:

\[ \Xi(z) = \sum_{n \geq 0} \frac{z^n}{n!} Z_n \]

- In the thermodynamic Limit \( |\Lambda| \to \infty \), we have the pressure

\[ \beta P = \lim_{|\Lambda| \to \infty} \frac{1}{|\Lambda|} \log \Xi(z) \]

- We assume the existence of such a limit

- Expansion for pressure \( P \) in terms of fugacity \( z \) is the cluster expansion \( \beta P(z) = \sum_{n \geq 1} \frac{z^n}{n!} b_n \)

- We have \( \rho = z \frac{\partial}{\partial z} \beta P \), the density

- We may invert this equation and substitute for \( z \) to obtain a power series in \( \rho \)

- The virial development of the Equation of State is the power series

\[ \beta P = \sum_{n=1}^{\infty} c_n \rho^n \] called the virial expansion.
We have the contour integral representation (Lagrange-Bürmann Inversion) of the nth term in this expansion as:

\[ c_n = \oint_C \frac{\partial \beta P}{\partial \rho} \frac{\rho^n}{n} \, d\rho \]

We may change integration variables to \( z \) and rearrange to:

\[ c_n = \oint_{C'} \frac{1}{zn\rho^{n-1}} \, dz \]
We write a general bound on the cluster coefficients as:

\[ |nb_n| \leq ab^n n^{n-1} \]

where \( a, b > 0 \) are functions of inverse temperature \( \beta \).

Since the first term of cluster expansions is always \( z \) (or we may rescale our variables to make this the case), we obtain the bound:

\[ |\rho - z| \leq \sum_{n \geq 2} \frac{|nb_n|}{n!} |z|^n \]

upon substituting the bounds:

\[ |\rho - z| \leq a \sum_{n \geq 2} \frac{n^{n-1}}{n!} (b|z|)^n \]
We define the function:

\[ f(x) := \sum_{n \geq 1} \frac{n^{n-1}}{n!} x^n \]

and cast the inequality for \( |\rho - z| \) in the form:

\[ |\rho| \geq |z|(1 + ab) - af(b|z|) \]

We make the change of variables \( b|z| = se^{-s} \), motivated by the fact \( f(se^{-s}) = s \):

\[ |\rho| \geq b^{-1}se^{-s}(1 + ab) - as \]
Tree Approximations and the Lambert Function

- Optimising over the value of $s$ and substituting into the Cauchy Integral formula, we obtain:

$$|c_n| \leq \frac{1}{n} \left( a^{-1} \frac{W(\mu)}{W(\mu) - 1} \right)^{n-1}$$

where $W$ is the Lambert W-function, defined by $W(z)e^{W(z)} = z$ and $\mu := \frac{eab}{1+ab}$

- We obtain improved bounds for the radius of convergence of the virial expansion \cite{T. 13}

$$R_{\text{vir}} \geq a \left( \frac{W(\mu) - 1}{W(\mu)} \right)^2$$

where $R_{\text{vir}}$ is the radius of convergence for the virial expansion.
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**Combinatorial Species of Structure - Definition**

**Definition**

A Combinatorial Species of Structure is a rule $F$, which

**I** for every finite set $U$ gives a finite set of structures $F[U]$  

**II** for every bijection $\sigma : U \to V$ gives a bijection $F[\sigma] : F[U] \to F[V]$  

Furthermore, the bijections $F[\sigma]$ are required to satisfy the functorial properties:

**I** If $\sigma : U \to V$ and $\tau : V \to W$, then $F[\tau \circ \sigma] = F[\tau] \circ F[\sigma]$  

**II** For the identity bijection: $Id_U : U \to U$, $F[Id_U] = Id_{F[U]}$
The structures have labels (the elements of the set $U$)

The structures are characterised by sets $\{1, \cdots, n\} = [n]$, so characterisation by size of set

Our collection of structures must be finite

Relabelling the elements in the structure must behave well (functorial property)
The important examples I will be using are those of graphs $\mathcal{G}$, connected graphs $\mathcal{C}$, two-connected graphs $\mathcal{B}$, and trees $\mathcal{T}$. 

Example (An Example of a Graph and a Connected Graph)
**Articulation Points**

An articulation point in a connected graph $C$ is a vertex such that its removal and the removal of all incident edges renders the graph disconnected.

**Two-connected Graph**

A two-connected graph is a connected graph with no articulation points.

**Blocks in Connected Graphs**

A maximal two-connected subgraph of a connected graph is called a *Block*.
The (Exponential) Generating function of a species of structure $F$ is:

$$F(z) = \sum_{n=1}^{\infty} \frac{f_n z^n}{n!}$$

where $f_n = \#F[n]$
We may also add weights to our objects and we have the corresponding generating function: If each structure $s \in F[\mathcal{U}]$ is given a weight, $w(s)$, we have the weighted generating function:

**Weighted Generating Function**

If $f_{n,w} = \sum_{s \in F[n]} w(s)$, then the weighted generating function is:

$$F_w(z) = \sum_{n=0}^{\infty} f_{n,w} \frac{z^n}{n!}$$
For (formal) power series we have useful operations such as:

- **Addition** \((F + G)(z) = F(z) + G(z)\)
- **Multiplication** \((F \ast G)(z) = F(z) \times G(z)\)
- **Substitution** \((F(G))(z) = F \circ G(z)\)
- **Differentiation** \(F'(z)\)
- **Euler Derivative (rooting)** \(F^\bullet(z) = z \frac{d}{dz} F(z)\)

There is a corresponding operation on the level of species for each of the above.
### The Classical Gas

With pair potential interactions, we have the Hamiltonian

\[ H_n = \sum_{i=1}^{n} \frac{p_i^2}{2m} + \sum_{i<j} \varphi(x_i, x_j) \]

If we use Mayer’s trick of setting \( f_{i,j} = \exp(-\beta \varphi(x_1, x_j)) - 1 \), we may express the interaction as:

\[
\prod_{i<j} \exp(-\beta \varphi(x_i, x_j)) = \prod_{i<j} (f_{i,j} + 1)
\]

\[
= \sum_{g \in G[n]} \prod_{\{i,j\} \in E(g)} f_{i,j}
\]

It thus makes sense to define our weights on a graph as:

\[
w(g) := \prod_{e \in E(g)} f_e
\]

which is edge multiplicative.
If we define $\tilde{w}(g) = \int \cdots \int w(g) \, dx_1 \cdots dx_N$, then we have that the grand canonical partition function can be identified as the generating function of weighted graphs in the parameter $z$.

**Grand Canonical Partition Function as Graph Generating Function**

$$\Xi(z) = G_{\tilde{w}}(z)$$
From the relationship $\mathcal{G} = \mathcal{E}(\mathcal{C})$ and noting that the generating function for $\mathcal{E}$ is the exponential function, we have that:

$$\log \Xi(z) = \tilde{C}_\tilde{w}(z)$$

We recognise that $\beta P = \log \Xi(z)$, so that:

**The Pressure as Connected Graph Generating Function**

$$\beta P = C_\tilde{w}(z)$$
The Density

We use the relationship for the density: \( \rho = z \frac{d}{dz} \beta P \), to get the combinatorial interpretation:

**Generating Function for Density**

\[
\rho(z) = C_{\tilde{w}}(z)
\]
If we let $C$ represent the species of connected graphs and $B$ the species of 2-connected graphs, then we have the combinatorial relationship:

$$C + B^\bullet(C^\bullet) = C^\bullet + B(C^\bullet)$$

Furthermore, the combinatorial relationship gives it as a generating function relationship:

$$C(z) + B^\bullet(C^\bullet(z)) = C^\bullet(z) + B(C^\bullet(z))$$

We can also add appropriate weights to get a weighted identity:

$$C_w(z) + B^\bullet_w(C^\bullet_w(z)) = C^\bullet_w(z) + B_w(C^\bullet_w(z))$$
We have the density \( \rho = C^\bullet_w(z) \) and \( \beta P = C_w(z) \) and so, using the dissymmetry theorem, we get:

\[
\beta P = \rho + \sum_{n=2}^{\infty} \frac{\beta_n,\tilde{w}}{n!} \rho^n - \sum_{n=2}^{\infty} \frac{n\beta_n,\tilde{w}}{n!} \rho^n
\]

\[
= \rho - \sum_{n=2}^{\infty} \frac{(n-1)\beta_n,\tilde{w}}{n!} \rho^n
\]

where \( \beta_n,\tilde{w} = \sum_{g \in B[n]} \tilde{w}(g) \)
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For a one-particle hard-core model, we have that the potential:
\[
\varphi(x_i, x_j) := \infty \quad \forall x_i \neq x_j
\]
The factor \( e^{-\beta \varphi(x_i, x_j)} = 0 \) and hence the edge factor is \( f_{i,j} = -1 \) for all \( i, j \).
The grand canonical partition function is:
\[
\Xi(z) = 1 + z
\]
giving the pressure as:
\[
\beta P = \log(1 + z) = \sum_{n \geq 1} \frac{(-1)^{n+1} z^n}{n}
\]
upon comparison with the combinatorial version (in terms of weighted connected graphs) we have:
\[
\frac{1}{2} n(n-1) \sum_{k=n-1} (-1)^k c_{n,k} = (-1)^{n-1} (n - 1)!
\]
**The one-particle hard-core model**

Furthermore, we may take the Euler derivative and obtain density:

\[ \rho = \frac{z}{1 + z} \]

which may be inverted

\[ z = \frac{\rho}{1 - \rho} \]

and then substituted to obtain pressure in terms of density:

\[ \beta P = - \log(1 - \rho) = \sum_{n \geq 1} \frac{\rho^n}{n} \]

Upon comparison with the combinatorial version (in terms of weighted two-connected graphs) we have:

\[ \frac{1}{2} n(n-1) \sum_{k=n} \frac{(-1)^k b_{n,k}}{k} = -(n-2)! \]
Combinatorial Puzzle from Mayer’s Theory of Cluster Integrals

Theorem (Bernardi 08)

Let \(c_{n,k}\) denote the number of connected graphs with \(n\) vertices and \(k\) edges, then

\[
\frac{1}{2} n(n-1) \sum_{k=n-1} (-1)^k c_{n,k} = (-1)^{n-1} (n - 1)!
\]

The cancellations coming from a graph involution \(\Psi : \mathcal{C} \to \mathcal{C}\), fixing only increasing trees.

- Involution involves adding or removing edges to a graph
- Created a pairing of graphs \(G\) with \(\Psi(G)\) for those which aren’t fixed
- May be generalised to the case of the Tonks Gas
We have from the virial expansion:

**Theorem (T. - In preparation)**

If \( b_{n,k} \) = number of **two-connected graphs** with \( n \) vertices and \( k \) edges, then:

\[
\frac{1}{2} n(n-1) \sum_{k=n}^{\infty} (-1)^k b_{n,k} = -(n-2)!
\]

The cancellations coming from a graph involution \( \Psi : B \rightarrow B \) fixing only the two-connected graphs which are formed from an increasing tree on the indices \([1, n-1]\) and has vertex \( n \) connected to all the other vertices. This method can also be generalised to the Tonks Gas
The Tonks Gas

The appropriate weight for this model is:

$$w(g) = (-1)^{e(g)} \text{Vol}(\Pi_g)$$

Where $\Pi_g$ is the polytope of the graph $g$, which is defined by:

$$\Pi_g := \{ x_{[2,n]} \in \mathbb{R}^{n-1} | |x_i - x_j| \leq 1 \forall (i,j) \in g \: x_1 = 0 \}$$

The identities arising from this are:

$$\sum_{g \in \mathcal{C}[n]} (-1)^{e(g)} \text{Vol}(\Pi_g) = (-1)^{n-1}(n)^{n-1}$$

$$\sum_{g \in \mathcal{B}[n]} (-1)^{e(g)} \text{Vol}(\Pi_g) = -n(n-2)!$$

The key technique in proving both of these is a splitting of each polytope into subpolytopes of equal volume. This first appeared in the paper by Ducharme, Labelle and Leroux, but is attributed to Lass.
The Tonks Gas

These also have combinatorial interpretations:

- Those fixed for an involution on connected graphs are rooted trees
- Those fixed for two-connected graphs can be understood as having one special vertex, which has edges to all the others. There is then a given order on the rest of the vertices and with respect to this order we have an increasing tree.

In the proof of the above, the key idea is to split the polytope into degree $n - 1$ simplices, represented by a pair $(h, \sigma)$ for $h \in \mathbb{Z}^{n-1}$ and $\sigma \in S_{[2,n]}$. 
The Tonks Gas

- The key difference in this case is to consider the vector \( \vec{h} = (h_i + \frac{\sigma(i)}{n}) \) providing an order to the edges in the graph which may be different from the usual lexicographical ordering provided by the labels on the graph.
- For the two-connected version it is necessary to first order the edges by the differences \( |\vec{h}_i - \vec{h}_j| \)
- We achieve a suitable modification of the one particle hard-core case, which gives a different involution for each pair \((h, \sigma)\) providing all cancellations.
- In the connected graph case, we end up with an identification with the rooted connected graphs.
- In the two-connected case, we actually obtain more cancellations and have only fixed graphs for \( h = (0, \cdots, 0, -1, \cdots, -1) \). We have \( n \) such vectors and have the same interpretation for the fixed graphs.
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Considering how to implement such a model was studied by Fuchs [42]

Initial difficulty: going from a single type particle to two different types gives three degrees of freedom (one for each of the ‘single types’ and one for the mixture)

Paper implicitly uses Lagrange-Good inversion and tree-like relationships

Notion of generalised radii of convergence (Borel)
For a complex power series in countable many variables \( \{z_i\}_{i \in I} \), we may define the region of convergence as a polydisc: \( z_i < R_i \ \forall i \in I \)
Combinatorial Tools

Approaching the Multispecies Cluster Expansion, we come armed with tools developed in Combinatorics:

- The Lagrange-Good Inversion [Good65] provides the way in which we can (formally) invert power series in the form:

\[
\rho(z) = z + \sum_{n \geq 2} nb_n z^n
\]

- The Dissymmetry Theorem for Connected Graphs (and also trees) [Bergeron Labelle Leroux 98]

- The notion of coloured graphs and an extension of the Dissymmetry Theorem - Application of this to the multivariate virial expansion [Faris 12]

- There is a lack of attention on the convergence of such expansions - only as formal power series
The context of the applications is on the multispecies generalisation of the paper by Poghosyan and Ueltschi [09].

We emphasise that there are subtleties in achieving the expansion in infinitely many variables, which require the need to restrict to rigid molecules, rather than being able to have continuous internal degrees of freedom.

We begin with a collection of fugacity parameters \( \{z_i\}_{i \in \mathbb{N}} \) with \( z_i \) being the activity of the species \( i \).

We assume the achievement of a ‘cluster expansion’ for the pressure and understand conditions to achieve a convergent virial expansion.

We start from the ‘formal’ power series representation (Cluster Expansion):

\[
P(z) = \sum_{n} b(n)z^n \quad \text{(CE)}
\]
\[ P(z) = \sum_{n} b(n)z^n \quad \text{(CE)} \]

- We may formally define:

\[ \rho_k := z_k \frac{\partial}{\partial z_k} P \quad \text{(R1)} \]

or via the power series:

\[ \rho_k := \sum_{n} n_k b(n)z^n \quad \text{(R2)} \]

- We wish to invert (R2), substitute for \( z \) in (CE) to obtain:

\[ P(\rho) = \sum_{n} c(n)\rho^n \quad \text{(VE)} \]
Convergence Conditions

**Theorem (Jansen, T., Tsagkarogiannis, Ueltschi)**

Assume that there exist $0 < r_i < R_i$ and $a_i \geq 0$, $i \in \mathbb{N}$, such that

- $p(z)$ converges absolutely in the polydisc $D = \{z \in \mathbb{C}^N \mid \forall i \in \mathbb{N} : |z_i| < R_i\}$.
- $\left| \log \frac{\partial p}{\partial z_i}(z) \right| < a_i$ for all $i \geq 1$ and all $z \in D$.
- $\sum_{i \geq 1} \sqrt{\frac{r_i}{R_i}} < \infty$ and $\sum_{i \geq 1} \frac{r_i a_i^2}{R_i} < \infty$.

Then there exists a constant $C < \infty$ (which depends on the $r_i$, $R_i$, $a_i$, but not on $n$) such that

$$|c(n)| \leq C \sup_{z \in D} |p(z)| \prod_{i \geq 1} \left( \frac{e^{a_i}}{r_i} \right)^{n_i}. \quad (C1)$$
The estimate for $c(n)$ guarantees convergence of the series $\sum_n c(n)\rho^n$ for all $\rho$ in the polydisc:

$$D' = \left\{ \rho \in \mathbb{C}^\mathbb{N} \mid \forall i \in \mathbb{N} : |\rho_i| < r_i e^{-a_i}, \sum_{i \in \mathbb{N}} |\rho_i| \frac{e^{a_i}}{r_i} < \infty \right\}.$$
Lagrange-Good Inversion

**Theorem**

Let $z(\rho)$ be a summable collection of power series and $G(\rho)$ be a collection of formal power series, such that $\forall i \in \mathbb{N}$

$$z_i(\rho) = \rho_i G_i(z(\rho)) \quad (LI1)$$

Let $J = \{i \in \mathbb{N} \mid n_i \neq 0\}$ and $n \geq k$, then we have that:

$$[\rho^n]z(\rho)^k = [z^{n-k}]\left| \delta_{i,j} G_i(z)^{n_i} - z_j \frac{\partial G_i}{\partial z_j} G_i(z)^{n_i-1} \right|_{i,j \in J}$$
Let $z(\rho)$ be a summable collection of power series and $G(\rho)$ be a collection of formal power series, such that $\forall i \in \mathbb{N}$

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Recall that:

$$\rho_i(z) := z_i \frac{\partial P}{\partial z_i} \quad (\text{R})$$
**Theorem**

Let $\mathbf{z}(\rho)$ be a summable collection of power series and $\mathbf{G}(\rho)$ be a collection of formal power series, such that $\forall i \in \mathbb{N}$

$$z_i(\rho) = \rho_i G_i(\mathbf{z}(\rho)) \quad \text{(LI1)}$$

Let $J = \{i \in \mathbb{N} \mid n_i \neq 0\}$ and $n \geq k$, then we have that:

$$[\rho^n] \mathbf{z}(\rho)^k = [\mathbf{z}^{n-k}] \left. \delta_{i,j} G_i(\mathbf{z})^{n_i} - z_j \frac{\partial G_i}{\partial z_j} G_i(\mathbf{z})^{n_i-1} \right|_{i,j \in J}$$

Recall that:

$$\rho_i(\mathbf{z}) := z_i \frac{\partial P}{\partial z_i} \quad \text{(R)}$$

So we have that $G_i = \frac{1}{\frac{\partial P}{\partial z_i}}$
**Lagrange-Good Inversion**

**Theorem**

Let $z(\rho)$ be a summable collection of power series and $G(\rho)$ be a collection of formal power series, such that $\forall i \in \mathbb{N}$

$$z_i(\rho) = \rho_i G_i(z(\rho)) \quad (LI1)$$

Let $J = \{ i \in \mathbb{N} \mid n_i \neq 0 \}$ and $n \geq k$, then we have that:

$$[\rho^n]z(\rho)^k = [z^{n-k}] \left| \delta_{i,j} G_i(z)^{n_i} - z_j \frac{\partial G_i}{\partial z_j} G_i(z)^{n_i-1} \right|_{i,j \in J}$$

This gives us the Lagrange Inversion Formula:

$$[\rho^n]P(\rho) = [z^n]P(z) \left| \delta_{i,j} \left( \frac{1}{\partial P / \partial z_i} \right)^{n_i} - z_j \frac{\partial}{\partial z_j} \left( \frac{1}{\partial P / \partial z_i} \right) \left( \frac{1}{\partial P / \partial z_i} \right)^{n_i-1} \right|_{i,j \in J} \quad (LI3)$$
This gives us the Lagrange Inversion Formula:

\[
\left[ \rho^n \right] P(\rho) = \left[ z^n \right] P(z) \left| \delta_{i,j} \left( \frac{1}{\partial P/\partial z_i} \right)^{n_i} - z_j \frac{\partial}{\partial z_j} \left( \frac{1}{\partial P/\partial z_i} \right)^{n_i-1} \right|_{i,j \in J} \tag{LI3}
\]

We rearrange this to:

\[
\left[ \rho^n \right] P(\rho) = \left[ z^n \right] P(z) \frac{1}{\left( \partial P/\partial z \right)^n} \left| \delta_{i,j} + z_j \frac{\partial}{\partial z_j} \ln \left( \frac{\partial P}{\partial z_i} \right) \right|_{i,j \in J} \tag{LI4}
\]
Lagrangian-Good Inversion

We rearrange this to:

\[
[r^nP](r) = [z^n]P(z) \frac{1}{(\frac{\partial P}{\partial z})^n} \left| \delta_{i,j} + z_j \frac{\partial}{\partial z_j} \ln \frac{\partial P}{\partial z_i} \right|_{i,j \in J} \tag{LI4}
\]

Recall the bound we have:

\[
|c(n)| \leq C \sup_{z \in D} |P(z)| \prod_{i \geq 1} \left( \frac{e^{a_i}}{r_i} \right)^{n_i}. \tag{C1}
\]

We can therefore see where the bound comes from - the \(C\) as uniform bound on determinant, the final product from bounds on the derivative in the assumption.
Conclusions

- Using the tree majorant of cluster expansions and inverting the series through Cauchy integral formula, to obtain the virial expansion, gives lower bound improvements on the radius of convergence.

- We have the combinatorial identities which provide us with a simple way of recognising the cluster and virial coefficients.

- The explanation of the virial coefficients representing two-connected coloured graphs is possible in some circumstances (block factorisation for multispecies case).

- This connection of weighted graphs to the coefficients of the two expansions provides useful mutual exchanges between combinatorics and statistical mechanics.
Conclusions

- Statistical Mechanics provides motivation for combinatorial identities.
- Langrange inversion and the Dissymmetry Theorem run in parallel to provide in the former case a method of computing coefficients exactly and in the latter case an interpretation of the coefficients in terms of combinatorial structures.
- We have obtained convergence conditions for infinitely many species in the virial expansion.
- Lagrange-Good inversion generalises precisely what one needs to do to get a virial expansion from the cluster expansion in the multispecies case.
- How to understand the difficulties with non-rigid molecules and what the possible expansions are.
Open Questions

- Other physical models/problems to apply combinatorial species of structure - renormalisation in QFT?
- Can the cancellations be understood in a larger framework/context? (posets, matroids - improved bounds)
- How can we use this knowledge and understanding of combinatorics to make effective cancellations in inequalities for our expansions?
- What are the general properties of convergence of functions related by Lagrange inversion?
- Further work could be done in understanding what models can precisely fit the requirements of the multispecies paper