COMBINATORIAL SPECIES
LABELLED AND UNLABELLED ENUMERATION
MAYER GRAPH WEIGHTS

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Based on the paper:

P.Leroux,
Enumerative problems inspired by Mayers' theory of cluster integrals,
Electronic Journal of Combinatorics, 11 (2004), #R32, 1–28.
[http://www.combinatorics.org/Volume11/Abstracts/v11i1r32.html]

Functional equations for connected graphs and blocks

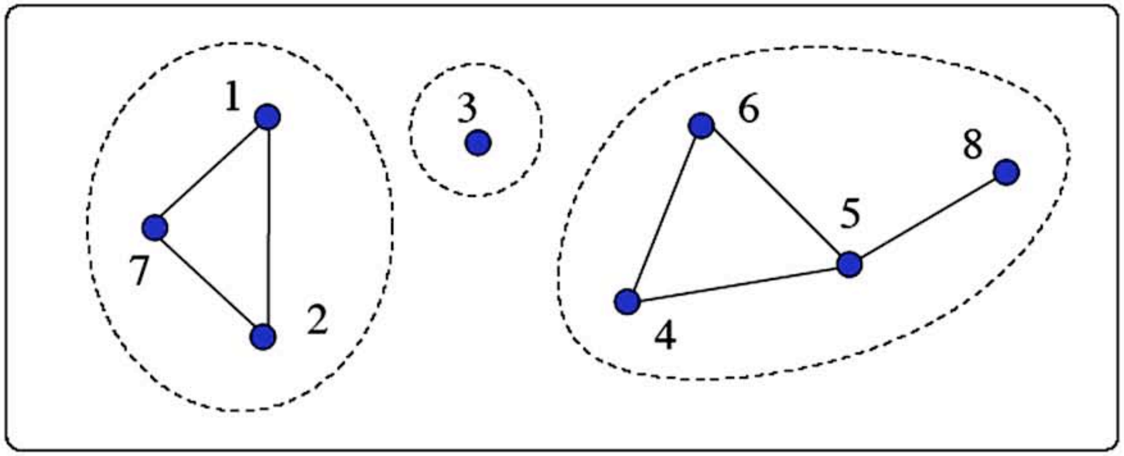


Figure 1: A simple graph g and its connected components

$$\mathcal{G} = E(\mathcal{C}),$$

$$\mathcal{G}(x) = \exp(\mathcal{C}(x)),$$

$$\widetilde{\mathcal{G}}(x) = Z_E(\widetilde{\mathcal{C}}(x), \widetilde{\mathcal{C}}(x^2), \ldots) = \exp\left(\sum_{k\geq 1} \frac{1}{k} \widetilde{\mathcal{C}}(x^k)\right).$$

Definitions. A *cutpoint* (or *articulation point*) of a connected graph g is a vertex of g whose removal yields a disconnected graph. A connected graph is called *2-connected* if it has no cutpoint. A *block* in a simple graph is a maximal 2-connected subgraph. The *block-graph* of a graph g is a new graph whose vertices are the blocks of g and whose edges correspond to blocks having a common cutpoint. The *block-cutpoint tree* of a connected graph g is a graph whose vertices are the blocks and the cutpoints of g and whose edges correspond to incidence relations in g. See Figure 2.

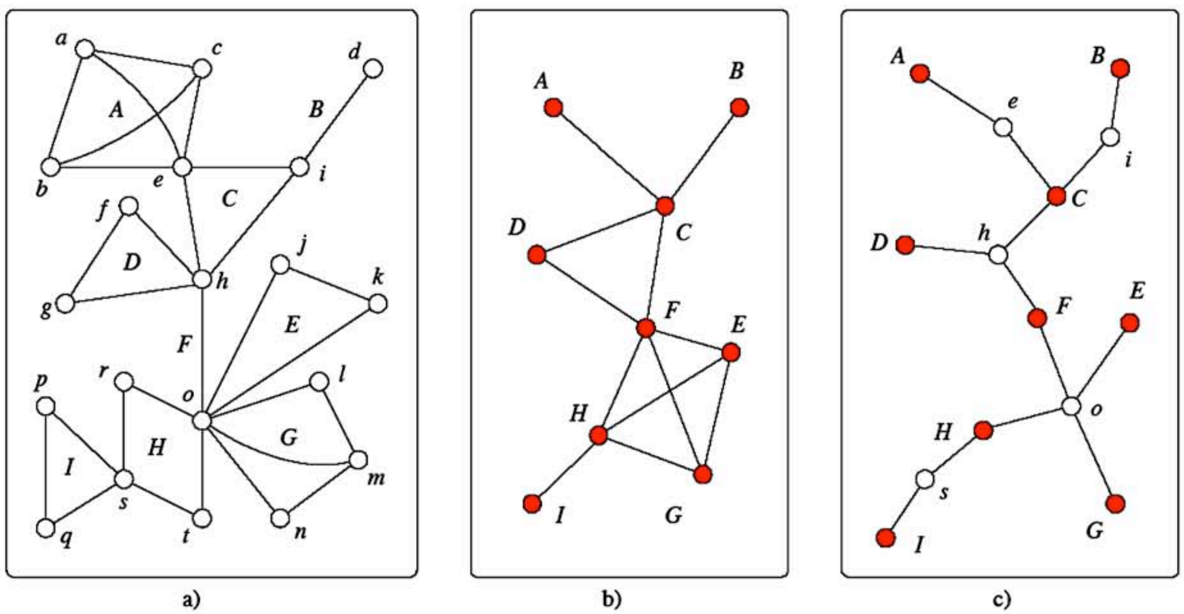


Figure 2: a) A connected graph g, b) the block-graph of g, c) the block-cutpoint tree of g

Now let $\mathcal{B}$ be a given species of 2-connected graphs. We denote by $C_{\mathcal{B}}$ the species of connected graphs all of whose blocks are in $\mathcal{B}$, called *$C_{\mathcal{B}}$-graphs*.

Examples 1.1. Here are some examples for various choices of $\mathcal{B}$:

1. If $\mathcal{B} = \mathcal{B}_a$, the class of *all* 2-connected graphs, then $C_{\mathcal{B}} = \mathcal{C}$, the species of (all) connected graphs.

2. If $\mathcal{B} = K_2$, the class of "edges", then $C_{\mathcal{B}} = \mathfrak{a}$, the species of (unrooted, free) trees ($\mathfrak{a}$ for French *arbres*).

3. If $\mathcal{B} = \{P_m, m \geq 2\}$, where P_m denotes the class of size-m polygons (by convention, $P_2 = K_2$), then $C_{\mathcal{B}} = \mathrm{Ca}$, the species of cacti. A *cactus* can also be defined as a connected graph in which no edge lies in more than one cycle. Figure 3, a), represents a typical cactus.

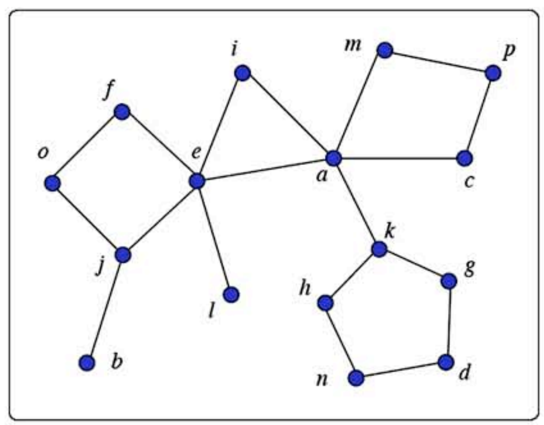


Figure 3: a) a typical cactus

4. If $\mathcal{B} = K_3 = P_3$, the class of "triangles", then $C_{\mathcal{B}} = \delta$, the class of triangular cacti.

5. If $\mathcal{B} = \{K_n, n \geq 2\}$, the family of complete graphs, then $C_{\mathcal{B}} = \mathrm{Hu}$, the species of *Husimi graphs*; that is, of connected graphs whose blocks are complete graphs. They were first (informally) introduced by Husimi in [12]. A Husimi graph is shown in Figure 2, b). See also Figure 7. It can be easily shown that any Husimi graph is the block-graph of some connected graph.

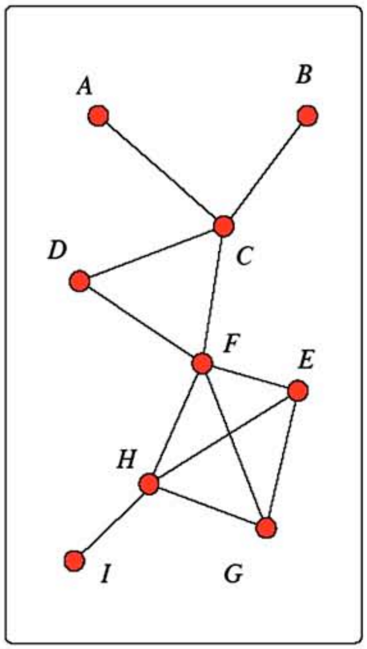


Figure 2: **b)**

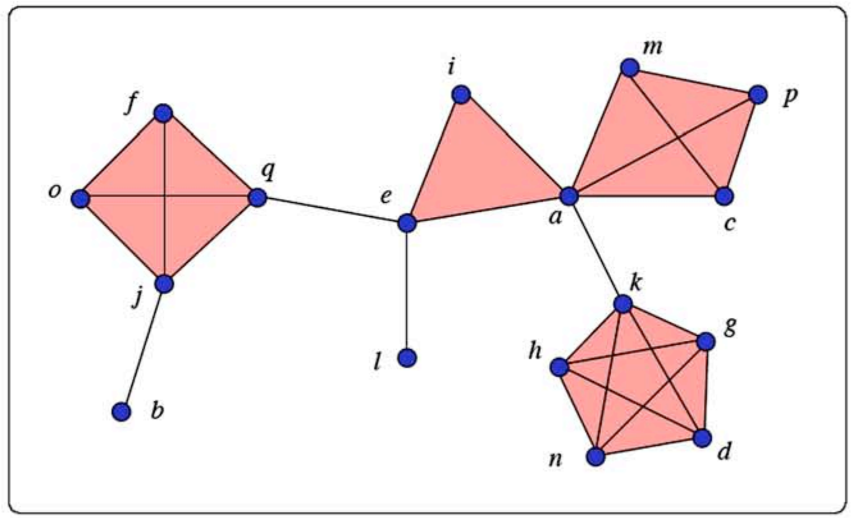


Figure 7: A Husimi graph with block-size distribution $(2^4 3^1 4^2 5^1 6^0 \cdots)$

6. If $\mathcal{B} = \{C_n, n \geq 2\}$, the family of oriented cycles, then $C_{\mathcal{B}} = \mathrm{Oc}$, the species of *oriented cacti*. Figure 3, b) shows a typical oriented cactus. These structures were introduced by C. Springer [29] in 1996.

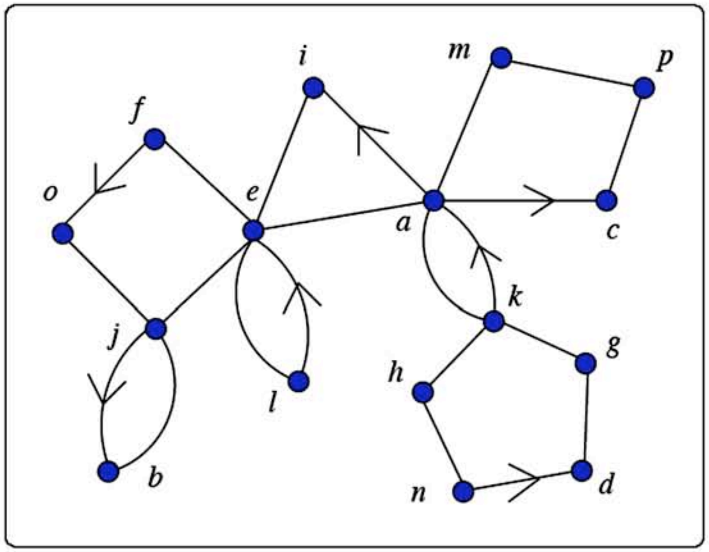


Figure 3: b) a typical oriented cactus

Theorem 1.1 *Let $\mathcal{B}$ be a class of 2-connected graphs and $C_{\mathcal{B}}$ be the species of connected graphs all of whose blocks are in $\mathcal{B}$. We then have the functional equation*

$$C'_{\mathcal{B}} = E(\mathcal{B}'(C^{\bullet}_{\mathcal{B}})).$$

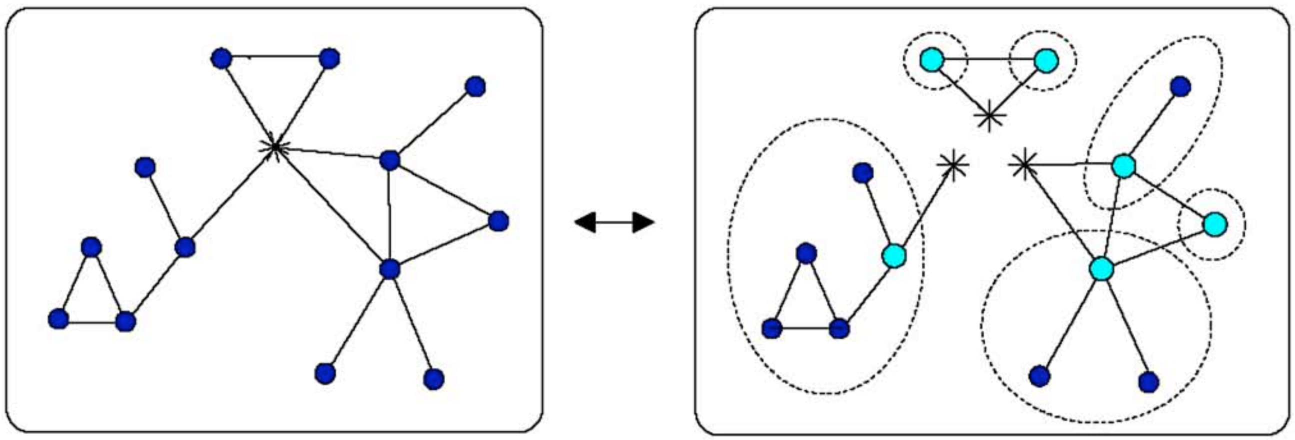


Figure 4: $C'_{\mathcal{B}} = E(\mathcal{B}'(C^{\bullet}_{\mathcal{B}}))$

$$C^{\bullet}_{\mathcal{B}} = X \cdot E(\mathcal{B}'(C^{\bullet}_{\mathcal{B}})),$$

$$C^{\bullet}_{\mathcal{B}}(x) = x \cdot \exp(\mathcal{B}'(C^{\bullet}_{\mathcal{B}}(x))).$$

Definition. A weight function w on the species $\mathcal{G}$ of graphs is said to be *multiplicative on the connected components* if for any graph $g \in \mathcal{G}[U]$, whose connected components are $c_1, c_2, \ldots, c_k$, we have

$$w(g) = w(c_1)w(c_2)\cdots w(c_k).$$

Examples 1.2. The following weight functions w on the species of graphs are multiplicative on the connected components.

1. $w_1(g) := y^{e(g)}$, where $e(g)$ is the number of edges of g.
2. $w_2(g) =$ graph complexity of $g :=$ number of maximal spanning forests of g.
3. $w_3(g) := x_0^{n_0} x_1^{n_1} x_2^{n_2} \cdots$, where n_i is the number of vertices of degree i.

Theorem 1.2 *Let w be a weight function on graphs which is multiplicative on the connected components. Then we have*

$$\mathcal{G}_w = E\left(\mathcal{C}_w\right).$$

For the exponential generating functions, we have

$$G_w(x) = \exp(\mathcal{C}_w(x)).$$

Definition. A weight function on connected graphs is said to be *block-multiplicative* if for any connected graph c, whose blocks are $b_1, b_2, \ldots, b_k$, we have

$$w(c) = w(b_1)w(b_2)\cdots w(b_k).$$

Examples 1.3. The weight functions $w_1(g) = y^{e(g)}$ and $w_2(g) =$ graph complexity of g of Examples 1.2 are block-multiplicative, but the function $w_3(g) = x_0^{n_0}x_1^{n_1}x_2^{n_2}\cdots$ is not. Another example of a block-multiplicative weight function is obtained by introducing formal variables y_i $(i \geq 2)$ marking the block sizes. In other terms, if the connected graph c has n_i blocks of size i, for $i = 2, 3, \ldots$, one sets

$$w(c) = y_2^{n_2}y_3^{n_3}\cdots.$$

Theorem 1.3. Let w be a block-multiplicative weight function on connected graphs whose blocks are in a given species B. Then we have

$$(C_{\mathcal{B}}^{\bullet})_w = X \cdot E(\mathcal{B}'_w((C_{\mathcal{B}}^{\bullet})_w)).$$

Partition functions for the non-ideal gas

Consider a non-ideal gas, formed of N particles interacting in a vessel $V \subseteq \mathbb{R}^3$ (whose volume is also denoted by V) and whose positions are $\overrightarrow{x_1}, \overrightarrow{x_2}, \ldots, \overrightarrow{x_N}$.

The Hamiltonian of the system:

$$H = \sum_{i=1}^{N} \left(\frac{\overrightarrow{p_i}^2}{2m} + U(\overrightarrow{x_i}) \right) + \sum_{1 \leq i < j \leq N} \varphi(|\overrightarrow{x_i} - \overrightarrow{x_j}|)$$

$\overrightarrow{p_i}$ is the linear momentum vector

$\frac{\overrightarrow{p_i}^2}{2m}$ is the kinetic energy of the i^{th} particle

$U(\overrightarrow{x_i})$ is the potential at position $\overrightarrow{x_i}$ due to outside forces (e.g., walls)

$|\overrightarrow{x_i} - \overrightarrow{x_j}| = r_{ij}$ is the distance between the particles $\overrightarrow{x_i}$ and $\overrightarrow{x_j}$

it is assumed that the particles interact only pairwise through the central potential $\varphi(r)$.

$$H = \sum_{i=1}^{N} \left(\frac{\overrightarrow{p_i}^2}{2m} + U(\overrightarrow{x_i}) \right) + \sum_{1 \le i < j \le N} \varphi(|\overrightarrow{x_i} - \overrightarrow{x_j}|)$$

The potential function φ has a typical form:

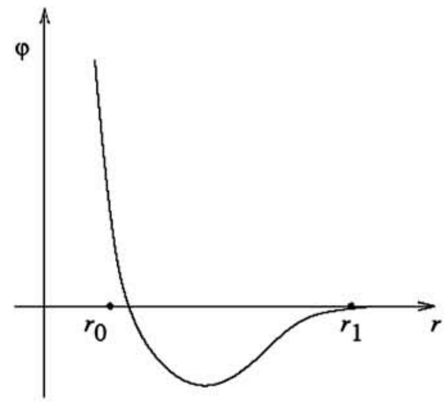


Figure 5: a) the function $\varphi(r)$

The *canonical partition function* $Z(V, N, T)$ is defined by

$$Z(V, N, T) = \frac{1}{N! h^{3N}} \int_{\Gamma} \exp\left(-\beta H\right) d\Gamma$$

h is Planck's constant

$\beta = \frac{1}{kT}$, T is the absolute temperature

k is Boltzmann's constant

Γ represents the state space $\overrightarrow{x_1}, \ldots, \overrightarrow{x_N}, \overrightarrow{p_1}, \ldots, \overrightarrow{p_N}$ of dimension $6N$.

$$H = \sum_{i=1}^{N} \left(\frac{\overrightarrow{p_i}^2}{2m} + U(\overrightarrow{x_i}) \right) + \sum_{1 \le i < j \le N} \varphi(|\overrightarrow{x_i} - \overrightarrow{x_j}|)$$

(Hamiltonian)

$$Z(V, N, T) = \frac{1}{N! h^{3N}} \int_{\Gamma} \exp(-\beta H) d\Gamma$$

(canonical partition function)

Γ represents the state space $\overrightarrow{x_1}, \ldots, \overrightarrow{x_N}, \overrightarrow{p_1}, \ldots, \overrightarrow{p_N}$ of dimension $6N$.

First simplification: assume that the potential energy $U(\overrightarrow{x_i})$ is negligible or null.
Second simplification: the integral over the momenta $\overrightarrow{p_i}$ is a product of Gaussian integrals which are easily evaluated,

so that the canonical partition function can now be written as

$$Z(V, N, T) = \frac{1}{N! \lambda^{3N}} \int_V \cdots \int_V \exp\left(-\beta \sum_{i<j} \varphi(|\overrightarrow{x_i} - \overrightarrow{x_j}|) \right) d\overrightarrow{x_1} \cdots d\overrightarrow{x_N},$$

where $\lambda = h(2\pi m k T)^{-\frac{1}{2}}$.

$$Z(V,N,T) = \frac{1}{N!\lambda^{3N}} \int_V \cdots \int_V \exp\left(-\beta \sum_{i<j} \varphi(|\overrightarrow{x_i} - \overrightarrow{x_j}|)\right) d\overrightarrow{x_1} \cdots d\overrightarrow{x_N},$$

where $\lambda = h(2\pi mkT)^{-\frac{1}{2}}$. **(canonical partition function)**

The *grand-canonical distribution*

is the generating function for the canonical partition functions,

$$Z_{\text{gr}}(V,T,z) = \sum_{N=0}^{\infty} Z(V,N,T)(\lambda^3 z)^N,$$

where the variable z is called the *fugacity* or the *activity*.

Macroscopic parameters :

$$\frac{P}{kT} = \frac{1}{V} \log Z_{\text{gr}}(V,T,z), \qquad \overline{N} = z\frac{\partial}{\partial z} \log Z_{\text{gr}}(V,T,z), \qquad \rho := \frac{\overline{N}}{V}.$$

pressure P, the average number of particles $\overline{N}$, and the *density* ρ.

$$Z(V,N,T) = \frac{1}{N!\lambda^{3N}} \int_V \cdots \int_V \exp\left(-\beta \sum_{i<j} \varphi(|\overrightarrow{x_i} - \overrightarrow{x_j}|)\right) d\overrightarrow{x_1} \cdots d\overrightarrow{x_N}$$

$$Z_{\mathrm{gr}}(V,T,z) = \sum_{N=0}^{\infty} Z(V,N,T)(\lambda^3 z)^N \qquad \frac{P}{kT} = \frac{1}{V} \log Z_{\mathrm{gr}}(V,T,z)$$

The virial expansion:

$$\frac{P}{kT} = \frac{\overline{N}}{V} + \gamma_2(T)\left(\frac{\overline{N}}{V}\right)^2 + \gamma_3(T)\left(\frac{\overline{N}}{V}\right)^3 + \cdots$$

(proposed by Kamerlingh Onnes, 1901)

It is the starting point of Mayer's theory of "cluster integrals":

(around 1930)

$$Z(V,N,T) = \frac{1}{N!\lambda^{3N}} \int_V \cdots \int_V \exp\left(-\beta \sum_{i<j} \varphi(|\vec{x_i} - \vec{x_j}|)\right) d\vec{x_1} \cdots d\vec{x_N}$$

Mayer's theory of "cluster integrals"

Mayer's idea consists of setting

$$1 + f_{ij} = \exp\left(-\beta\varphi(|\vec{x_i} - \vec{x_j}|)\right), \qquad f_{ij} = f(r_{ij}).$$

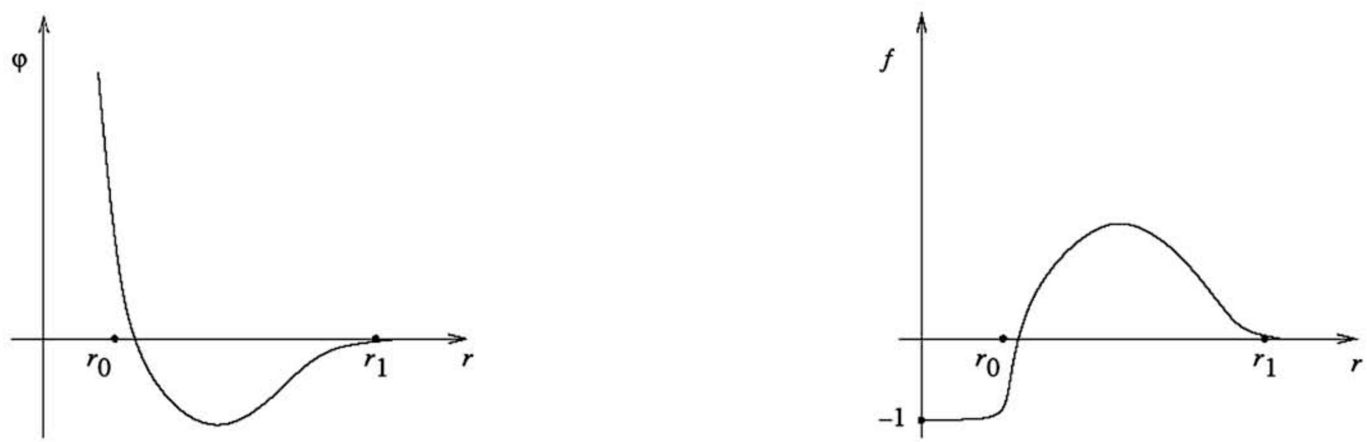


Figure 5: a) the function $\varphi(r)$ b) the function $f(r) = \exp(-\beta\varphi(r)) - 1$

$$
\begin{aligned}
Z(V,N,T) &= \frac{1}{N!\lambda^{3N}} \int_V \cdots \int_V \exp\left(-\beta \sum_{i<j} \varphi(|\overrightarrow{x_i} - \overrightarrow{x_j}|)\right) d\overrightarrow{x_1} \cdots d\overrightarrow{x_N} \\
&= \frac{1}{N!\lambda^{3N}} \int_V \cdots \int_V \prod_{1\le i<j\le N} (1 + f_{ij})\, d\overrightarrow{x_1} \cdots d\overrightarrow{x_N}. \\
&= \frac{1}{N!\lambda^{3N}} \sum_{g\in\mathcal{G}[N]} \int_V \cdots \int_V \prod_{\{i,j\}\in g} f_{ij}\; d\overrightarrow{x_1} \cdots d\overrightarrow{x_N} \\
&= \frac{1}{N!\lambda^{3N}} \sum_{g\in\mathcal{G}[N]} W(g),
\end{aligned}
$$

where the weight $W(g)$ of a graph g is given by the integral

$$
W(g) = \int_V \cdots \int_V \prod_{\{i,j\}\in g} f_{ij} d\overrightarrow{x_1} \cdots d\overrightarrow{x_N}.
$$

$$W(g) = \int_V \cdots \int_V \prod_{\{i,j\} \in g} f_{ij} d\overrightarrow{x_1} \cdots d\overrightarrow{x_N}$$

For the grand canonical function, we then have

$$\begin{aligned} Z_{\mathrm{gr}}(V,T,z) &= \sum_{N=0}^{\infty} Z(V,N,T)(\lambda^3 z)^N \\ &= \sum_{N=0}^{\infty} \frac{1}{N!\lambda^{3N}} \sum_{g \in \mathcal{G}[N]} W(g)(\lambda^3 z)^N \\ &= \sum_{N=0}^{\infty} \frac{1}{N!} \sum_{g \in \mathcal{G}[N]} W(g) z^N \\ &= \mathcal{G}_W(z). \end{aligned}$$

This is the exponential generating series of the species $\mathcal{G}_W$ of W-weighted graphs.

$$W(g) = \int_V \cdots \int_V \prod_{\{i,j\} \in g} f_{ij} d\overrightarrow{x_1} \cdots d\overrightarrow{x_N}$$

Proposition 2.1 *The weight function W is multiplicative on the connected components.*

For example, for the graph g of Figure 1, we have

$$\begin{aligned} W(g) &= \int_{V^8} f_{12} f_{17} f_{27} f_{45} f_{46} f_{56} f_{58} d\overrightarrow{x_1} \cdots d\overrightarrow{x_8} \\ &= \int f_{12} f_{17} f_{27} d\overrightarrow{x_1} d\overrightarrow{x_2} d\overrightarrow{x_7} \int d\overrightarrow{x_3} \int f_{45} f_{46} f_{56} f_{58} d\overrightarrow{x_4} d\overrightarrow{x_5} d\overrightarrow{x_6} d\overrightarrow{x_8} \\ &= W(c_1) W(c_2) W(c_3). \end{aligned}$$

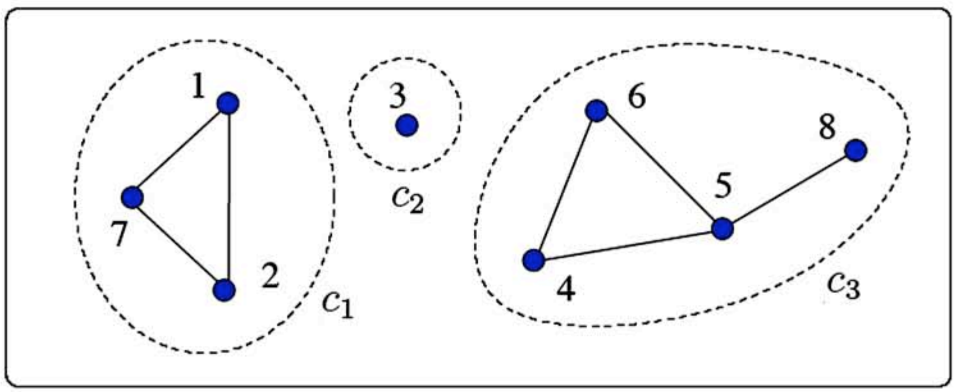


Figure 1: A simple graph g and its connected components

We deduce that

$$\mathcal{G}_W(z) = \exp\left(\mathcal{C}_W(z)\right),$$

where $\mathcal{C}_W$ denotes the weighted species of connected graphs, with

$$\mathcal{C}_W(z) = \sum_{n \geq 1} |\mathcal{C}[n]|_W \frac{z^n}{n!},$$

and

$$|\mathcal{C}[n]|_W = \sum_{c \in \mathcal{C}[n]} \int_V \cdots \int_V \prod_{\{i,j\} \in c} f_{ij} \, d\overrightarrow{x_1} \cdots d\overrightarrow{x_n}.$$

Historically, the quantities $b_n(V) = \frac{1}{Vn!}|\mathcal{C}[n]|_W$ are precisely the *cluster integrals* of Mayer.

We then have a combinatorial interpretation of the quantity $\frac{P}{kT}$ **:**

$$\frac{P}{kT} \quad = \quad \frac{1}{V} \log Z_{\text{gr}}(V, T, z) \quad = \quad \frac{1}{V} \log \mathcal{G}_W(z) \quad = \quad \frac{1}{V} \mathcal{C}_W(z).$$

$$\frac{P}{kT} = \frac{1}{V}\mathcal{C}_W(z)$$

Proposition 2.2 *For large V, the weight function $w(c) = \frac{1}{V}W(c)$, defined on the species of connected graphs, is block-multiplicative.*

Proof. First observe that for any connected graph c on the set of vertices $[k] = \{1, 2, \ldots k\}$, the value of the partial integral

$$I = I(\overrightarrow{x_k}) = \lim_{V\to\infty} \int_V \cdots \int_V \prod_{\{i,j\}\in c} f_{ij} d\overrightarrow{x_1} \cdots d\overrightarrow{x_{k-1}}$$

The integrand lies in a ball of radius at most $(k-1)r_1$ centered at $\overrightarrow{x_k}$

is in fact independent of $\overrightarrow{x_k}$. **For large V:**

$$W(c) = \int_V \cdots \int_V \prod_{\{i,j\}\in c} f_{ij} d\overrightarrow{x_1} \cdots d\overrightarrow{x_{k-1}} \int_V d\overrightarrow{x_k} = \int_V \cdots \int_V \prod_{\{i,j\}\in c} f_{ij} d\overrightarrow{x_1} \cdots d\overrightarrow{x_{k-1}} \cdot V.$$

$$\lim_{V\to\infty} \int_V \cdots \int_V \prod_{\{i,j\}\in c} f_{ij} d\overrightarrow{x_1} \cdots d\overrightarrow{x_{k-1}} = \lim_{V\to\infty} \frac{1}{V} W(c) = w(c)$$

------->

Now if a connected graph is decomposed into blocks $b_1, b_2, \ldots, b_k$, we have

$$w(c) = w(b_1)w(b_2)\cdots w(b_k).$$

For example, for the graph c shown in Figure 6, we have

$$\begin{aligned} w(c) &= \int_{V^7} f_{12}f_{13}f_{23}f_{34}f_{56}f_{37}f_{36}f_{67}f_{68}f_{78}d\vec{x_1}d\vec{x_2}\cdots d\vec{x_7} \\ &= \int f_{12}f_{13}f_{23}d\vec{x_1}d\vec{x_2}\, f_{34}d\vec{x_4}\, f_{56}d\vec{x_5}\, f_{37}f_{36}f_{67}f_{68}f_{78}d\vec{x_3}d\vec{x_6}d\vec{x_7} \\ &= w(b_1)w(b_2)w(b_3)w(b_4). \end{aligned}$$

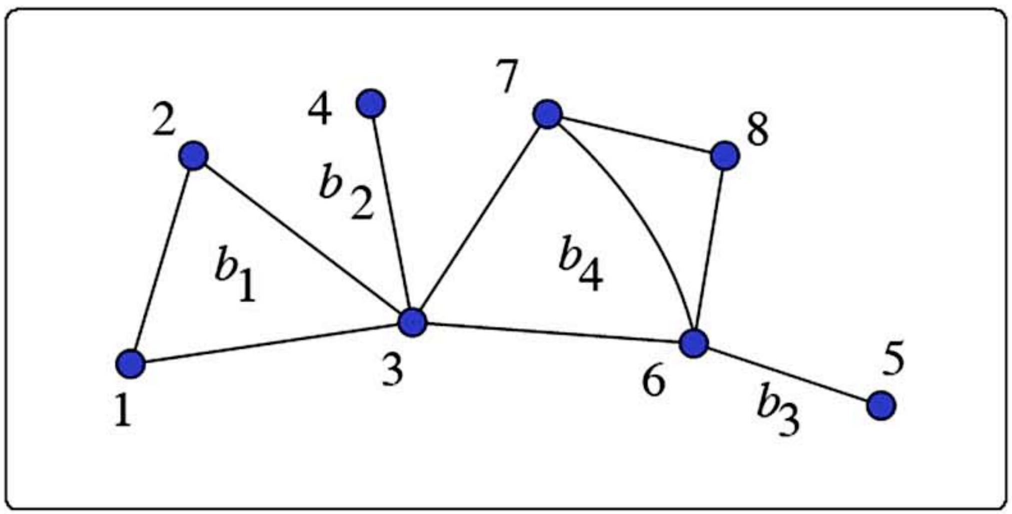


Figure 6: A connected graph with blocks b_1, b_2, b_3, b_4

NOTE : It can be shown that the thermodynamic $\lim_{V\to\infty} \frac{1}{V} W(c) = w(c)$ exists (and is block-multiplicative) under the following integrability conditions:

Proposition *If the function* $f : [0,\infty) \to \mathbb{R}$ *is integrable and bounded and if*

$$\int_0^\infty r^{d+\epsilon-1} |f(r)| \, dr < \infty,$$

(for example if $|f(r)| = \mathrm{O}(1/r^{d+2\epsilon}),\ r \to \infty$*), then for any fixed* $\vec{x}_N \in \mathbb{R}^d$*, the function* $F_{\vec{x}_N} : \mathbb{R}^{d\cdot(N-1)} \to \mathbb{R}$*, defined by*

$$F_{\vec{x}_N}(\vec{x}_1, \ldots, \vec{x}_{N-1}) = \prod_{\{i,j\}\in c} f(|\vec{x}_i - \vec{x}_j|) = \prod_{\{i,j\}\in c} f_{ij}$$

is integrable over $(\mathbb{R}^d)^{N-1}$ *and its integral is independent of* $\vec{x}_N$*. Moreover the limit* $\lim_{V\to\infty} \frac{1}{V} W(c) = w(c)$ *exists and is equal to*

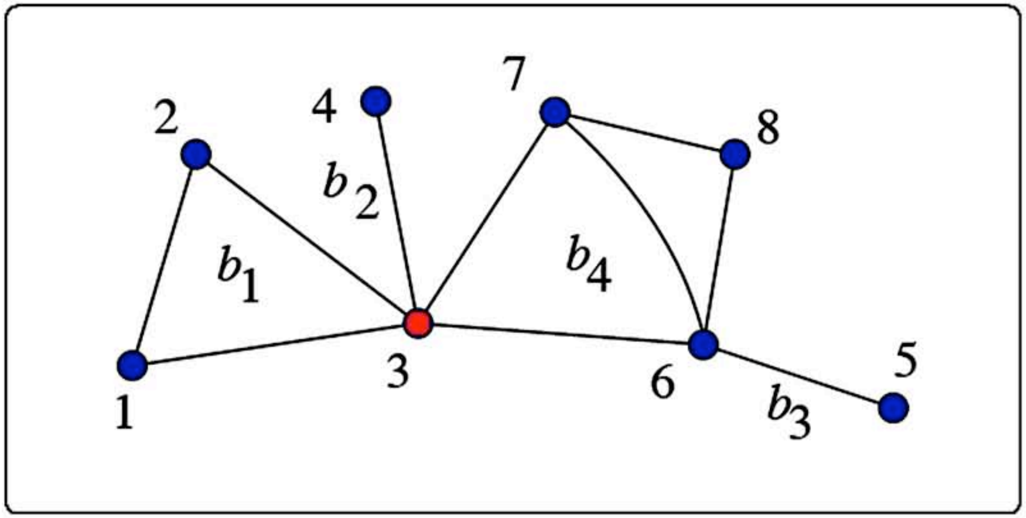
$$w(c) = \int_{(\mathbb{R}^d)^{N-1}} \prod_{\{i,j\}\in c;\ \vec{x}_N = \vec{0}} f_{ij} \, d\vec{x}_1 \ldots d\vec{x}_{N-1}.$$

It follows that

$$\mathcal{C}_w^\bullet = X \cdot E(\mathcal{B}'_w(\mathcal{C}_w^\bullet)),$$

where $\mathcal{B} = \mathcal{B}_a$ is the species of all 2-connected graphs, and for the exponential generating functions,

$$\mathcal{C}_w^\bullet(z) = z\exp(\mathcal{B}'_w(\mathcal{C}_w^\bullet(z))).$$



Computation of the virial expansion (following Uhlenbeck and Ford)

We have, for the density $\rho(z) = z\frac{\partial}{\partial z}\frac{1}{V}\log Z_{\text{gr}}(V,T,z) \;=\; z\frac{\partial}{\partial z}\mathcal{C}_w(z) \;=\; \mathcal{C}^{\bullet}_w(z).$

Since $\mathcal{C}^{\bullet}_w(z) = z\exp(\mathcal{B}'_w(\mathcal{C}^{\bullet}_w(z)))$ it follows that $\rho(z) = z\exp\mathcal{B}'_w(\rho(z)).$

$$\frac{P}{kT} \;=\; \frac{1}{V}\log Z_{\text{gr}}(V,T,z) \;=\; \mathcal{C}_w(z) \;=\; \int_0^z \mathcal{C}'_w(t)\,dt \;=\; \int_0^z \frac{\rho(t)}{t}\,dt.$$

Let us make the change of variable $t = t(r) = r\exp(-\mathcal{B}'_w(r)),$ inverse function of $r = \rho(t).$

Note that $\rho(0) = 0$ and $\rho(z) = \rho$, and also that $dt = [\exp(-\mathcal{B}'_w(r)) - r\exp(-\mathcal{B}'_w(r))\cdot\mathcal{B}''_w(r)]dr.$

$$\frac{P}{kT} \;=\; \int_0^z \frac{\rho(t)}{t}\,dt \;=\; \int_0^\rho (1 - r\mathcal{B}''_w(r))\;dr \;=\; \rho - \int_0^\rho r\mathcal{B}''_w(r)\;dr$$

$$= \rho - \int_0^\rho \sum_{n\geq 1} n\beta_{n+1}\frac{r^n}{n!}\,dr \;=\; \rho - \sum_{n\geq 2}(n-1)\beta_n\frac{\rho^n}{n!},$$

where we have set $\mathcal{B}_w(r) = \sum_{n\geq 2}\beta_n\frac{r^n}{n!}$. This is precisely the virial expansion, with $\rho = \frac{N}{V}$.

Hence the n^{th} virial coefficient, for $n \geq 2$, is given by $\gamma_n(T) \;=\; -\frac{(n-1)}{n!}\beta_n \;=\; -\frac{(n-1)}{n!}|\mathcal{B}[n]|_w.$

Virial expansion (combinatorial form)

$$\frac{P}{kT} = \frac{\overline{N}}{V} + \gamma_2(T)\left(\frac{\overline{N}}{V}\right)^2 + \gamma_3(T)\left(\frac{\overline{N}}{V}\right)^3 + \cdots$$

where

$$\gamma_n(T) \quad = \quad -\frac{(n-1)}{n!}|\mathcal{B}[n]|_w.$$

and $\mathcal{B} = \mathcal{B}_a$ is the species of all 2-connected graphs weighted by

$$w(c) = \int_{(\mathbb{R}^d)^{n-1}} \prod_{\{i,j\}\in c;\ \vec{x}_n=\vec{0}} f_{ij}\, d\vec{x}_1 \ldots d\vec{x}_{n-1}.$$

The following combinatorial equations hold

$$\mathcal{C}_w^\bullet = X \cdot E(\mathcal{B}'_w(\mathcal{C}_w^\bullet)), \qquad \mathcal{G}_w = E(\mathcal{C}_w)$$

where $\mathcal{G}_w$ is the species of all graphs

and $\mathcal{C}_w$ is the species of all connected graphs.

Gaussian model

It is interesting, mathematically, to consider a Gaussian model, where

$$f_{ij} = -\exp\left(-\alpha||\overrightarrow{x_i} - \overrightarrow{x_j}||^2\right),$$

which corresponds to a soft repulsive potential, at constant temperature. In this case, all cluster integrals can be explicitly computed:

The weight $w(c)$ of a connected graph c has value

$$w(c) = (-1)^{e(c)} \left(\frac{\pi}{\alpha}\right)^{\frac{3}{2}(n-1)} \gamma(c)^{-\frac{3}{2}},$$

where

$e(c)$ is the number of edges of c

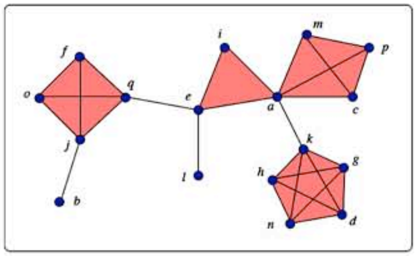
and

$\gamma(c)$ is the graph complexity of c, that is, the number of spanning subtrees of c.

Enumerative results

Labelled enumeration

The species Hu of Husimi graphs is of the form $C_{\mathcal{B}}$ with $\mathcal{B} = K_{\geq 2}$



Proposition 3.1 *The number* $\mathrm{H}_n = |\,\mathrm{Hu}[n]|$ *of (labelled) Husimi graphs on* $[n]$*, for* $n \geq 1$*, is given by*

$$\mathrm{H}_n = \sum_{k\geq 0} S(n-1,k)\, n^{k-1},$$

where k *represents the number of blocks and* $S(m,k)$ *denotes the Stirling number of the second kind.*

Proposition 3.2 (Mayer [23], Husimi [12]) *Let* $(n_2, n_3, \ldots)$ *be a sequence of non-negative integers and* $n = \sum_{i\geq 2} n_i(i-1)+1$*. Then the number* $\mathrm{Hu}(n_2, n_3, \ldots)$ *of Husimi graphs on* $[n]$ *having* n_i *blocks of size* i *is given by*

$$\mathrm{Hu}(n_2, n_3, \ldots) = \frac{(n-1)!}{(1!)^{n_2} n_2! (2!)^{n_3} n_3! \cdots}\, n^{k-1},$$

where $k = \sum_{i\geq 2} n_i$ *is the total number of blocks.*

Take now $\mathcal{B} = \sum_{k \geq 2} C_k$, the species of oriented cycles of size $k \geq 2$

Proposition 3.3 *The number* $\mathrm{Oc}_n = |\,\mathrm{Oc}[n]|$ *of oriented cacti on* $[n]$, *for* $n \geq 2$, *is given by*

$$\mathrm{Oc}_n = \sum_{k \geq 1} \frac{(n-1)!}{k!} \binom{n-2}{k-1} n^{k-1},$$

where $k = \sum_{i \geq 2} n_i$ *is the number of cycles.*

Proposition 3.4 [29] *Let* $(n_2, n_3, \ldots)$ *be a sequence of non-negative integers and* $n = \sum_{i \geq 2} n_i(i-1) + 1$. *Then the number* $\mathrm{Oc}(n_2, n_3, \ldots)$ *of oriented cacti on* $[n]$ *having* n_i *cycles of size* i *for each* i, *is given by*

$$\mathrm{Oc}(n_2, n_3, \cdots) = \frac{(n-1)!}{n_2! n_3! \cdots} n^{k-1},$$

where $k = \sum_{i \geq 2} n_i$ *is the number of cycles.*

Take now $\mathcal{B} = \sum_{k\geq 2} P_k$, the species of oriented polygons. size $k \geq 2$.

Proposition 3.5 (Ford and Uhlenbeck [5]) *Let* $(n_2, n_3, \ldots)$ *be a sequence of non-negative integers and* $n = \sum_{i\geq 2} n_i(i-1)+1$. *Then the number* $\mathrm{Ca}(n_2, n_3, \ldots)$ *of cacti on* $[n]$ *having* n_i *polygons of size* i *for each* i, *is given by*

$$\mathrm{Ca}(n_2, n_3, \cdots) = \frac{1}{2^{\sum_{j\geq 3} n_j}} \frac{(n-1)!}{\prod_{j\geq 2} n_j!}\, n^{k-1},$$

where $k = \sum_{i\geq 2} n_i$ *is the number of polygons.*

Proposition 3.6 *The number* $\mathrm{Ca}_n = |\,\mathrm{Ca}[n]|$ *of (labelled) cacti on* $[n]$, *for* $n \geq 2$, *is given by*

$$\mathrm{Ca}_n = \sum_{k\geq 0} \sum_{\substack{n_2+n_3+\cdots=k \\ n_2+2n_3+\cdots=n-1}} \frac{(n-1)!\; n^{k-1}}{2^{n_3+n_4+\cdots}\; n_2! n_3! \cdots} \;.$$

Unlabelled enumeration

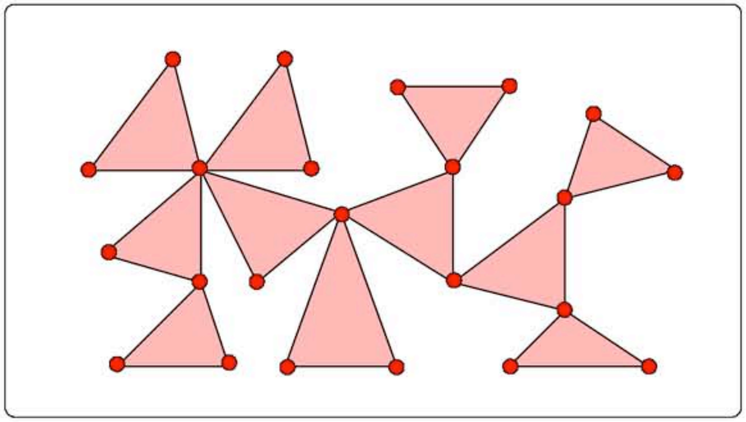
1. $C_{\mathcal{B}}^{\diamondsuit}$ is the species of $C_{\mathcal{B}}$-graphs with a distinguished block,
2. $C_{\mathcal{B}}^{\bullet\diamondsuit}$ is the species of $C_{\mathcal{B}}$-graphs with a distinguished vertex-rooted block.

Theorem 3.7 (Dissymmetry Theorem for Graphs [19], [20], [2]). *The species $C_{\mathcal{B}}$ of connected graphs whose blocks are in $\mathcal{B}$ and its associated rooted species are related by the following isomophism:*

$$C_{\mathcal{B}}^{\bullet} + C_{\mathcal{B}}^{\diamondsuit} = C_{\mathcal{B}} + C_{\mathcal{B}}^{\bullet\diamondsuit}.$$

This identity can also be written as

$$C_{\mathcal{B}}^{\bullet} + \mathcal{B}(C_{\mathcal{B}}^{\bullet}) = C_{\mathcal{B}} + C_{\mathcal{B}}^{\bullet} \cdot \mathcal{B}'(C_{\mathcal{B}}^{\bullet}).$$



Proposition 3.8 *The numbers D_n, of unlabelled rooted triagular cacti on n vertices satisfy $D_1 = 1$ and the recurrence formula, for $n \geq 1$,*

$$D_{n+1} = \frac{1}{n} \sum_{m=1}^{n} D_{n-m+1} \left(\sum_{\substack{d|m \\ d \geq 2}} \sum_{j=1}^{d} j D_{d-j} D_j + \sum_{\substack{d|m \\ d \text{ even}}} \frac{d}{2} D_{\frac{d}{2}} \right).$$

Proposition 3.9 *The numbers d_n, of unlabelled (unrooted) triangular cacti on n vertices satisfy, for $n \geq 1$,*

$$d_n = D_n + \frac{1}{3} \left(\chi(3|n) D_{\frac{n}{3}} - \sum_{i+j+k=n} D_i D_j D_k \right).$$

Proposition 3.10 *The numbers H_n, of unlabelled rooted Husimi graphs on n vertices can be computed by the following recursive scheme:* $\varphi_1 = 1, \quad H_1 = 1,$ *and, for* $n \geq 1$,

$$\begin{aligned} b_n &= \sum_{d|n} \sum_{h=1}^{d} \sum_{l|d-h+1} l H_l \, \varphi_h, \\ H_{n+1} &= \frac{1}{n} \sum_{k=1}^{n} H_{n-k+1} b_k, \\ \varphi_{n+1} &= \frac{1}{n} \sum_{m=1}^{n} \varphi_{n-m+1} \sum_{d|m} d H_d. \end{aligned}$$

Proposition 3.11 *The numbers h_n, of unlabelled Husimi graphs on n vertices satisfy*

$$h_n = \varphi_{n+1} - \sum_{k=1}^{n-1} \varphi_{k+1} H_{n-k},$$

where the numbers H_n and φ_n are given by Proposition 3.10.

Molecular expansions

Maple Package Devmol, developed at LaCIM by Pierre Auger:

P. Auger, P. Leroux and G. Labelle, *Computing the molecular expansion of species with the Maple Package Devmol*, Séminaire Lotharingien de Combinatoire, B49z (2003), 34 pp.
`http://euler.univ-lyon1.fr/home/slc`

```
> n := 6;
```

$$n := 6$$

```
> ajoutvv(seq(y[k], k = 1..n));
```

$$\{t,\, y_1,\, y_2,\, y_3,\, y_4,\, y_5,\, y_6\}$$

```
> BB := sum(y[k]*E[k](X), k = 2..n);
```

$$BB := y_2\, E_2(X) + y_3\, E_3(X) + y_4\, E_4(X) + y_5\, E_5(X) + y_6\, E_6(X)$$

```
> HuW := CBgraphes(BB,n):
> affichertable(tablephom(HuW));
```

$$1$$
$$X$$
$$2$$
$$y_2\, E_2(X)$$
$$3$$
$$X\, {y_2}^2\, E_2(X) + y_3\, E_3(X)$$
$$4$$
$$y_2\, X^2\, y_3\, E_2(X) + X\, {y_2}^3\, E_3(X) + {y_2}^3\, E_2(X^2) + y_4\, E_4(X)$$
$$5$$
$$(y_3\, {y_2}^2 + {y_2}^4)\, X^3\, E_2(X) + X\, {y_2}^2\, E_2(X)^2\, y_3 + (y_3\, {y_2}^2 + {y_2}^4)\, X\, E_2(X^2)$$
$$+X\, {y_2}^4\, E_4(X) + X\, {y_3}^2\, E_2(E_2(X)) + y_5\, E_5(X) + y_2\, X^2\, y_4\, E_3(X)$$
$$6$$
$${y_2}^5\, X^2\, E_2(X^2) + ({y_2}^2\, y_4 + y_3\, y_4 + y_3\, {y_2}^3)\, X\, E_2(X)\, E_3(X)$$
$$+y_4\, E_2(X)\, {y_2}^2\, E_2(X^2) + ({y_3}^2\, y_2 + {y_2}^5 + 3\, y_3\, {y_2}^3)\, X^4\, E_2(X)$$
$$+{y_2}^5\, E_2(X^3) + ({y_3}^2\, y_2 + {y_2}^5)\, E_2(X\, E_2(X)) + y_2\, {y_3}^2\, X^2\, E_2(E_2(X))$$
$$+y_3\, {y_2}^3\, E_3(X^2) + y_2\, y_5\, X^2\, E_4(X) + y_6\, E_6(X) + y_3\, {y_2}^3\, X^2\, E_2(X)^2$$
$$+ y_3\, {y_2}^3\, X^6 + ({y_2}^5 + {y_2}^2\, y_4)\, X^3\, E_3(X) + {y_2}^5\, X\, E_5(X)$$

$$5$$

$$(y_3\, {y_2}^2 + {y_2}^4)\, X^3\, E_2(X) + X\, {y_2}^2\, E_2(X)^2\, y_3 + (y_3\, {y_2}^2 + {y_2}^4)\, X\, E_2(X^2)$$
$$+X\, {y_2}^4\, E_4(X) + X\, {y_3}^2\, E_2(E_2(X)) + y_5\, E_5(X) + y_2\, X^2\, y_4\, E_3(X)$$

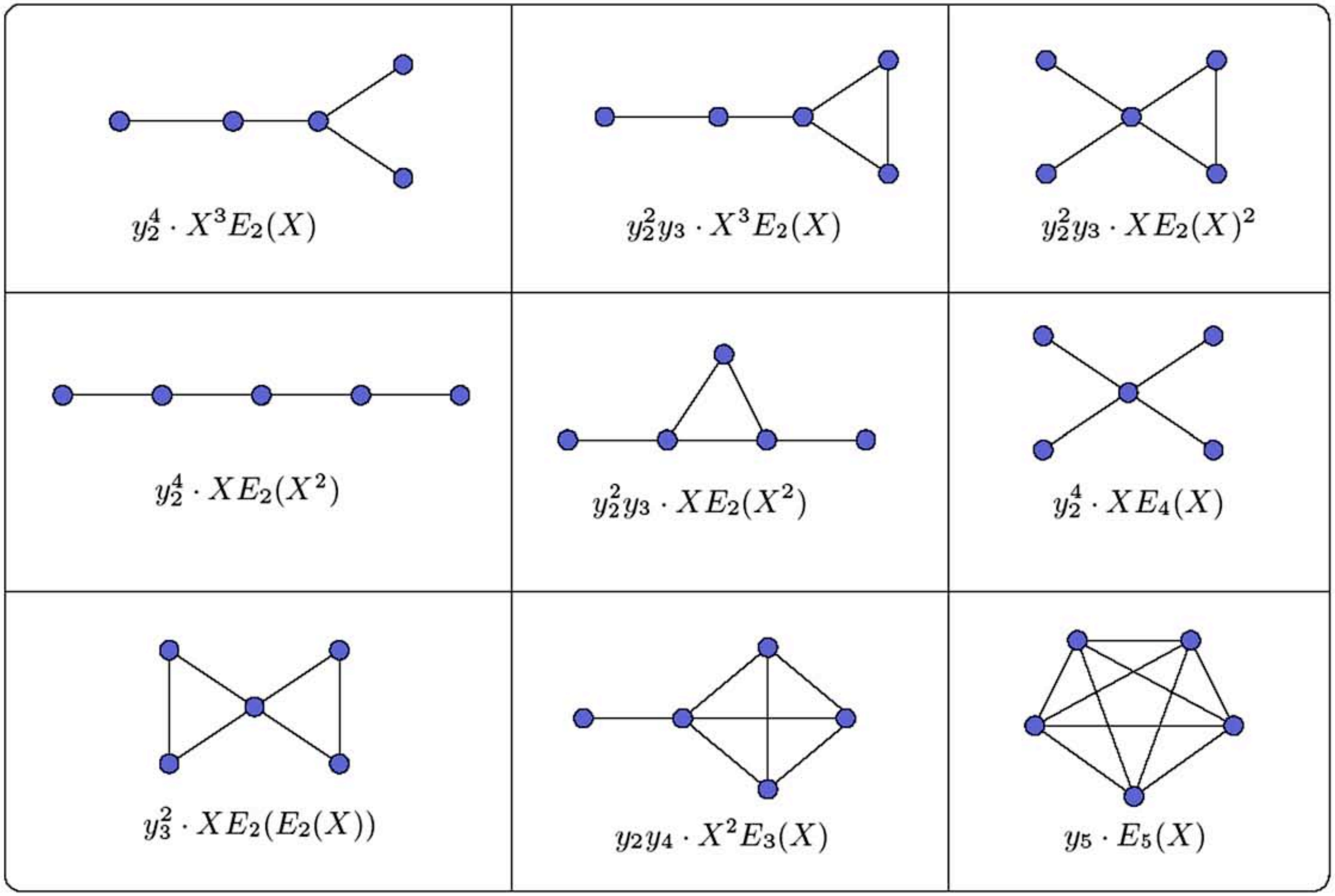


Figure 10: Husimi graphs of size 5

what is this 3 ???

6

$$y_2{}^5\,X^2\,E_2(X^2) + (y_2{}^2\,y_4 + y_3\,y_4 + y_3\,y_2{}^3)\,X\,E_2(X)\,E_3(X)$$
$$+y_4\,E_2(X)\,y_2{}^2\,E_2(X^2) + (y_3{}^2\,y_2 + y_2{}^5 + 3\,y_3\,y_2{}^3)\,X^4\,E_2(X)$$
$$+y_2{}^5\,E_2(X^3) + (y_3{}^2\,y_2 + y_2{}^5)\,E_2(X\,E_2(X)) + y_2\,y_3{}^2\,X^2\,E_2(E_2(X))$$
$$+y_3\,y_2{}^3\,E_3(X^2) + y_2\,y_5\,X^2\,E_4(X) + y_6\,E_6(X) + y_3\,y_2{}^3\,X^2\,E_2(X)^2$$
$$+\,y_3\,y_2{}^3\,X^6 + (y_2{}^5 + y_2{}^2\,y_4)\,X^3\,E_3(X) + y_2{}^5\,X\,E_5(X)$$

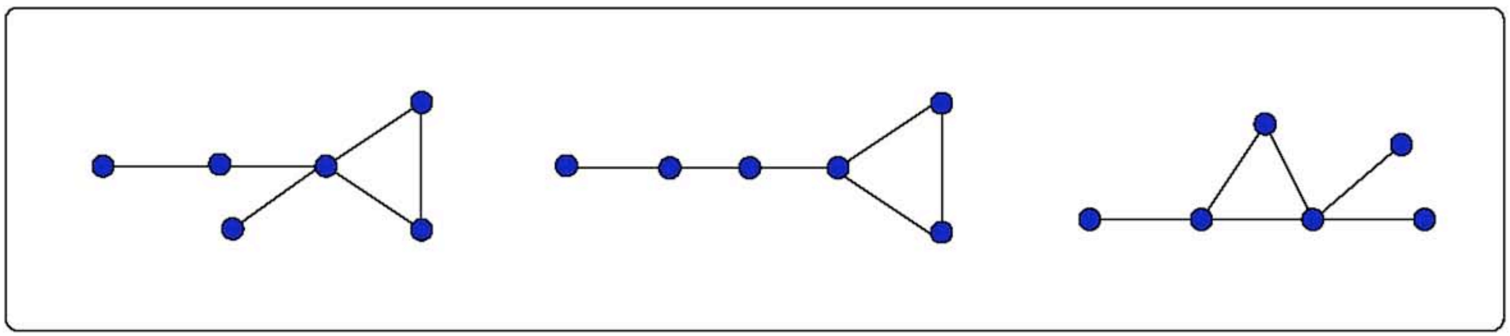


Figure 11: The three unlabelled Husimi graphs of molecular type $y_2^3 y_3 \cdot X^4 E_2(X)$

END

Thank You !!