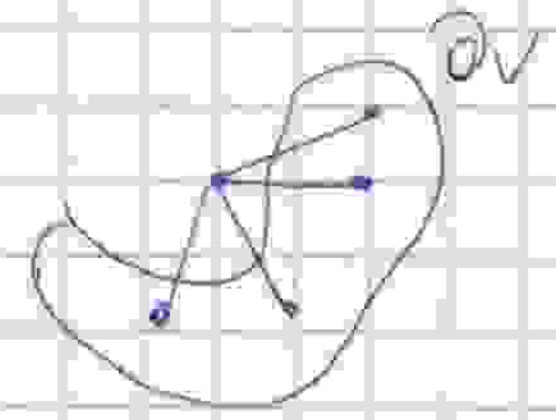
Monomer-Dimer-Model

Matchings

Graph $G = (E, V)$

$v \in V$, ∂v = set of neighbors of v / edges incident to v.



matching $\underline{B} = (B_e, e \in E)$, $B_e \in \{0,1\}$

for all $\sum_{e \in \partial v} B_e \leq 1$

$G =$ 

(matching number $= 2$)

Size of a matching $\sum_e B_e$

$\nu(G)$ = matching number = $\max\{\sum_e B_e\}$

$m_k(G)$ = # of matchings of size k

$P_G(z) = \sum_{k=0}^{\nu(G)} m_k(G) z^k$ - matching generating function.

Example

$P_\Delta(z) = 1 + 3z$

$P_{\Delta\!\_}(z) = 1 + 5z + 4z^2$

A littlebit of statistical physics

Gibbs distribution over matchings

$$\mu_G^z(\underline{B} = \underline{b}) = \frac{z^{\sum_e b_e} \cdot \mathbb{1}(\underline{b} \text{ is a matching})}{P_G(z)}$$

$\underline{b} = (b_e, e \in E)$

Internal energy $U_G(z) = -\sum_{e \in E} \mu_G^z(B_e = 1) = -\langle \sum_{e \in E} B_e \rangle_{\mu_G^z}$

$\langle \cdot \rangle_{\mu_G^z}$ - expectation w.r.t. μ_G^z

$$U_G(z) = -\left\langle \sum_{e\in E} B_e \right\rangle_{\mu_G^z} = -\sum_{e\in E}\langle B_e\rangle_{\mu_G^z} = -\sum_{e\in E}\mu_G^z(B_e=1)$$

Canonical entropy

$$S_G(z) = -\sum_{\underline{b}} \mu_G^z(\underline{B}=\underline{b})\ln\mu_G^z(\underline{B}=\underline{b}) = -\langle \ln\mu_G^z(\underline{B})\rangle_{\mu_G^z}$$

$$\Phi_G(z) = -U_G(z)\ln z + S_G(z)$$

? Q: Show that $\Phi_G(z)=\ln P_G(z)$
①

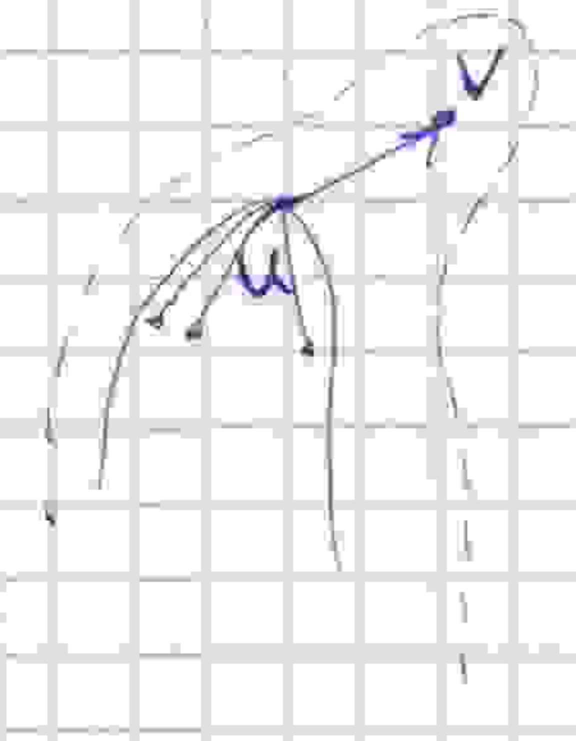
$$\Phi_G(z) = -\ln z\, U_G(z) + S_G(z) = -\ln z \sum_k m_k(G)\frac{kz^k}{P_G(z)} - \sum_k m_k(G)\frac{z^k}{P_G(z)}\ln\left(\frac{z^k}{P_G(z)}\right)$$

$$= \sum_k m_k(G)\, z^k / P_G(z) \ln P_G(z) = \ln P_G(z)$$

? Q: $\Phi_G'(z) = -\dfrac{U_G(z)}{z}$
②

2 Local recursions on finite graphs

First assume that G is a tree.



$T_{u\to v}$

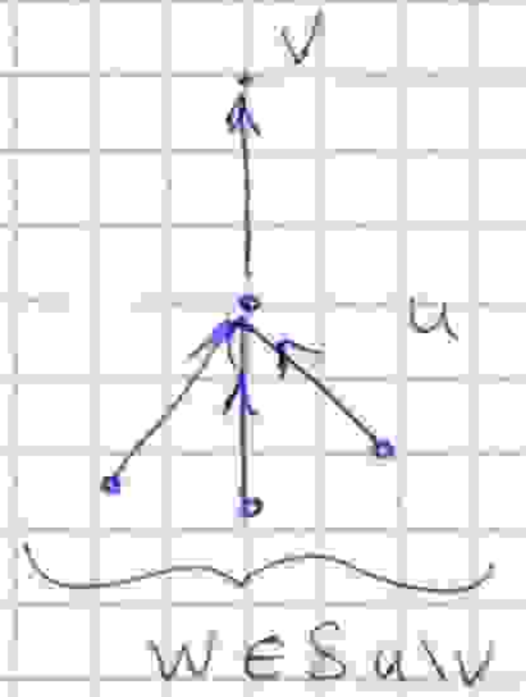
$$\underbrace{\frac{\mu^z_{T_{u\to v}}(B_{uv}=1)}{\mu^z_{T_{u\to v}}(B_{uv}=0)}}_{\text{LHS}} = \frac{z\prod_{w\in\partial u\setminus v}\mu^z_{T_{w\to u}}(B_{wu}=0)}{\prod_{w\in\partial u\setminus v}\mu^z_{T_{w\to u}}(B_{wu}=0) + \sum_{w'\in\partial u\setminus v}\mu^z_{T_{w'\to u}}(B_{w'u}=1)\cdot\prod_{\substack{w\neq w'\\ w\in\partial u\setminus v}}\mu^z_{T_{w\to u}}(B_{wu}=0)}$$

$$\text{LHS} = \frac{z}{1 + \sum_{w \in \partial u \setminus v} \frac{\mu^z_{T_{w\to u}}(B_{wu}=1)}{\mu^z_{T_{w\to u}}(B_{wu}=0)}}$$

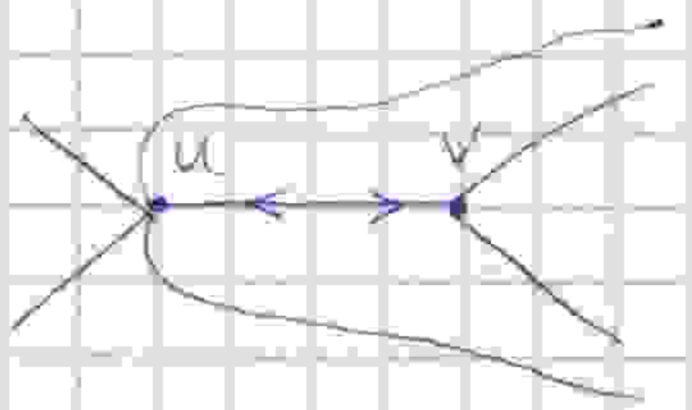
$$Y_{u\to v}(z) = \frac{\mu^z_{T_{u\to v}}(B_{uv}=1)}{\mu^z_{T_{u\to v}}(B_{uv}=0)}$$

$$Y_{u\to v}(z) = \frac{z}{1 + \sum_{w \in \partial u \setminus v} Y_{w\to u}(z)}$$

$Y_{u\to v}(z)$



? Q : ③ $$\frac{\mu^z_T(B_{uv}=1)}{\mu^z_T(B_{uv}=0)} = \frac{Y_{u\to v}(z)\, Y_{v\to u}(z)}{z}$$



Proposition 1

G-finite, $z>0$, the fixed point eq $\underline{Y} = z R_E(\underline{Y})$ defined by:

$$Y_{u\to v} = \frac{z}{1 + \sum_{w\in\partial u\setminus v} Y_{w\to u}} \qquad \forall (u,v) \in \vec{E}$$

has a unique attractive solution $\underline{Y}(z) \in (0,z)^{\vec{E}}$

Proof
$$\begin{cases} Y^{t+1}_{u\to v}(z) = \dfrac{z}{\underbrace{1 + \sum_{w\in\partial u\setminus v} Y^t_{w\to u}(z)}_{=: z R_{u\to v}(\underline{Y}^t(z))}}, & t \geq 0 \\ Y^0_{u\to v}(z) = 0 \end{cases}$$

$$0 \leq \underline{Y}^{2t}(z) \leq \underline{Y}^{2t+1}(z) \leq z$$

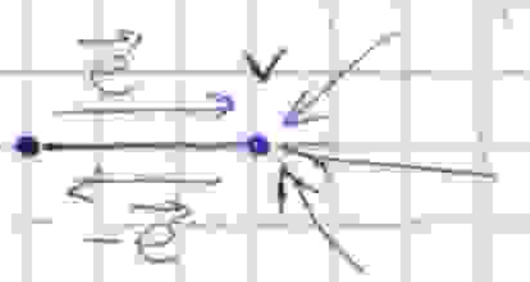
$$0 \leq \vec{\underline{Y}}^{2t}(z) \leq \underline{Y}^-(z) \leq \underline{Y}^+(z) \leq \vec{\underline{Y}}^{2t+1}(z) \leq z \quad \text{for any fixed point } \underline{Y}(z)$$

$$0 \leq \underline{Y}^{2t}(z) \leq \underline{Y}^-(z) \leq \underline{Y}(z) \leq \underline{Y}^+(z) \leq \underline{Y}^{2t+1}(z) \leq z$$

We now prove that $Y^-(z) = Y^+(z)$

$v \in V$:

$$D_v(\underline{Y}) = \sum_{\vec e \in \partial v} \frac{Y_{\vec e}\, R_{\vec e}(\underline{Y})}{1 + Y_{\vec e}\, R_{\vec e}(\underline{Y})}$$



$$R_{\vec e}(\underline{Y}) = \frac{1}{1 + \sum_{\substack{\vec e' \in \partial v \\ \vec e' \neq \vec e}} Y_{\vec e'}}$$

$$\left\{ \vec e ,\ -\vec e \right\}$$

$$D_v(\underline{Y}) = \frac{\sum_{\vec e \in \partial v} Y_{\vec e}}{1 + \sum_{\vec e \in \partial v} Y_{\vec e}}$$

$$\underline{Y}^+(z) = z\, R_G(\underline{Y}^-(z))$$

$$\underline{Y}^-(z) = z\, R_G(\underline{Y}^+(z))$$

$$\sum_v D_v(\underline{Y}^+(z)) = \sum_v D_v(\underline{Y}^-(z)) \Rightarrow \underline{Y}^+(z) = \underline{Y}^-(z) \qquad \square$$

$$\mu_T^z(B_e = 1) = x_e(z) = \frac{Y_{\vec e}(z)\, Y_{-\vec e}(z)}{z + Y_{\vec e}(z)\, Y_{-\vec e}(z)} \qquad \left(\begin{array}{l} \text{Graph is a tree} \\ \text{Trivial} \end{array} \right)$$

~~Repreme~~

<u>~~Representation~~ of the Gibbs measure</u>

<u>Reparametrization</u>

For any vector $\underline{b} \in \{0,1\}^E$

$$\underline{b}_{\partial v} = (b_e, e \in \partial v) \in \{0,1\}^{\partial v}, \quad v \in V$$

marginal prob

$$\mu_{\partial v}(\underline{b}_{\partial v}) = \left(1 - \sum_{e \in \partial v} x_e(z)\right)^{1 - \sum_{e \in \partial v} b_e} \prod_{e \in \partial v} x_e(z)^{b_e}$$

$$\mu_e(b_e) = x_e(z)^{b_e} (1 - x_e(z))^{1 - b_e}$$

$$\mu_G^z(\underline{B}=\underline{b}) = \frac{z^{\sum b_e}}{P_G(z)}$$

$$\Phi_G(z) = \ln P_G(z) = -\underbrace{U_G(z)}_{\text{energy}} \ln z + \underbrace{S_G(z)}_{\text{entropy}}$$

When G is a tree, local recursion

$$Y_{u\to v}(z) = \frac{z}{1 + \sum_{w \in \partial u \setminus v} Y_{w\to u}(z)}$$

$$x_e(z) = \frac{Y_{\vec{e}}(z)\, Y_{-\vec{e}}(z)}{z + Y_{\vec{e}}(z)\, Y_{-\vec{e}}(z)} = \mu_G^z(B_e = 1)$$

($x_e(z)$ is a very important parameter. If you can compute it, then you can compute everything ☺)

The question is can we construct Gibbs measure, if we have just the marginals? Yes (if the graph is a ~~the~~ tree)

Given a graph $G = (V, E)$, some set $F \subset E$,

$d_F(v)$ is the degree of v in the subgraph induced by F.

A generalized loop is any subset F such that

$$d_F(v) \neq 1 \quad \forall v \in V$$

<u>Theorem</u> (Reparametrization of the Gibbs measure)

For <u>any graph</u> G, $z > 0$

$$\mu_G^z(\underline{b}) = \frac{1}{Z_R} \frac{\prod_{v \in V} \mu_{\partial v}(b_{\partial v})}{\prod_{e \in E} \mu_e(b_e)}$$

with

$$Z_R = 1 + \sum_{\emptyset \neq F \subset E} (-1)^{V(F)} \prod_{v \in V} (d_F(v) - 1) \prod_{e \in F} \frac{x_e(z)}{1 - x_e(z)}$$

(for a tree  $Z_R \Rightarrow 1$)

3. Variational Formulation

$\boxed{\text{Bethe}}$

$$U_G^B(\underline{x}) = -\sum_{e\in E} x_e$$

If G is a tree $U_G(z) = U_z^B(\underline{x}(z))$

fractional matching polytope: $FM(G) = \{ \underline{x} \in \mathbb{R}^E,\ \underset{\forall e \in E}{x_e \geq 0},\ \sum_{e\in\partial v} x_e \leq 1 \}$

$$S_G^B(\underline{x}) = \frac{1}{2}\sum_{v\in V}\Big\{ \sum_{e\in\partial v}(-x_e \ln x_e + (1-x_e)\ln(1-x_e)) - \quad \text{(we know: } \sum_{e\in\partial v} B_e \leq 1) $$

$$-2\Big(1-\sum_{e\in\partial v} x_e\Big)\ln\Big(1-\sum_{e\in\partial v} x_e\Big)\Big\}$$

and $S_G(z) = S_G^B(\underline{x}(z))$

Bethe free entropy $\underbrace{\Phi_G^B(\underline{x},z)}_{\text{concave fct in } x} = -\underbrace{U_G^B(\underline{x})}_{\text{linear in } x}\ln z + \underbrace{S_G^B(\underline{x})}_{\text{concave}}$

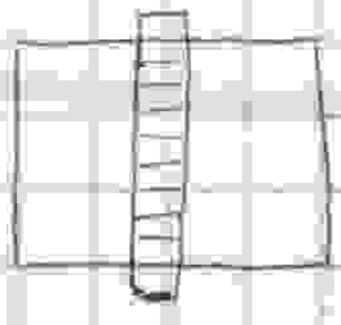
Proposition 2

$\Phi_G^B(\underline{x}(z), z) = \sup_{\underline{x}\in FM(G)} \Phi_G^B(\underline{x}, z)$ – for any graph G.

From finite graphs to infinite graphs
particular case of lifts

1) Gibbs measure on an infinite tree.

Markov Random field



for any finite graph G, μ_G^z has a global Markov property: any two subsets of variables are conditionally independent given a separating subset

T is infinite tree with bounded degree,

the ball of radius t centered at e T_e^t and ∂T_e^t - the set of boundary edges.

Take an arbitrary boundary condition

$\underline{b}_{\partial T_e^t} \in \{0,1\}^{\partial T_e^t}$

$$\mu_T^z(\underline{B}_{T_e^t} \mid \underline{B}_{\partial T_e^t} = \underline{b}_{\partial T_e^t}) \cong z^{\sum B_e} \mathbb{1}(\underline{B}_{\partial T_e^t} = \underline{b}_{\partial T_e^t})$$

Proposition 3

Prop 1 is still correct, when G is an infinite tree

~~Example~~ Proof: $[0,z]^E$ Schauder fixed point + contraction $h_{u\to v} = \ln(y_{u\to v}(z)/z)$

$$h_{u\to v} = \ln\left(1 + z\sum_{w\in\partial u\setminus v} e^{-h_{w\to u}}\right)$$

T - infinite tree, $z>0$, $Y(z) = (Y_{\vec{e}}(z), \vec{e} \in \vec{E})$ the solution of:

$$Y_{u\to v}(z) = \frac{z}{1 + \sum\limits_{w \in \partial u \setminus v} Y_{w \to u}(z)}$$

$$x_e(z) = \frac{Y_{\vec{e}}(z) \cdot Y_{-\vec{e}}(z)}{z + Y_{\vec{e}}(z) Y_{-\vec{e}}(z)} \quad \forall e$$

$\forall e$: $\mu^{z}_{T^{t}_{e}}(B_e = 1) \xrightarrow[t\to\infty]{} x_e(z)$ (with Kolmogorov consisting theorem)

Example:

20.08.2016

$$\mu^z_G(\underline{B} = \underline{b}) = \frac{z^{\sum b_e}}{P_G(z)} \qquad G\text{ - finite Graph}$$

$$\forall v \in V \quad \sum_{e \in \partial v} b_e \le 1$$

L ∞-line

1) G finite $\quad \mu^z_G\left(\sum\limits_{e \in \partial v} B_e = 0\right) = \dfrac{P_{G\setminus\{v\}}(z)}{P_G(z)}$

$\mu^z_G(\forall e \in \partial v, B_e = 0) = \mu^z_G(v \text{ is uncovered}) =$

$$= \sum_{\substack{\underline{b} \text{ such that} \\ v \text{ is uncovered}}} \mu^z_G(\underline{B} = \underline{b}) = \sum_{\underline{b},\, s.t.\ v\text{-uncovered}} \frac{z^{\sum b_e}}{P_G(z)}$$

$$P_{G\setminus\{v\}}(z) = \sum_{\substack{\underline{b}\text{-matching} \\ \text{in } G\setminus\{v\}}} z^{\sum b_e}$$

2) Show, that if v has degree 2, then

$$P_G(z) = P_{G\setminus\{v\}}(z) + z P_{G\setminus\{v,l\}}(z) + z P_{G\setminus\{v,n\}}(z)$$

Define $$R_{G,v}(z) = \frac{P_{G\setminus\{v\}}(z)}{P_G(z)} = \mu_G^z(v \text{ is uncovered})$$

$$R^{-1}_{G,v}(z) = 1 + z R_{G\setminus\{v\},\mathrm{left}} + z R_{G\setminus\{v\},\mathrm{right}}(z)$$

$$R_{L,v}(z) = \frac{1}{1+2zR_{SL,s}(z)}$$

$$P_G(z) = P_{G\setminus\{s\}}(z) + z P_{G\setminus\{s,s+1\}}(z)$$

$$R_{SL,s}(z) = \frac{1}{1+zR_{SL,s}(z)}$$

$$R_{SL,s}(z) = \frac{\sqrt{1+4z}-1}{2z}$$

$$\mu_L^z\Big(\sum_{e\in\partial v} B_e = 0\Big) = \frac{1}{\sqrt{1+4z}}$$

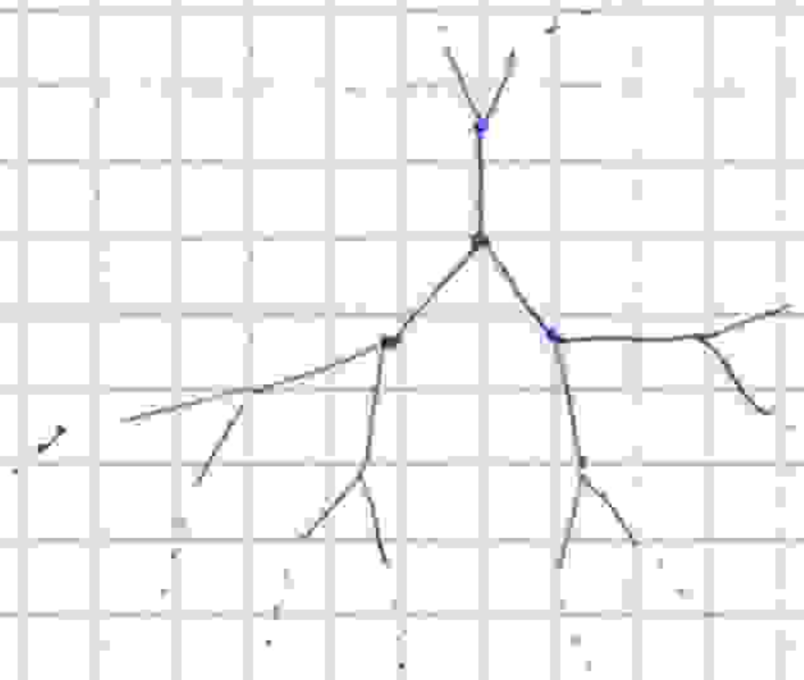
$$Y(z) = \frac{z}{1+Y(z)} \Rightarrow Y(z) = \frac{\sqrt{1+4z}-1}{2}$$

$$x_e(z) = \frac{Y(z)^2}{z+Y(z)^2} = \frac{1+2z-\sqrt{1+4z}}{1+4z-\sqrt{1+4z}}$$

$$\mu_{\partial v}(\underline{B}_{\partial v}) = \Big(1-\sum_{e\in\partial v} x_e(z)\Big)^{1-\sum_{e\in\partial v} b_e} \prod_{e\in\partial v} x_e(z)^{b_e}$$

$$\mu_{\partial v}\Big(\sum_{e\in\partial v} B_e = 0\Big) = 1 - 2x_e(z) = \frac{\sqrt{1+4z}-1}{1+4z-\sqrt{1+4z}} = \frac{1}{\sqrt{1+4z}}$$

$$D_v(\underline{Y}) = \frac{2Y(z)}{1+2Y(z)} = 1 - \frac{1}{\sqrt{1+4z}}$$



d-regular tree
(in this case 3-reg tree)

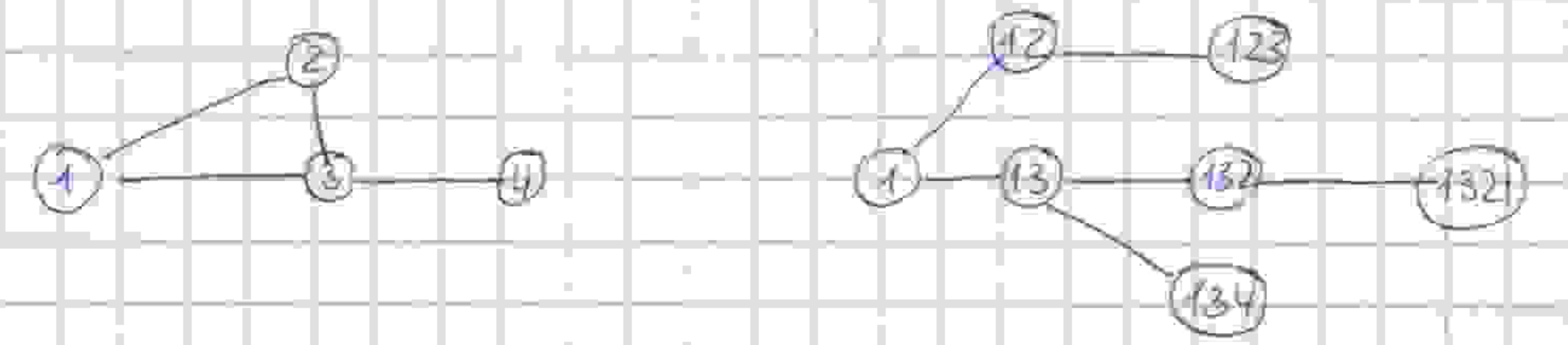
$$Y(z) = \frac{z}{1+(d-1)Y(z)}$$

$$Y(z) = \frac{1}{2(d-1)}\left(\sqrt{1+4(d-1)z}-1\right)$$

$$a = \frac{z}{1+z+\frac{z}{1+a}}$$

$$\frac{z}{1+\frac{2z}{1+a}}$$

Given a finite graph G with a distinguished vertex $v \in V$, we construct the rooted tree $(T(G), v)$ of non backtraking walks in G, starting in v.



$T(G)$ is the universal cover of G.

If G is a graph and $v \in V(G)$, the 1-neighbourhood of r is the subgraph consisting of all edges incident to r.

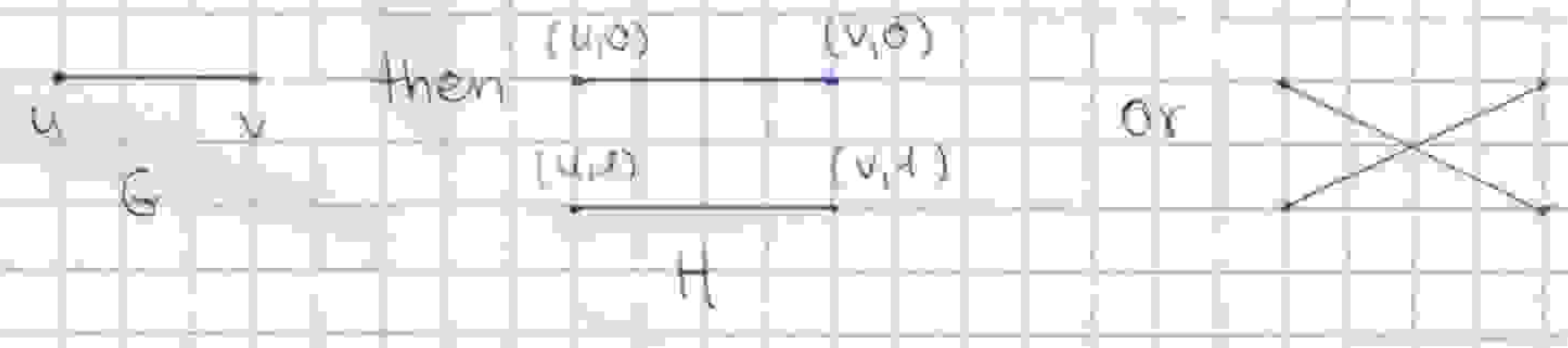
A graph homomorphism
$\pi G' \to G$ is a covering map if for each $v' \in V(G)$ π gives a bijection of the edges of the 1-neighb. of v with those of $v = \pi(v')$. G' is a cover / lift of G.

Definition

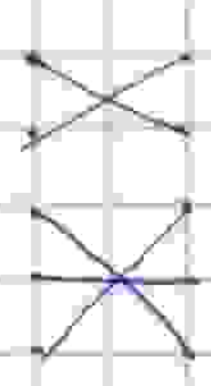
G with no loop ($\cancel{\circlearrowleft}$)

H is a 2-lift of G if $V(H) = V(G) \times \{0,1\}$

if



k-lift:



1) Gibbs measure on ∞ tree

2) Rooted graphs

(G, o) graph with distinguished vertex $o \in V$, called the root

G_* = set of all localy finite conected rooted graphs
considered up to rooted isomorphism

$(G, o) \equiv (G', o')$ if there exists a bijection $\gamma : V \to V'$
that preserves the root $\gamma(o) = o'$ adjacency
$$(i,j) \in E \Leftrightarrow (\gamma(i), \gamma(j)) \in E'$$

We write $[G, o]_h$ for the finite rooted subgraph induced by vertices at graph-dist at most h from the root o

The distance

$$\mathrm{DIST}((G,o),(G',o')) = \frac{1}{1+n} \quad \text{where}$$

$M = \sup\{h, [G,o]_h \equiv [G',o']_h\}$ turns G_* into ~~a~~ a complete separable metric space.

(G, o) = equivalence class of rooted graph
(unlabeled)

Proposition 4

For any graph $G=(V,E)$ there exists a graph sequence $\{G_n\}_{n\in\mathbb{N}}$ such that $G_0=G$, G_n is a 2-lift of G_{n-1} for $n\geq 1$.
G_n is a 2^n-lift of G, $\pi_n : G_n \to G$ the corresponding covering.
$\forall v \in V$, if $v_n \in \pi_n^{-1}(v)$ $(G_n, v_n) \to (T(G), v)$ in G_*.

Proof. a random 2-lift H of G is the random graph obtained by choosing between  and  with prob. 1/2, each choice independent

Let G be a graph with girth* γ and let k be the number of cycles in G of size γ. (*: girth - minimum size of a cycle)
Let X be the number of γ-cycles in H a random 2-lift of G. The girth of H must be at least γ. A γ-cycle in H must be a lift of a γ-cycle in G.

$\mathbb{E}[X] = k$

$G \cup G$ - trivial lift, $2k$ γ-cycles

$\Rightarrow$ there exists a 2-lift with strictly less than k γ-cycles.

$\square$

3. Thermodynamic limit

$\frac{1}{n} \ln P_{G_n}(z)$ conv ? $\mu^z_{T(G)}$?

Lemma If $(G_n, o_n) \to (T, o)$ in G_*, then

$$\sum_{e \in \partial o_n} \mu^z_{G_n}(B_e = 1) \longrightarrow \sum_{e \in \partial o} \mu^z_T(B_e = 1)$$

Theorem

$$\lim_{n \to \infty} \frac{1}{|V_n|} \ln P_{G_n}(z) = \frac{1}{|V|} \Phi^B_G(\underline{x}(z), z)$$

entropy

$$\max_{\underline{x} \in FM(G)} \Phi^B_G(\underline{x}, z)$$

Proposition 5

G - bipartite graph.

H a 2-lift of G, then $P_G(z)^2 \geq P_H(z)$

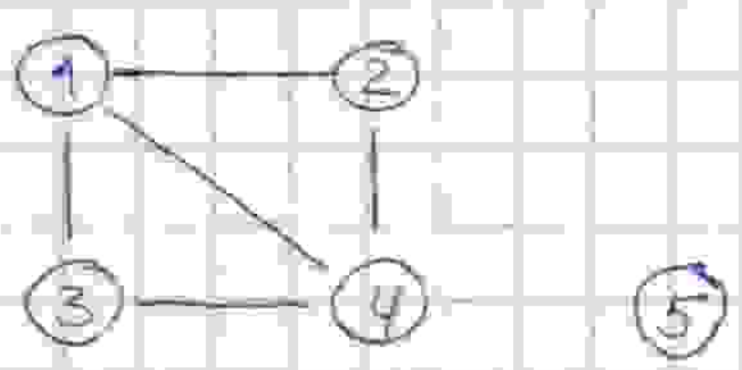
$$\left\{ \frac{1}{|V|} \ln P_G(z) \geq \frac{1}{|V|} \max_{\underline{x} \in FM(G)} \Phi^B_G(\underline{x}, z) \right\}$$

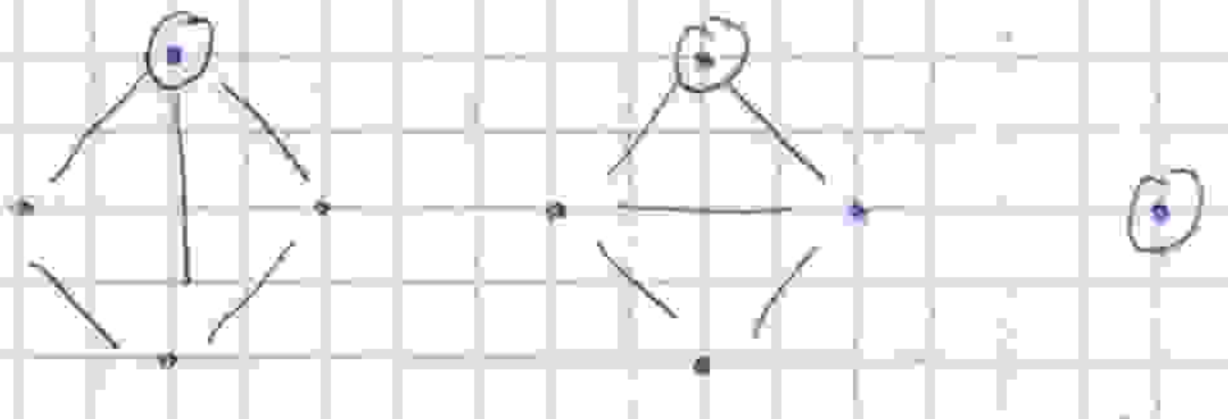
4 The framework of Local Weak Convergence

$P(G_*)$ set of prob. measure on G_*. $\mathcal{L} \in P(G_*)$ is the law of (G, o) a random rooted graph.

Given a finite Graph $G = (V, E)$, we constructed a random element of G_* by choosing uniformly at random a vertex $o \in V$ to be the root and restricting G to the connected component of o the resulting law is $U(G) \in P(G_*)$.

Example





$2/5 \qquad 2/5 \qquad 1/5$

$\mathcal{G}_*$ is a Polish space (Polish = complete separable)
$\to P(\mathcal{G}_*)$ with topology of weak convergence

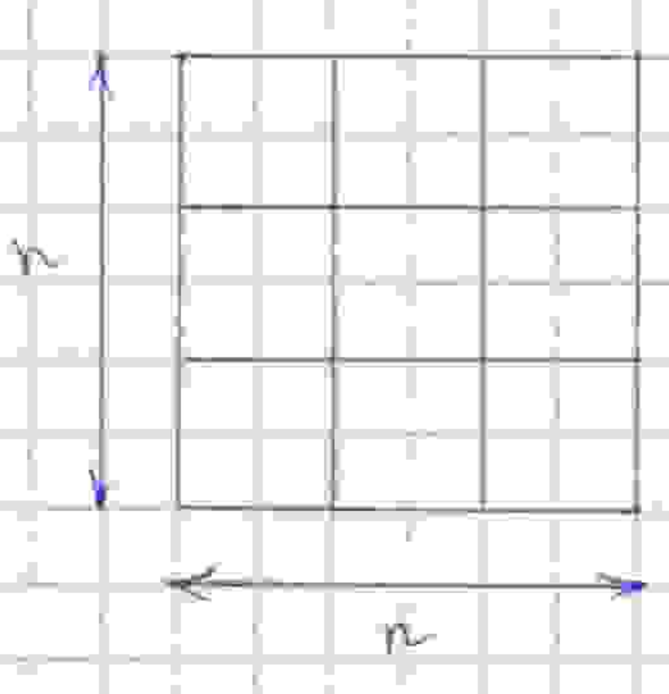
If (G_n) is a sequence of finite graphs, we say that (G_n) has a local weak limit $\mathcal{L} \in P(\mathcal{G}_*)$
if $U(G_n) \Rightarrow \mathcal{L}$ weakly in $P(\mathcal{G}_*)$
(Sometimes one can write it: $G_n \rightsquigarrow (G, o)$, where $(G,o) \sim \mathcal{L}$

$$\mathbb{E}_{(G,o)}[f(G,o)] = \int_{\mathcal{G}_*} f(G,o)\, d\mathcal{L}(G,o)$$)

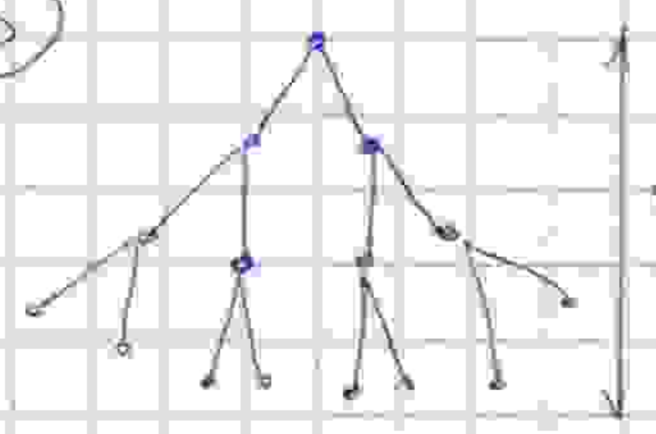
Example

1. 

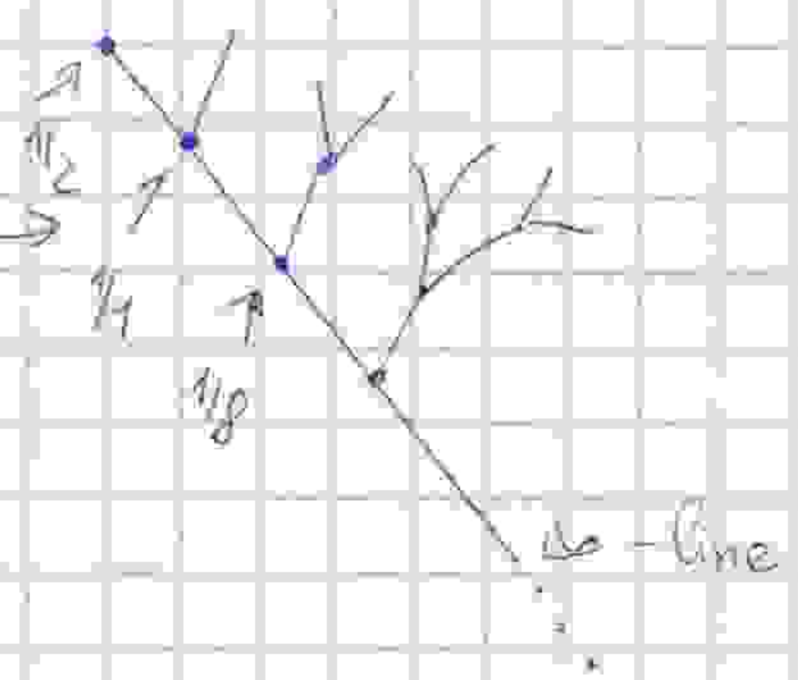
$\to \mathbb{Z}$

2. 

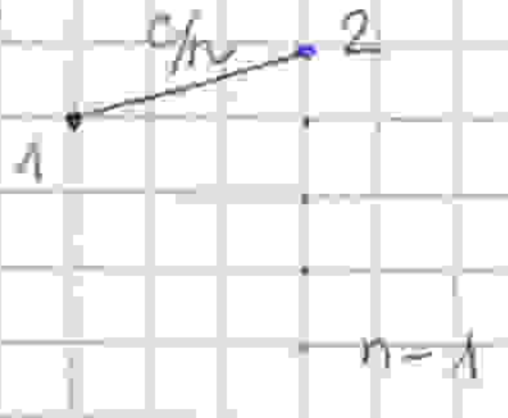
$\to \mathbb{Z}^2$

3. 

$$\left.\begin{matrix} 2^0 \\ 2 \\ \vdots \\ 2^{n-1} \\ 2^n \end{matrix}\right\} \Sigma = 2^{n+1} - 1 \longrightarrow \begin{matrix} 1/8 \\ 1/4 \\ 1/2 \end{matrix} \longrightarrow$$



④ Erdös - Renyi - Graph $\quad G(n, \frac{c}{n})$



$Bin(n-1, \frac{c}{n}) \xrightarrow[n\to\infty]{} Poi(c)$

$G_n \rightsquigarrow (T, o)$ a.s., where $T \sim PGWT$

5 Application to mathings

(G_n) seq. of graphs $|V_n| = n$

$$\frac{1}{n} U_{G_n}(z) = -\frac{1}{2n} \sum_{v \in V_n} \mu_{G_n}^z (v \text{ is cov.}) = -\frac{1}{2} \mathbb{E}_{U(G_n)} \left[\mu_{G_n}^z (o \text{ is covered}) \right]$$

$G_n \rightsquigarrow (T, o)$.

If $G_n \rightsquigarrow (T, o)$, then $\mathbb{E}_{U(G_n)} [\mu_{G_n}^z (o \text{ is covered})] \longrightarrow \mathbb{E}_{(T,o)} [\mu_T^z (o \text{ is covered})]$

$$= \mathbb{E}_{(T,o)} \left[\sum_{e \in \partial o} x_e(z) \right]$$

$$\Phi_G'(z) = U_G(z)/z$$

$$\frac{1}{n} \ln P_{G_n}(z) \longrightarrow \mathbb{E}_{(T,o)} \Big[\frac{\ln z}{z} \sum_{e \in \partial o} x_e(z) + \frac{1}{2} \sum_{e \in \partial o} \big(-x_e(z) \ln x_e(z) +$$

$$+ (1 - x_e(z)) \ln (1 - x_e(z)) \big) - \big(1 - \sum_{e \in \partial o} x_e(x)\big) \ln \big(1 - \sum_{e \in \partial o} x_e(z)\big) \Big]$$

$$Y_{u \to v}(z) = \frac{z}{1 + \sum_{w \in \partial u \setminus v} Y_{w \to u}(z)}$$

Recursive distributional equation:

$$Y(z) \overset{d}{=} \frac{z}{1 + \sum_{i=1}^{N} Y_i(z)},$$

wher $N \sim Poi(c)$, $(Y(z), Y_1(z), \ldots)$ i.i.d.

An algorithmic perspective 21.08.2016

Sum-Product algorithm

Belief Propagation

1) Distributive law

$a, b \in \mathbb{F}: \quad ab + bc = b(a+c)$

Example: $f(x_1, x_2, x_3, x_4, x_5, x_6) = f_1(x_1, x_2, x_3) f_2(x_1, x_4, x_6) f_3(x_4) f_4(x_4, x_5)$

x_i variables $\in \mathcal{X}$ finite alphabet ($|\mathcal{X}|$)

$$f(x_1) = \sum_{\substack{x_2, x_3, x_4 \\ x_5, x_6}} f(x_1 \dots x_6) = \sum_{\sim x_1} f(x_1 \dots x_6) \qquad \forall x_1 \in \mathcal{X}$$

all marginals $\Theta(|\mathcal{X}|^6)$

$$f(x_1) = \Big[\sum_{x_2, x_3} f_1(x_1, x_2, x_3) \Big] \Big[\underbrace{\sum_{x_4} f_3(x_4) \Big(\sum_{x_6} f_2(x_1, x_4, x_6) \Big) \Big(\sum_{x_5} f_4(x_4, x_5) \Big)}_{\Theta(|\mathcal{X}|^2)} \Big]$$

x_1 - fixed $\qquad \Theta(|\mathcal{X}^2|)$

$\hookrightarrow \Theta(|\mathcal{X}^3|)$

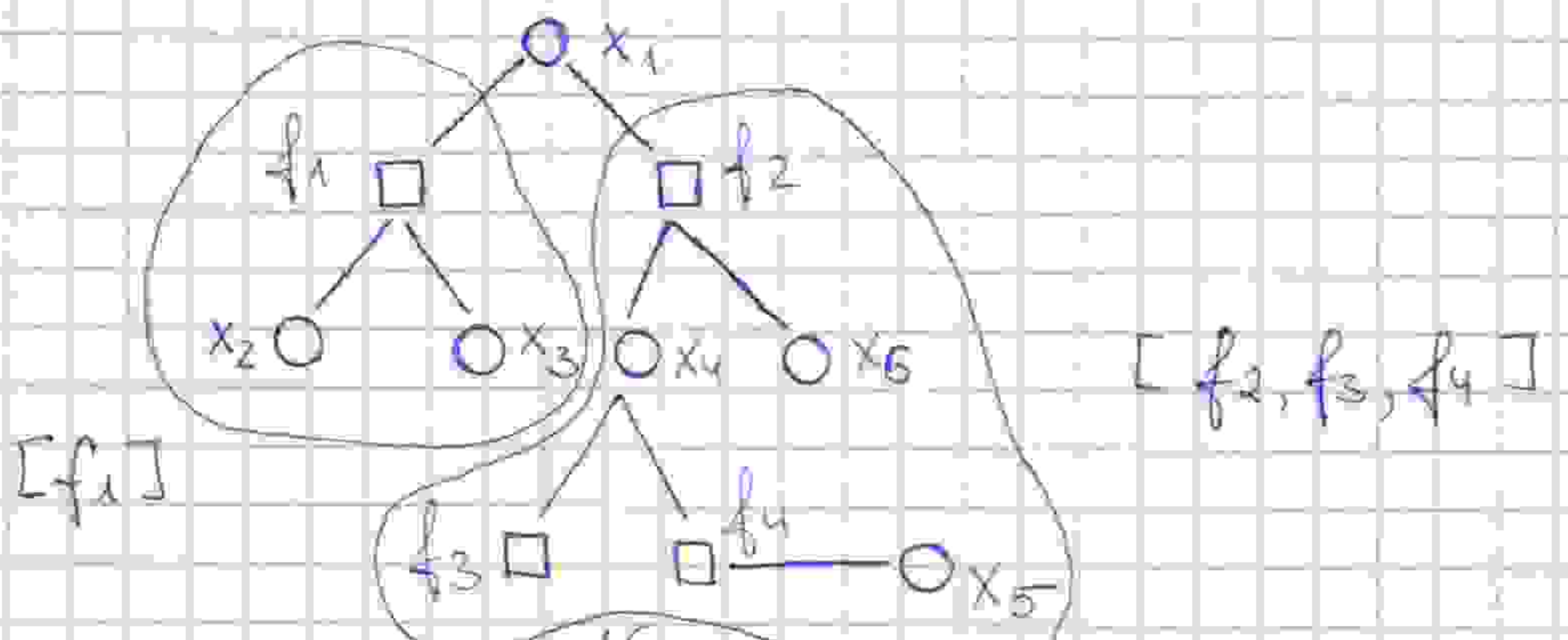
2) Graphical (model) interpretation of factorization

each variable $\longrightarrow$ variable node $\bigcirc$

each factor $\longrightarrow$ factor node $\square$

Connect a variable node to a factor node by an edge, iff the corresponding variables appears in the

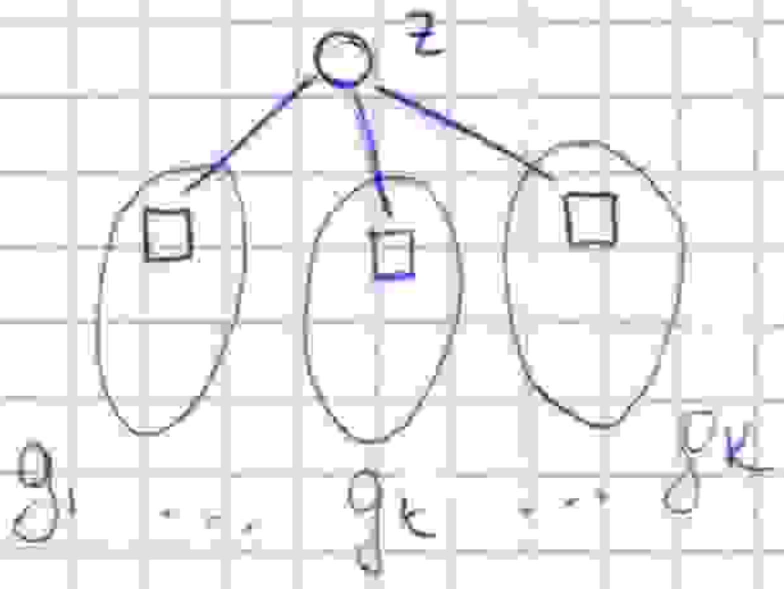
$\rightarrow$ factor graph is bipartite



3. Recursive determination of marginals

Generic function g and suppose the associated factor graph is a tree

$$g(z) = \sum_{\sim z} g(z, \dots)$$



$$g(z, \dots) = \prod_{k=1}^{K} [g_k(z, \dots)]$$

for some K with the following property:

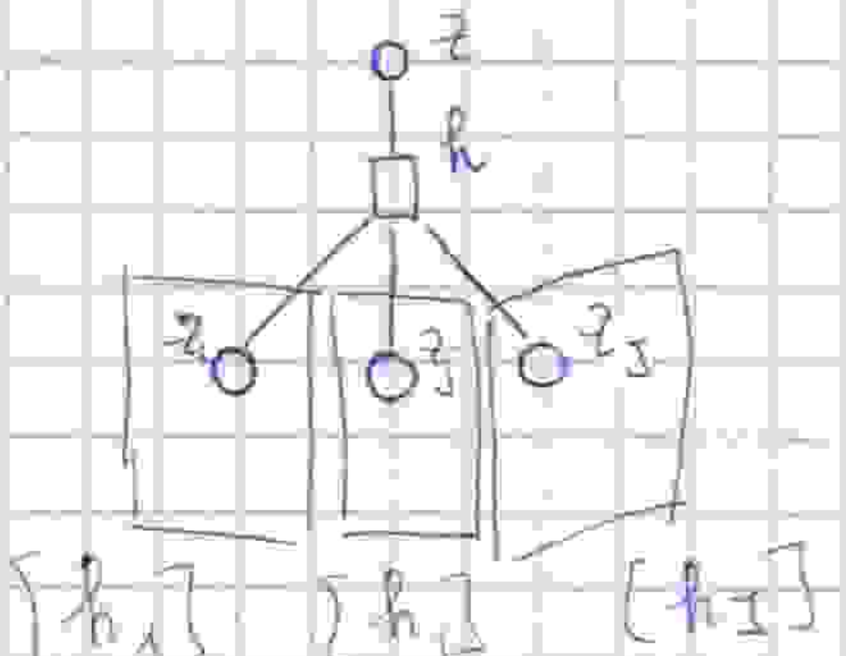
z appears on each of the factors g_k, but all other variables appear in only one factor.

Application of the distributive law

$$\sum_{\sim z} g(z, \dots) = \prod_{k=1}^{K} \Big[\sum_{\sim z} g_k(z, \dots) \Big]$$

$$g_k(z, \dots) = \underset{\text{kernel}}{h(z, z_1 \dots z_J)} \cdot \prod_{j=1}^{J} \underbrace{[h_j(z_j \dots)]}_{\text{factors}}$$

z appears only in the kernel. Each of the z_j appears posibly in the kernel and in at most one of the factors

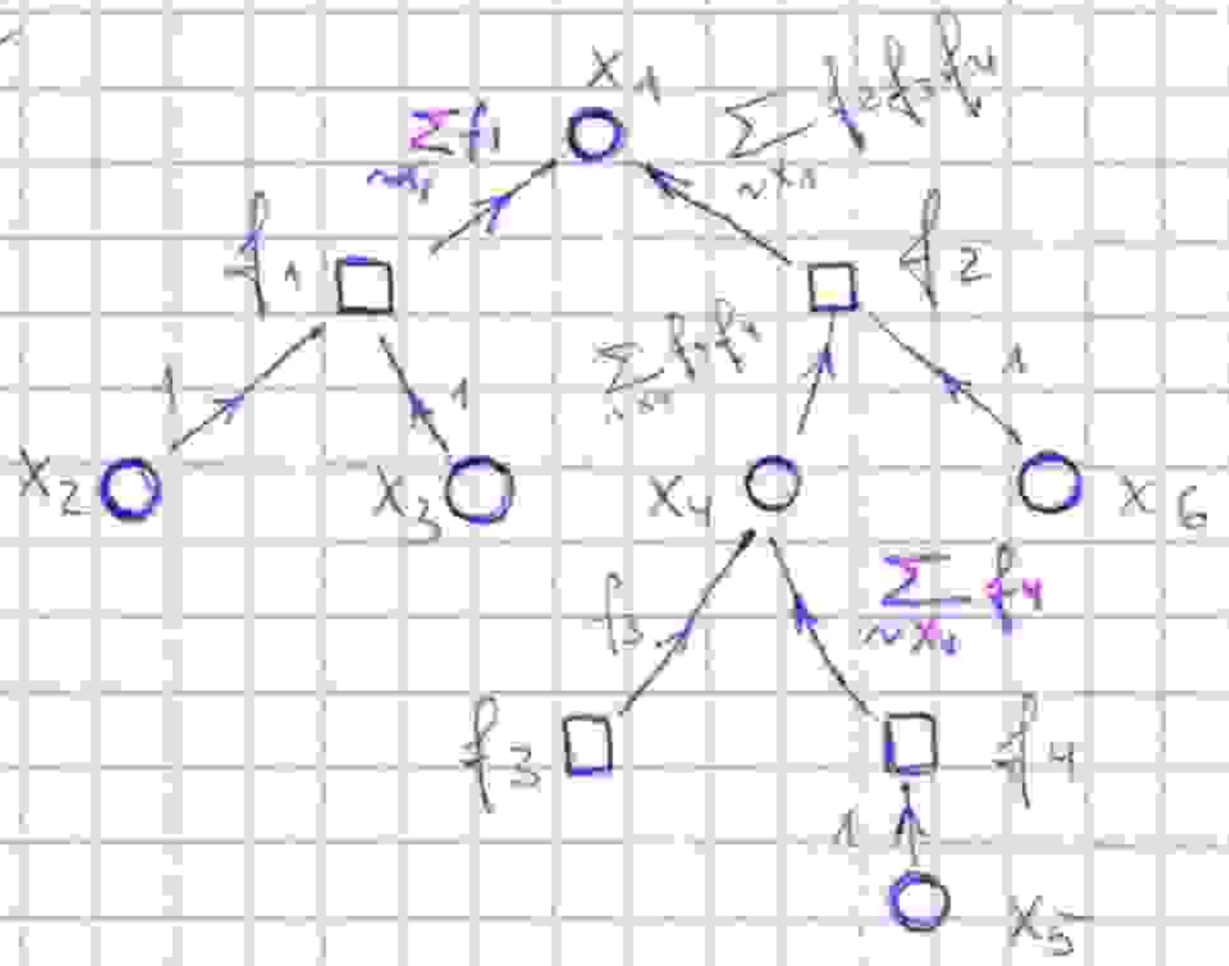


$$\sum_{\sim z} g_k(z, \dots) = \sum_{\sim z} h(z, z_1 \dots z_J) \prod_{j=1}^{J} [h_j(z_j, \dots)] = \sum_{z} h(z, z_1 \dots z_J) \cdot$$
$$\cdot \prod_{j=1}^{J} \Big[\sum_{\sim z_j} h_j(z_j, \dots) \Big]$$

4 Marginalisation via message passing

Nodes in the graph compute marginals, which are functions over $\mathcal{X}$ and pass these on to the next level along the edges of the tree

Example



factor leaf node f_3 sends the function f_3.

x_2, x_3, x_5, x_6 send the constant function 1

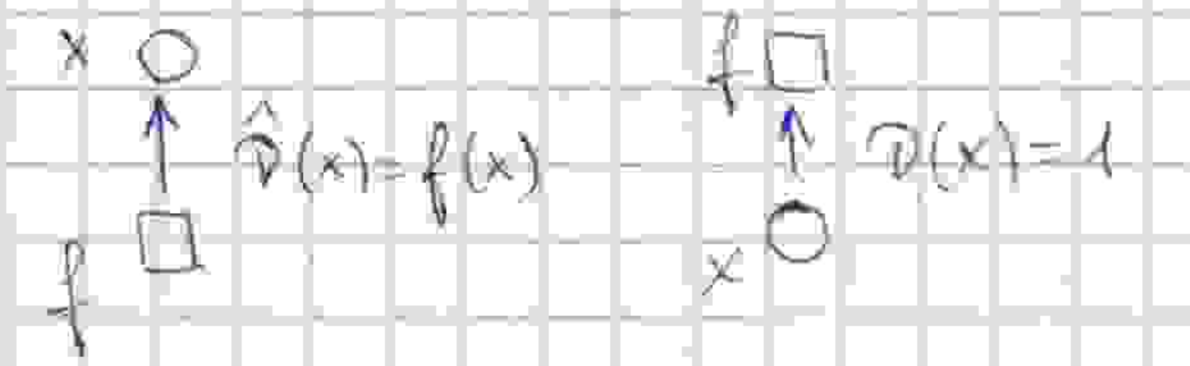
f_1 sends to its parent x_1

$$\sum_{\sim x_1} f_1(x_1, x_2, x_3)\; 1 \cdot 1$$

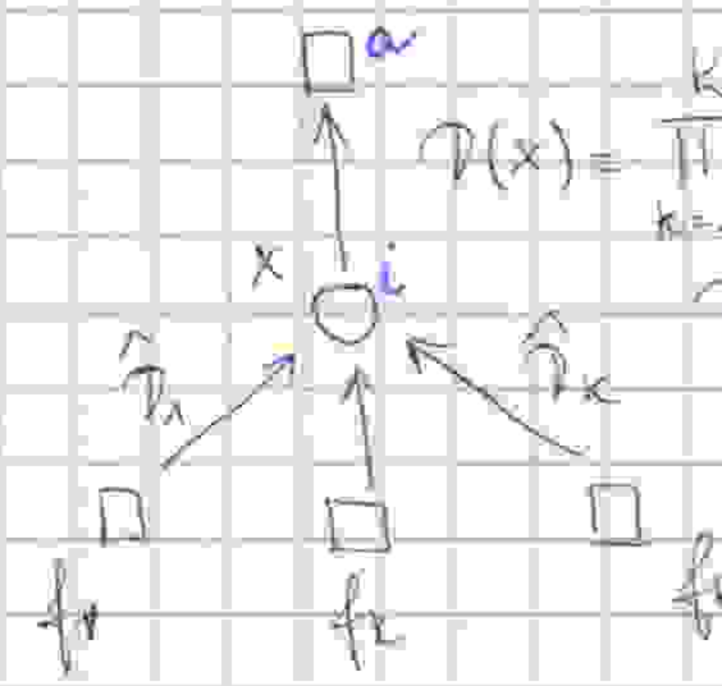
variable node x_4 forwards to its parent node f_2 the product of its incoming messages. This message is a function of x_4 given by:

$$f_3(x_4) \sum_{\sim x_4} f_4(x_4, x_5)$$

- messages $\overset{\square}{\underset{\bigcirc}{\uparrow}}\ \nu$ and $\overset{\bigcirc}{\underset{\square}{\uparrow}}\ \hat{\nu}$ are functions on $\mathcal{X}$
- marginals are denoted μ
- Initialisation at leaf nodes

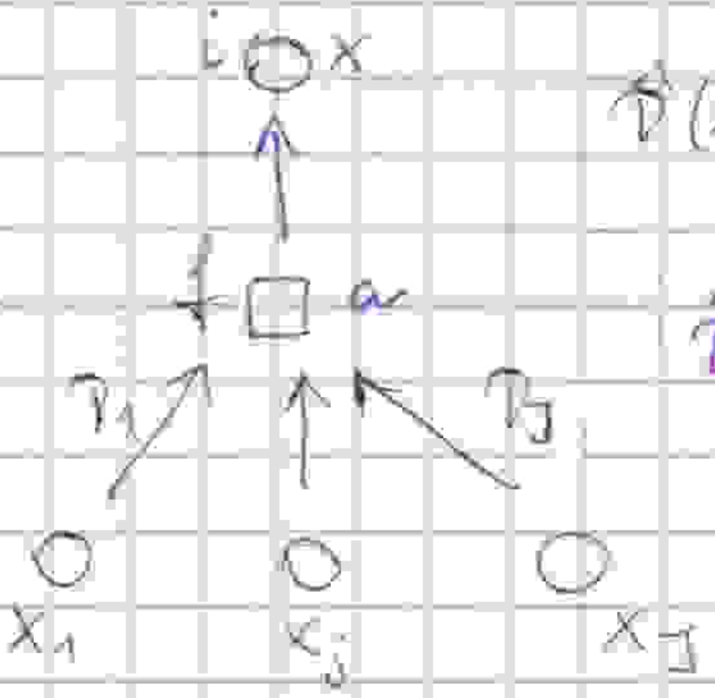


variable / function node processing (Monomer-dimer Notation)



$$\nu(x) = \prod_{k=1}^{K} \hat{\nu}_k(x)$$

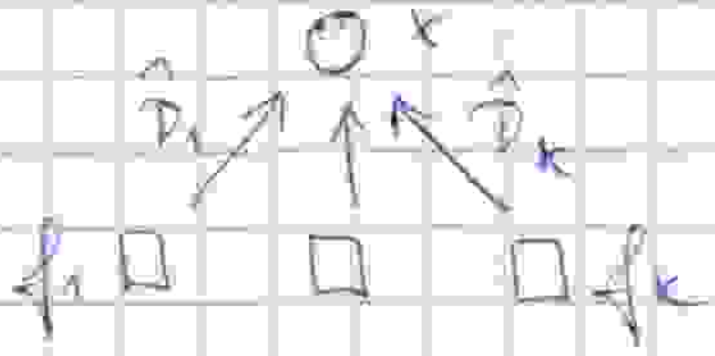
$$\nu_{i\to a}(x_i) = \prod_{b\in\partial i \setminus a} \hat{\nu}_{b\to i}(x)$$



$$\hat{\nu}(x) = \sum_{\sim x} f(x, x_1, \dots x_J) \prod_{j=1}^{J} \nu_j(x_j)$$

$$\hat{\nu}_{a\to i}(x) = \sum_{\sim x_i} f_a(x_{\partial a}) \prod_{j\in\partial a\setminus i} \nu_{j\to a}(x_j)$$

Recall:



$$\mu(x) = \prod_{k=1}^{K} \hat{\nu}_k(x)$$

Sum-product algo is exact on trees

$\oplus$ = min / max

$\otimes$ = +

$a \otimes b \oplus a \otimes c = a \otimes (b \oplus c)$

Gibbs measure of the form

$$\mu(\underline{x}) = \frac{1}{Z} \prod_a f_a(x_{\partial a})$$

→ with variables $x_i \in \mathcal{X}$, $1 \leq i \leq n$

→ kernel function f_a, $1 \leq a \leq h$

→ Z - normalization function

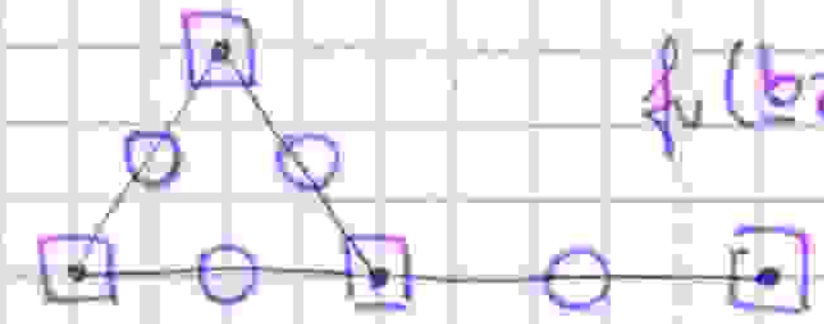
{Monomer - Dimer - Notation :

$$\mu_i(x_i) = \frac{\prod_{a\in\partial i} \hat{\nu}_{a\to i}(x_i)}{\sum_{x_i}\prod_{a\in\partial i} \hat{\nu}_{a\to i}(x_i)} \qquad x_i \in \mathcal{X}$$

$$\mu_{\partial a}(\underline{x}_{\partial a}) = \frac{f_a(\underline{x}_{\partial a})\prod_{i\in\partial a} \nu_{i\to a}(x_i)}{\sum_{\underline{x}_{\partial a}} f_a(\underline{x}_{\partial a})\prod_{i\in\partial a} \nu_{i\to a}(x_i)}$$

$$\mu_G^z(\underline{B}=\underline{b}) = \frac{z^{\sum_e b_e}}{P_G(z)} \quad \sum_{e\in\partial v} b_e \leq 1 \quad , \quad G=(V,E)$$

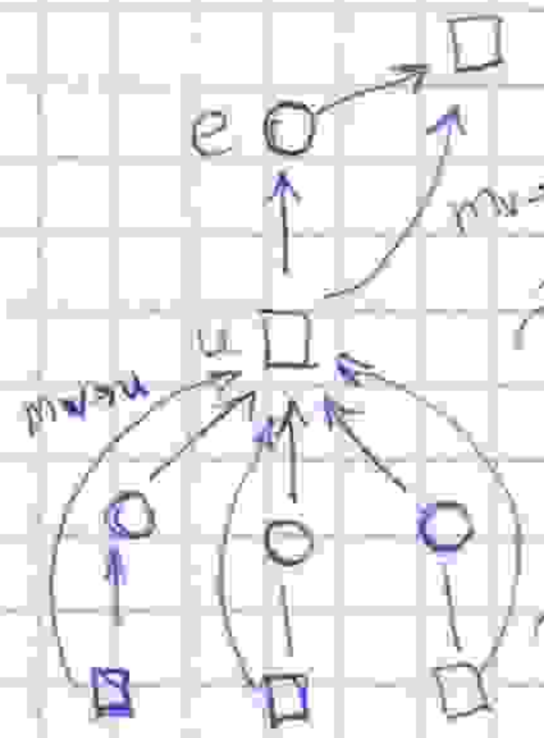
variables $(b_e,\ e\in E) \in \{0,1\}^E$



$$f_v(\underline{b}_{\partial v}) = \mathbb{1}\Big(\sum_{e\in\partial v} b_e \leq 1\Big)\sqrt{z}^{\sum_{e\in\partial v} b_e}$$

$$\boxed{\nu_{e\to v}(b_e) = \hat{\nu}_{u\to e}(b_e)}$$

$m_{u\to v}(\cdot) = \hat{\nu}_{u\to e}(\cdot)$ with $e=(u,v)$



$$\hat{\nu}_{u\to e}(b_e) = \sum_{\underline{b}',\, b'_e=b_e} \mathbb{1}\Big(\sum_{e'\in\partial u} b'_{e'} \leq 1\Big)\sqrt{z}^{\sum_{e'\in\partial u} b'_{e'}} \prod_{\substack{e'\in\partial u\\ e'\neq e}} \nu_{e'\to u}(b'_{e'})$$

$$\hat{\nu}_{u\to e}(1) = \sqrt{z}\prod_{\substack{e'\in\partial u\\ e'\neq e}} \nu_{e'\to u}(0)$$

$$\hat{\nu}_{u\to e}(0) = \prod_{\substack{e'\in\partial u\\ e'\neq e}} \nu_{e'\to u}(0) + \sqrt{z}\sum_{\substack{e'\in\partial u\\ e'\neq e}} \nu_{e'\to u}(1)\prod_{\substack{e''\in\partial u\\ e''\neq e,e'}} \nu_{e''\to u}(0)$$

$$m_{u\to v}(1) = \sqrt{z} \prod_{w' \in \partial u \setminus v} m_{w' \to u}(0)$$

$$m_{u\to v}(0) = \prod_{w' \in \partial u \setminus v} m_{w' \to u}(0) + \sqrt{z} \sum_{w \in \partial u \setminus v} m_{w\to u}(1) \prod_{\substack{w' \in \partial u \setminus v \\ w' \neq w}} m_{w' \to u}(0)$$

$$\frac{m_{u\to v}(1)}{m_{u\to v}(0)} = \frac{\sqrt{z}}{1 + \sqrt{z} \sum_{w \in \partial u \setminus v} \frac{m_{w\to u}(1)}{m_{w\to u}(0)}}$$

$$Y_{u\to v}(z) = \sqrt{z}\, \frac{m_{u\to v}(1)}{m_{u\to v}(0)}$$

$$Y_{u\to v}(z) = \frac{z}{1 + \sum_{w \in \partial u \setminus v} Y_{w\to u}(z)}$$

$$\mu_i(x_i) = \sum_{\sim x_i} \mu(x_1 \dots x_n)$$

$$\mu_{\partial a}(\underline{x}_{\partial a}) = \sum_{\sim \underline{x}_{\partial a}} \mu(x_1 \dots x_n)$$

If a factor graph is a tree

$$\mu(\underline{x}) = \frac{1}{Z} \prod_a f_a(\underline{x}_{\partial a}) = \prod_a \mu_{\partial a}(\underline{x}_{\partial a}) \prod_i (\mu_i(x_i))^{1-d_i},$$

where d_i is the degree of node i

The free energy on trees

Statistical physics

$$\mu(\underline{x}) = \frac{1}{Z(\beta)} \exp(-\beta \cdot \overset{\text{Hamiltonian}}{H}(\underline{x}))$$

$$\beta H(x) = -\sum_a \ln f_a(x_{\partial a})$$

$$\Phi(\beta) = \log Z(\beta)$$

internal energy $U(\beta) = -\frac{\partial}{\partial \beta}\left(\Phi(\beta)\right)$

canonical entropy $S(\beta) = -\beta^2 \frac{\partial}{\partial \beta}\left(\frac{\Phi_G(\beta)}{\beta}\right)$

Example

→ $U(\beta) = \langle H \rangle = \sum_{\underline{x}} \mu(\underline{x}) H(\underline{x})$

→ $S(\beta) = -\sum_{\underline{x}} \mu(\underline{x}) \log \mu(\underline{x})$

→ $\Phi(\beta) = -\beta U(\beta) + S(\beta)$

$$\log Z = \sum_a \sum_{\underline{x}_{\partial a}} \mu_a(\underline{x}_{\partial a}) \log \frac{\mu_a(\underline{x}_{\partial a})}{f_a(\underline{x}_{\partial a})} + \sum (1-d_i) \sum_{x_i} \mu_i(x_i) \ln \mu_i(x_i)$$

true on
a tree graphical
model