## In Memoriam Ralf Koetter


(10/10/1963-02/02/2009)

A Graph-Dynamics Interpretation of the Sum-Product Algorithent
Pascal O. Vontobel Information Theory Reseärch Groúp Hewlett-Packard Laboratories Palo Alto
ITA Workshop, UC San Diego, CA, Februrary 9,2009

## (p)

## Overview of Talk

- Introductory example
- Review of some basics (factor graphs / SPA / fixed points of the SPA / graph covers)
- Re-interpretation of fixed points of the SPA in terms of graph covers and valid configurations therein
- Re-interpretation of the transient part of the SPA in terms of a graph-dynamical system


# Introductory Example 

## Particles in a Box

Experiment: let us place $M$ particles in a uniformly and independently distributed manner on a very fine lattice bounded by a box.


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Which one of the above two outcomes is more likely to happen?

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## Particles in a Box

Experiment: let us place $M$ particles in a uniformly and independently distributed manner on a very fine lattice bounded by a box.


This experiment has many possible outcomes. Here are two of them:


Better question: when doing this experiment again, is the outcome more likely "to look nearly like" outcome 1 or like outcome 2 ?

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The results of the previous experiment:



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microstate $=$ Coordinates of all $M$ particles

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## Particles in a Box

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$\frac{1}{47}$| 2 | 2 | 2 | 1 | 0 | 0 | 0 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3 | 2 | 3 | 3 | 0 | 0 | 0 | 0 |
| 1 | 2 | 1 | 2 | 0 | 0 | 0 | 0 |
| 3 | 2 | 2 | 1 | 0 | 0 | 0 | 0 |
| 1 | 3 | 1 | 3 | 0 | 0 | 0 | 0 |
| 2 | 2 | 2 | 1 | 0 | 0 | 0 | 0 |

microstate $=$ Coordinates of all $M$ particles

## Particles in a Box

The results of the previous experiment:

$\frac{1}{47}$| 2 | 1 | 1 | 1 | 1 | 1 | 2 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 1 | 1 | 1 | 1 | 1 | 1 |
| 1 | 1 | 1 | 0 | 1 | 1 | 1 | 1 |
| 1 | 1 | 1 | 1 | 2 | 0 | 1 | 1 |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 0 | 1 | 0 | 2 | 1 | 1 | 0 | 1 |
| 0 |  |  | 1 |  |  |  |  |


$\frac{1}{47}$| 2 | 2 | 2 | 1 | 0 | 0 | 0 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3 | 2 | 3 | 3 | 0 | 0 | 0 | 0 |
| 1 | 2 | 1 | 2 | 0 | 0 | 0 | 0 |
| 3 | 2 | 2 | 1 | 0 | 0 | 0 | 0 |
| 1 | 3 | 1 | 3 | 0 | 0 | 0 | 0 |
| 2 | 2 | 2 | 1 | 0 | 0 | 0 | 0 |
| 2 |  |  |  |  |  |  |  |

$$
\begin{aligned}
\text { microstate } & =\text { Coordinates of all } M \text { particles } \\
\text { macrostate } & =\text { "Summary" of a microstate }
\end{aligned}
$$

## Particles in a Box


microstate
$\varphi \downarrow$
macrostate

## Particles in a Box



Note: $\varphi$ is usually a many-to-one mapping.

## Particles in a Box


microstate
macrostate

If $P($ microstate $)=$ const. for all microstates then
$P($ macrostate $) \propto \#\{$ microstate $: \varphi($ microstate $)=$ macrostate $\}$

$$
=\# \varphi^{-1} \text { (macrostate) }
$$

## Particles in a Box


microstate
$\varphi \downarrow$
macrostate

Here: $\# \varphi^{-1}$ (macrostate 1) $\gg \varphi^{-1}$ (macrostate 2)

## Particles in a Box


microstate
$\varphi \downarrow$
macrostate

Here: $\# \varphi^{-1}$ (macrostate 1) $\gg \# \varphi^{-1}$ (macrostate 2)

$$
\Rightarrow P(\text { macrostate } 1) \gg P(\text { macrostate } 2)
$$

Particles in a Box with Gradient Field

## Particles in a Box with Gradient Field



Particles in a Box with Gradient Field


## Particles in a Box with Gradient Field

$\left.\frac{1}{47} \begin{array}{|c|c|c|c|c|c:c|c|}\hline 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ \hdashline 0 & 1 & 0 & 0 & 1 & 1 & 0 & 1 \\ \hdashline 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ \hdashline 1 & 2 & 2 & 1 & 1 & 1 & 1 & 1 \\ \hdashline 2 & 1 & 1 & 2 & 2 & 1 & 1 & 1 \\ \hdashline 1 & 2 & 3 & 2 & 1 & 1 & 3 & 1 \\ \hline\end{array}\right] \Downarrow g$

## Particles in a Box with Gradient Field



If $P($ microstate $) \propto \exp (-M \cdot E(\varphi($ microstate $)))$

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- $\#\{$ microstate $: ~ \varphi($ microstate $)=$ macrostate $\}$


## Particles in a Box with Gradient Field



If $P($ microstate $) \propto \exp (-M \cdot E(\varphi($ microstate $)))$ then $P($ macrostate $) \propto \exp (-M \cdot E($ macrostate $))$

- \#\{microstate : $\varphi($ microstate $)=$ macrostate $\}$
$=\exp (-M \cdot E($ macrostate $)) \cdot \# \varphi^{-1}($ macrostate $)$


## Particles in a Box with Gradient Field

$\frac{1}{47}$| 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0 | 1 | 0 | 0 | 1 | 1 | 0 | 1 |
| 1 | 0 | 1 | 0 | 1 | 1 | 0 | 1 |
| 1 | 2 | 2 | 1 | 1 | 1 | 1 | 1 |
| 2 | 1 | 1 | 2 | 2 | 1 | 1 | 1 |
| 1 | 2 | 3 | 2 | 1 | 1 | 3 | 1 |

## Particles in a Box with Gradient Field



Let

$$
H_{M}(\text { macrostate }) \triangleq \frac{1}{M} \log \left(\# \varphi^{-1}(\text { macrostate })\right)
$$

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$\Rightarrow P($ macrostate $) \propto \exp (-M \cdot E($ macrostate $)) \cdot \# \varphi^{-1}($ macrostate $)$

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Let

$$
H_{M}(\text { macrostate }) \triangleq \frac{1}{M} \log \left(\# \varphi^{-1}(\text { macrostate })\right)
$$

$\Rightarrow P($ macrostate $) \propto \exp (-M \cdot E($ macrostate $)) \cdot \# \varphi^{-1}($ macrostate $)$

$$
=\exp \left(M \cdot\left(-E(\text { macrostate })+H_{M}(\text { macrostate })\right)\right)
$$

## Static vs. Dynamic Setup

Static setup:

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$$
P(\mathrm{M}) \propto \exp (-M \cdot E(\mathrm{M})) \cdot \# \varphi^{-1}(\mathrm{M})
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Dynamic setup:

$$
\begin{aligned}
& P(\mathrm{M}(t+\Delta t) \mid \mathrm{m}(t)) \\
& \quad \propto \exp (-M \cdot E(\mathrm{M}(t+\Delta t) \mid \mathrm{m}(t))) \cdot \# \varphi^{-1}(\mathrm{M}(t+\Delta t) \mid \mathrm{m}(t))
\end{aligned}
$$

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"Better" dynamic setup:

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## Static vs. Dynamic Setup

Static setup: will model fix points of the SPA

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\end{aligned}
$$

"Better" dynamic setup: will model the transient part of the SPA

$$
\begin{aligned}
& P(\mathrm{M}(t+\Delta t) \mid \mathrm{M}(t)) \\
& \quad \propto \exp (-M \cdot E(\mathrm{M}(t+\Delta t) \mid \mathrm{M}(t))) \cdot \# \varphi^{-1}(\mathrm{M}(t+\Delta t) \mid \mathrm{M}(t))
\end{aligned}
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Forney-style Factor Graphs (FFGs)
$\left[\right.$ Labs $\left.^{\text {hp }}\right]$

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- Normal (factor) graphs were defined in [Forney:01].


## Forney-style Factor Graphs (FFGs)



- Factor graphs were defined in [Kschischang:Frey:Loeliger:01].
- Normal (factor) graphs were defined in [Forney:01].
$\Rightarrow$ We will call them Forney-style Factor graphs (FFGs).


## Forney-style Factor Graphs (FFGs)



The above FFG has

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- the local functions $f_{\mathrm{A}}, f_{\mathrm{B}}$, and $f_{\mathrm{C}}$,


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## Forney-style Factor Graphs (FFGs)



The above FFG has

- the local functions $f_{\mathrm{A}}, f_{\mathrm{B}}$, and $f_{\mathrm{C}}$,
- the edges corresponding to the variables $X$ and $Z$,
- the half edges corresponding to the variables $U, W$, and $Y$,
- and finally the global function $f_{\mathrm{A}}(u, w, x) \cdot f_{\mathrm{B}}(x, y, z) \cdot f_{\mathrm{C}}(z)$.


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## Forney-style Factor Graphs (FFGs)



- A configuration is a particular assignment of values to all variables.
- The configuration space $\Omega$ is the set of all configurations.
- A configuration $\boldsymbol{\omega} \in \Omega$ is called valid if $f(\boldsymbol{\omega}) \neq 0$.
- System variable: $X: \Omega \rightarrow A_{X}: \boldsymbol{\omega} \mapsto x=X(\boldsymbol{\omega})$.


## The Sum-Product Algorithm (SPA)

## SPA: Update Rule



$$
\begin{aligned}
& \mu_{f_{4} \rightarrow f_{5}}\left(x_{5}\right) \\
& \quad=\frac{1}{Z_{f_{4} \rightarrow f_{5}}} \sum_{x_{1}} \sum_{x_{2}} \sum_{x_{3}} f_{4}\left(x_{1}, x_{2}, x_{3}, x_{5}\right) \cdot \mu_{f_{1} \rightarrow f_{4}}\left(x_{1}\right) \cdot \mu_{f_{2} \rightarrow f_{4}}\left(x_{2}\right) \cdot \mu_{f_{3} \rightarrow f_{4}}\left(x_{3}\right)
\end{aligned}
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\end{aligned}
$$

Note: $\frac{1}{Z_{f_{4} \rightarrow f_{5}}}$ is suitably chosen depending on the setup.

## SPA: Computing Marginals



$$
\begin{aligned}
& \eta_{f_{4}}\left(x_{1}, x_{2}, x_{3}, x_{5}\right) \\
& \quad=\frac{1}{Z_{f_{4}}} f_{4}\left(x_{1}, x_{2}, x_{3}, x_{5}\right) \cdot \mu_{f_{1} \rightarrow f_{4}}\left(x_{1}\right) \cdot \mu_{f_{2} \rightarrow f_{4}}\left(x_{2}\right) \cdot \mu_{f_{3} \rightarrow f_{4}}\left(x_{3}\right) \cdot \mu_{f_{5} \rightarrow f_{4}}\left(x_{5}\right)
\end{aligned}
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$$

Note: $\frac{1}{Z_{f_{4}}}$ is suitably chosen depending on the setup.

## Fixed Points of the SPA

Theorem (Yedidia/Freeman/Weiss, 2000)
Fixed points of the SPA correspond to stationary points of the Variational Bethe free energy (VBFE).

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- If it is an approximation, how is it possible that we obtain an exact result like in the above theorem?


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Note that the VBFE is an approximation of the Var. Gibbs free energy:

- If it is an approximation, how is it possible that we obtain an exact result like in the above theorem?
- What is the meaning of the VBFE?


## Graph Covers and

## Counting Valid Configurations Therein

## Graph Covers


original graph

(a possible)
double cover of the original graph

.. -

## Graph Covers


original graph

(possible)
$M$-fold cover of original graph

An $M$-fold cover is also called a cover of degree $M$. Do not confuse this degree with the degree of a vertex!
Note: there are many possible $M$-fold covers of a graph.

## Graph Covers


$\left(\right.$ LABS $\left.^{\text {hp }}\right)$

## Graph Covers



Note: the above graph has $2!\cdot 2!\cdot 2!\cdot 2!\cdot 2!=32$ double covers.

## Graph Covers



Note: the above graph has $2!\cdot 2!\cdot 2!\cdot 2!\cdot 2!=32$ double covers.
In general: $\# \widetilde{\mathcal{G}}_{M}=\#(M$-covers of G$)=(M!)^{\# \operatorname{Edges}(\mathrm{G})}$.

## Graph Covers <br> and Valid Configurations Therein



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The components of the pseudo-codeword

$$
\omega=\left(\omega_{1}, \ldots, \omega_{n}\right)
$$

associated to $\tilde{\mathrm{x}}$ are given by

$$
\omega_{i} \triangleq \frac{1}{M} \sum_{m \in[M]} \tilde{x}_{i, m}
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$$

$$
\begin{aligned}
& \omega_{1}=\frac{2}{2}\left\{\begin{array}{l}
\frac{y_{1}}{y_{1}} \boldsymbol{\square} \begin{array}{l}
\tilde{X}_{1,1}=1 \\
\tilde{X}_{1,2}=1 \\
\text { 目 }
\end{array} \\
\hline
\end{array}\right. \\
& \omega_{2}=\frac{1}{2}\left\{\begin{array}{l}
y_{2}-\begin{array}{l}
\tilde{X}_{2,1}=0 \\
y_{2} \\
\tilde{X}_{2,2}=1
\end{array} \\
\hline
\end{array}\right. \\
& \begin{array}{l}
\omega_{3}=\frac{1}{2}\left\{\begin{array}{l}
\frac{y_{3}}{y_{3}} \square_{\tilde{X}_{3,2}=1}^{\tilde{X}_{3,2}=1} \\
\omega_{4}=\frac{0}{2}\left\{\begin{array}{l}
y_{4} \square \tilde{X}_{4,1}=0 \\
y_{4} \square
\end{array}\right. \\
\tilde{X}_{4,2}=0
\end{array}\right.
\end{array}
\end{aligned}
$$

## Graph Covers and Valid Configurations Therein

Using the language of the first part of this talk, let us consider the following setup.

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(Finally, we are mostly interested in the limit $M \rightarrow \infty$.)


## Graph Covers and Valid Configurations Therein

Using the language of the first part of this talk, let us consider the following setup.

- Fix some positive integer $M$.
(Finally, we are mostly interested in the limit $M \rightarrow \infty$.)
- Set of microstates $\triangleq$ set of microstates ${ }_{M}$

$$
\triangleq\left((\widetilde{\mathrm{G}}, \widetilde{\mathbf{x}}) \mid \widetilde{\mathrm{G}} \in \widetilde{\mathcal{G}}_{M}, \widetilde{\mathbf{x}} \text { is a valid configuration in } \widetilde{\mathcal{G}}_{M}\right)
$$

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$$

- Mapping $\varphi_{M}$

$$
\operatorname{maps}(\widetilde{G}, \widetilde{\mathrm{x}}) \text { to } \omega(\widetilde{\mathrm{x}})
$$

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Using the language of the first part of this talk, let us consider the following setup.

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$$

- Mapping $\varphi_{M}$

$$
\operatorname{maps}(\widetilde{G}, \widetilde{\mathrm{x}}) \text { to } \omega(\widetilde{\mathrm{x}})
$$

- Set of macrostates $\triangleq$ set of macrostates $M_{M}$

$$
\triangleq \varphi_{M}(\text { set of microstates })
$$

## Graph Covers

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# Graph Covers <br> and Valid Configurations Therein 

- Note:
$\#($ set of macrostates $)=\operatorname{poly}(M)$


## Graph Covers <br> and Valid Configurations Therein

- Note:

$$
\#(\text { set of macrostates })=\operatorname{poly}(M)
$$

- Note:

$$
\operatorname{closure}\left(\lim _{M \rightarrow \infty}(\text { set of macrostates })\right)=\text { fundamental polytope }
$$

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Re-interpretation in terms of graph covers:
Let

$$
P(\text { microstate }) \triangleq \exp \left(-M \cdot\left\langle\boldsymbol{\varphi}_{M}(\text { microstate }), \boldsymbol{\lambda}\right\rangle\right)
$$

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Let

$$
P(\text { microstate }) \triangleq \exp \left(-M \cdot\left\langle\boldsymbol{\varphi}_{M}(\text { microstate }), \boldsymbol{\lambda}\right\rangle\right)
$$

Then

$$
\begin{aligned}
P(\text { macrostate })= & \exp (-M \cdot\langle\text { macrostate }, \boldsymbol{\lambda}\rangle) \\
& \cdot \# \varphi^{-1}(\text { macrostate })
\end{aligned}
$$

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## Re-interpretation in terms of graph covers:

A fixed point of the SPA corresponds to a macrostate $\omega$, i.e., a pseudo-codeword $\omega$, that is a stationary point of

$$
P(\boldsymbol{\omega}) \propto \exp (-M \cdot\langle\boldsymbol{\omega}, \boldsymbol{\lambda}\rangle) \cdot \# \varphi^{-1}(\boldsymbol{\omega})
$$

when $M$ goes to infinity.

## Fixed Points of the SPA

Theorem (Yedidia/Freeman/Weiss, 2000)
Fixed points of the SPA correspond to local minima of the Variational Bethe free energy (VBFE).

Re-interpretation in terms of graph covers:
A fixed point of the SPA corresponds to a macrostate $\omega$, i.e., a pseudo-codeword $\omega$, that is a local maximimum of

$$
P(\boldsymbol{\omega}) \propto \exp (-M \cdot\langle\boldsymbol{\omega}, \boldsymbol{\lambda}\rangle) \cdot \# \varphi^{-1}(\boldsymbol{\omega})
$$

when $M$ goes to infinity.

## Justifying this Result (Ingredient 1)

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Theorem: For any macrostate $\omega$, i.e., pseudocodeword $\omega$,

$$
\lim _{M \rightarrow \infty} \frac{1}{M} \log \frac{\# \boldsymbol{\varphi}_{M}^{-1}(\boldsymbol{\omega})}{\# \widetilde{\mathcal{G}}_{M}}=H_{\text {Bethe }}(\omega)
$$

## Justifying this Result (Ingredient 1)

Theorem: For any macrostate $\omega$, i.e., pseudocodeword $\boldsymbol{\omega}$,

$$
\lim _{M \rightarrow \infty} \frac{1}{M} \log \frac{\# \boldsymbol{\varphi}_{M}^{-1}(\boldsymbol{\omega})}{\# \widetilde{\mathcal{G}}_{M}}=H_{\text {Bethe }}(\omega)
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- Similarly to the computation of the asymptotic growth rate of average Hamming spectra one has to be somewhat careful in formulating the above limit; we leave out the details.


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- Similarly to the computation of the asymptotic growth rate of average Hamming spectra one has to be somewhat careful in formulating the above limit; we leave out the details.
- Note: The ratio

$$
\frac{\# \varphi_{M}^{-1}(\omega)}{\# \widetilde{\mathcal{G}}_{M}}
$$

represents the average number of valid configurations $\tilde{\mathrm{x}}$ per $M$-fold cover with associated pseudo-codeword $\omega$. Therefore, $H_{\text {Bethe }}(\omega)$ gives the asymptotic growth rate of that quantity.

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- [Fogal/McEliece/Thorpe, 2005],
- papers by Divsalar, Ryan, et al. (2005-).
- To the best of our knowledge, the above interpretation of the Bethe entropy cannot be found in the literature (besides the talk that we gave at the 2008 Allerton Conference.)


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\end{aligned}
$$

with

$$
\begin{aligned}
& -U_{\text {Bethe }}(\boldsymbol{\omega})=\langle\boldsymbol{\omega}, \boldsymbol{\lambda}\rangle \\
& +H_{\text {Bethe }}(\boldsymbol{\omega})=\lim _{M \rightarrow \infty}\left(\frac{1}{M} \log \# \boldsymbol{\varphi}_{M}^{-1}(\boldsymbol{\omega})-\frac{1}{M} \log \# \widetilde{\mathcal{G}}_{M}\right)
\end{aligned}
$$

## The Transient Part of the SPA

## Graph-Dynamical Systems

We want to show that the transient part of the SPA can be expressed in terms of a graph-dynamical system.

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Graph-dynamical system (e.g., [Prisner:95]):

- Let $\Gamma$ be a set of graphs.
- Let $\Psi$ be some (possibly random) mapping from $\Gamma$ to $\Gamma$.
- Because the domain and the range of $\Psi$ are equal, it makes sense to study the repeated application of the mapping $\Psi$ :

$$
\Gamma \xrightarrow{\Psi} \Gamma \quad \xrightarrow{\Psi} \quad \cdots \quad \xrightarrow{\Psi} \quad \Gamma
$$

## Review

(of the setup used in the re-interpretation of f.p.s of the SPA)

- Set of microstates

$$
\triangleq\left((\widetilde{\mathrm{G}}, \widetilde{\mathbf{x}}) \mid \widetilde{\mathrm{G}} \in \widetilde{\mathcal{G}}_{M}, \widetilde{\mathbf{x}} \text { is a valid configuration in } \widetilde{\mathcal{G}}_{M}\right)
$$

- Mapping $\varphi_{M}$

$$
\text { maps }(\widetilde{G}, \widetilde{\mathrm{x}}) \text { to } \omega(\widetilde{\mathrm{x}})
$$

- Set of macrostates

$$
\triangleq \varphi_{M}(\text { set of microstates })
$$

# Corresponding Setup for the <br> Transient Part of the SPA 

- Set of microstates
???
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???
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# Corresponding Setup for the Transient Part of the SPA 

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Note: $\Gamma=$ set of $M$-covers of $G$ and valid configurations therein is obviously not sufficient.


## Corresponding Setup for the Transient Part of the SPA

- Set of microstates
$\Rightarrow \Gamma=$ set of what we call colored hypergraph $M$-cover
or colored twisted $M$-cover
- Mapping $\varphi_{M}$
- Set of macrostates


## Corresponding Setup for the Transient Part of the SPA

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or colored twisted $M$-cover
- Mapping $\varphi_{M}$
???
- Set of macrostates
set of all possible marginals on the LHS function nodes
$\times$ set of all possible marginals on the RHS function nodes


## Comment on Microstates



## Comment on Microstates



## Comment on Microstates



## Comment on Macrostates



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$\boldsymbol{\eta}_{\text {left }}(0)$
$\eta_{\text {right }}(-.5)$$\rightarrow\left[\begin{array}{c}\boldsymbol{\eta}_{\text {left }}(0) \\ \boldsymbol{\eta}_{\text {right }}(0.5)\end{array} \rightarrow \begin{array}{c}\boldsymbol{\eta}_{\text {left }}(1) \\ \boldsymbol{\eta}_{\text {right }}(0.5)\end{array} \rightarrow \begin{array}{c}\begin{array}{c}\boldsymbol{\eta}_{\text {left }}(1) \\ \boldsymbol{\eta}_{\text {right }}(1.5)\end{array}\end{array} \rightarrow \begin{array}{|}\begin{array}{c}\boldsymbol{\eta}_{\text {left }}(2) \\ \boldsymbol{\eta}_{\text {right }}(1.5)\end{array}\end{array}\right.$.

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Cf. "Message-free version of belief-propagation" in [Wainwright/Jaakkola/Willsky, 2003].

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- Talked about microstates, macrostates, and their uses.
- Given a re-interpretation of fixed points of the SPA in terms of graph covers and valid configurations therein.
- Touched upon a re-interpretation of the transient part of the SPA in terms of a graph-dynamical system.


## Thank you!

