Stat 375: Inference in Graphical Models
Lectures 1-2

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Stanford University

April 2, 2012

Logistics

Mon-Wed 9:30AM-10:45PM, Green Earth Sciences 131

Andrea Montanari (montanari)

http://www.stanford.edu/ montanar/TEACHING/Stat375/stat375.html

Homework due on Mon (starting 4/9/2012).
Take-home final.

Topics

- Probability distributions that are 'local' wrt a graph
- Random variables sit on vertices.
- Strongly dependent if they are nearby.
- *Images, philogenies, error-correcting codes, Bayes networks...*

Topics

Emphasis on computational and mathematical aspects.

Topics

- Equivalent graphical representations.
- Polynomial reductions between various probabilistic inference tasks. Computational hardness.
- Models on trees. Belief propagation.
- Variational inference: naive mean field, Bethe free energy, generalized BP and convex relaxations.
- Gaussian graphical models.
- Learning graphical model form data.
- Correlation decay. The Markov Chain Monte Carlo method.
- Applications to clustering and classification.

Why you should not take this class

- Emphasis on fundamental challenges.
- There is no textbook.
- We'll use the P-word.

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Let us start: Families of graphical models

General theme

Probability distribution over $x = (x_1, x_2, \dots, x_n)$

$$\mu(x_1, x_2, \dots, x_n)$$

Family # 1: Undirected Pairwise Graphical Models

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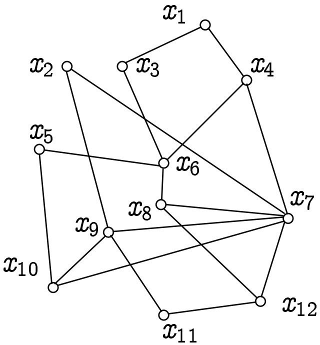
(aka Markov Random Fields)



$G = (V, E)$, $V = [n]$, $x = (x_1, \dots, x_n)$, $x_i \in \mathcal{X}$

$$\mu(x) = \frac{1}{Z} \prod_{(ij) \in E} \psi_{ij}(x_i, x_j) \, .$$

Undirected Pairwise Graphical Models

Specified by

- Graph $G = (V, E)$.
- Alphabet $\mathcal{X}$.
- Compatibility functions $\psi_{ij} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_+$, $(i, j) \in E$.

Alphabet

Typically $|\mathcal{X}| < \infty$.

Occasionally $\mathcal{X} = \mathbb{R}$ and

$$\mu(\mathrm{d}x) = \frac{1}{Z} \prod_{(ij)\in E} \psi_{ij}(x_i, x_j)\, \mathrm{d}x$$

(all formulae interpreted as densities)

Key challenge: $n \gg 1$ (space dimension).

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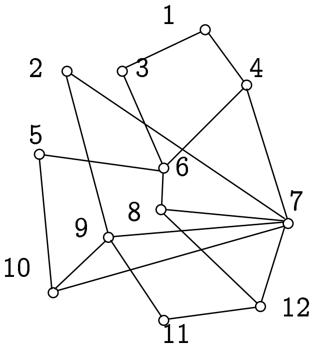
Key challenge: $n \gg 1$ (space dimension).

Partition function

$$Z \equiv \sum_{x \in \mathcal{X}^V} \prod_{(ij) \in E} \psi_{ij}(x_i, x_j)$$

[Plays a crucial role!]

Notations



$$\partial i \equiv \{\text{neighbors of vertex } i\}, \qquad \deg(i) = |\partial i|,$$
$$\partial 9 = \{10, 2, 11\}, \qquad \deg(9) = 3,$$

$$x_U \equiv (x_i)_{i \in U},$$
$$x_{\{1,7,10\}} = (x_1, x_7, x_{10}).$$

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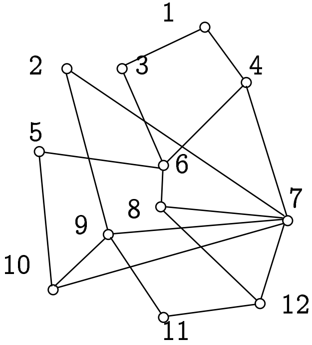

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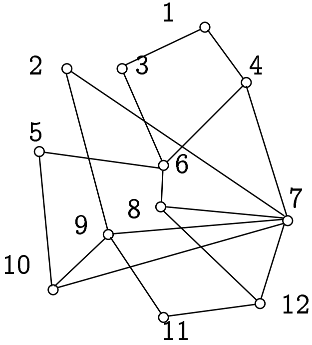

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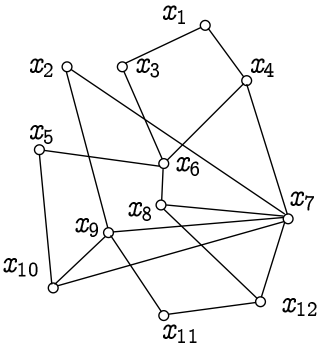
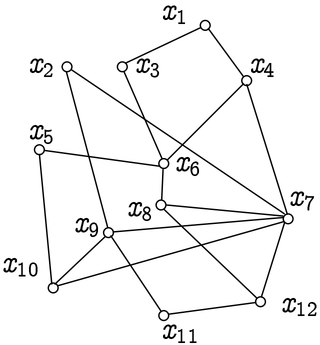
Example: Ising models



$G = (V, E)$, $V = [n]$, $x = (x_1, \dots, x_n)$, $x_i \in \{+1, -1\}$

$$\mu(x) = \frac{1}{Z} \prod_{(ij) \in E} \psi_{ij}(x_i, x_j) \, .$$

Example: Ising models



$G = (V, E)$, $V = [n]$, $x = (x_1, \dots, x_n)$, $x_i \in \{+1, -1\}$

$$\mu(x) = \frac{1}{Z} \, \exp\Big\{ \sum_{(i,j)\in E} \theta_{ij} x_i x_j \, + \sum_{i \in V} \theta_i x_i \Big\} \, .$$

A motivation: Boltzmann Machines

Can we train a computer to do handwriting?

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MNIST dataset: $60,000$ handwritted digits (28×28 pixels)

Can we learn $\mu(x_I)$, $x_I \in \{+1,-1\}^I$, $I = [28] \times [28]$ that generates samples as above?

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An attempt

(R. Salakhutdinov, G. Hinton, AISTATS 2009)

What's the magic?

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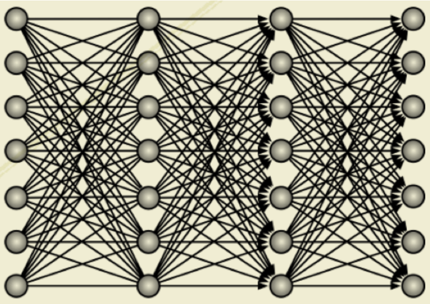
Hidden variables



Image

$$\mu(x_I) = \sum_{x_{H(1)},x_{H(2)},x_{H(3)}} \mu_{G,\theta}(x_I, x_{H(1)}, x_{H(2)}, x_{H(3)})$$

$\mu_{G,\theta}(\cdot)$ Ising model on $G = (V, E)$

$$V = (I, H(1), H(2), H(3))$$

What's the magic?

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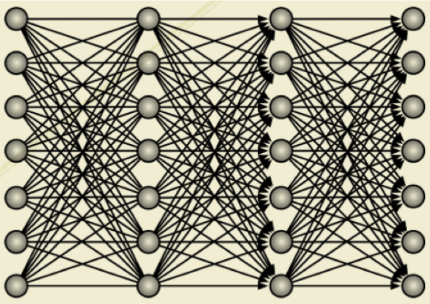

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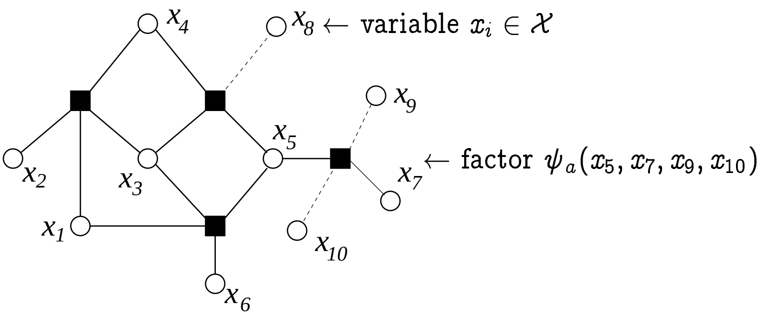

$G = (V, F, E)$, $V = [n]$, $x = (x_1, \ldots, x_n)$, $x_i \in \mathcal{X}$

$$\mu(x) = \frac{1}{Z} \prod_{a \in F} \psi_a(x_{\partial a}) .$$

Factor graph models

Terminology

- Variable nodes: $i, j, k, \cdots \in V$.
- Function nodes: $a, b, c \cdots \in F$.

Specified by

- Factor graph $G = (V, F, E)$.
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Factor graphs are as powerful as pairwise models

A pairwise model on $G = (V, E)$ with alphabet $\mathcal{X}$ can be represented by a factor graph model on $G' = (V', F', E')$ with $V' = V$, $F' \simeq E$, $|E'| = 2|E|$, $\mathcal{X}' = \mathcal{X}$.

- Put a factor node on each edge.

A factor model on $G = (V, F, E)$ with alphabet $\mathcal{X}$ can be represented by a pairwise model on $G' = (V', F')$ with $V' = V \cup F$, $E' = E$, $\mathcal{X}' = \mathcal{X}^{\Delta}$, $\Delta \equiv \max_{a \in F} \deg(a)$.

- Represent at a factor node the state of its neighbors,

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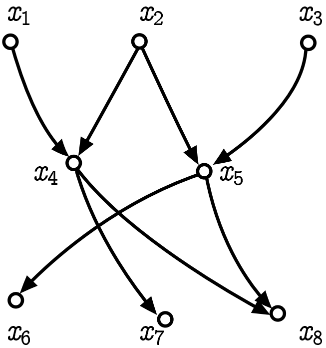

$G = (V, D)$, directed $V = [n]$, $x = (x_1, \dots, x_n)$, $x_i \in \mathcal{X}$
$D = \{$ directed edges $\}$

$$\mu(x) \;=\; \prod_{i \in V} \mu_i(x_i | x_{\pi(i)}) \,, \qquad\qquad \pi(i) = \{ \text{ parents of } i \ \} \,.$$

Bayesian Networks

Specified by

- Directed acyclic graph $G = (V, D)$, $\quad ((i,j) \neq (j,i))$.
- Alphabet $\mathcal{X}$.
- Conditional probability tables $\mu_i(\,\cdot\,|\,\cdot\,) : \mathcal{X} \times \mathcal{X}^{\pi(i)} \to \mathbb{R}_+$, $i \in F$:

$$\sum_{x_i \in \mathcal{X}} \mu_i(x_i|x_{\pi(i)}) = 1 \quad \text{for all } x_{\pi(i)} \in \mathcal{X}^{\pi(i)}\,.$$

Bayes networks are as powerful as factor graphs

A Bayes network $G = (V, D)$ with alphabet $\mathcal{X}$ can be represented by a factor graph model on $G' = (V', F', E')$ with $V' = V$, $|F'| = |V|$, $|E'| = |D| + |V|$, $\mathcal{X}' = \mathcal{X}$.

- Represent by a factor node each CPT.

A factor model on $G = (V, F, E)$ with alphabet $\mathcal{X}$ can be represented by a Bayes network $G' = (V', D')$ with $V' = V$ and $\mathcal{X}' = \mathcal{X}$.

- Choose a total ordering of $V' = V$ and write μ in terms of conditional probabilities.

In general the resulting Bayes network is dense.

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In general the resulting Bayes network is dense.

Bayes networks with observed variables

$$\begin{aligned} V &= H \cup O\,, \\ x &= (x_i)_{i\in H} = (x_1,\dots,x_n) = (\text{ Hidden Variables })\,, \\ y &= (y_i)_{i\in O} = (y_1,\dots,y_m) = (\text{ Observed Variables }) \end{aligned}$$

$$\mu(x,y) = \prod_{i\in H} \mu(x_i | x_{\pi(i)\cap H}, y_{\pi(i)\cap O}) \prod_{i\in O} \mu(y_i | x_{\pi(i)\cap H}, y_{\pi(i)\cap O})$$

Of interest $\mu_y(x) = \mu(x|y)$

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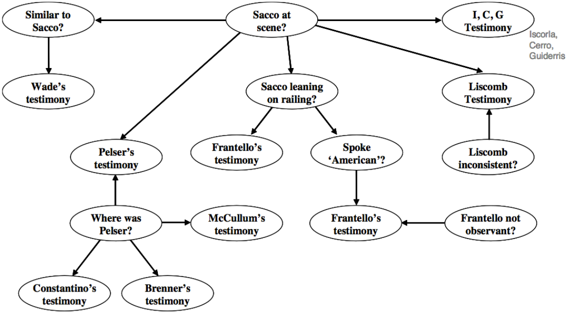
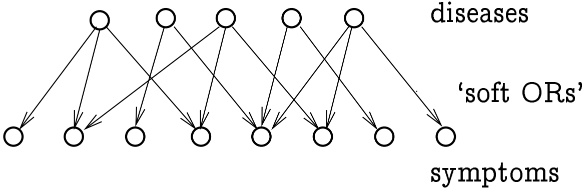
Example 1: Forensic science



[Kadane, Shum, *A probabilistic analysis of the Sacco and Vanzetti evidence*, 1996]
[Taroni et al., *Bayesian Networks and Probabilistic Inference in Forensic Science*, 2006]

Example 2: Diagnostic network



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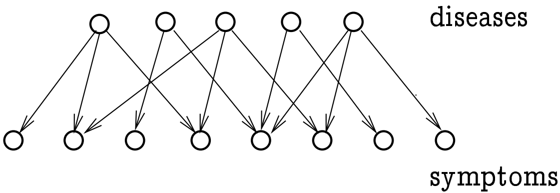
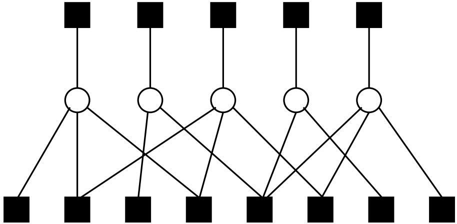
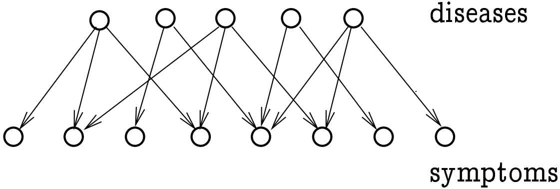
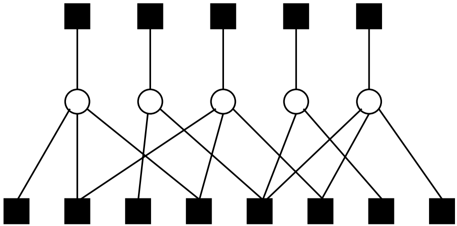




Bayes networks are as powerful as factor graphs

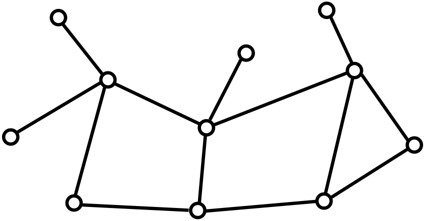




With observed variables graph remains unchanged

Markov property

Global Markov Property



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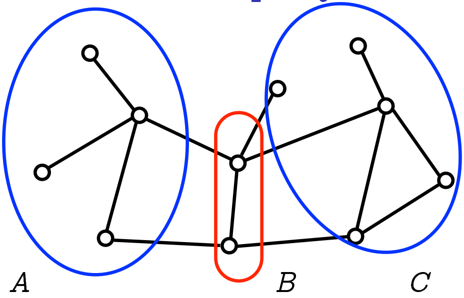
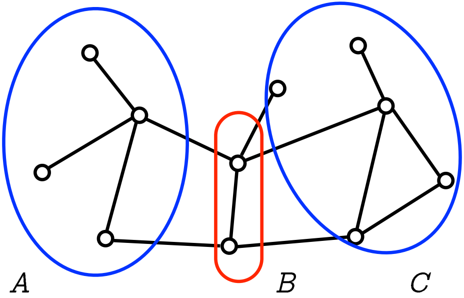


Definition

Let $A \cup B \cup C$ be a partition of V. We say that B separates A from C if any path starting in A and terminating in C has at least one node in B.

Global Markov Property



Definition

The probability distribution μ over $\mathcal{X}^V$ satisfies the global Markov property on G if for any partition $V = A \cup B \cup C$ such that B separates A from C,

$$\mu(x_A, x_C | x_B) = \mu(x_A | x_B)\, \mu(x_C | x_B)$$

The most general

Theorem (Hammersley, Clifford, 1971)

Let $\mu(\,\cdot\,)$ be a probability distribution on $\mathcal{X}^V$, and $G = (V, E)$ be a graph such that

- *μ is Markov with respect to G.*
- *$\mu(x) > 0$ for all $x \in \mathcal{X}^V$.*
- *G does not contain triangles.*

Then μ is a pairwise graphical model on G.

Proof sketch (Grimmett, Bull. London Math. Soc. 1973)

For every $S \subseteq V$, define

$$\widetilde{\psi}_S(x_S) \equiv \prod_{U \subseteq S} \mu(x_U, 0_{V \setminus U})^{(-1)^{|S \setminus U|}}$$

Example: For $S = \{i, j\}$ (not necessarily edge) let $\mu_{ij,+}(\,\cdot\,) \equiv \mu(\,\cdot\,, 0_{V \setminus \{i,j\}})$

$$\widetilde{\psi}_{ij}(x_i, x_j) = \mu_{ij,+}(x_i, x_j)\, \mu_{ij,+}(x_i, 0)^{-1} \mu_{ij,+}(0, x_j)^{-1}\, \mu_{ij,+}(0, 0)\,.$$

Exercise: If $V = \{i, j\} \ldots$

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Exercise: If $V = \{i, j\}$...

Proof sketch (Grimmett, 1973)

- **Claim 1:** $\mu(x) = \mu(0_V) \prod_{S\subseteq V} \widetilde{\psi}_S(x_S)$

- **Claim 2:** For $S \neq \{i,j\} \in E$, $\{i\}$, $\widetilde{\psi}_S(x_S)$ =const.

Given μ, can construct G!

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Given μ, can construct G!

Useful facts

Fact

$$\sum_{K\subseteq W} (-1)^{|K|} = \mathbb{I}(W = \emptyset)\,.$$

(Sum includes the empty set.)

Fact

If f is a set function, $W' \subseteq W$ proper subset, then

$$\sum_{K\subseteq W} (-1)^{|K|} f(K\cap W') = 0\,.$$

(Sum includes the empty set.)

If G contains triangles

$$\mu(x) = \frac{1}{Z} \prod_{\mathcal{C} \in \text{cliques}(G)} \psi_{\mathcal{C}}(x_{\mathcal{C}})\,.$$

Footnote #1

Definition (Global Markov)

For any partition $V = A \cup B \cup C$ such that B separates A from C,

$$\mu(x_A, x_C | x_B) = \mu(x_A | x_B) \, \mu(x_C | x_B)$$

Local Markov: Required only for $A = \{i\}$, $B = \partial i$, $C = V \setminus \{i\} \cup \partial i$.

Pairwise Markov: Required only for $A = \{i\}$, $B = V \setminus \{i, j\}$, $C = \{j\}$.

They are in fact equivalent

Obviously

$$(G) \Rightarrow (L) \Rightarrow (P)$$

Less obviously: (P) $\Rightarrow$ (G)

By induction over $s \equiv |V \setminus B|$:

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Induction step: The Intersection Lemma

We write A–B–C if x_A is conditionally independent of x_C given x_B.

Lemma

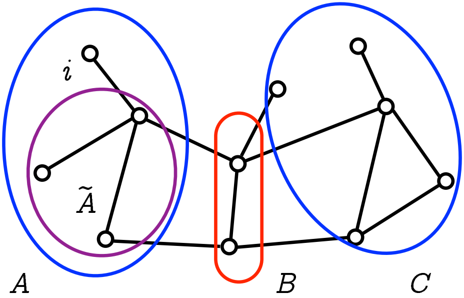
If μ is strictly positive and

$$A\text{–}(C \cup D)\text{–}B, \qquad A\text{–}(B \cup D)\text{–}C,$$

then

$$A\text{–}D\text{–}(B \cup C).$$

Induction step



$$A = \widetilde{A} \cup \{i\}$$

by induction assumption $\quad C \text{–} (B \cup i) \text{–} \widetilde{A}$

$$C \text{–} (B \cup \widetilde{A}) \text{–} \{i\}$$

By the intersection lemma

$$C \text{–} B \text{–} (\widetilde{A} \cup i) = A$$

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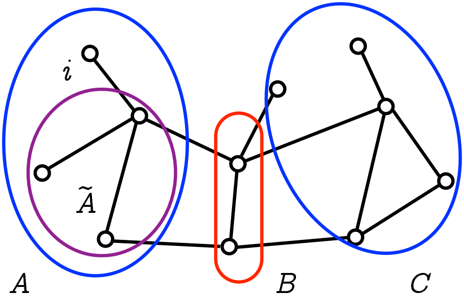

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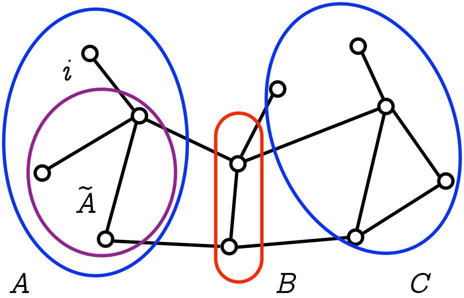

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BTW: How do you define a MRF on an infinite graph?

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Footnote #2

Where does the $(-1)^{|S \setminus U|}$ come from?

Möbius inversion formula

$$2^V = \{ \text{ subsets of } V \},$$

Theorem

Let $f, g : 2^V \to \mathbb{R}$. Then the following are equivalent

$$\begin{aligned} f(S) &= \sum_{U \subset S} g(U), \quad \textit{for all } S \subseteq V, \\ g(S) &= \sum_{U \subset S} (-1)^{|S \setminus U|} f(U), \quad \textit{for all } S \subseteq V. \end{aligned}$$

Proof: Exercise.

[see also G.C.Rota, Prob. Theor. Rel. Fields, 2 (1964) 340-368]

Relation with what we did

$$
\begin{aligned}
f(S) &= \log \mu(x_S, 0_{V\setminus S}), \\
g(S) &= \sum_{U\subset S} (-1)^{|S\setminus U|} \log \mu(x_U, 0_{V\setminus U}) = \tilde{psi}_S(x)
\end{aligned}
$$

Claim 1 in the proof ← Möbius