Learning and Inference for Graphical and Hierarchical Models: A Personal Journey

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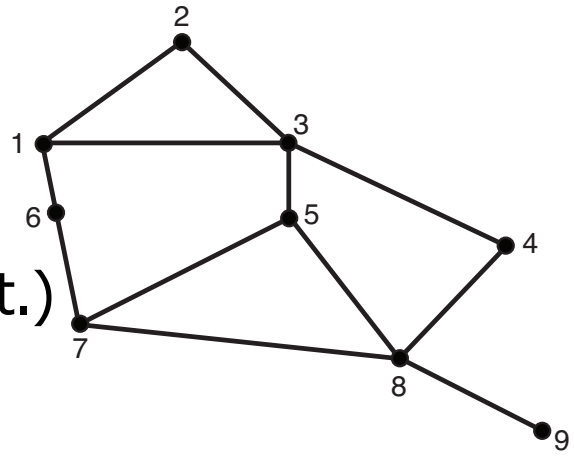
Undirected graphical models



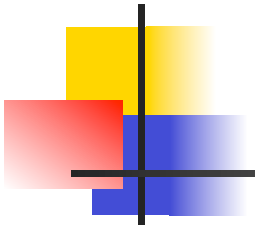
- $\boldsymbol{G} = (V, E)$ (V=vertices; $E \subset V \times V$ = edges)
- Markovianity on $\boldsymbol{G}$
  - Hammersley-Clifford (NASC for positive dist.)
    - $\mathbf{C}$ = Set of all cliques in $\boldsymbol{G}$

$$p(x) = \frac{1}{Z} \exp\left\{ \sum_{C \in \mathbf{C}} \varphi_C(x_C) \right\}$$

    - φ_c = Clique potential Z = partition function
- Pairwise graphical models

$$p(x) = \frac{1}{Z} \exp\left\{ \sum_{s \in V} \varphi_s(x_s) + \sum_{(s,t) \in E} \varphi_{st}(x_s, x_t) \right\}$$

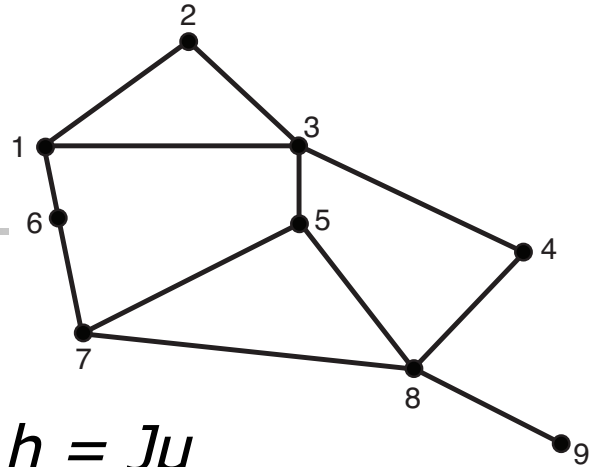
$$p(x) = \frac{1}{Z} \prod_{s \in V} \psi_s(x_s) \prod_{(s,t) \in E} \psi_{st}(x_s, x_t)$$



Directing/undirecting the graphs?

- Undirected models: Factors are ***not*** typically probabilities
  - Although they ***can*** be for cycle-free graphs (see BP), i.e., ***trees***
- Directed models: Specify in terms of transition probabilities (parents to children)
- Directed to undirected: Easy (after moralization)
- Undirected to directed: Hard (and often a mistake) unless the graph is a tree (see BP)

Gaussian models



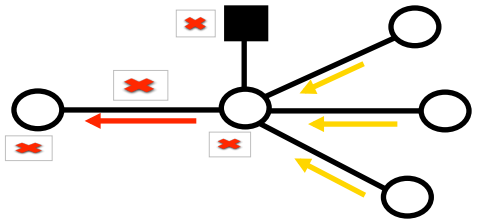
- $X \sim N(\mu, P)$ or $N^{-1}(h, J)$, with $J = P^{-1}$ and $h = J\mu$
- The sparsity structure of J determines graph structure
  - I.e., $J_{st} = 0$ if (s, t) is not an edge
- Directed model (0-mean for simplicity):

$$AX = w$$

  - $W \sim N(0, I)$
  - A – Lower triangular
- $A = J^{1/2}$ ➔ In general we get lots of ***fill***, unless the graph structure is a tree
- And it's even more complicated for non-Gaussian models, as higher-order cliques are introduced

Belief Propagation: Message passing for pairwise models on ***trees***

- Fixed point equations for likelihoods from disjoint parts of the graph:



$$m_{ts}(x_s) = \alpha \int_{x_t} \psi_{s,t}(x_s, x_t)\psi_t(x_t) \prod_{u \in \mathcal{N}(t)\setminus s} m_{ut}(x_t)dx_t$$

$$P_s(x_s) = \alpha\psi_s(x_s) \prod_{u \in \mathcal{N}(s)} m_{us}(x_s)$$

$$P_{st}(x_s, x_t) = \alpha\psi_{st}(x_s, x_t)\psi_s(x_s)\psi_t(x_t) \prod_{u \in \mathcal{N}(s)/t} m_{us}(x_s) \prod_{u \in \mathcal{N}(t)/s} m_{ut}(x_t)$$

BP on trees

- Gives factored form for distribution in terms of probability distributions

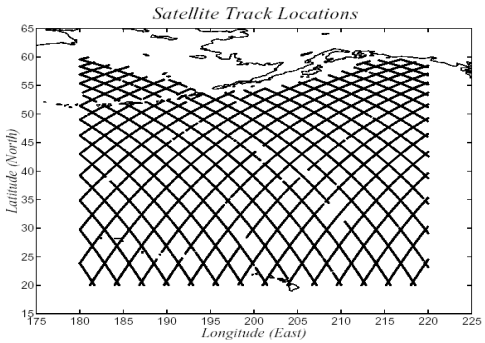
$$P(\{x_s | s \in V\}) = \prod_{s \in V} P_s(x_s) \prod_{(s,t) \in E} \frac{P_{st}(x_s, x_t)}{P_s(x_s) P_t(x_t)}$$

- Great flexibility in message-scheduling
  - Leaves-root-leaves = Rauch-Tung-Striebel
  - Completely parallel messaging, convergence in number of steps = diameter of the graph

Modeling of ***structure***: Four questions

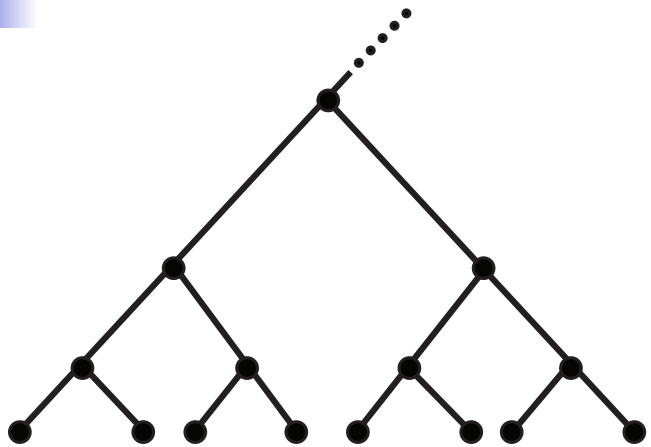
- What should the structure of the graph be?
- Which variables go where?
- What about adding hidden (unobserved) nodes (and variables)?
- What should the dimensions of the various variables be?

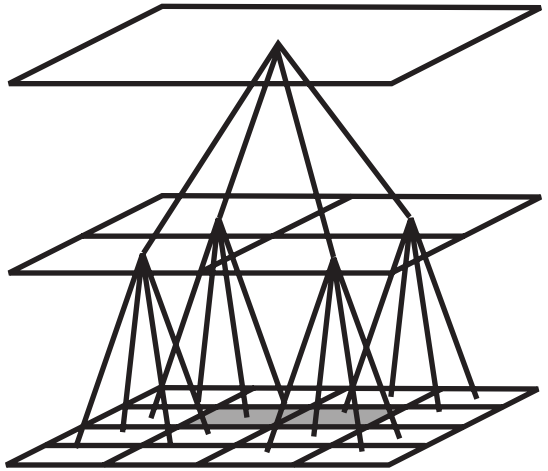
Our initial foray (with thanks to Michèle Basseville and Albert Benveniste): Multiresolution Models



- What can be multiresolution?
  - The ***phenomenon*** being modeled
  - The ***data*** that are collected
  - The ***objectives*** of statistical inference
  - The ***algorithms*** that result
- Some applications that motivated us (and others)
  - Oceanography
  - Groundwater hydrology
  - "Fractal priors" in regularization formulations in computer vision, mathematical physics, …
  - Texture discrimination
  - Helioseismology (?) …

Specifying MR models on trees





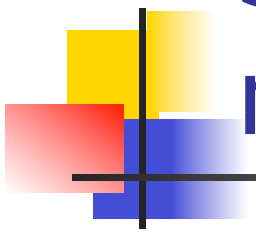
- MR ***synthesis***, leads, as with Markov chains, to thinking about ***directed trees***:
- E.g.: $x(s) = A(s)x(s\gamma) + w(s)$
  - E.g.: Midpoint deflection is such a model
- Note that the ***dimension*** of the variables comes into play
- But let's assume we pre-specify the tree structure

A control theorist's idea: **Internal models**

- Variables at coarser nodes are ***linear functionals*** of the finest-scale variables
  - Some of these may be measured or important quantities to be estimated
  - The rest are to be ***designed***
    - To approximate the condition for tree-Markovianity
    - To yield a model that is "close" to the true fine-scale statistics
  - Scale-recursive algebraic design
    - Criterion used: Canonical correlations or predictive efficiency
  - Alternate using midpoint deflection or wavelets**
- Confounding the control theorist
  - Internal models need not have minimal state dimension

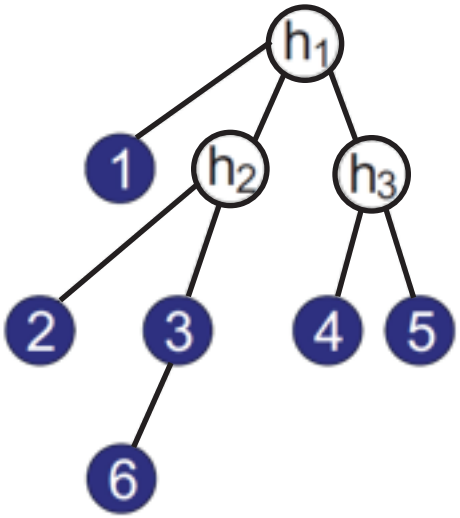
$$x(s) = x(s\overline{\gamma}) + w(s)$$

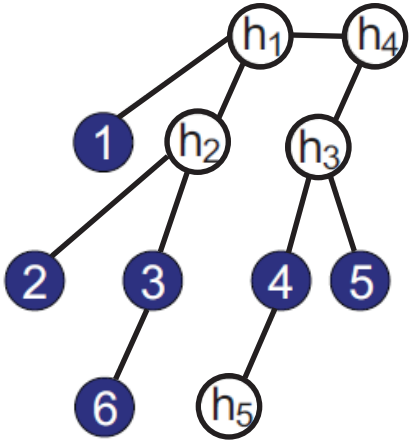
So, what if we want a tree but not necessarily a hierarchical one



- One approach: Construct the maximum likelihood tree given sample data (or the full second-order statistics)
- ***NOTE:*** This is quite different from what system theorists typically consider
  - There is no "state" to identify: All of the variables in the model we desire are observed
  - It is the ***index set*** that we get to play with
- Chow-Liu found a very efficient algorithm
  - Form graph with each observed variable at a different node
  - Edge weight between any two variables is their mutual information
  - Compute max-weight spanning tree
- What if we want hidden/latent "states"?

Reconstruction of a Latent Tree





- Reconstruct a latent tree using exact statistics (first) or samples (to follow) of observed nodes only
- Exact/consistent recovery of ***minimal*** latent trees
  - Each hidden node has at least 3 neighbors
  - Observed variables are neither perfectly dependent nor independent
- Other objectives:
  - Computational efficiency
  - Low sample complexity

Information Distance

- Gaussian distributions

$$d_{ij} := -\log |\rho_{ij}|$$

$$\rho_{ij} := \frac{\mathrm{Cov}(X_i, X_j)}{\sqrt{\mathrm{Var}(X_i)\mathrm{Var}(X_j)}}$$

- Discrete distributions

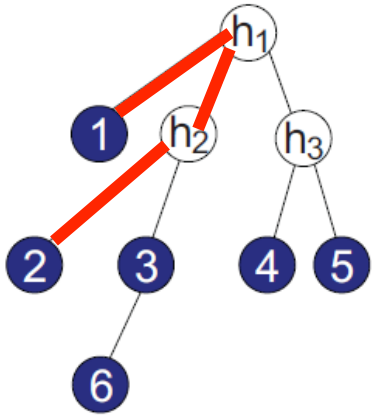
$$d_{ij} := -\log \frac{|\det \mathbf{J}^{ij}|}{\sqrt{\det \mathbf{M}^i \det \mathbf{M}^j}}$$

$\mathbf{J}^{ij}$ Joint probability matrix

$\mathbf{M}^i$ Marginal probability matrix (diagonal)

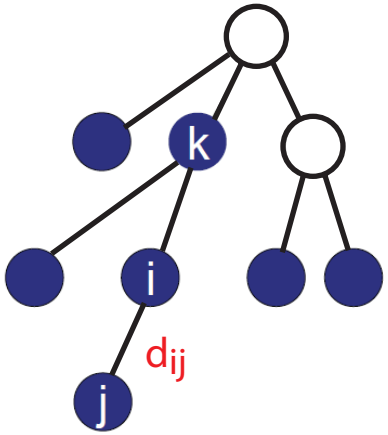
Additivity

$$d_{k,l} = \sum_{(i,j)\in \mathrm{Path}((k,l);E_p)} d_{i,j}$$



$$d_{12} = d_{1h_1} + d_{h_1h_2} + d_{2h_2}$$

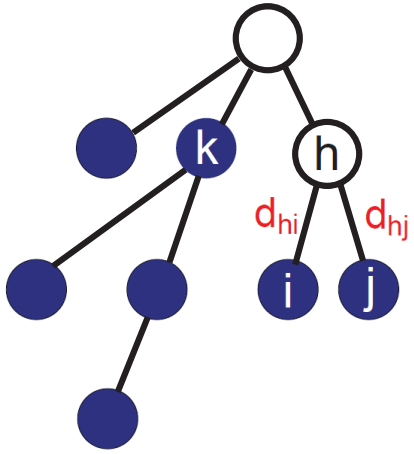
Testing Node Relationships



Node j – a leaf node Node i – parent of j

$\Leftrightarrow$ for all $k \neq i, j$ $d_{jk} - d_{ik} = d_{ij}$

Can identify (parent, leaf child) pair

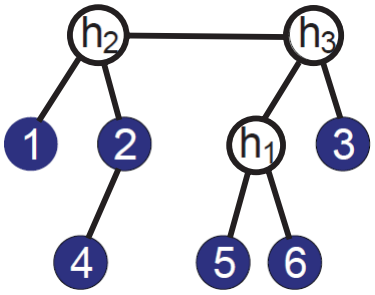


Node i and j – leaf nodes and share the same parent (sibling nodes)

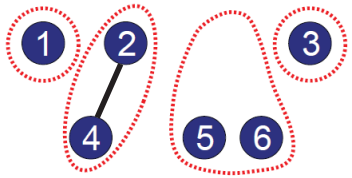
$\Leftrightarrow$ for all $k \neq i, j$ $d_{jk} - d_{ik} = d_{hj} - d_{hi}$

Can identify leaf-sibling pairs.

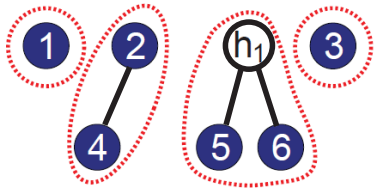
Recursive Grouping (exact statistics)



Step 1. Compute $d_{jk} - d_{ik}$ for all observed nodes (i, j, k).

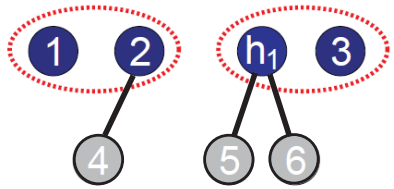


Step 2. Identify (parent, leaf child) or (leaf siblings) pairs.



Step 3. Introduce a hidden parent node for each sibling group without a parent.

Step 4. Compute the information distance for new hidden nodes. E.g.: $d_{5h_1} = \frac{1}{2}(d_{56} + d_{53} - d_{63})$



Step 5. Remove the identified child nodes and repeat Steps 2-4.

Recursive Grouping

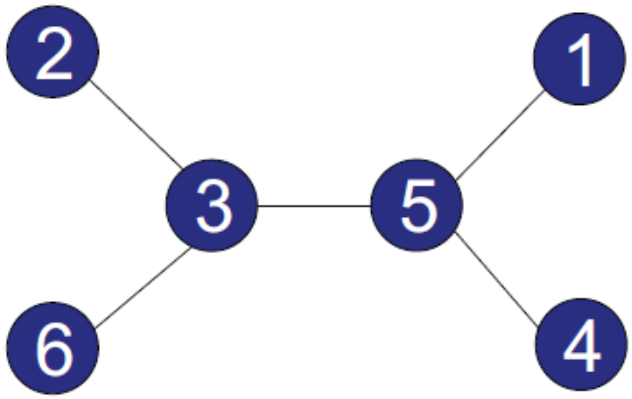
- Identifies a group of family nodes at each step.
- Introduces hidden nodes recursively.
- Correctly recovers all minimal latent trees.

- Computational complexity $O(\text{diam}(T)\, m^3)$.

Worst case $O(m^4)$

Chow-Liu Tree

$$\mathrm{MST}(V; \mathbf{D})$$



Minimum spanning tree of V

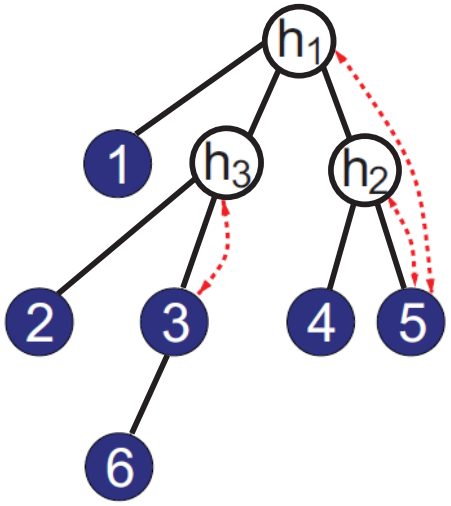
using D as edge weights

V = set of observed nodes

D = information distances

- Computational complexity $O(m^2 \log m)$

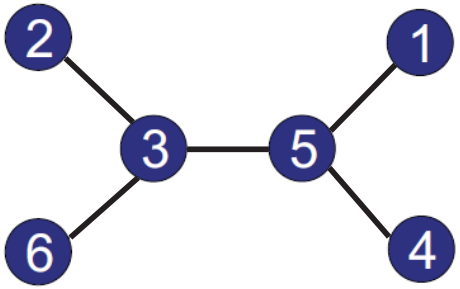
Surrogate Nodes and the C-L Tree



V = set of observed nodes

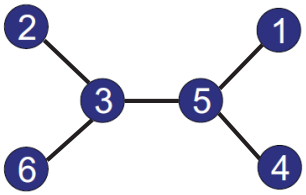
Surrogate node of i

$$\mathrm{Sg}(i) := \operatorname*{argmin}_{j \in V} d_{ij}$$

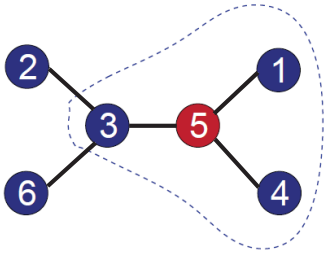


If (*i*, *j*) is an edge in the latent tree, then (Sg(*i*), Sg(*j*)) is an edge in the Chow-Liu tree

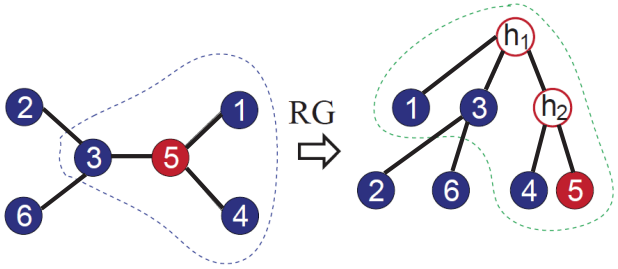
CLGrouping Algorithm



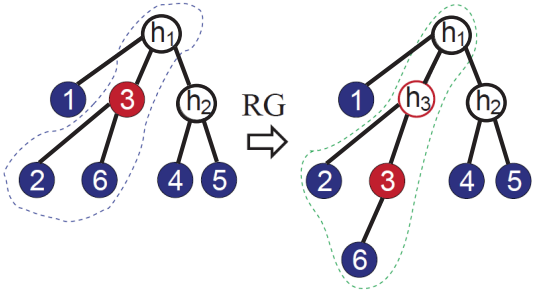
Step 1. Using information distances of observed nodes, construct MST(V; D). Identify the set of internal nodes.



Step 2. Select an internal node and its neighbors, and apply the recursive-grouping (RG) algorithm.



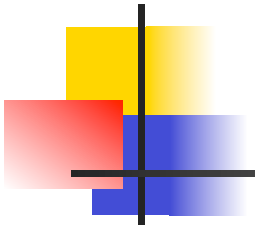
Step 3. Replace the output of RG with the sub-tree spanning the neighborhood.



Repeat Steps 2-3 until all internal nodes are operated on.

Computational complexity

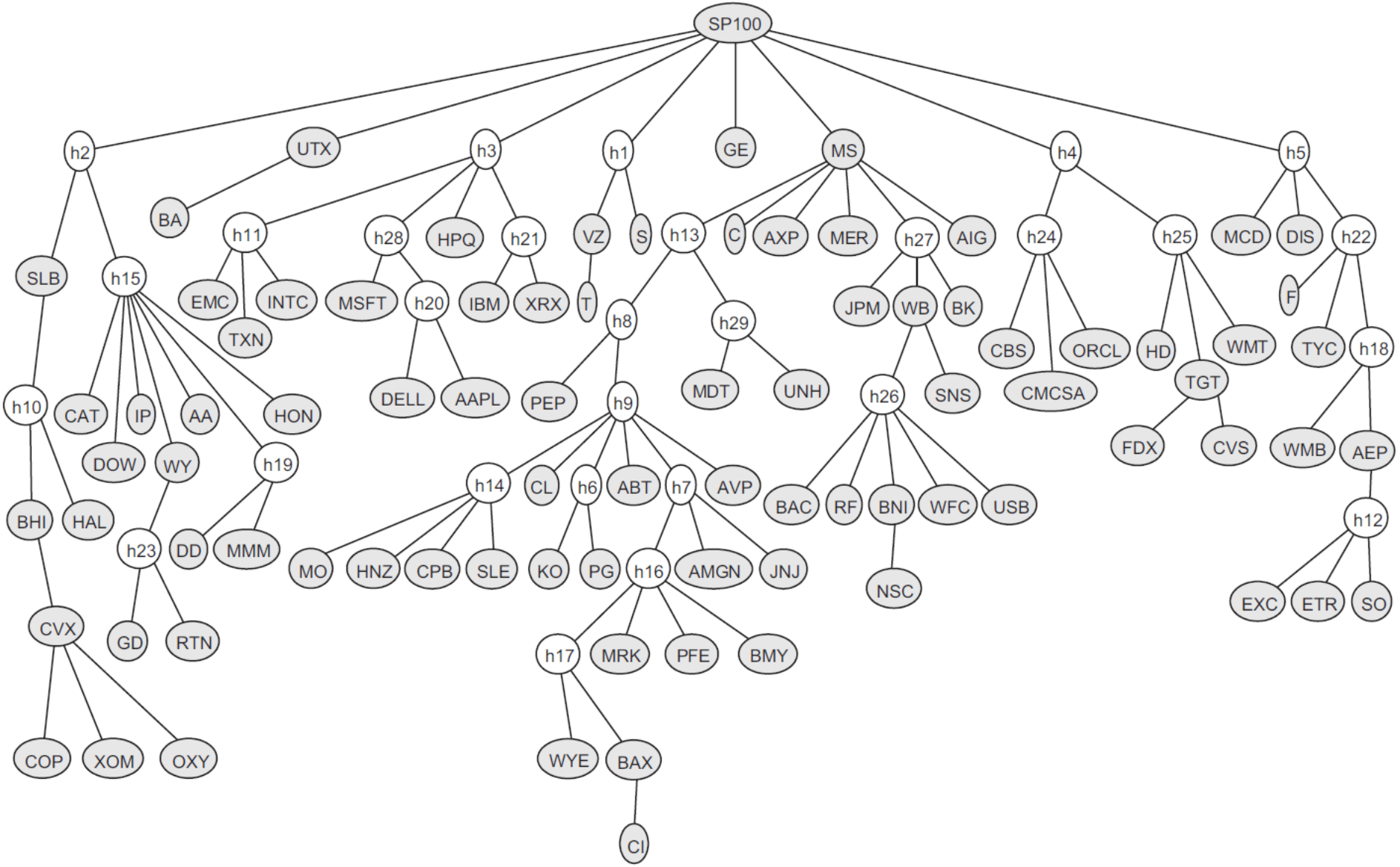
$O(m^2 \log m + (\#\text{internal nodes})\,(\text{maximum degree})^3)$



Sample-based Algorithms

- Compute the ML estimates of information distances.
- Relaxed constraints for testing node relationships.
- Consistent (only in structure for discrete distributions)

- Regularized CLGrouping for learning latent tree approximations.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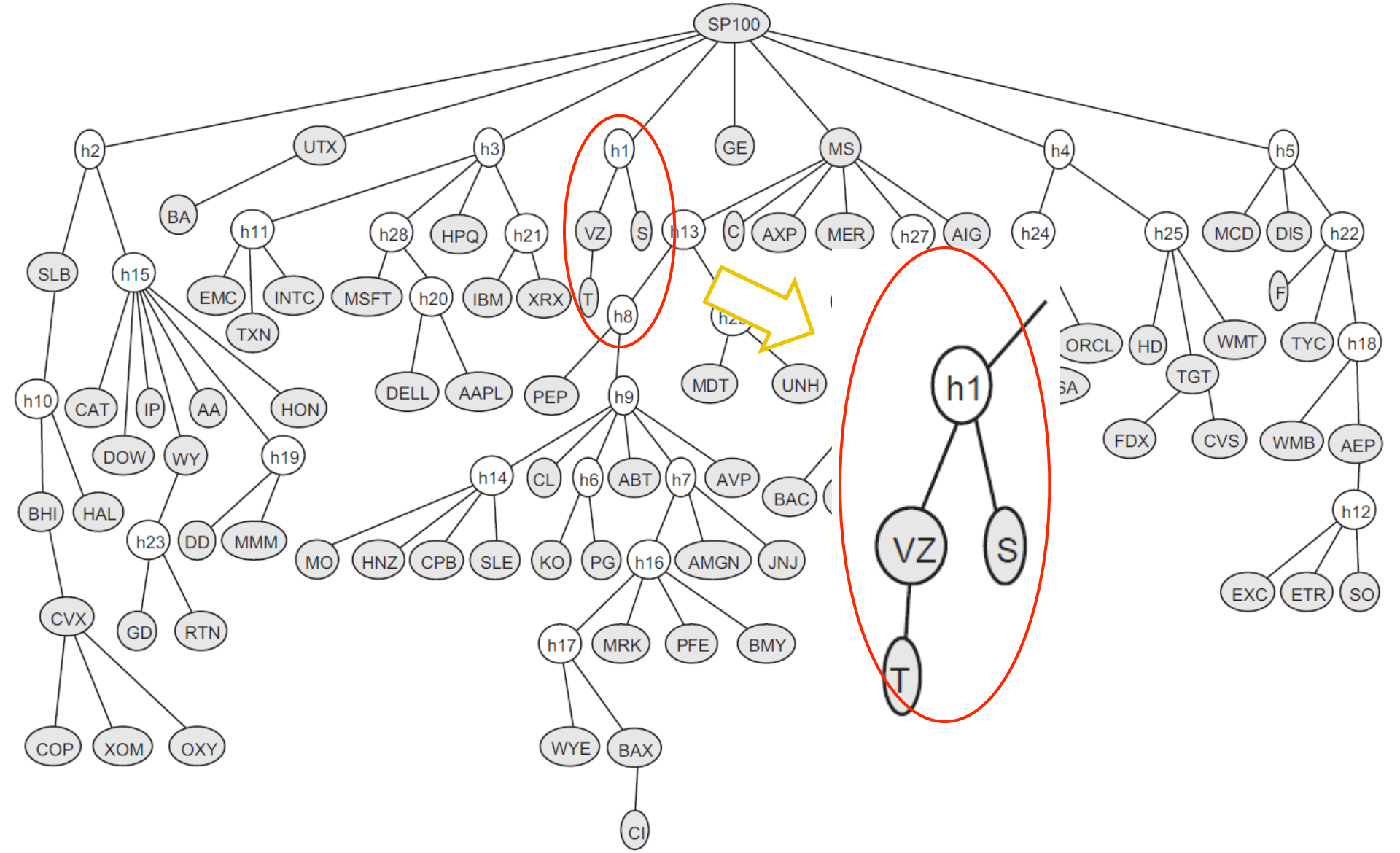
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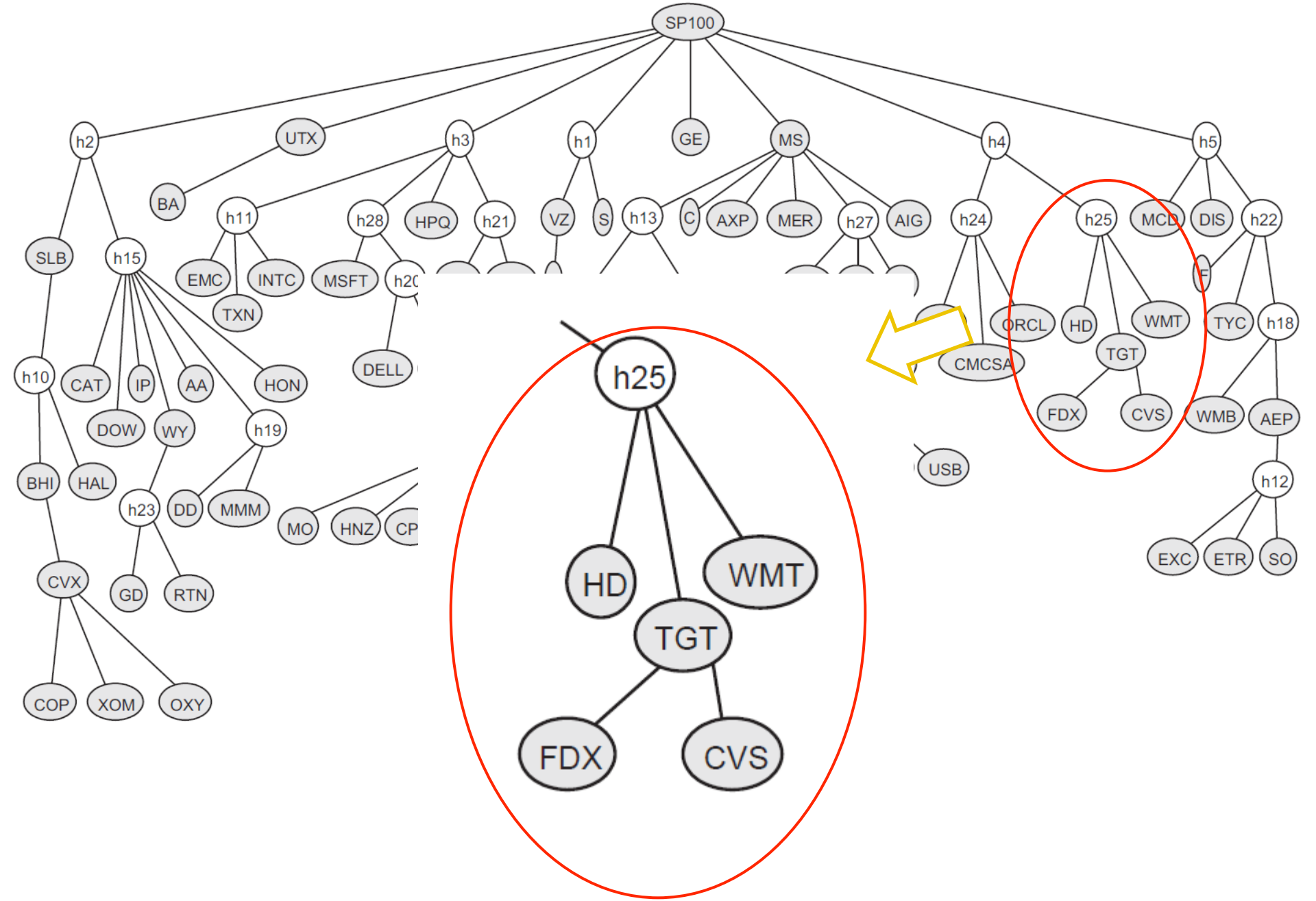
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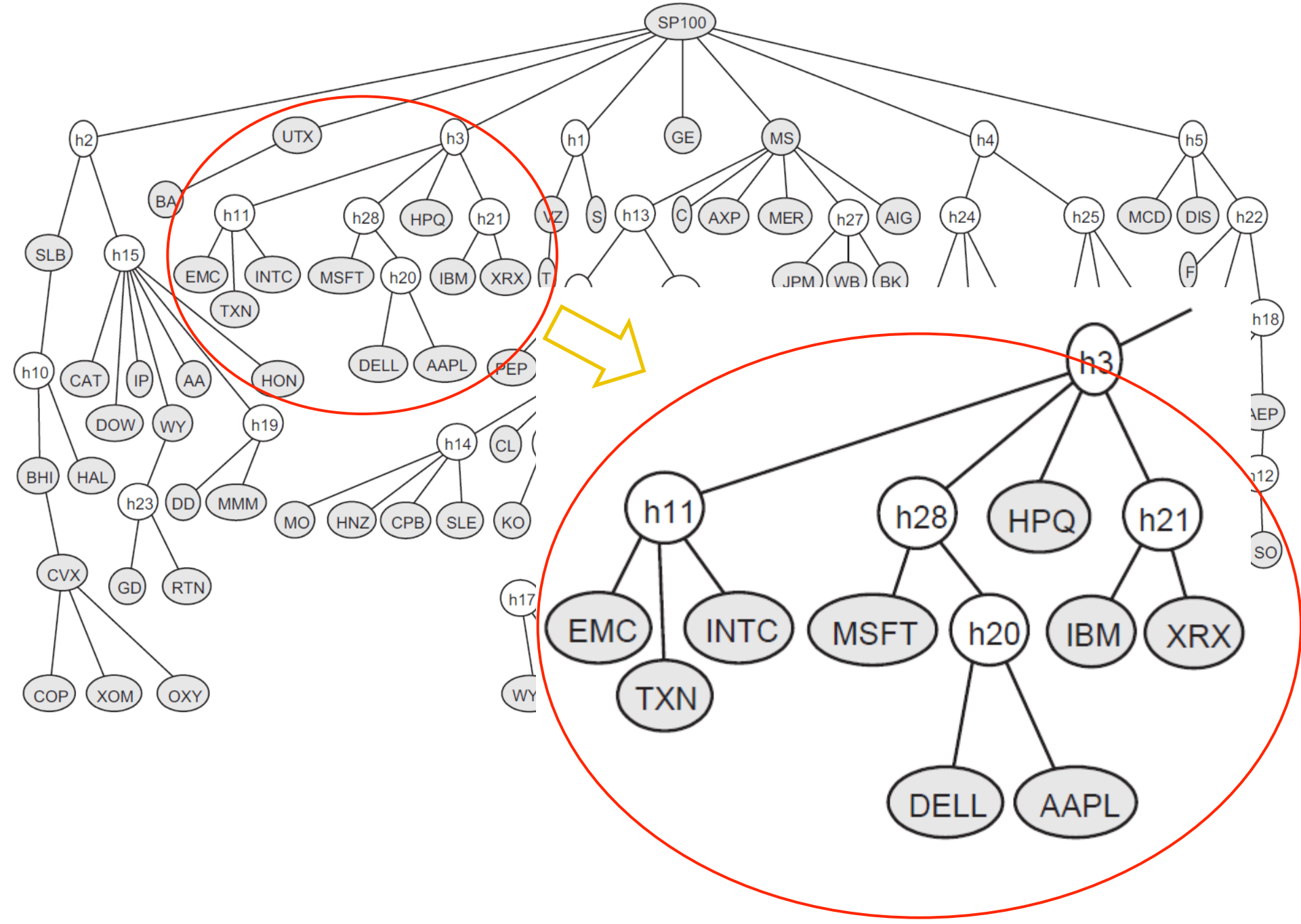
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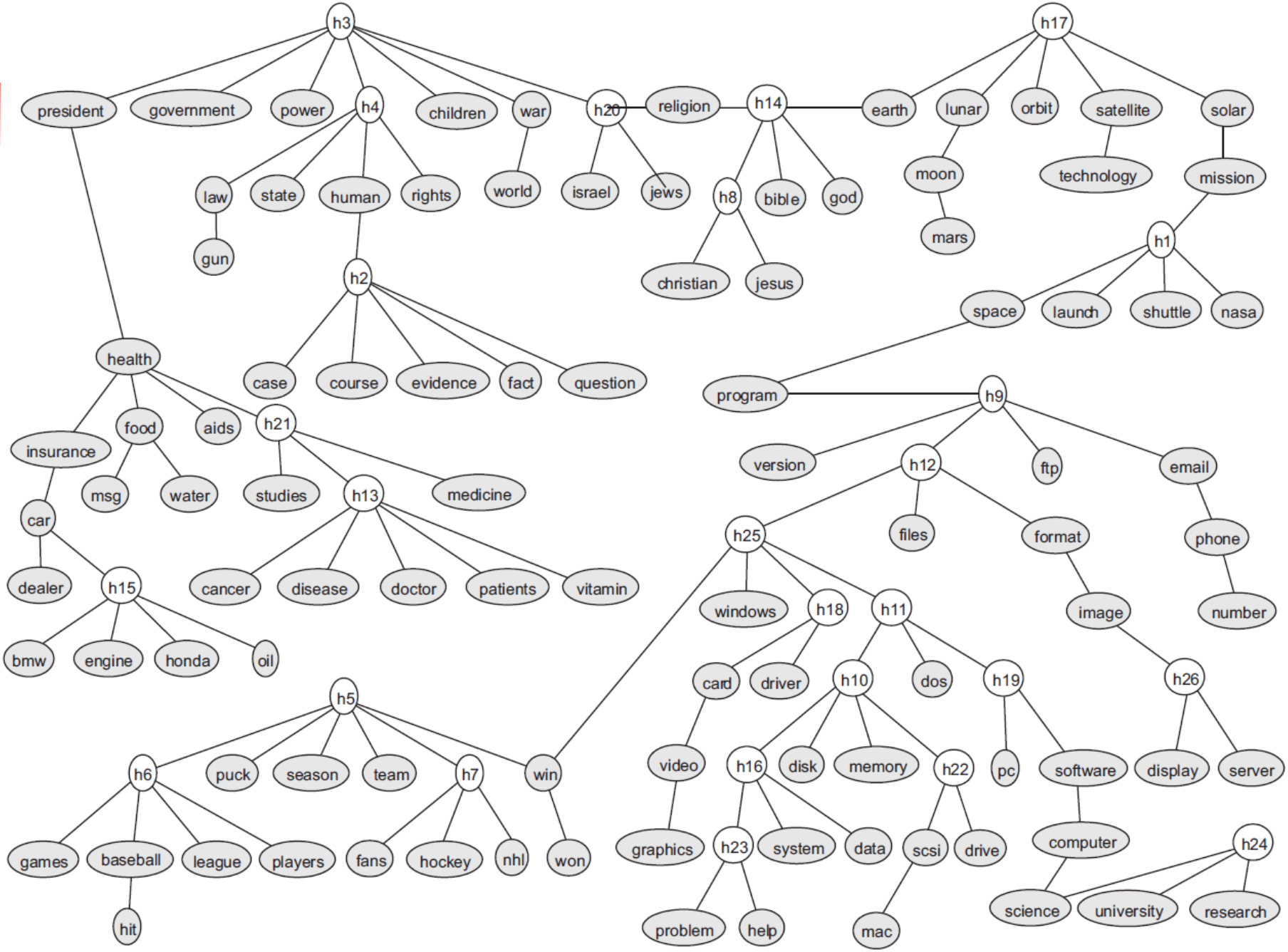
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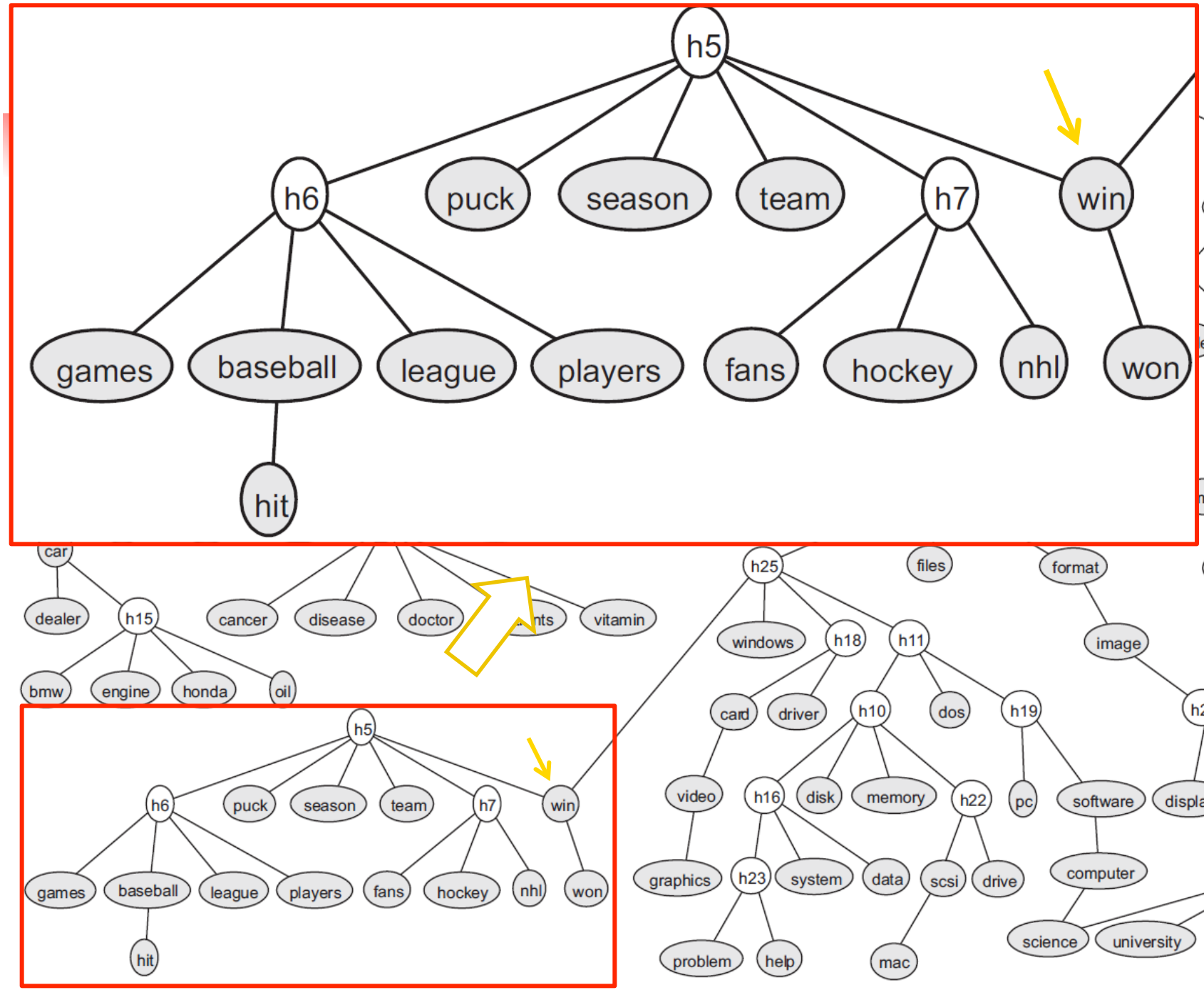
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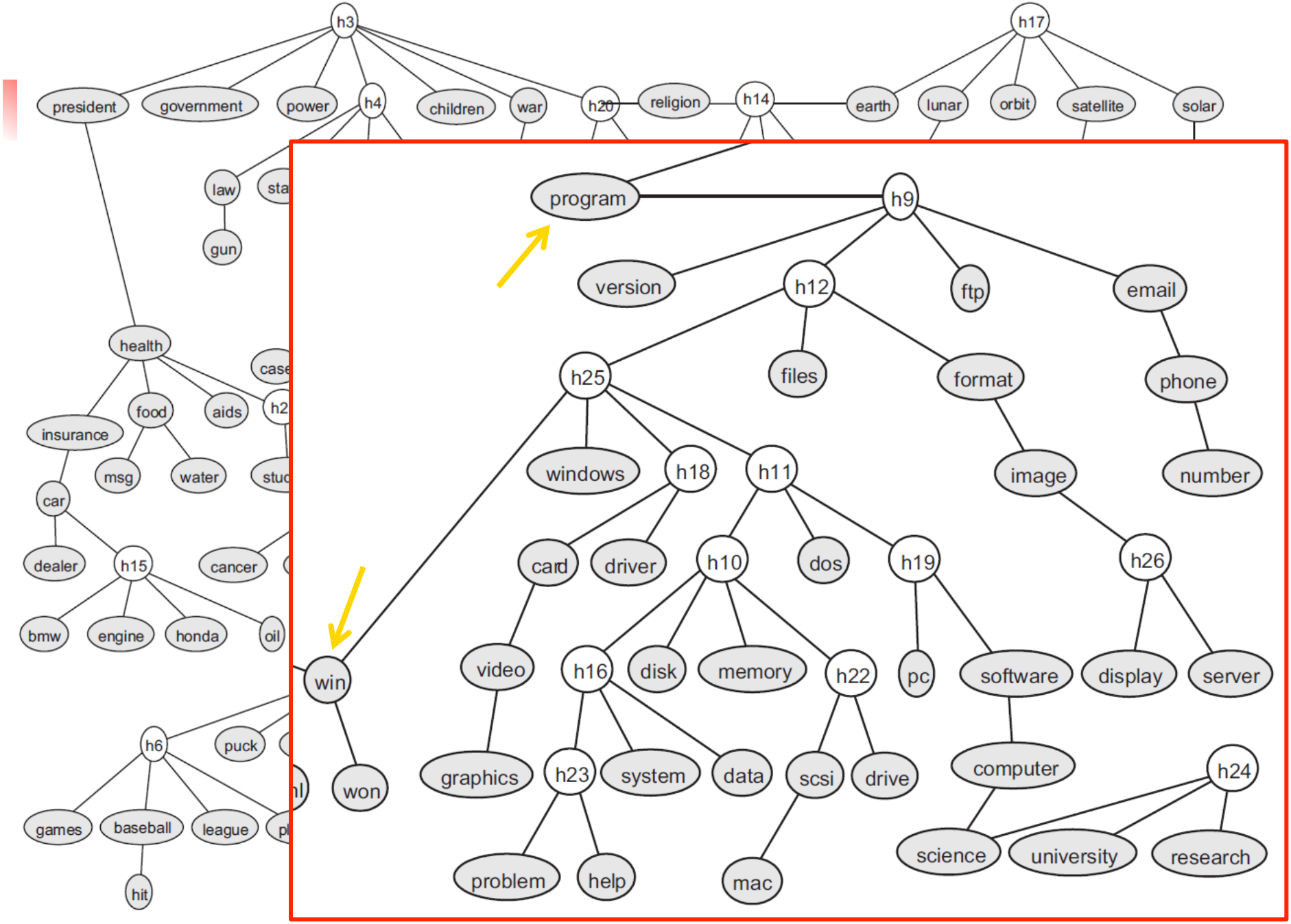
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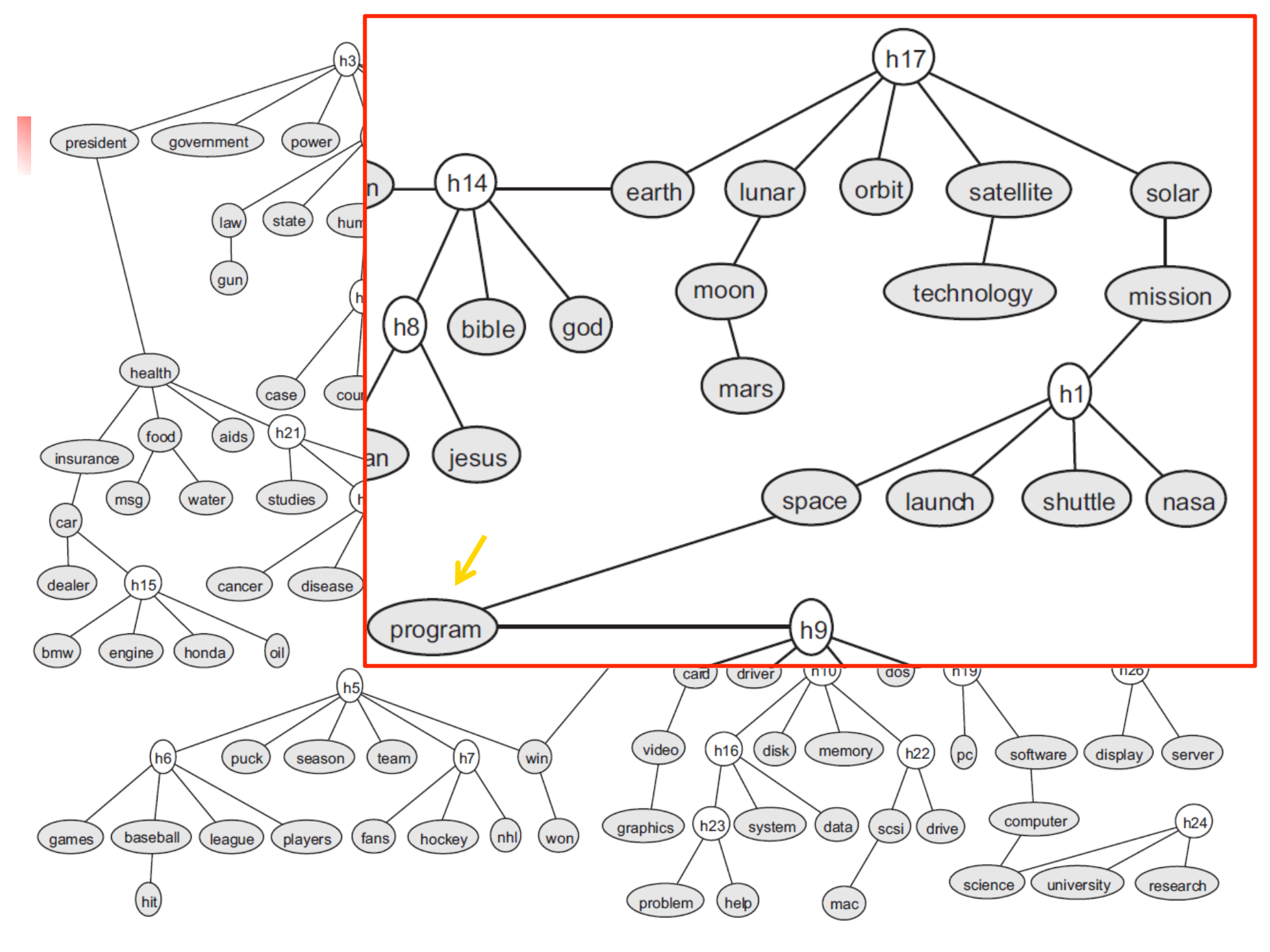
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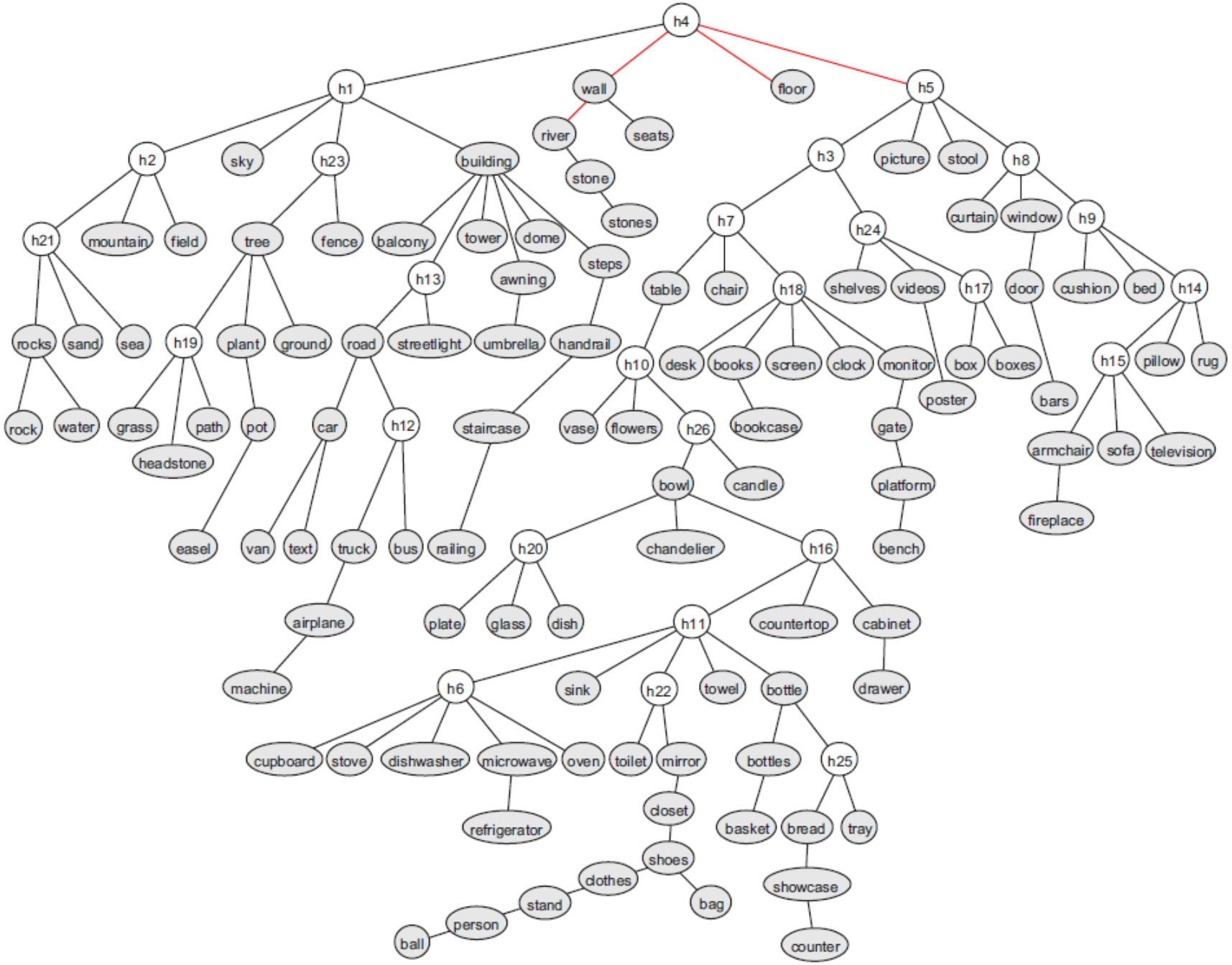
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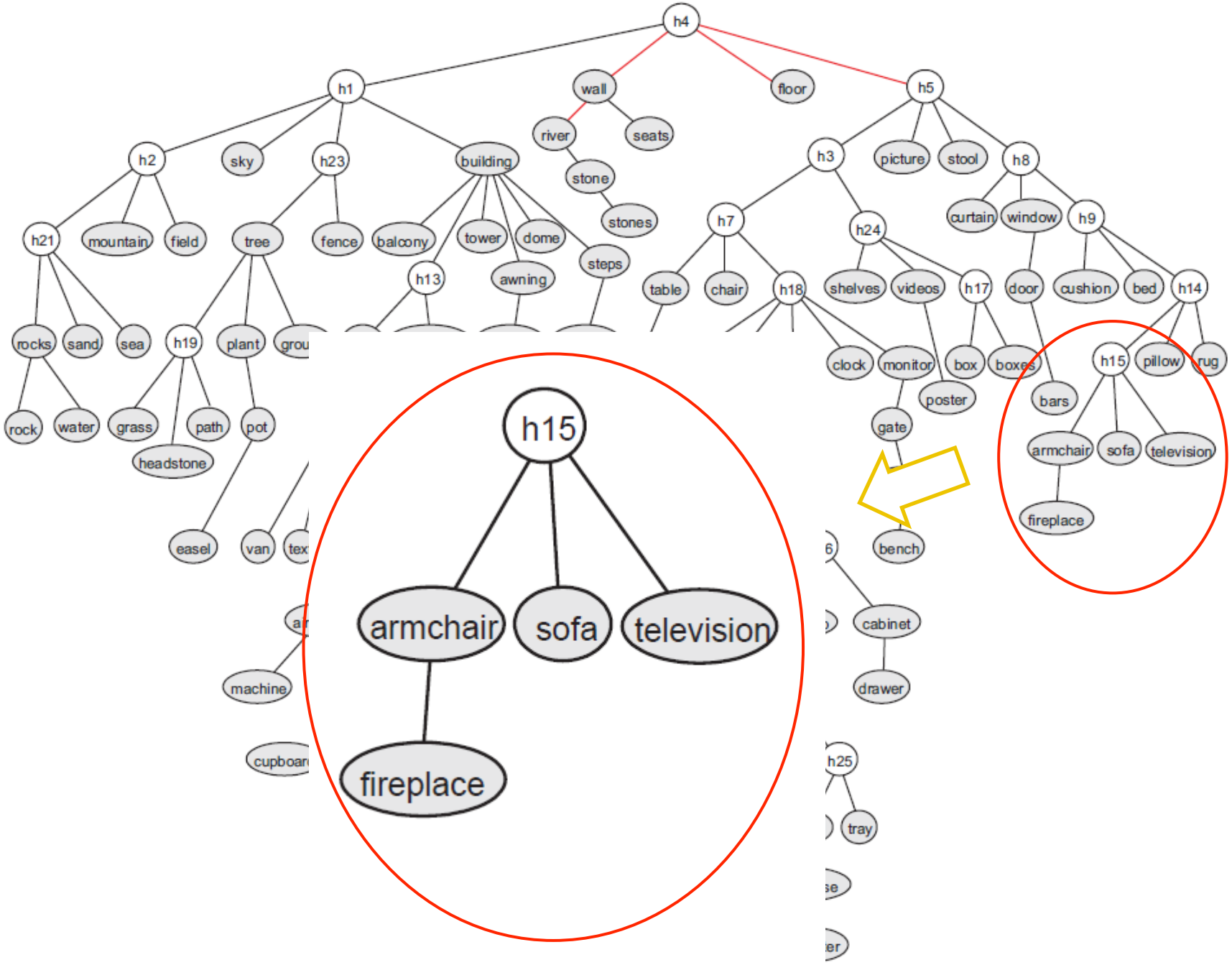
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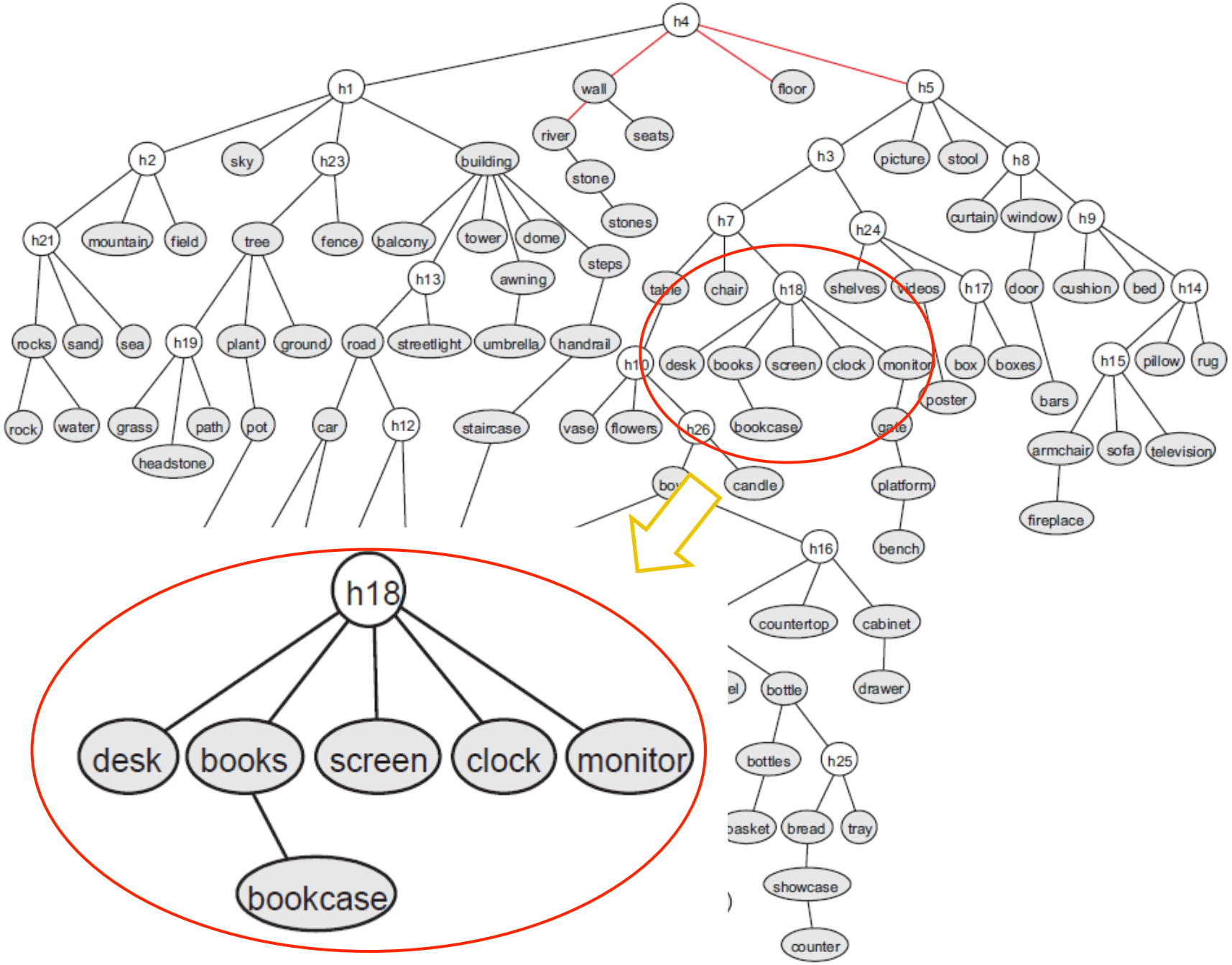
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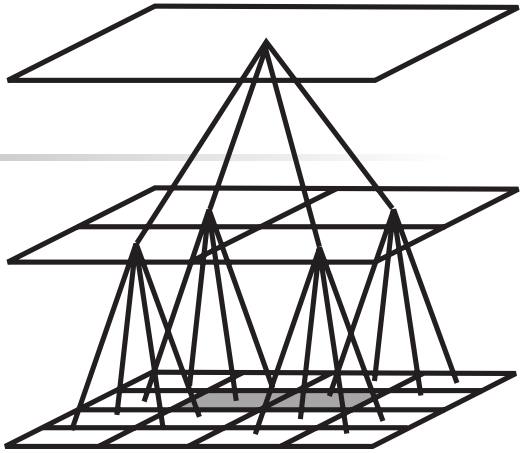
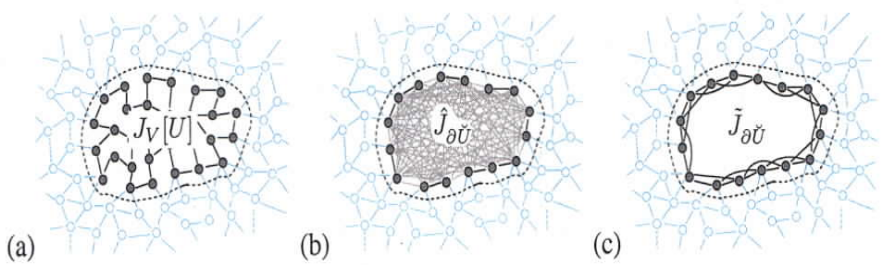
The dark side of trees = The bright side: No loops



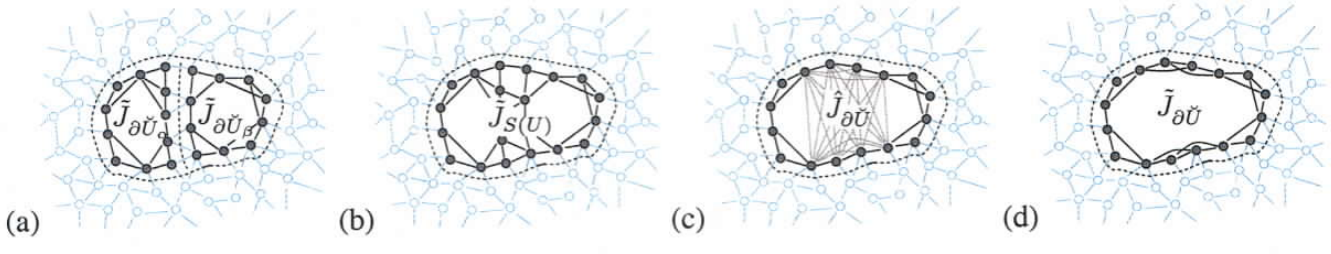
- So, what do we do?
- Try #1: Turn it into a junction tree
  - Not usually a good idea, but …
- Try #2: Pretend the problem isn't there and use a tree
  - If the real objectives are at coarse scales, then fine-scale artifacts may not matter
- Try #3: Pretend it's a tree and use (Loopy) BP
- Try #4: Think!
  - What does LBP ***do?***
  - Better algorithms?
  - Other graphs for which inference is scalable?

Recursive Cavity Models: "Reduced-order" modeling as part of estimation

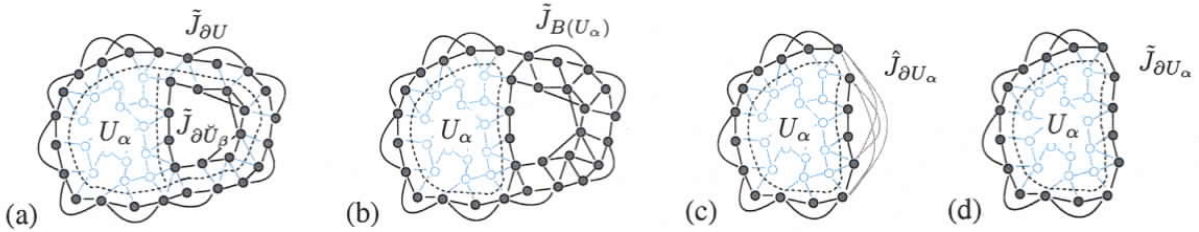
- Cavity thinning



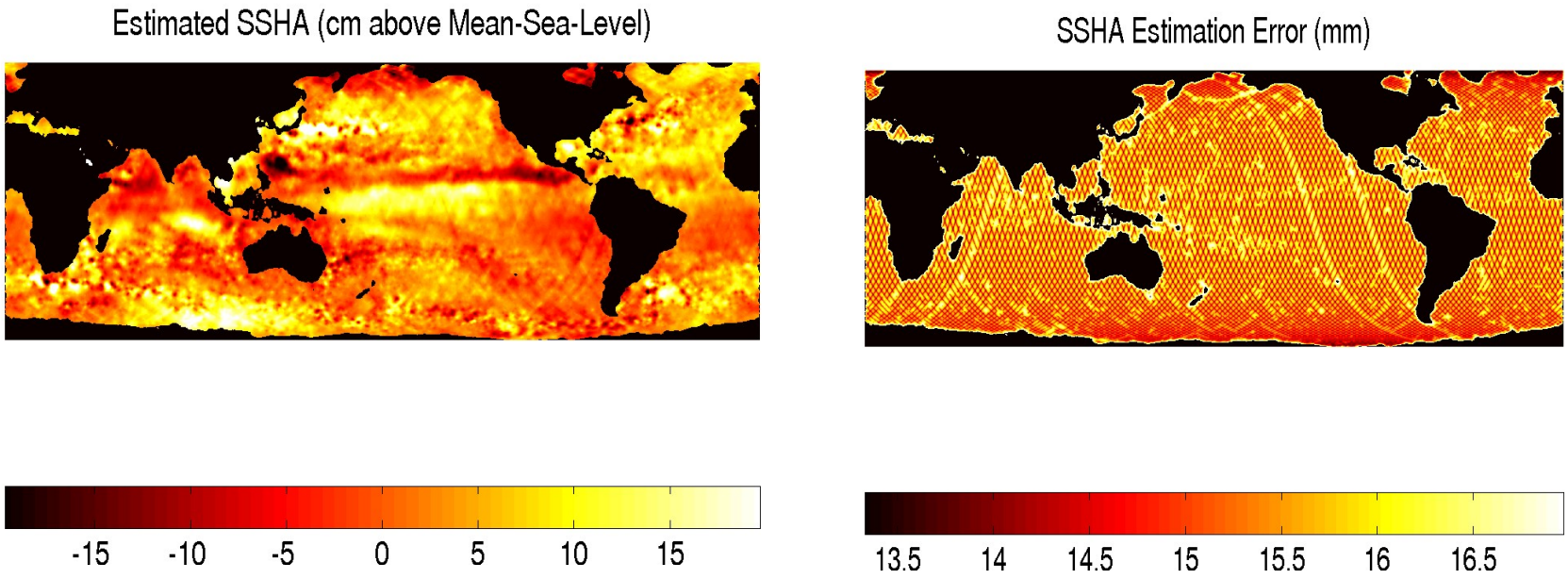
- Collision



- Reversing the process (bring your own blanket)



RCM in action: We are the world



- This is the information-form of RTS, with a thinning approximation at each stage
- How do the thinning errors propagate?
  A control-theoretic stability question

Walk-sums and Gaussian models

$$J = P^{-1} \qquad\qquad h = P^{-1}\mu$$

- Assume *J* normalized to have unit diagonal

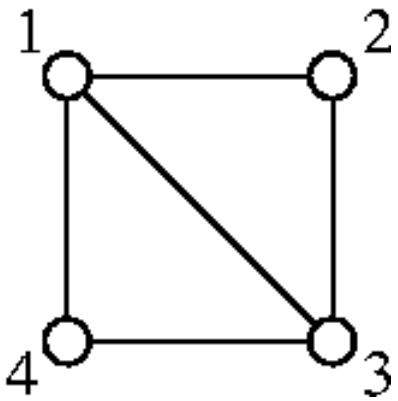
$$J^{-1} = (I - R)^{-1} = I + R + R^2 + \dots$$

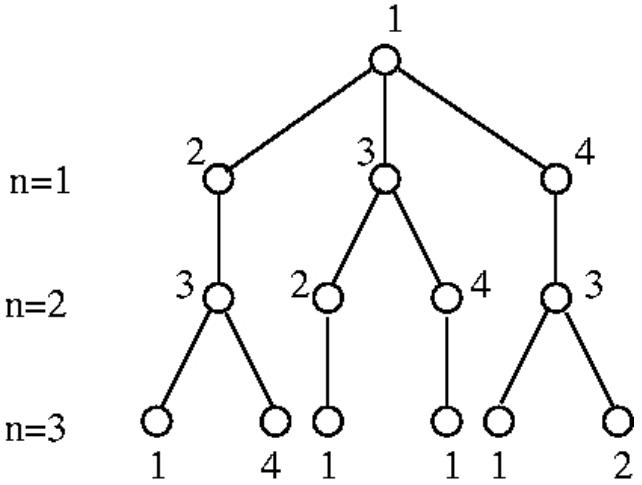
  - *R* is the matrix of ***partial correlation coefficients***
  - $(R^\ell)_{s,t}$ =***sum over weighted length-ℓ walks*** from *s* to *t* in graph

$$P_{s,t} = \phi(s \to t), \quad \mu_t = \sum_{s \in V} h_s \phi(s \to t)$$

- Inference algorithms may "collect" walks in different ways
- Walk-summability, corresponding to $\varrho(\bar{R}) < 1$, guarantees
  - Collection in any order is OK
  - LBP converges
  - If LBP converges it collects all walks for μ_i but only ***some*** of the ***self-return walks*** required for P_{ii}
  - There are lots of interesting/important models that are non-WS (and for which BP goes haywire)

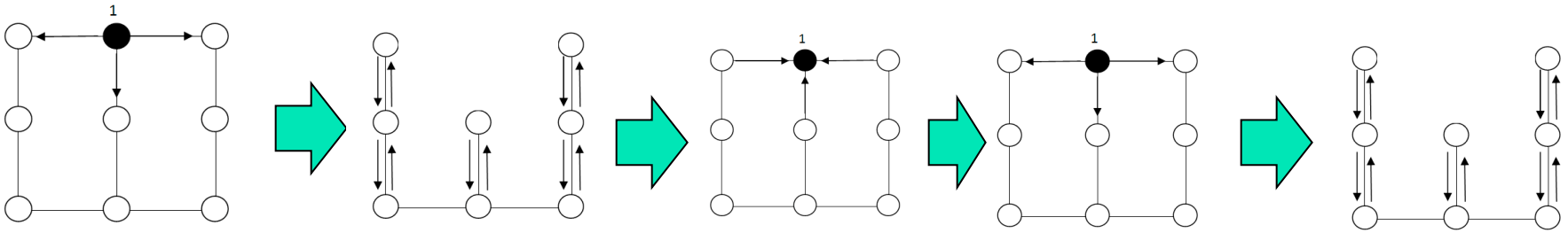
A computation tree





- BP includes the ***back-tracking self-return*** walk (1,2,3,2,1)
- BP does ***not*** include the walk (1,2,3,1)
- **BUT:** For Non-WS models, the tree **may be nonsensical**
- There are ways to collect some or all of the missed walks
  - Embedded subgraphs as preconditioners
    - Convergence for WS models always
  - A method that works also for non-WS models, recognizing that not all nodes are created equal

An alternate approach: Using (Pseudo-) ***Feedback Vertex Sets***

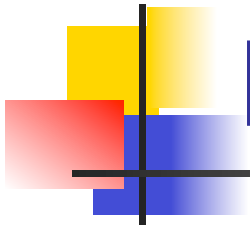


- Provide additional potentials to allow computation of quantities needed in mean/variance/covariance computation in the FVS
- Run BP with both original potentials and the additional set(s)
- Feed back information to FVS to allow computation of exact variance and mean within the FVS
- Send modified information potentials to neighbors of FVS
- Run BP with modified information potentials
  - Yields exact means immediately
  - Combining with results from Steps 2, 3 yields exact variances

Approximate FVS

- Complexity is $\mathcal{O}(k^2 n)$, where $k = |\mathcal{F}|$
- If k is too large
  - Use a pseudo- (i.e., partial) FVS, breaking only some loops
  - On the remaining graph, run LBP (or some other algorithm)
- Assuming convergence (which does ***not*** require WS)
  - Always get the correct means and variances on $\mathcal{F}$, exact means on $\mathcal{T}$, and (for LBP) approximate variances on $\mathcal{T}$
  - The approximate variances collect *more walks* than LBP on full graph
- Local (fast) method for choosing nodes for the pseudo-FVS to:
  - Enhance convergence
  - Collect the most important wants
- Theoretical and empirical evidence show $k \approx \mathcal{O}(\log n)$ works

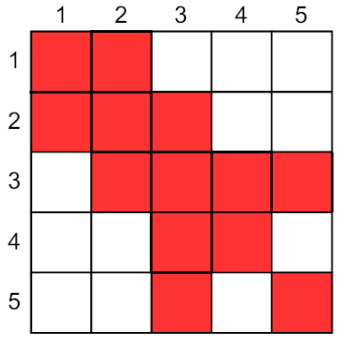
Motivation from PDEs: **MultiPOLE Models**

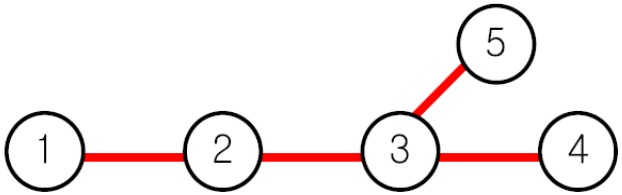


- Motivation from methods for efficient preconditioners for PDEs
  - Influence of variables at a distance are well-approximated by coarser approximation
  - We then only need to do ***LOCAL*** smoothing and correction
- The idea for statistical models:
  - Pyramidal structure in scale
  - However, when conditioned on neighboring scales, ***the remaining correlation structure at a given scale is sparse and local***

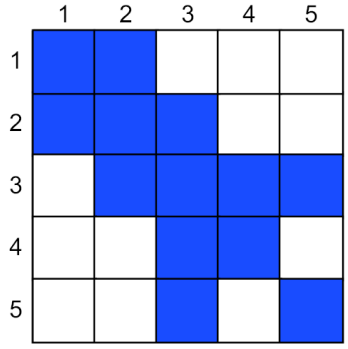
Models on graphs and on ***conjugate graphs***

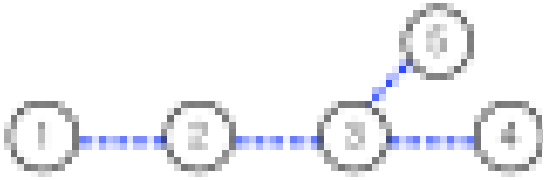
Garden variety graphical model: sparse ***inverse*** covariance

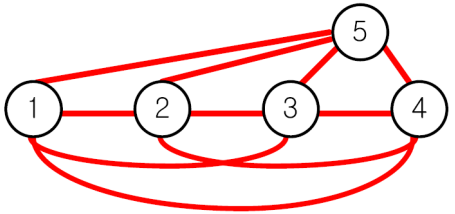




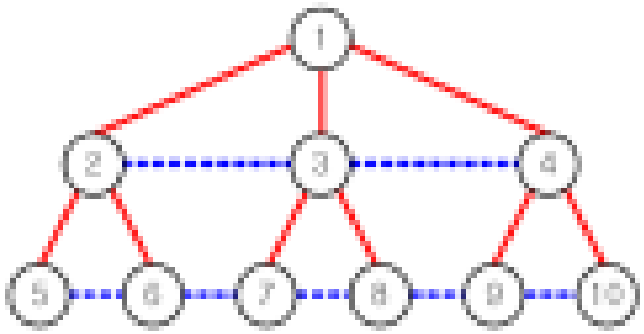
Conjugate models: sparse ***covariance***





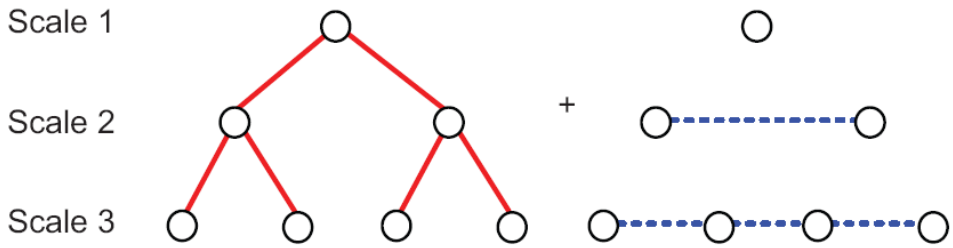


Inspiration from Multipole Methods for PDEs: Allow ***Sparse Residual Correlation*** Within Each Scale



- Conditioned on scale 1 and scale 3, x_2 is independent of x_4.

$$J = \begin{pmatrix} J_{[1]} & J_{[1,2]} & 0 \\ J_{[2,1]} & J_{[2]} & J_{[2,3]} \\ 0 & J_{[3,2]} & J_{[3]} \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & J_{[1,2]} & 0 \\ J_{[2,1]} & 0 & J_{[2,3]} \\ 0 & J_{[3,2]} & 0 \end{pmatrix}}_{J^h} + \underbrace{\begin{pmatrix} J_{[1]} & 0 & 0 \\ 0 & J_{[2]} & 0 \\ 0 & 0 & J_{[3]} \end{pmatrix}}_{J^c = (\Sigma^c)^{-1}}$$

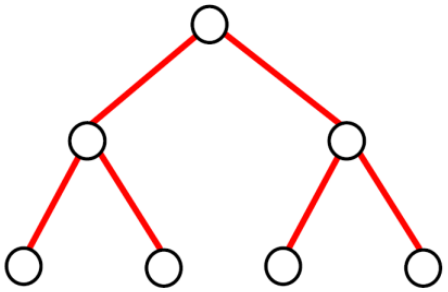


Learning such models:

"Dual" convex optimization problems

Multipole Estimation

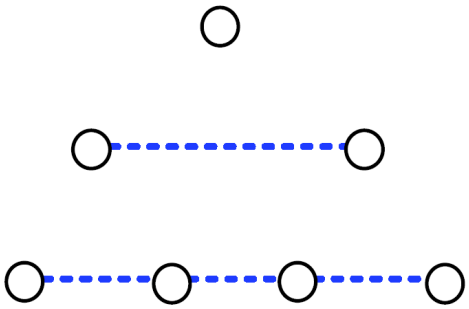
- Richardson Iteration to solve $(J^h + (\Sigma^c)^{-1})x = h$
  - Global tree-based inference
  - Sparse matrix multiplication for in-scale correction



$$J^h x_{new} = h - (\Sigma^c)^{-1} x_{old}$$

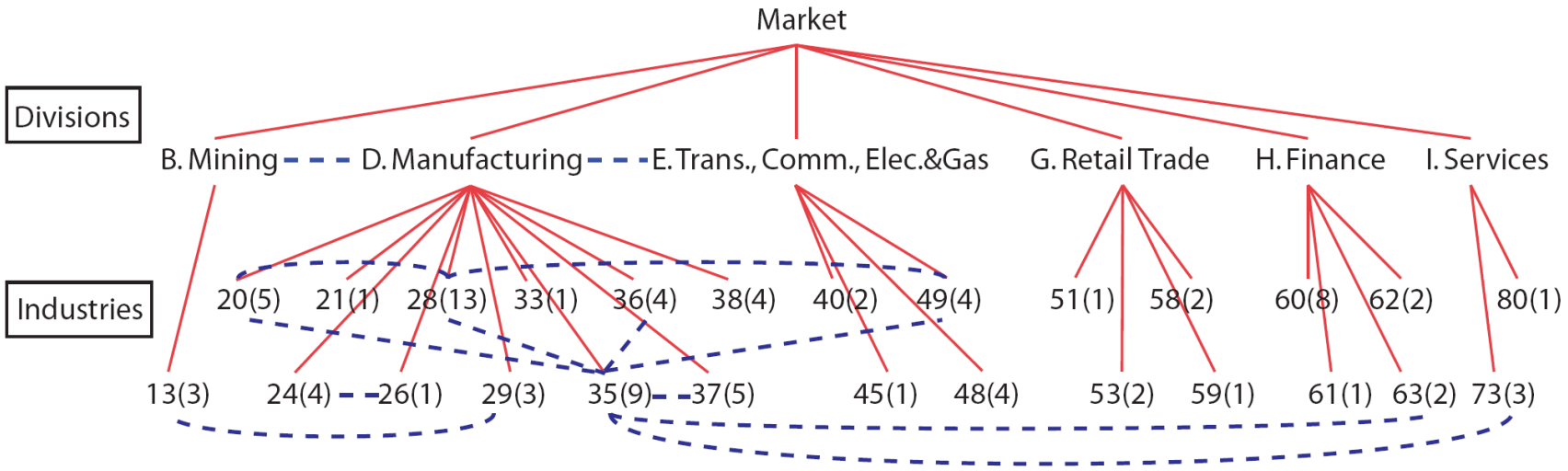
Compute last term via sparse equation

$$\Sigma^c z = x_{old}$$



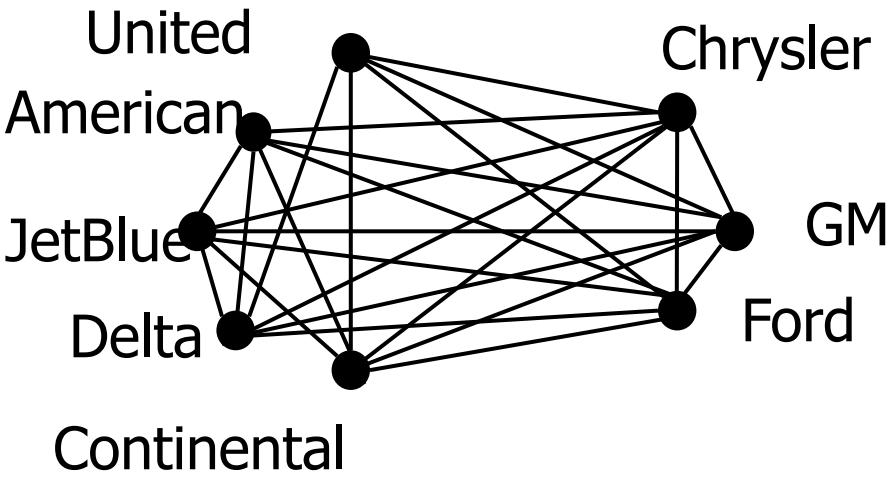
$$x_{new} = \Sigma^c (h - J^h x_{old})$$

Stock Returns Example

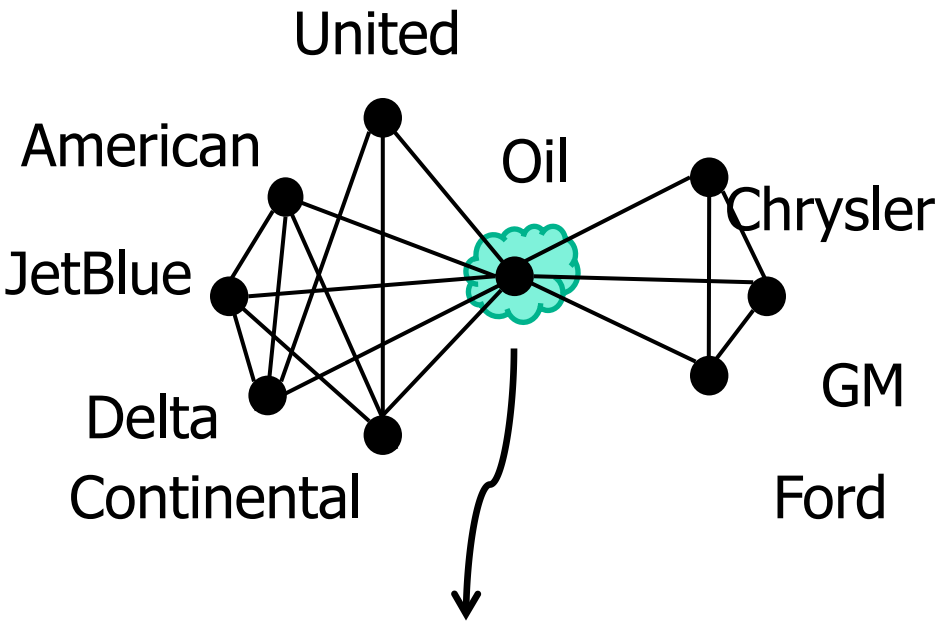


- Monthly returns of 84 companies in the S&P 100 index (1990-2007)
- Hierarchy based on the Standard Industrial Classification system
- Market, 6 divisions, 26 industries, and 84 individual companies
- Conjugate edges find strong residual correlations
  - Oil service companies (Schlumberger,…) and oil companies
  - Computer companies, Software companies, electrical equipment
  - …

What If Some Phenomena Hidden?



- **Many dependencies among observed variables**
- Less concise model



- **Hidden variables**
  - Hedge fund investments,
  - Patent accepted/rejected,
  - Geopolitical factors,
  - Regulatory issues, …

Graphical Models With Hidden Variables: Sparse Modeling Meets PCA

$$X = (X_O, X_H) \sim \mathcal{N}(0, \Sigma)$$

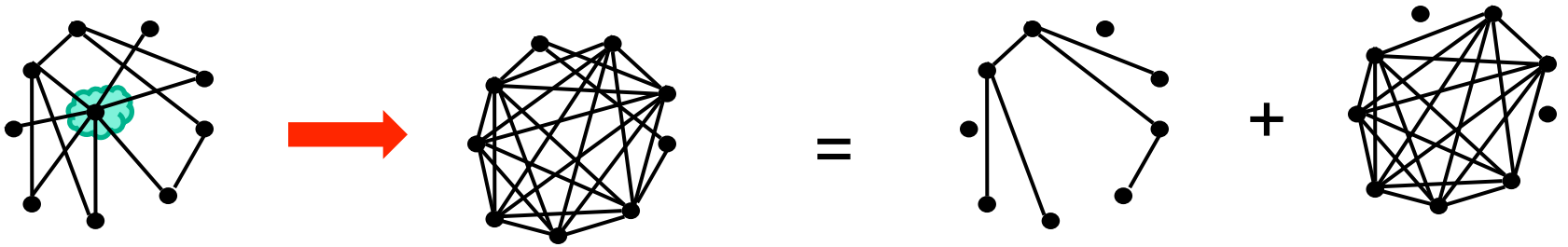
$$\Sigma = \begin{bmatrix} \Sigma_O & \Sigma_{O,H} \\ \Sigma_{H,O} & \Sigma_H \end{bmatrix} \qquad \Sigma^{-1} = K = \begin{bmatrix} K_O & K_{O,H} \\ K_{H,O} & K_H \end{bmatrix}$$

Marginal concentration matrix

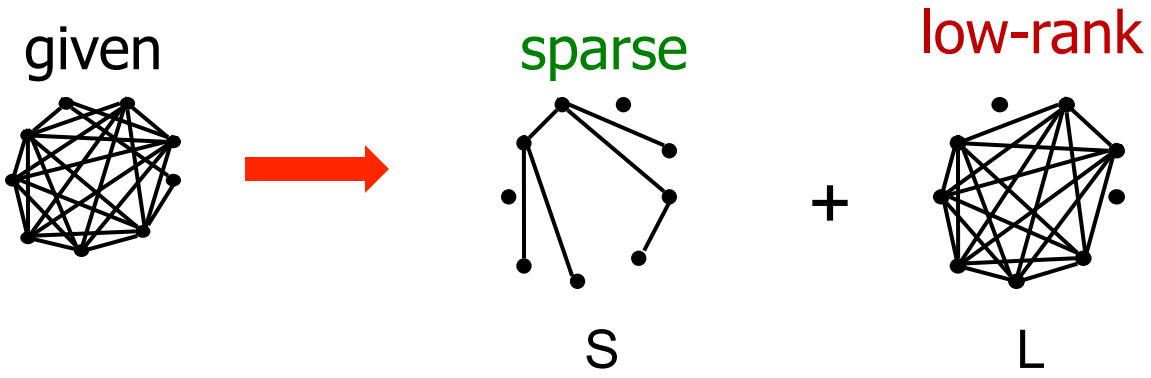
$$(\Sigma_O)^{-1} = K_O - K_{O,H} K_H^{-1} K_{H,O}$$

Sparse

Low-rank



Convex Optimization for Modeling



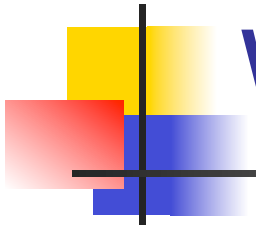
- Samples of obs. vars.: $\mathcal{D}_n = \{X_O^1, \ldots, X_O^n\}$

$$(\hat{S}_n, \hat{L}_n) = \arg\min_{S,L} \; -\tfrac{1}{n} \log \text{lik.}\,(S\text{–}L;\; \mathcal{D}_n) \;+\; \lambda_n \left[\gamma \|S\|_1 + \text{trace}(L)\right]$$

$$\text{s.t.} \quad S - L \succ 0, \;\; L \succeq 0.$$

- Last two terms provide convex regularization for sparsity in *S* and low-rank in *L*
- Weights allow tradeoff between sparsity and rank

When does this work?



- Identifiability conditions
  - The sparse part can't be low rank and the low rank part can't be sparse
- There are precise conditions (including conditions on regularization weights) that guarantee
  - Exact recovery if exact statistics are given
  - Consistency results if samples are available ("with high probability" scaling laws on problem dimension and available sample size)

On the way: Construct richer classes of models for which inference is ***easy***

- We have
  - Methods to learn hidden trees with fixed structure but unknown variable dimensions
  - Method to learn hidden trees with unknown structure but fixed (scalar) variable dimension
- Can we do both at the same time?
- We have method for recovering sparse plus low rank
  - How about ***tree*** plus low rank (i.e., small FVS)?
- Message-passing algorithms are distributed dynamic systems. How about designing better ones than LBP?