Probabilistic Logic and Deep Learning

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Research Proficiency Examination

Agenda

- **Deep Learning**
- Logical Student-Teacher Network
- Probabilistic Logic Programming
- TensorLog
- Conclusion

Deep Neural Networks

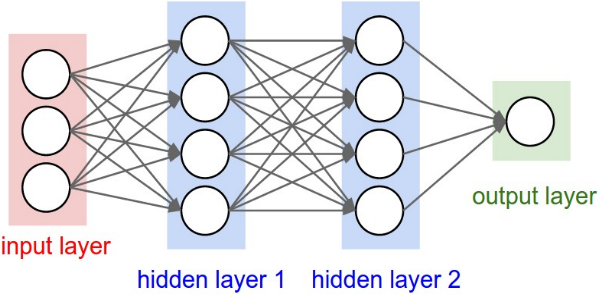

Figure: A two layer neural network $g(\mathbf{x}) = o(h_2(h_1(x)))$.

- $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{y} \in \mathbb{R}$
- $h_1(\mathbf{x}) = \phi_1(W_1\mathbf{x} + b_1)$
- $h_2(h_1(\mathbf{x})) = \phi_2(W_2 h_1(\mathbf{x}) + b_2)$
- $o(h_2(h_1(\mathbf{x}))) = \psi(W_3\phi_2(\phi_1(\mathbf{x})) + b_3)$

Deep Neural Networks

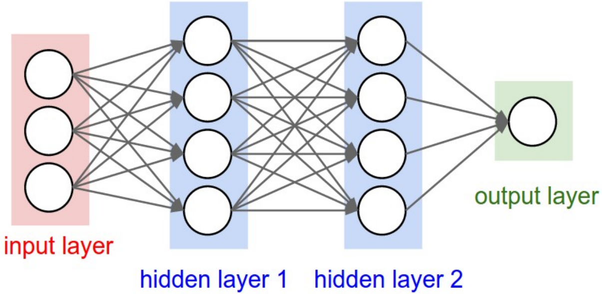

Figure: A two layer neural network $g(\mathbf{x}) = o(h_2(h_1(x)))$.

- Each ϕ_i is a nonlinear function applied element-wise to the hidden layer output.
- Ex: tanh, ReLu, logistic sigmoid
- ψ_j is a function applied to the output layer output.
- Ex: identity, softmax

Deep Neural Networks

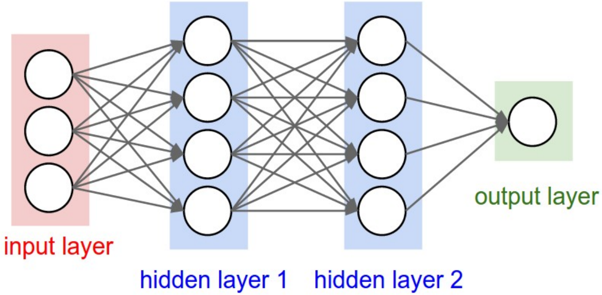

Figure: A two layer neural network $g(\mathbf{x}) = o(h_2(h_1(x)))$.

- A loss (objective, reward, etc) function is defined with respect to the output of the network and the ground truth label.
- Ex: MSE is $\sum_i (\mathbf{y}^{(i)} - g(\mathbf{x}^{(i)}))^2$

Deep Neural Networks

Data: Training data $\mathcal{S} = \{(\mathbf{x}^{(n)}, \mathbf{y}^{(n)})\}_{n=1}^{N}$,
Hyperparameters: η learning rate
Result: $\boldsymbol{\theta}^*$ which minimizes $\mathcal{L}$

Initialize DNN parameters $\boldsymbol{\theta}$
while $\neg$ *converged* **do**
    Sample a minibatch $(X, Y) \subset \mathcal{S}$
    Set $g \leftarrow 0$
    for $(\mathbf{x}, \mathbf{y}) \in (X, Y)$ **do**
        Compute gradient: $g \leftarrow g + \nabla_\theta \mathcal{L}(f_\theta(\mathbf{x}), \mathbf{y}; \boldsymbol{\theta})$
    end
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta g$
end

Algorithm 1: Stochastic Gradient Descent

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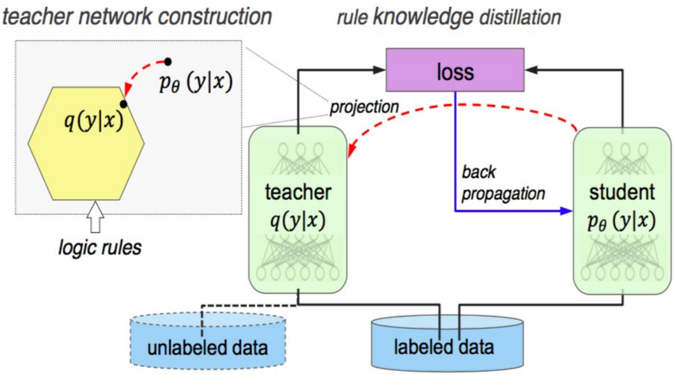
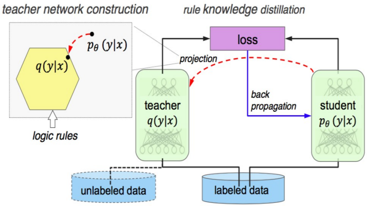
Architecture



Loss Function



$$\theta^{(t+1)} = \operatorname*{argmin}_{\theta \in \Theta} \frac{1}{N} \sum_{n=1}^{N} (1-\pi)\mathcal{L}(\mathbf{y}_n, \boldsymbol{\sigma}_\theta(\mathbf{x}_n)) + \pi \mathcal{L}(s_n^{(t)}, \boldsymbol{\sigma}_\theta(\mathbf{x}_n)) \quad (1)$$

- $\mathbf{x}_n, \mathbf{y}_n$: *nth* sample
- $\mathcal{L}$ is an arbitrary loss (assume cross-entropy)
- π is the mixture weight between student and teacher networks
- $\boldsymbol{\sigma}_\theta(\mathbf{x}_n)$ is the output from the student network (assumed to be a softmax vector)
- $s_n^{(t)}$: teacher network output at iteration t

Logic Rules

- $\mathcal{R} = \{(R_l, \lambda_l)\}_{l=1}^{L}$ where each R_l is a first-order logic formula with an associated confidence $\lambda_l \in [0, \infty]$.
- These rules are encoded using a continuous logic called soft logic which allows continuous truth values $\in [0, 1]$ with the following semantics:

$$\begin{aligned} \neg A &= 1 - A \\ A \& B &= \max\{A + B - 1, 0\} \\ A \vee B &= \min\{A + B, 1\} \\ A_1 \wedge \ldots \wedge A_N &= \sum_i A_i / N \end{aligned} \tag{2}$$

Teacher Network Construction

Loss function

$$
\begin{aligned}
&\min_{q,\xi \geq 0} \mathrm{KL}(q(Y|X)||p_\theta(Y|X)) + C \sum_{l,g_l} \xi_{l,g_l} \\
&\text{s.t. } \lambda_l(1 - \mathbf{E}_q[r_{l,g_l}(X,Y)]) \leq \xi_{l,g_l} \\
&g_l = 1, ..., G_l, l = 1, ..., L.
\end{aligned} \tag{3}
$$

- Intuitively, we want the teacher network distribution q to be close to the student network p_θ, so we use a KL term.
- Additionally we want the soft logic rules to approximately hold, so we use an expectation term in the constraints and introduce slack variables ξ.

Teacher Network Construction

Dual Lagrangian

Rewrite (3) in standard form.

$$\min_{q,\xi} \mathrm{KL}(q(Y|X)||p_\theta(Y|X)) + C\sum_{l,g_l}\xi_{l,g_l}$$

$$\text{s.t. } \lambda_l(1 - \mathbf{E}_q[r_{l,g_l}(X,Y)]) - \xi_{l,g_l} \leq 0$$

$$-\xi_{l,g_l} \leq 0$$

$$\sum_Y q(Y|X) - 1 = 0$$

$$g_l = 1, ..., G_l, l = 1, ..., L$$

Then add Lagrange multipliers and simplify (algebra)

$$\max_{\eta\geq 0,\mu\geq 0,\alpha\geq 0}\min_{q,\xi} \mathrm{KL}(q(Y|X)||p_\theta(Y|X)) + C\sum_{l,g_l}\xi_{l,g_l}$$

$$+\sum_{l,g_l}\eta_{l,g_l}(\mathbf{E}_q[\lambda_l(1 - r_{l,g_l}(X,Y))] - \xi_{l,g_l}) - \sum_{l,g_l}\mu_{l,g_l}\xi_{l,g_l} + \alpha(\sum_Y q(Y|X)$$

Teacher Network Construction

Teacher Construction Rule

By solving the dual Lagrangian we obtain the teacher network construction rule:

$$q^*(Y|X) \propto p_\theta(Y|X) \exp\left\{ -\sum_{l,g_l} C\lambda_l (1 - r_{l,g_l}(X,Y)) \right\}. \quad (4)$$

- $q^*(Y|X)$ can be computed efficiently for a given example $\mathbf{x}$
- We simply feed $\mathbf{x}$ as input to the student network and use the output vector $\boldsymbol{\sigma}_\theta(\mathbf{x})$ as $p_\theta(Y|X)$ in the above expression.
- Thus an inference step in the teacher network will have complexity of the order $O(lg_l + \mathcal{I})$ where $\mathcal{I}$ is the complexity of inference in the student network.

Learning Algorithm

Data: Training data $\mathcal{S} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$,
Rule set $\mathcal{R} = \{(R_l, \lambda_l)\}_{l=1}^L$,
Hyperparameters: π imitation parameter,
C regularization strength

Result: Trained networks p_θ and q

Initialize DNN parameters $\boldsymbol{\theta}$
while $\neg$ *converged* **do**
  Sample a minibatch $(X, Y) \subset \mathcal{S}$
  Construct teacher network q using (4)
  Update $\boldsymbol{\theta}$ using (1)
end

Algorithm 2: Teacher and Student Network Training

Sentence Level Sentiment Analysis

Student Network Architecture

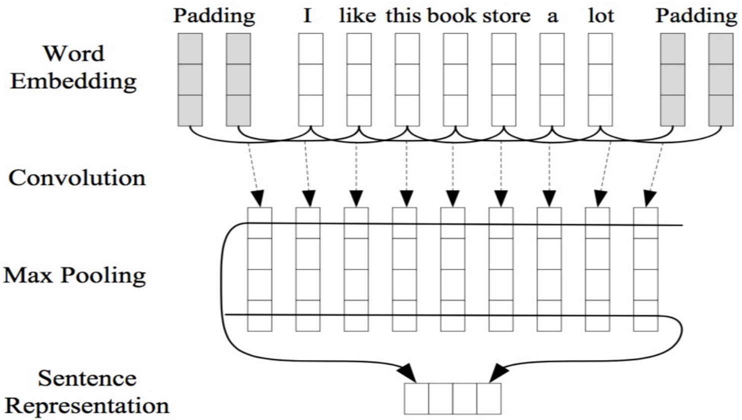


Figure: CNN architecture using Word2Vec vectors.

Sentence Level Sentiment Analysis

Logic Rule

$$\text{has-A-but-B-structure}(S) \Rightarrow$$
$$(\mathbf{1}(y=+) \Rightarrow \boldsymbol{\sigma}_\theta(B)_+ \wedge \boldsymbol{\sigma}_\theta(B)_+ \Rightarrow \mathbf{1}(y=+)),$$

- Intuitively, if a sentence has a "but" in it we should take the sentiment of the subsentence after the "but".
- "At first I thought the movie was great but it turned out to be derivative and boring."

Sentence Level Sentiment Analysis

Results

	Model	SST2	MR	CR
1	CNN (Kim, 2014)	87.2	81.3±0.1	84.3±0.2
2	CNN-Rule-*p*	88.8	81.6±0.1	85.0±0.3
3	CNN-Rule-*q*	89.3	**81.7±0.1**	**85.3±0.3**
4	MGNC-CNN (Zhang et al., 2016)	88.4	–	–
5	MVCNN (Yin and Schutze, 2015)	**89.4**	–	–
6	CNN-multichannel (Kim, 2014)	88.1	81.1	85.0
7	Paragraph-Vec (Le and Mikolov, 2014)	87.8	–	–
8	CRF-PR (Yang and Cardie, 2014)	–	–	82.7
9	RNTN (Socher et al., 2013)	85.4	–	–
10	G-Dropout (Wang and Manning, 2013)	–	79.0	82.1

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Logical Inference and Neural Networks

- Logical specifications allow one to model aspects of the world and perform **logical inference**.
- In Prolog this is done using SLD-resolution, which is a search procedure over proofs for a query.
- Discrete search is not a differentiable function, and thus cannot directly be integrated in gradient-based learning systems.

TensorLog

- TensorLog proposes a differentiable (probabilistic) logical inference procedure.
- This algorithm can be seen as an instance of the Belief Propagation algorithm for probabilistic graphical models.
- Thus TensorLog offers a method of incorporating traditional logical inference as a component of a DNN.
- Alternatively, TensorLog offers a method of incorporating DNNs for traditional logical inference.

Example TensorLog Model

```
% Theory T
uncle(X, Y) :- child(X, Z), brother(Z, Y).
uncle(X, Y) :- aunt(X, W), husband(W, Y).
status(X, tired) :- child(W, X), infant(W).

% Knowledge Base DB
0.99 :: child(liam, eve).      0.7 :: infant(liam).
0.99 :: child(dave, eve).      0.1 :: infant(dave).
0.75 :: child(liam, bob).      0.9 :: aunt(joe, eve).
0.9 :: husband(eve, bob).      0.9 :: brother(eve, chip).
```

Figure: Example $\mathcal{DB}$ and $\mathcal{T}$.

Logical Preliminaries

- A **database** $\mathcal{DB} = \{f_1, ..., f_N\}$ where each f_i is a ground **fact**.
- A fact is of the form $p(a, b)$ or $q(c)$ where p and q are predicate symbols and $a, b, c \in \mathcal{C}$ are constant symbols from domain $\mathcal{C}$.
- A theory $\mathcal{T}$, is a set of function-free Horn clauses.
- The least model for $(\mathcal{DB}, \mathcal{T})$ is written $Model(\mathcal{DB}, \mathcal{T})$.
- A fact f is true iff $f \in Model(\mathcal{DB}, \mathcal{T})$

Probabilistic Logical Preliminaries

- Θ is a parameter vector over the facts $f \in \mathcal{DB}$ s.t. $\theta_f \in [0, 1]$.
- The semantics of this parameter vary in different probabilistic deductive database models
- Θ defines a distribution $Pr(f|\mathcal{T}, \mathcal{DB}, \Theta)$ over facts in $Model(\mathcal{T}, \mathcal{DB})$.

TensorLog Logical Restrictions

- TensorLog is function free.
- Predicates in TensorLog have arity at most 2.
- Queries are of the form $q(a, X) \leftarrow b_1(a, c), ..., b_k(z, b)$. or $q(X, b) \leftarrow b_1(a, c), ..., b_k(z, b)$.
- Thus we are interested in all relationships between some constant a and all other constants b s.t. $q(a, X)[X/b]$ holds in the theory.
- TensorLog only models restricted Datalog programs of this form and does so using matrix representations of predicates and constants.

TensorLog Matrix Representation

- It is assumed that there is some arbitrary order on $c \in C$ corresponding to indices $[1, ..., |C|]$ which holds in all matrices and vectors.
- Constants $c \in C$ are represented using a one-hot row-vector $\mathbf{u} \in \mathbf{R}^{|C|}$.
- Binary predicates are represented as a sparse matrix $\mathbf{M}_r$ where $\mathbf{M}_r[i, j] = \theta_{r(i,j)}$ if $r(i, j) \in \mathcal{DB}$, and 0 otherwise.
- A unary predicate q is represented analogously as a row-vector $\mathbf{v}_q$.

TensorLog Matrix Representation Example

```
% Knowledge Base DB
0.99 :: child(liam, eve).      0.7 :: infant(liam).
0.99 :: child(dave, eve).      0.1 :: infant(dave).
0.75 :: child(liam, bob).      0.9 :: aunt(joe, eve).
0.9 :: husband(eve, bob).      0.9 :: brother(eve, chip).
```

When the order is [*liam*, *eve*, *dave*, *bob*, *joe*, *chip*],

$$\mathbf{M}_{child} = \begin{bmatrix} \theta_{child(liam,liam)} & \theta_{child(liam,eve)} & \cdots & \theta_{child(liam,chip)} \\ \theta_{child(eve,liam)} & \theta_{child(eve,eve)} & \cdots & \theta_{child(eve,chip)} \\ \hdotsfor{4} \\ \theta_{child(chip,liam)} & \theta_{child(chip,eve)} & \cdots & \theta_{child(chip,chip)} \end{bmatrix}$$

$$\mathbf{v}_{infant} = \begin{bmatrix} 0.7 & 0 & 0.1 & 0 & 0 & 0 \end{bmatrix}$$

We will use matrix multiplication to implement logical inference.

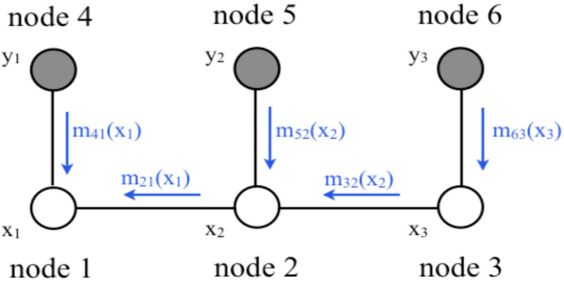
Probabilistic Graphical Models I

- A probabilistic graphical model (PGM) represents the joint probability distribution of a set of random variables $Pr(X)$.
- Naively the joint factorizes as $Pr(X = x_1, x_2, ..., x_n) = Pr(x_1) \times Pr(x_2|x_1) \times ... \times Pr(x_n|x_{n-1}, x_{n-2}, ..., x_2, x_1)$
- Generally, we want factorizations which minimize the number of parameters. We achieve this by introducing conditional independence relations.
- Ex: Bayesian networks (directed graphical models) encode the factorization as

$$p(X) = \prod_i p(x_i|\pi(x_i))$$

where $\pi(x) = \{x' : (x', x) \in E\}$.

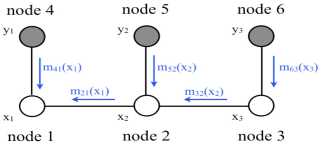
Probabilistic Graphical Models II



Markov chain with three observed variables y_1, y_2, y_3 and three hidden variables x_1, x_2, x_3. The factorization of this example is:

$$p(X, Y) = \frac{1}{Z}\psi_{12}(x_1, x_2)\psi_{23}(x_2, x_3)\phi_1(x_1, y_1)\phi_2(x_2, y_2)\phi_3(x_3, y_3).$$

Probabilistic Graphical Models III

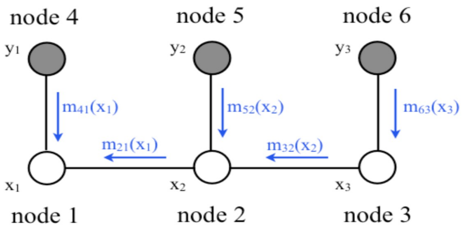


- In practice we will be interested in using a PGM to perform inference over some subset of the random variables; ie. computing the probability of the subset $p(X' \subseteq X)$.
- Assume that we wish to compute the marginal probability of x_1 given Y:

$$p(x_1|Y) = \frac{1}{p(Y)} \sum_{X_2} \sum_{X_3} p(X, Y),$$

where the equation is due to the fact that $p(X|Y) = \frac{p(X,Y)}{p(Y)}$.

Belief Propagation I



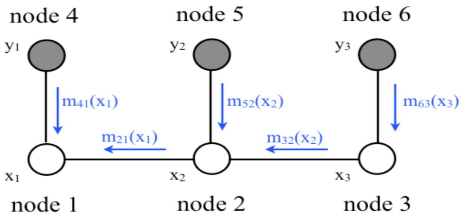
$$p(x_1|Y) = \frac{1}{p(Y)} \sum_{X_2} \sum_{X_3} p(X, Y)$$

$$= \frac{1}{p(Y)} \sum_{X_2} \sum_{X_3} \psi_{12}(x_1, x_2)\psi_{23}(x_2, x_3)\phi_1(x_1, y_1)\phi_2(x_2, y_2)\phi_3(x_3, y_3).$$

$$= \frac{1}{p(Y)} \phi_1(X_1, y_1) \sum_{X_2 = x_2} \psi_{12}(X_1, x_2)\phi_2(x_2, y_2) \sum_{X_3 = x_3} \psi_{23}(x_2, x_3)\phi_3(x_3, y_3)$$

$$= \frac{1}{p(Y)} m_{41}(x_1) \sum_{X_2 = x_2} \psi_{12}(X_1, x_2) m_{52}(x_2) \sum_{X_3 = x_3} \psi_{23}(x_2, x_3) m_{63}(x_3)$$

Belief Propagation II



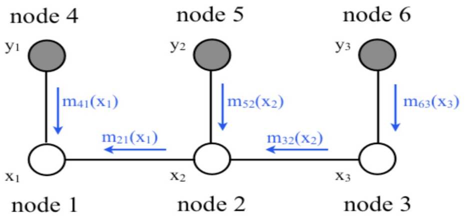
$$\frac{1}{p(Y)} m_{41}(x_1) \sum_{X_2=x_2} \psi_{12}(X_1, x_2) m_{52}(x_2) \sum_{X_3=x_3} \psi_{23}(x_2, x_3) m_{63}(x_3)$$

Let's take a closer look at these messages.

- $m_{41}(x_1) = \phi_1(x_1, y_1)$
- $m_{52}(x_2) = \phi_2(x_2, y_2)$
- $m_{63}(x_3) = \phi_3(x_3, y_3)$

All of these messages are scalars which are known.

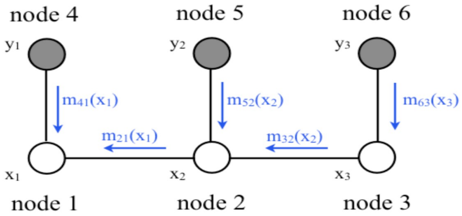
Belief Propagation III



$$
\begin{aligned}
&\frac{1}{p(Y)} m_{41}(x_1) \sum_{X_2=x_2} \psi_{12}(X_1, x_2) m_{52}(x_2) \sum_{X_3=x_3} \psi_{23}(x_2, x_3) m_{63}(x_3) \\
&= \frac{1}{p(Y)} m_{41}(x_1) \sum_{X_2=x_2} \psi_{12}(X_1, x_2) m_{52}(x_2) m_{32}(x_2) \\
&= \frac{1}{p(Y)} m_{41}(x_1) m_{21}(x_1).
\end{aligned}
$$

Finally, if we were to compute say $p(x_2|Y)$ we would be able to reuse many of these messages.

Belief Propagation IV

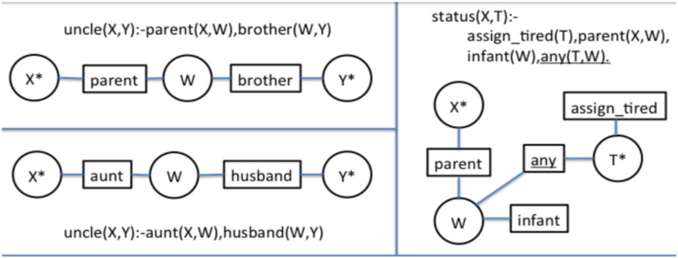


- BP for undirected graphical models is defined as follows:
  1. Convert the PGM to an equivalent PGM with only pairwise potentials.
  2. Compute $m_{ji}(x_i)$ as:

$$m_{ji}(x_i) = \sum_{X_j = x_j} \psi_{ij}(x_i, x_j) \prod_{k \in N(j) \setminus i} m_{kj}(x_j).$$

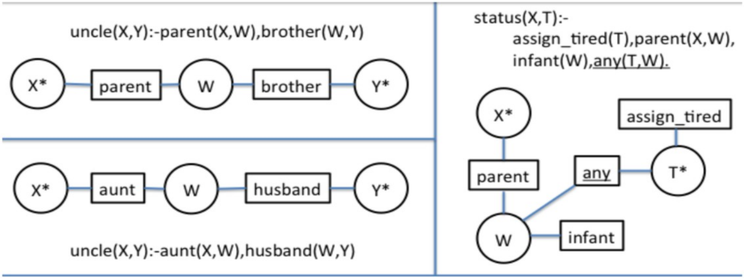
- In English: The message from some x_j to x_i is computed as the sum over products of all neighbors of n_j (except n_i) and then weighted by the "compatibility" between n_j and n_i.

TensorLog Factor Graphs I



- TensorLog converts rules $r \in \mathcal{T}$ into factor graphs G_r.
- A factor graph is like an undirected graphical model which explicitly represents factors as nodes.
- Predicate symbols become factors which have edges connected to logical variables which are the arguments of the predicate.
- The matrix of a factor node for predicate p is exactly $\mathbf{M}_p$.

TensorLog Factor Graphs II



- Special `any/2` and `assign/1` predicates are introduced.
- `any/2` holds for any two constants in the language with probability 1. It is used to connect disjoint factor graphs.
- `assign/1` is a syntactic restriction which is "algorithmically convenient".

TensorLog Inference I

G_r defines a distribution over possible groundings of the variables in r. Let $X_1, ..., X_m$ be the variables in r. Then:

$$Pr_{G_r}(X_1 = c_1, ..., X_m = c_m) = \frac{1}{Z} \prod_{(c_i, c_j) \in E_r} \phi_r(c_i, c_j) = \prod_{(c_i, c_j) \in E_r} \theta_{r(c_i, c_j)}.$$

If $r(c_i, c_j) \notin \mathcal{DB}$ any substitution $r(X_i, X_j)\{X_i/c_i, X_j/c_j\}$ will have 0 probability.

TensorLog Inference II

Assume that we are interested in the query `uncle(c, Y)` for some $c \in C$. We will perform BP over G_{uncle} conditioned on $X = c$. This corresponds to the following linear transformation:

$$(\mathbf{u}_c \mathbf{M}_{parent}) \mathbf{M}_{brother}.$$

Recall that $\mathbf{u}_c$ is a one-hot vector which encodes the position of the constant $c \in C$. Then $\mathbf{v}_W = \mathbf{u}_c \mathbf{M}_{parent}$ is a vector where $\mathbf{v}_W[c'] = \theta_{parent(c,c')}$. Finally $\mathbf{v}_Y = \mathbf{v}_W \mathbf{M}_{brother}$ computes the marginal probability for Y which is exactly what BP does in the message passing steps.

TensorLog Inference III

- BP in G_r corresponds to simple linear transformations of the probability vector representations over $\mathcal{KB}$.
- In the case where some predicate is defined in multiple rules we simply return the sum of the response vectors for the individual definitions.
- For example, $g_{io}^{\texttt{uncle}}(\mathbf{u}_c) = g_{io}^{\texttt{uncle}_1}(\mathbf{u}_c) + g_{io}^{\texttt{uncle}_2}(\mathbf{u}_c)$ where $\texttt{uncle}_i$ is the *ith* definition for the predicate.
- If a predicate r is defined by some $r' \in \mathcal{T}$ (as opposed to some $r' \in \mathcal{DB}$) we replace $\mathbf{v}_{F,X} \leftarrow \mathbf{v}_i \mathbf{M}_r$ with $\mathbf{v}_{F,X} \leftarrow g_{io}^{r'}(\mathbf{v}_i)$ in compileMessage($F \rightarrow X$).

TensorLog BP Algorithm

Function *compileMessage*($F \to X$)*:*

Data: Factor F representing $r(X)$ or $r(X_i, X_o)$,
Random variable X representing the logical variable

Result: Message from F to X: $\mathbf{v}_{F,X}$

if $F = r(X)$ **then**
  $\mathbf{v}_{F,X} \leftarrow \mathbf{v}_r$
else if X *is the output variable* X_o *of* F **then**
  $\mathbf{v}_i \leftarrow \text{compileMessage}(X_i \to F)$
  $\mathbf{v}_{F,X} \leftarrow \mathbf{v}_i \mathbf{M}_r$
else if X *is the input variable* X_i *of* F **then**
  $\mathbf{v}_o \leftarrow \text{compileMessage}(X_o \to F)$
  $\mathbf{v}_{F,X} \leftarrow \mathbf{v}_o \mathbf{M}_r^\top$
end
return $\mathbf{v}_{F,X}$

TensorLog BP Algorithm

Function *compileMessage*$(X \to F)$:

Data: Random variable X representing the logical variable,
Factor F representing $r(X)$ or $r(X_i, X_o)$

Result: Message from X to F: $\mathbf{v}_{X,F}$

if *X is the given variable to the query* **then**
  $\mathbf{v}_{X,F} \leftarrow \mathbf{u}_c$ // return the one-hot vector
// if the only factor which has X as an argument is F:
else if $\eta(X) = \{F\}$ **then**
  $\mathbf{v}_{X,F} \leftarrow \mathbf{1}$ // return a vector of all 1's
else
  // loop over all k of X's neighbor literals F_i except F
  foreach $F_i \in \eta(X) \setminus F$ **do**
    $\mathbf{v}_i \leftarrow$ compileMessage$(F_i \to X)$
  end
  $\mathbf{v}_{X,F} \leftarrow \mathbf{v}_1 \circ \ldots \circ \mathbf{v}_k$ // $\circ$ is the element-wise product
end
return $\mathbf{v}_{X,F}$

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