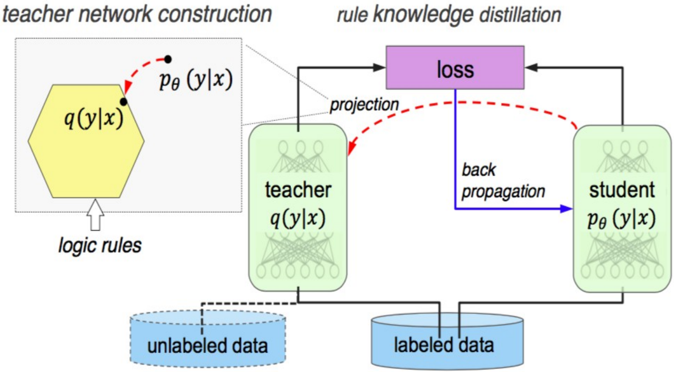
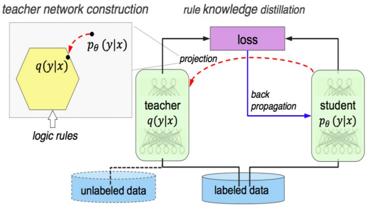
TensorLog: A Differentiable Deductive Database

William W. Cohen
Presenter: Tim Zhang

Architecture



Loss Function



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

- $\mathbf{x}_n, \mathbf{y}_n$: *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

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

- 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.

Note: the strange indexing has to do with the set of groundings of the first-order logic rules and can simply be ignored without hurting understanding.

Teacher Network Construction

Dual Lagrangian

Rewrite (3) in standard form.

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

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

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

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

$$g_l = 1, \ldots, G_l, l = 1, \ldots, L$$

Then add Lagrange multipliers and simplify (algebra)

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

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

Teacher Network Construction

Teacher Construction Rule

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

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

It is immediately apparent that $q^*(Y|X)$ 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 1: Teacher and Student Network Training

Sentence Level Sentiment Analysis

Student Network Architecture

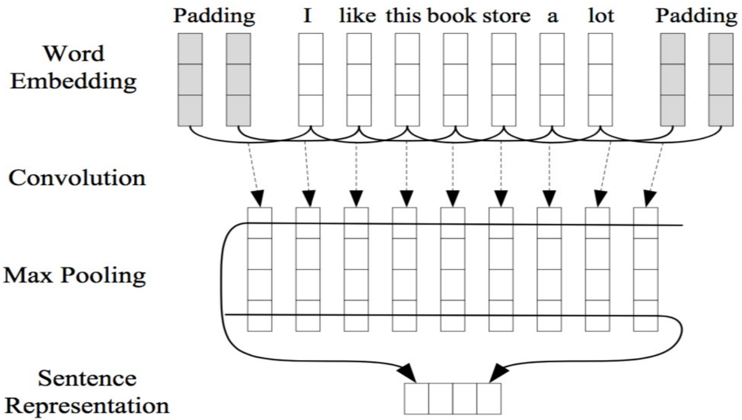


Figure: CNN architecture using Word2Vec vectors.

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 terrible.

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

Logic 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.

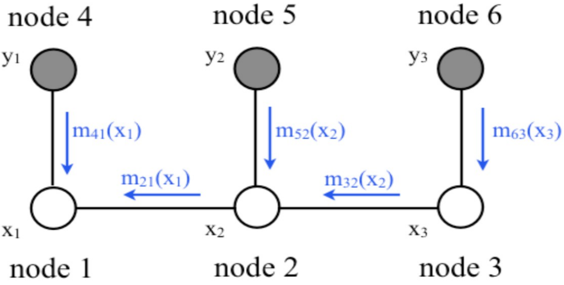
Probabilistic Graphical Models I

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

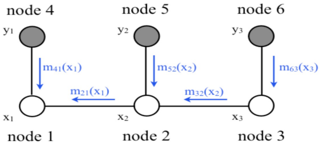
Probabilistic Graphical Models II



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

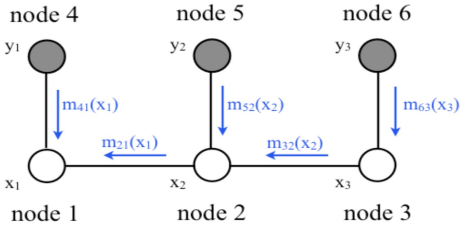


- In practice we will be interested in using a PGM to perform inference over some subset of the random variables; ie. computing the probability of the subset $p(X' \subseteq X)$.
- Assume that we wish to compute the marginal probability of x_1 given Y:

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

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

Belief Propagation I



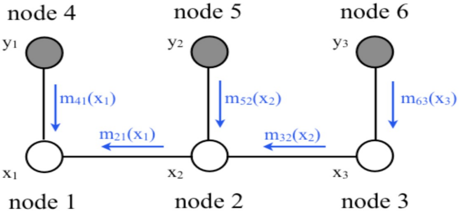
$$p(x_1|Y) = \frac{1}{p(Y)} \sum_{X_2} \sum_{X_3} p(X, Y)$$

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

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

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

Belief Propagation II



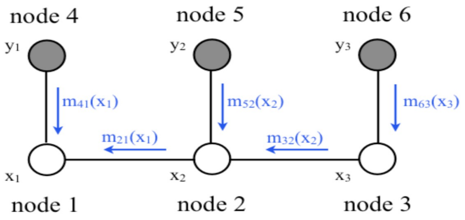
$$\frac{1}{p(Y)} m_{41}(x_1) \sum_{X_2=x_2} \psi_{12}(X_1, x_2) m_{52}(x_2) \sum_{X_3=x_3} \psi_{23}(x_2, x_3) m_{63}(x_3)$$

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.

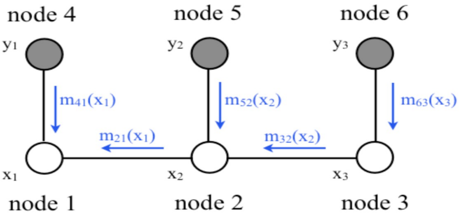
Belief Propagation III



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

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

Belief Propagation IV

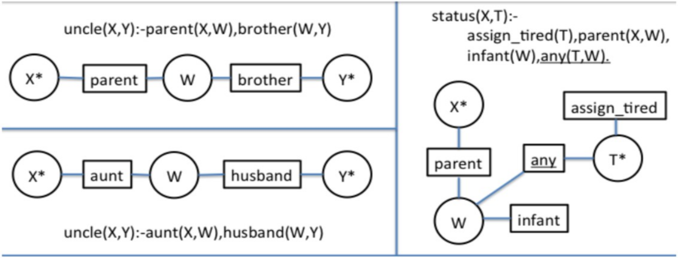


- BP for undirected graphical models is defined as follows:
  1. Convert the PGM to an equivalent PGM with only pairwise potentials.
  2. Compute $m_{ji}(x_i)$ as:

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

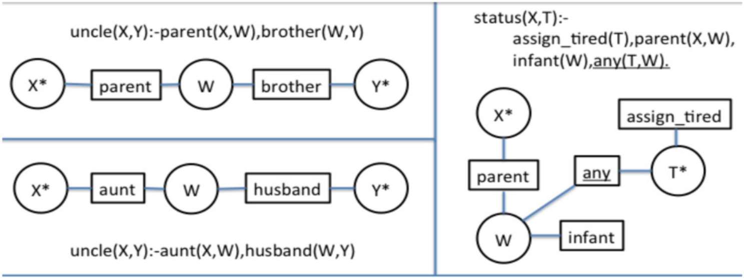
- In English: The message from some x_j to x_i is computed as the sum over products of all neighbors of n_j (except n_i) and then weighted by the "compatibility" between n_j and n_i.

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, $g_{io}^{\mathtt{uncle}}(\mathbf{u}_c) = g_{io}^{\mathtt{uncle}_1}(\mathbf{u}_c) + g_{io}^{\mathtt{uncle}_2}(\mathbf{u}_c)$ where $\mathtt{uncle}_i$ 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*($X \rightarrow F$):

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($F_i \rightarrow X$)
  end
  $\mathbf{v}_{X,F} \leftarrow \mathbf{v}_1 \circ \ldots \circ \mathbf{v}_k$ // $\circ$ is the element-wise product
end
return $\mathbf{v}_{X,F}$