Learning to Reason: From Theory to Practice

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Outline

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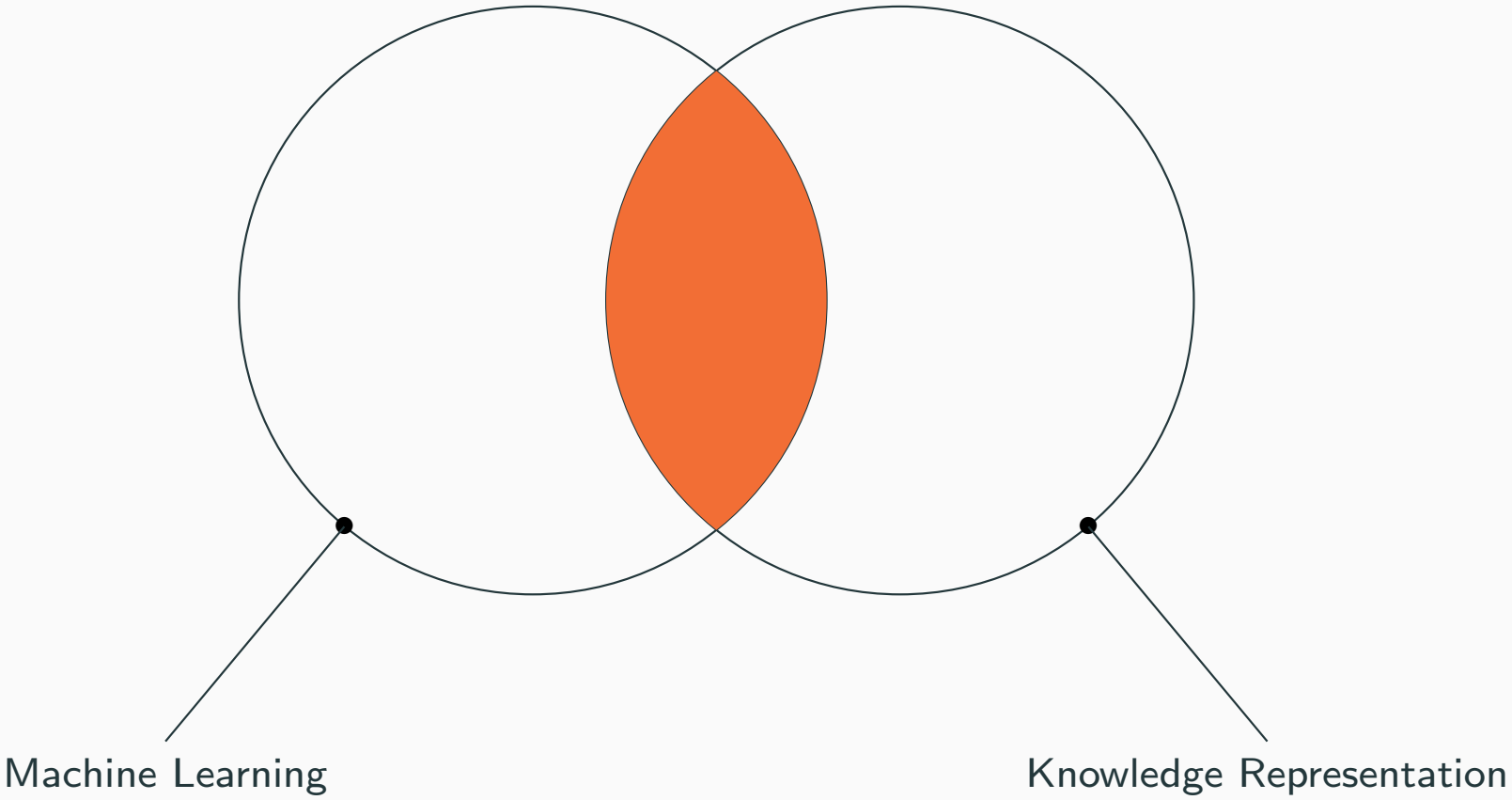

Learning to Reason (L2R) is a research topic that lies at the intersection of Machine Learning and Knowledge Representation. The key challenge is to develop algorithms capable of performing inference tasks from experience.

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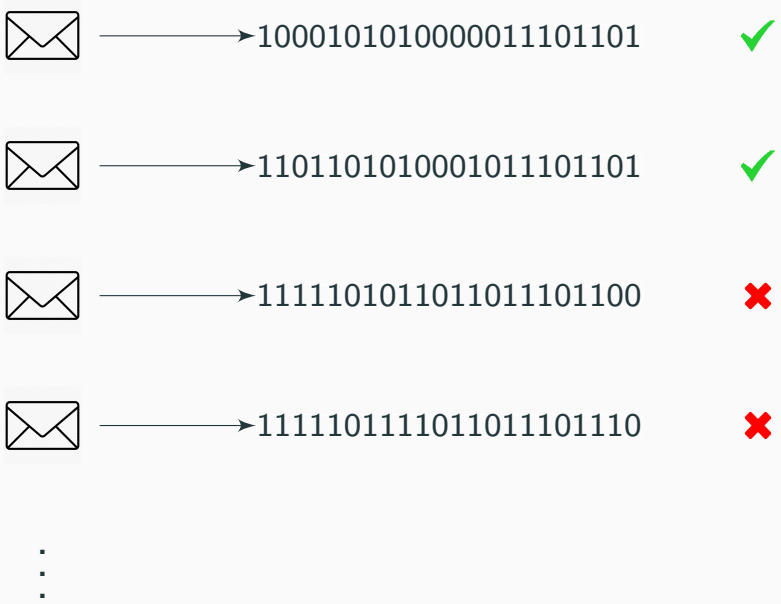
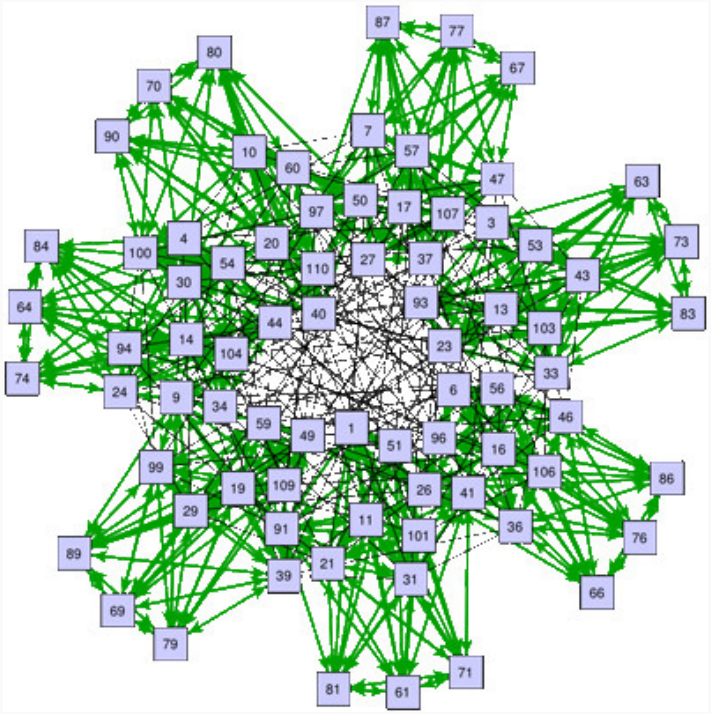
- **Computational Barrier:** Many, if not most, reasoning tasks are related to NP-hard problems. Learning useful patterns from observed instances can be relevant for solving - or helping a solver in handling - new instances.
- **Adaptivity:** In many tasks, the distribution of instances is susceptible to change over time (ex: visual scenes). Online learning algorithms are, by nature, adaptative to those changes.



Consider a spam filtering problem: the goal is to predict whether each incoming message, characterized by its feature vector x, is a spam (✓) or not (✖).

This is a standard classification task.



01**1100011***** ✓

*1*011*1100011**110000 ✓

000100*1000011**1*1001 ✗

111111*1100001***1010* ✗

1*00*1*1*00000**110000 ✓

100010*0*00000**101101 ✓

⋮

Suppose we have a (fixed) constraint network representing our knowledge about some application (scheduling, planning, etc.). The goal is to predict whether each incoming *partial assignment* x can be extended (✓) to a *total satisfying assignment*, or not (✗).

This is a much more difficult global consistency task.

$(x_1 \vee x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee \overline{x}_3) \wedge (x_1 \vee \overline{x}_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee x_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee x_3) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee \overline{x}_3)$ ✖

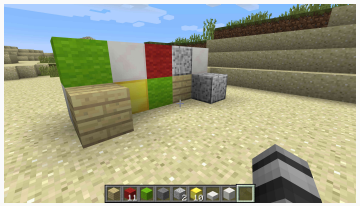
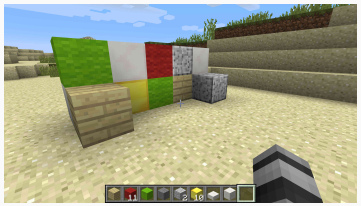
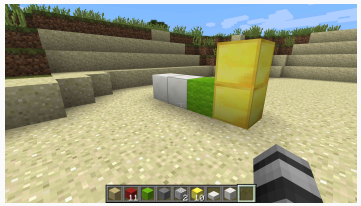
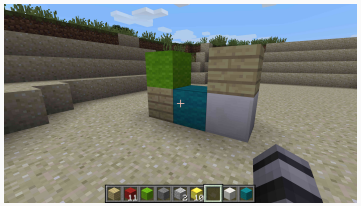
$(x_1 \vee x_2 \vee x_4) \wedge (x_1 \vee x_2 \vee \overline{x}_3) \wedge (x_1 \vee \overline{x}_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee x_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee \overline{x}_4 \vee x_3) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee \overline{x}_3)$ ✔

$(x_1 \vee x_2) \wedge (x_1 \vee \overline{x}_2) \wedge (\overline{x}_1 \vee x_2) \wedge (\overline{x}_1 \vee \overline{x}_2) \wedge (\overline{x}_1 \vee x_4 \vee \overline{x}_5) \wedge (\overline{x}_1 \vee \overline{x}_4 \vee x_5) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee \overline{x}_5)$ ✖

$\vdots$

Suppose we have a generator of SAT instances, like **SR**(n), where n is the number of boolean variables. The goal is to predict whether each generated CNF formula is SAT or UNSTAT.

This again a difficult satisfiability task.

. . .

⟨ red,above-of,green ⟩ ⟨ green,below-of,red ⟩ ⟨ green,below-of,red ⟩ ⟨ green,above-of,blue ⟩

✓ ✓ ✗ ✗

Suppose we are observing images (ex: Minecraft scenes), each labeled by a yes/no question involving a relation between objects. The goal is to predict the answer of each incoming visual question.

This is once again a difficult task called Visual Question Answering.

Outline

Machine learning problems are specified by:

- a task we wish to solve, characterized by its instance space $\mathcal{Z}$;
- a hypothesis class (prediction models) $\mathcal{H}$ for solving this task;
- a loss function $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}$ for measuring the performance of a model at solving the task.

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For statistical learning problems, it is further assumed that task instances are i.i.d. according to a fixed, but *hidden*, probability distribution $\mathcal{D}$. The (true) risk of any hypothesis $h \in \mathcal{H}$ is given by

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The learning algorithm cannot have access to $\mathcal{D}$, but it has access to a *training sample*, that is, a sequence of instances S drawn according to $\mathcal{D}$. So, the main question is

How can we find a model $h \in \mathcal{H}$ with small risk using only S?

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What is the loss function? A natural choice is the zero-one loss (i.e. error) function:

$$\ell^{\mathrm{ERR}}(h_{\boldsymbol{w}}, (\boldsymbol{x}, y)) = \begin{cases} 1 & \text{if } h_{\boldsymbol{w}}(\boldsymbol{x}) \neq y \\ 0 & \text{otherwise.} \end{cases}$$

But the separation problem is here NP-hard! So, an alternative choice is a convex loss function, such as the hinge loss:

$$\ell^{\mathrm{HINGE}}(h_{\boldsymbol{w}}, (\boldsymbol{x}, y)) = \max\{0, 1 - y(\boldsymbol{w}^\top \boldsymbol{x})\}$$

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What is the hypothesis class? The problem is generally not linearly separable. So, we can start with polynomial zero-threshold functions of degree k:

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = \operatorname{sign}(\boldsymbol{w}^\top \boldsymbol{\phi}(\boldsymbol{x}))$$

where $\boldsymbol{w} \in \mathcal{W} \subseteq \mathbb{R}^d$, and $\boldsymbol{\phi} : \{0, *, 1\}^n \to \{0, 1\}^d$ is a *feature expansion operator*. Namely, $\boldsymbol{\phi}$ can be described by a set $\{f_1, \cdots, f_d\}$ of monomials with degree at most k, and $\phi_i(\boldsymbol{x}) = 1$ iff $\boldsymbol{x}$ can be extended to a total assignment satisfying f_i.

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What is the loss function? Again, a natural choice is the zero-one loss. But the separation problem is also NP-hard here. So, convex loss functions might be more appropriate.

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What is the loss function? For deep learning models, common loss functions for binary labels are the convex and differentiable logistic loss, and sigmoid cross-entropy loss.

A definition of Learnability:

- $\mathcal{S}$ is the set of all finite training sets, i.e. $\mathcal{S} = \bigcup_{m \in \mathbb{N}} \mathcal{Z}^m$.
- A learning algorithm is a map $A : \mathcal{S} \to \mathcal{H}$ that takes as input a training set S and returns as output a prediction model $A(S)$.
- A learning rate is a monotone decreasing map $\epsilon : \mathbb{N} \to \mathbb{R}$ that converges to 0 as m tends to infinite.

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Let $\mathcal{Z}$ be an instance space, $\mathcal{H}$ be a hypothesis class, and $\ell : \mathcal{H} \times \mathcal{Z} \to \mathbb{R}$ be a loss function. Then, $\mathcal{H}$ is learnable with respect to ℓ if there is a learning algorithm A and a rate ϵ such that, for any distribution $\mathcal{D}$ over $\mathcal{Z}$ and any integer $m \in \mathbb{N}$:

$$\mathbb{E}_{S \in \mathcal{Z}^m}[L_{\mathcal{D}}(A(S))] - \inf_{h \in \mathcal{H}} L_{\mathcal{D}}(h) \leq \epsilon(m) \tag{1}$$

Any algorithm A satisfying (1) is called statistically efficient (aka statistically consistent).

This definition is quite standard in statistical computational learning. Notably it generalizes the concept of (agnostic) PAC learnability.

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Bias-Variance Dilemma. The main inequality:

$$\mathbb{E}_{S \in \mathcal{Z}^m}[L_{\mathcal{D}}(A(S))] - \inf_{h \in \mathcal{H}} L_{\mathcal{D}}(h) \leq \epsilon(m)$$

indicates that the risk of our predictive model $A(S)$ must converge to the risk of the best possible hypothesis in $\mathcal{H}$. So,

- if $\mathcal{H}$ is small (simple models), the best hypothesis may perform poorly (large bias);
- if $\mathcal{H}$ is large (complex models), the convergence may be slow (large "variance").

Thus, choosing the right hypothesis class is critical for any task.

Accuracy-Complexity Dilemma. Recall that:

$$L_{\mathcal{D}}(h) = \mathbb{E}_{z \sim \mathcal{D}}[\ell(h, z)]$$

is measured with respect to a loss function ℓ which, for computational reasons, is often a convex surrogate of the true objective function (e.g. zero-one loss).

Thus, choosing the right loss function is also critical for reasoning tasks.

Outline

Consider the global consistency task, in which we are given a constraint network, and the training set consists of partial assignments (the queries), labeled by ✓ or ✖ depending on whether they are globally consistent, or not.

For each partial assignment $\boldsymbol{x} \in \{0, *, 1\}^n$, we use $\textsc{ext}(\boldsymbol{x})$ to denote the set of all its total extensions in $\{0, 1\}^n$.

A Sampling Method.

1. Let T be the set of *total* assignments *labeled by* 1 in S.
2. For each incoming instance $\boldsymbol{x}$, predict ✓ if $\textsc{ext}(\boldsymbol{x}) \cap T \neq \varnothing$, and ✖ otherwise.

Now, consider the following assumption:

> Let W be the set of satisfying assignments of the constraint network, and $\mathcal{D}$ be a (hidden) probability distribution over $\{0, *, 1\}^n$. A partial assignment $\boldsymbol{x}$ is called γ-fair if either $\boldsymbol{x}$ is *not* globally consistent, or $\mathbb{P}_{\mathcal{D}}[W \cap \textsc{ext}(\boldsymbol{x}) \neq \varnothing] > \gamma$.

Theorem (Khardon & Roth, 1997)

Under the assumption that any partial assignment $\boldsymbol{x}$ drawn by $\mathcal{D}$ is γ-fair, the sampling algorithm is consistent.

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Proof

1. Clearly, if $\boldsymbol{x}$ is not GC, the algorithm will answer ✖.

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Proof

1. Clearly, if $\boldsymbol{x}$ is not GC, the algorithm will answer ✖.
2. The algorithm makes a mistake only if $\boldsymbol{x}$ is GC, but a total assignment in $W \cap \mathrm{EXT}(\boldsymbol{x})$ is not sampled.
3. However, by γ-fairness such an assignment is drawn with probability greater than γ.
4. So, after m trials, the expected error on this instance is bounded by:
$$\mathbb{E}_{S \in \mathcal{Z}^m}[\ell^{\mathrm{ERR}}(T; (\boldsymbol{x}, 1))] \leq (1-\gamma)^m$$
5. Now, let $\mathcal{X} = \{0, *, 1\}^n$. By extending the previous inequality to all instances in $\mathcal{X}$,
$$\mathbb{E}_{S \in \mathcal{Z}^m}[L_{\mathcal{D}}(T)] \leq |\mathcal{X}|(1-\gamma)^m$$
6. Therefore, by taking more than
$$m = \frac{1}{\gamma}\left(\ln|\mathcal{X}| + \ln\frac{1}{\delta}\right)$$
samples, and using the fact that $\ln(1-\gamma) \leq -\gamma$, we get that
$$\mathbb{E}_{S \in \mathcal{Z}^m}[L_{\mathcal{D}}(T)] \leq \delta$$
Finally, since $|\mathcal{X}| = 3^n$, the algorithm is statistically consistent with sample complexity:
$$m = \frac{1}{\gamma}\left(n\ln 3 + \ln\frac{1}{\delta}\right)$$

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Let us try a convex optimization method, using the class of polynomial functions. Let $\{f_1, \cdots, f_d\}$ be the set of all monomials of degree at most k over n variables, where

$$d = \sum_{j=1}^{k} \binom{j}{n}$$

Stochastic Gradient Descent. Initialize θ_1 to $\mathbf{0}$.

For $t = 1$ to T

1. Let $\boldsymbol{w}_t = \frac{1}{\lambda t}\theta_t$
2. Choose the tth sample $(\boldsymbol{x}_t, y_t)$ uniformly over the training set S
3. if $y_t(\boldsymbol{w}_t^\top \phi(\boldsymbol{x}_t) < 1)$ set $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + y_t\phi(\boldsymbol{x}_t)$
4. otherwise set $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t$

Output $\boldsymbol{w} = \frac{1}{T}\sum_{t=1}^{T} \boldsymbol{w}_t$

Theorem (Shalev-Shwartz & Ben David, 2014)

Let $\mathcal{D}$ be a distribution on $\mathcal{X} \times \{0, 1\}$, where $\|\phi(\boldsymbol{x})\| \leq \rho\}$. Consider running the SGD algorithm on a training set $S \sim \mathcal{D}^m$, and let $\boldsymbol{w}$ be the solution returned by SGD. Then for every $\boldsymbol{u}$ such that $\|\boldsymbol{u}\| \leq B$, we have

$$\mathbb{E}_{S \sim \mathcal{D}^m}[L_{\mathcal{D}}^{\text{ERR}}(\boldsymbol{w})] \leq L_{\mathcal{D}}^{\text{HINGE}}(\boldsymbol{u}) + 2\rho B\sqrt{2/m}$$

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So, for the global consistency task, if the given constraint network is representable by a polynomial function of degree k, in which each weight in $\boldsymbol{u}$ statisfies $u_i \in [-c, +c]$, we have:

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Are we cheating here? Maybe so, because:

$$L_{\mathcal{D}}^{\text{HINGE}}(\boldsymbol{u}) \geq L_{\mathcal{D}}^{\text{ERR}}(\boldsymbol{u}) = 0$$

In fact, we don't know how to bound $L_{\mathcal{D}}^{\text{HINGE}}(\boldsymbol{u})$ without additional assumptions!

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Kernel Approaches. The above SGD algorithm is the core of Pegasos, a well-known soft-SVM technique which is kernelizable. Instead of computing $\boldsymbol{w}_t$ at each iteration, we may use the kernel trick by replacing the large vectors $\boldsymbol{w}_t$ with a kernel $K(\boldsymbol{x}, \boldsymbol{x}')$.

Open question: which kernel would be appropriate for global consistency tasks?

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Deep Approaches. Polynomial functions can be efficiently represented by sum-product networks, a deep architecture. Livni, Shalev-Shwartz and Shamir (2014) have proposed such an architecture for learning polynomial functions, in which the last layer uses SGD.

Open question: can we efficiently learn sum-product networks for global consistency tasks?

Outline

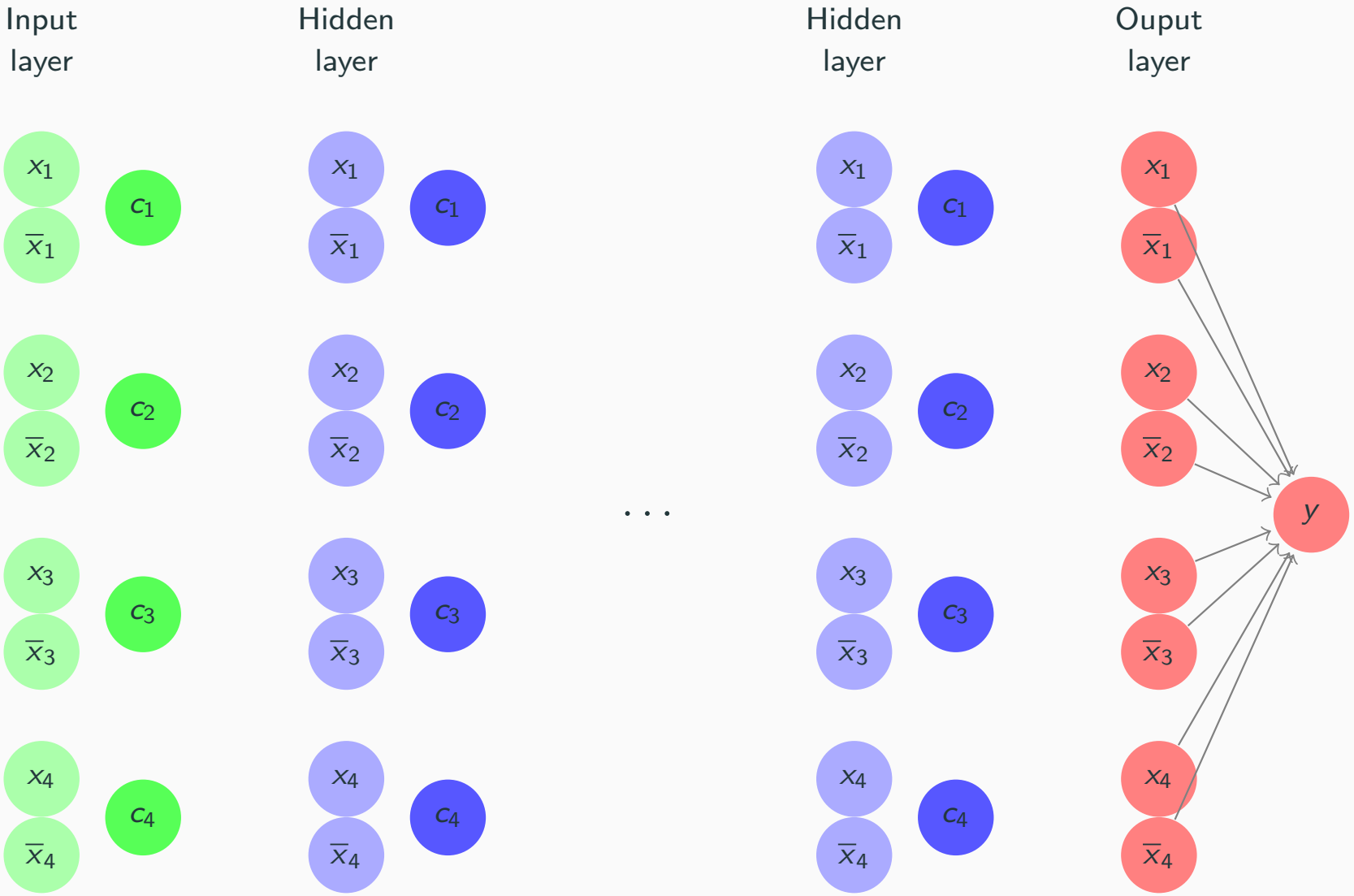
$(x_1 \vee x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee \overline{x}_3) \wedge (x_1 \vee \overline{x}_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee x_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee x_3) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee \overline{x}_3)$ ✖

$(x_1 \vee x_2 \vee x_4) \wedge (x_1 \vee x_2 \vee \overline{x}_3) \wedge (x_1 \vee \overline{x}_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee x_2 \vee \overline{x}_3) \wedge (\overline{x}_1 \vee \overline{x}_4 \vee x_3) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee \overline{x}_3)$ ✓

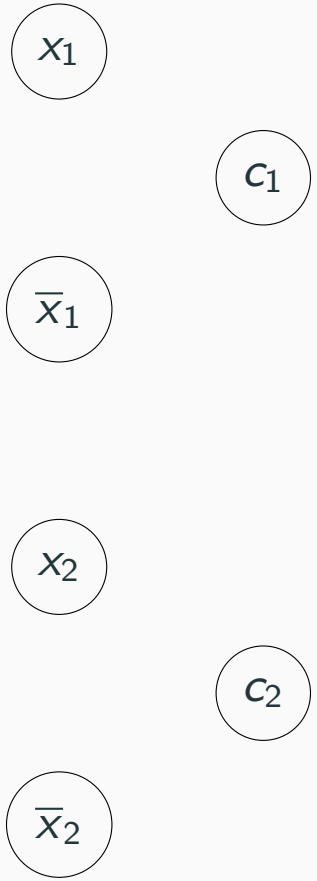
$(x_1 \vee x_2) \wedge (x_1 \vee \overline{x}_2) \wedge (\overline{x}_1 \vee x_2) \wedge (\overline{x}_1 \vee \overline{x}_2) \wedge (\overline{x}_1 \vee x_4 \vee \overline{x}_5) \wedge (\overline{x}_1 \vee \overline{x}_4 \vee x_5) \wedge (\overline{x}_1 \vee \overline{x}_2 \vee \overline{x}_5)$ ✖

⋮

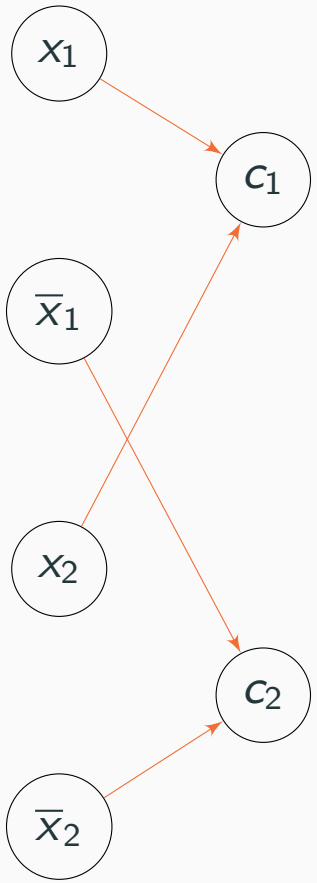
Recall that in the satisfiability task, we have a generator of SAT instances, and the goal is to predict whether each generated CNF formula is SAT or UNSTAT.



The NeuroSAT architecture (Selsam et. al, 2018) is a feedforward neural net in which the input layer and hidden layers are defined from literal embeddings and clause embeddings. The final layer use a vote among literals to determine the output y.

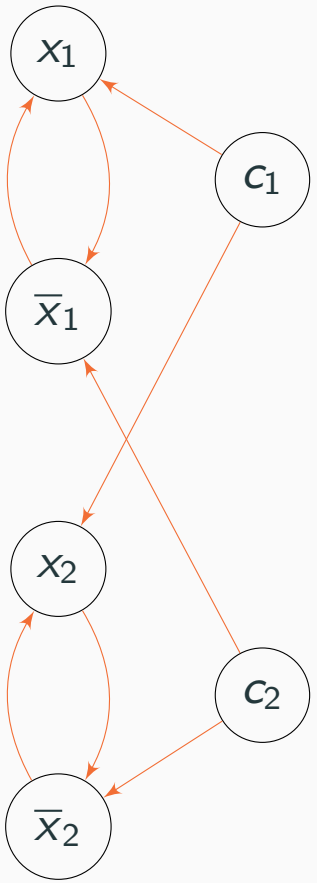


For each layer t, we have an embedding for every literal (l-node) and every clause (c-node). An iteration $t \to t + 1$ consists of two stages:



For each layer t, we have an embedding for every literal (l-node) and every clause (c-node). An iteration $t \to t+1$ consists of two stages:

- first, each c-node receives messages from its connected l-nodes, and updates its embedding accordingly;



For each layer t, we have an embedding for every literal (l-node) and every clause (c-node). An iteration $t \to t+1$ consists of two stages:

- first, each c-node receives messages from its connected l-nodes, and updates its embedding accordingly;
- next, each l-node receives message from its connected c-nodes, as well as its complement, and updates its embedding accordingly.

NeuroSAT is parameterized by:

- Two vectors $\boldsymbol{L}_{\text{INIT}}$ and $\boldsymbol{C}_{\text{INIT}}$
- Three multilayer percetrons $\boldsymbol{L}_{\text{MSG}}$, $\boldsymbol{C}_{\text{MSG}}$ and $\boldsymbol{L}_{\text{VOTE}}$
- Two layer-norm long-short term memory networks $\boldsymbol{L}_{\text{LSTM}}$ and $\boldsymbol{C}_{\text{LSTM}}$

Each layer t involves four matrices:

- $\boldsymbol{L}^{(t)} \in \mathbb{R}^{2n \times d}$ is the matrix storing each literal embedding.
- $\boldsymbol{C}^{(t)} \in \mathbb{R}^{m \times d}$ is the matrix storing each clause embedding.
- $\boldsymbol{L}^{(t)_h}$ and $\boldsymbol{C}_h^{(t)}$ are the corresponding hidden matrices initialized to zero.

The layers are updated as follows:

- $[\boldsymbol{C}^{(t+1)}, \boldsymbol{C}_h^{(t+1)}] = \boldsymbol{C}_{\text{LSTM}}[\boldsymbol{C}_h^{(t)}, \boldsymbol{M}^\top \boldsymbol{L}_{\text{MSG}}(\boldsymbol{L}^{(t)})]$
- $[\boldsymbol{L}^{(t+1)}, \boldsymbol{L}_h^{(t+1)}] = \boldsymbol{L}_{\text{LSTM}}[\boldsymbol{L}_h^{(t)}, F(\boldsymbol{L}^{(t)}), \boldsymbol{M}\boldsymbol{C}_{\text{MSG}}(\boldsymbol{C}^{(t)})]$

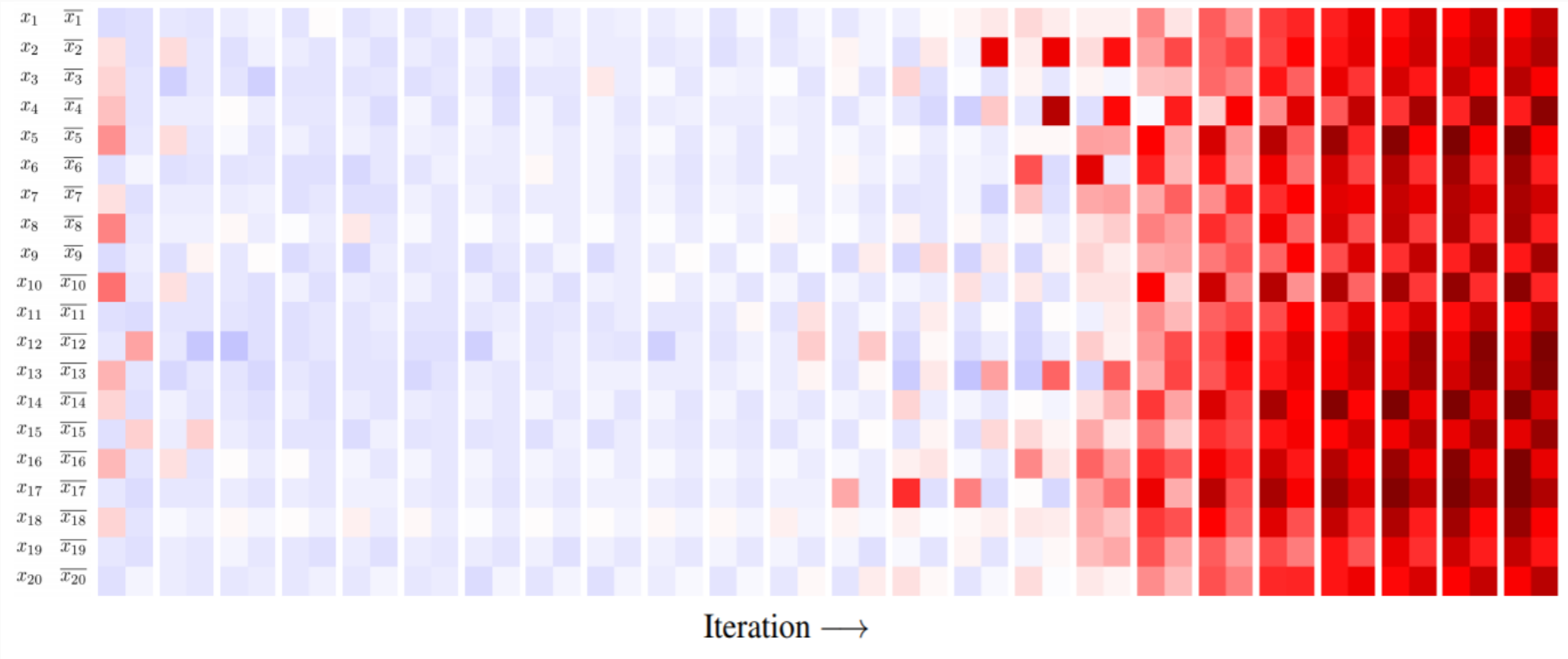
where

- $\boldsymbol{M}$ is the adjacency matrix, i.e. $M(i,j) = 1$ iff $l_i \in c_j$
- $F(\boldsymbol{L})$ swaps each row of $\boldsymbol{L}$ with the row of its complement.

For the output layer,

$$y = \text{mean}(\text{vote}(\boldsymbol{L}^{(T)}))$$

where $\text{vote}(\boldsymbol{L}^{(T)}) \in \mathbb{R}^n$ is the vote for the value of each variable, and y is the average of each vote.



When making a prediction about a new problem, NeuroSAT

- predicts UNSAT with low confidence (light blue) until it finds a satisfying assignment, at which point it guesses SAT with very high confidence (red).
- or keeps predicting UNSAT with low confidence (light blue) until T. It never becomes high confident for UNSAT.

For now, NeuroSAT makes 15 % mistakes in predicting the satisfiability of SR(20) instances. We are far below modern SAT solvers, but this is just the beginning of neuro-sat techniques.