

CQT 13/07/2018

#### Dario Poletti

Singapore University of Technology and Design









#### Machine learning

- supervised, unsupervised
- some tasks
- classical and quantum

#### Many body quantum physics

- using machine learning
- interpreting machine learning
- Novel algorithms

#### MPS for classification

MPO for sequence to sequence

Outlook

#### Machine learning

- supervised, unsupervised
- some tasks
- classical and quantum

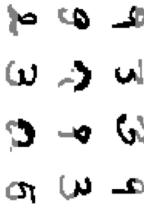
Supervised: you feed possible inputs and outputs to the model which tries to figure out which conditional probability they were extracted from

#### Machine learning

- supervised, unsupervised
- some tasks
- classical and quantum

which conditional probability they were extracted from Supervised: you feed possible inputs and outputs to the model which tries to figure out

an inner structure Unsupervised: you feed unlabeled data and the model infers a function that describes

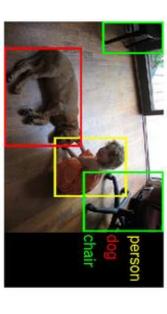


#### Machine learning

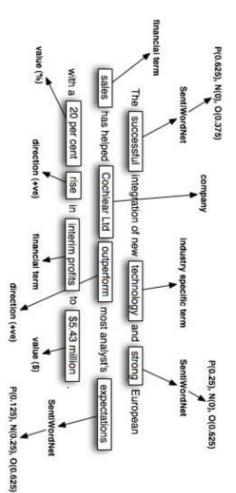
- supervised, unsupervised
- some tasks
- classical and quantum

#### 

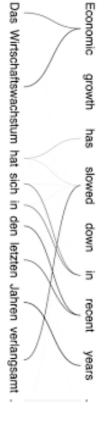
#### image recognition



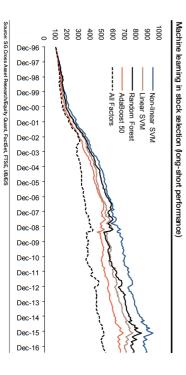
#### Natural language processing



#### translation



#### stock prediction



Machine learning

- supervised, unsupervised
- some tasks
- classical and quantum

You can use a classical computer or a quantum computer

use wave-functions, use quantum algorithms

Many body quantum physics

- using machine learning
- interpreting machine learning
- Novel algorithms

https://physicsml.github.io/pages/papers.html

#### Many body quantum physics

- using machine learning
- interpreting machine learning
- Novel algorithms

### Machine learning for phase recognitions

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J. Carrasquilla, and R.G. Melko, Nature Physics 13, 431 (2017).
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- Y. Zhang, and E.A. Kim, Phys. Rev. Lett. 118, 216401 (2017).
- K. Ch'ng, N. Vazquez, and E. Khatami, Phys. Rev. E 97, 013306 (2018).
- P. Zhang, H. Shen, and H. Zhai, Phys. Rev. Lett. 120, 066401 (2018)
- E. P. van Nieuwenburg, Y.-H. Liu, and S. D. Huber, Nat. Phys. 13, 435 (2017).
- P. Broecker, J. Carrasquilla, R. G. Melko, and S. Trebst, Scientific Reports 7, 8823 (2017).
- K. Ch'ng, J. Carrasquilla, R. G. Melko, and E. Khatami, Phys. Rev. X 7, 031038 (2017).

#### Many body quantum physics

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### Boost efficiency of codes or provide new codes

```
L.F. Arsenault, A. Lopez-Bezanilla, O.A. von Lilienfeld, and A.J. Millis, Phys. Rev. B 90, 155136 (2014).
L.-F. Arsenault, O. A. von Lilienfeld, and A. J. Millis, arXiv:1506.08858 (2015).
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G. Torlai and R. G. Melko, Phys. Rev. B 94, 165134 (2016).

M. H. Amin, E. Andriyash, J. Rolfe, B. Kulchytskyy, and R. Melko, arXiv:1601.02036.

J. Liu, Y. Qi, Z. Y. Meng, and L. Fu, Phys. Rev. B 95, 041101 (2017).

L. Huang and L. Wang, Phys. Rev. B 95, 035105 (2017).

K.-I. Aoki and T. Kobayashi, Mod. Phys. Lett. B, 1650401 (2016).

G. Carleo, and M. Troyer, Science 355, 602 (2017).

Y. Nomura, A.S. Darmawan, Y. Yamaji, and M. Imada, Phys. Rev. B 96, 205152 (2017).

S. Czischek, M. Garttner, and T. Gasenzer, arxiv:1803.08321.

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#### Many body quantum physics

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### Interpreting the networks and/or why they work

C. Beny, arXiv:1301.3124.

P. Mehta and D. J. Schwab, arXiv:1410.3831.

H.W. Lin, M. Tegmark, and D. Rolnick, Journal of Statistical Physics 168, 1223 (2017).

### Why does deep and cheap learning work so well?\*

Henry W. Lin, Max Tegmark, and David Rolnick

Dept. of Physics, Harvard University, Cambridge, MA 02138

Dept. of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139 and

Dept. of Mathematics, Massachusetts Institute of Technology, Cambridge, MA 02139

(Dated: July 21 2017)

n variables cannot be multiplied using fewer than  $2^n$  neurons in a single hidden layer. not be accurately approximated by shallow ones without efficiency loss; for example, we show that group. We prove various "no-flattening theorems" showing when efficient linear deep networks canpolynomial log-probability translate into exceptionally simple neural networks. We further argue how properties frequently encountered in physics such as symmetry, locality, compositionality, and mate arbitrary functions well, the class of functions of practical interest can frequently be approxiin physics and machine-learning, a deep neural network can be more efficient than a shallow one that when the statistical process generating the data is of a certain hierarchical form prevalent mated through "cheap learning" with exponentially fewer parameters than generic ones. We explore physics: although well-known mathematical theorems guarantee that neural networks can approxi-We formalize these claims using information theory and discuss the relation to the renormalization We show how the success of deep learning could depend not only on mathematics but also on

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Use quantum many body inspired algorithms to prepare new machine learning models

#### With MPS

E.M. Stoudenmire and D.J. Schwab, Advances In Neural Information Processing Systems 29, 4799 (2016).

Z.-Y. Han, J. Wang, H. Fan, L. Wang, and P. Zhang, arxiv:1709.01662.

E.M. Stoudenmire, Quantum Science and Technology (2018).

A. Novikov, M. Trofimov, and I. Oseledets, arxiv:1605.03795, ICLR (2017).

Huggins et al. arxiv:1803.11537

our work

BIG PROBLEM!!!

Size of  $|\psi>$  scales as  $d^L$  where d is the size of the local Hilbert space while L is the size of the system

$$|\psi\rangle = \sum_{\sigma_1,\sigma_2,\dots,\sigma_L} C^{\sigma_1,\sigma_2,\dots,\sigma_L} |\sigma_1,\sigma_2,\dots,\sigma_L\rangle$$

#### BIG PROBLEM!!!

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$$|\psi\rangle = \sum_{\sigma_1,\sigma_2,\cdots,\sigma_L} C^{\sigma_1,\sigma_2,\cdots,\sigma_L} |\sigma_1,\sigma_2,\cdots,\sigma_L\rangle$$

Rewrite  $|\psi>$  as the product of a series of 3-dimensional tensors

$$c_{\sigma_1,\dots,\sigma_L} = \sum_{a_1,a_2,\dots,a_{L+1}} M_{a_1,a_2}^{\sigma_1} M_{a_2,a_3}^{\sigma_2} \dots M_{a_L,a_{L+1}}^{\sigma_L}$$

Now it scales polynomial with system size  $\,dD^2L$ 

$$c_{\sigma_1,\dots,\sigma_L} = \sum_{a_1,a_2,\dots,a_{L+1}} M_{a_1,a_2}^{\sigma_1} M_{a_2,a_3}^{\sigma_2} \dots M_{a_L,a_{L+1}}^{\sigma_L}$$

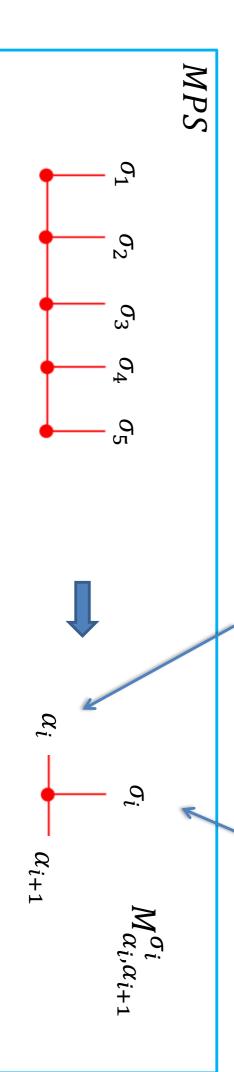
$$C_{\sigma_1,\dots,\sigma_L} = \sum_{a_1,a_2,\dots,a_{L+1}} M_{a_1,a_2}^{\sigma_1} M_{a_2,a_3}^{\sigma_2} \dots M_{a_L,a_{L+1}}^{\sigma_L}$$



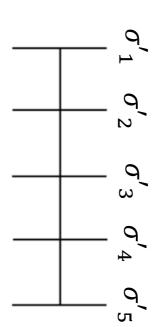


Physical dimension (size local Hilbert space)

Auxiliary dimension (size local bond dimension D)



#### MPO



 $\sigma_2$ 

 $\sigma_3$   $\sigma_4$   $\sigma_5$ 

 $\sigma_i$ 



$$\alpha'_{i+1}$$

 $W^{\sigma_i,\sigma'_i}_{lpha_i,lpha_{i+1}}$ 

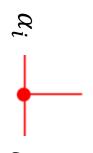


MPS

 $\sigma_2$ 

 $\sigma_3$   $\sigma_4$ 

 $\sigma_{5}$ 

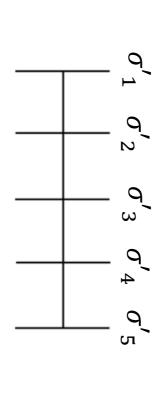


 $\sigma_{i}$ 

$$\sigma_{i} \qquad M_{\alpha_{i},\alpha_{i+1}}^{\sigma_{i}}$$

$$\alpha_{i+1}$$

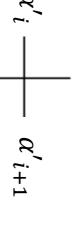
#### MPO



 $\sigma_2$ 

 $\sigma_3$   $\sigma_4$   $\sigma_5$ 





 $W^{\sigma_i,\sigma_i}_{lpha_i,lpha_{i+1}}$ 

 $oldsymbol{O}_i$ 

Auxiliary dimension (size local MPO bond dimension  $D_{W}$ )

#### MPS



$$\alpha_i \xrightarrow{\sigma_i} M_{\alpha_i,\alpha_{i+1}}^{\sigma_i}$$

$$\alpha_i \xrightarrow{\alpha_{i+1}} \alpha_{i+1}$$

#### MPO for sequence to sequence

- Method
- Cellular automata
- Analytical solutions
- Performance
- Comparison to Conditional Random Fields
- Discrete nonlinear maps
- Performance
- Comparison to LSTM
- Classification

Words, sentences, data, images can be written as a sequence

$$(x_{k,1},x_{k,2},\ldots,x_{k,L})$$

and there is some function which from the input sequence returns an output sequence

$$\vec{y_i} = f(\vec{x_i})$$

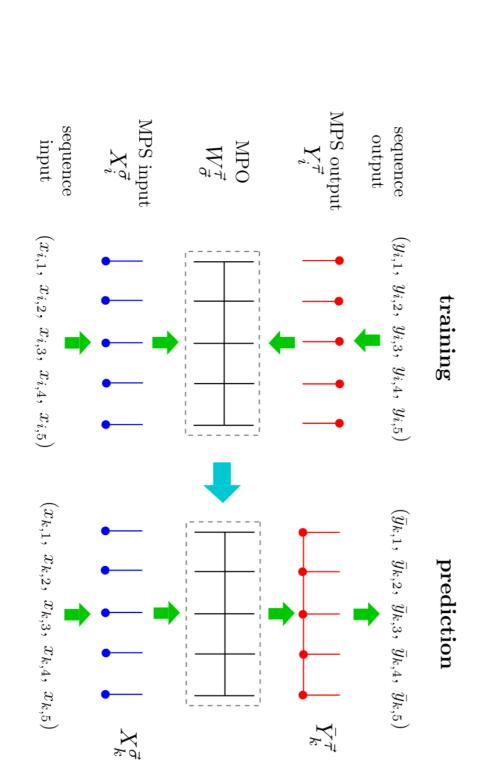
Can we train an MPO that would return an output

$$(ar{y}_{k,1},ar{y}_{k,2},\ldots,ar{y}_{k,L})$$

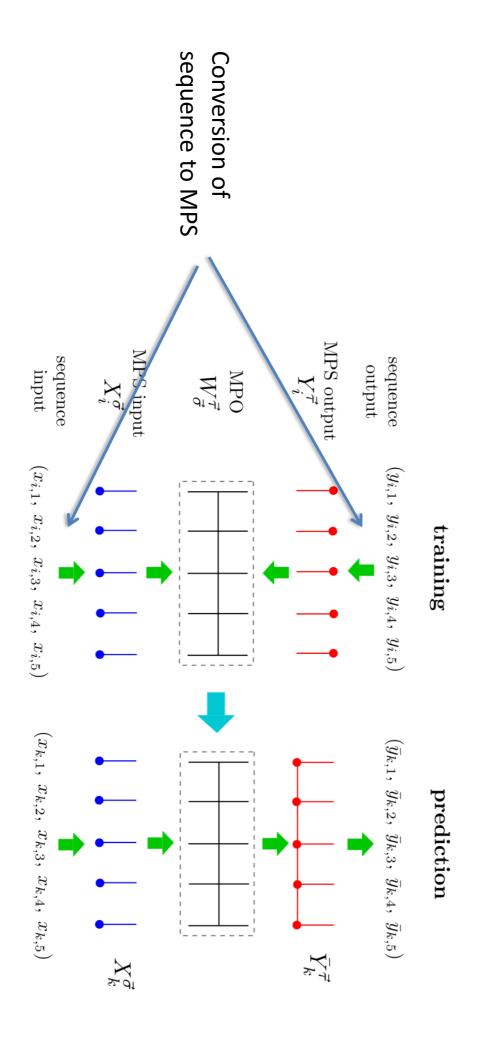
which is close to  $\ ec{y_i}$  ?

Here we will focus on equal input and output sizes L.

The main points of our MPO model are described in this figure



## From input/output sequences to input/output MPSs



For real number, for example from 0 to 1, we map each site to a vector

$$\left(\sqrt{1-x_{i,l}^2},x_{i,l}
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For integer numbers you choose a vector of the size given by the possible outcomes The you put a 1 in the location corresponding to the value

:

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For integer numbers you choose a vector of the size given by the possible outcomes The you put a f 1 in the location corresponding to the value

; د

3 -> (0,0,0,1,0,0)

:

Then

$$\vec{x}_i \to X_i^{\vec{\sigma}} = \sum_{i,a_0,a_1} X_{i,a_1,a_2}^{\sigma_2} \dots X_{i,a_{L-1},a_L}^{\sigma_L}$$

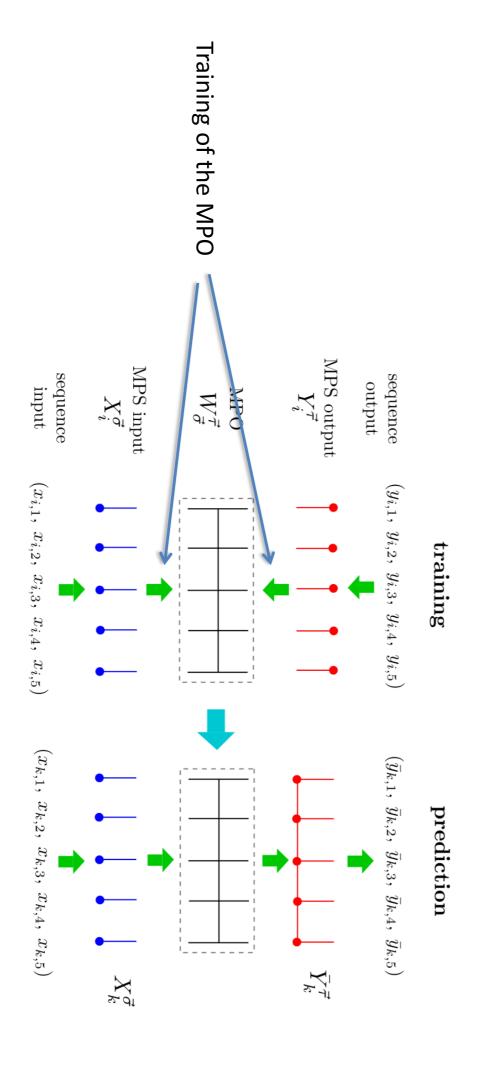
inputs

$$\vec{y}_i \to Y_i^{\vec{\tau}} = \sum_{c_0, \dots, c_L} Y_{i, c_0, c_1}^{\tau_1} Y_{i, c_1, c_2}^{\tau_2} \dots Y_{i, c_{L-1}, c_L}^{\tau_L}$$

outputs

where all the  $a_l = c_l = 1$  only.

### From input/output MPS to trained MPO



We define the cost function C

$$C(W_{\vec{\sigma}}^{\vec{\tau}}) = \sum_{i=1}^{N} \left( \bar{Y}_i^{\vec{\tau}^\dagger} - Y_i^{\vec{\tau}^\dagger} \right) \left( \bar{Y}_i^{\vec{\tau}} - Y_i^{\vec{\tau}} \right) + \alpha \operatorname{tr} \left( W_{\vec{\sigma}}^{\vec{\tau}^\dagger} W_{\vec{\sigma}}^{\vec{\tau}} \right)$$

 $\bar{Y}_i^{\vec{\tau}} = W_{\vec{\sigma}}^{\vec{\tau}} X_i^{\vec{\sigma}}$ 

Predicted output

Distance between predicted and output MPS

Regularization term

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Predicted output

Distance between predicted and output MPS

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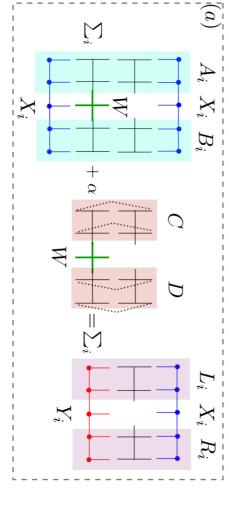
We minimize the cost function iteratively over the local MPOs W

$$\frac{\partial C(\hat{W})}{\partial W_{b_{l-1},b_{l}}^{\sigma_{l},\tau_{l}}} = 0.$$

Minimization is graphically depicted here

$$\frac{\partial C(\hat{W})}{\partial W_{b_{l-1},b_{l}}^{\sigma_{l},\tau_{l}}} = 0.$$

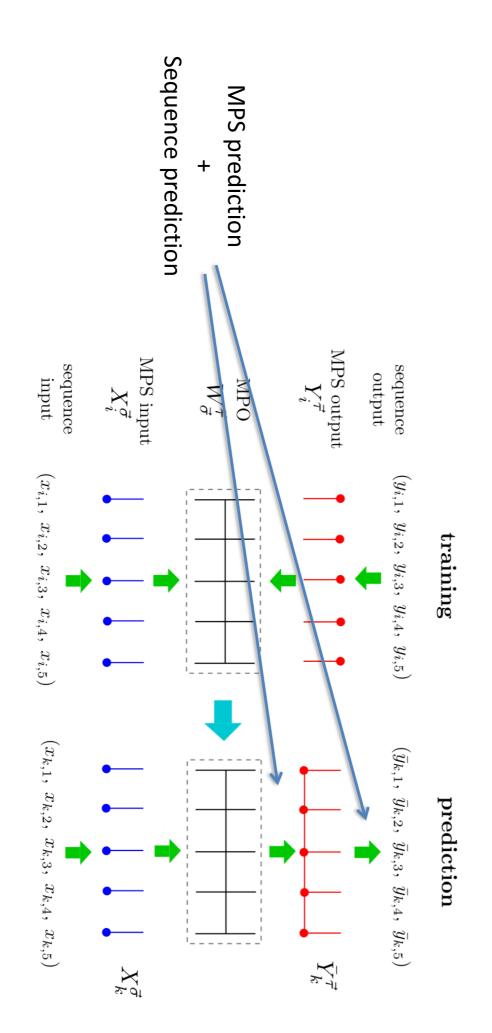




Fairly straightforward linear problem to solve

MW = V

Generation of output MPS and its conversion to sequence



The output MPS is simply given by the product of input MPS with the trained MPO

$$egin{aligned} ar{Y}_i^{ec{ au}} &= W_{ec{\sigma}}^{ec{ au}} X_i^{ec{\sigma}} &= \sum_{ar{c}_0,...,ar{c}_L} ar{Y}_{i,ar{c}_0,ar{c}_1} \ldots ar{Y}_{i,ar{c}_{L-1},ar{c}_L}^{ au_L}, \end{aligned}$$
 where  $ar{Y}_{i,ar{c}_1-1,ar{c}_1}^{ au_l} = \sum_i W_i$ 

ere  $ar{Y}_{i,ar{c}_l-1,ar{c}_l}^{ au_l} = \sum_{\sigma_l} W_{b_l-1,b_l}^{\sigma_l, au_l} X_{i,a_{l-1},a_l}^{\sigma_l}.$ 

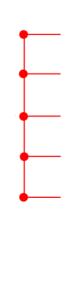
The **output MPS** is simply given by the product of **input MPS** with the **trained MPO** 



where  $\bar{Y}_{i,\bar{c}_{l-1},\bar{c}_{l}}^{\tau_{l}} = \sum W_{b_{l-1},b_{l}}^{\sigma_{l},\tau_{l}} X_{i,a_{l-1},a_{l}}^{\sigma_{l}}.$ 

#### Conversion of output MPS to sequence

- We convert the MPS to a bond dimension D=1 MPS
- We check with physical index  $\sigma_l$  has the largest occupation
- We chose this physical index as the value for the sequence













$$(x_{k,1}, x_{k,2}, x_{k,3}, x_{k,4}, x_{k,5})$$

We can now study the performance

We will study two sequence to sequence problems

- Evolution of cellular automata
- Discrete nonlinear maps

And one classification problem

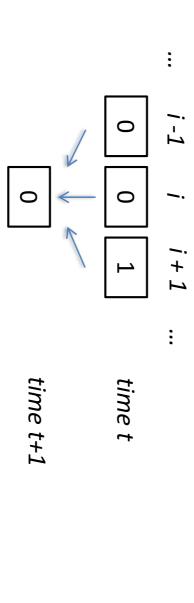
MNIST digits classification

Cellular automata

#### Cellular automata

256 rules have been classified (Wolfram1980)

time step is decided Given the value at one position and its nearest neighbors, the position at the next



#### Cellular automata

### 256 rules have been classified (Wolfram1980)

time step is decided Given the value at one position and its nearest neighbors, the position at the next

$$\begin{array}{c|cccc}
 & i-1 & i & i+1 & \dots \\
\hline
 & 0 & 0 & 1 & & time t \\
 & \downarrow & \downarrow & & \\
\hline
 & 0 & & time t+1 & \dots \\
\end{array}$$

with *d>1* We also consider long-range rules, where the evolution at site i depends on site i+d

does ... We focus on rules 153, 153-long-range, 18 and 30 ... easy to figure what each rule

written exactly using MPOs. The evolution of a string of 0s and 1s due to some cellular automata rules can be

For the 256 rules, the MPO bond dimension  $D_{\rm W}$  is at most 4.

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Example: Rule 153 (for which  $D_w = 2$ )

correct output sequence. The product of the MPOs chosen in this manner is only different from 0 for the

$$W^{0,0}_{b_{l-1},b_l} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad W^{0,1}_{b_{l-1},b_l} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$
 $W^{1,1}_{b_{l-1},b_l} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad W^{1,0}_{b_{l-1},b_l} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$ 

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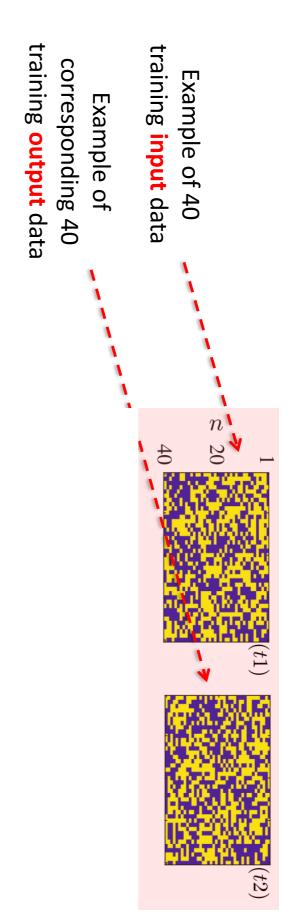
$$W_{b_{l-1},b_{l}}^{0,0} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad W_{b_{l-1},b_{l}}^{0,1} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$
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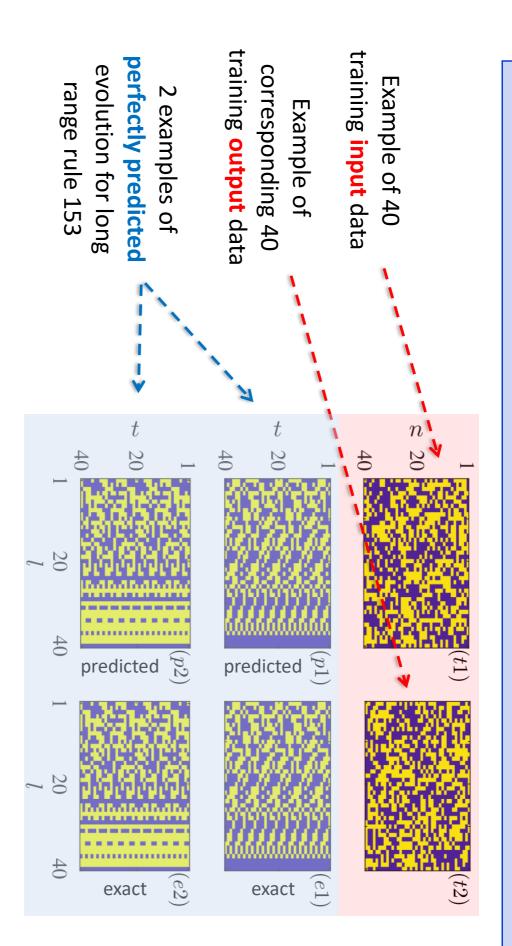
We use fix boundary conditions which translate to

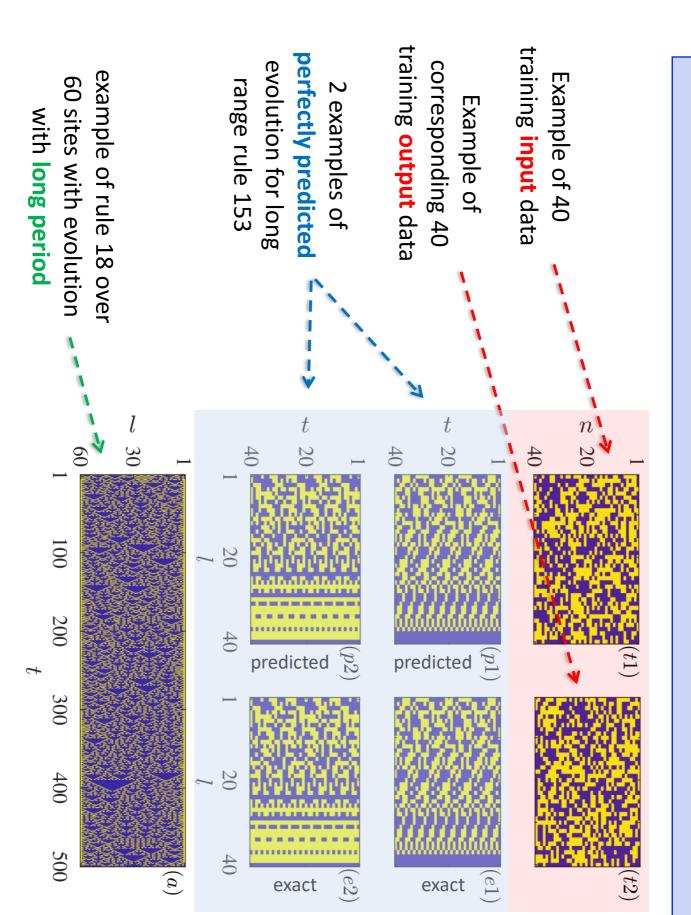
$$\begin{aligned} W^{0,0}_{b_0,b_1} &= [0,\,1]\,, \quad W^{0,1}_{b_0,b_1} &= [1,\,0] \end{aligned} \qquad W^{0,0}_{b_{L-1},b_L} &= \begin{bmatrix} 1\\0 \end{bmatrix}, \quad W^{0,1}_{b_{L-1},b_L} &= \begin{bmatrix} 0\\0 \end{bmatrix} \\ W^{1,1}_{b_0,b_1} &= [0,\,1]\,, \quad W^{1,0}_{b_0,b_1} &= [1,\,0] \end{aligned} \qquad W^{1,1}_{b_{L-1},b_L} &= \begin{bmatrix} 0\\0 \end{bmatrix}$$

First site

Last site





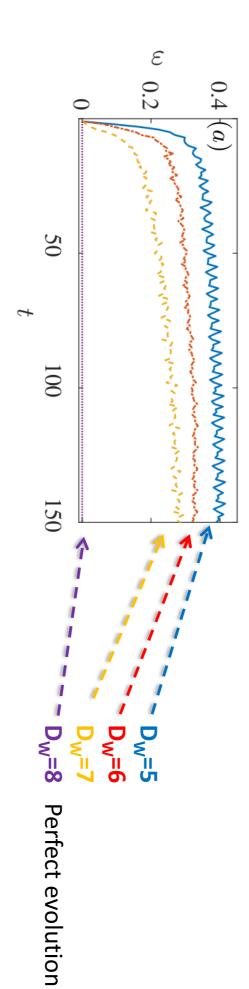


We quantify the error  $\varepsilon$  as

$$\varepsilon = \sum_{k,l} |y_{k,l}(t) - \bar{y}_{k,l}(t)|/(L N)$$

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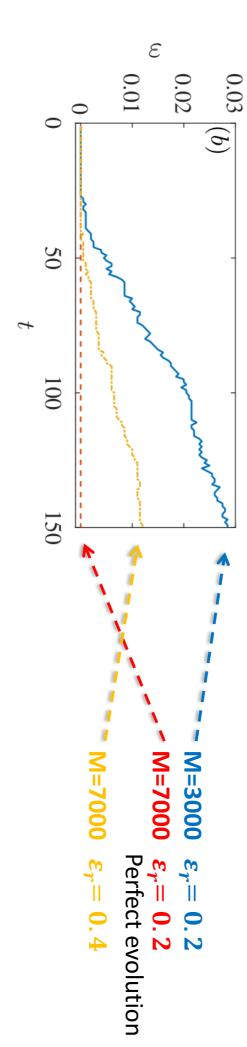


We consider N=100 initial conditions for a system of size L=40 and we evolve for 150 steps. We used M=7000 samples to train.

If the bond dimension is large enough, we get perfect predictions.

the percentage of output data which are chosen from uniform random distribution. We also consider the presence of wrong training data. The quantify the error  $arepsilon_r$  is

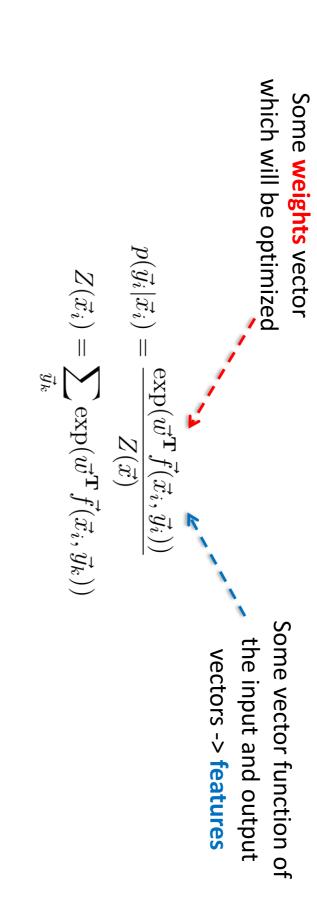
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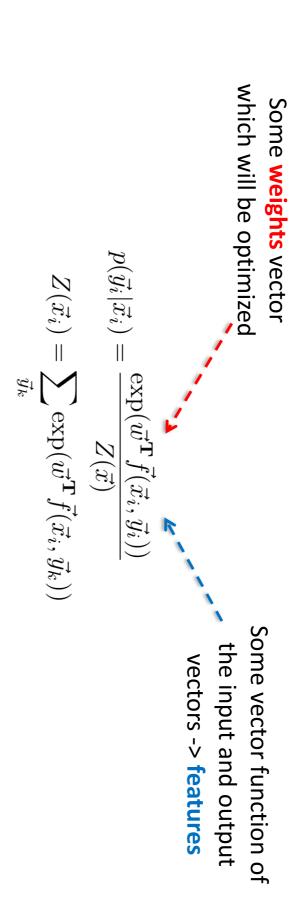
We consider N=100 initial conditions for a system of size L=40 and we evolve for 150 steps. We used  $D_{\rm W}$ =8 bond dimension.

Larger sample size can compensate for the errors in the training data.

Comparison to conditional random fields (CRF) model



Comparison to conditional random fields (CRF) model

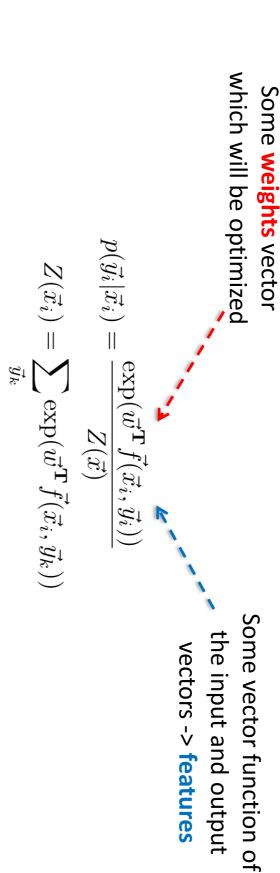


Minimize the log-likelihood to compute the parameters

$$\frac{\partial \mathcal{L}}{\partial w_k} = 0$$

$$\mathcal{L}(\vec{w}) = -\sum_i \log p(\vec{y}_i | \vec{x}_i) + \lambda \vec{w}^T \vec{w}$$

Comparison to conditional random fields (CRF) model



Minimize the log-likelihood to compute the parameters

$$\frac{\partial \mathcal{L}}{\partial w_k} = 0$$

$$\mathcal{L}(\vec{w}) = -\sum \log p(\vec{y}_i | \vec{x}_i) + \lambda \vec{w}^T \vec{w}$$

CRF can also give perfect predictions for the evolution of cellular automata.

However, this only occurs if the features are chosen correctly, otherwise the results could be completely random despite a large size of features vector.

The MPO model "finds" the relevant features.

Discrete nonlinear maps

Discrete nonlinear maps

We consider a nonlinear and beyond nearest-neighbor model for evolution of a probability distribution

$$P_{l,t+1} = P_{l,t} + g_1/2 \left[ (P_{l-1,t})^{m_1} + (P_{l+1,t})^{m_1} - 2 (P_{l,t})^{m_1} + g_2/2 \left[ (P_{l-2,t})^{m_2} + (P_{l+2,t})^{m_2} - 2 (P_{l,t})^{m_2} \right]$$

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and then the total probability is normalized) and their corresponding outputs. For training we use random inputs (each site is taken from uniform distribution [0,1]

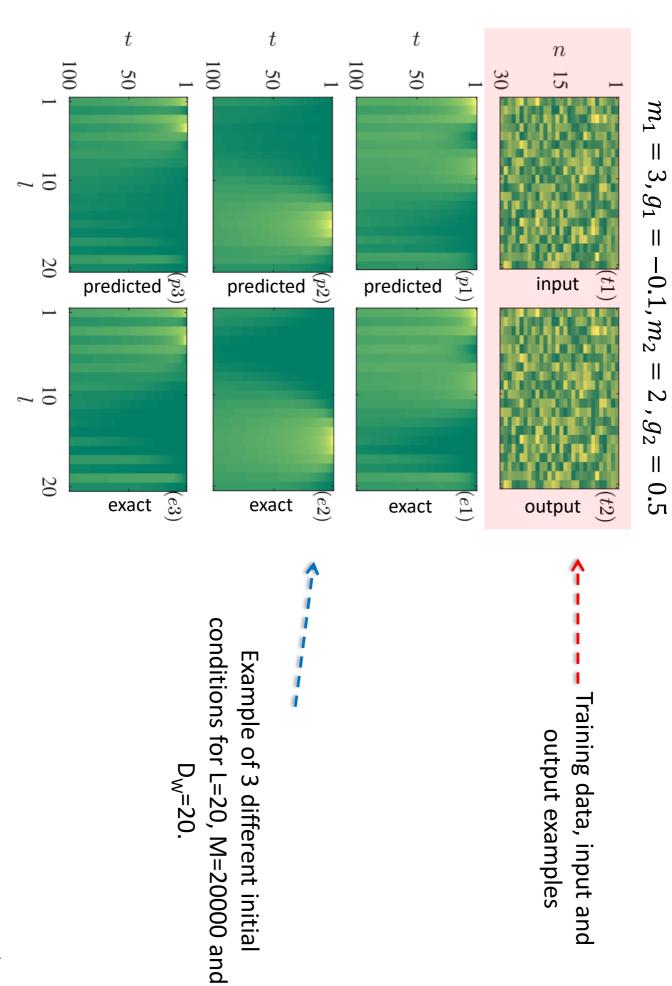
We then compare to 100 initial conditions chosen as

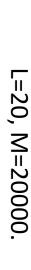
$$P_{l,t=1} = (1 + \cos(2\pi l\lambda/L)) \exp(-((l-l_0)^2)/(2v))/\Gamma$$

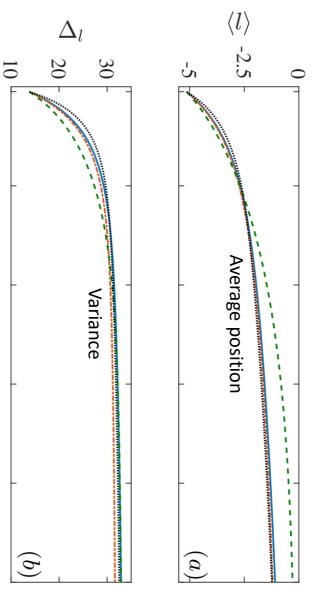
where  $\lambda, l_0$  and v are chosen randomly and  $\Gamma$  is the normalization.

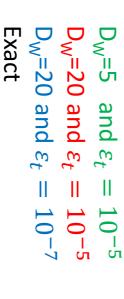
$$m_1 = 3, g_1 = -0.1, m_2 = 2, g_2 = 0.5$$
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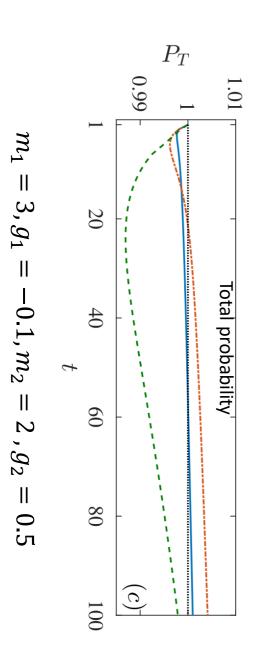
– – — Training data, input and output examples



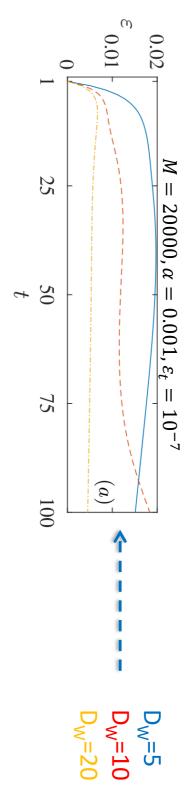






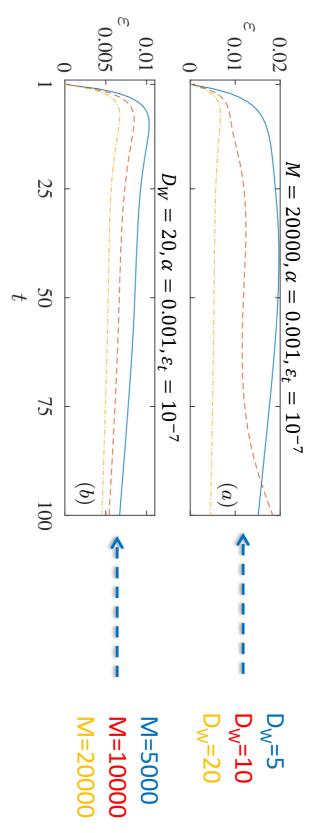


Comparison of performance for different hyperparameters. Average of N=100 initial conditions and L=20, M=20000.



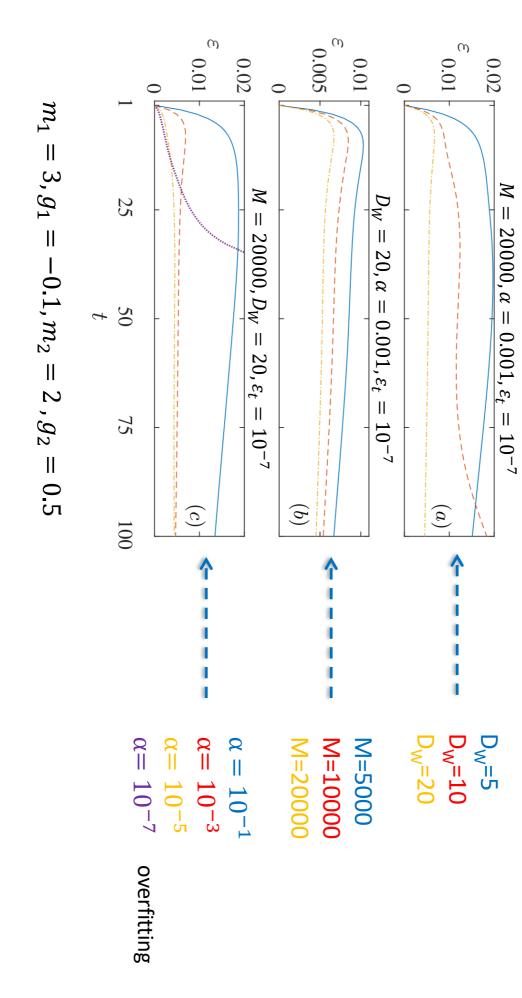
$$m_1=3$$
,  $g_1=-0.1$ ,  $m_2=2$  ,  $g_2=0.5$ 

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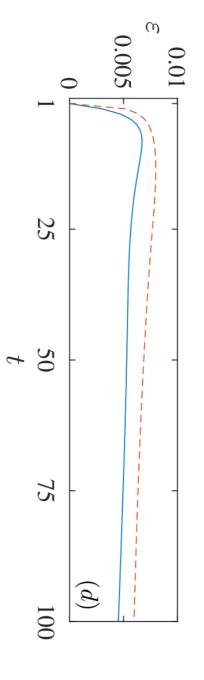


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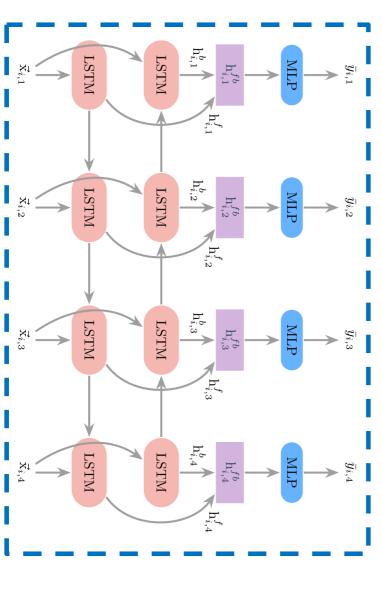
#### Comparison to LSTM bi-directional neural network



#### LSTM

MPO  $D_W$ =20 and  $\varepsilon_t = 10^{-7}$ 

#### LSTM bi-directional neural network



$$\begin{split} \vec{\mathbf{i}}_{i,l} &= \sigma \left( \mathbf{W}_{\mathrm{x}i} \ \vec{\mathbf{x}}_{i,l} + \vec{\mathbf{b}}_{\mathrm{x}i} + \mathbf{W}_{\mathrm{h}i} \ \vec{\mathbf{h}}_{i,l-1} + \vec{\mathbf{b}}_{\mathrm{h}i} \right) \\ \vec{\mathbf{f}}_{i,l} &= \sigma \left( \mathbf{W}_{\mathrm{x}f} \ \vec{\mathbf{x}}_{i,l} + \vec{\mathbf{b}}_{\mathrm{x}f} + \mathbf{W}_{\mathrm{h}f} \ \vec{\mathbf{h}}_{i,l-1} + \vec{\mathbf{b}}_{\mathrm{h}f} \right) \\ \vec{\mathbf{g}}_{i,l} &= \tanh \left( \mathbf{W}_{\mathrm{x}g} \ \vec{\mathbf{x}}_{i,l} + \vec{\mathbf{b}}_{\mathrm{x}g} + \mathbf{W}_{\mathrm{h}f} \ \vec{\mathbf{h}}_{i,l-1} + \vec{\mathbf{b}}_{\mathrm{h}g} \right) \\ \vec{\mathbf{o}}_{i,l} &= \sigma \left( \mathbf{W}_{\mathrm{x}o} \ \vec{\mathbf{x}}_{i,l} + \vec{\mathbf{b}}_{\mathrm{x}o} + \mathbf{W}_{\mathrm{h}o} \ \vec{\mathbf{h}}_{i,l-1} + \vec{\mathbf{b}}_{\mathrm{h}o} \right) \\ \vec{\mathbf{c}}_{i,l} &= \vec{\mathbf{f}}_{i,l} \odot \vec{\mathbf{c}}_{i,l-1} + \vec{\mathbf{i}}_{i,l} \odot \vec{\mathbf{g}}_{i,l} \\ \vec{\mathbf{h}}_{i,l} &= \vec{\mathbf{o}}_{i,l} \odot \tanh (\vec{\mathbf{c}}_{i,l}) \end{split}$$

C. Guo, et al. arxiv:1803.10908 (2018)

Classification tasks: the MPO algorithm can be used for this too.

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Key is to encode the few possible outputs in a way that can perform effectively.

MNIST  $\rightarrow$  28 x 28 pixels to 10 digits (training set 60000 images, development 10000)

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one-hot vectors in which the 1s are evenly spaced

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one-hot vectors in which the 1s are evenly spaced

We obtain:

 $D_{\rm W}$ =10 -> 93.9% accuracy on training set and 94.0% on development set

 $D_w$ =20 -> 97.6% accuracy on training set and 97.2% on development set

#### Conclusions and outlook

MPS and MPO approaches seem to carry some potential.

The MPO approach we introduced:

- Allows to perform sequence to sequence prediction
- Cellular automata
- Discrete nonlinear maps
- Seems to be comparable with some state-of-the-art ML models for different tasks
- It requires less previous knowledge than CRF
- It can perform faster than LSTM bi-directional NN
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#### Outlook

- Study of texts -> part-of-speech tagging, entity recognition inherently 1D problems
- Extend to sequences of variable and/or infinite length
- Probabilistic inputs and outputs
- Various optimizations
- Interpretation of machine learning



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