Unsupervised Learning of Phase Transitions

Seminar: Machine Learning Quantum Matter

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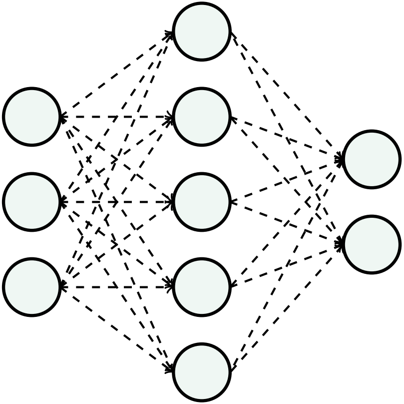
Unsupervised Compared to Supervised Methods

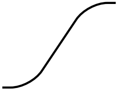
Supervised learning

Input Hidden layer Output



$\underline{x}$

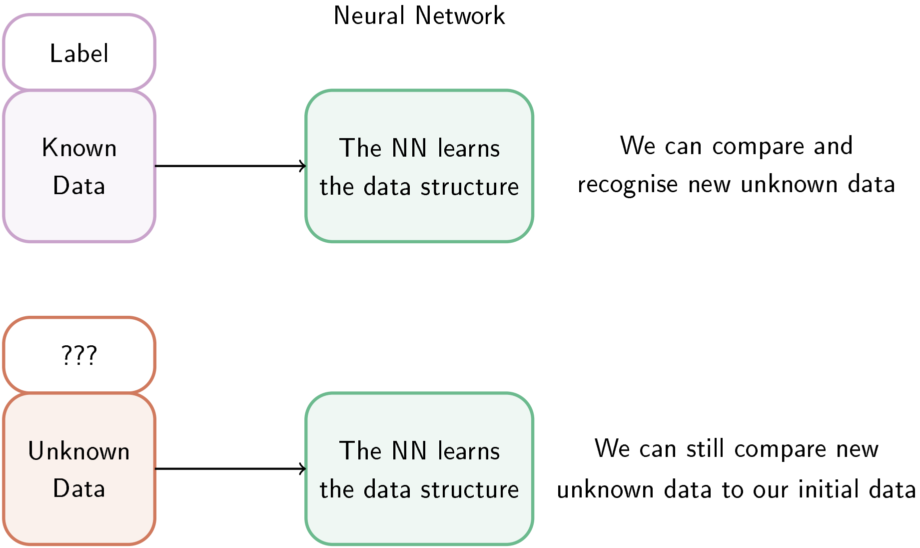
$$C \propto \sum_{\underline{x}} \left\| Label(\underline{x}) - Output(\underline{x}) \right\|^2 + l_2 \left\| \underline{\omega} \right\|^2$$



$\mathrm{Output}_i \in (0,1)$

$$\sigma\left(\underline{\omega}^{(i)} \cdot \underline{x} + b_i\right)$$

Unsupervised Compared to Supervised Methods

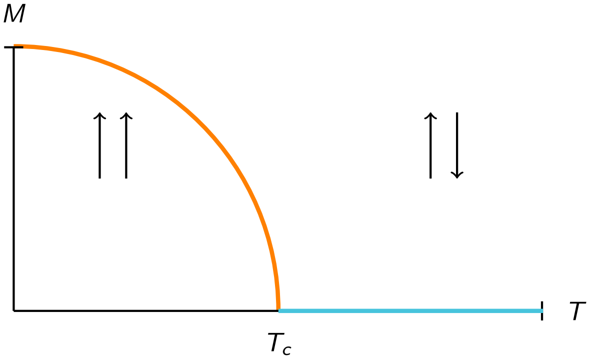


Learning Phase Transitions by Confusion

van Nieuwenburg, Evert P. L. and Liu, Ye-Hua and Huber, Sebastian D.

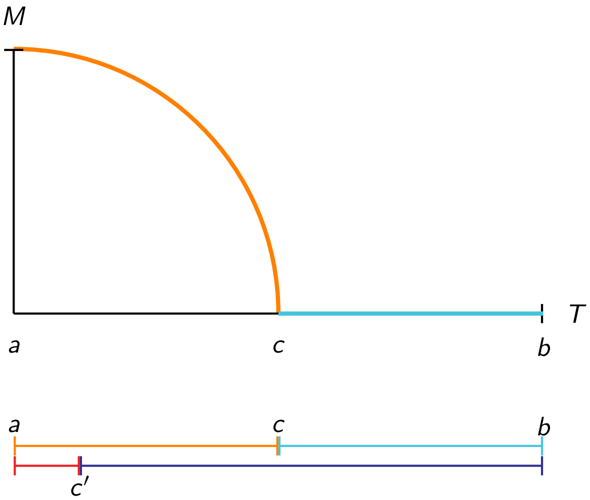
2017

Classical Ising model on L^2 grid

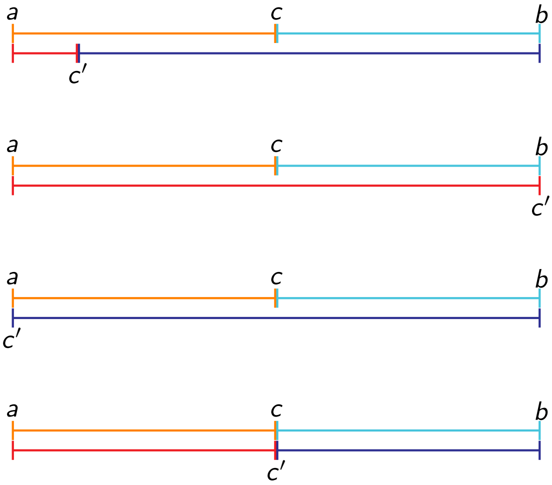


$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^Z$$

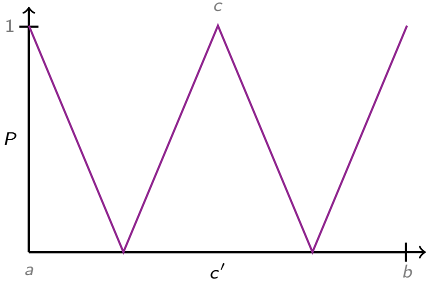
Learning Phase Transitions by Confusion



Learning Phase Transitions by Confusion

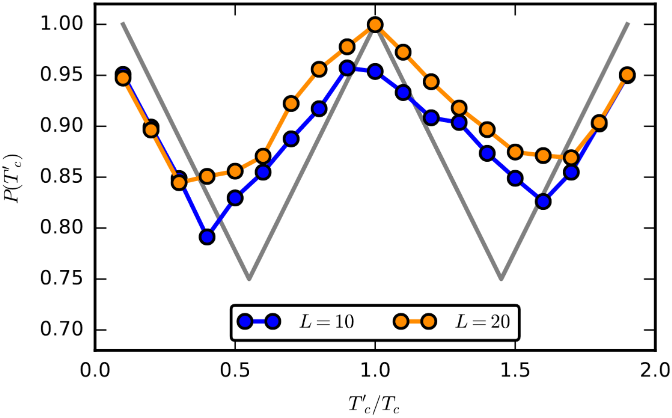


Learning Phase Transitions by Confusion



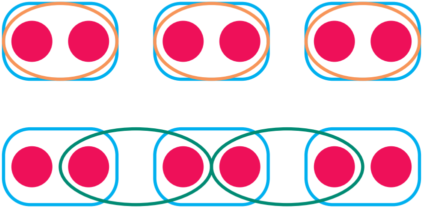
$$P\left(c'\right) = \begin{cases} 1 - \dfrac{\min\left(c-c', c'-a\right)}{c-a}, & c' < c \\ 1 - \dfrac{\min\left(c'-c, b-c'\right)}{b-c}, & c' > c \end{cases}$$

Classical Ising model on L^2 grid



Source: van Nieuwenburg et al. [1]

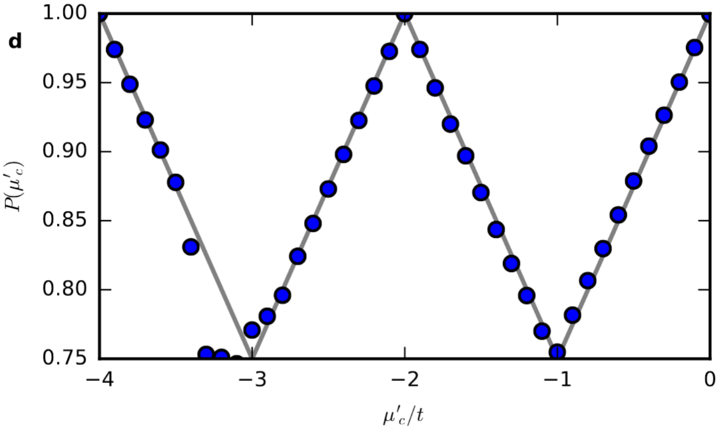
Kitaev chain



$$\hat{H} = -t \sum_{i=1}^{L} \left(\hat{c}_{i+1}^{\dagger} \hat{c}_i + \hat{c}_{i+1} \hat{c}_i + h.c. \right) - \mu \sum_{i=1}^{L} \hat{c}_i^{\dagger} \hat{c}_i$$

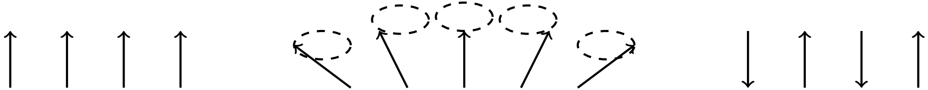
- 1 phase transition at $\mu_c = -2t$

Kitaev chain



Source: van Nieuwenburg et al. [1]

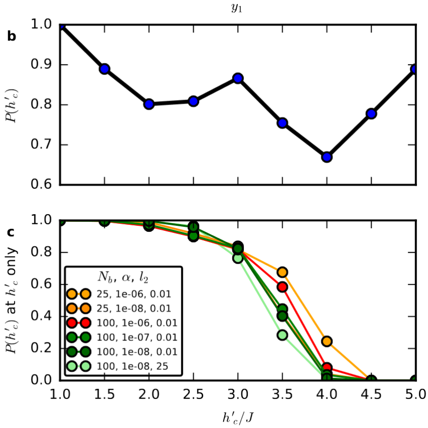
Heisenberg model



$$H = J \sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sum_{\alpha=x,y,z} \sum_{i=1}^{L} h_i^\alpha S_i^\alpha$$

- 1 phase transition at $h_c \approx 3J$

Heisenberg model



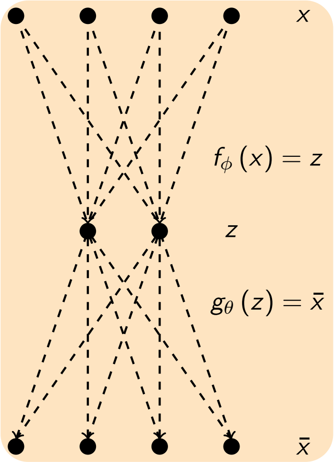
- The algorithm parameters are learning rate (α), regularization (adds $l_2 \sum |\omega|^2$ to cost the function) and batch size of training data (N_b)

Source: van Nieuwenburg et al. [1]

Unsupervised Phase Discovery with Deep Anomaly Detection

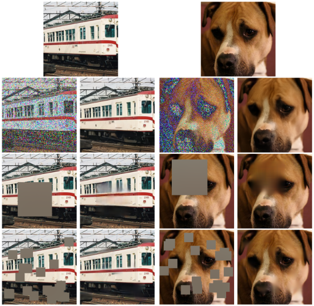
Kottmann, Korbinian and Huembeli, Patrick and Lewenstein, Maciej and Acín, Antonio
2020

Auto encoder



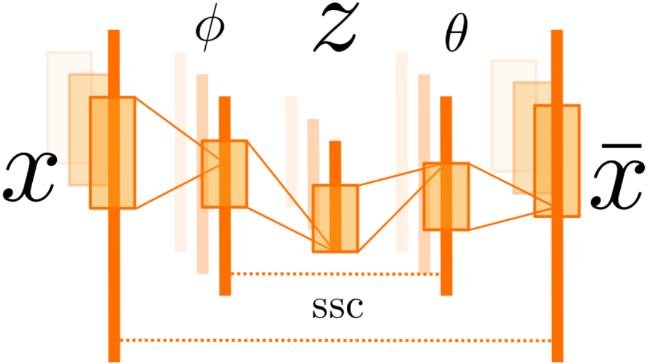
$$L(x, \bar{x}) = \frac{|x - \bar{x}|^2}{dim(x)}$$

$$dim(x) = dim(\bar{x})$$



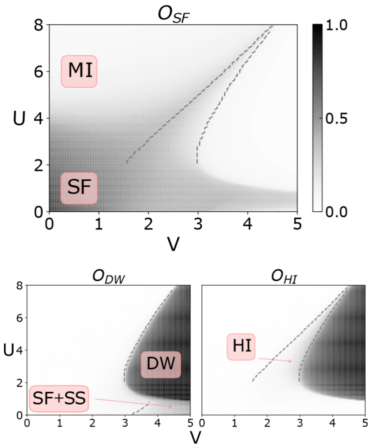
Source: Jianfeng Dong et al. [3]

Symmetric shortcut connections



Source: Kottmann et al. [2]

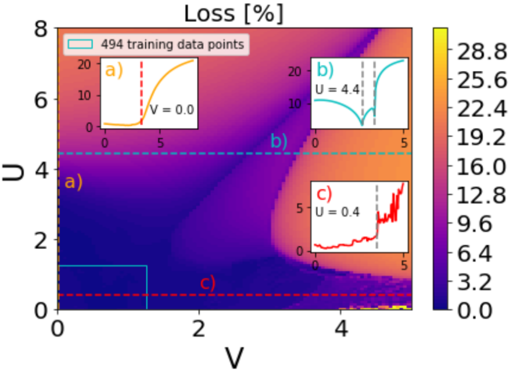
Extended Bose-Hubbard Model

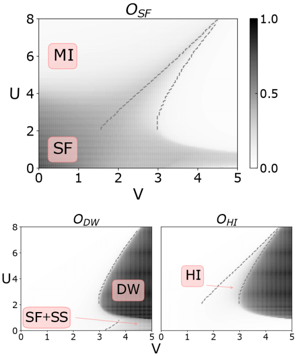


$$H = -t \sum_i \left(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right) + \frac{U}{2} \sum_i b_i^\dagger b_i \left(b_i^\dagger b_i - 1 \right) + V \sum_i b_i^\dagger b_i b_{i+1}^\dagger b_{i+1}$$

Source: Kottmann et al. [2]

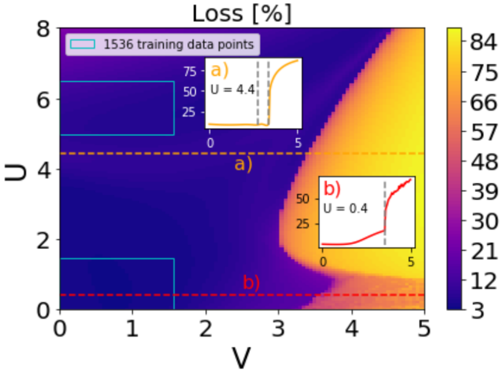
Extended Bose-Hubbard Model





Source: Kottmann et al. [2]

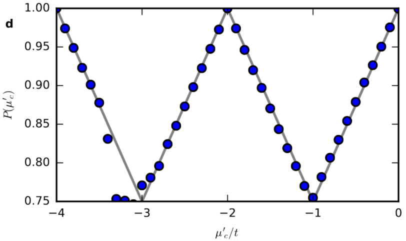
Extended Bose-Hubbard Model



Source: Kottmann et al. [2]

Summary

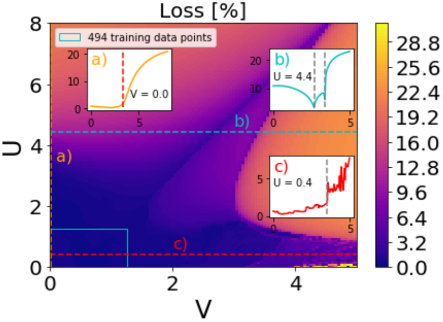
Learning Phase Transitions by Confusion



- No knowledge over phases needed
- Sampling over the dataset gives a robust tool to find transitions
- But each sample needs a training cycle and is more costly than our second method

Source: van Nieuwenburg et al. [1]

Unsupervised Phase Discovery with Deep Anomaly Detection



- One training over only a small region is sufficient
- Spans a whole phase diagram
- Runs on different kinds of input data type

Source: Kottmann et al. [2]

References

van Nieuwenburg, Evert P. L. and Liu, Ye-Hua and Huber, Sebastian D.: *Learning phase transitions by confusion*. In: *Nature Physics*. Springer Science and Business Media LLC. 2017

Kottmann, Korbinian and Huembeli, Patrick and Lewenstein, Maciej and Acín, Antonio: *Unsupervised Phase Discovery with Deep Anomaly Detection*. In: *Physical Review Letters*. American Physical Society (APS). 2020

Jianfeng Dong and Xiao-Jiao Mao and Chunhua Shen and Yu-Bin Yang: *Learning Deep Representations Using Convolutional Auto-encoders with Symmetric Skip Connections*. 2017