Machine learning phase transitions: Connections to the Fisher information

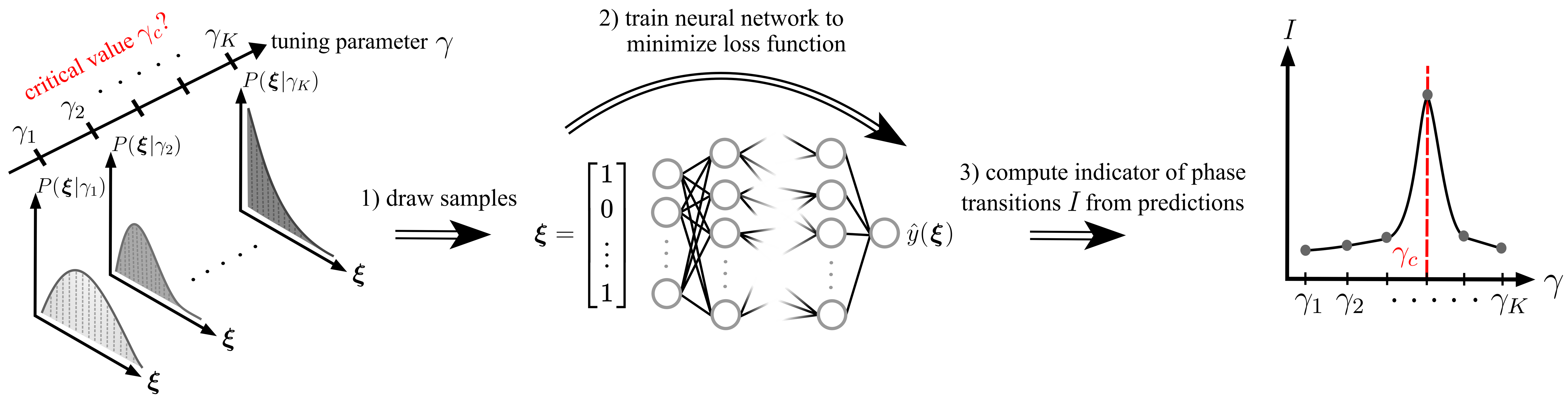
Julian Arnold,[1] Niels Lörch,[1] Flemming Holtorf,[2] and Frank Schäfer[2]

① University of Basel

② Massachusetts Institute of Technology

Automated detection of phase transitions from data

requires minimal explicit knowledge of the system's underlying physics and could enable the discovery of new phases of matter



Approach 1 ("Supervised learning")

- pick a set of points Γ_0 and Γ_1 lying within each of the two phases
- each sample $\boldsymbol{\xi}$ drawn in Γ_y is assigned the label y

$\Rightarrow$ $I_1(\gamma) = \left|\frac{\partial \hat{y}(\gamma)}{\partial \gamma}\right|$, where $\hat{y}(\gamma) = \mathbb{E}_{\boldsymbol{\xi}\sim P(\cdot|\gamma)}\left[\hat{y}(\boldsymbol{\xi})\right]$

Approach 2 ("Learning by confusion")

- split parameter space at γ into two neighboring regions Γ_0 and Γ_1
- each sample $\boldsymbol{\xi}$ drawn in Γ_y is assigned the label y

$\Rightarrow$ $I_2(\gamma) = 1 - 2p_{\rm err}(\gamma)$, where $p_{\rm err}(\gamma)$ is mean unbiased error rate

Approach 3 ("Prediction-based method")

- each sample $\boldsymbol{\xi}$ drawn at γ is assigned the label $y = \gamma$

$\Rightarrow$ $I_3(\gamma) = \frac{\partial \hat{\gamma}(\gamma)/\partial\gamma}{\sigma(\gamma)}$, where $\sigma(\gamma)$ is standard deviation of estimator at γ

Relation to the Fisher information

Classical Fisher information matrix $\mathcal{F}(\boldsymbol{\gamma})$ measures how quickly a probability distribution $P(\cdot|\boldsymbol{\gamma})$ changes w.r.t. its parameters $\boldsymbol{\gamma}$

$$\mathcal{F}_{i,j}(\boldsymbol{\gamma}) = \mathcal{F}_{i,j}\left[P(\cdot|\boldsymbol{\gamma})\right] = \mathbb{E}_{\boldsymbol{\xi}\sim P(\cdot|\boldsymbol{\gamma})}\left[\left(\frac{\partial \log\left[P(\cdot|\boldsymbol{\gamma})\right]}{\partial\gamma_i}\right)\left(\frac{\partial \log\left[P(\cdot|\boldsymbol{\gamma})\right]}{\partial\gamma_j}\right)\right]$$

Main result:

Machine-learned indicators of phase transitions are underapproximators to the square root of the system's (classical) Fisher information

$$I(\boldsymbol{\gamma}) \leq \sqrt{\mathrm{tr}\left[\mathcal{F}(\boldsymbol{\gamma})\right]}$$

Proof sketch:

Approach 1

use Cauchy-Schwarz inequality with constraints

$\Rightarrow$ indicator is maximal iff $\hat{y}$ is perfectly correlated with score $\frac{\partial \log[P(\cdot|\gamma)]}{\partial\gamma}$

Approach 2

equivalent to single-shot binary symmetric hypothesis testing task

$\Rightarrow$ $I_2^{\rm opt} = \mathrm{TV}[P_{\rm I}, P_{\rm II}] = \frac{1}{2}\sum_{\boldsymbol{\xi}} |P_{\rm I}(\boldsymbol{\xi}) - P_{\rm II}(\boldsymbol{\xi})|$

$\Rightarrow$ related to Fisher information to 1st order $\mathrm{TV}[P(\cdot|\gamma), P(\cdot|\gamma+\delta\gamma)] \leq \frac{1}{2}\sqrt{\mathcal{F}(\gamma)}\delta\gamma + \mathcal{O}(\delta\gamma^2)$

Approach 3

equivalent to parameter estimation task

$\Rightarrow$ apply Cramér-Rao bound

$$\sigma^2(\gamma) \geq \frac{(\partial\psi(\gamma)/\partial\gamma)^2}{\mathcal{F}(\gamma)},$$

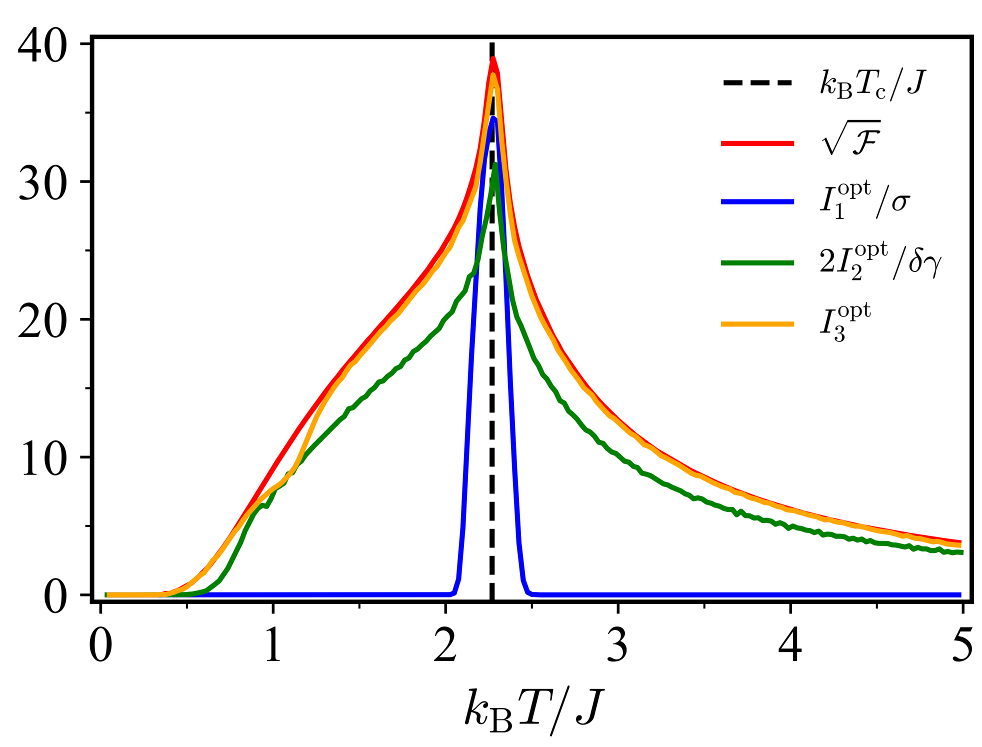
where σ^2 and ψ are variance and expected value of estimator $\hat{y}$

Classical example: 2D Ising model

Hamiltonian $H = -J\sum_{\langle ij\rangle}\sigma_i^z\sigma_j^z$

$\Rightarrow$ consider system in thermal state $\rho(\gamma) = e^{-H/k_{\rm B}T}/Z$ with $\gamma = k_{\rm B}T/J$ measured in z-basis: $P(\boldsymbol{z}|\gamma) = \mathrm{tr}\left[|\boldsymbol{z}\rangle\langle\boldsymbol{z}|\rho(\gamma)\right]$

$\Rightarrow$ Fisher information is proportional to heat capacity C: $\mathcal{F}(\gamma) = CJ^2/k_{\rm B}^3T^2$

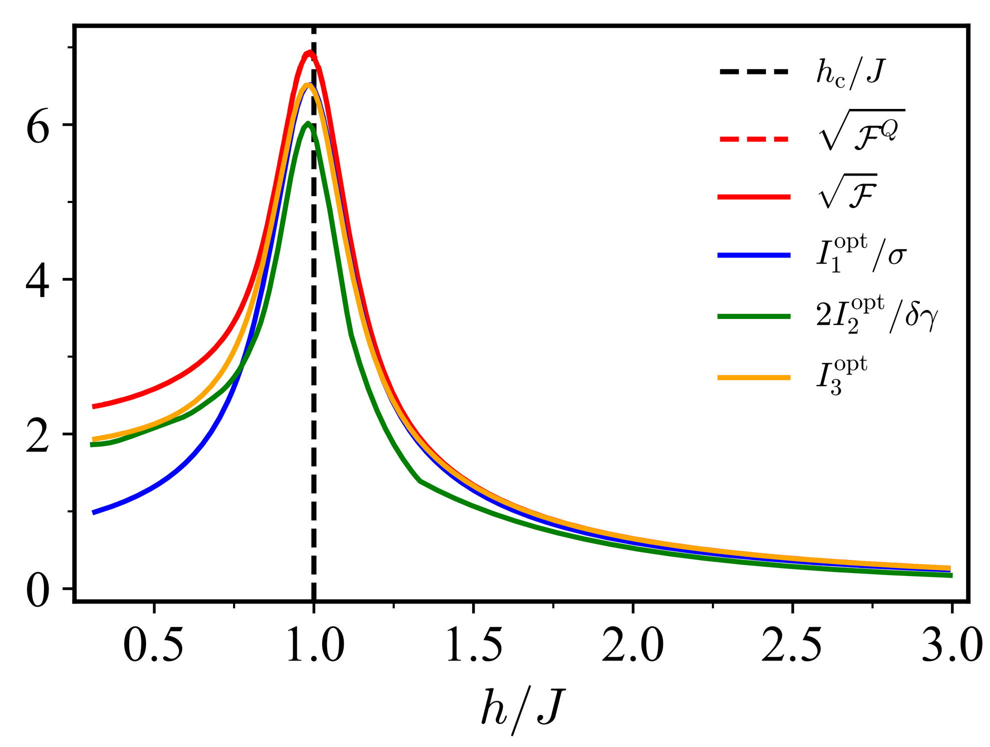


Quantum example: 1D TFIM

Hamiltonian $H = -J\sum_{\langle ij\rangle}\sigma_i^z\sigma_j^z - h\sum_i\sigma_i^x$

$\Rightarrow$ consider system in ground state $|\Psi(\gamma)\rangle$ with $\gamma = h/J$ measured in x-basis: $P(\boldsymbol{x}|\gamma) = |\langle\boldsymbol{x}|\Psi(\gamma)\rangle|^2$

$\Rightarrow$ indicators also lower-bound square root of quantum Fisher information $\mathcal{F}^Q(\gamma) = \max_{\{\Pi_{\boldsymbol{\xi}}\}_{\boldsymbol{\xi}}}\mathcal{F}\left(\mathrm{tr}\left[\Pi_{\boldsymbol{\xi}}\rho(\gamma)\right]\right)$



References

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Contact

julian.arnold@unibas.ch

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