



Методы машинного обучения в анализе фазовых переходов моделей статистической механики



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Рабочее совещание "ОИЯИ-ВШЭ"
14.06.2024, Дубна



Фазовые переходы – универсальные механизмы



1. Физика твердого тела
 - Магнетизм
 - Сверхтекучесть
 - Сверхпроводимость
2. Конформации полимеров
3. Свертываемость белков
4. Космология и астрофизика
5. Геология, противогаз, кофемашина

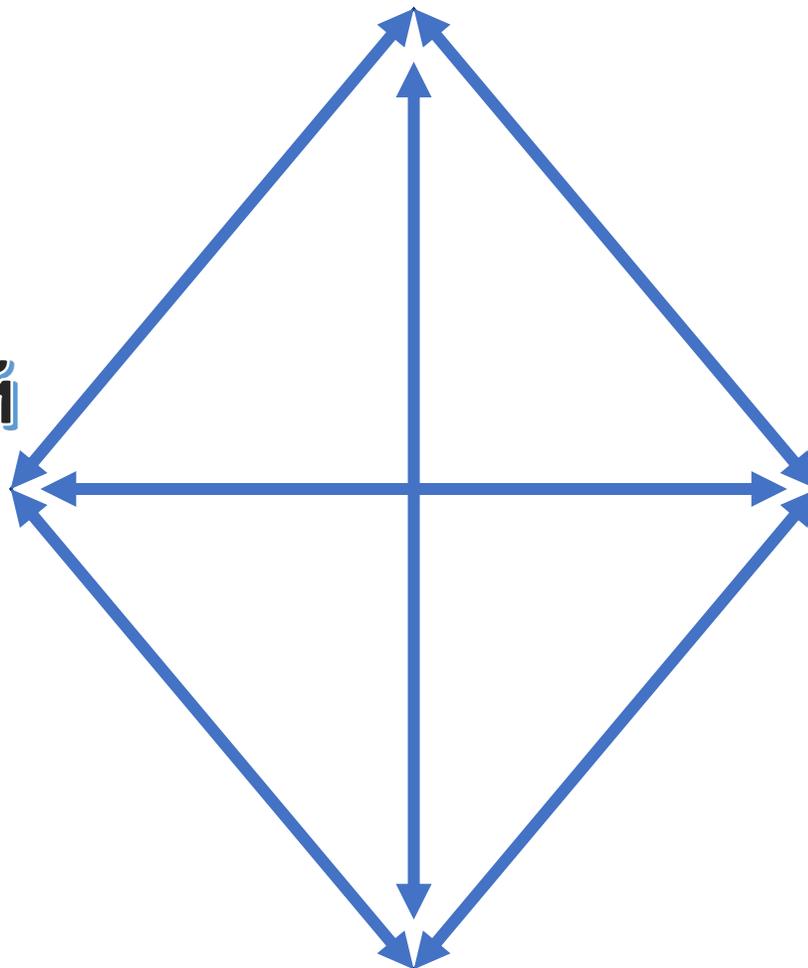


Эксперимент

**Вычислительный
эксперимент**

**Машинное
обучение**

Теория



Рабочее совещание "ОИЯИ-ВШЭ"
14.06.2024, Дубна

Finite-size analysis in neural network classification of critical phenomena

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NN	$\#_{\text{params}}^{L=48} \cdot 10^6$	$\#_{\text{params}}^{L=216} \cdot 10^6$	$\#_{\text{params}}^{L=243} \cdot 10^6$
FCNN	0.59	11.9	15.1
CNN	0.59	11.9	14.7
ResNet10	4.9	4.9	4.9
ResNet18	11.2	11.2	11.2
ResNet34	21.3	21.3	21.3
ResNet50	23.5	23.5	23.5

TABLE II: Number of adjustable parameters in NNs. $L = 48$ is the minimum lattice size for the Ising and the BW models, $L = 216$ and $L = 243$ are the maximum lattice sizes for Ising and BW models, respectively.

NN	Train	Valid	Acc	AUC-ROC
FCNN	0.38(1)	0.34(2)	0.85(1)	0.94(1)
CNN	0.27(2)	0.25(3)	0.87(1)	0.96(1)
ResNet10	0.26(2)	0.25(3)	0.87(1)	0.96(1)
ResNet18	0.26(2)	0.25(2)	0.87(1)	0.96(1)
ResNet34	0.27(2)	0.25(2)	0.87(1)	0.96(1)
ResNet50	0.28(3)	0.27(2)	0.87(1)	0.96(1)

TABLE III: Training protocol for the Ising model. Train and Valid are measured by BCE on the training and validation datasets, respectively.

NN	Train	Valid	Acc	AUC-ROC
FCNN	0.24(4)	0.20(4)	0.93(2)	0.97(1)
CNN	0.18(4)	0.16(4)	0.93(2)	0.98(1)
ResNet10	0.17(4)	0.16(4)	0.94(2)	0.98(1)
ResNet18	0.17(4)	0.16(4)	0.93(2)	0.98(1)
ResNet34	0.17(5)	0.16(5)	0.93(2)	0.98(1)
ResNet50	0.18(5)	0.17(4)	0.93(2)	0.98(1)

TABLE IV: Training protocol for the BW model, same as for the Ising model in the Table III.

Вероятность принадлежности к ферромагнитной фазе и ее вариация

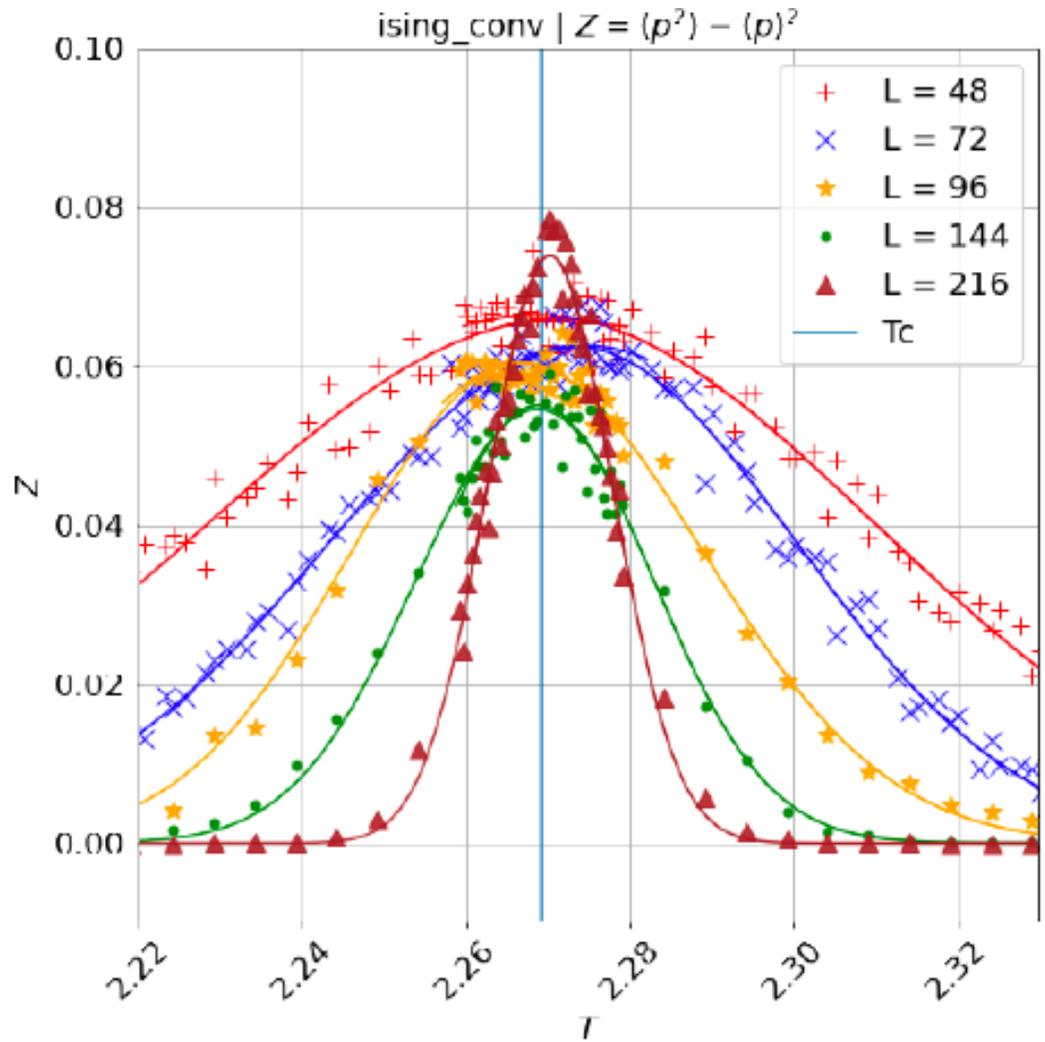
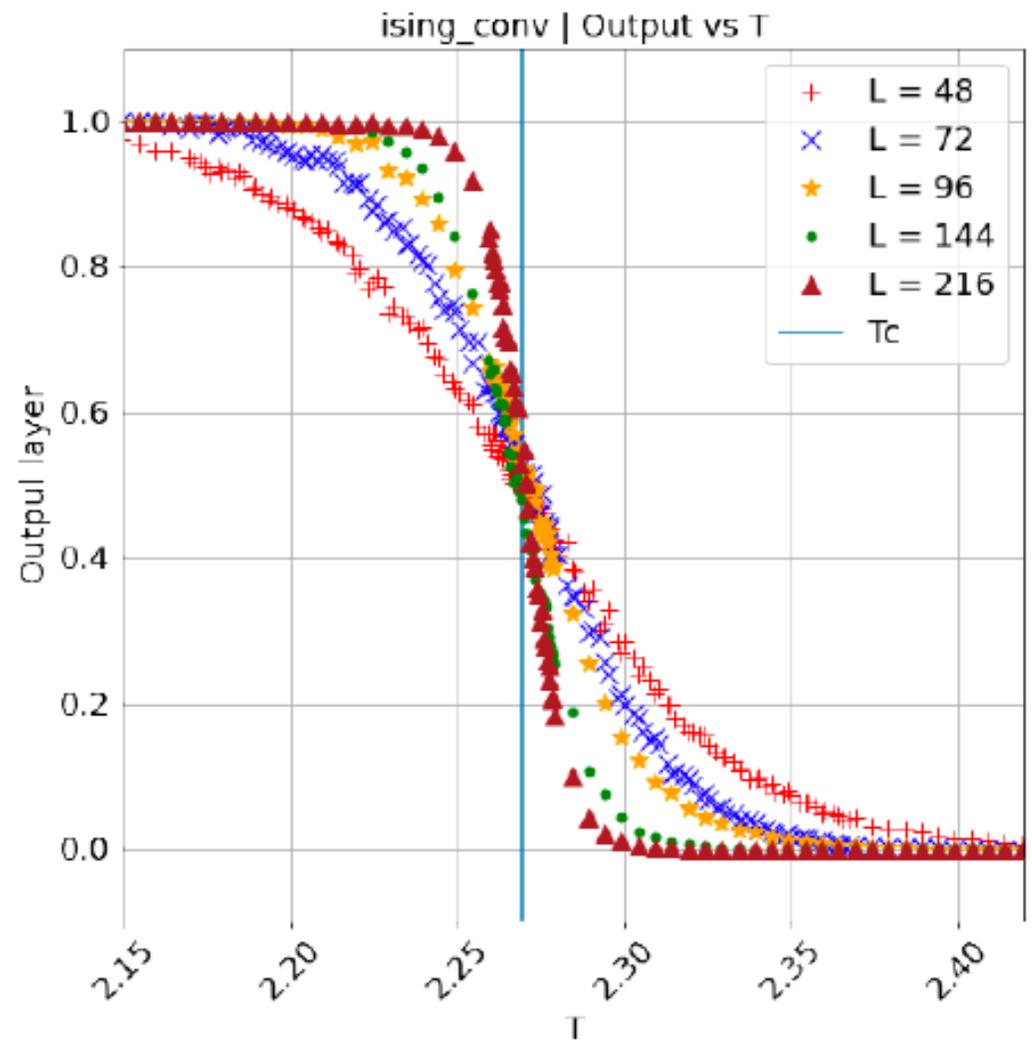
Averaging over the **testing** dataset, we define the average prediction, F^T ,

$$F^T = \frac{1}{N} \sum_{i=1}^N f_i^T \quad (1)$$

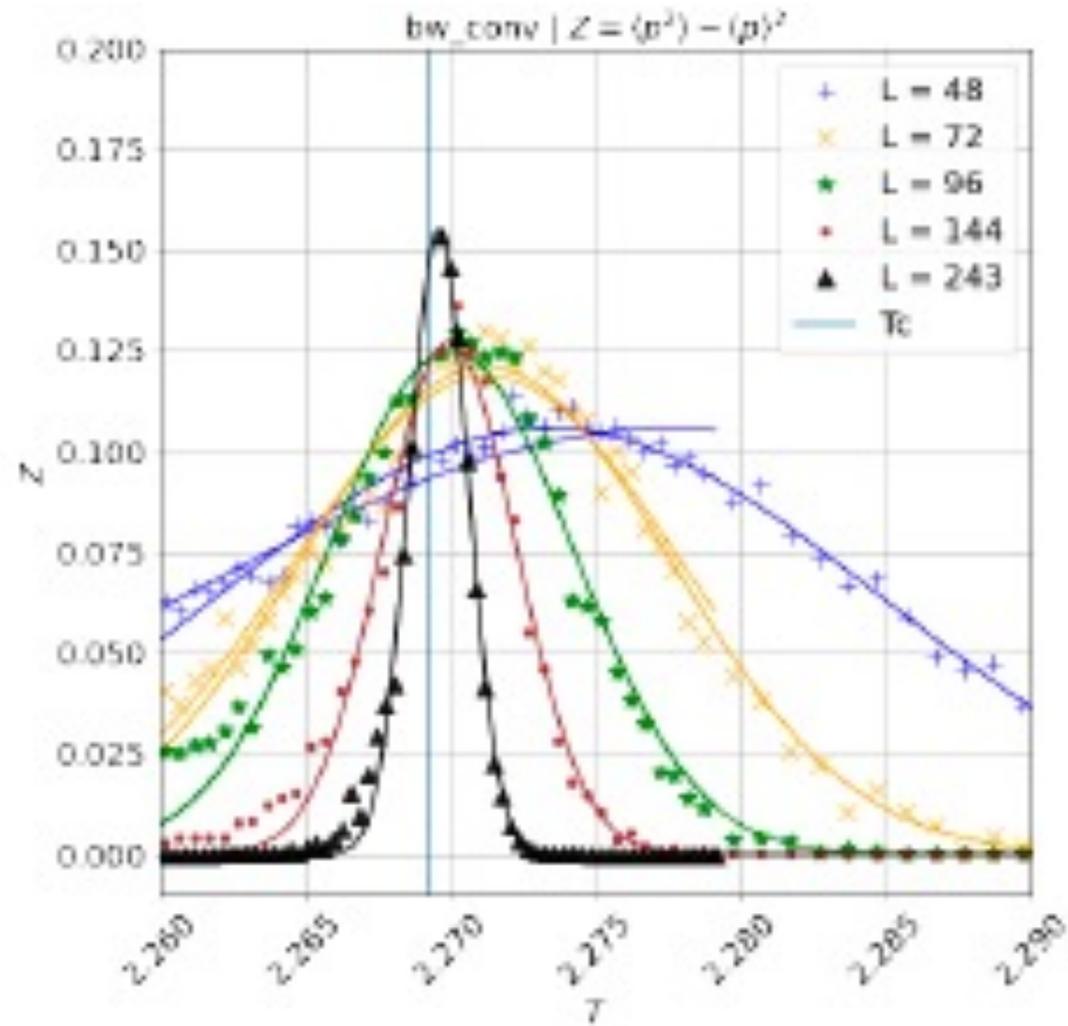
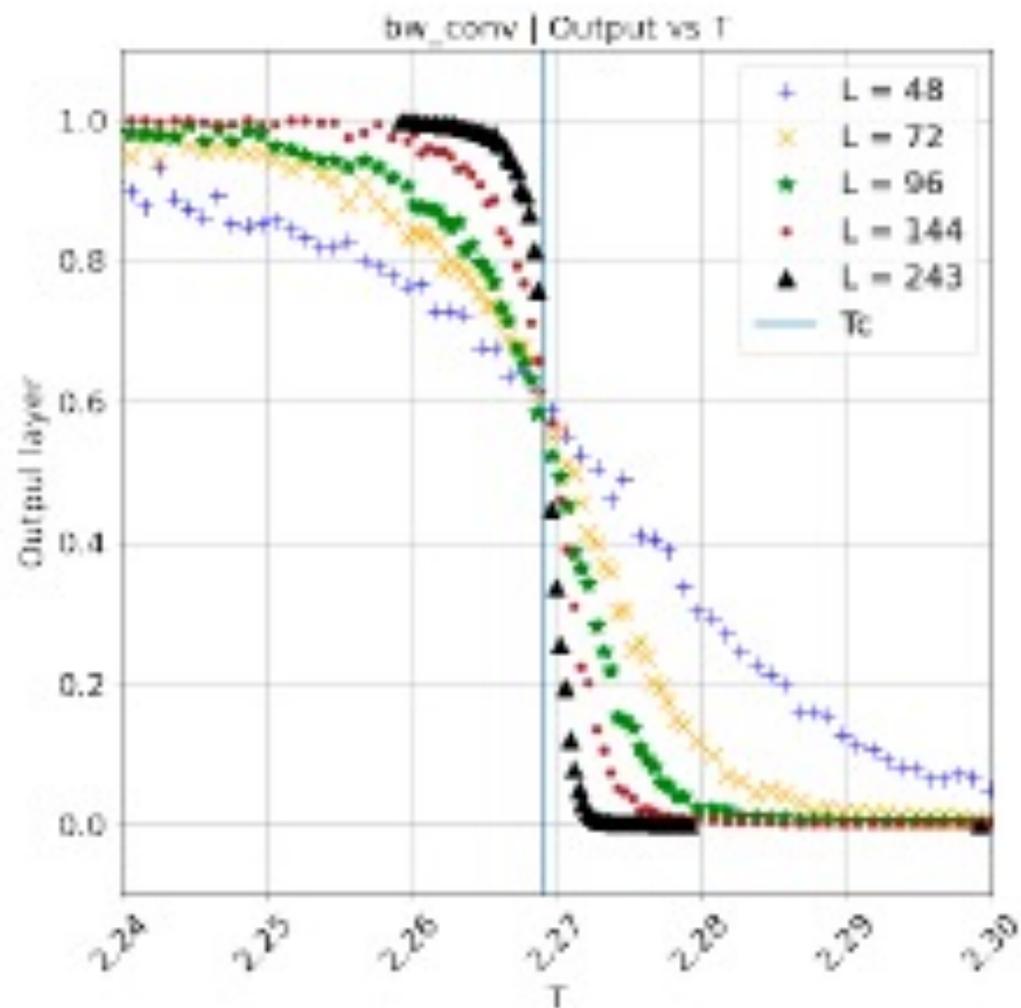
and its variance, V^T ,

$$V^T = \frac{1}{N} \sum_{i=1}^N (f_i^T)^2 - \left(\frac{1}{N} \sum_{i=1}^N f_i^T \right)^2. \quad (2)$$

Модель Изинга и CNN



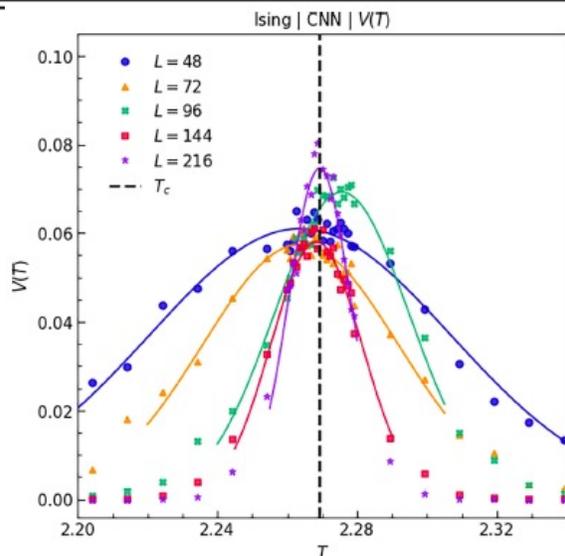
Модель Бакстера-Ву и CNN



Результаты тестирования – модель Изинга

TABLE I. Peak widths for the Ising model. Here v_σ is the estimate from fitting the Gaussian profile to the V^T . v_σ^+ and v_σ^- are similar estimates where we only fit the right-hand side (resp., left-hand side) of the V^T curves. See the text for discussion.

NN	$1/v_\sigma$	$1/v_{\sigma^-}$	$1/v_{\sigma^+}$
FCNN	1.01(1)	1.02(13)	0.98(4)
CNN	1.06(3)	1.11(5)	1.07(2)
ResNet-10	1.25(3)	1.24(7)	1.24(3)
ResNet-18	1.17(11)	1.41(6)	1.08(10)
ResNet-34	1.15(16)	1.26(7)	1.12(24)
ResNet-50	1.20(5)	1.21(5)	1.31(6)



Точное значение = 2.269185...

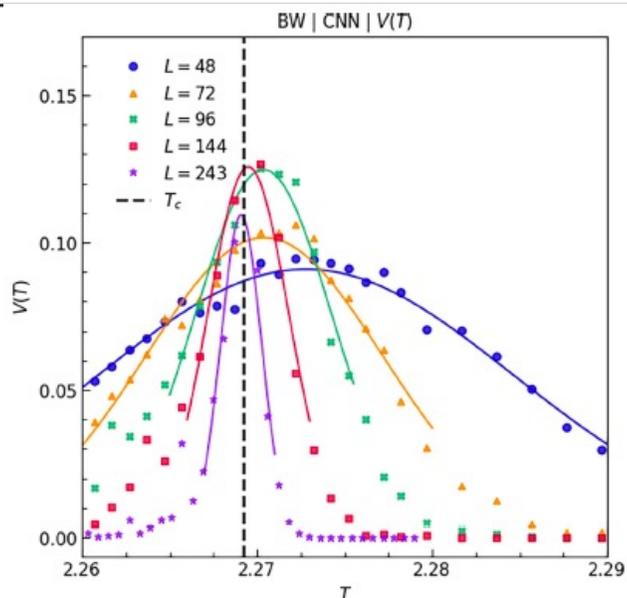
TABLE III. Ising model: Estimation of the critical temperature from the VOT width using Ferdinand-Fisher law. The last column is the difference between the estimated critical temperature and the exact critical temperature $\Delta = |T^* - T_c|$ divided by the statistical error σ_T of the weighted linear fit.

NN	T^*	Δ/σ_T
FCNN	2.2699(5)	1
CNN	2.2727(6)	5
ResNet-10	2.2667(6)	4.2
ResNet-18	2.2688(6)	0.7
ResNet-34	2.2659(6)	5.5
ResNet-50	-	-

Результаты тестирования – модель Бакстера-Ву

TABLE II. Peak widths for the Baxter-Wu model. Here v_σ , v_σ^+ , and v_σ^- are the same as in Table I.

NN	$1/v_\sigma$	$1/v_{\sigma^-}$	$1/v_{\sigma^+}$
FCNN	1.49(3)	1.57(2)	1.38(8)
CNN	1.45(5)	1.55(6)	1.49(5)
ResNet-10	1.48(5)	1.65(13)	1.47(4)
ResNet-18	1.32(11)	1.36(14)	1.40(7)
ResNet-34	1.54(6)	1.76(5)	1.47(3)
ResNet-50	1.43(9)	1.69(16)	1.47(5)



Точное значение = 1.5

Точное значение = 2.269185...

TABLE IV. Baxter-Wu model: Estimation of the critical temperature from the VOT width using Ferdinand-Fisher law. The last column is the difference between the estimated critical temperature and the exact critical temperature $\Delta = |T^* - T_c|$ divided by the statistical error σ_T of the weighted linear fit.

NN	T^*	Δ/σ_T
FCNN	2.2691(4)	0
CNN	2.2687(4)	1.25
ResNet-10	2.2690(4)	0.25
ResNet-18	2.2684(4)	2
ResNet-34	2.2694(4)	0.5
ResNet-50	2.2688(4)	1



Заключение

1. Предложена методика оценки критической температуры и критического индекса корреляционной длины, основанная на обучении с учителем
2. Применение методов глубокого машинного обучения представляется новым и перспективным методом исследования