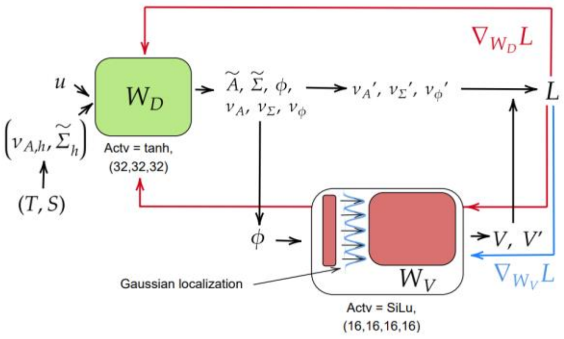
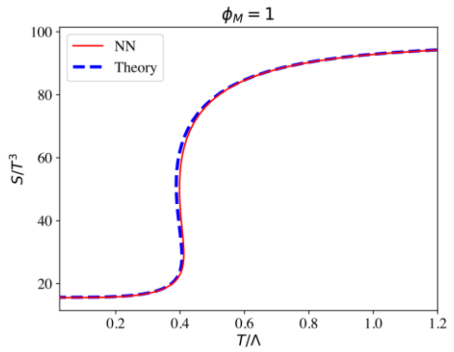
Solving an inverse problem using neural networks

Yago Bea

University of Barcelona





Based on: 2403.14763

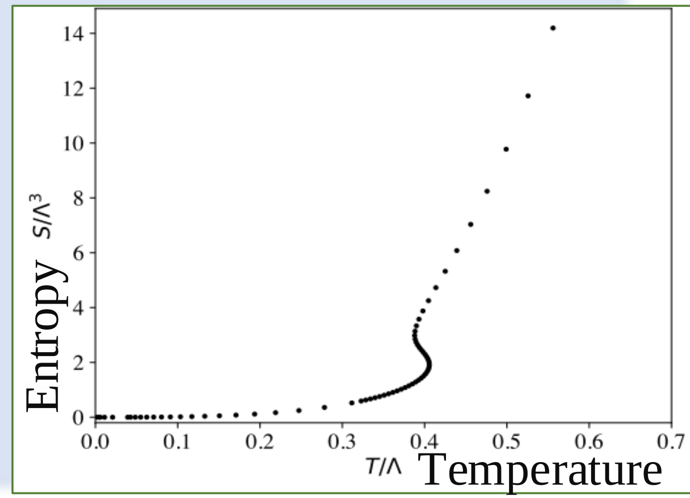
With Raul Jiménez, David Mateos, Shuheng Liu,
Pavlos Protopapas, Pedro Tarancón and Pablo Tejerina

Main idea

Einstein eqs.

$$S = \frac{2}{\kappa_5^2} \int dx^5 \sqrt{-g} \left[\frac{1}{4} R - \frac{1}{2} (\nabla \phi)^2 - V(\phi) \right]$$

Direct problem



Main idea

Holography

Gravity 4+1

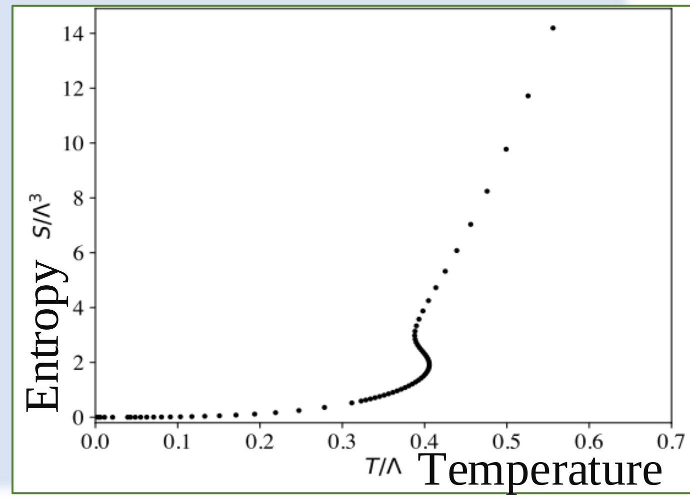
QFT 3+1

Einstein eqs.

Direct problem →

Equation of state

$$S = \frac{2}{\kappa_5^2} \int dx^5 \sqrt{-g} \left[\frac{1}{4} R - \frac{1}{2} (\nabla \phi)^2 - V(\phi) \right]$$



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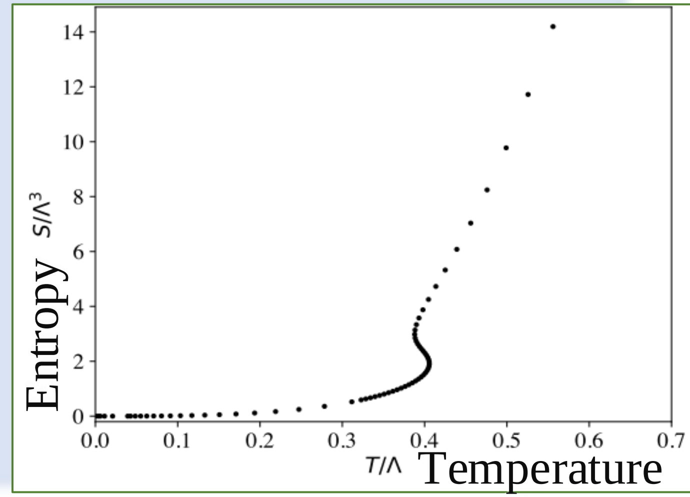
Direct problem →

← Inverse problem

Equation of state



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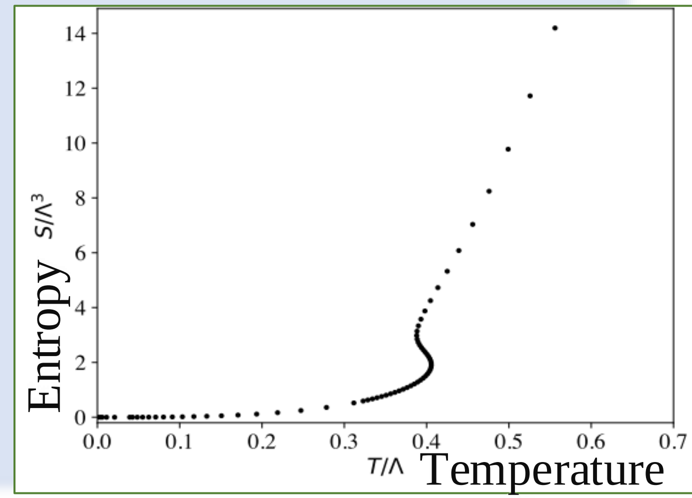
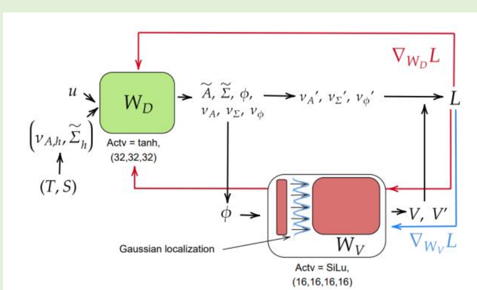


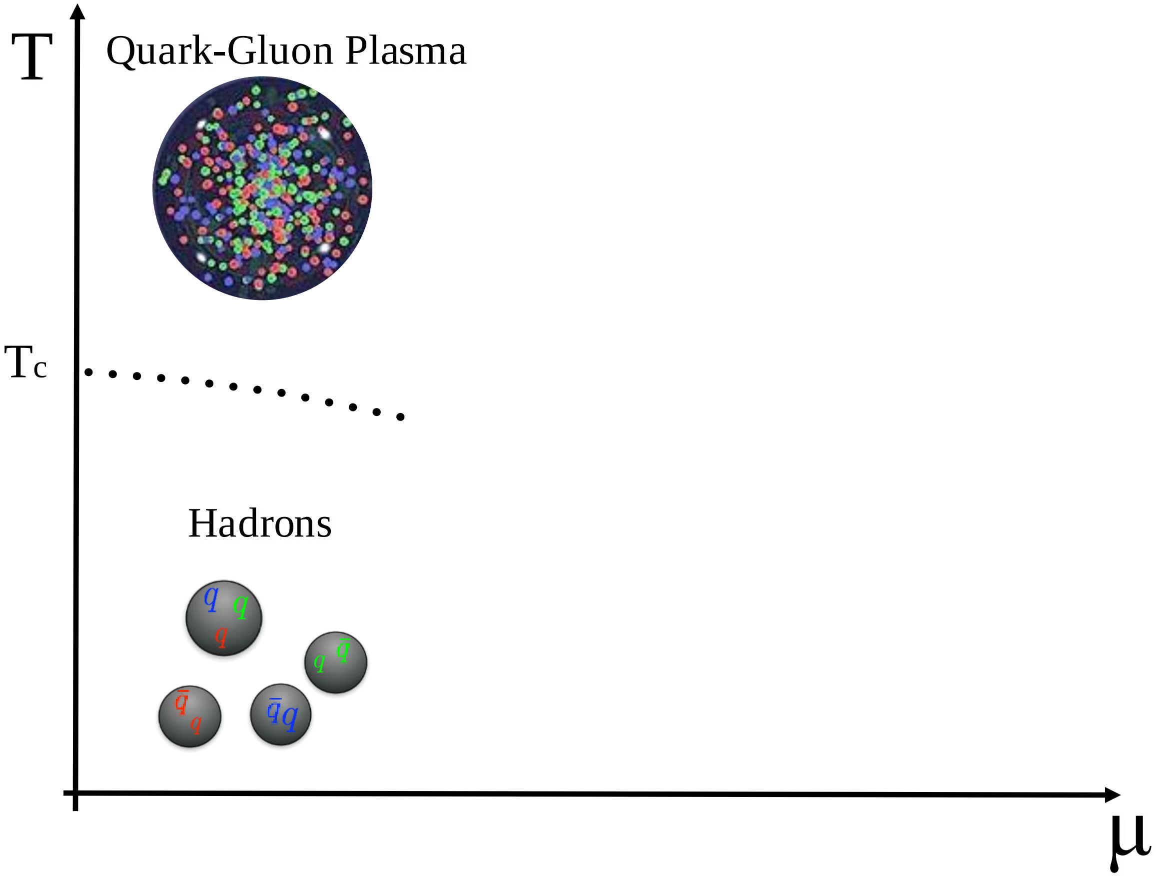
Neural Networks



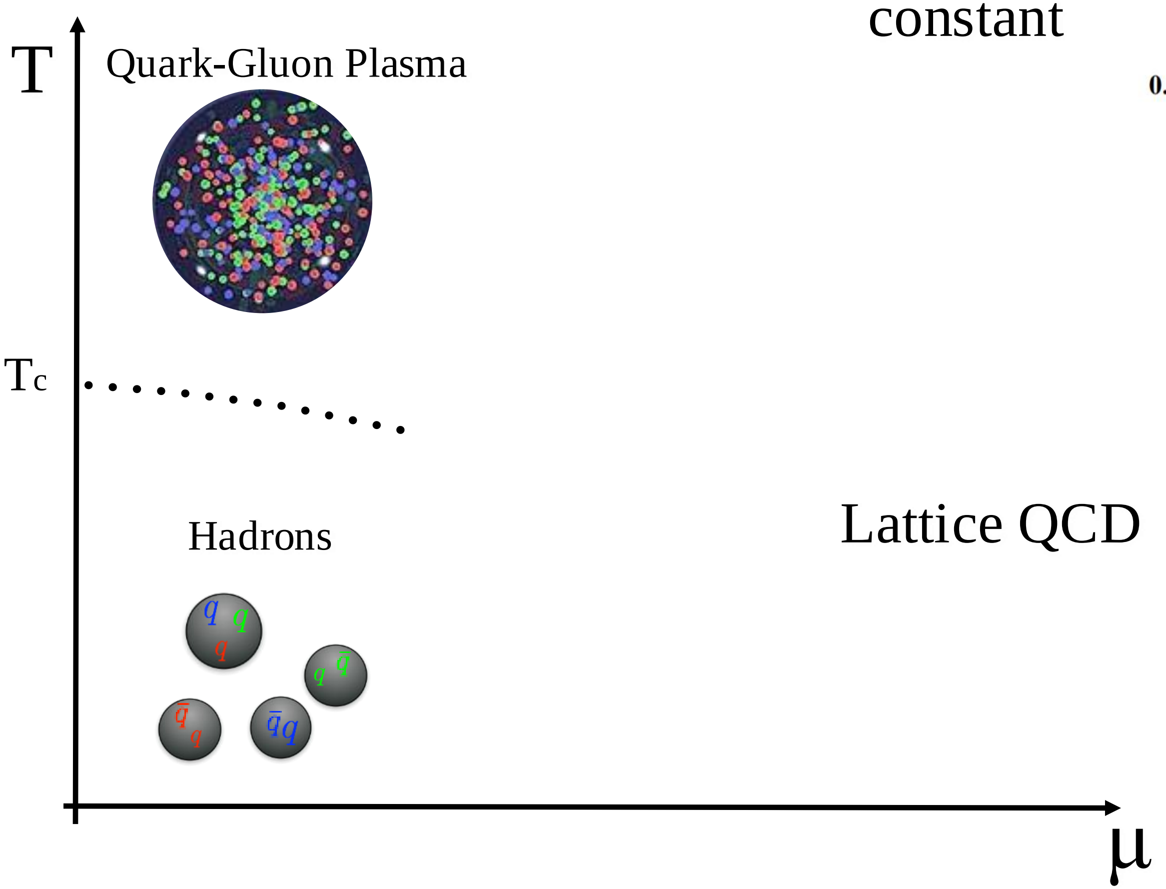
→ We use NN to solve a problem not addressed before

Holography: motivation

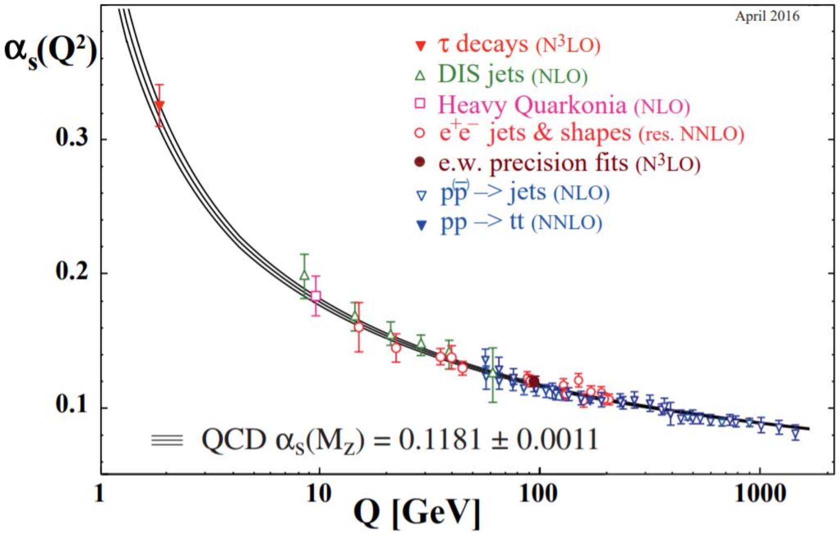
QCD & Holography



QCD & Holography

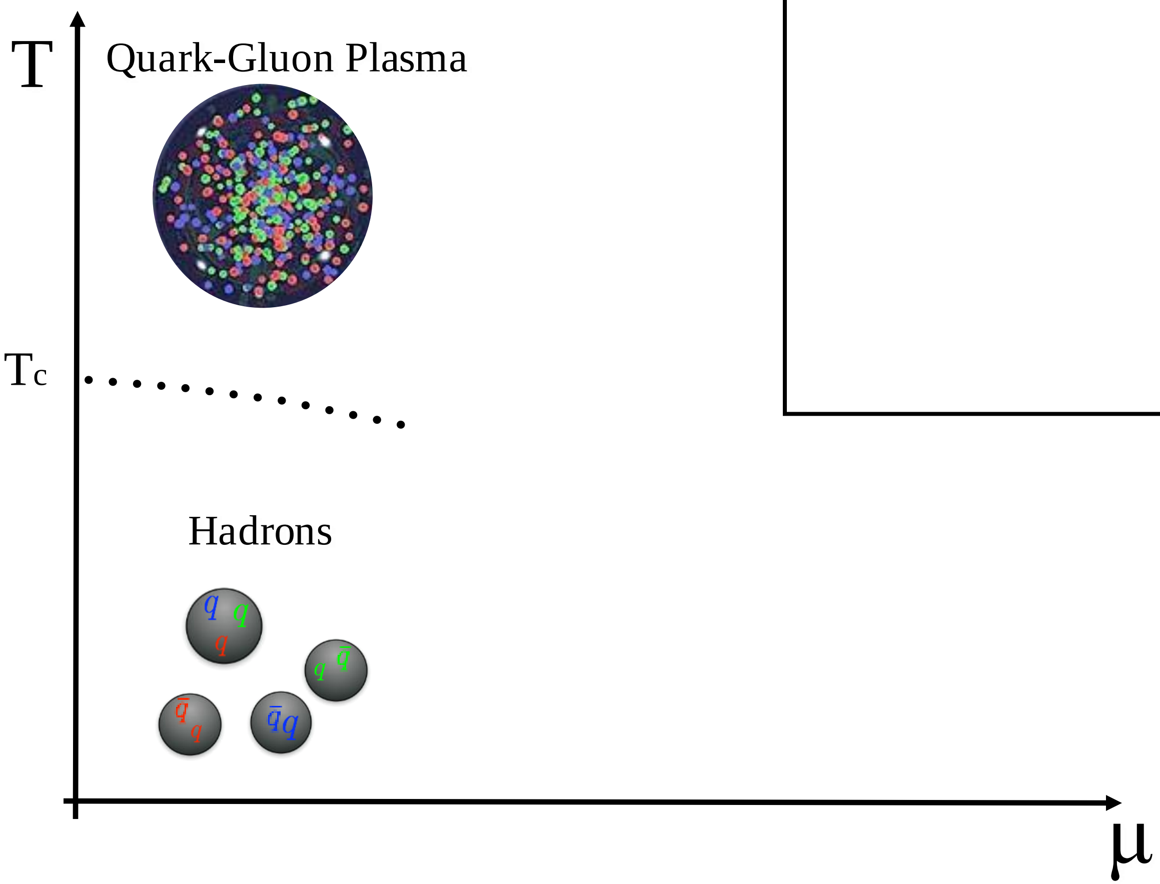


QCD coupling constant



Lattice QCD

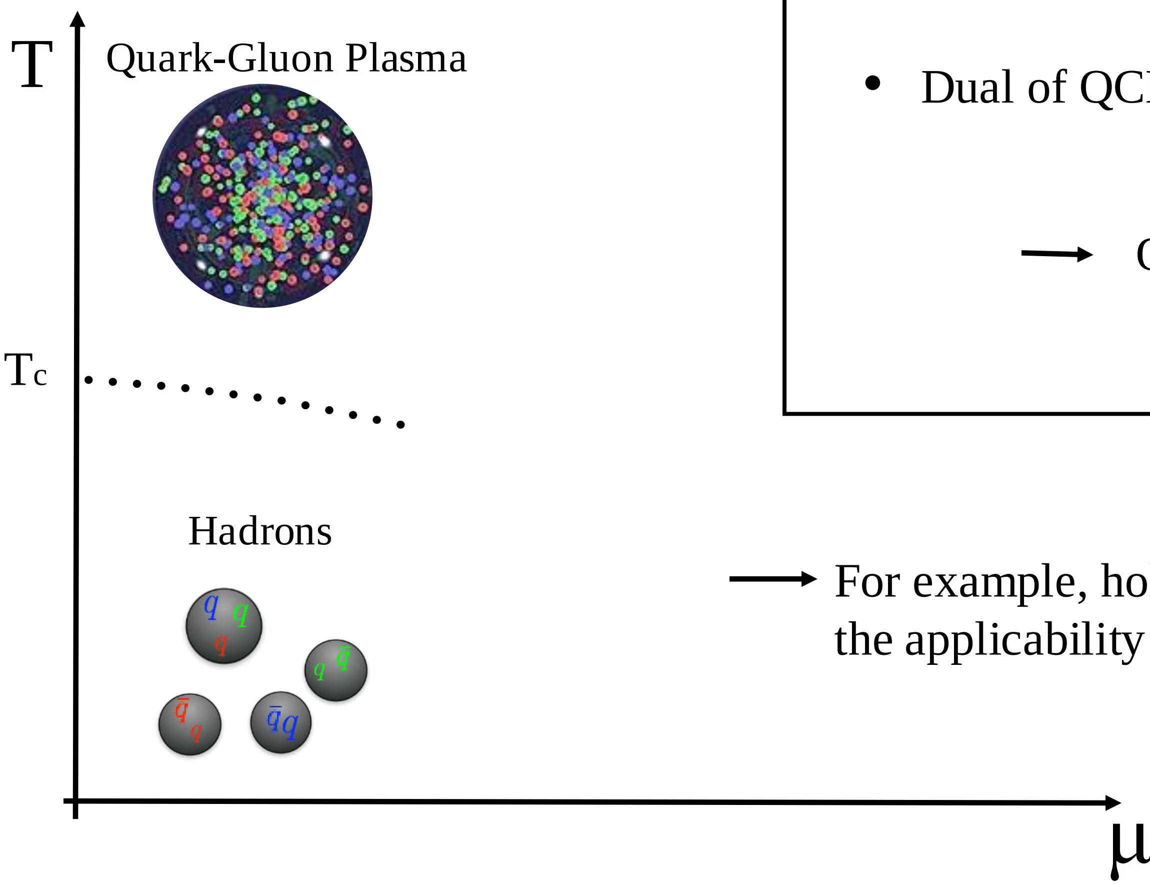
QCD & Holography



Holography

- Strongly coupled QFT
- Out of equilibrium physics

QCD & Holography



Holography

- Strongly coupled QFT
- Out of equilibrium physics
- Dual of QCD not known…

→ Qualitative insights

→ For example, holography as a laboratory to study the applicability of hydrodynamics.

Holography: Our model

- Gravity in 4+1 dim :

$$S \sim \int d^{3+1}x \sqrt{-g}\,(R - 2\Lambda)$$

Holography: Our model

- CFT on Minkowski in 3+1 dim
- Decoupled sector of the stress tensor $T^{\mu\nu}$

Holography

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- QFT on Minkowski in 3+1 dim
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Holography

We want to make contact with phenomenology so we proceed to break conformality:

→ We introduce a scalar field

- Gravity in 4+1 dim :

$$S \sim \int d^{3+1}x\,\sqrt{-g}\,(R - \frac{1}{2}(\partial\phi)^2 - V(\phi))$$

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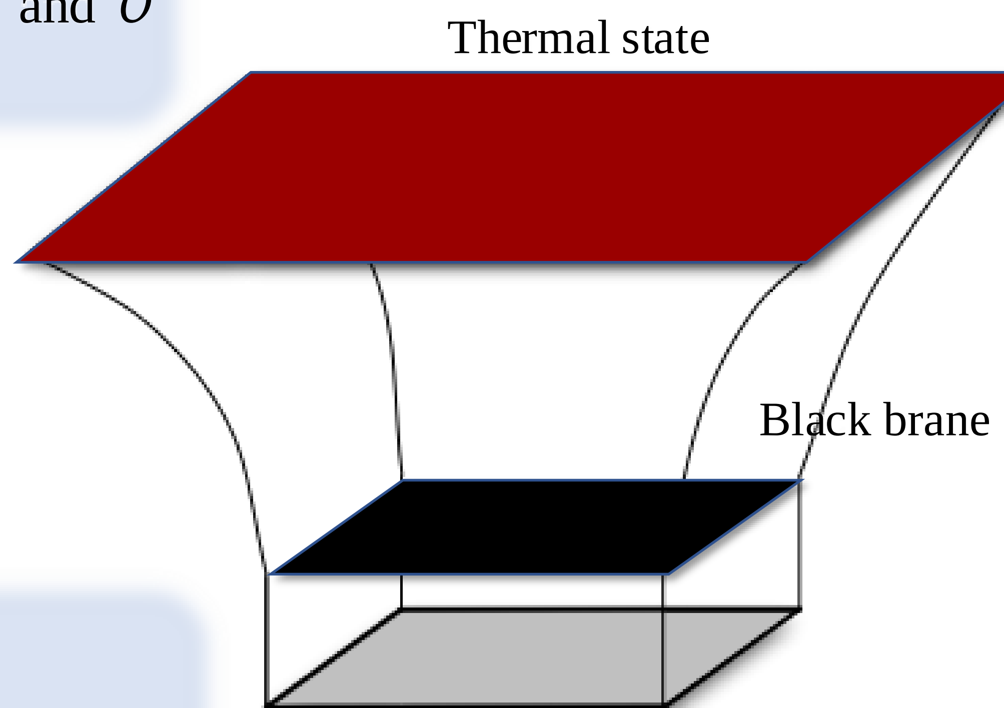
Holography



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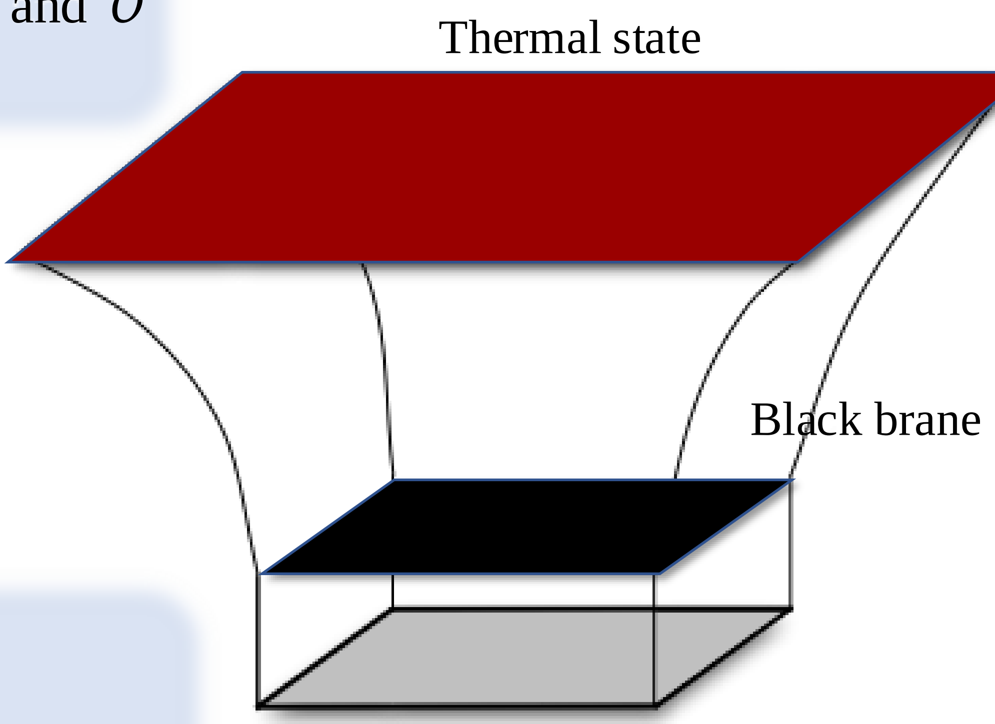

Bekenstein-Hawking entropy S

Hawking temperature T

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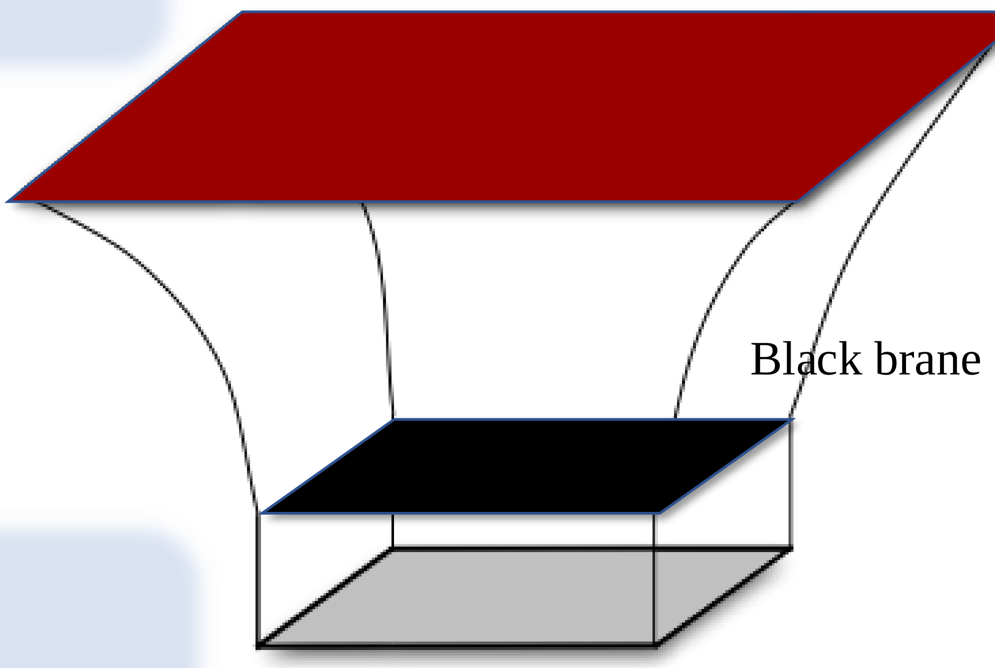
Holography

- Gravity in 4+1 dim :

$$S \sim \int d^{3+1}x \sqrt{-g}\,(R - \frac{1}{2}(\partial\phi)^2 - V(\phi))$$

By constructing all black branes, we reconstruct the equation of state S(T)



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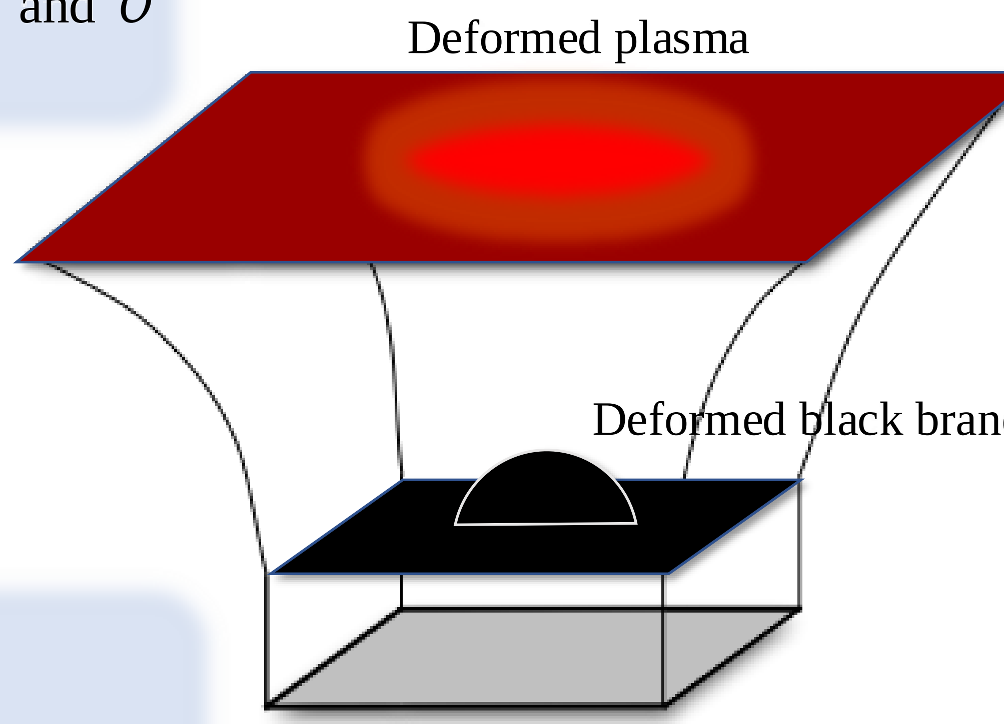

Holography: Our model

- QFT on Minkowski in 3+1 dim
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Real-time quantum dynamics

Holography

Numerical Relativity

Dynamical classical gravity

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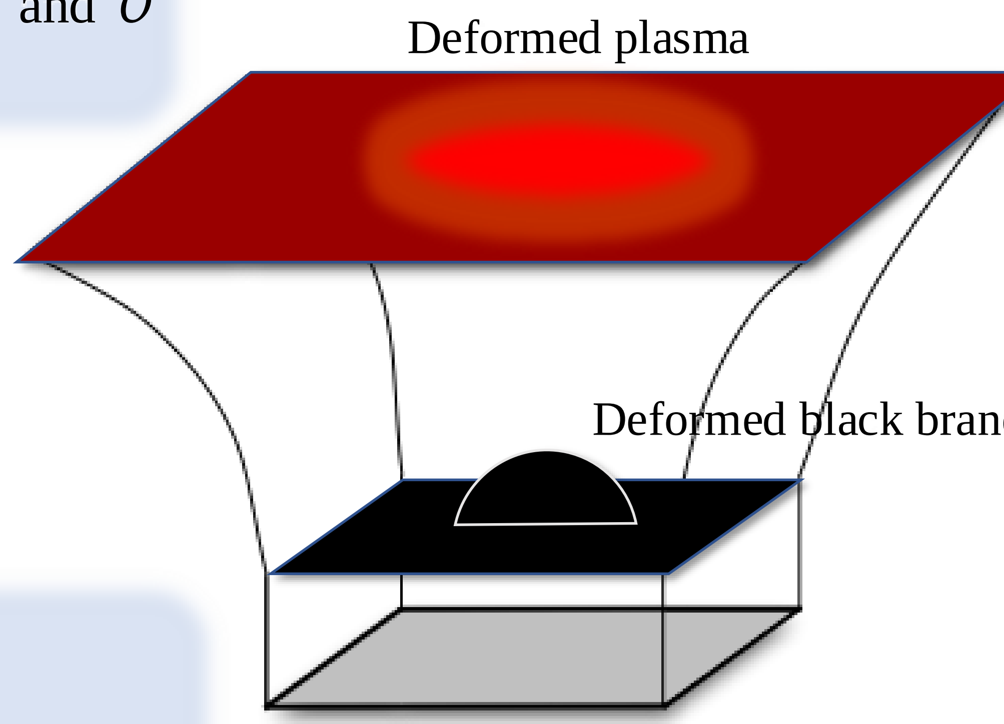

Holography: Our model

- QFT on Minkowski in 3+1 dim
- Decoupl

Numerica

Relativity

- Gravity

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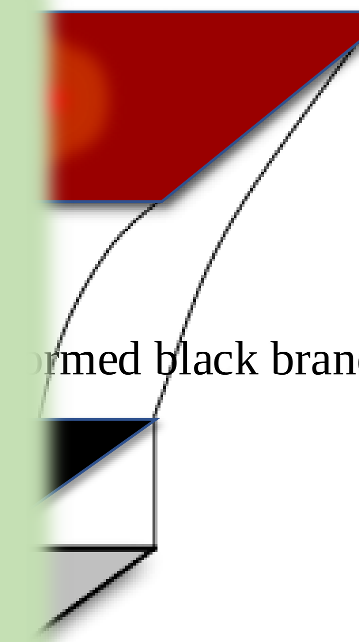
- We have explored the real time dynamics in different context by using holography
- Applications in QGP, phase transitions, cosmology

sma



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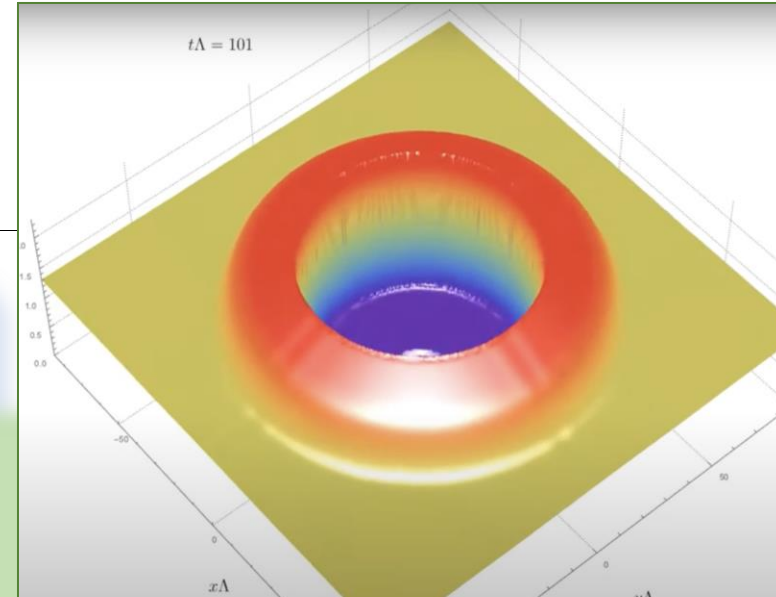

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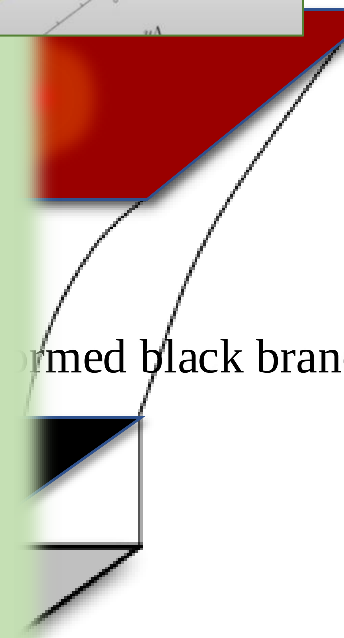

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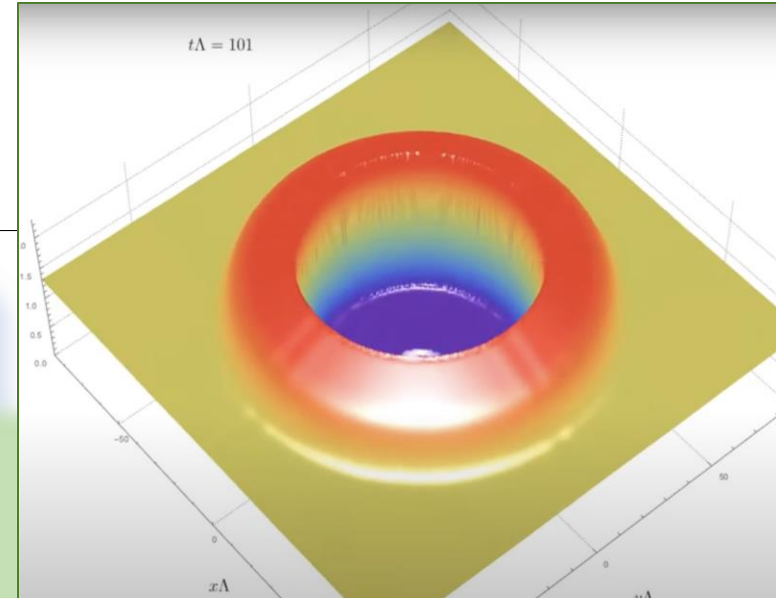

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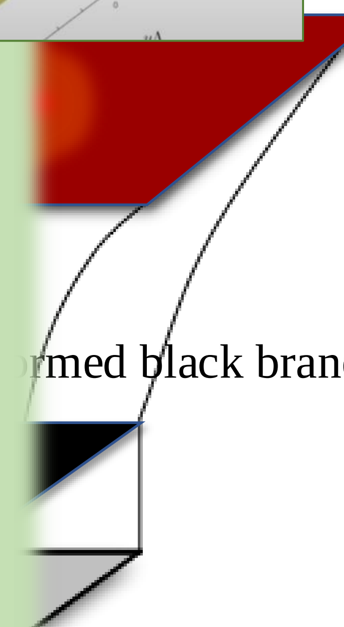
- We would like to perform evolutions in a holographic theory with a given eq. of state



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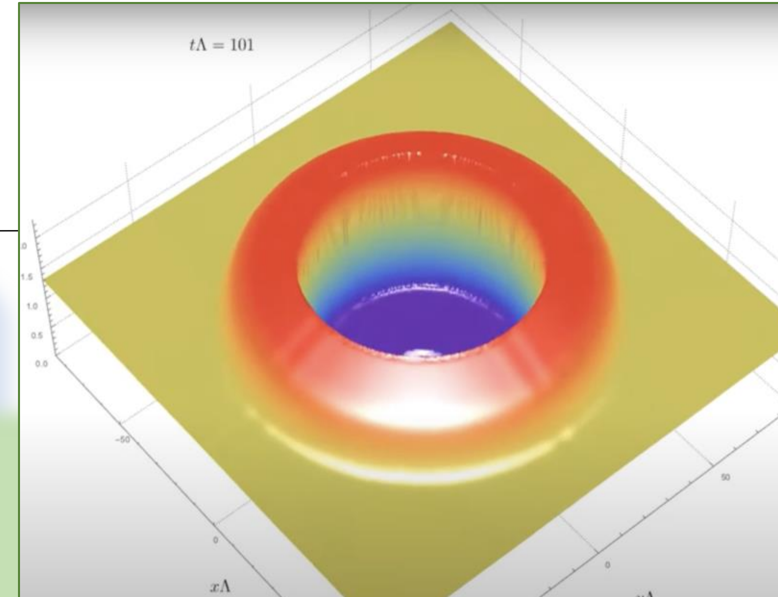

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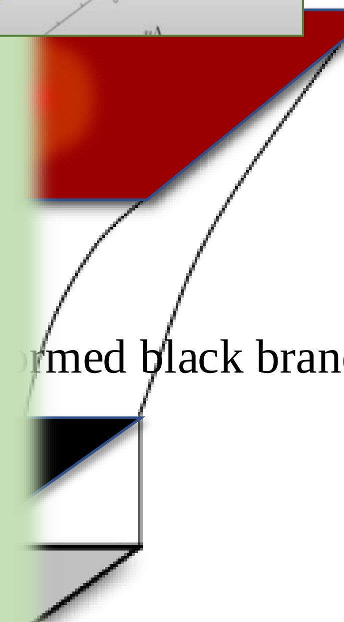


- We would like to perform evolutions in a holographic theory with a given eq. of state
- This is why we want to find the potential that gives rise to a given eq. of state $\longrightarrow$ inverse problem

Holography: A simple model

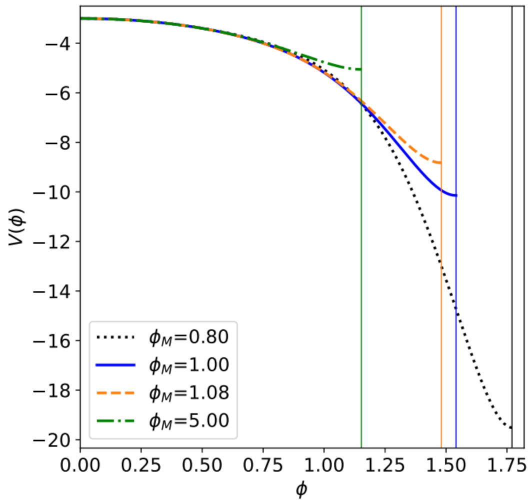
$$S = \frac{2}{\kappa_5^2} \int dx^5 \sqrt{-g} \left[\frac{1}{4} R - \frac{1}{2} (\nabla \phi)^2 - V(\phi) \right]$$

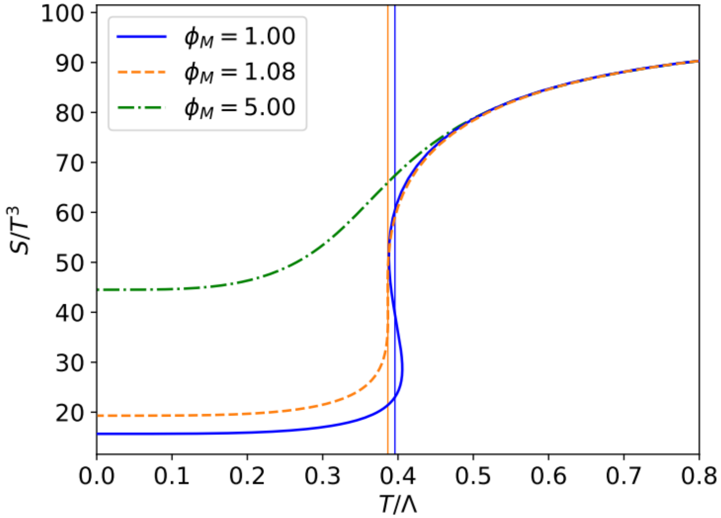
$$V_{\text{theory}}(\phi) = -\frac{4}{3} \mathcal{W}(\phi)^2 + \frac{1}{2} \mathcal{W}'(\phi)^2 \,,$$

$$\mathcal{W}(\phi) = -\frac{3}{2} - \frac{\phi^2}{2} - \frac{\phi^4}{4\phi_M^2} + \frac{\phi^6}{10} \,.$$

Bea, Mateos ‘18

- Simple, smooth at IR, captures first order/2nd order/crossover
- RG flow from CFT at the UV to a CFT at the IR





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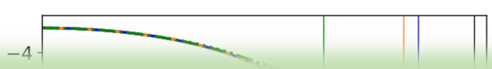

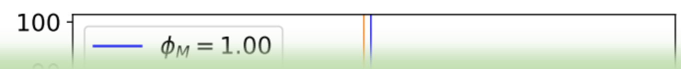

- This model has been used in several contexts in holography:
  ⟶ cosmology, dynamics of phase transitions...

Casalderrey-Solana, Mateos, Serantes ‘23
Ares, Henriksson, Hindmarsh, Hoyos, Jokela ‘21
Bea, Casalderrey-Solana, Gianakopoulos, Mateos, Sanchez-Garitaonandia, Zilhao ‘21
.....

The inverse problem

Einstein eqs.

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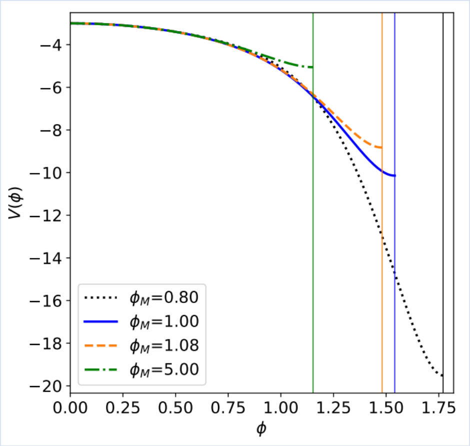
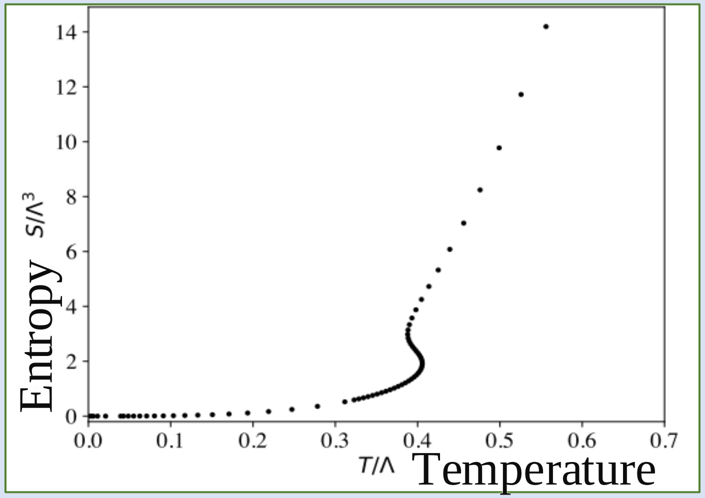


Direct problem

Inverse problem

Equation of State



→ We address the inverse problem by using **Neural Networks**

Neural Networks

Neural Networks

I will present neural networks from the perspective of our problem

Neural Networks

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We use **P**hysics **I**nformed **N**eural **N**etwoks, **PINNs**

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→ The Neural Network is informed by the physical equations

→ In our case, Einstein's equations

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→ The Neural Network is informed by the physical equations

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Other uses: training on known solutions ("supervised training"; "recognizing faces")
....but not in our work

Neural Networks

For our purposes, we can understand a NN as a **function**:

Neural Networks

For our purposes, we can understand a NN as a **function**:

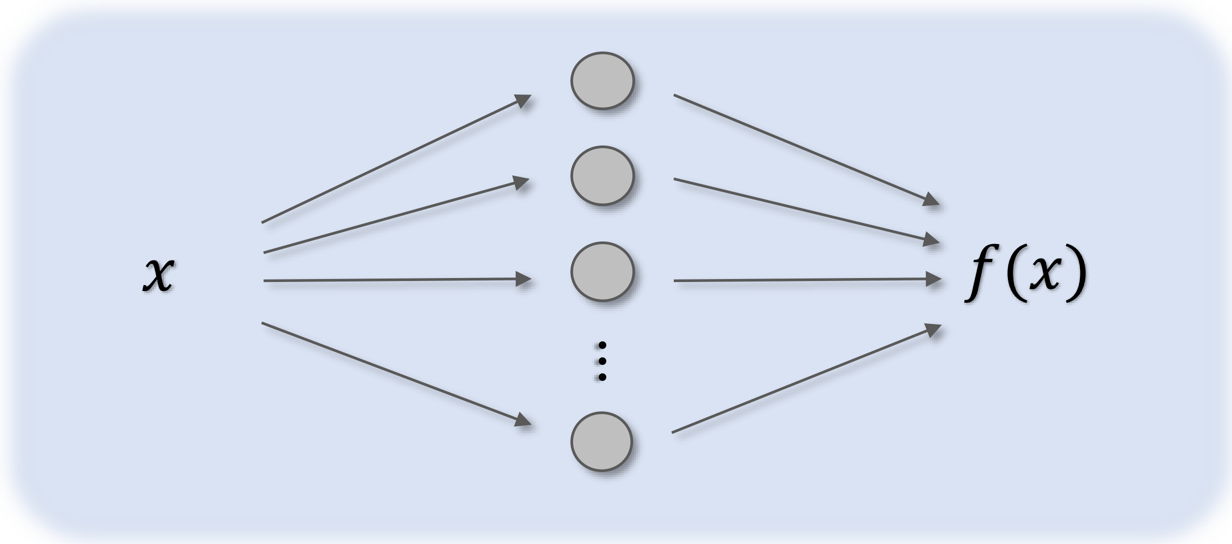
→ Cos(x)

→ Exp(x)

→ A solution to our equations

Neural Networks

For our purposes, we can understand a NN as a **function**:



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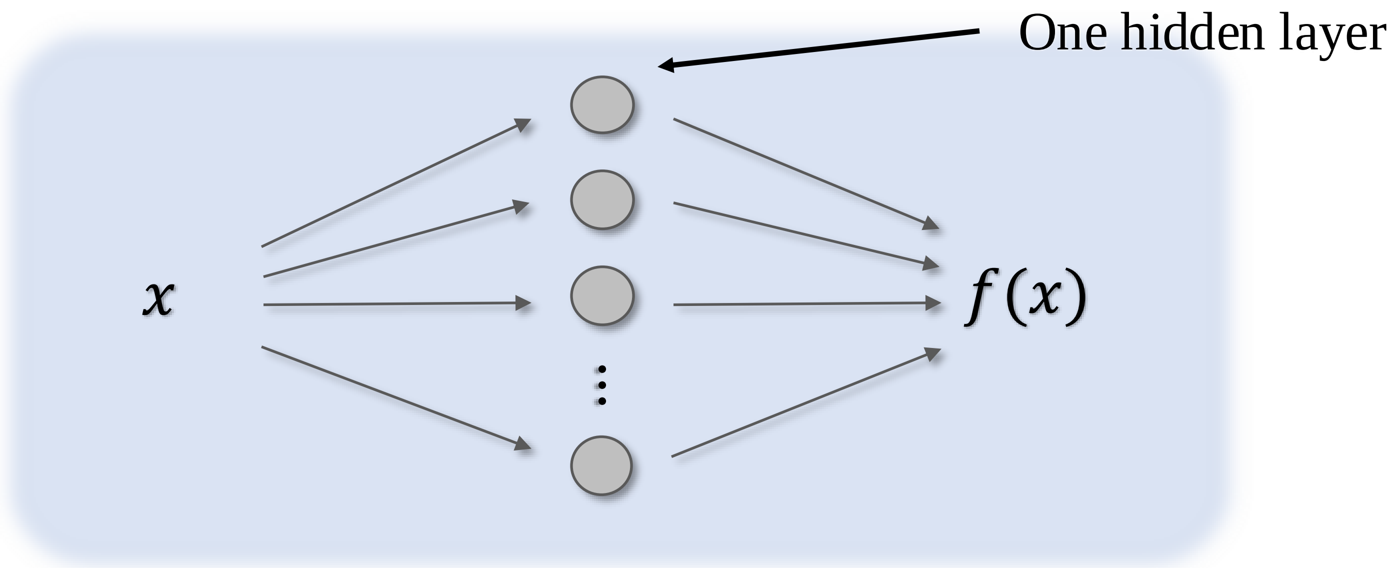

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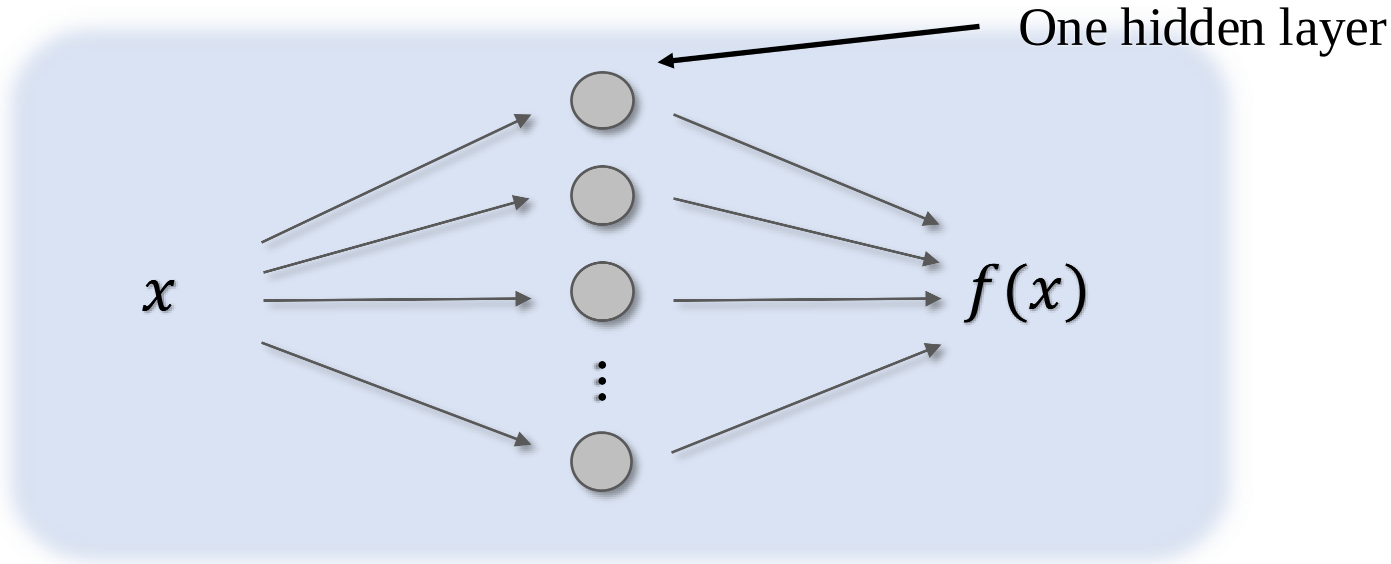

In each neuron

x_i

Neural Networks

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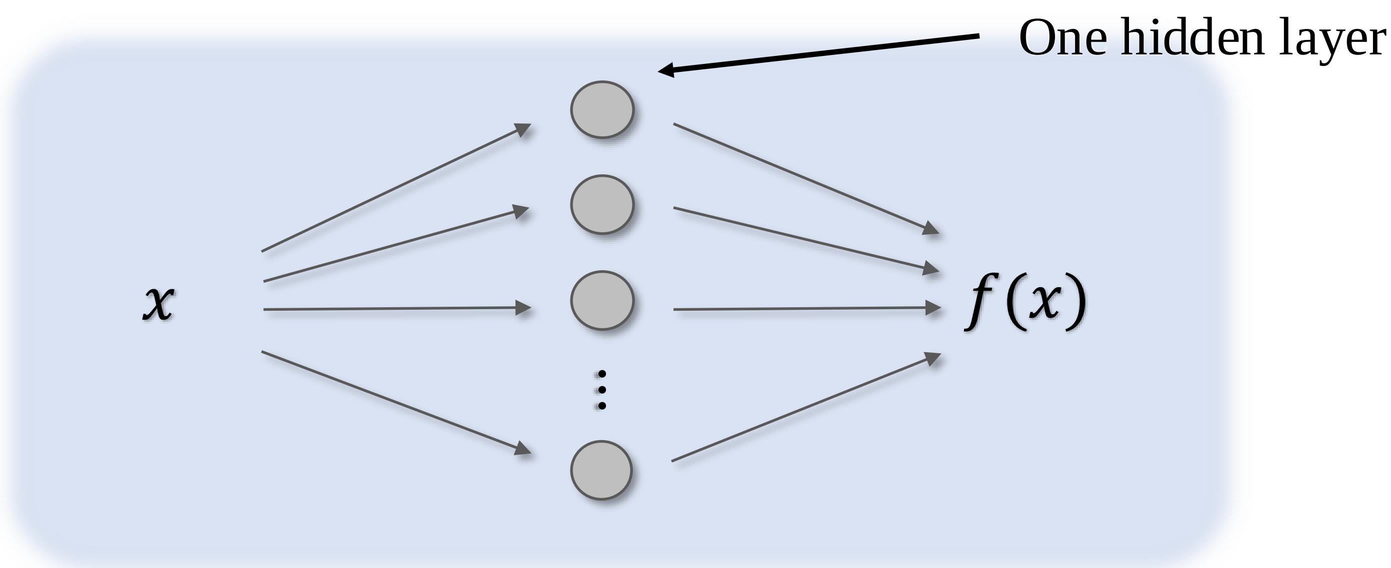

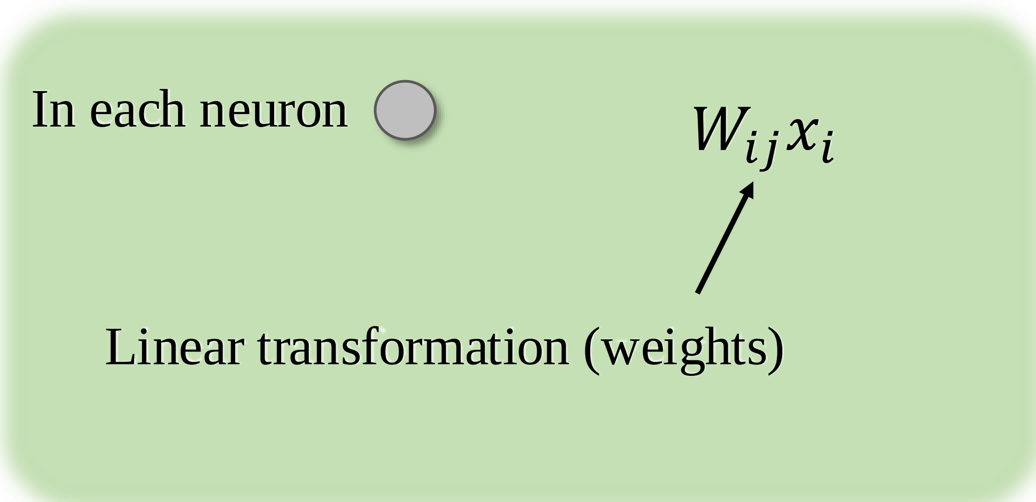

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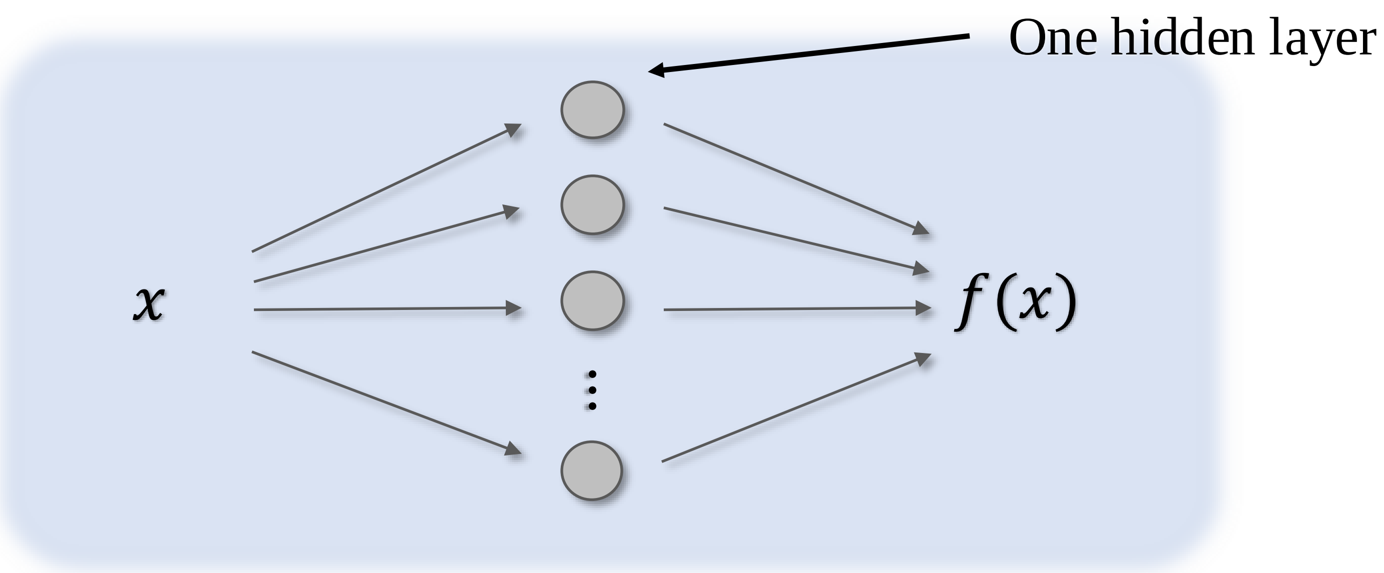

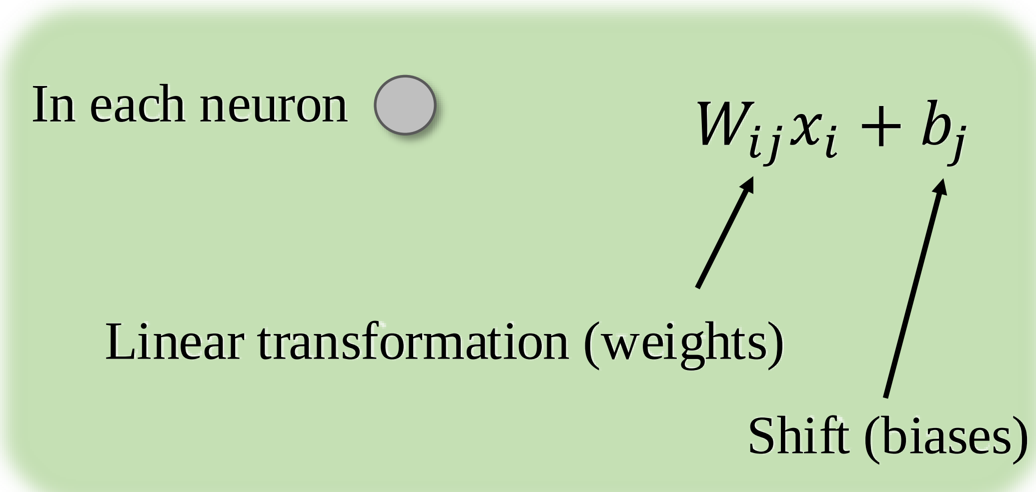

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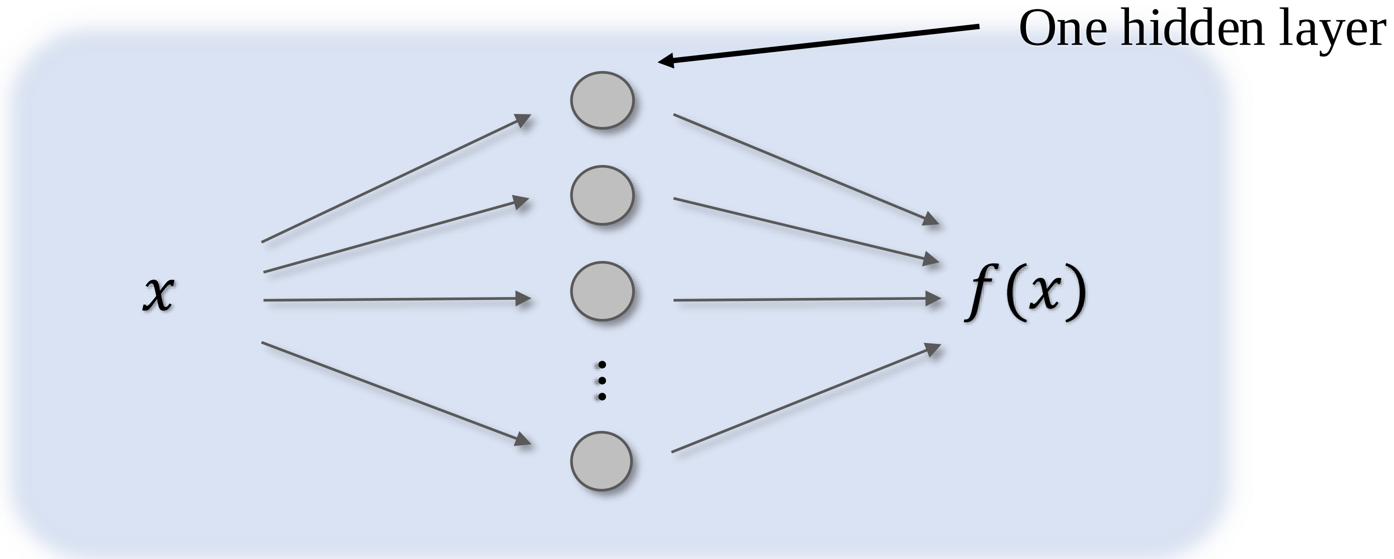

In each neuron

$$Tanh(W_{ij}x_i + b_j)$$

Activation function

Linear transformation (weights)

Shift (biases)

Neural Networks

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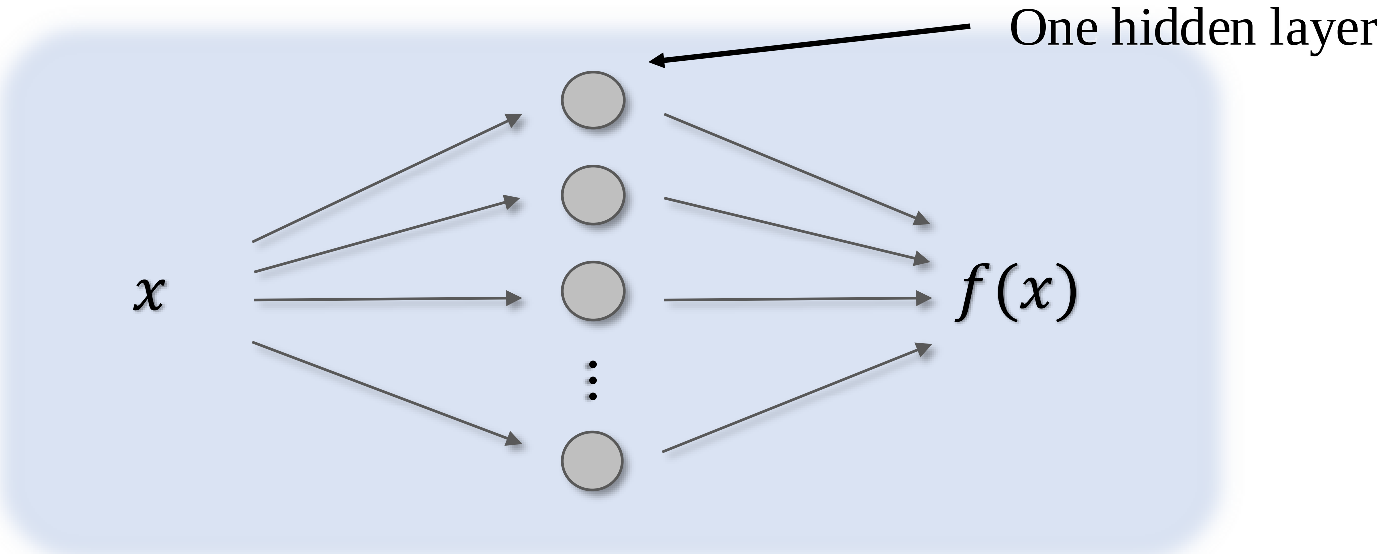

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Internally is **analytical**

Just a combination of tanh's...

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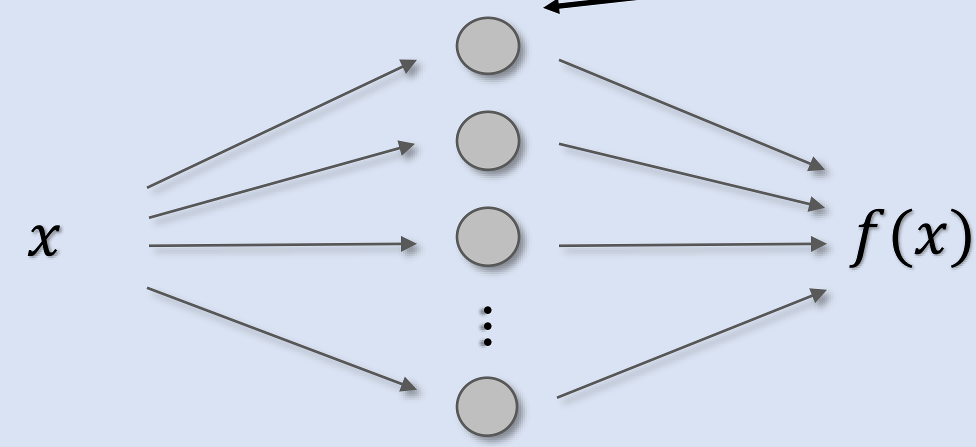
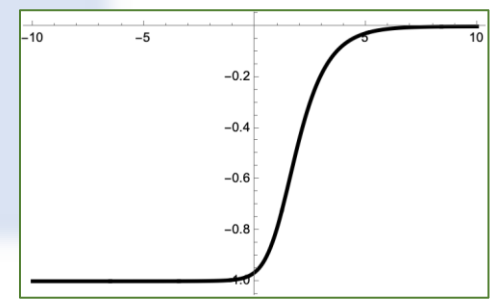
One hidden layer



Tanh[2Tanh[0.5x]-2]



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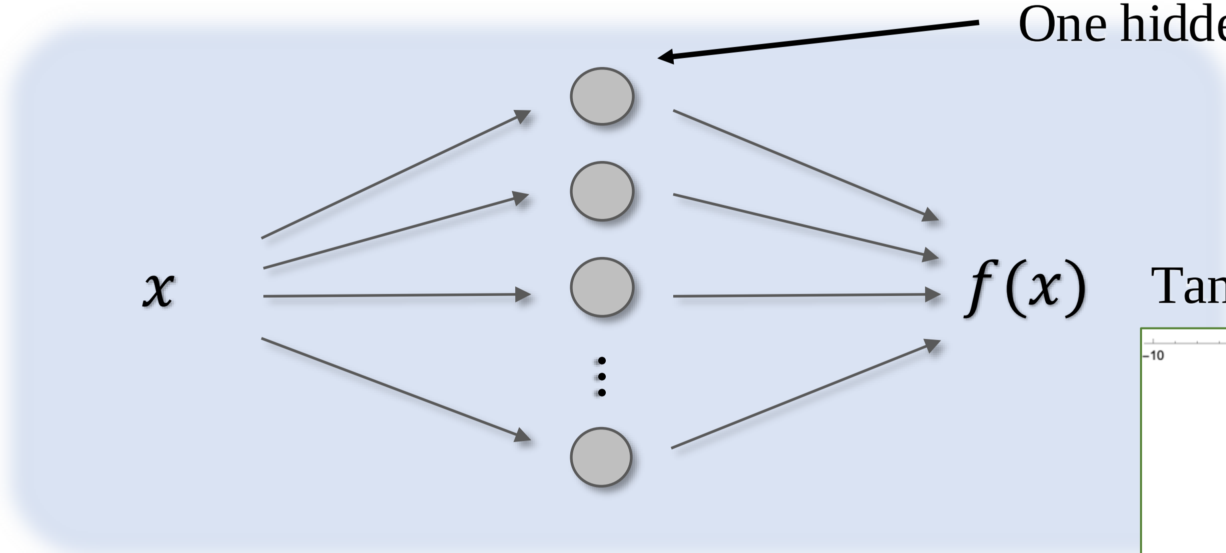

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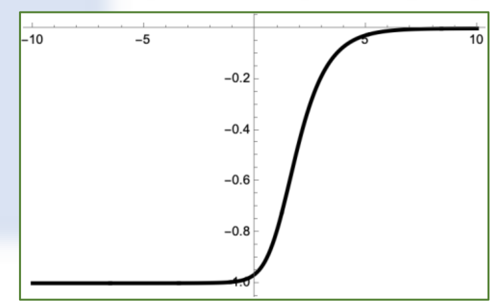

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Finite but large number of parameters
(in our case 15.000)

Neural Networks

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But.......why is this useful?

In each n

Activati

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on of tanh's...

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- **NN can learn**

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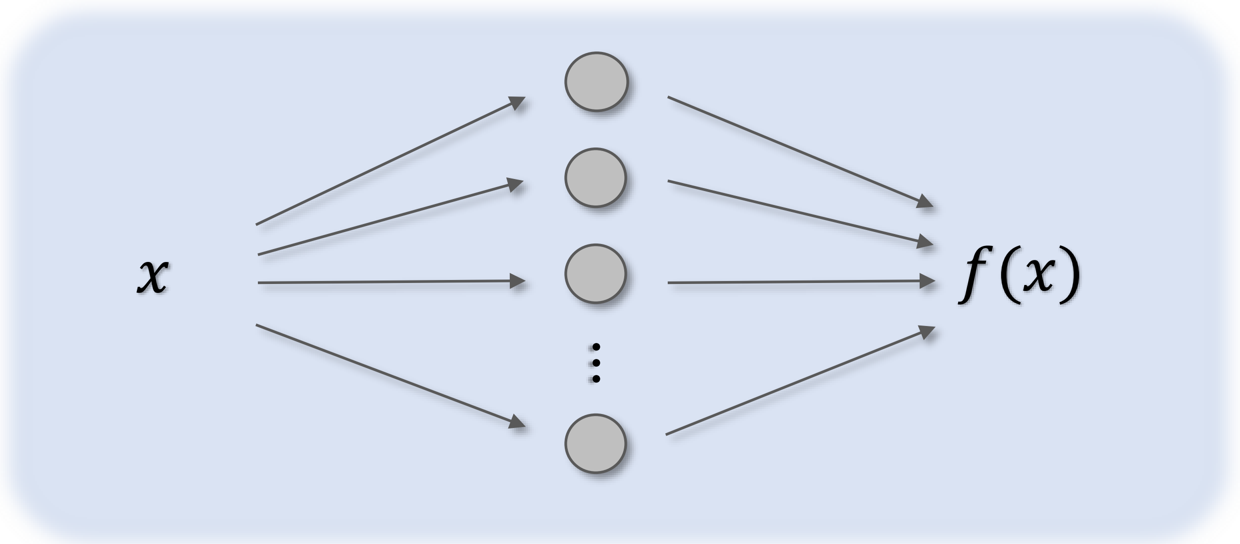
Universal approximation theorems

NN are supported on mathematical theorems



Universal approximation theorems

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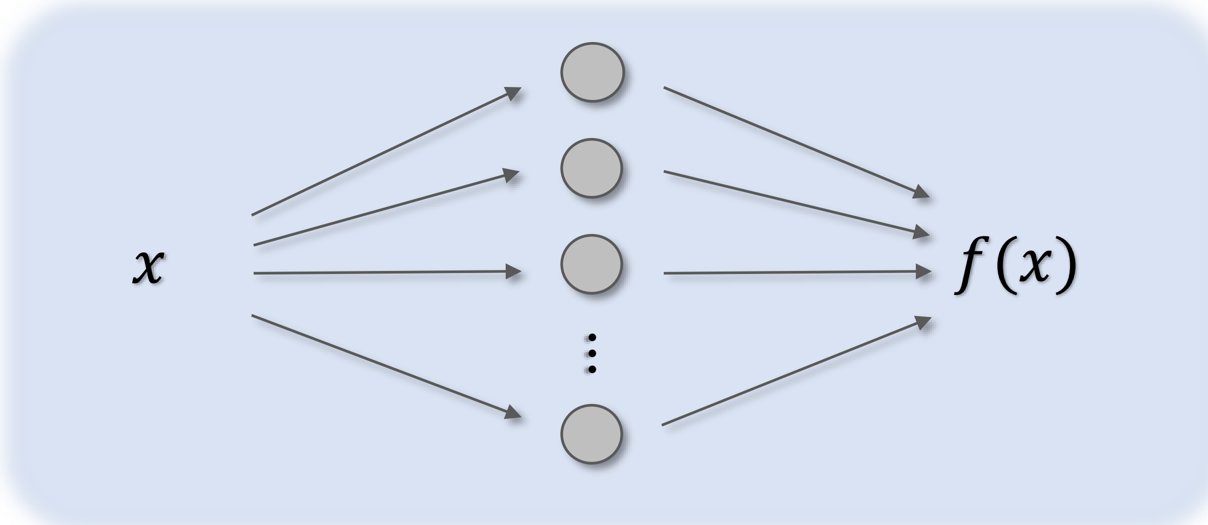

Universal approximation theorem

"With enough neurons, we can recover a given function to a certain accuracy"

Universal approximation theorems

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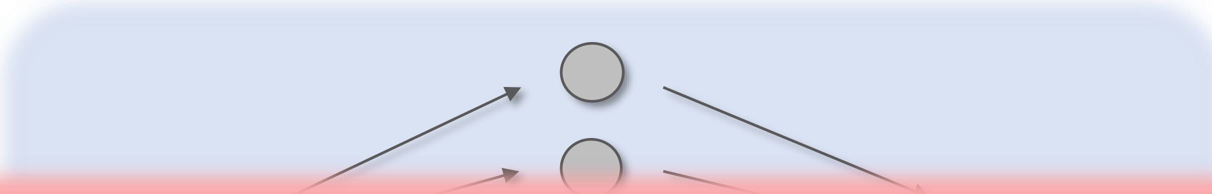

This means, that, in particular, that a NN can represent a solution to our equations

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Universal approximation theorems

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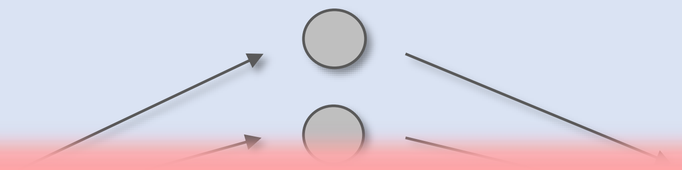


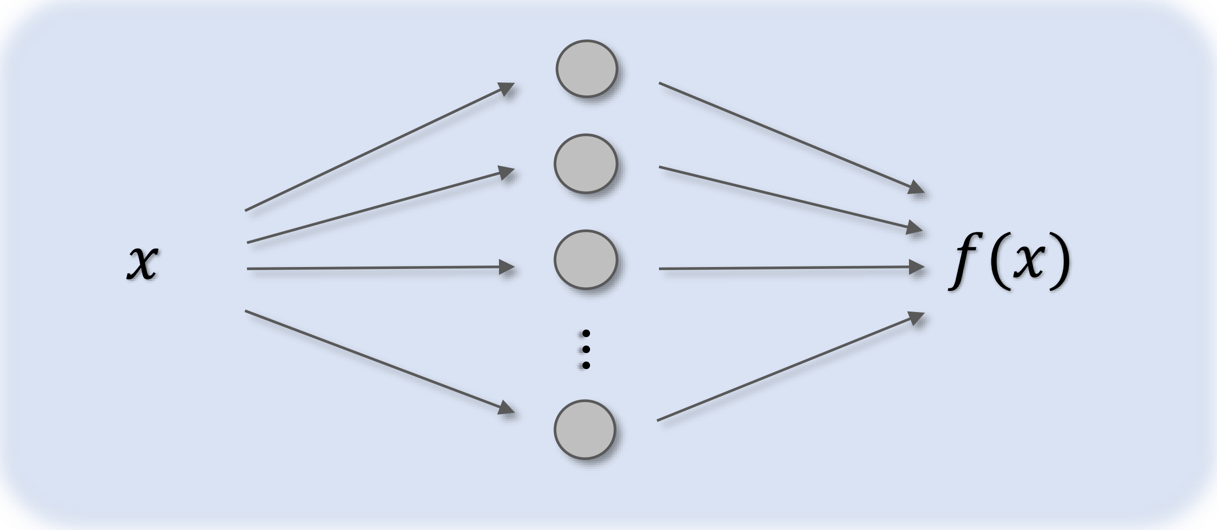
This means, that, in particular, that a NN can represent a solution to our equations

But.... how do we get to that NN?

“With enough neurons, we can recover a given function to a certain accuracy”

Definition of Loss

We now want this NN to be a solution to our equations



Loss function   L := (residual of Einstein's equations)^2

We want to minimize the loss function

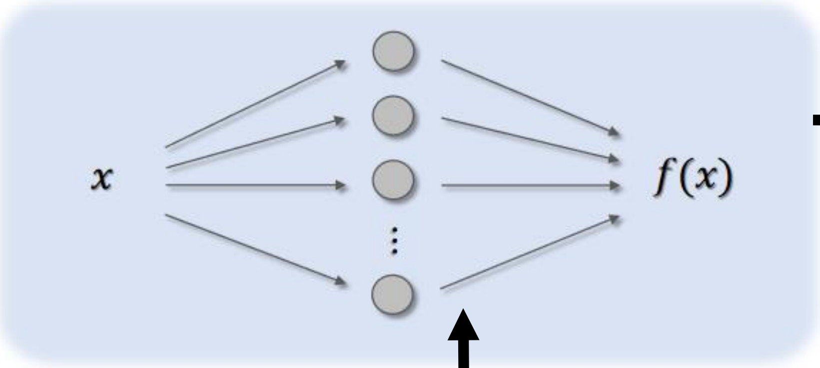
This is our definition of PINNs

Neural Networks: learning process

But..... how does it learn?

Neural Networks: learning process

But..... how does it learn?



Loss=(Eqs residuals)^2

Analytical expression with params W, b

“$Tanh(Wx + b)$”

Gradient $\nabla_{W,b} L$

Neural Networks: learning process

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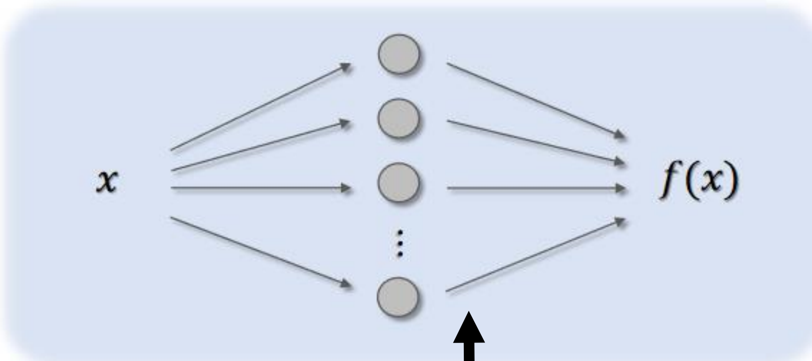

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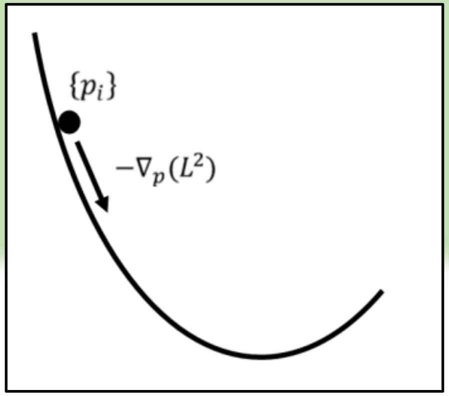
Gradient $\nabla_{W,b} L$

Gradient descent



Our set up

Einstein-Klein Gordon

$$S = \frac{2}{\kappa_5^2} \int dx^5 \sqrt{-g} \left[\frac{1}{4} R - \frac{1}{2} (\nabla \phi)^2 - V(\phi) \right]$$

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Metric ansatz

$$ds^2 = -A dt^2 + \Sigma^2 (dx^2 + dy^2 + dz^2) - \frac{2}{u^2} dt du$$

$A(u), \Sigma(u), \phi(u) \longrightarrow$ Unknown functions

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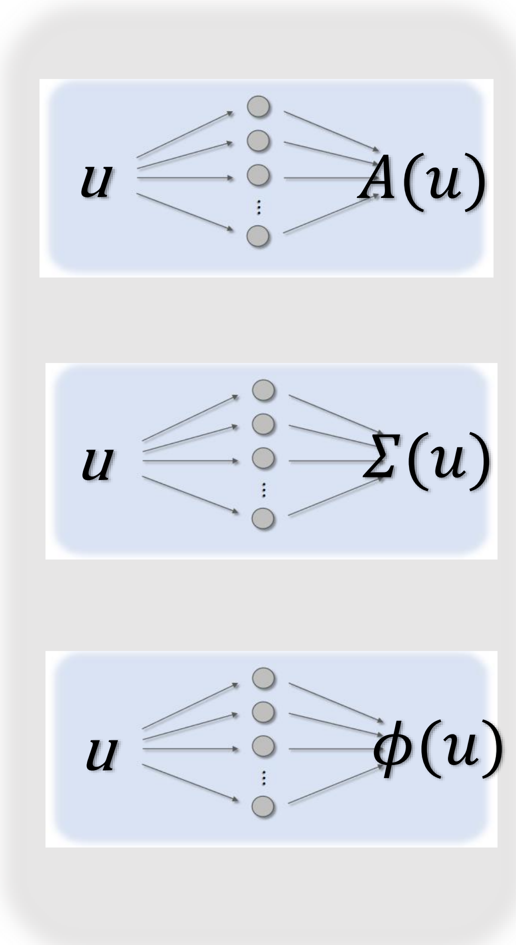
$A(u), \Sigma(u), \phi(u) \longrightarrow$ Unknown functions

$u \longrightarrow$ Holographic variable

$u \in [0,1]$

The direct problem



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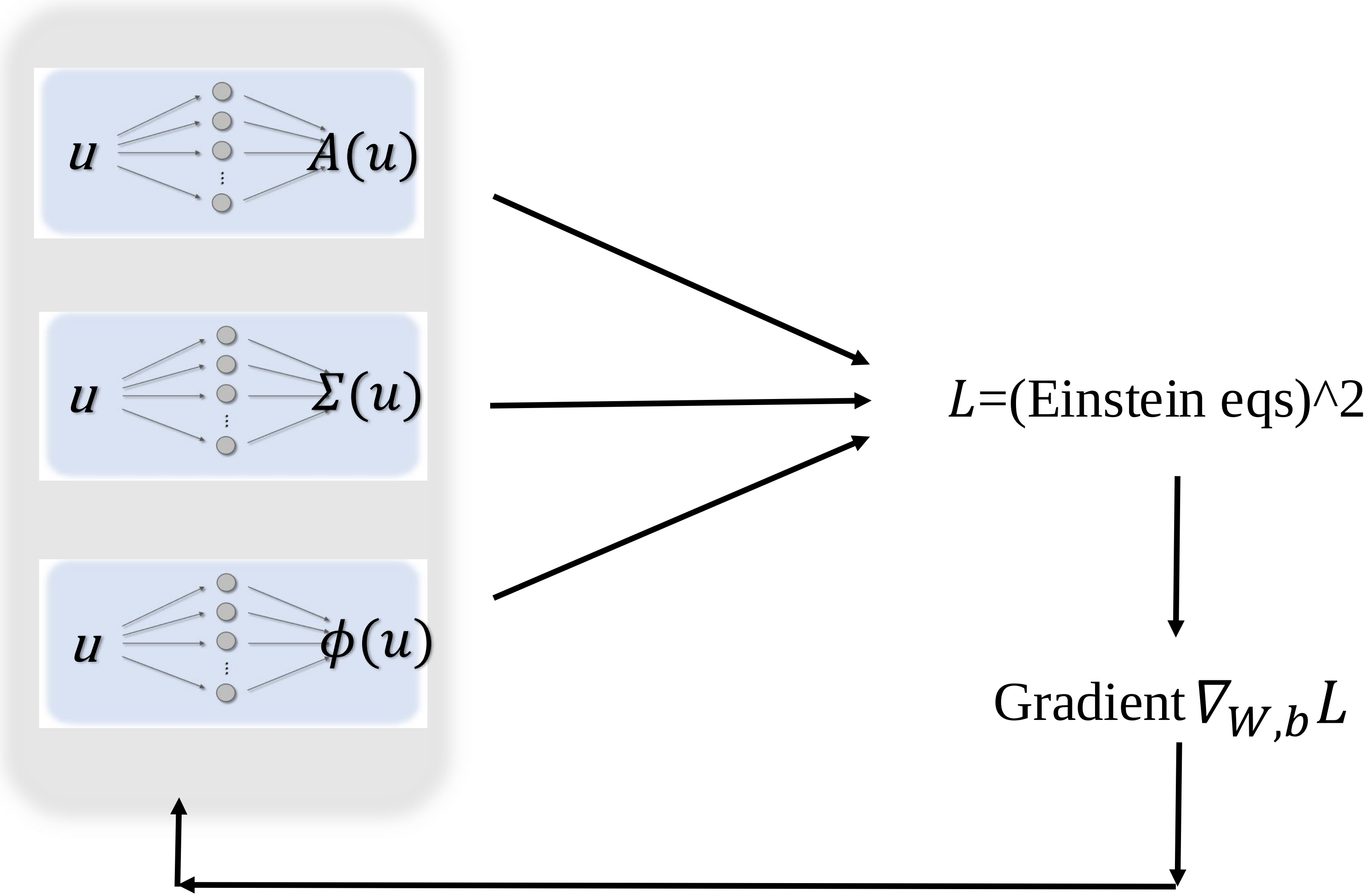

The direct problem

we solve the direct problem as a **test**

u

u s)^2

u $_b L$

The direct problem

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-We fix the potential V(φ)

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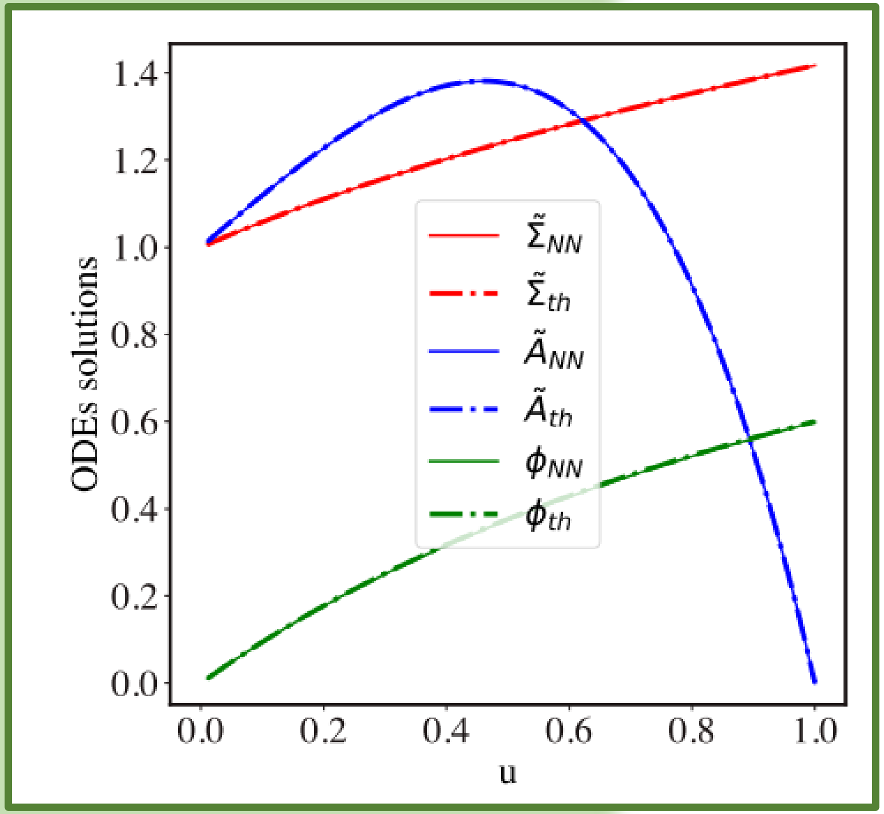

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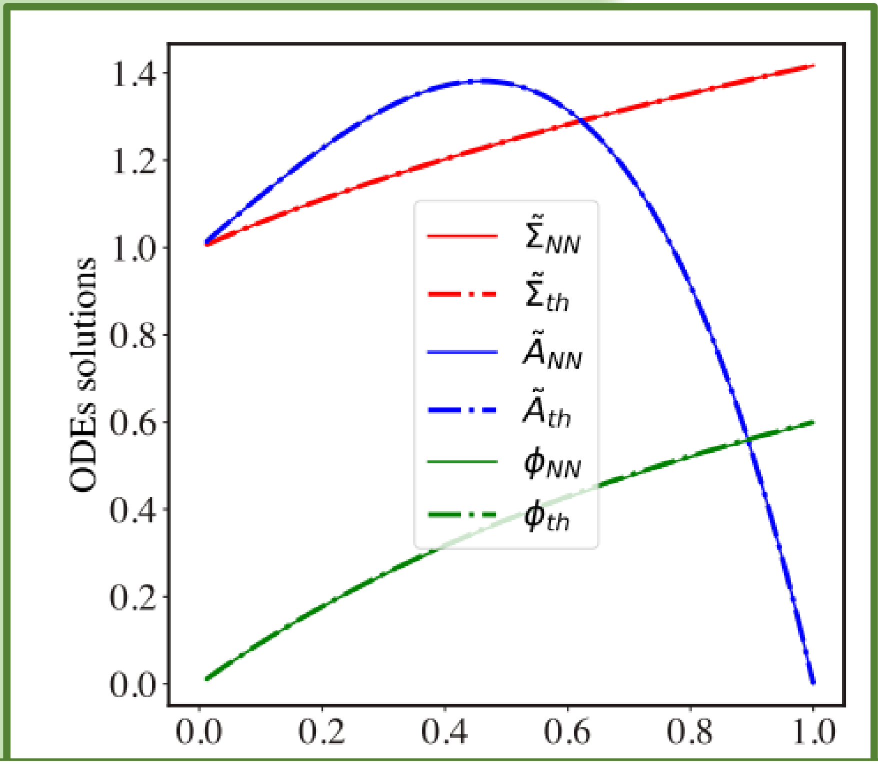


Direct problem works very well!

The direct problem

we solve the direct problem as a **test**

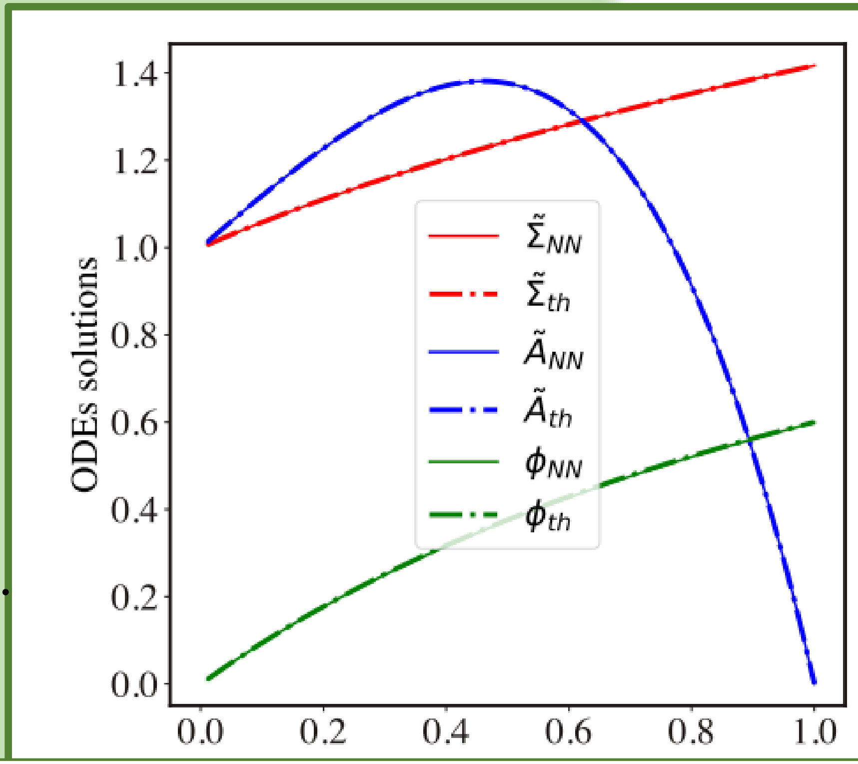
-We fix the potential V(φ)

- Run for ~million iterations

- Compare with traditional methods

-This corresponds to one black brane solution, i.e., one (T,S) point.

-We have control on the solution: more iteration, reduce the loss



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The inverse problem

We are given the potential V(φ)
We construct the thermodynamics S(T)

Einstein eqs.

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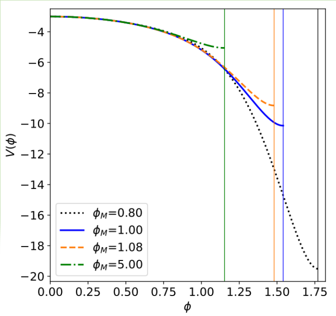
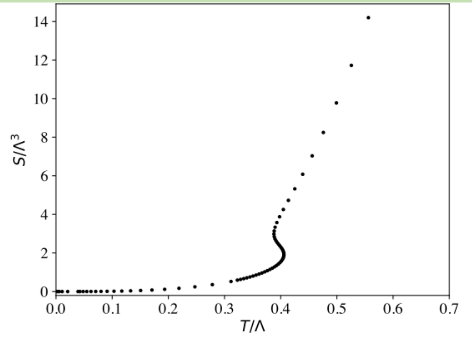


Direct problem

Equation of state



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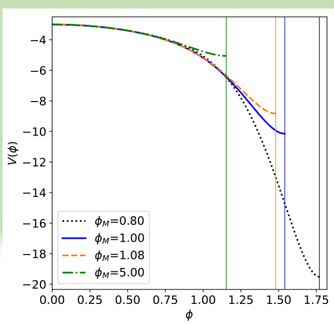

Direct problem

Inverse problem

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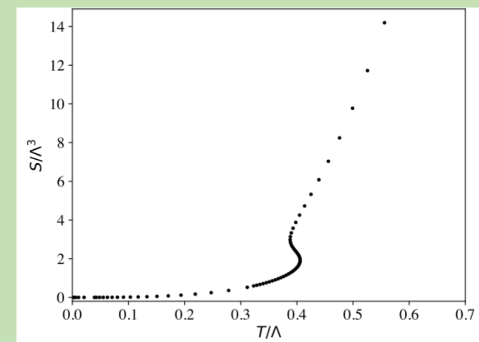

We are given an equation of state S(T)
and we want to reconstruct V(φ)

→ This corresponds to reconstructing the theory

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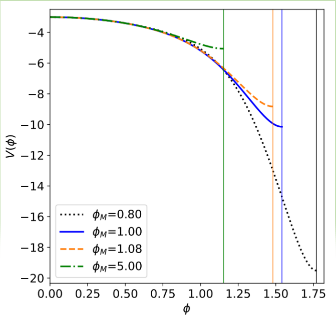

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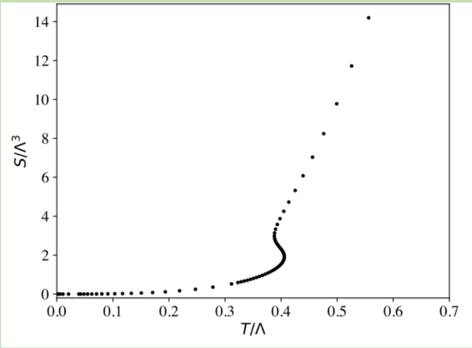
Equation of state



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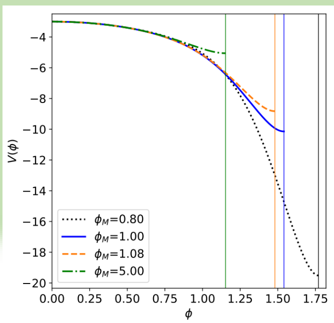

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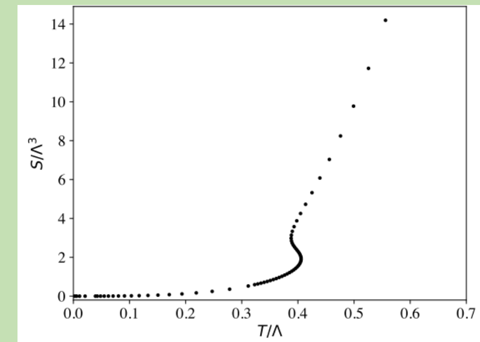

-Sampling of the eq. of state S(T), ~70 points

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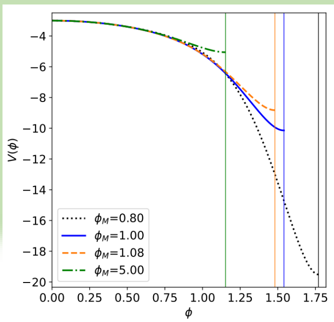

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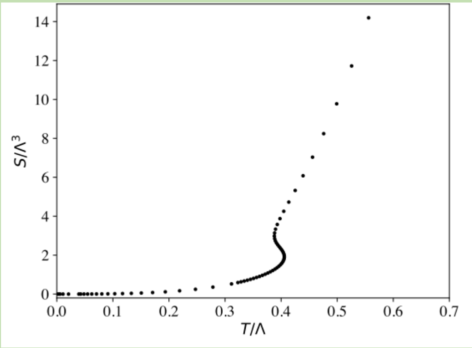

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-Each point in the sampling corresponds to a black brane

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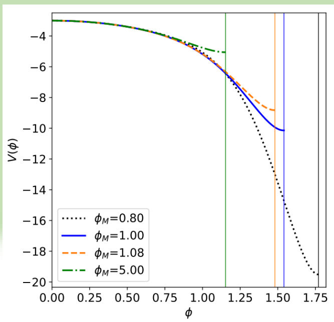

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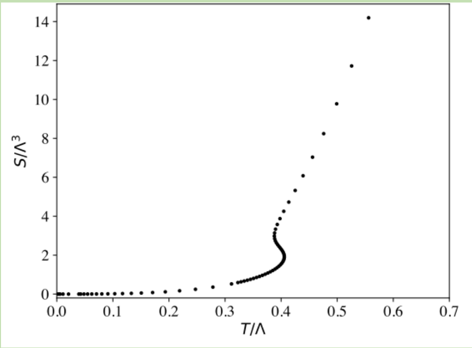

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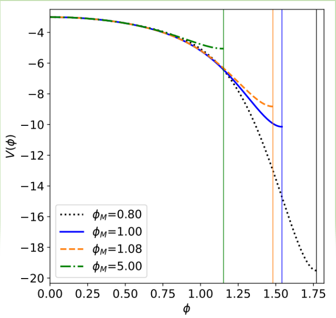

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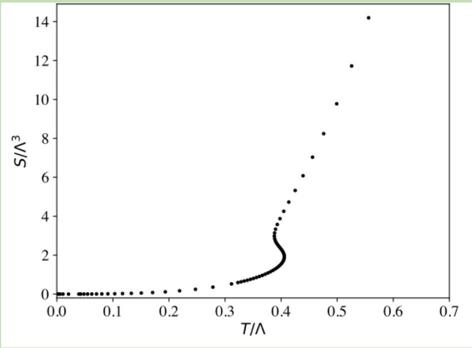

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-We introduce an additional NN for V(φ) (now it is an unknown)

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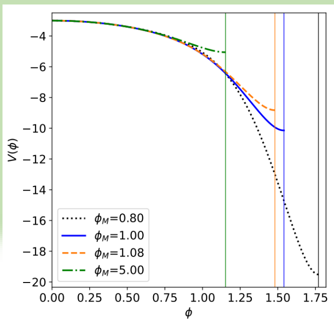

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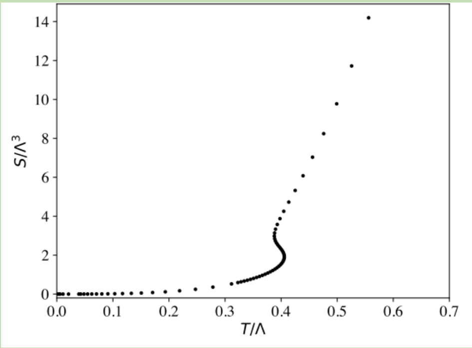

-Loss= Σ(residuals Einstein eqs)^2 (sum over branes)

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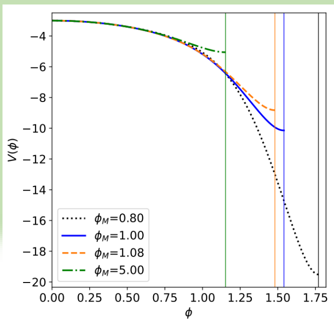

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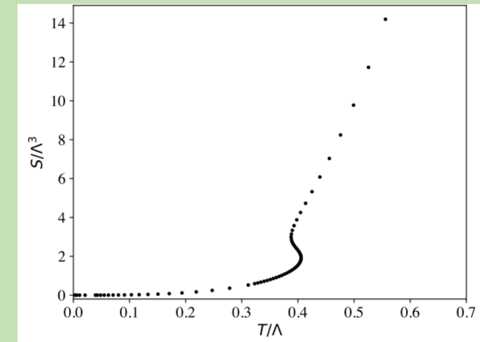

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-For each black brane, S and T enter as boundary conditions at the horizon

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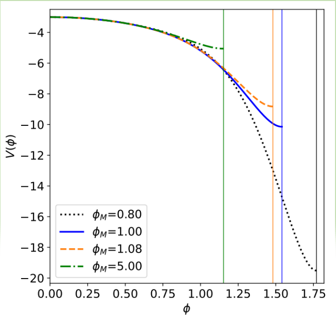

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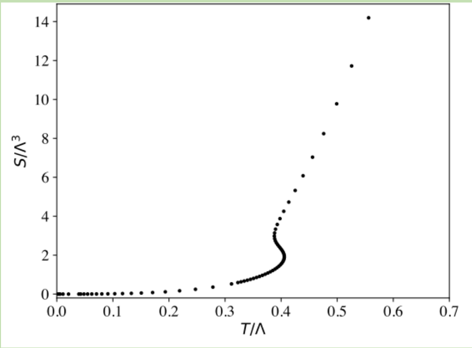

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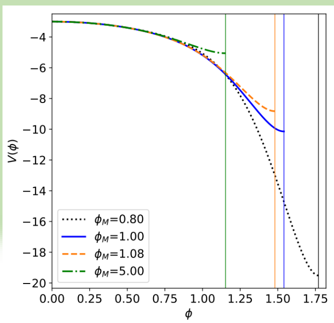

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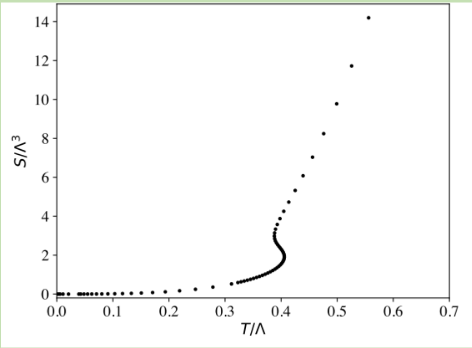

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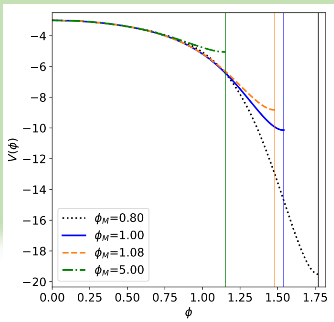

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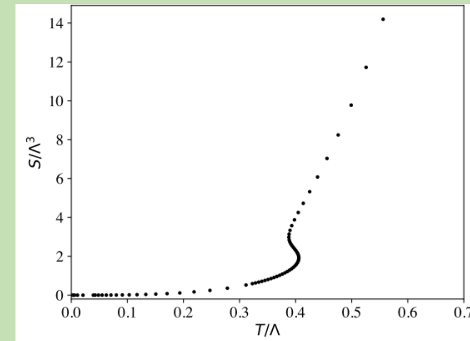

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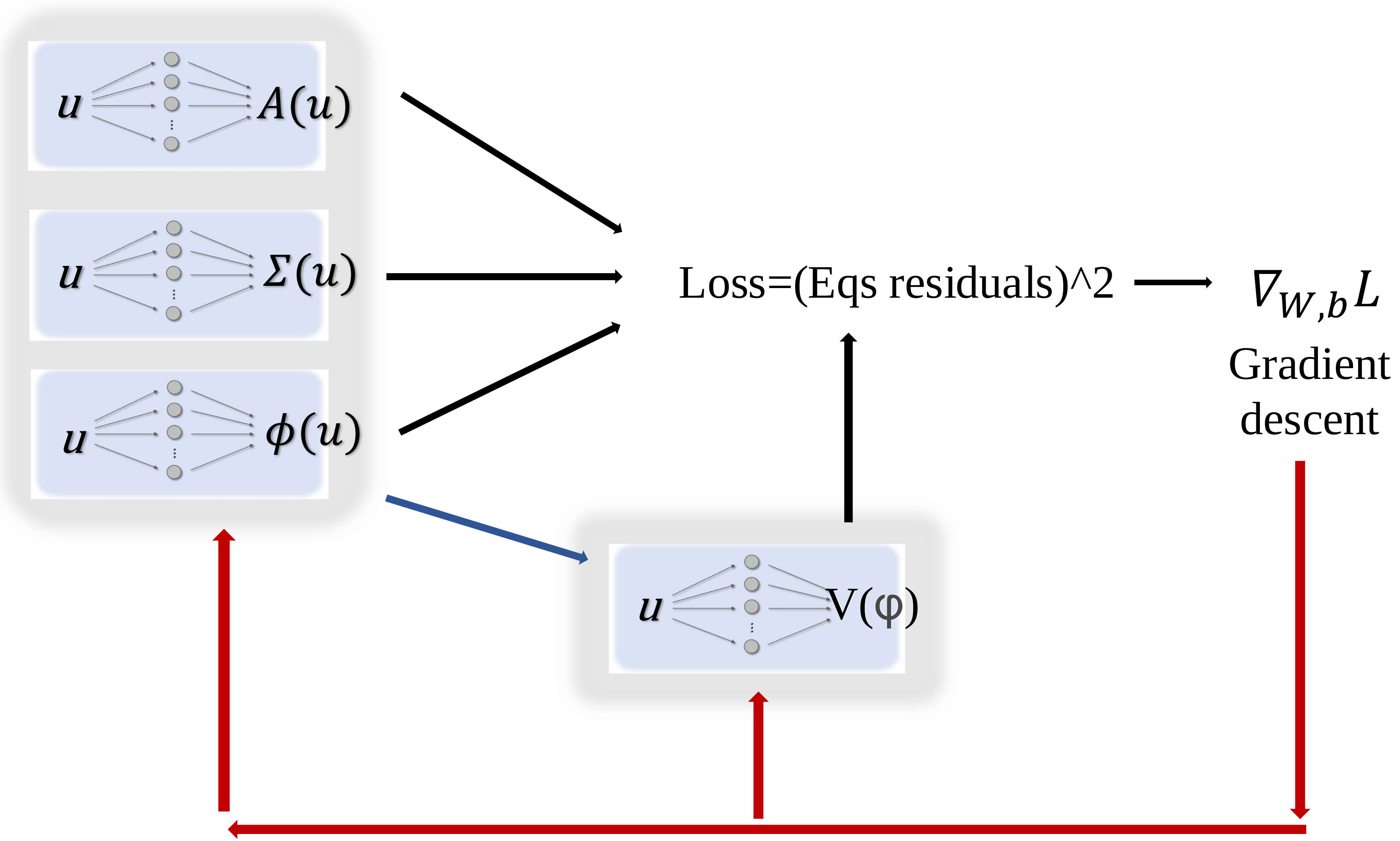
-The range of phi's is found by the NN

Architecture summary



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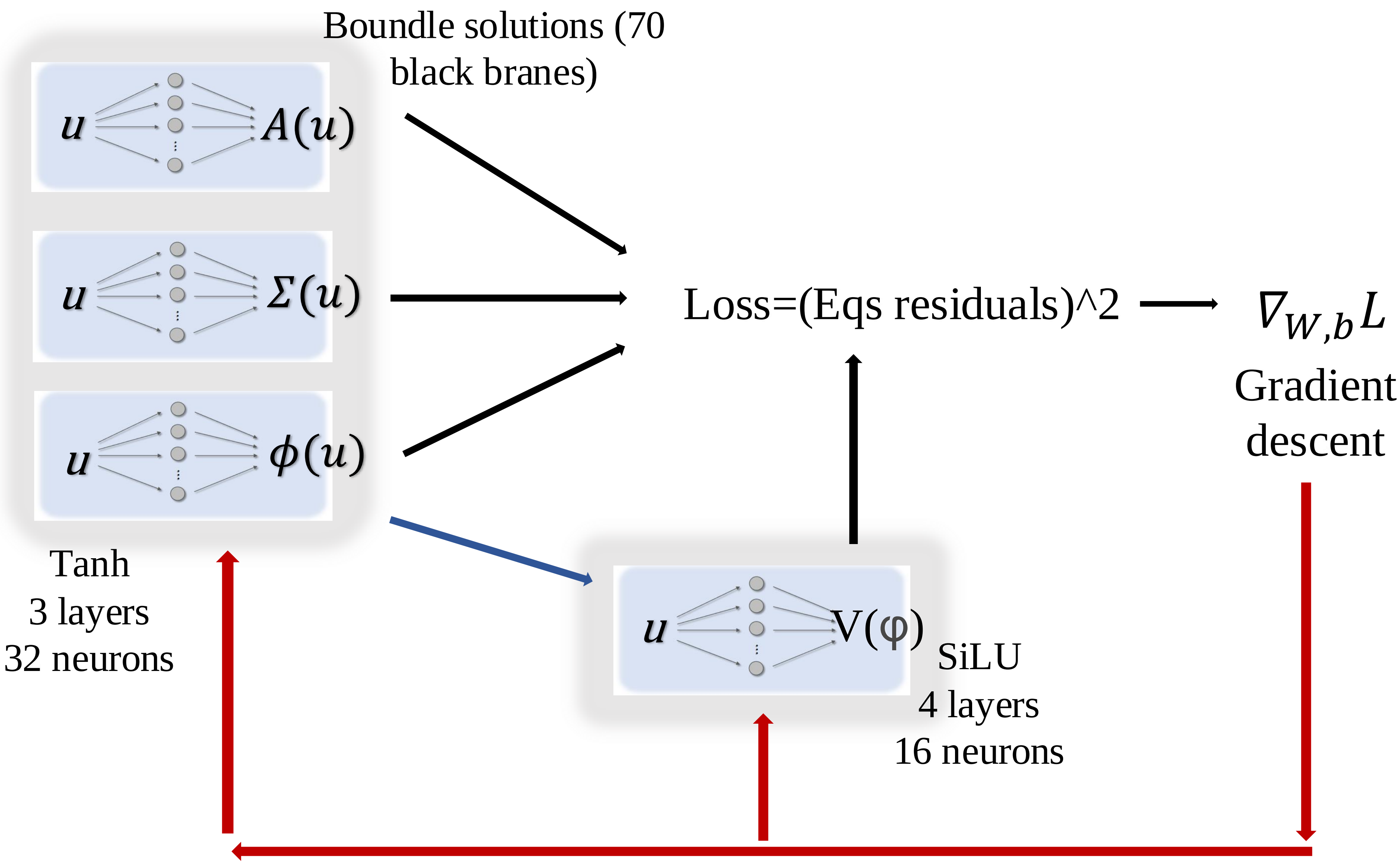

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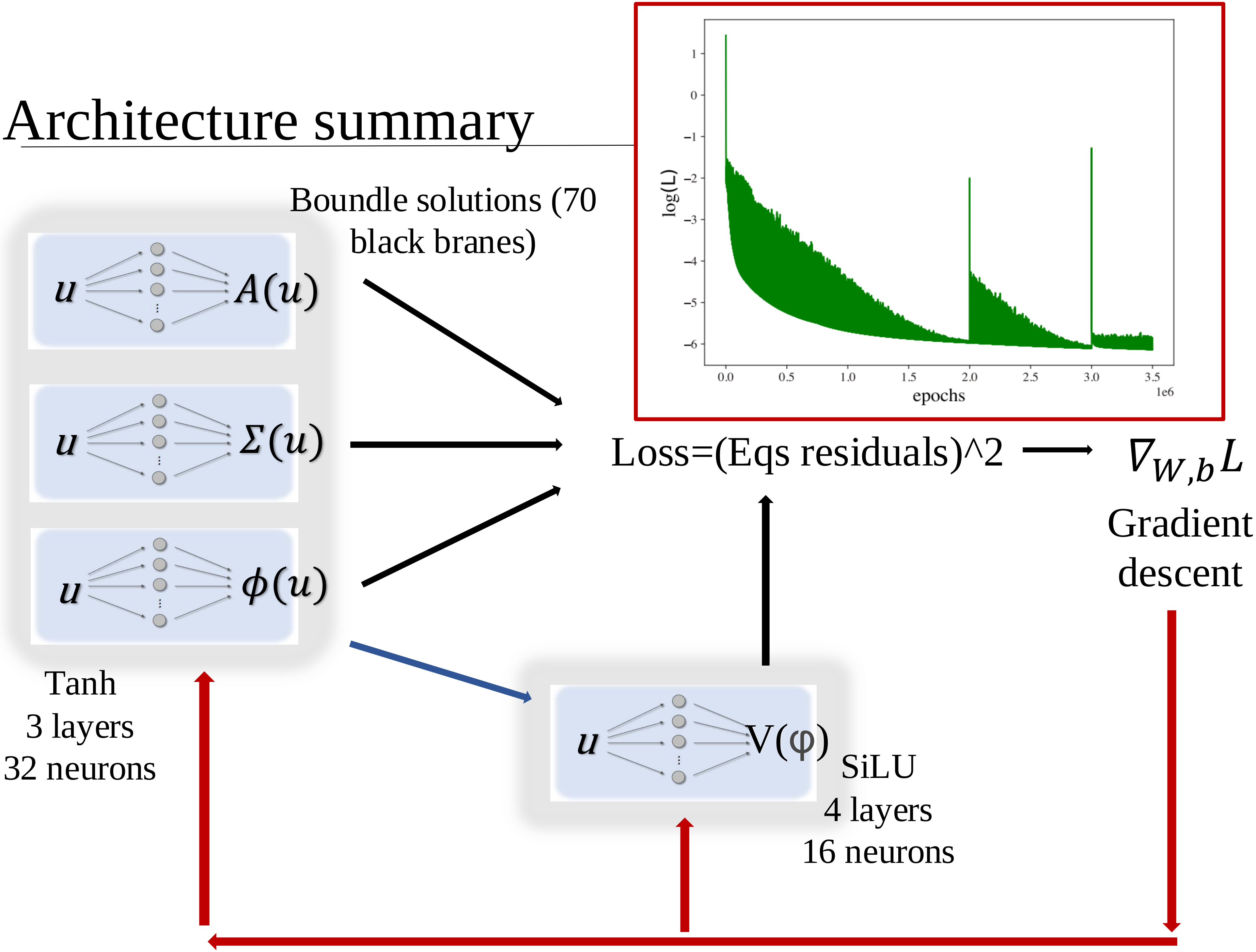
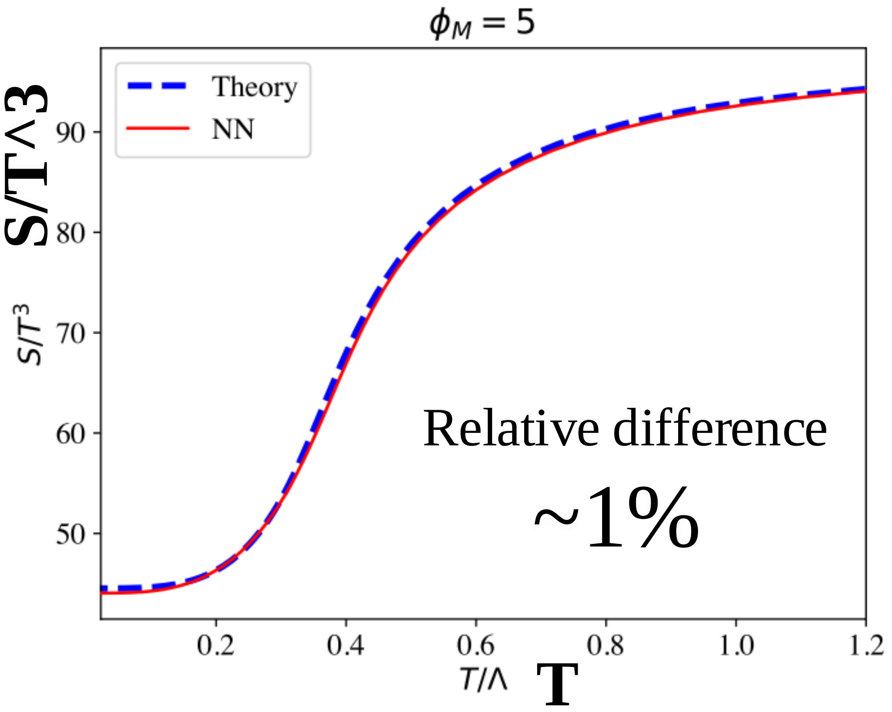


Main results

Solving the inverse problem

Crossover second order first order



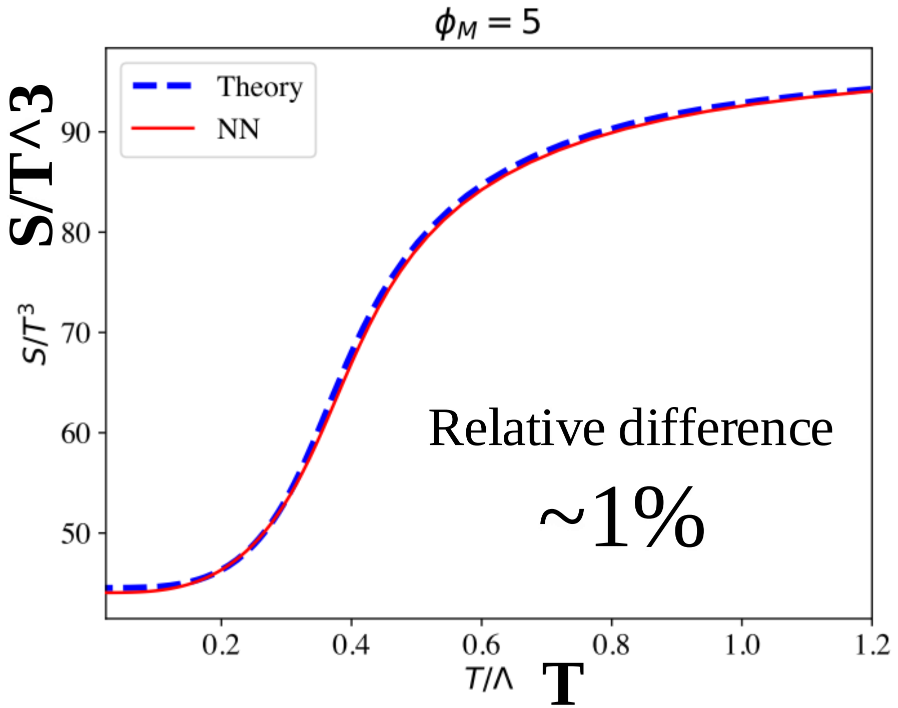
Main conclusion

We have solved the inverse problem using NN within ~1%, not solved before with other methods

Solving the inverse problem

Crossover second order first order

As we known the original potential,
we can perform a further check:



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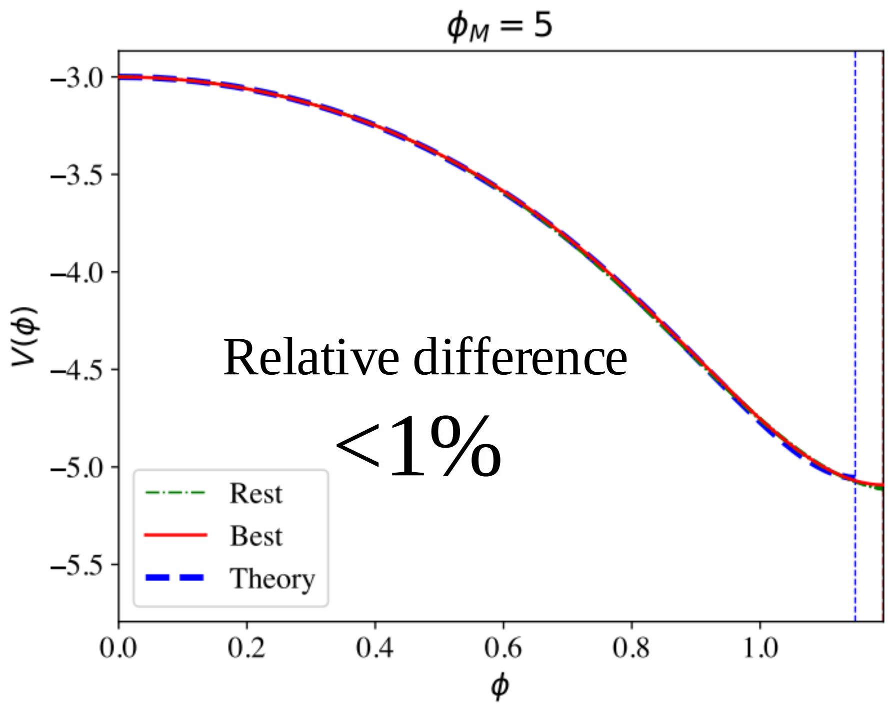

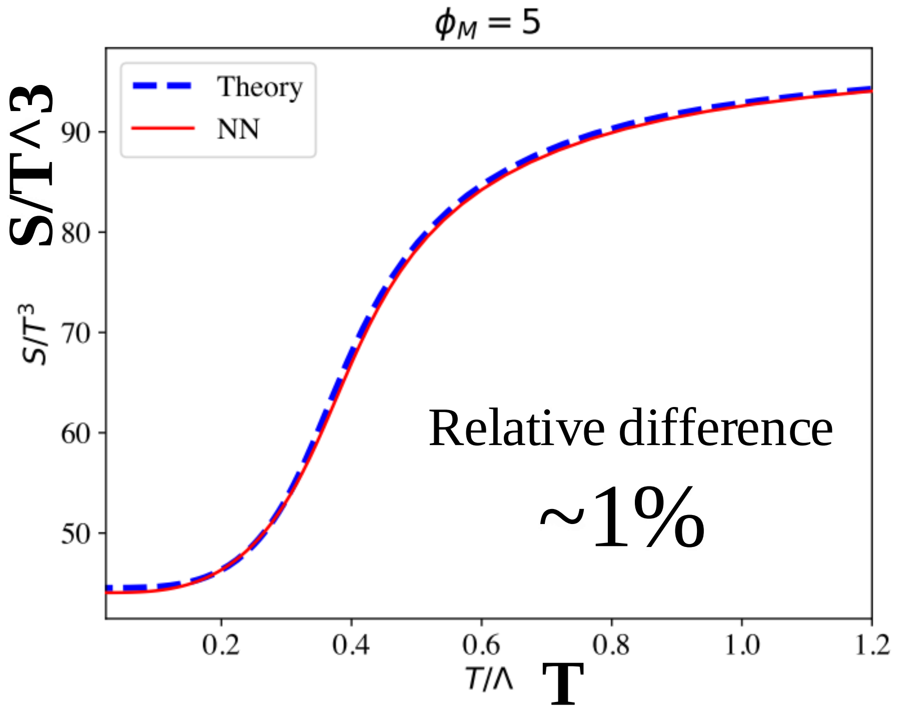

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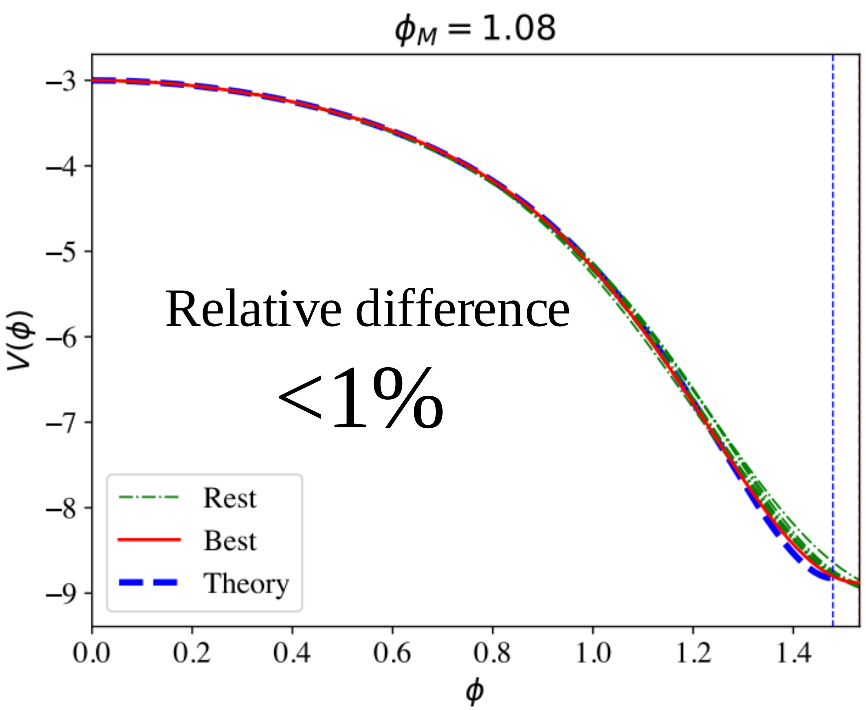

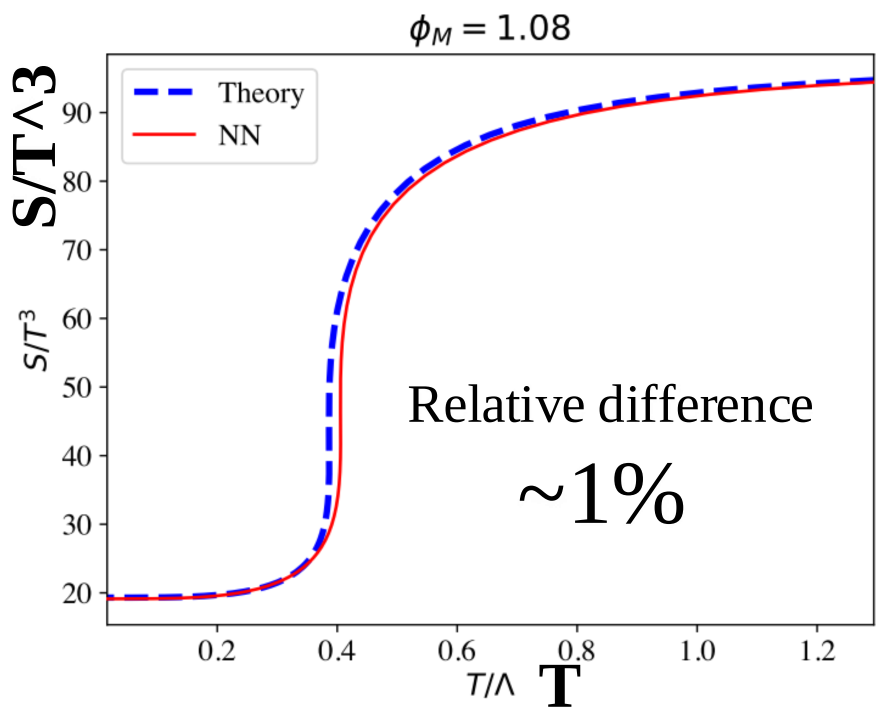

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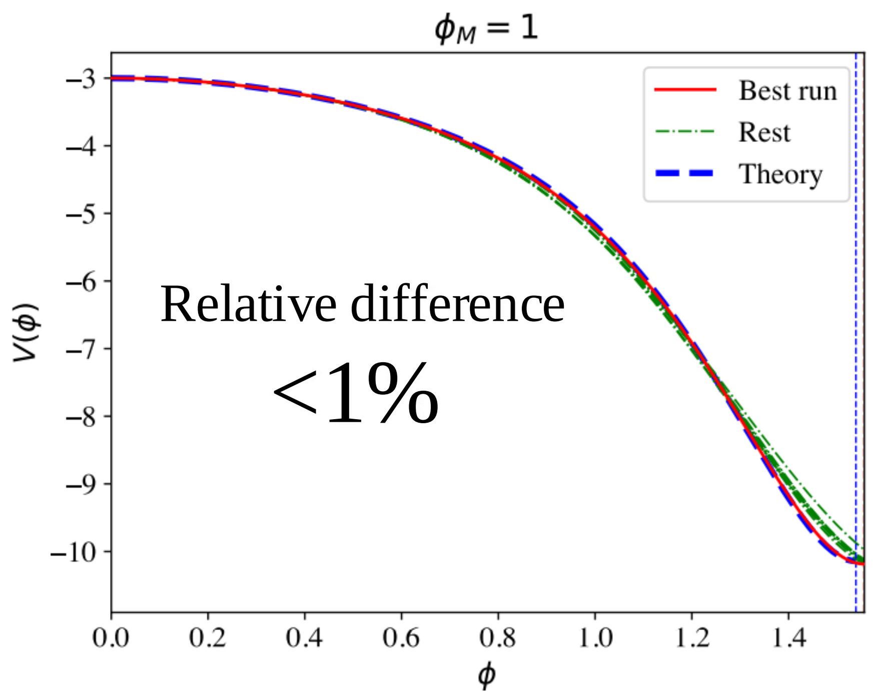
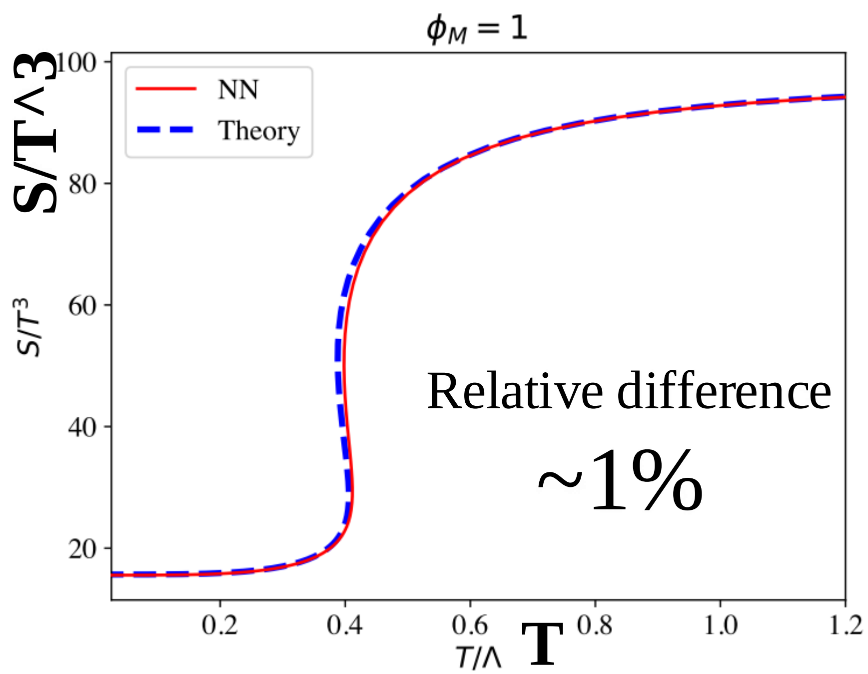
Solving the inverse problem

Crossover　　second order　　**first order**





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Additional comments

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- Choose specific architecture, number of neurons, layers, etc
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→ There is some stochasticity:
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→ Our method is general and applicable in generic inverse problems

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- Choose s
- Samplin
- Samplin

→ The

Thank you!

→ Our method is general and applicable in generic inverse problems

Backup Slides

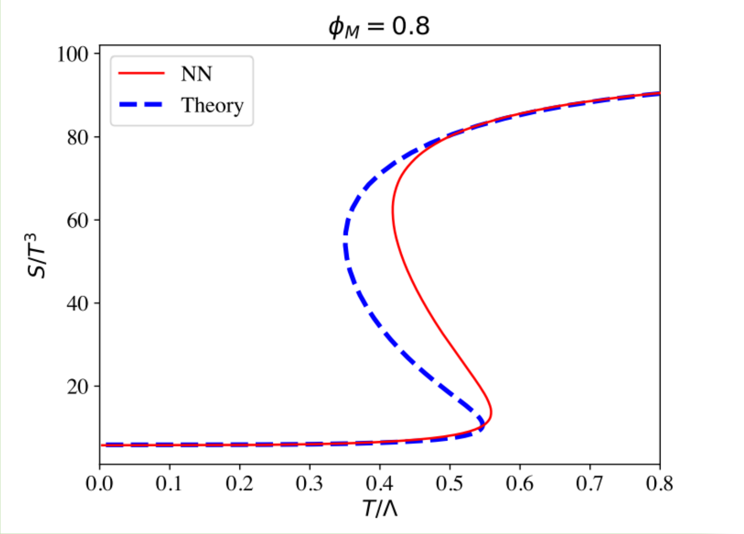
Future directions

This is just a first paper, a lot of room for improvement and extensions

→ Next step: improve accuracy

We are currently increasing the number of neurons and layers

We want to improve the resolution in problems with large separation of scales



→ We are also exploring transfer learning

Our potential

$$S = \frac{2}{\kappa_5^2} \int dx^5 \sqrt{-g} \left[\frac{1}{4} R - \frac{1}{2} (\nabla \phi)^2 - V(\phi) \right]$$

$$V_{\text{theory}}(\phi) = -\frac{4}{3} \mathcal{W}(\phi)^2 + \frac{1}{2} \mathcal{W}'(\phi)^2 \,,$$

$$\mathcal{W}(\phi) = -\frac{3}{2} - \frac{\phi^2}{2} - \frac{\phi^4}{4\phi_M^2} + \frac{\phi^6}{10} \,.$$

Einstein equations

$$E_1 = \nu_\Sigma - \tilde{\Sigma}' \,, \tag{4.3a}$$

$$E_2 = \nu_A - \tilde{A}' \,, \tag{4.3b}$$

$$E_3 = \nu_\phi - \phi' \,, \tag{4.3c}$$

$$E_4 = \nu_\Sigma' + \frac{2}{3}\tilde{\Sigma}\,\nu_\phi^2 \,, \tag{4.3d}$$

$$E_5 = u^2\,\tilde{\Sigma}\,\nu_A' + \frac{8}{3}V(\phi)\,\tilde{\Sigma} + \nu_A\,\left(3u^2\,\nu_\Sigma - 5u\,\tilde{\Sigma}\right) + \tilde{A}\left(8\tilde{\Sigma} - 6u\,\nu_\Sigma\right)\,, \tag{4.3e}$$

$$E_6 = u^2\,\tilde{\Sigma}\,\tilde{A}\,\nu_\phi' - \tilde{\Sigma}\,\frac{dV}{d\phi} + \nu_\phi\left(-3u\,\tilde{A}\,\tilde{\Sigma} + u^2\,\tilde{\Sigma}\,\nu_A + 3u^2\,\nu_\Sigma\,\tilde{A}\right)\,, \tag{4.3f}$$

$$E_7 = \left(u\,\nu_\Sigma - \tilde{\Sigma}\right)\left(u^2\,\tilde{\Sigma}\,\nu_A + 2u^2\,\tilde{A}\,\nu_\Sigma - 4u\tilde{A}\tilde{\Sigma}\right) - \frac{2}{3}u\,\tilde{\Sigma}^2\left(u^2\tilde{A}\,\nu_\phi^2 - 2V(\phi)\right)\,. \tag{4.3g}$$

Boundary conditions

$$\tilde{A}|_{u=0} = 1 \ ,$$

$$\tilde{\Sigma}|_{u=0} = 1 \ ,$$

$$\phi|_{u=0} = 0 \ ,$$

$$\nu_\phi|_{u=0} = 1 \ ,$$

$$\tilde{A}|_{u=1} = 0 \ ,$$

$$\nu_A|_{u=1} = -4\pi T \ ,$$

$$\tilde{\Sigma}_{u=1} = (S/\pi)^{1/3} \ .$$

Libraries

We have chosen the `Adam` optimizer[2] for the optimization process, which uses stochastic gradient descent with information about higher-order momenta (see [49] for details).

The described NN system has been implemented in the `Python` language through the open source `neurodiffeq` library [50], built on `PyTorch`.

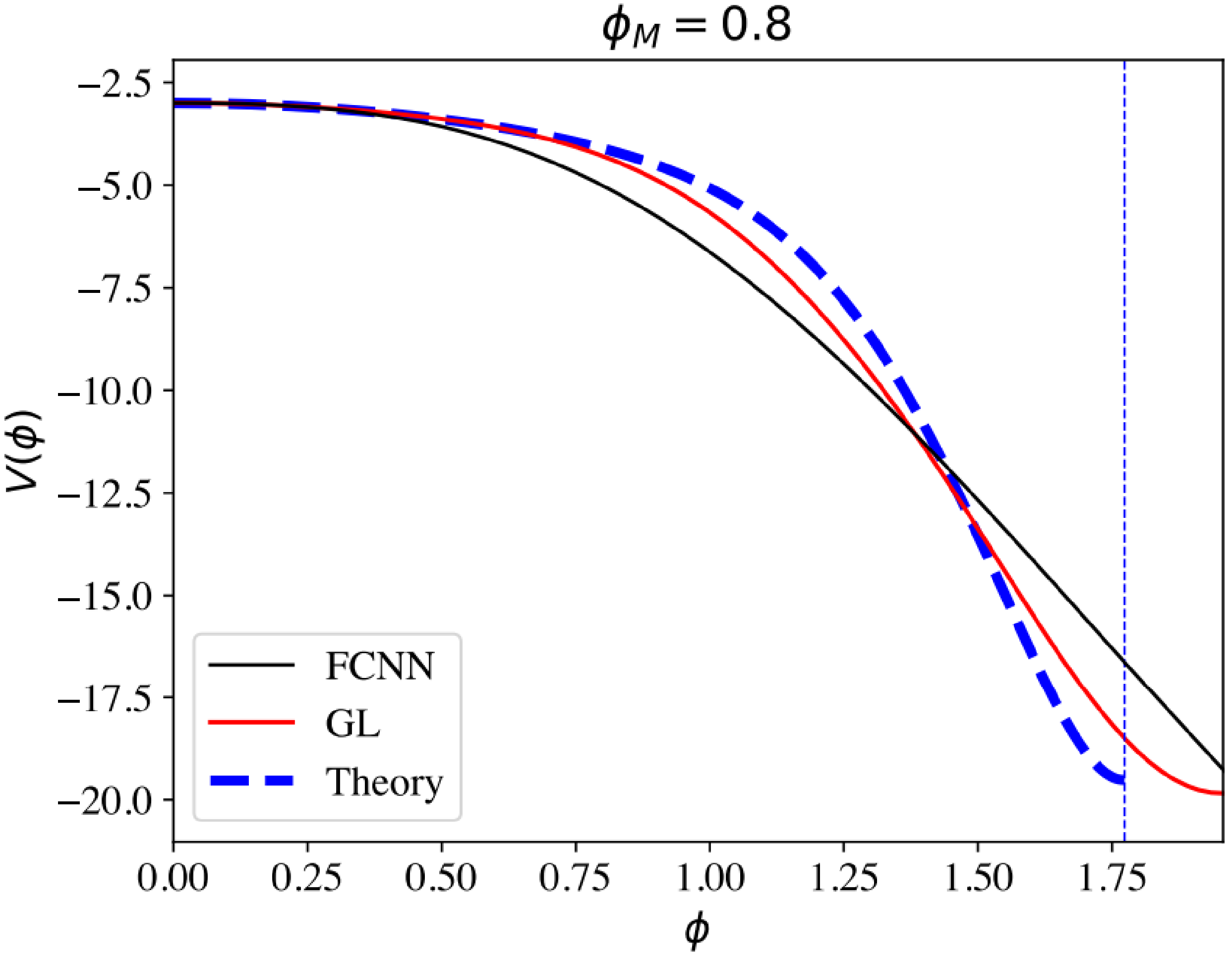
[49] D.P. Kingma and J. Ba, *Adam: A method for stochastic optimization*, 2017.

[50] F. Chen, D. Sondak, P. Protopapas, M. Mattheakis, S. Liu, D. Agarwal et al., *Neurodiffeq: A python package for solving differential equations with neural networks*, *Journal of Open Source Software* **5** (2020) 1931.

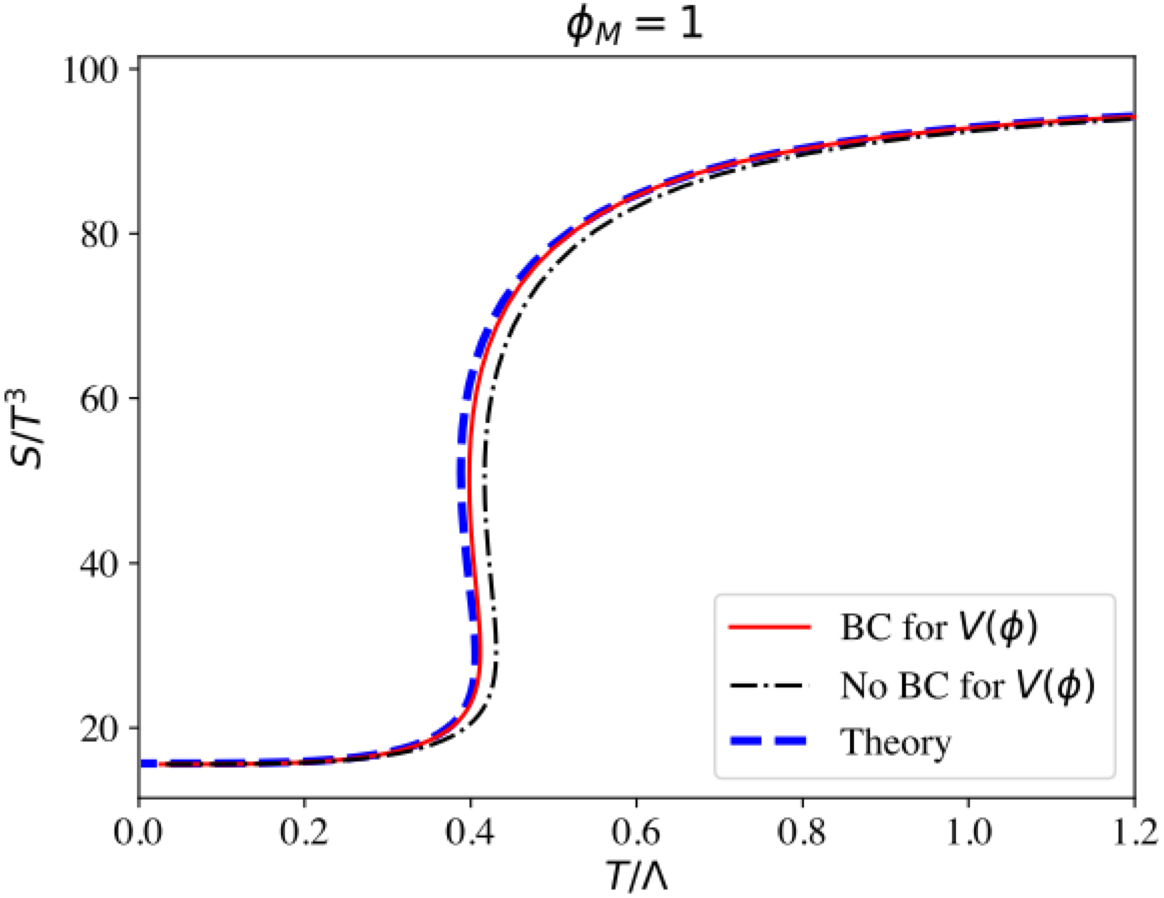
Computational considerations

Training and discovery of a solution with sub-per cent precision in the potential and per cent precision in the recovered equation of state requires about 8-16 hours and a couple of million epochs in a dedicated NVidia A40 GPU. As explained above, we performed ten

Gaussian localization vs fully connected



Additional loss



References NN in holography

The only papers that reconstruct the theory:

[8] K. Hashimoto, K. Ohashi and T. Sumimoto, *Deriving the dilaton potential in improved holographic QCD from the meson spectrum*, *Phys. Rev. D* **105** (2022) 106008 [2108.08091].

[9] K. Hashimoto, K. Ohashi and T. Sumimoto, *Deriving the dilaton potential in improved holographic QCD from the chiral condensate*, *PTEP* **2023** (2023) 033B01 [2209.04638].

[10] X. Chen and M. Huang, *Machine learning holographic black hole from lattice QCD equation of state*, 2401.06417.

Other papers (reconstruct solutions):

[12] Y.-Z. You, Z. Yang and X.-L. Qi, *Machine Learning Spatial Geometry from Entanglement Features*, *Phys. Rev. B* **97** (2018) 045153 [1709.01223].

[13] K. Hashimoto, S. Sugishita, A. Tanaka and A. Tomiya, *Deep learning and the AdS/CFT correspondence*, *Phys. Rev. D* **98** (2018) 046019 [1802.08313].

[14] K. Hashimoto, S. Sugishita, A. Tanaka and A. Tomiya, *Deep Learning and Holographic QCD*, *Phys. Rev. D* **98** (2018) 106014 [1809.10536].

[15] H.-Y. Hu, S.-H. Li, L. Wang and Y.-Z. You, *Machine Learning Holographic Mapping by Neural Network Renormalization Group*, *Phys. Rev. Res.* **2** (2020) 023369 [1903.00804].

[16] K. Hashimoto, *AdS/CFT correspondence as a deep Boltzmann machine*, *Phys. Rev. D* **99** (2019) 106017 [1903.04951].

......+ 15 references