Unification of Symmetries Inside Neural Networks: Transformer, Feedforward and Neural ODE

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ArXiv:2402.02362 (w/ Yuji Hirono, Akiyoshi Sannai)

Unification of Symmetries Inside Neural Networks

[Hirono, Sannai, KH 2402.02362]

1. Motivation: gauge sym in NN — 2 pages
2. Candidates for diffeo in NN — 4 pages
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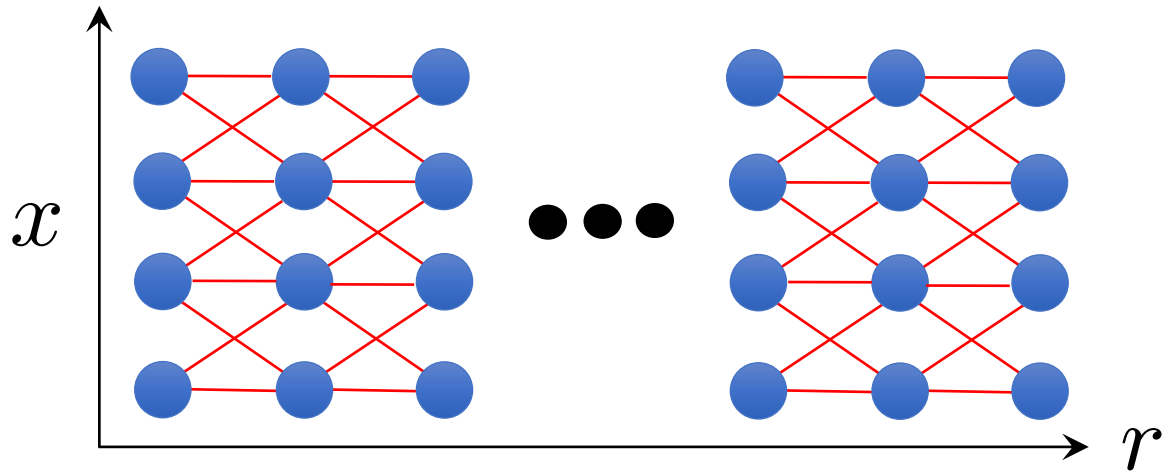
1. Motivation: gauge sym in NN

There should be diffeo, a la AdS/DL

Deep feedforward NN = AdS spacetime



Bulk reconstruction by entanglement [Lam You] [You Yang Qi] …

Bulk reconstruction by QFT correlators

[Tanaka Tomiya Sughishita KH] [Akutagawa Sumimoto KH] [Hu You KH] [Tan Chen] [Song Oh Ahn Kim] [Yan Wu Ge Tian] …

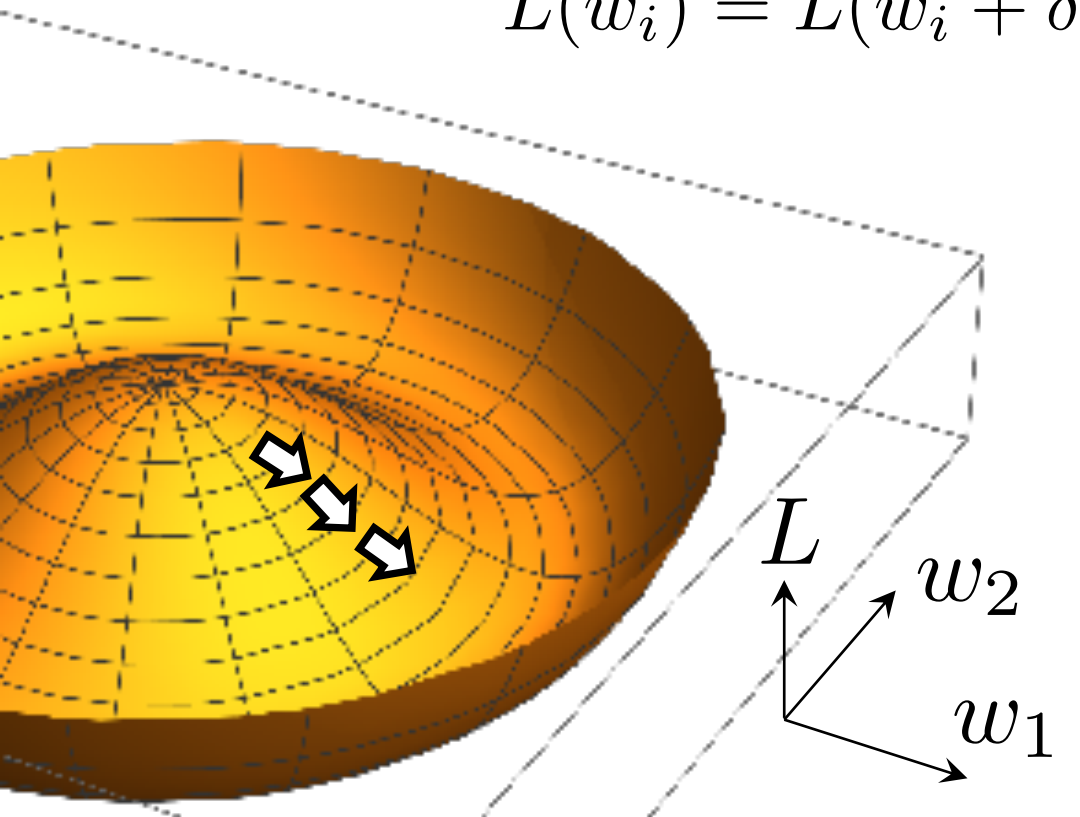
Deep Boltzmann machine = AdS/CFT [KH]

1. Motivation: gauge sym in NN

Symmetries = redundancy → trainability

NN symmetry : Invariance of loss function $L(w_i)$ under a transformation on weights w_i

$$L(w_i) = L(w_i + \delta_i(w))$$



Learning dynamics may depend on symmetries.

[Amari] [Amari Ozeki Karakida Yoshida Okada]
[Badrinarayanan Mishra Cipolla]
[Neyshabur Salakhutdinov Srebro]
[Ziyin 2023] …

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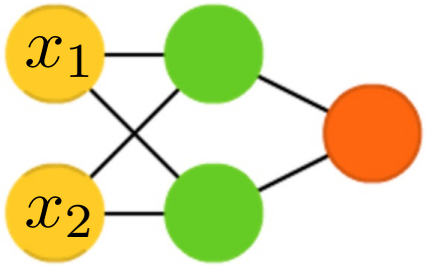
2. Candidates for diffeo in NN

Review of Feedforward NN

Perceptron model



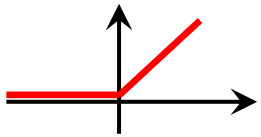
$W_i^{(2)}\varphi(W_{ij}^{(1)}x_j)$

"Unit" (circles) : Vector components

"Weight" W (lines) : Linear transformation to be optimized

"Activation function" φ (hidden line-end) : Nonlinear component-wise transf.

$$\mathrm{ReLU}(x) = x\,\theta(x)$$

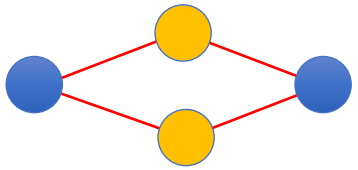


- Training protocol :
  1) Prepare many sets $\{(x_j, f)\}$: input and output
  2) Train the network (adjust W) by lowering

"Loss function" $E \equiv \sum_{\text{data}} \left| f - W_i^{(2)}\varphi\left(W_{ij}^{(1)}x_j\right)\right|$

2. Candidates for diffeo in NN

1. Permutation symmetry



$$f(x) = w_1\varphi(\tilde{w}_1 x + \tilde{b}_1) + w_2\varphi(\tilde{w}_2 + \tilde{b}_2) + b$$

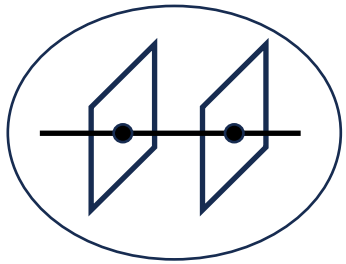
Multi-Layer
Perceptron

NN symmetry : swapping of neurons

$$w_1 \leftrightarrow w_2, \quad \tilde{w}_1 \leftrightarrow \tilde{w}_2, \quad \tilde{b}_1 \leftrightarrow \tilde{b}_2$$

Note : this Z_2 sym enhances at singularity

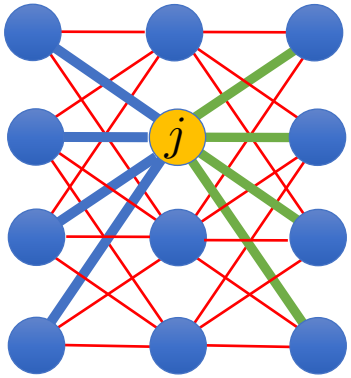
[Amari Ozeki Karakida Yoshida Okada 2016]



2. Candidates for diffeo in NN

2. Rescaling symmetry

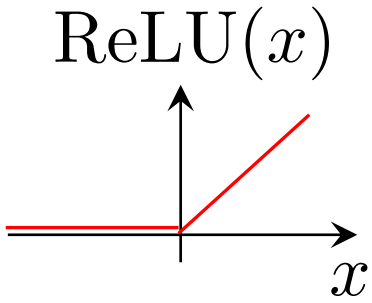
x_k



$$f_i = w_{ij}\varphi(\tilde{w}_{jk}x_k + \tilde{b}_j) + b_i$$

ReLU activation

$\varphi(x) = \mathrm{ReLU}(x)$



NN symmetry : For any fixed j, rescale

$$w_{ij} \mapsto \alpha w_{ij}, \quad \tilde{w}_{jk} \mapsto \alpha^{-1}\tilde{w}_{jk}, \quad \tilde{b}_j \mapsto \alpha^{-1}\tilde{b}_j$$

due to ReLU scaling property

$$\mathrm{ReLU}(\alpha^{-1}x) = \alpha^{-1}\mathrm{ReLU}(x)$$

2. Candidates for diffeo in NN

3. Self-attention in transformers

$$h_i = \sum_{j=1}^{n} \mathrm{ReLU}\left((xw^{(q)})_i (xw^{(k)})_j^{\mathrm{T}} \right) (xw^{(v)})_j$$

$x \in \mathbf{R}^{n\times d}$: set of data $x_i \in \mathbf{R}^d (i = 1, 2, \cdots, n)$

$w^{(q),(k),(v)} \in \mathbf{R}^{d\times d}$: query, key and value weights

NN sym 1 : rescaling $w^{(a)} \mapsto \alpha^{(a)} w^{(a)}, \quad \alpha^{(q)}\alpha^{(k)}\alpha^{(v)} = 1$

NN sym 2 : Internal sym

$$w^{(q)} \mapsto w^{(q)} A, \quad w^{(k)} \mapsto w^{(k)} (A^{-1})^T, \quad A \in SL(d, \mathbf{R})$$

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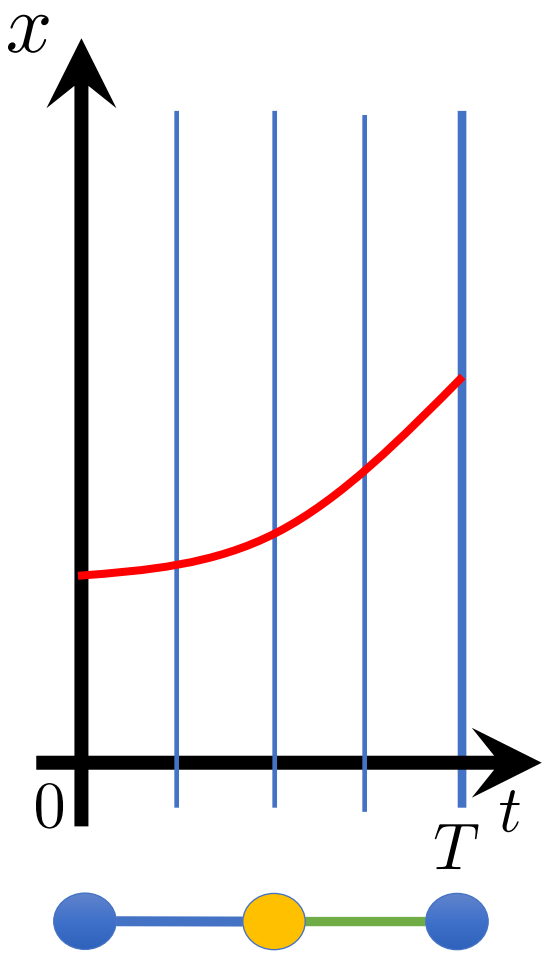
3. Diffeos in neural ODEs

Neural ODEs = continuous ver. of NN

Chen, Rubanova, Bettencourt, Duvenaud
ArXiv:1806.07366 [cs.LG]



$$\dot{x}(t) = F(t, x(t))$$

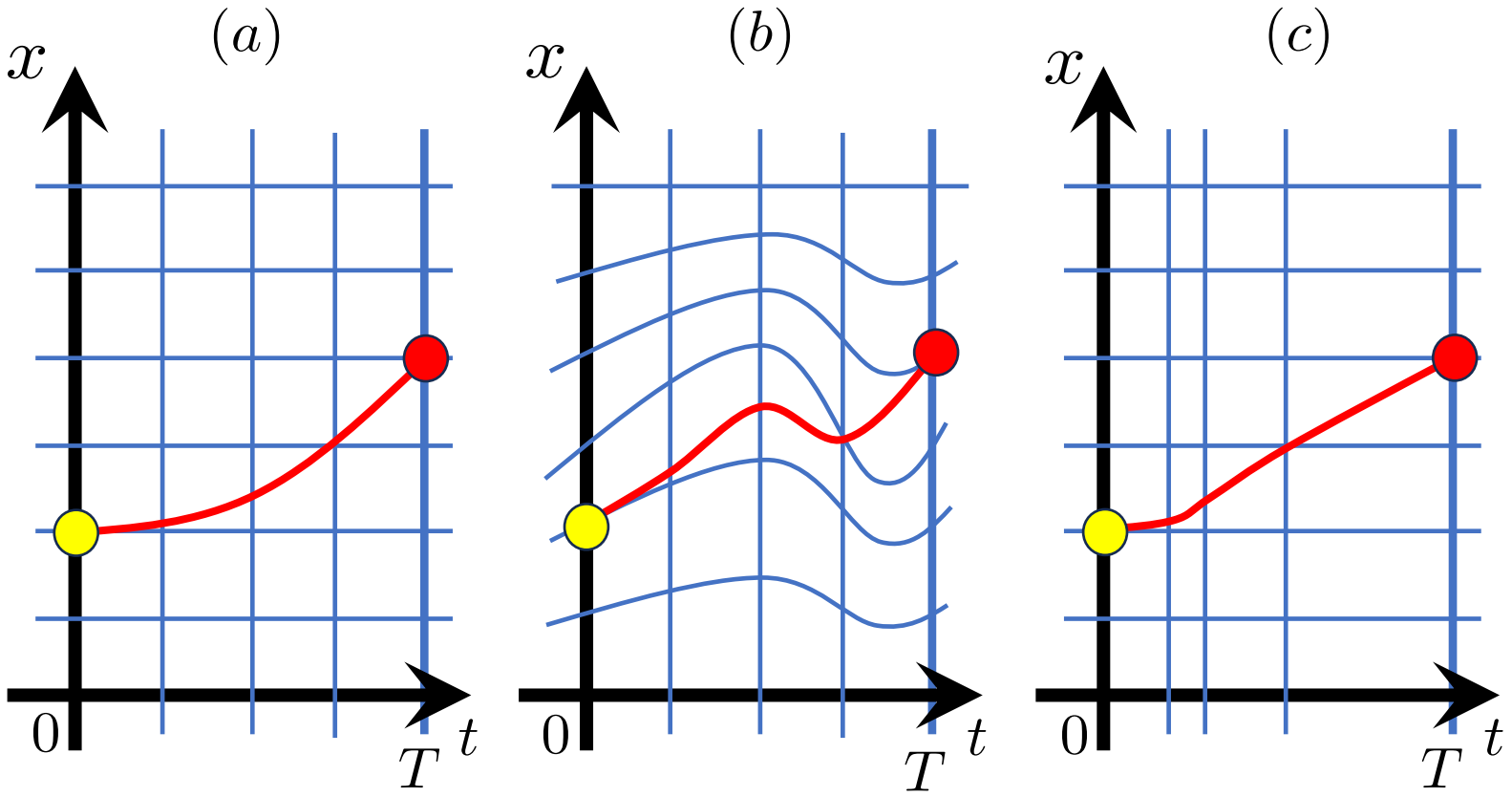
Training : train $F(t, x)$ such that the relation $(x(0), x(T))$ reproduces given set of data $\{(x_i, x_f)\}$.

Discretizing it gives a residual NN :

$$x(t + \delta t) = x(t) + F(t, x(t))\delta t$$

3. Diffeos in neural ODEs

Diffeos in ADM-like decomposition in neural ODE



Original frame

Spatial diffeo

$x(t) \mapsto x(t) + \epsilon(t, x(t))$

Time reparam.

$t \mapsto t + f(t)$

3. Diffeos in neural ODEs

Linear neural ODE can be solved

Linear neural ODE : $\dot{x}(t) = w(t)x(t) + b(t)$

Explicit solution of the ODE

$$x(T) = e^{\int_0^T w(t')dt'} x(0) + \left(\int_0^T e^{-\int_0^{t'} w(t'')dt''} b(t')dt' \right) e^{\int_0^T w(t'')dt''}$$

"Wilson loop"

Spatial diffeo $x(t) \mapsto x(t) - g(t)x(t)$ is weight transf.

$$w(t) \mapsto w(t) + \dot{g}(t), \quad b(t) \mapsto e^{g(t)-g(t=0)}\, b(t)$$

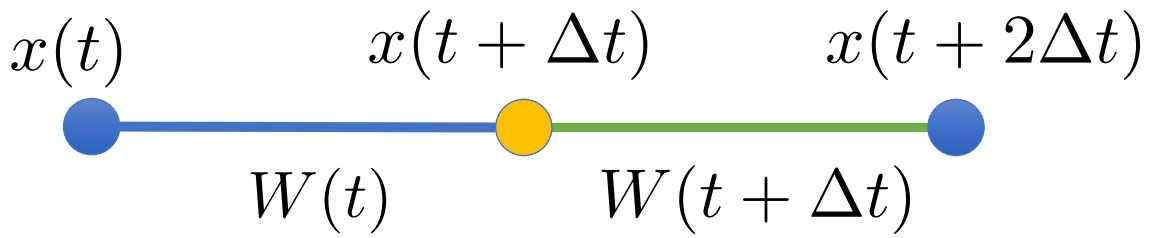
"Gauge field" "Higgs field"

Time reparam. $t \mapsto t + f(t)$ is weight transf.

$$w(t) \mapsto w(t) - \frac{d}{dt}(w(t)f(t)), \quad b(t) \mapsto b(t) - \frac{d}{dt}(b(t)f(t))$$

3. Diffeos in neural ODEs

Rescaling = a spatial diffeo



Spatial diffeo : Integrated weight transforms as Wilson line

$$W(t) \mapsto e^{-g(t)} W(t) e^{g(t+\Delta t)}$$

$$W(t+\Delta t) \mapsto e^{-g(t+\Delta t)} W(t) e^{g(t+2\Delta t)}$$

which reproduces the rescaling symmetry

$$w_{ij} \mapsto \alpha w_{ij}, \quad \tilde{w}_{jk} \mapsto \alpha^{-1} \tilde{w}_{jk}$$

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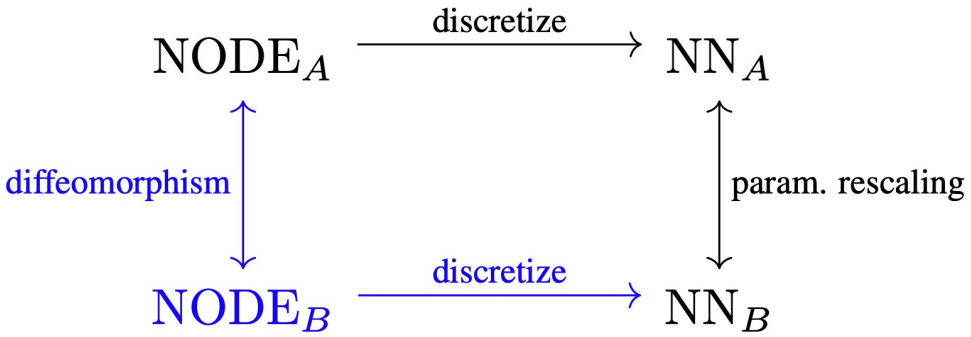
4. Physics of NN symmetries?

NN gauge symmetries are broken in general

- Discretization breaks spacetime sym, as in lattice QFT.



- Other than (leaky) ReLU, no rescaling symmetry.

[Godfrey Brown Emerson Kvinge 2205.14258(cs.LG)]

- Special neural ODE allows a metric interpretation.

"Neural geodesic equation"
$$\begin{cases} \dot{x}^i = v^i \\ \dot{v}^i = -\Gamma^i_{jk}(x) v^j v^k \end{cases}$$

4. Physics of NN symmetries?

Training and symmetry breaking

Nevertheless, amusing to see similarities to gauge theory!

- Weights = gauge field, Biases = Higgs field
- Weight decay = Gauge mass term

$$\sum_{i,j} w_{ij}^2 \sim \int dt\, w(t)^2$$

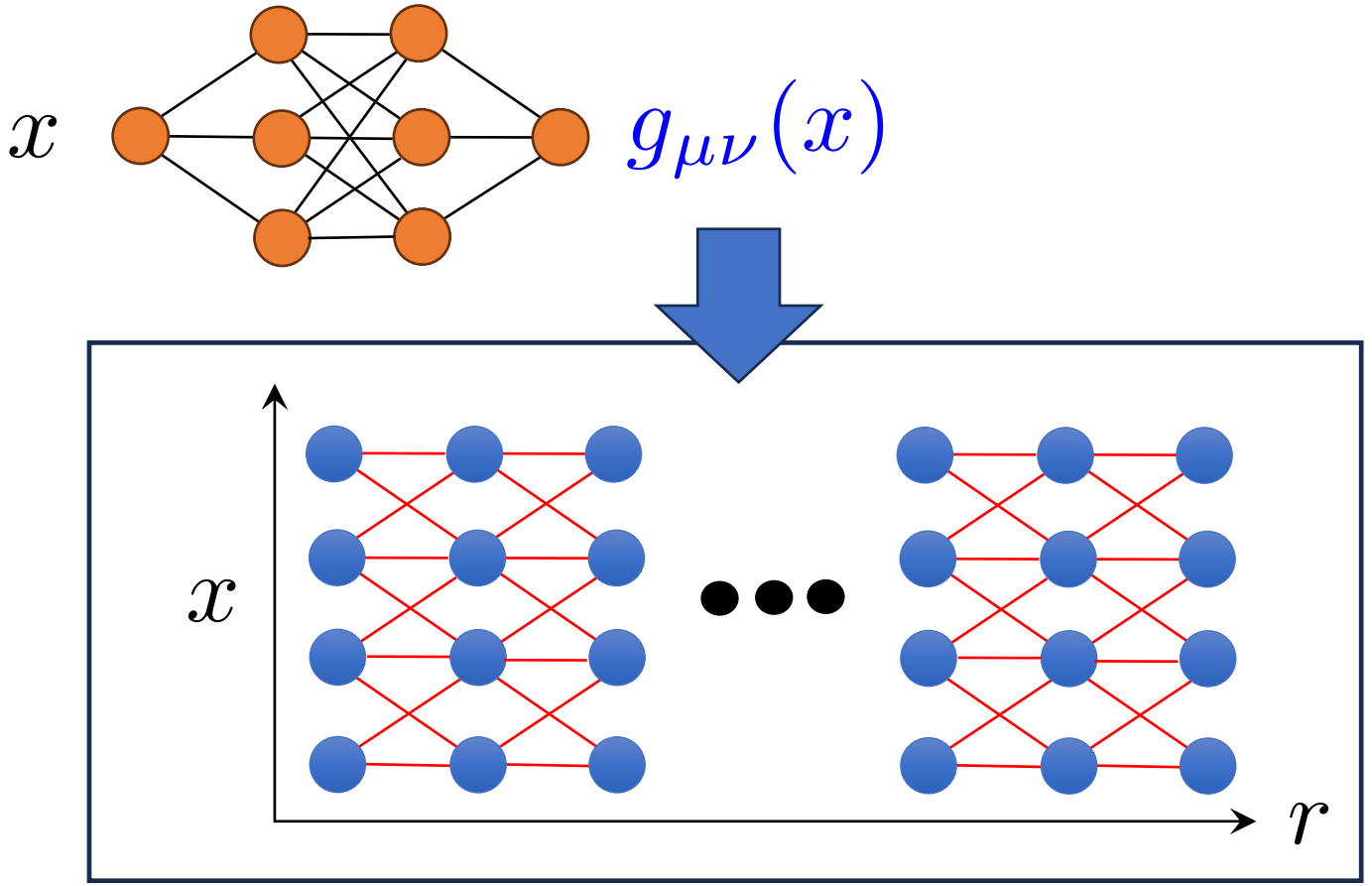
- Linear transport condition = Lorentz gauge fixing term

$$L_{\mathrm{R}} = \lambda \int_0^T dt \left[(\dot{w} + w^2)^2 + \left[(\partial_t + w) b \right]^2 \right]$$

4. Physics of NN symmetries?

Generative spacetimes

We may add other NN to generate the spacetime lattice



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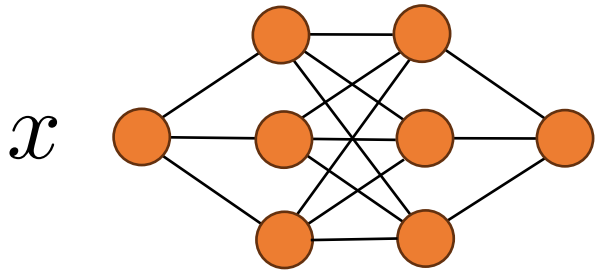
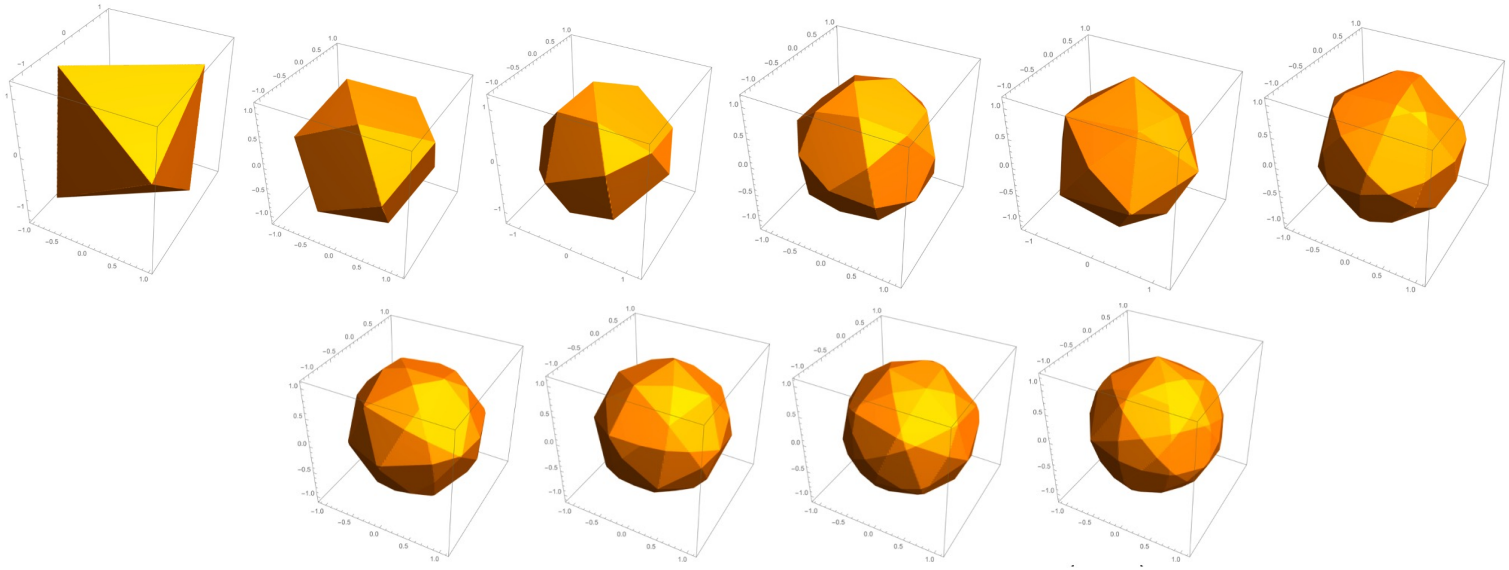


$g_{\mu\nu}(x)$

Naito, Naito, KH
ArXiv:2307.00721 [cs.LG]



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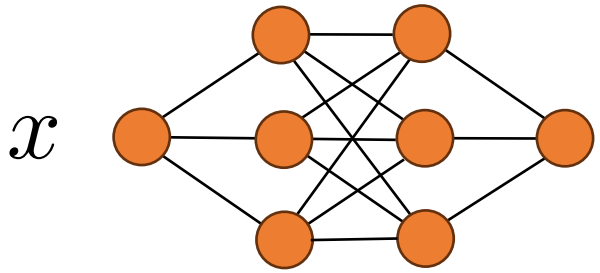

$$g_{\mu\nu}(x)$$

Naito, Naito, KH
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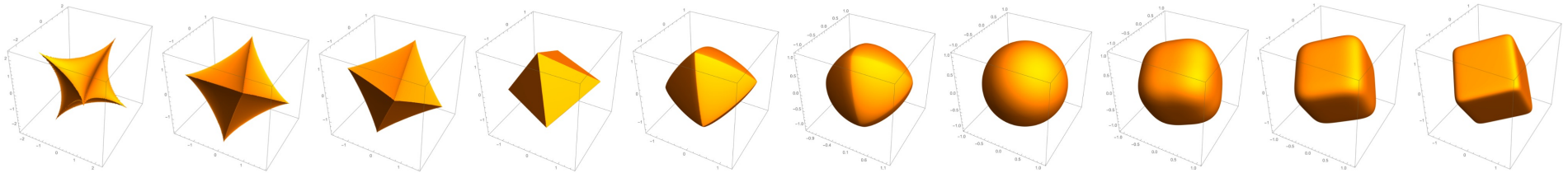

"Neural Polytopes" :
Continuous generalization of polytopes

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