Machine-learning of topological defects and deconfinement transition on the lattice

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Approximate plan of the talk

— Very brief overview of confinement problem in QCD

— Motivation: mechanism of confinement with machine learning?

— Overview of machine learning and artificial neural networks
  (here and in other places in the text)

— Recognizing confinement from dynamics of topological objects?
  Example: compact U(1) gauge theory in (2+1)d as a toy model

— Guessing Getting physics from unphysics with neural networks:
  Finding physical deconfinement temperature in
  lattice Yang-Mills theories via a hint from
  outside the scaling window (if we have time).
  In collaboration with D. Boyda (MIT, USA & Vladivostok, Russia),
  N. Gerasimenyuk, S. Lyubimov (Vladivostok, Russia)

— Future developments

[2006.09113]
[to appear]
Very brief overview of the confinement problem in QCD

— At zero temperature, quarks and gluons form bound states (confined inside colorless states: hadrons, glueballs.)

— The confinement of color is due to dynamics of gluons not quarks

— To study the problem (as well as the accompanying mass-gap generation), concentrate on pure gluonic system, Yang-Mills theory

— Yang-Mills theory is confining at low temperature (phase) and deconfining at high temperature (gluon plasma phase)

— The mechanism of confinement is not well understood.

— Could be caused by dynamics of certain (topological) objects such as center vortices, abelian monopoles, non-abelian calorons, instanton-dyons + many more ideas.

— Many assuring signatures (mainly, from the lattice), no solid proof.
— We see the color confinement in first-principle lattice simulations.

— The mechanism of confinement is hidden somewhere inside those (typically, very large) configurations of gluons produced by various Monte Carlo algorithms.

However:

In the machine learning field of computer science, artificial neural networks can successfully recognize and classify hidden patterns in (typically, huge) data sets.

**Motivation of the talk:**
can we recognize mechanism of color confinement with machine learning?

*) this is the motivation but not the aim of this talk
Many developments in the field (ML + QFT + …)

... +
1605.01735, Carrasquilla-Melko;
1608.07848, Broecker et al.;
1703.02435, Wetzel;
1705.05582, Wetzel-Scherzer;
1805.11058, Abe et al.;
1801.05784, Shanahan-Trewartha-Detmold;
1807.05971, Yoon-Bhattacharya-Gupta;
1810.12879, Zhou-Endrõdi-Pang;
1811.03533, Urban-Pawlowski;
1904.12072, Albergo-Kanwar-Shanahan;
1908.00281 Fukushima-Funai-lida;
1909.06238, Matsumoto-Kitazawa-Kohno;
2004.14341 Bachtis-Aarts-Lucini
+ ...
Machine learning and artificial neural networks

Definitions:

**Machine learning (Arthur Samuel, 1959):**

The field of study that gives computers the ability to learn without being explicitly programmed.

**Machine learning (Tom Mitchell, 1997)**

A computer program is said to learn from experience $E$ with respect to some class of tasks $T$ and performance measure $P$ if its performance at tasks in $T$, as measured by $P$, improves with experience $E$.

Surely, besides these two extremes, one has more in between.
Machine learning and artificial neural networks

Features:

— pattern recognition (without explicit programming)
— flexible (wide range of applications)
— very general (no theory is needed, black box problem)
— for some, possesses some “creative” and “predictive” power

Applications, some of (General idea = pattern recognition):

— classification / clustering
— regression (prediction)
— transcription / translation
— anomaly detection
— de-noising
— synthesis and sampling

Applications in industry: computer vision, language processing, medical diagnosis, fraud detection, recommendation system, autonomous driving, …
Machine learning and artificial neural networks

Examples (media):

- **MuZero, AlphaZero (DeepMind):**
  play chess, shogi, Go [https://deepmind.com/](https://deepmind.com/)

- **GPT-2 (OpenAI):** conditional synthetic text sampling (+ question answering, reading comprehension, summarization, translation) [https://openai.com/](https://openai.com/)

- **YOLO:** real-time object detection [1804.02767]

- **Grammarly:** AI-enhanced text processing (clarity, concision, vocabulary, delivery style) [https://grammarly.com/](https://grammarly.com/)

Examples (science):

- **AlphaFold (DeepMind):** protein folding


- **astronomy** [1904.07248]

- **geometrical structures** [https://geometricdeeplearning.com/](https://geometricdeeplearning.com/)
Machine learning and artificial neural networks

Comparisons:

— results comparable and sometimes superior to human experts (cancer diagnosis, traffic sign recognition. . . )

— generally, performance is much better compared to any other machine algorithm

Drawbacks:

— black box

— magic

— numerical

(= how to extract analytical / exact results?)

For us, Machine Learning algorithms will upgrade the standard Monte Carlo
Deep neural network

Layered structure

(1) Input layer is the first layer of neurons which receives data (bits that encode colored pixels from an image, values of gauge fields in an MC-generated SU(N) field configuration)

(2) Hidden layer is a layer of neurons that gets information from the input layer, modifies it, and passes to the output (or, next) layer.

Terminology: A neural network that contains more than one hidden layer is a deep neural network.

(3) The final layer of a neural network which contains the answer(s).

Sometimes the answer is “42”.

→ Link: is a matrix operation which acts on a vector from \( n \)th layer and gives an input to the \((n+1)\)th layer. The matrix elements are weights to be tuned.

\[
\mathbf{x}_{i}^{(n+1)} = G_{i}^{(n+1)}(y_{i}^{(n)})
\]

Activation function. Examples:

- **ReLU**
  \[
  G(\xi) = \xi \Theta(\xi) \equiv \begin{cases} 
  \xi, & \xi > 0 \\
  0, & \text{otherwise}
  \end{cases}
  \]

- **Sigmoid**
  \[
  G(\xi) = \frac{1}{1 + e^{-\xi}} \in (0, 1)
  \]
Deep neural network

Operations:

— **convolution** = Reduces matrix (database) size.
  Takes a convolution (“selective blurring”) across an area.

— **pooling** = Reduces matrix (database) size.
  Takes the maximum / average value across the pooled area.

— **dropout** = A form of regularization useful in training neural networks.
  Removes a random selection of a fixed number of the units

Supervision:

— supervised network: teach network at a set of examples using mean squared error as a validation (= examination)

— un-supervised network: leave network alone and let it classify features of the system (of the database) itself.
Question: can we “learn confinement” in QCD?

— Big aim: Assuming that some (topological, semi-classical) structures are responsible for confinement, can we find (determine, describe) them in gluon configurations?

— Modest (intermediate) aim: first take a well-known toy model; make test, tune the artificial network, and compare with (expected) results.
Compact U(1) gauge theory in (2+1)d
(also known as “compact electrodynamics”, cU(1) or cQED, despite the absence of matter fields)

Formulation in continuum spacetime

Lagrangian:
\[ \mathcal{L} = \frac{1}{4} F_{\mu\nu}^2 \]

Field strength tensor:
\[ F_{\mu\nu} = F_{\mu\nu}^{ph} + F_{\mu\nu}^{mon} \]

Photon–field strength tensor
\[ F_{\mu\nu}^{ph}[A] = \partial_\mu A_\nu - \partial_\nu A_\mu \]

Field-strength vector
\[ \tilde{F}_\mu = \frac{1}{2} \epsilon^{\mu\alpha\beta} F_{\alpha\beta} \]

Dual field-strength vector

Monopole strength tensor
\[ \partial_\mu \tilde{F}_\mu^{mon,\mu} = \rho \]

Density of magnetic monopoles
Compact U(1) gauge theory in (2+1)d

Magnetic monopoles

- appear in the singular/monopole part of the field-strength tensor

\[ \partial_{\mu} \tilde{F}^{\mu} = \partial_{\mu} \tilde{F}^{\text{mon,}\mu} = \rho \]

- carry magnetic charge

\[ \partial_{\mu} F^{\mu \nu} = j^{\nu} \]

\[ \partial_{\mu} \tilde{F}^{\mu} = \rho \]

- magnetic monopoles are instantons in (2+1)d

\[ \rho(\mathbf{x}) = \sum_{a} q_{a} \delta^{(3)}(\mathbf{x} - \mathbf{x}_a) \]

\[ \tilde{F}^{\mu} = \frac{1}{2} \epsilon^{\mu \alpha \beta} F_{\alpha \beta} \]

dual field-strength vector

a typical monopole configuration

magnetic charge density

magnetic charge of \( a \)th monopole

position of \( a \)th monopole

magnetic charge density
Compact U(1) gauge theory in (2+1)d
(easier to work in Euclidean space-time via Wick transformation)

Magnetic (singular) part the field strength:

\[
F^{\text{mon}}_{\mu\nu}(x) = -g_{\text{mon}}\epsilon_{\mu\nu\alpha}\partial_\alpha \int d^3y D(x - y)\rho(y)
\]

\[
g_{\text{mon}} = \frac{2\pi}{g}
\]

Dirac quantization condition

\[
-\Delta D(x) = \delta(x)
\]

Action decouples into two parts:

\[
S[A, \rho] = \frac{1}{4} \int d^3x \left( F^{\text{ph}}_{\mu\nu}[A] + F^{\text{mon}}_{\mu\nu}[\rho] \right)^2 \equiv S^{\text{ph}}[A] + S^{\text{mon}}[\rho]
\]

monopole density

elementary magnetic charge

Green’s function of Laplacian in 3D

monopole density
Compact U(1) gauge theory in (2+1)d

Monopole partition function

Action for $N$ monopoles:

$$S^{\text{mon}}[\rho] = \frac{g_{\text{mon}}^2}{2} \sum_{a,b=1 \atop a \neq b}^N q_a q_b D(x_a - y_b) + N S_0$$

Coulomb gas of monopoles

$$D(x) = \int \frac{d^3 k}{(2\pi)^3} \frac{e^{ikx}}{k^2} = \frac{1}{4\pi |x|}$$

The partition function of monopoles:

$$Z_{\text{mon}} = \oint_{\text{mon}} e^{-S_{\text{mon}}[\rho]} \rightarrow \int \mathcal{D}\chi \exp \left\{ - \int d^3 x \mathcal{L}_s(\chi) \right\}$$

fugacity controls mean monopole density

Sine-Gordon model with the scalar field $\chi$

$$\mathcal{L}_s = \frac{1}{2g_{\text{mon}}^2} (\partial_\mu \chi)^2 - 2\zeta \cos \chi$$

photon-monopole decoupling

$$Z = Z_{\text{ph}} \cdot Z_{\text{mon}}$$

measure of monopole integration

$$\oint_{\text{mon}} = \sum_{N=0}^{\infty} \frac{1}{N!} \prod_{a=1}^N \left( \sum_{q_a = \pm 1} \zeta \int d^3 x_a \right)$$
Compact U(1) gauge theory in (2+1)d

Photon becomes massive. Debye mass:

\[ m_{\text{ph}} = \frac{2\pi \sqrt{\varrho_{\text{mon}}}}{g} \]

mass of the sine-Gordon field

Finite Debye length

\[ \lambda_D = m_{\text{ph}}^{-1} \]

non-perturbative

\[ \mathcal{L}_S = \frac{1}{2g_{\text{mon}}^2} \left[ (\partial_\mu \chi)^2 + m_{\text{ph}}^2 \chi^2 \right] + O(\chi^4) \]

Mean monopole density:

\[ \varrho_{\text{mon}} = 2\zeta \]

(average number of monopoles plus antimonopoles)

Applicability: dilute gas approximation

\[ \varrho_{\text{mon}}^{1/2} g_{\text{mon}}^3 \ll 1 \]

The number of monopoles in a unit Debye volume is sufficiently high:

\[ \varrho_{\text{mon}} \lambda_D^3 \gg 1 \]
Compact U(1) gauge theory in (2+1)d

— Confinement: test electric charges are confined by a linear potential

\[ V(R) = \sigma R \]

String tension

\[ \sigma = \frac{8\sqrt{2\zeta}}{g_{\text{mon}}} \equiv \frac{4g\sqrt{\xi_{\text{mon}}}}{\pi} \]

valid at the distances \( R \gg \lambda_D \)

Notice:

in (2+1)d, the standard photon exchange gives to a logarithmically rising confining, also confining potential

Confinement is a result of the monopole dynamics
Compact U(1) gauge theory in (2+1)d

— Finite-temperature deconfinement transition

Phase transition of the BKT type

in agreement with the Svetitsky-Yaffe conjecture
— symmetry breaking pattern determines the order of the phase transition
— the order parameter: U(1) Polyakov loop
— universality class corresponds to a two-dimensional spin system with U(1) global symmetry group (XY model)
— the BKT phase transition is a smooth transition of an infinite order
— high-temperature phase of the compact U(1) gauge theory is described by the conformal-field theory corresponding to the low-temperature phase of XY in 2d

\[ L = \exp \left\{ i \int dx_3 A_3 \right\} \]

circle closed via compactified Euclidean time direction \((x_3)\)

Hamiltonian of XY model:

\[ H = -J \sum_{\langle i,j \rangle} s_i \cdot s_j \]
Compact U(1) gauge theory in (2+1)d

— Monopole dynamics at the phase transition

\[ D(x) = \begin{cases} \frac{1}{4\pi|x|} & \text{low-}T \\ -2T \log |\vec{x}|T & \text{high-}T \end{cases} \quad (|\vec{x}|T \gg 1) \]

Essentially the dimensional reduction due to shrinking length of Euclidean time direction

Monopole action:

\[ S^{\text{mon}}[\rho] = \frac{g_{\text{mon}}^2}{2} \sum_{a,b=1 \atop a \neq b}^N q_a q_b D(x_a - y_b) \]

Confinement is lost because free monopoles disappear. Monopoles and anti-monopoles become logarithmically confined into magnetically neutral dipole pairs at the critical temperature.

Similarity with the mechanism of the BKT transition in the 2d XY model (the vortices are bound in vortex-antivortex pairs in the low-T phase of the XY model)
Compact $U(1)$ gauge theory in (2+1)d

Similarities with $SU(N)$ Yang-Mills theories:

- Mass gap generation
- Linear confinement
- Presence of instantons (instanton-like objects)
- Finite-temperature deconfinement

Differences with $SU(N)$ Yang-Mills theories (some of):

- Photons are not confined. Contrary to gluons.
- Monopoles in $cU(1)$ are not exactly “instantons”.
- Different type of phase transition
  - In $SU(N)$ Yang-Mills: either second ($N=2$) or first ($N>2$) order-phase transition.
- Trivial high-temperature limit.
  - Massless photon in two Euclidean dimensions.
  - However, spatial Wilson loop obeys area law (which is trivial in 2d).
cU(1) gauge theory on the lattice

— Lattice action

\[ S[\theta] = \beta \sum_P (1 - \cos \theta_P) \]

\[ \beta = \frac{1}{g^2 a} \]

— Plaquette angle

\[ \theta_{P_{x,\mu\nu}} = \theta_{x,\mu} + \theta_{x+\hat{\mu},\nu} - \theta_{x+\hat{\nu},\mu} - \theta_{x,\nu} \]

— Compactness

\[ \theta_{x,\mu} \in [-\pi, +\pi) \]

— Density of abelian monopoles

\[ \rho_x = \frac{1}{2\pi} \sum_{P \in \partial C_x} \bar{\theta}_P \]

\[ \bar{\theta}_P = \theta_P + 2\pi k_P \in [-\pi, \pi), \quad k_P \in \mathbb{Z} \]

Monopoles are defined on the cubes of the lattice
cU(1) gauge theory on the lattice

— Finite-temperature deconfinement transition

\[
0 \quad T = T_c \quad \beta = \beta_c \quad T
\]

\[x_3 \text{ (time)} \quad x_2 \quad x_1 \text{ (space)}\]

lattice coupling

\[
\beta = \frac{1}{g^2 a}
\]

temperature

\[
T = \frac{1}{N_t a}
\]

lattice size \( N_t \times N_s \times N_s \)

lattice spacing \( a \)

continuum \( \frac{T}{g^2} = \frac{\beta}{N_t} \)

lattice
cU(1) gauge theory on the lattice

Finite-temperature deconfinement transition seen by/via monopoles

Confinement

Deconfinement

\[ T = T_c \]

\[ \beta = \beta_c \]

A BKT-type transition in three Euclidean dimensions

Low temperature

Dense gas of monopoles and anti-monopoles (surely)

High temperature

Dilute gas of magnetic dipoles (surely)

around transition

(????)
cU(1) gauge theory on the lattice

— Finite-temperature deconfinement transition seen by/via monopoles

Confinement  \( T = T_c \)  Deconfinement  \( \beta = \beta_c \)

A BKT-type transition in three Euclidean dimensions

Low temperature

Dense gas of monopoles and anti-monopoles  (surely)

High temperature

Dilute gas of magnetic dipoles  (surely)

Can we recognize the confining property?
Machine learning monopoles and confinement

Summary. The artificial neural network (ANN):

—uses the supervised learning technique to acquire knowledge about monopole configurations generated by the standard Monte-Carlo technique

—processes the monopole configurations as 3d holograms

—studies how to associate these monopole holograms with the vacuum expectation value of the Polyakov loop

—after training, uses the monopole configurations at larger-volume lattices to distinguish confinement and deconfinement phases

—neglects the renormalization effects: while the predicted Polyakov loop differs from the original order parameter, the critical inflection points are close to each other.

—the best criterion for locating the phase transition: the degree of the confusion experienced by the neural network.

the last point agrees with [1610.02048]
Machine learning monopoles and confinement

We should learn how to machine learn physical effects:
- vast diversity of different architectures
- choice of architecture depends on a specific problem (empirical)

Our objectives:
- train ANN at small lattice volumes \((Lt, Ls) = (4,16)\)
- predict for larger lattices \((Lt = 4, 6, 8, Ls = 16, 32)\):
  - the nature of the phase (confinement/deconfinement)
  - values of Polyakov loop, \(|L|\)
  - the critical temperature, \(T_c\)

Input:
- Lattice monopole configurations

Neural network:
- network: convolution + dense layers
- supervised learning technique
- 1.28M parameters … more than just fitting
Machine learning monopoles and confinement

Architecture:

\((L_1, L_2, L_3)\)

- conv 3D: 128 units
- activation: leaky ReLU (\(\alpha = 0.1\))
- batch normalisation (\(\pi = 0.9\))
- pooling 3D: max, size \([2, 4, 4]\)

\((L_{1/2}, L_{2/4}, L_{3/4}, 128)\)

- conv 3D: 256 units
- activation: leaky ReLU (\(\alpha = 0.1\))
- batch normalisation (\(p = 0.9\))

\((L_{1/2}, L_{2/4}, L_{3/4}, 256)\)

- global pooling: max
- dropout (\(p = 0.25\))

\((256)\)

- dense: 256 units
- activation: ReLU

\((256)\)

- dense: 128 units
  - activation: ReLU
  - dropout: \(p = 0.5\)

\((128)\)

- dense: 1 unit
  - activation: sigmoid

\(p(\phi)\)

- \(|L|, \text{Re } L, \text{Im } L\)

- dense: 3 units
  - activation: none

- dense: 1 unit
  - activation: none

- \(\rho\)

(de)confinement

Polyakov loop

Monopole characteristics
Machine learning monopoles and confinement

Architecture:

- vast diversity of different architectures
- choice of architecture depends on a specific problem (empirical)

https://xkcd.com/1838
Machine learning monopoles and confinement

Classifying the phases using the monopole configurations

\( \beta \)

1.5

1.6

1.7

1.8

1.9

confinement

\( \beta \)

2.0

2.1

2.2

2.3

2.35

deconfinement

\( \beta_c \)
Machine learning monopoles and confinement

How fast does this ANN learn?

Training curve

Epoch = A full “training course" using the full dataset

Learning curve

Uses the Adam optimization algorithm (an extension to stochastic gradient descent)

training: about 2000 configurations
validation: 200 configurations
Machine learning monopoles and confinement

The neural network was trained at a small volume and asked to make predictions at larger volumes (never seen configurations).

Predicting the value of the Polyakov loop and the phase

- (a) $6 \times 16^2$ – real
- (b) $6 \times 16^2$ – predicted
- (c) $8 \times 32^2$ – real
- (d) $8 \times 32^2$ – predicted
Machine learning monopoles and confinement

Predicting the value of the Polyakov loop and the monopole density

(c) $6 \times 16^2$

(d) $6 \times 32^2$

Predicting the critical temperature

Locating the phase transition by the degree of the confusion experienced by the neural network
Machine learning monopoles and confinement

Summary again:

— the neural network uses the supervised learning technique to make reasonable predictions about the phase diagram

— we learned that the network may learn about the confinement.

— we did not ask yet “how?” It’s, however, possible.

— after a successful training, one may ask the neural network what exactly it learned to distinguish the phases.

  - What the most considerable weight corresponds to?

  = How the decision is made? (check the “decision function”)

— the task for the next steps + generalization to SU(N) Yang-Mills.
Learning physics from “unphysics”

Motivation: we know very-well a result at an unphysical or not-so-interesting point, but we want to get some information about a physical/interesting point.

Example: finite baryonic chemical potential in QCD

Important feature: de-noising (technically) or renormalization (physically). The neural network removes uninteresting UV fluctuations and leaves only non-perturbative physics → the Polyakov loop in compact electrodynamics
Learning physics from “unphysics”

Simplified example: lattice Yang-Mills at strong coupling

[D. Boyda, N. Gerasimenyuk, V. Goy, S. Lyubimov, A. Molochkov, M.C., to appear]

Input: We know the value of the order parameter at unphysical coupling(s)
- bad version No. 1: lattice Yang-Mills at very strong coupling, no relation to the continuum limit
- bad version No. 2: lattice Yang-Mills at very weak coupling, purely perturbative finite-volume physics

Output: We want to know the value of the order parameter for any value of the coupling including the scaling region in lattice Yang-Mills theory

We take the bad choice No. 2:
SU(N_c) gauge theory on the lattice with \( \beta=4 \) (for \( N_c=2 \)) and \( \beta=10 \) (for \( N_c=3 \)); on the lattices with spatial extensions \( N_s=8,16,32 \)

Our choices are really very bad: physical spatial lattice size is \( \sim 0.01 \) fm.

P.S. We also checked that a good ANN can treat the bad choice No. 1 very well as well.
Learning physics from “unphysics”

Architecture of the neural network

<table>
<thead>
<tr>
<th>Layer</th>
<th>Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>InputLayer</td>
<td>In $(N_t = 4, Ns \times Ns, Ns, Dim \times Mtx)$</td>
</tr>
<tr>
<td></td>
<td>Out $(N_t = 4, Ns \times Ns, Ns, Dim \times Mtx)$</td>
</tr>
<tr>
<td>Conv3D</td>
<td>In $(4, Ns \times Ns, Ns, Dim \times Mtx)$</td>
</tr>
<tr>
<td></td>
<td>Out $(2, Ns \times Ns, Ns, 256)$</td>
</tr>
<tr>
<td>Conv3D</td>
<td>In $(2, Ns \times Ns, Ns, 256)$</td>
</tr>
<tr>
<td></td>
<td>Out $(1, Ns \times Ns, Ns, 32)$</td>
</tr>
<tr>
<td>AveragePooling3D</td>
<td>In $(1, Ns \times Ns, Ns, 32)$</td>
</tr>
<tr>
<td></td>
<td>Out $(1, 1, 1, 32)$</td>
</tr>
<tr>
<td>Flatten</td>
<td>In $(1, 1, 1, 32)$</td>
</tr>
<tr>
<td></td>
<td>Out $(32)$</td>
</tr>
<tr>
<td>Dense</td>
<td>In $(32)$</td>
</tr>
<tr>
<td></td>
<td>Out $(1)$</td>
</tr>
</tbody>
</table>

Example: Architecture of the artificial neural network for the Polyakov Loop prediction in the SU(2)/SU(3) gauge theory with the lattice temporal size $N_t = 4$.

Input: raw configuration of SU(N) gauge field.

Hidden layers

Output: expectation value of the Polyakov loop

Train in the unphysical region:
known value of the Polyakov loop for a set of SU(N) configurations at unphysically small lattices ~$(0.01 \text{ fm})^3$
Learning physics from “unphysics”

Results:

The neural network is able to find a “proper expression” of the order parameter in the unphysical point. We restore it in the whole parameter space, including the transition region.

*) preliminary, to be beautified later
Future developments (very briefly)

Use artificial neural network, together with Monte Carlo to find

— gluonic field configurations responsible for color confinement in Yang-Mills theory.

— QCD endpoint at real baryonic chemical potential.