Classifying Topological Sector via Machine Learning

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MK, Kohno, Matsumoto, to appear

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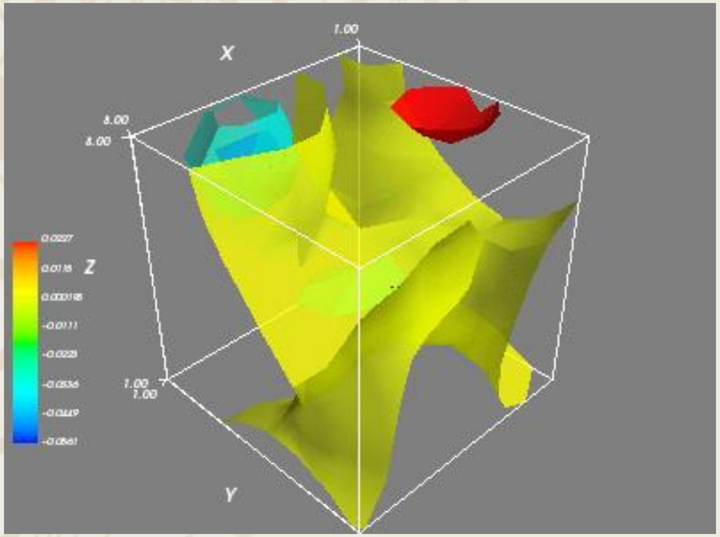
Topological Charge in YM Theory

$$Q = \int d^4x q(x) \quad \text{: integer}$$

$$q(x) = -\frac{1}{32\pi^2}\mathrm{tr}[F_{\mu\nu}\tilde{F}_{\mu\nu}]$$

q(x) in SU(3) YM,
β=5.8, 8^4, t/a^2=2.0



- **Interests / applications**
  - Instantons
  - Axial U(1) anomaly
  - Axion cosmology
  - Topological freezing

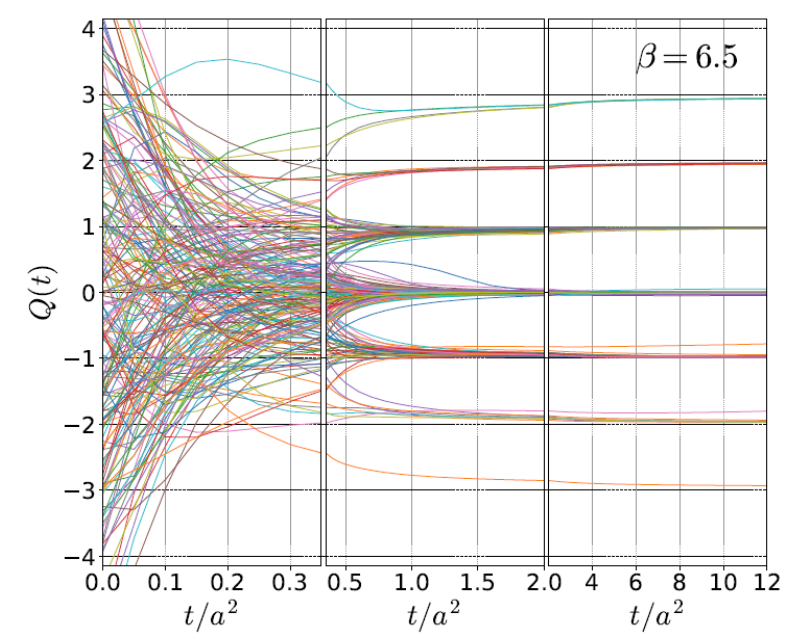
Topology on the Lattice

- Distinct topological sectors on sufficiently fine lattices

Luscher, 1981

- Definitions of Q on the lattice:
  - fermionic: Atiyah-Singer index theorem
  - gluonic: q(x) after smoothing
    - cooling, smearing
    - **gradient flow**

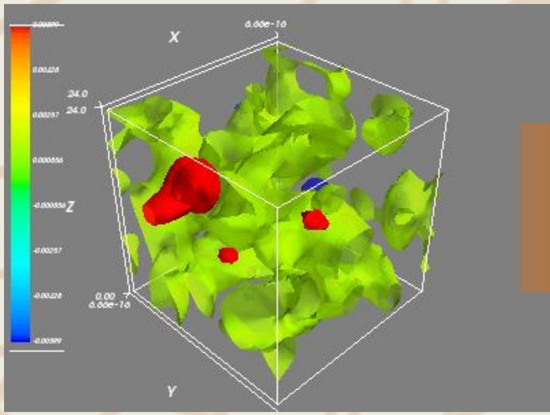
Luscher, Weisz, 2011



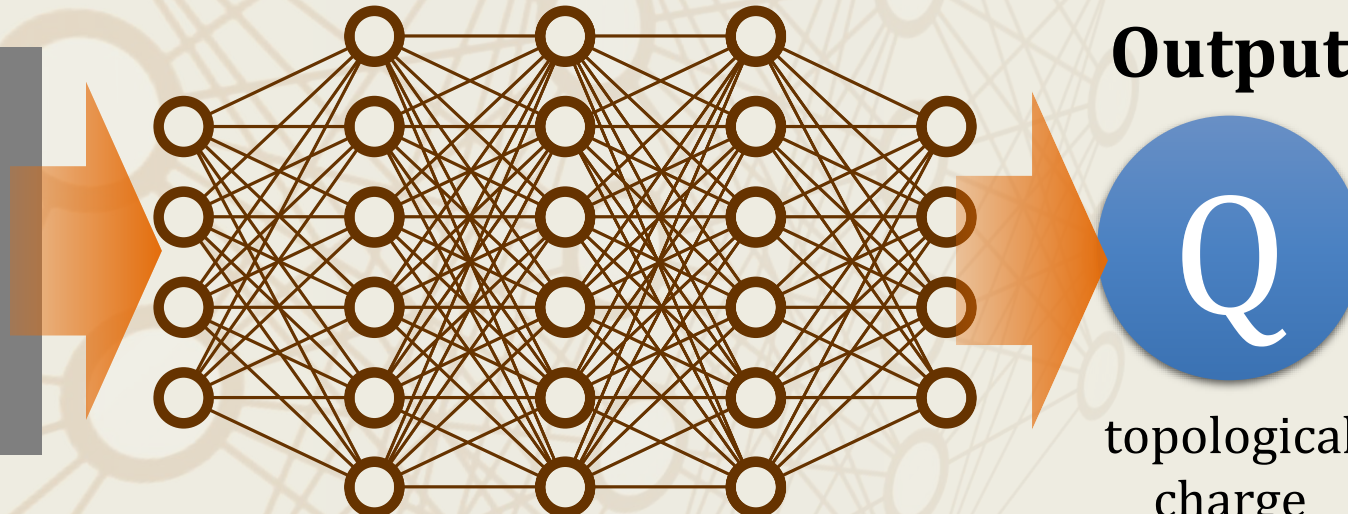
- Good agreement b/w various definitions
- **Faster algorithm is desirable!**

Machine Learning

Input: q(x)



4-dimensional field



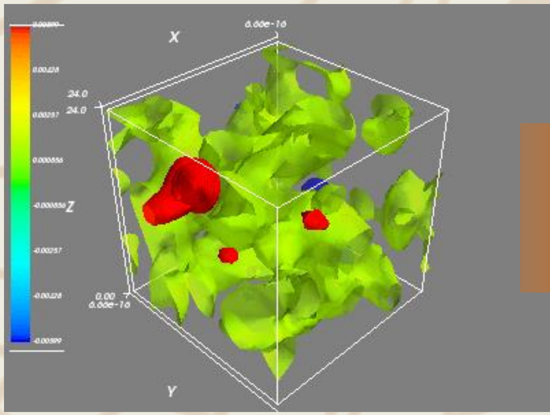
Output

topological
charge

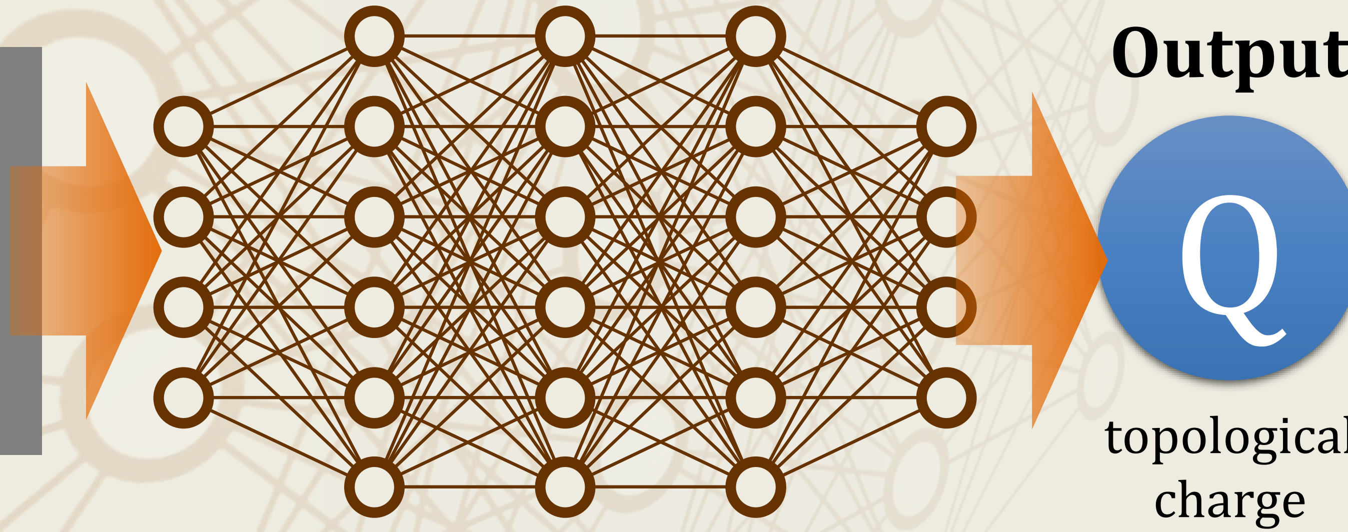
- **Capture "instanton"-like structure?**
- **Acceleration of the analysis of Q?**

Machine Learning

Input: q(x)



4-dimensional field



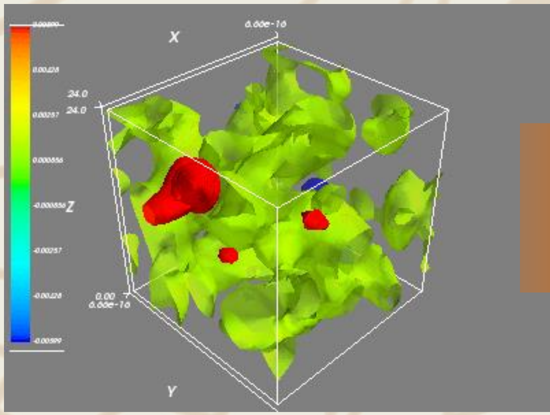
Output

topological charge

- **Capture "instanton"-like structure?** 
- **Acceleration of the analysis of Q?** 

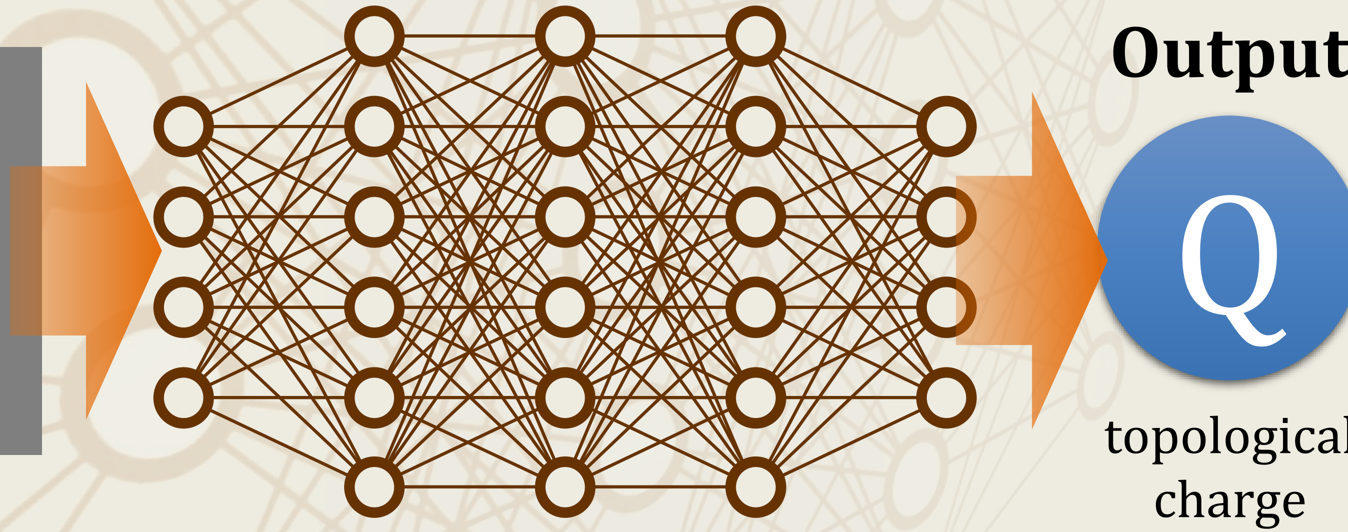
Machine Learning

Input: q(x)



4-dimensional field

Output



topological charge

- **Why q(x) rather than link variables?**
  - to reduce the input data
  - to skip teaching SU(N) and gauge invariance

Lattice Setting

- **SU(3) Yang-Mills**
- **Wilson gauge action**
- 2 lattice spacings with **same physical volume**
- $LT_c \sim 0.63$
- $\langle Q^2 \rangle \simeq 1.1$

- **Gradient flow** for smoothing

β	N^4	N_{conf}
6.2	16^4	20,000
6.5	24^4	20,000

20,000 confs. in total

Training: 10,000

Validation: 5,000

Test: 5,000

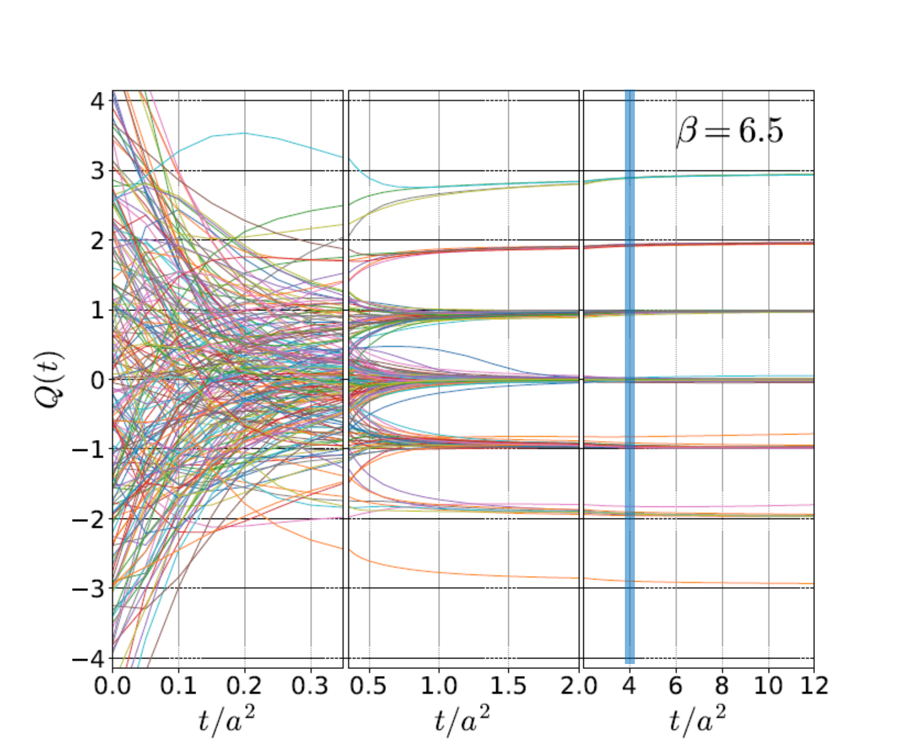
distribution of Q

Q	-5	-4	-3	-2	-1	0	1	2	3	4	5
$\beta = 6.2$	2	17	235	1325	4571	7474	4766	1352	240	18	0
$\beta = 6.5$	0	5	105	1080	4639	8296	4621	1039	202	13	0

Neural Network Setting

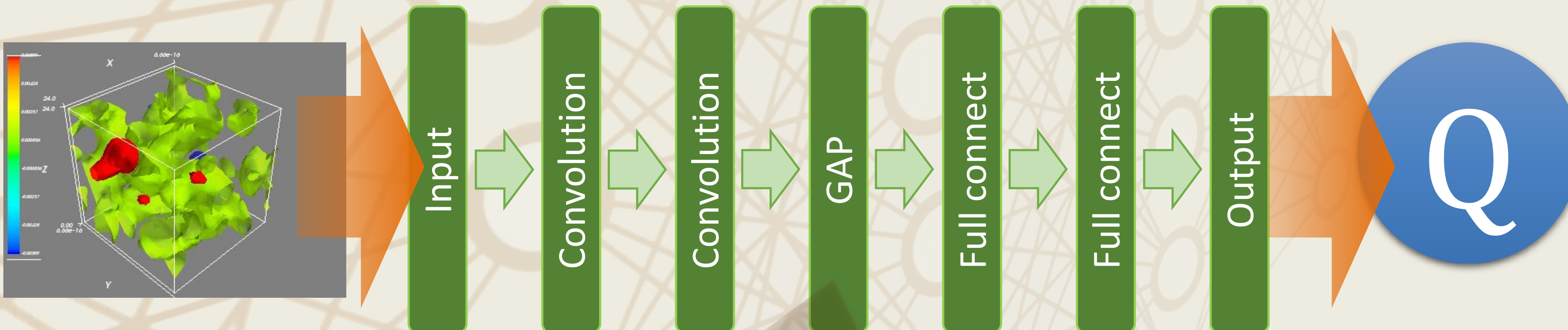
- convolutional neural network by **CHAINER framework**
- supervised learning
- convolutional layer: 4-dim., periodic BC
- regression analysis / round off to obtain integer
- activation: logistic

- answer of Q
  - Q(t) @ t/a^2=4.0
  - round off



Trial 1: Topol. Charge Density

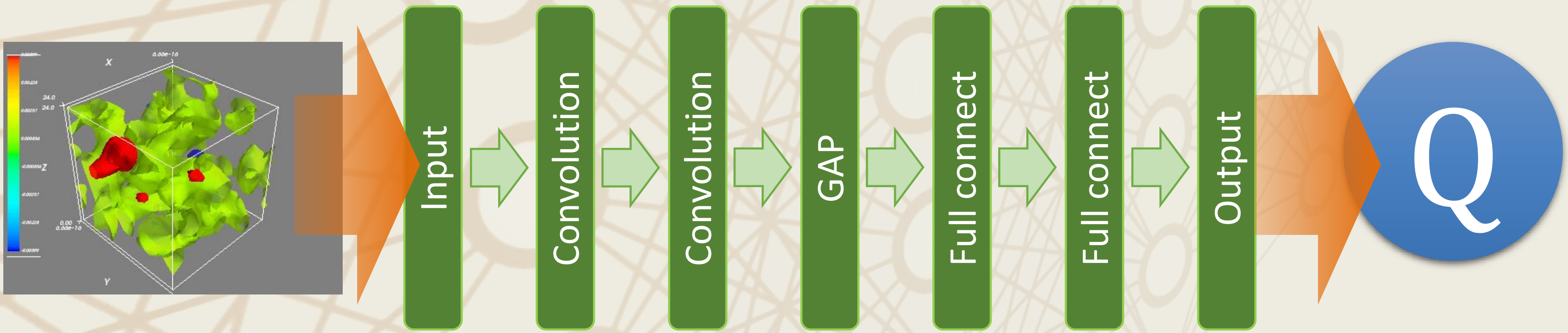
- Input: q(x) in 4-dim space
- Data reduction to 8^4 (average pooling)



GAP=Global Average Pooling
Translational invariance is respected in this NN.

Trial 1: Topol. Charge Density

- Input: q(x) in 4-dim space
- Data reduction to 8^4 (average pooling)



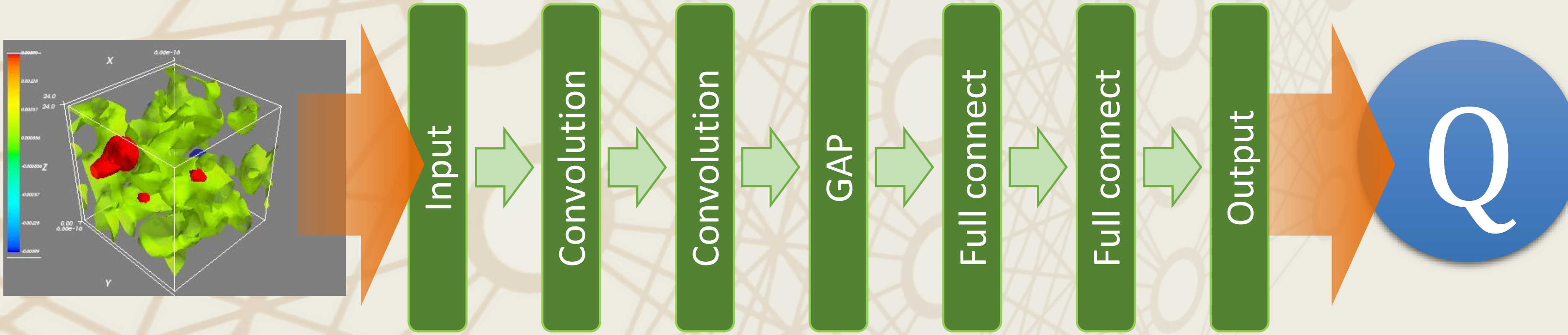
- **Result: best accuracy for β=6.2: 37.0%**

Accuracy of each topological sector (%)

Q	-4	-3	-2	-1	0	1	2	3	4	total
$t/a^2=0$	0	0	0	0	37.2	0	0	0	0	37.0

Trial 2: Topol. Density @ t>0

- Input: $q(x,t)$ in 4-dim space at nonzero flow time
- Data reduction to 8^4 (average pooling)



Accuracy of each topological sector (%)

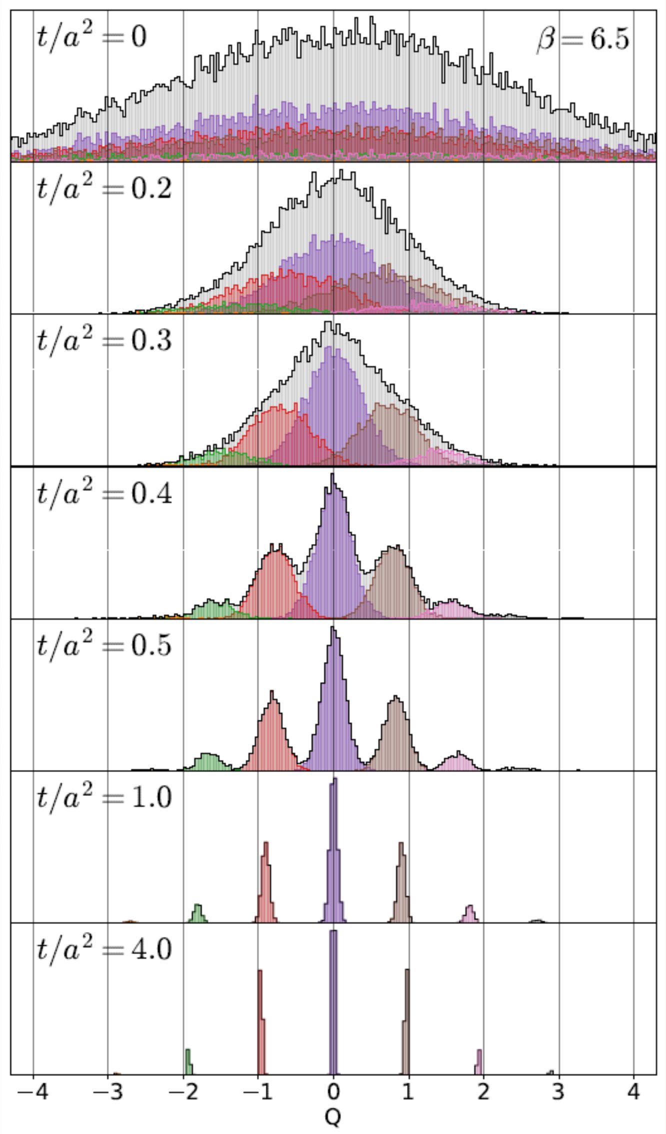
Q	-4	-3	-2	-1	0	1	2	3	4	total
$t/a^2=0$	0	0	0	0	37.2	0	0	0	0	**37.0**
$t/a^2=0.1$	0	0	31.6	39.1	41.4	38.9	19.0	0	0	**40.3**
$t/a^2=0.2$	0	40.0	46.4	53.8	55.9	52.3	48.1	50.0	0	**53.7**
$t/a^2=0.3$	0	91.3	72.9	76.3	79.0	74.8	68.1	70.0	50.0	**76.1**

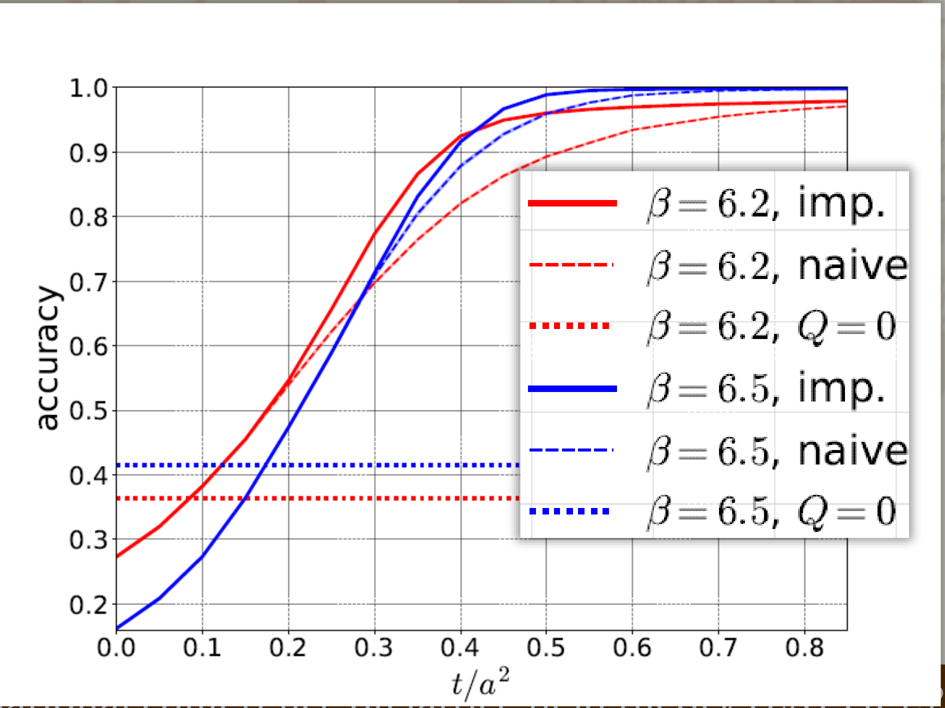
Benchmark

□ Simple estimator from Q(t)

1) Naïve: $Q = \mathrm{round}[Q(t)]$
2) Improved: $Q = \mathrm{round}[cQ(t)]$
c>1: optimization param.
3) zero: $Q = 0$

Distribution of Q(t)





Comparison: NN vs Benchmark

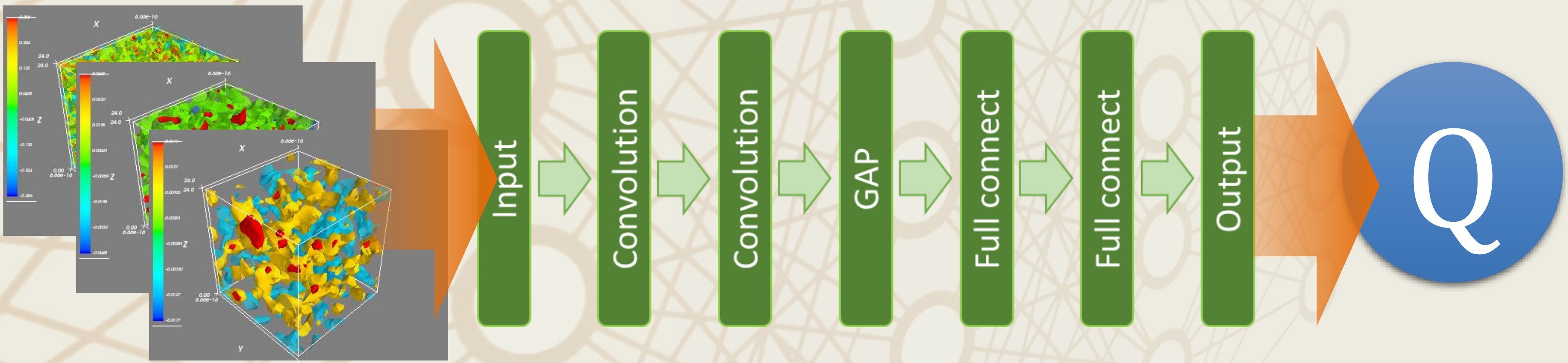
accuracy at β=6.2

	ML (Trial 2)	naïve	improved
$t/a^2=0$	37.0	27.3	27.3
$t/a^2=0.1$	40.3	38.3	38.3
$t/a^2=0.2$	53.7	54.0	54.6
$t/a^2=0.3$	76.1	69.8	77.3

- Machine learning cannot exceed the benchmark value.
- NN would be trained to answer the “improved” value.
- **No useful local structures found by the NN.**

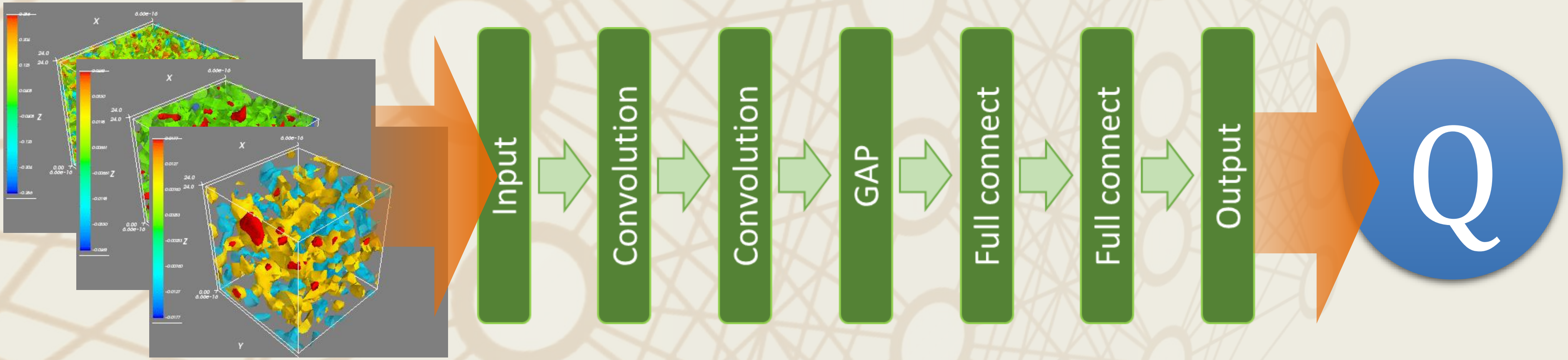
Trial 3: Multi-Channel Analysis

- Input: q(x,t) in four-dimensional space **at t/a^2=0.1, 0.2, 0.3**



Trial 3: Multi-Channel Analysis

- Input: q(x,t) in four-dimensional space **at t/a^2=0.1, 0.2, 0.3**



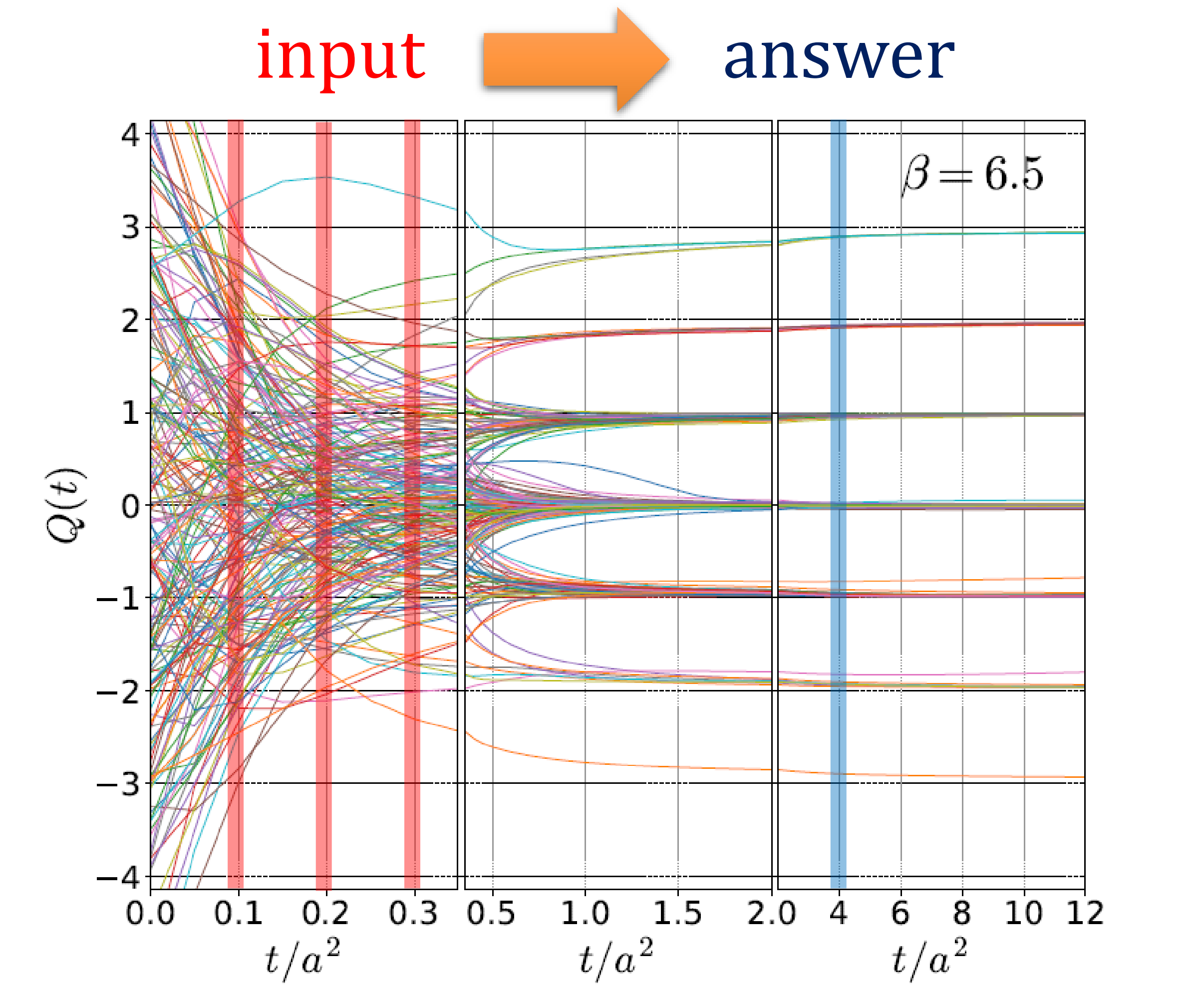
- **Result**

machine learning | benchmark @ t/a^2=0.3

	machine learning	benchmark @ t/a^2=0.3
β=6.2	**93.8**	77.3
β=6.5	**94.1**	71.3

- **non-trivial improvement from the benchmark!!**

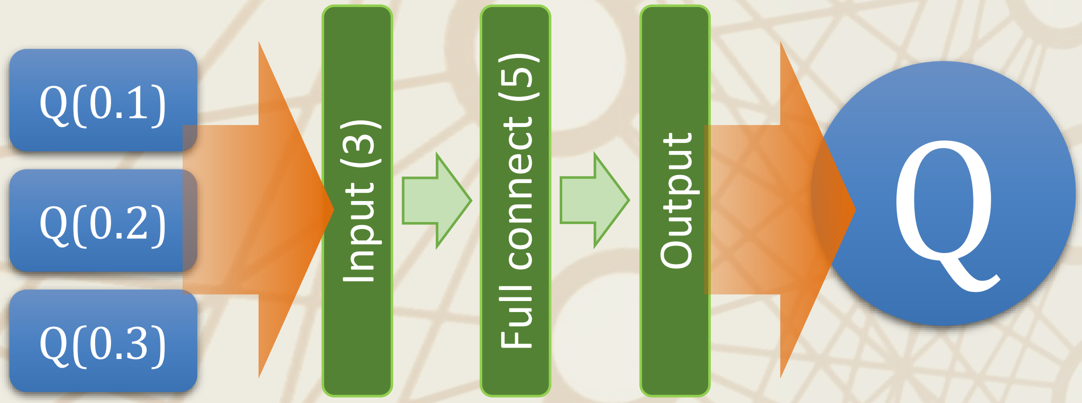
Is this a non-trivial result?

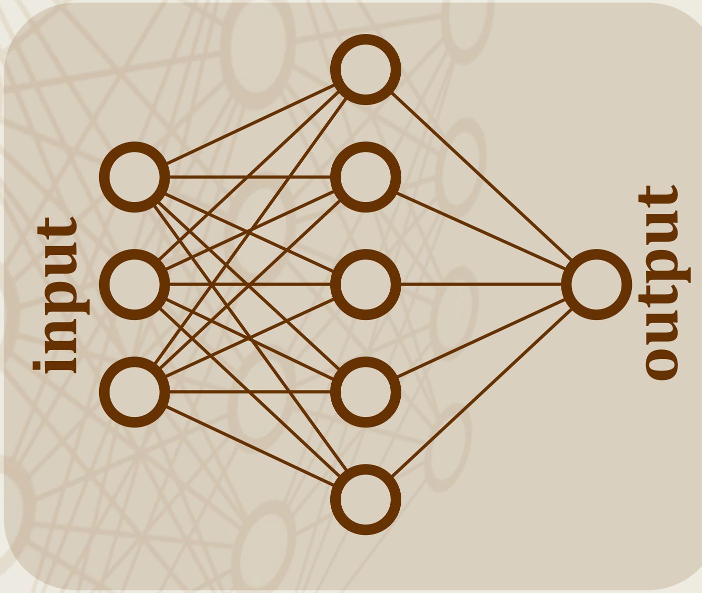


We can estimate the answer from Q(t) by our eyes…

Trial 4: Feed Q(t) [0-dim]

- Input: Q(t) at t/a^2=0.1, 0.2, 0.3





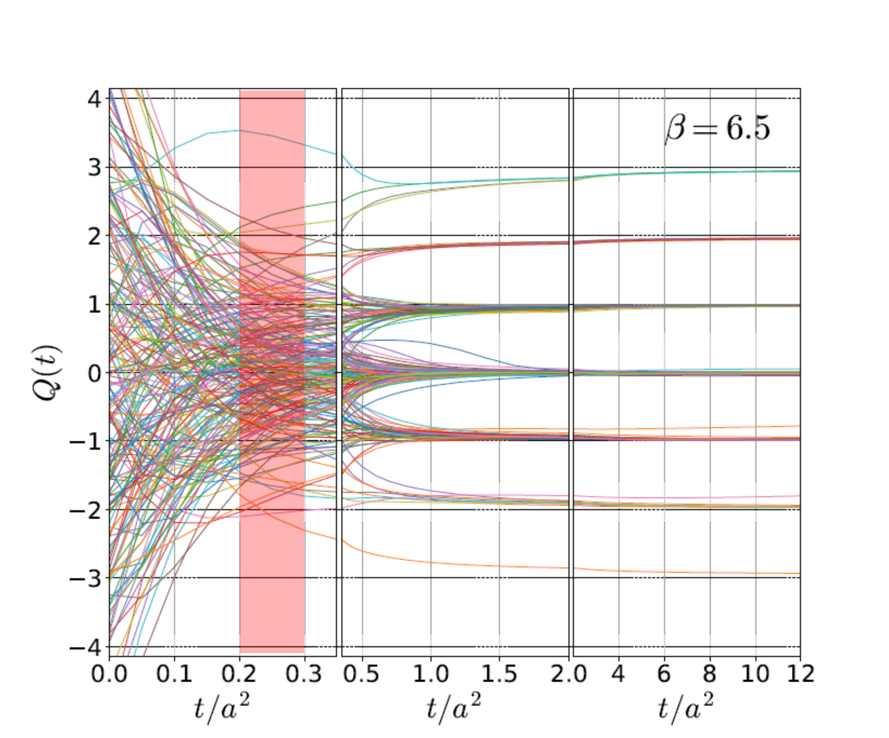
- **Result**

	Q(t)	Trial 3 (4dim)	benchmark
β=6.2	**95.5**	93.8	77.3
β=6.5	**95.7**	94.1	71.3

- Good accuracy is obtained only from Q(t)

Using different flow times

t/a^2	β=6.2	β=6.5
0.3, 0.25, 0.2	**95.9(2)**	**99.0(2)**
0.3, 0.2, 0.1	95.5(2)	95.7(2)
0.25, 0.2, 0.15	95.1(3)	95.0(2)
0.2, 0.15, 0.1	86.9(3)	83.1(4)
0.2, 0.1, 0	75.6(5)	68.2(4)
0.15, 0.1, 0.05	71.8(4)	65.2(4)
0.1, 0.05, 0	54.8(5)	49.9(3)



- t/a^2=0.3, 0.25, 0.2 gives the best accuracy.
- Better accuracy on the finer lattice.
- More than three t values do not improve accuracy.
  - error: variance in 10 independent trainings

Reducing the Training Data

- Smaller training data will reduce numerical cost for the training.

Training data	10,000	5,000	1,000	500	100
β=6.2	**95.9(2)**	**95.9(2)**	**95.9(2)**	95.5(3)	90.3(7)
β=6.5	**99.0(2)**	**99.0(2)**	**98.9(2)**	98.9(1)	90.2(8)

- 1000 configurations are enough to train the NN successfully!
- Numerical cost for the training is small.

Versatility

- Analyze configurations with a different parameter set

training data	analyzed data: β=6.2	analyzed data: β=6.5
β=6.2	95.9(2)	98.6(2)
β=6.5	95.6(2)	99.0(2)

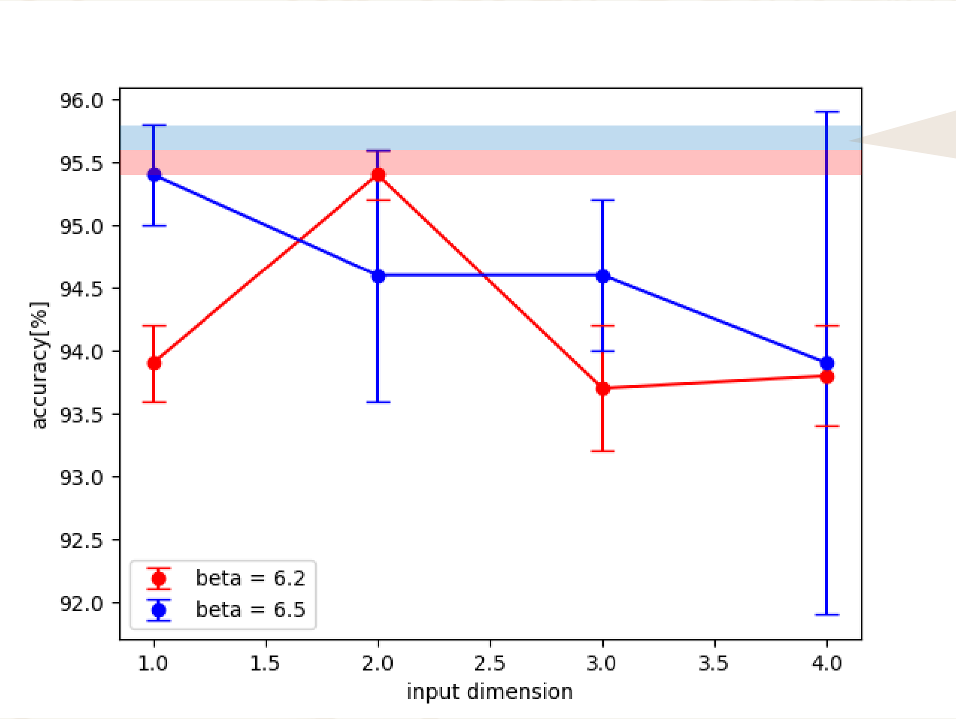
- NNs trained for β=6.2 and 6.5 can be used for another parameter successfully.
- **Universal NN would be developed!**
- Note: same physical volume

Trial 5: Dimensional Reduction

- Optimal dimension between d=0 and 4?
- d-dimensional CNN
- Input: $q_d(x)$ after dimensional reduction
- 3-channel analysis: t/a^2=0.1, 0.2, 0.3

$$q_3(x,y,z) = \int d\tau q(x)$$

$$q_2(x,y) = \int d\tau dz q(x)$$



Accuracy of Trial 4

Summary and Outlook

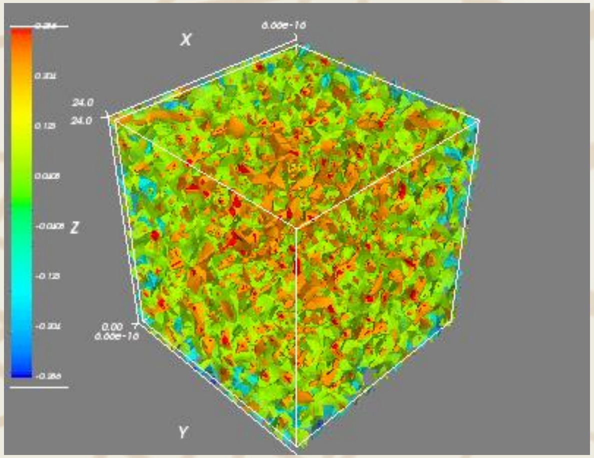
- **Topological charge can be estimated with high accuracy from Q(t) at $0.2<t/a^2<0.3$ with the aid of the machine learning technique.**
- On the finer lattices, the better accuracy.
- Applications: checking topological freezing, etc.

- No local structure captured by NN
- No "Instanton"-like structure? Or too noisy data?

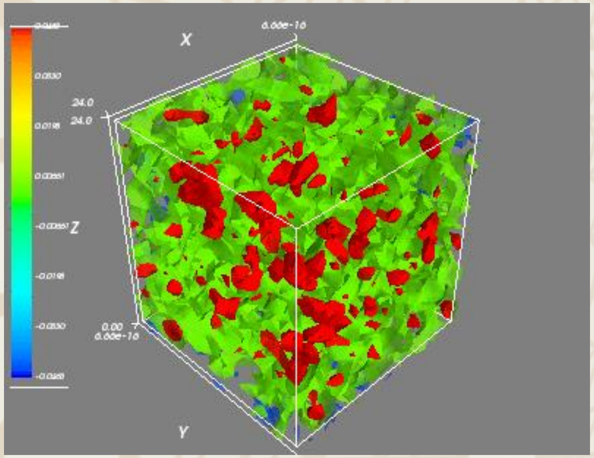
- Future Study
  - Continuum limit / volume dependence
  - High T configurations where DIGA is valid

Topological Charge Density

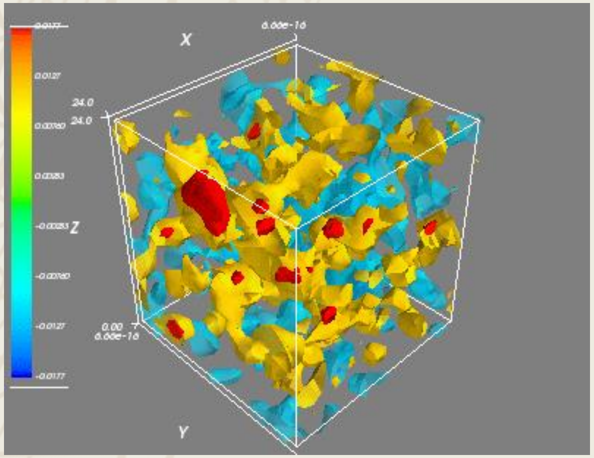
$t/a^2 = 0.1$



$t/a^2 = 0.2$



$t/a^2 = 0.3$



No isolated instanton structure…

backup

Details of NN

Trial 1~3

Layer	Filter size	Output size	Activation
input		$8^4 \times 1$	
convolution	$3^4 \times 5$	$8^4 \times 5$	Logistic
convolution	$3^4 \times 5$	$8^4 \times 5$	Logistic
average pooling	$8^4 \times 1$	5×1	
full connect		5	Logistic
full connect		1	

Trial 4

Layer	Output size	Activation
input	3	
full connect	5	Logistic
full connect	1	

Trial 5

Layer	Filter size	Output size	Activation
input		$12^d \mathrm{or} 8^d \times 3$	
convolution	$3^d \times 5$	$12^d \mathrm{or} 8^d \times 5$	Logistic
convolution	$3^d \times 5$	$12^d \mathrm{or} 8^d \times 5$	Logistic
convolution	$3^d \times 5$	$12^d \mathrm{or} 8^d \times 5$	Logistic
average pooling	$12^d \mathrm{or} 8^d \times 1$	5×1	
full connect		5	Logistic
full connect		1