Estimation of the Lattice QCD Observables using Machine Learning

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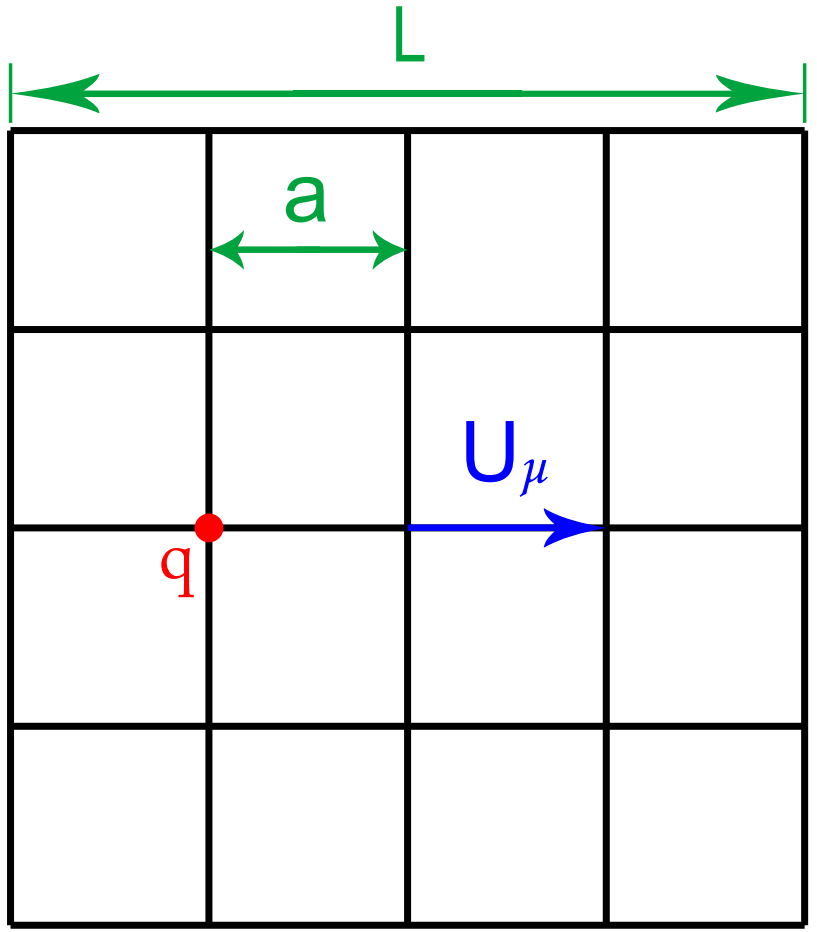
Outline

1. Lattice QCD
2. Machine learning (ML) on Lattice QCD observables (statistical data)
3. Correction of the Prediction Bias
4. Applications
5. ML regression on D-Wave quantum annealer

Lattice QCD

- Non-perturbative approach to understand QCD
- Formulated on discretized Euclidean space-time
  - Hypercubic lattice
  - Lattice spacing a
  - Quark fields placed on sites
  - Gauge fields on the links between sites; U_μ



Lattice QCD

- Correlation functions

$$\langle O \rangle = Z^{-1} \int dU dq d\bar{q}\, O(U, q, \bar{q}) e^{-S_g - \bar{q}(D+m_q)q}$$

$$= Z^{-1} \int dU \left[O\left(U, (D+m_q)^{-1}\right) e^{-S_g} \det(D+m_q) \right]$$

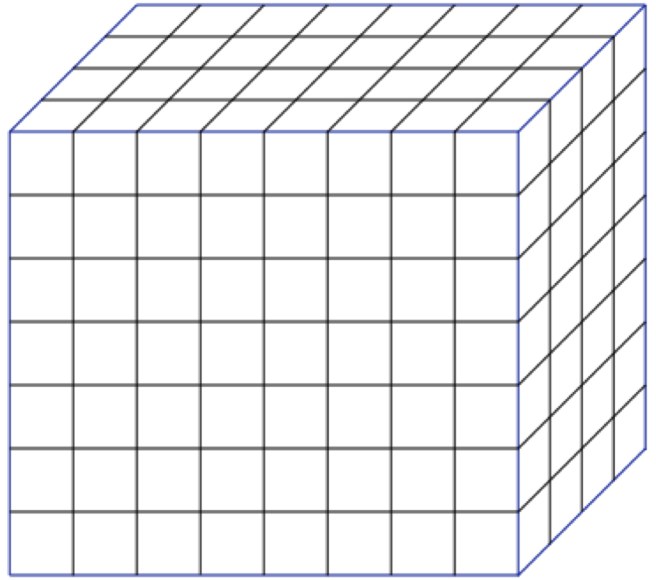
- Monte-Carlo integration
  - Integration variable U is huge

$$N_s^3 \times N_t \times 4 \times 8 \sim 10^9$$

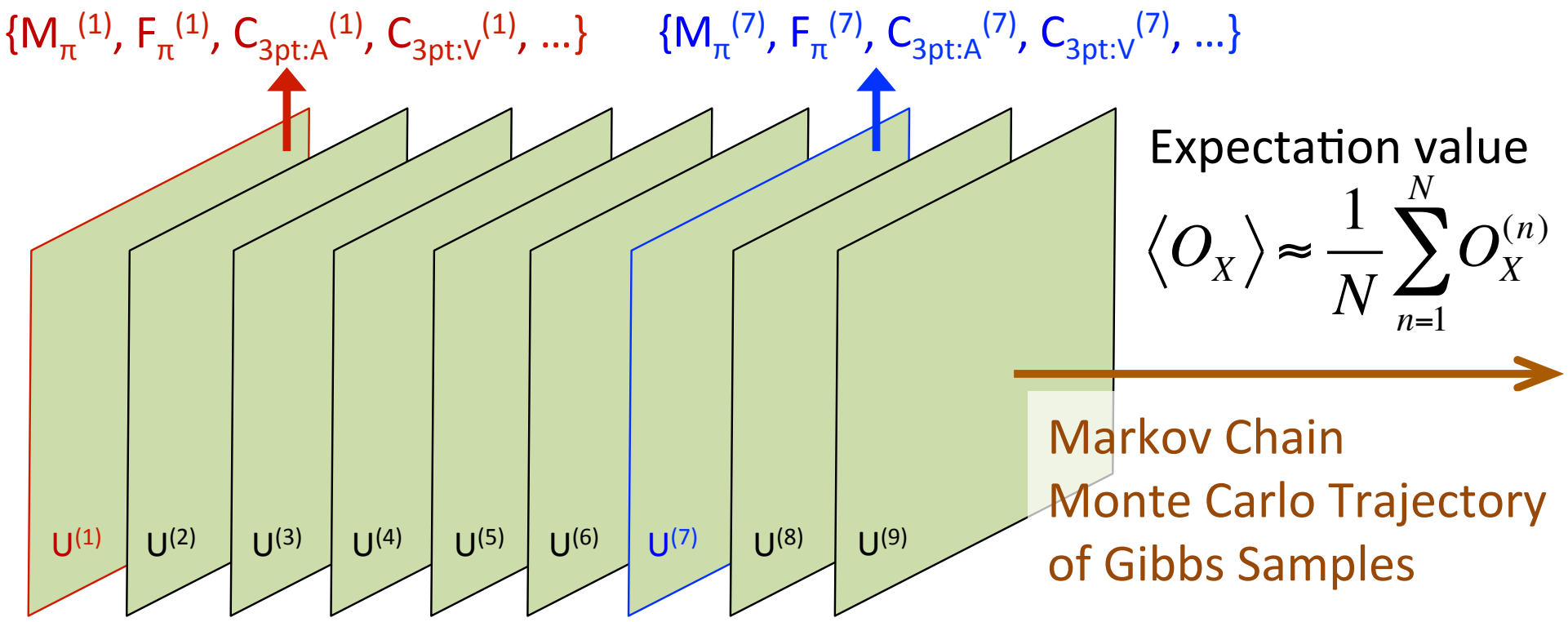
  - Generate Markov chain of gauge configurations U
  - Calculate average as expectation value

$$\langle O \rangle \approx \frac{1}{N} \sum_i O_i \left(U, (D+m_q)^{-1}\right)$$

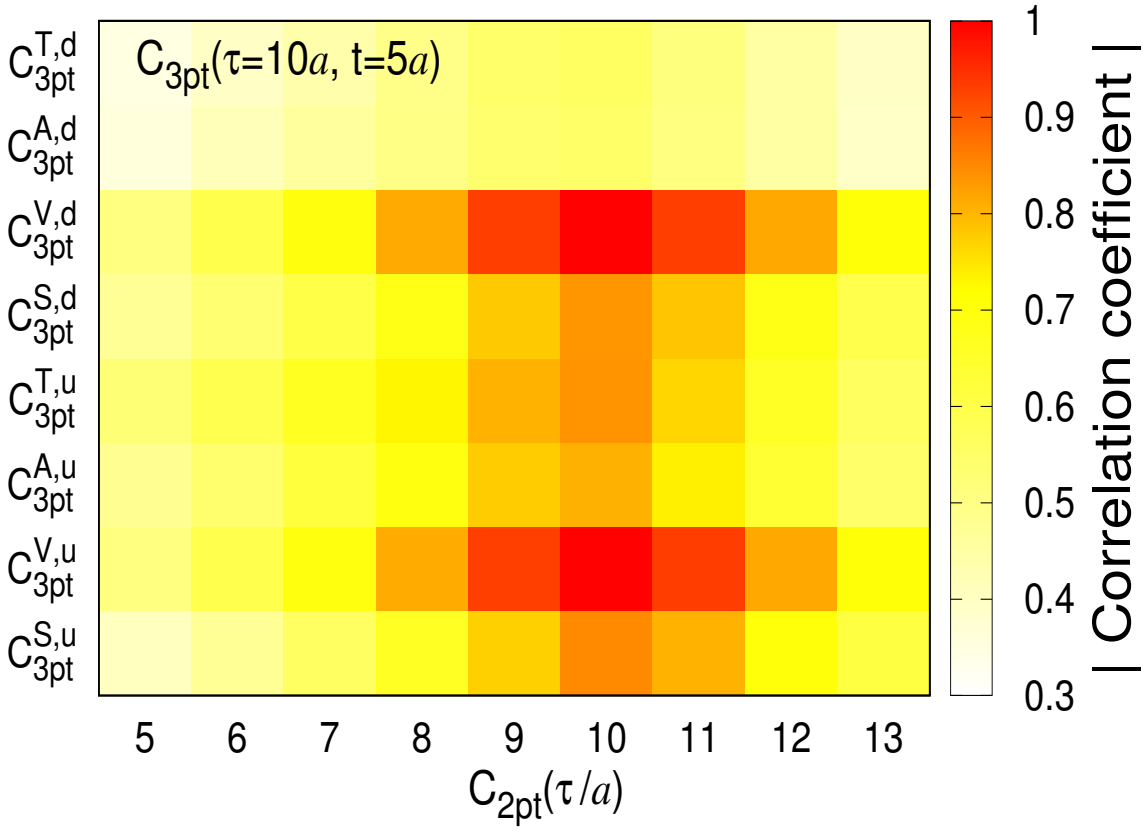
  - Calculation of $O_i \left(U, (D+m_q)^{-1}\right)$: measurement
  - $(D+m)^{-1}$ is computationally expensive



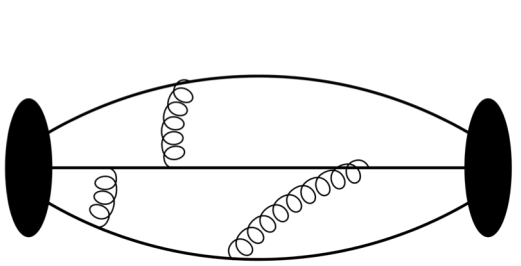
Lattice QCD Observables are Correlated

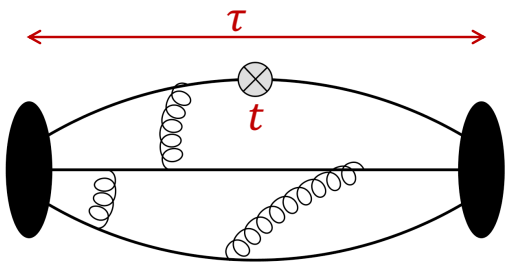


Correlation Map of Nucleon Observables



- Correlation between proton(uud) 3-pt and 2-pt correlation functions





$C_{2pt} \sim \langle N(\tau)N^{\dagger}(0)\rangle$ $C_{3pt}^{A,S,T,V} \sim \langle N(\tau)O(t)N^{\dagger}(0)\rangle$

- Using these correlations, C_{3pt} can be estimated from C_{2pt} on each configuration

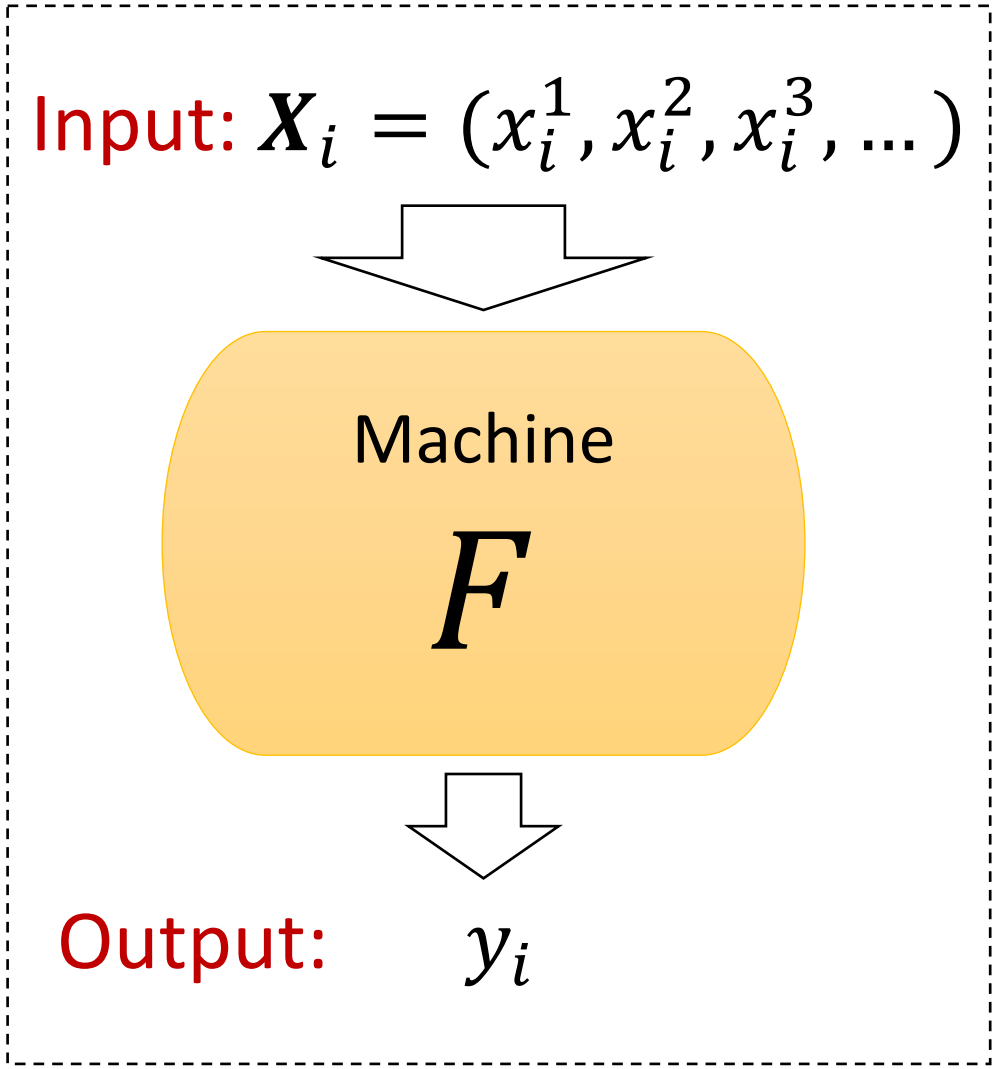
Machine Learning on Lattice QCD Observables

Machine Learning

- One can consider the machine learning (ML) process as a data fitting
- The machine F has very general fitting functional form with huge number of free parameters
- The free parameters are determined from large number of training data:

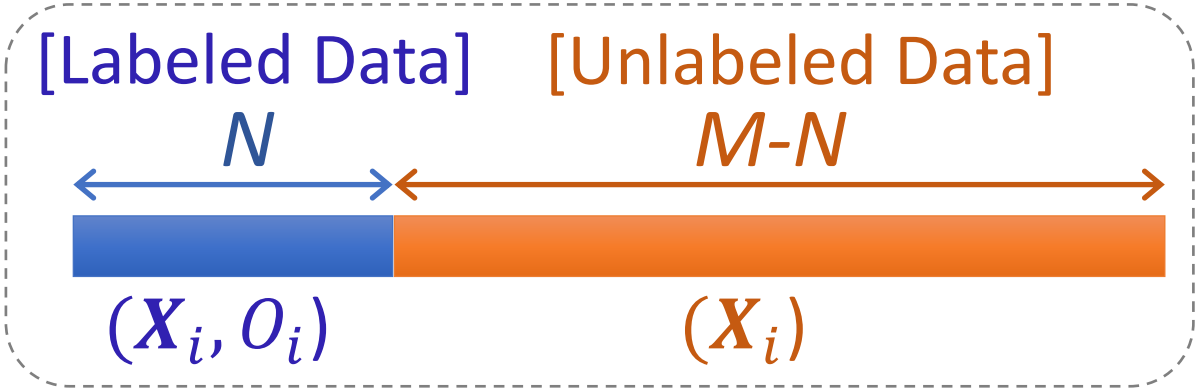
$$F(\boldsymbol{X}_i) \approx y_i$$

- For example,
  $\boldsymbol{X}_i$: pixels of a picture
  y_i : "***cat***" or "***dog***"



Machine Learning on Lattice QCD Observables

- Assume *M* indep. measurements
- Common observables $\boldsymbol{X}_i$ on all *M*
  Target observable O_i on first *N*



1) **Train** machine ***F*** to yield O_i from $\boldsymbol{X}_i$
on the Labeled Data

2) **Predict** O_i of the Unlabeled data from $\boldsymbol{X}_i$

$$\boldsymbol{F}(\boldsymbol{X}_i) = O_i^P \approx O_i$$

Input: $\boldsymbol{X}_i = (o_i^1, o_i^2, o_i^3, \dots)$

Machine

$\boldsymbol{F}$

Output: O_i

Prediction Bias

- $\boldsymbol{F}(\boldsymbol{X}_i) = O_i^P \approx O_i$
- Simple average

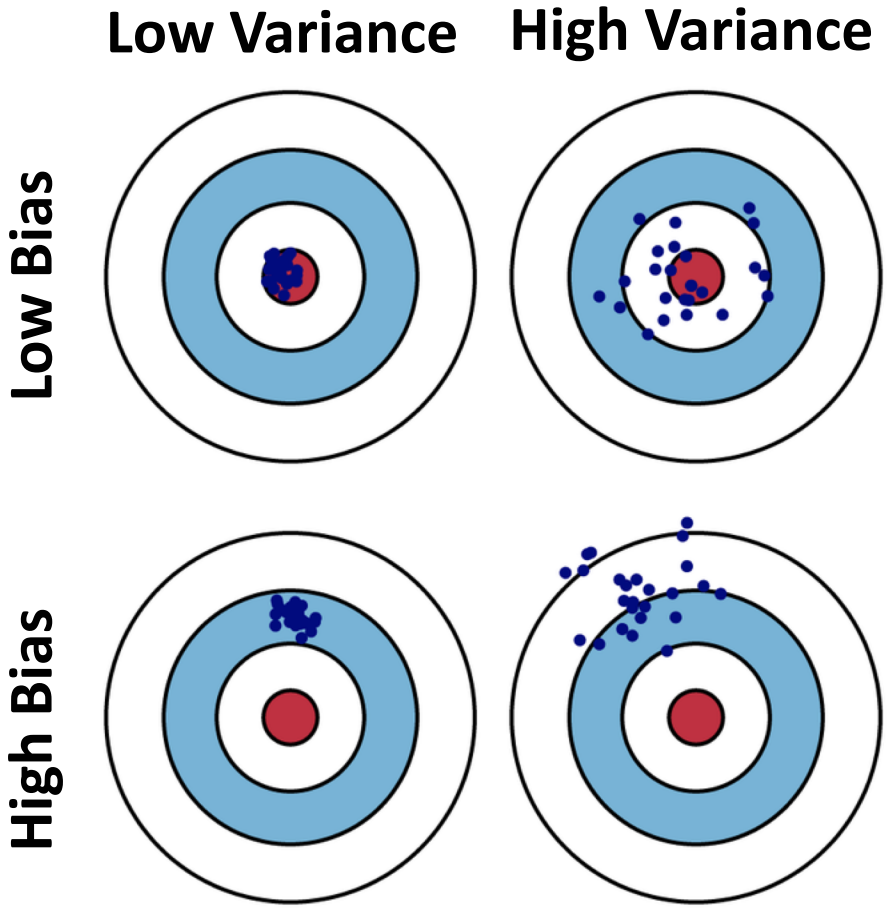
$$\overline{O} = \frac{1}{M-N} \sum_{i \in \text{Unlabeled}} O_i^P$$

  is not correct due to prediction bias

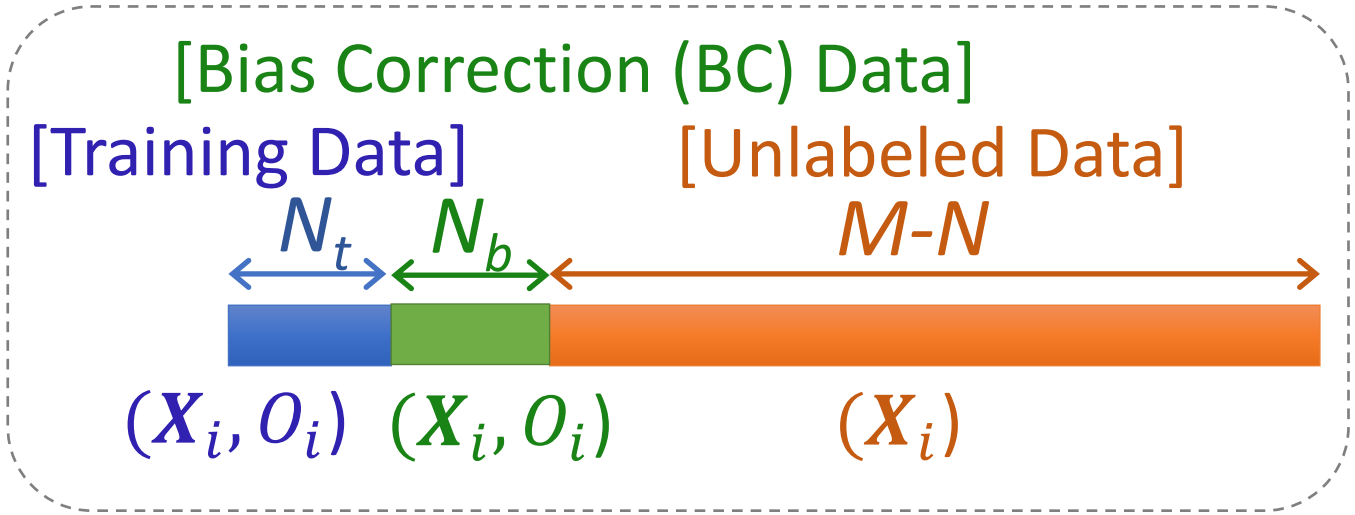
- Prediction = TrueAnswer + Noise + Bias
- ML prediction may have bias

$$\langle O_i^P \rangle \neq \langle O_i \rangle$$

$$\text{Bias} = \langle O_i^P \rangle - \langle O_i \rangle$$



Bias Correction



- Split labeled data $N = N_t + N_b$
- Average of predictions on test data with bias correction

$$\overline{O} = \frac{1}{M-N} \sum_{i \in \text{Unlabeled}} O_i^P + \frac{1}{N_b} \sum_{i \in BC} \left(O_i - O_i^P \right)$$

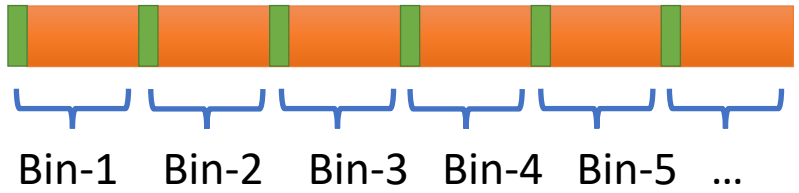
- Expectation value, $\langle \overline{O} \rangle = \langle O_i^P \rangle + \langle O_i - O_i^P \rangle = \langle O_i \rangle$
- BC term converts systematic error of prediction to statistical uncertainty

Incorporating Labeled Data

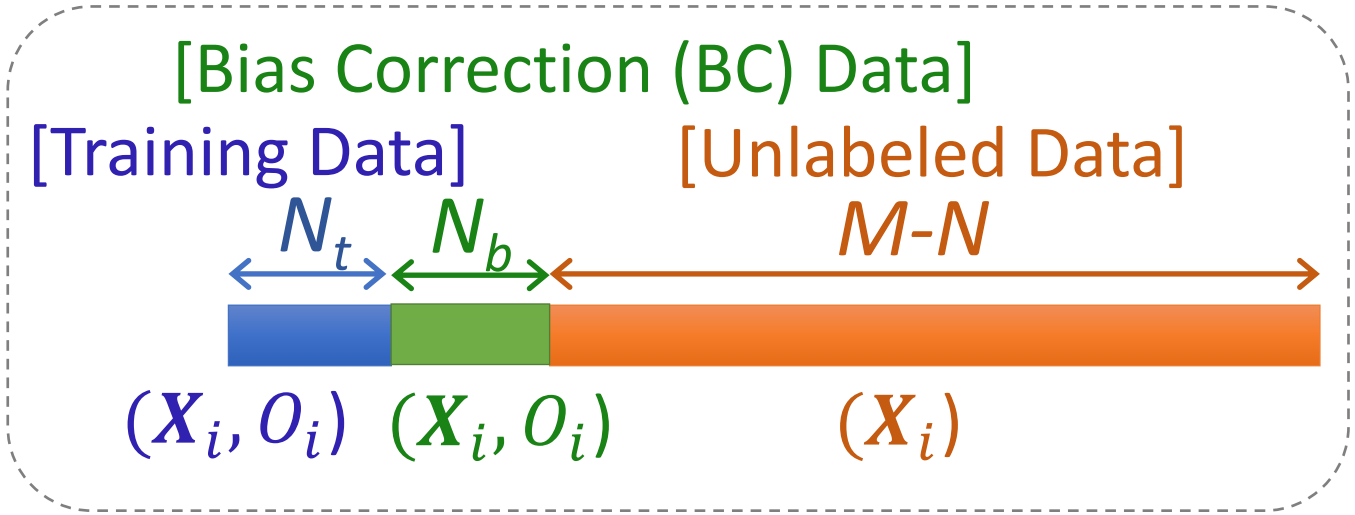
- Include directly measured values O_i from labeled data

$$\overline{O}^{\text{imp}} = w_1 \times \left(\frac{1}{N} \sum_{i \in \text{Labeled}} O_i \right) + w_2 \times \left(\frac{1}{M-N} \sum_{i \in \text{Unlabeled}} O_i^P + \frac{1}{N_b} \sum_{i \in BC} \left(O_i - O_i^P \right) \right)$$

- w_1, w_2: weights determined based on the (co)variance of two terms
- If you need more than just a simple average in data analysis
  - two different data, O_i on labeled and O_i^P on unlabeled samples
  - simultaneous fit on these two data sets with the same fit parameters
  - O_i and O_i^P have the same mean after BC but may have different variance
- Binning and BC for each bin is another option for complicated data analysis



Error Estimation



- Training, bias correction and predictions are made on statistical data
- Final estimates, including the trained ML algorithm, inherit uncertainties
- We use **bootstrap resampling** for error estimation
  - Random choice of bootstrap samples (labeled and unlabeled data set, separately)
  - Split training, BC data in labeled data
  - Train, BC and obtain estimates on each bootstrap sample

Applications

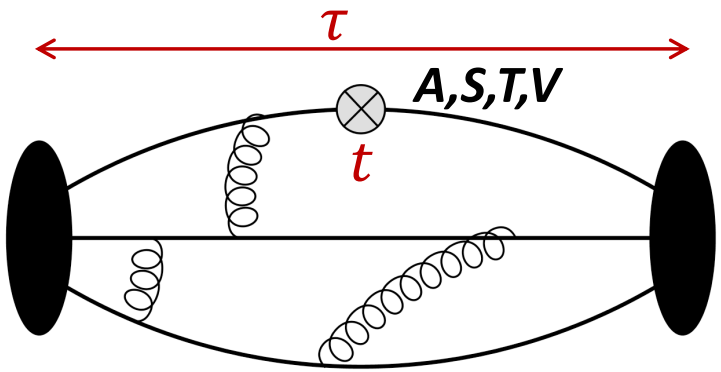
Nucleon Isovector Charges $g_{A,S,T,V}$

$$\langle p|\bar{u}\Gamma d|n\rangle = g_\Gamma \bar{\psi}_p \Gamma \psi_n$$

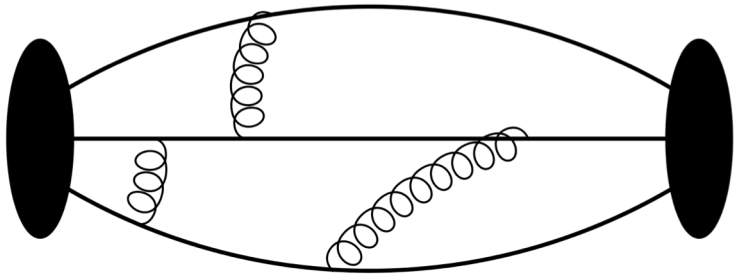
- $g_A = 1.2772(20)$ [Expt]
- g_T: quark EDM

- On lattice,

$$\frac{C_{3pt}}{C_{2pt}} \rightarrow g_\Gamma$$



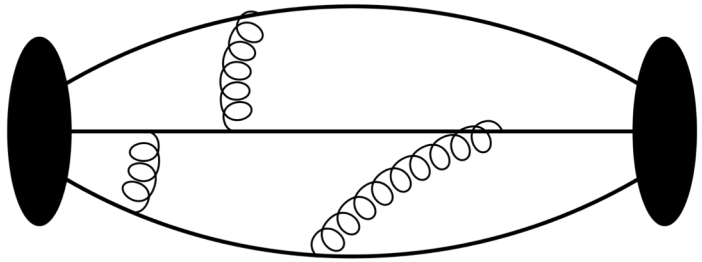
$C_{3pt}(\tau, t)$

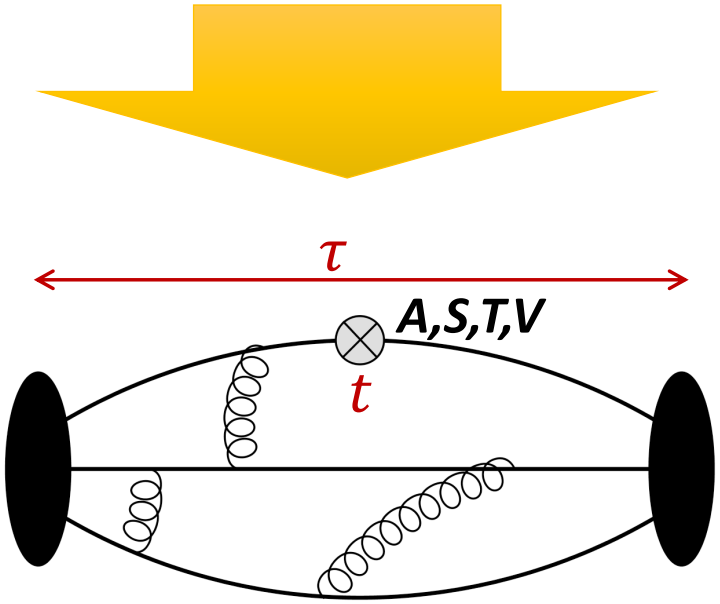


$C_{2pt}(\tau)$

Prediction of C_{3pt} from C_{2pt}

$C_{2pt}(\tau)$





$C_{3pt}(\tau, t)$

Input: $\boldsymbol{X}_i = \{C_{2pt}(0 \leq \tau/a \leq T_{\max})\}$

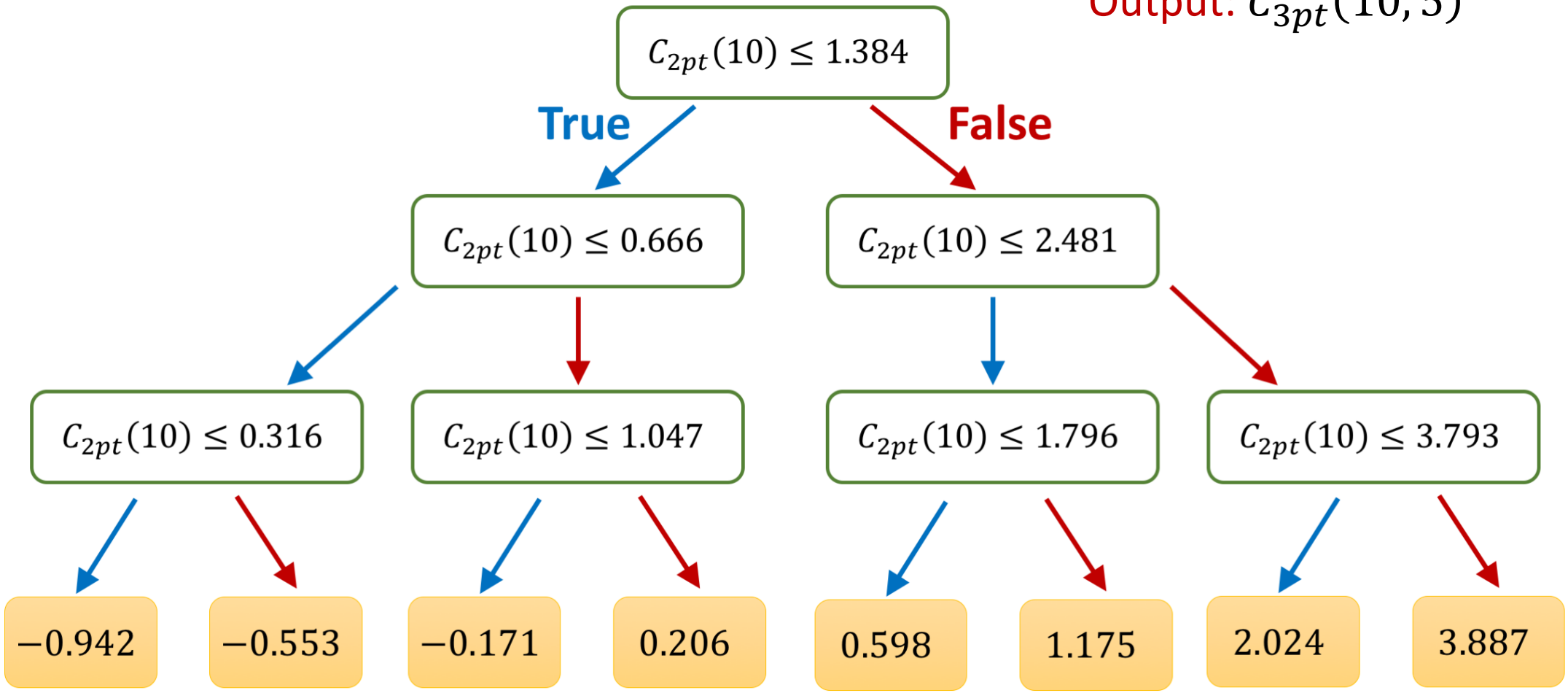
Boosted Decision Tree Regression

Output: $C_{3pt}^{A,S,T,V}(\tau, t)$

Decision Tree Regression

Input: $\{C_{2pt}(0 \leq \tau/a \leq 20)\}$

Output: $C_{3pt}^{A}(10,5)$



$$C_{3pt}^{A}(\tau/a = 10, t/a = 5)$$

Boosted Decision Tree (BDT)

- **Iterative boosting**

$F_0 =$ [Simple DT h_0]
$F_1 = F_0$ + [Simple DT h_1 that corrects residual error of F_0]
$F_2 = F_1$ + [Simple DT h_2 that corrects residual error of F_1]
$F_3 = F_2$ + [Simple DT h_3 that corrects residual error of F_2]
…
$F_n = F_{n-1} + h_n$

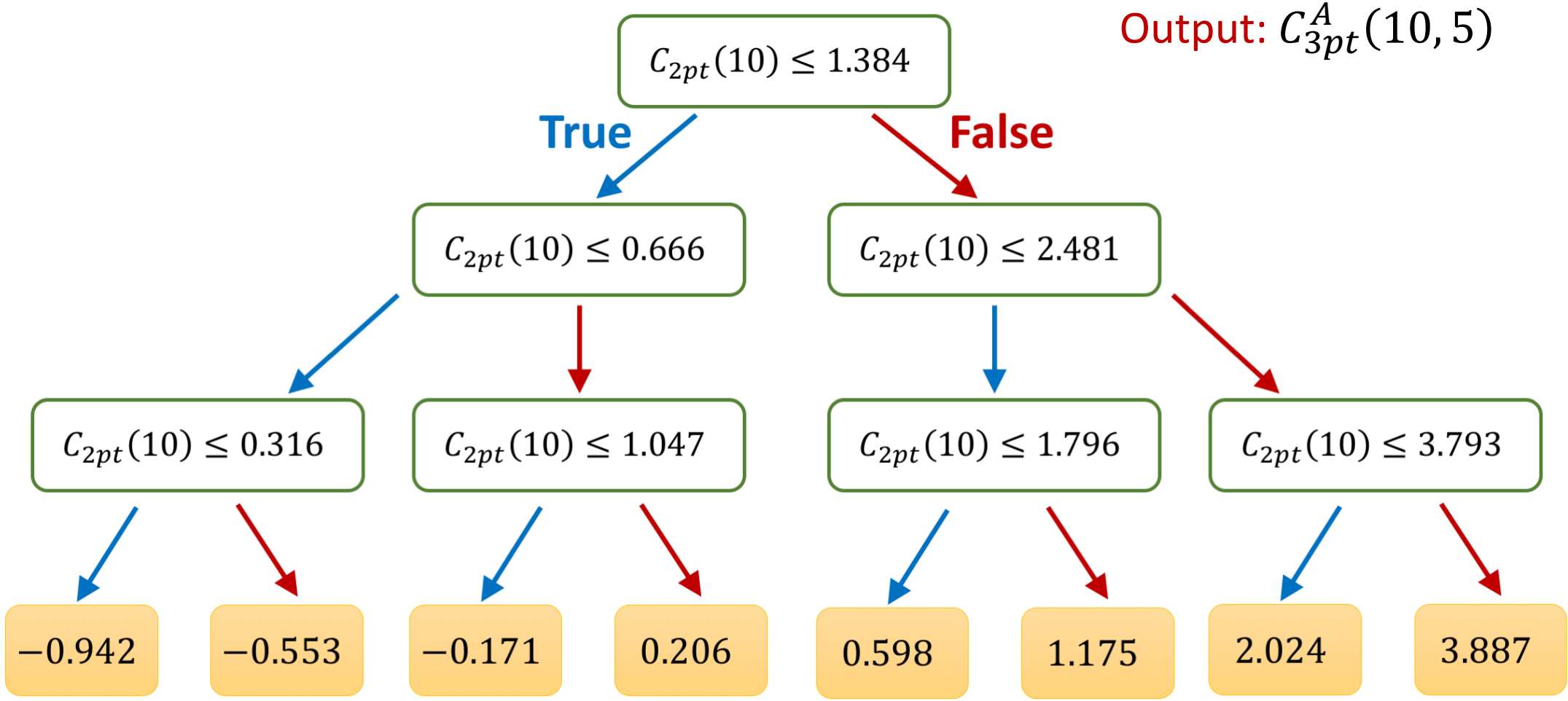
$$F(\boldsymbol{X}) = F_{N_{boost}}(\boldsymbol{X})$$

- Usually, $F_n = F_{n-1} + \nu \cdot h_n$ with "learning rate" $\nu \sim 0.1$
- In this study, $N_{boost} = 100 - 500$

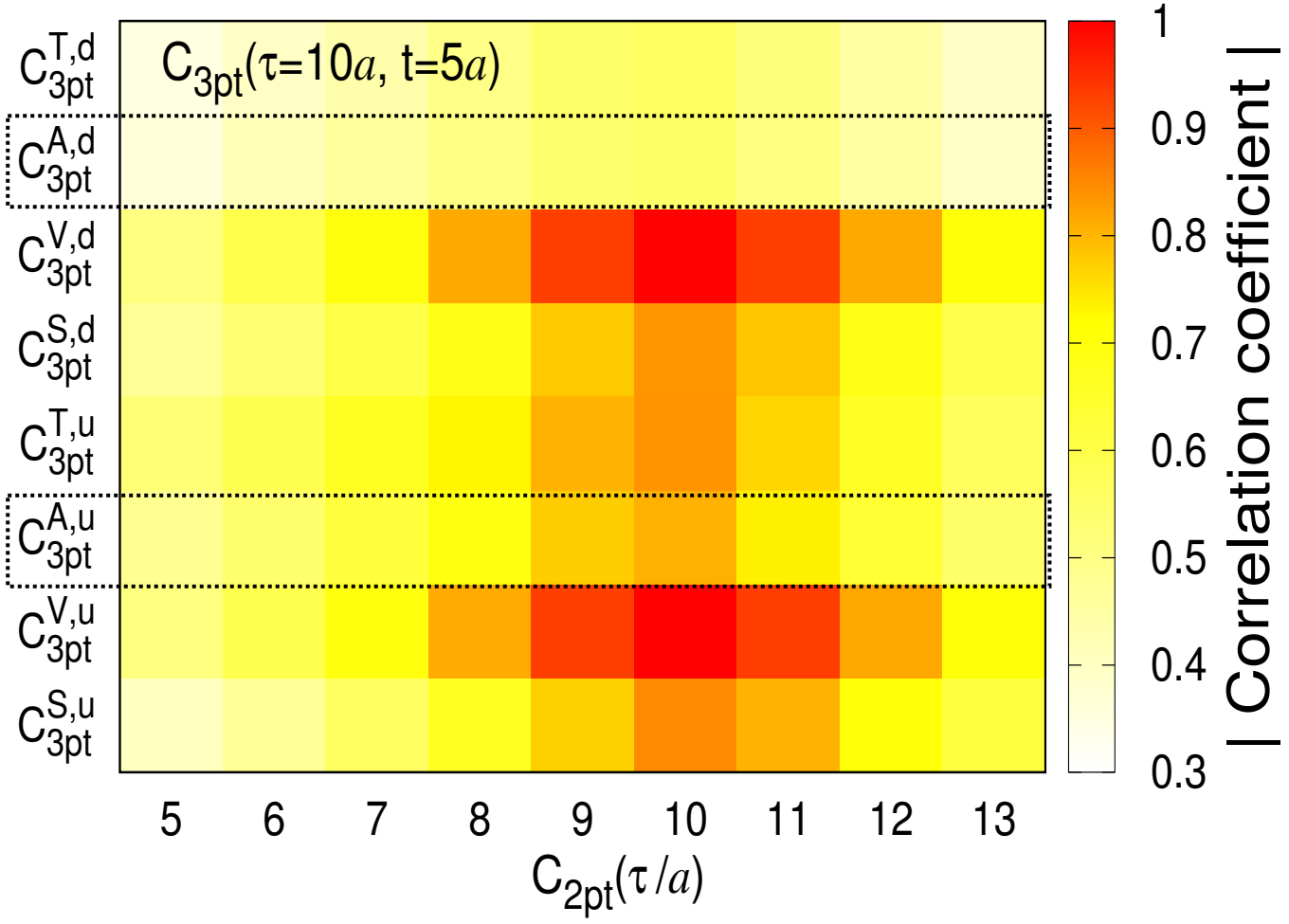
Decision Tree h_0 for $C_{3pt}^{A}(10, 5)$

Input: $\{C_{2pt}(0 \leq \tau/a \leq 20)\}$

Output: $C_{3pt}^{A}(10, 5)$



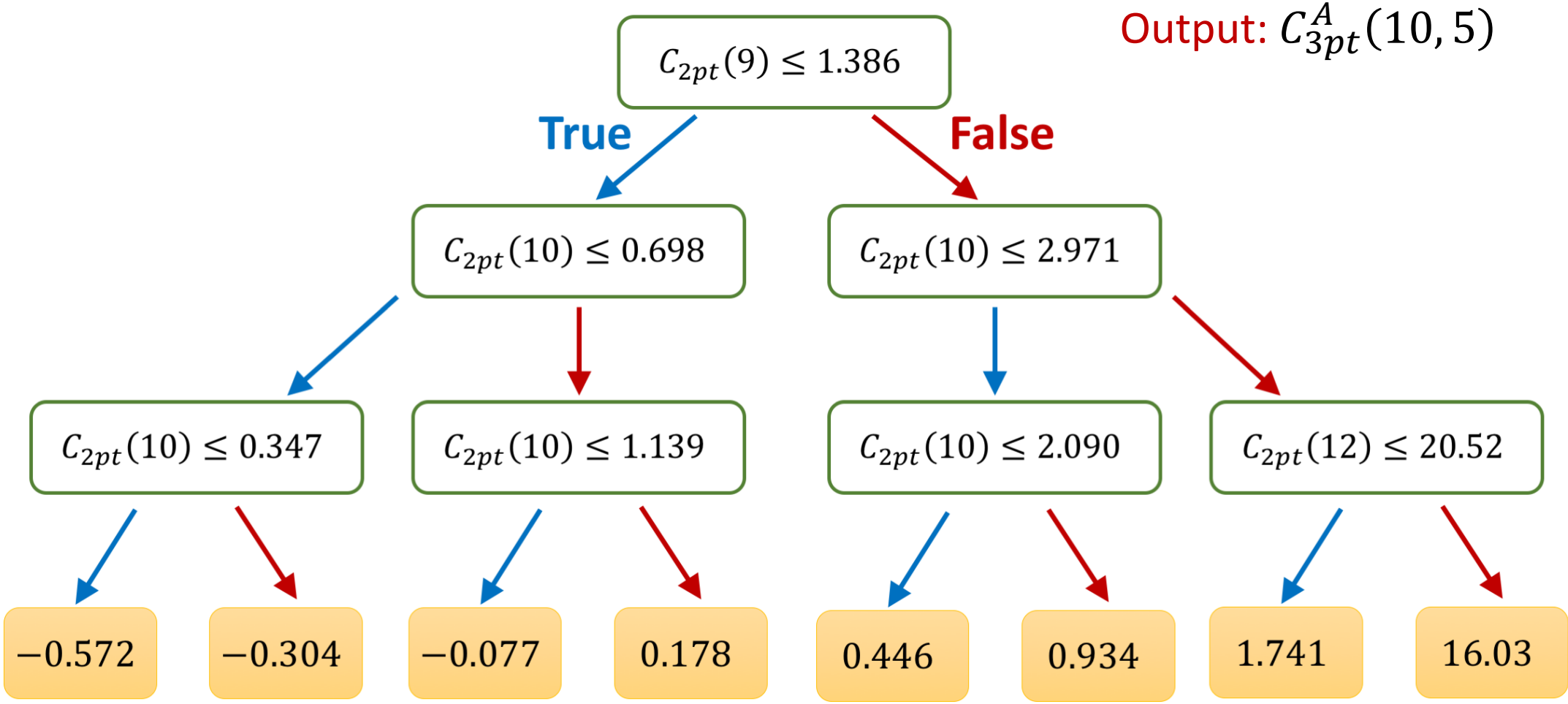
Revisit: Correlation Map of Nucleon Observables



Decision Tree h_5 for $C_{3pt}^{A}(10, 5)$

Input: $\{C_{2pt}(0 \leq \tau/a \leq 20)\}$

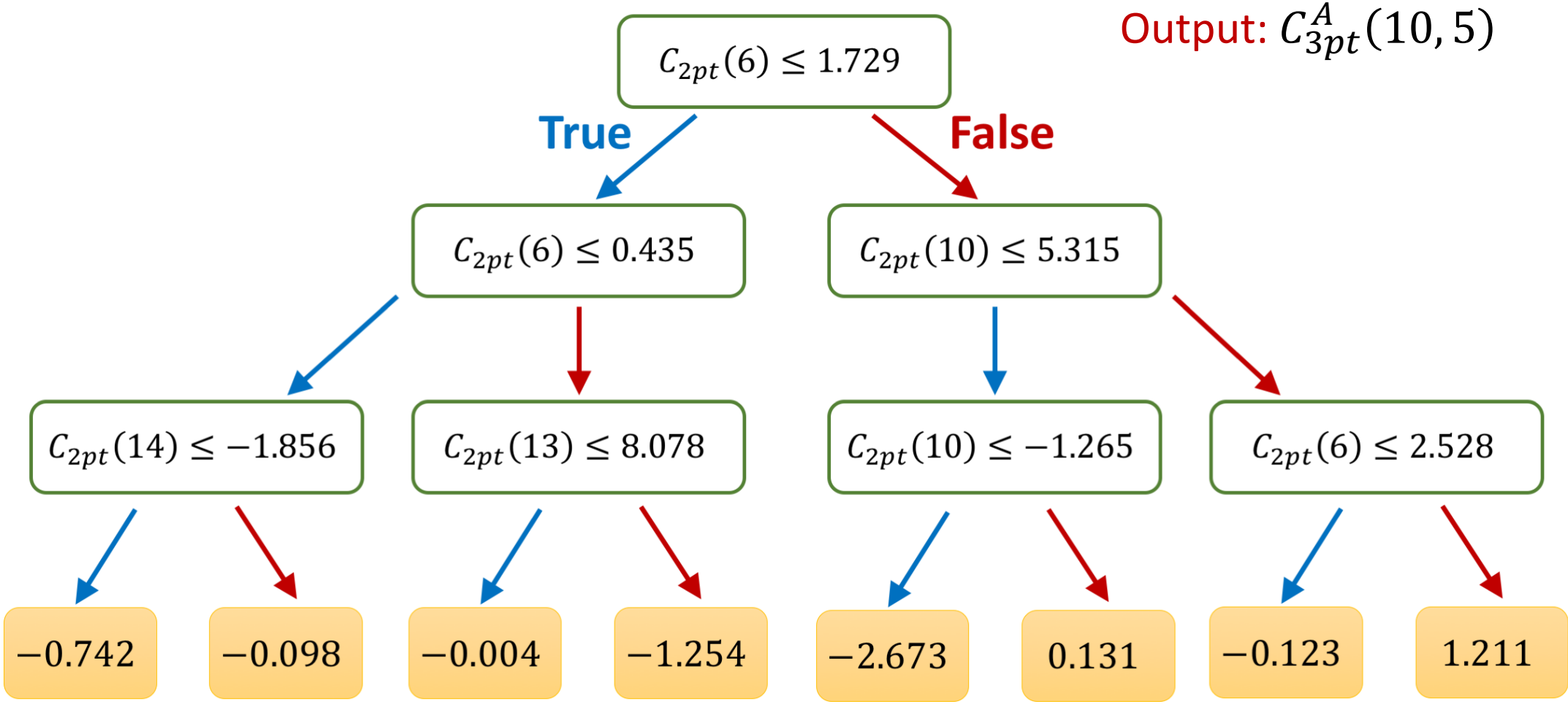
Output: $C_{3pt}^{A}(10, 5)$



Decision Tree h_{30} for $C_{3pt}^{A}(10,5)$

Input: $\{C_{2pt}(0 \leq \tau/a \leq 20)\}$

Output: $C_{3pt}^{A}(10,5)$



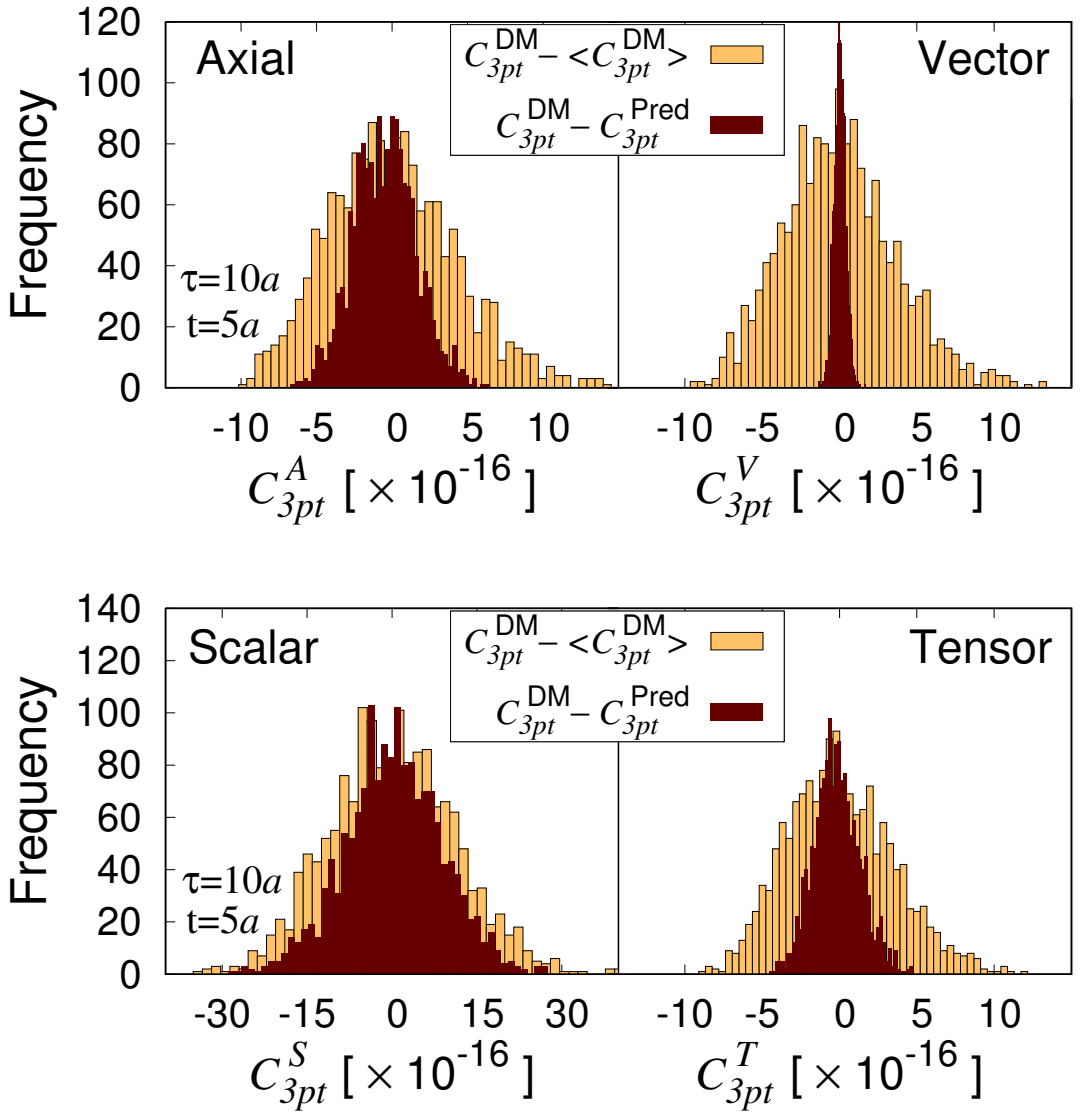
Prediction of C_{3pt} from C_{2pt}

- Training and Test performed for
  - Clover-on-HISQ
  - $a = 0.089$fm, $M_\pi = 313$ MeV
  - Measurements: 2263 confs × 64 srcs
- # of training data: 60 confs
  # of BC data: 620 confs
  # of unlabeled data: 1583 confs
- Prediction error

$$\mathrm{PE} = C_{3pt}^{\mathrm{DirectMeas.}} - C_{3pt}^{\mathrm{Pred}}$$

- Prediction quality for $C_{3pt}^{\Gamma}(10,5)$

$$\frac{\sigma_{PE}}{\sigma_{DM}} = 0.79\ (S), 0.49\ (A), 0.44\ (T), 0.12\ (V)$$



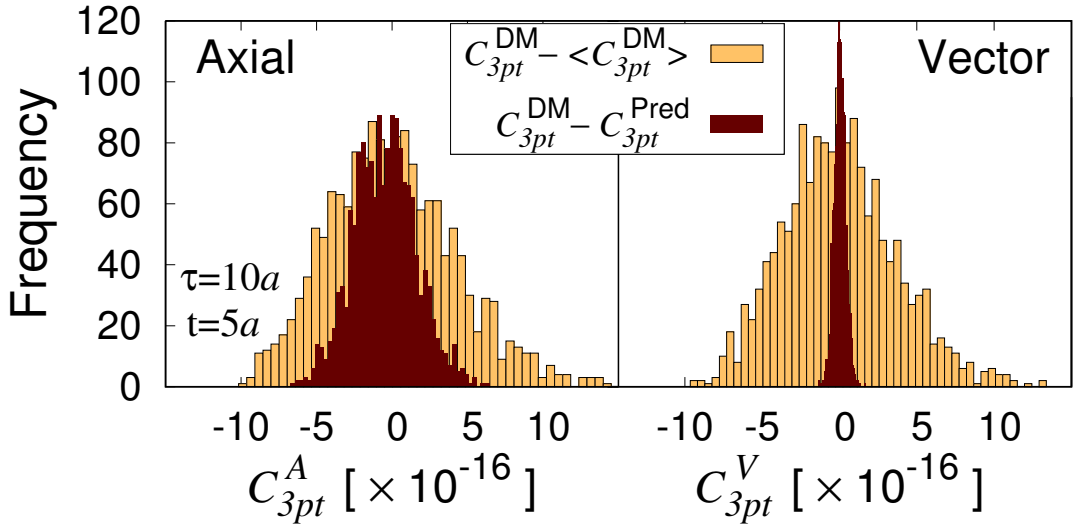
Prediction of C_{3pt} from C_{2pt}

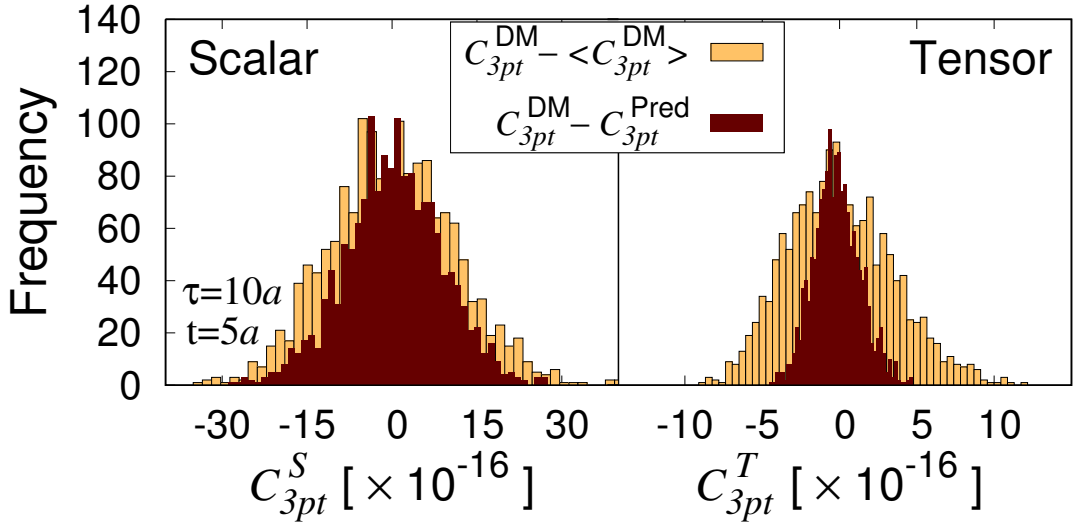
- Prediction quality $C^{\Gamma}_{3pt}(10,5)$

$$\frac{\sigma_{PE}}{\sigma_{DM}} = 0.79\ (S), 0.49\ (A), 0.44\ (T), 0.12\ (V)$$

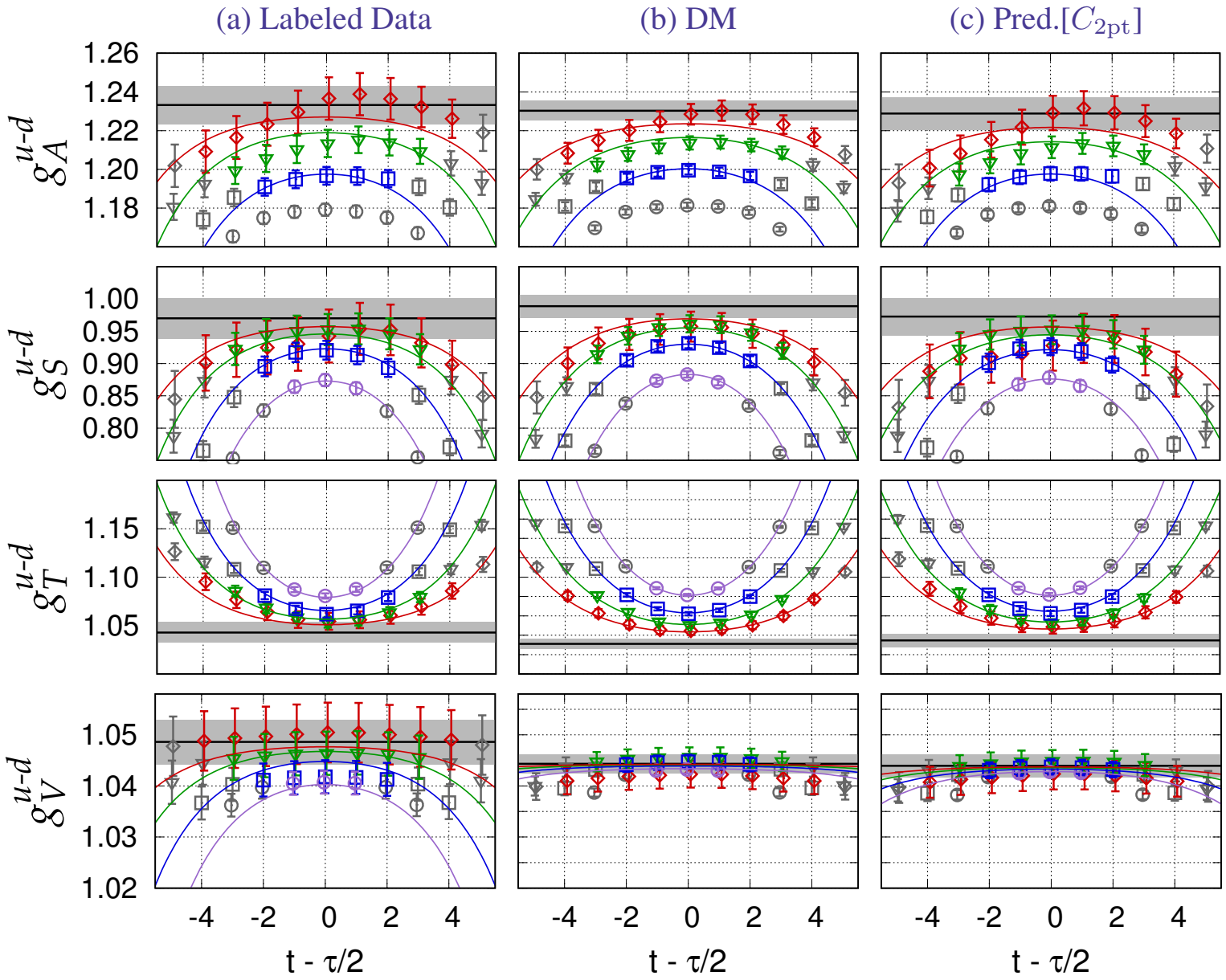
- Predictions of $C^{\Gamma}_{3pt}(10,5)/\langle C_{2pt}(10)\rangle$

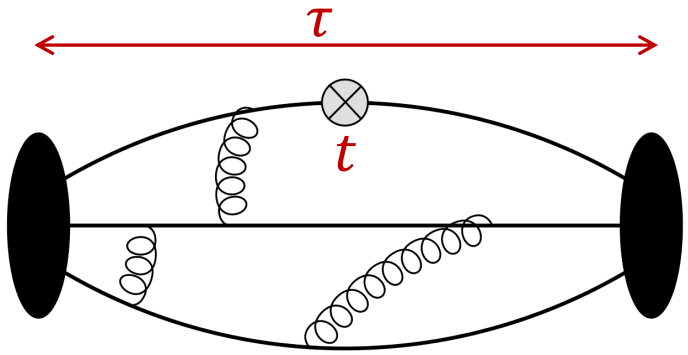
Γ	DM	BC-Prediction	Raw-Prediction	Bias
S	0.936(10)	0.933(15)	0.931(45)	+0.002(46)
A	1.2011(41)	1.1997(48)	1.1999(109)	−0.0003(105)
T	1.0627(34)	1.0638(39)	1.0642(79)	−0.0004(78)
V	1.0462(36)	1.0455(36)	1.0453(39)	+0.0002(20)





Prediction of C_{3pt} from C_{2pt}





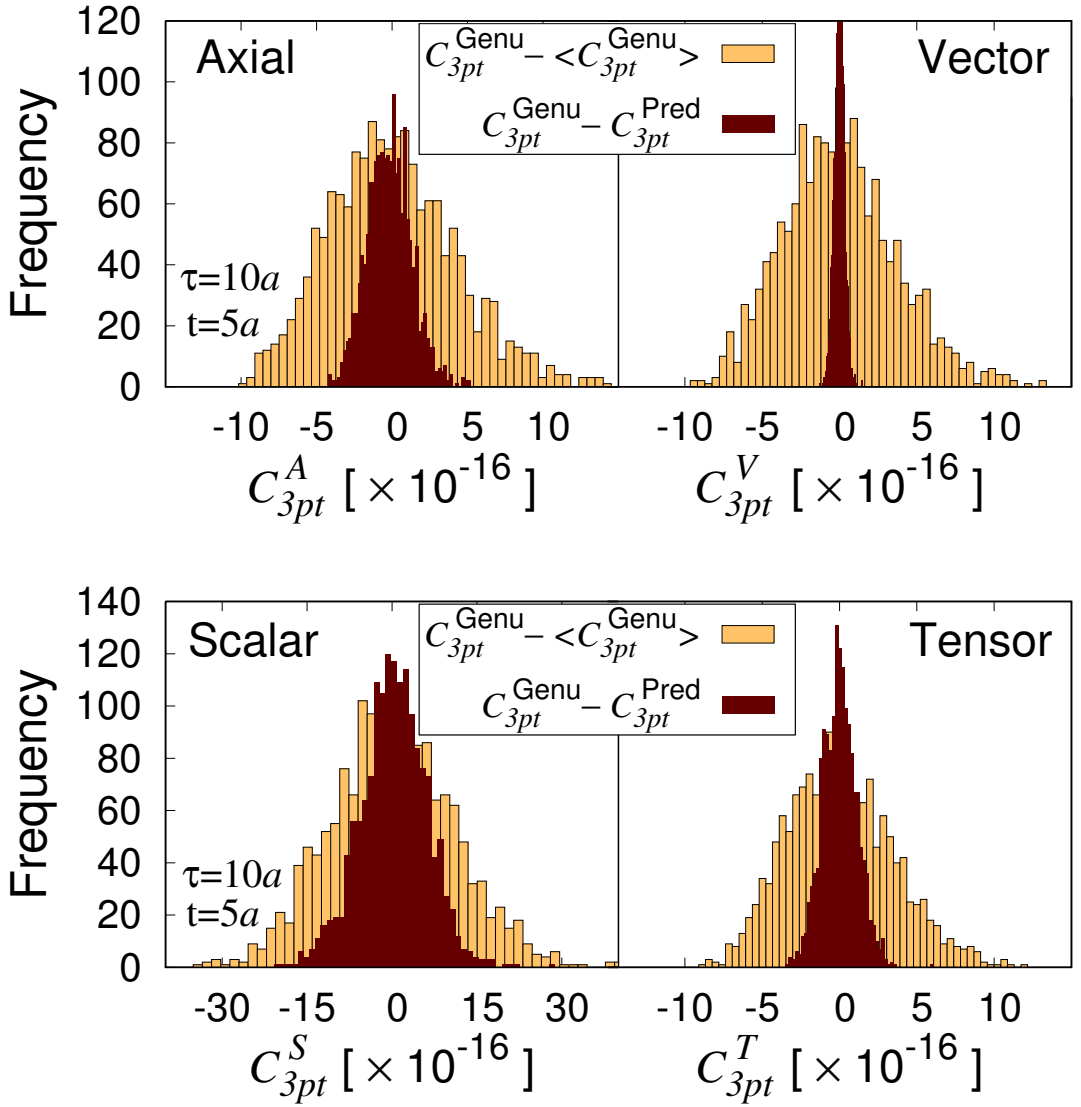
τ=14 τ=12 τ=10 τ=8

Prediction of $\boldsymbol{C_{3pt}(8,10,14)}$ from $\boldsymbol{C_{2pt}}$ and $\boldsymbol{C_{3pt}}(12)$

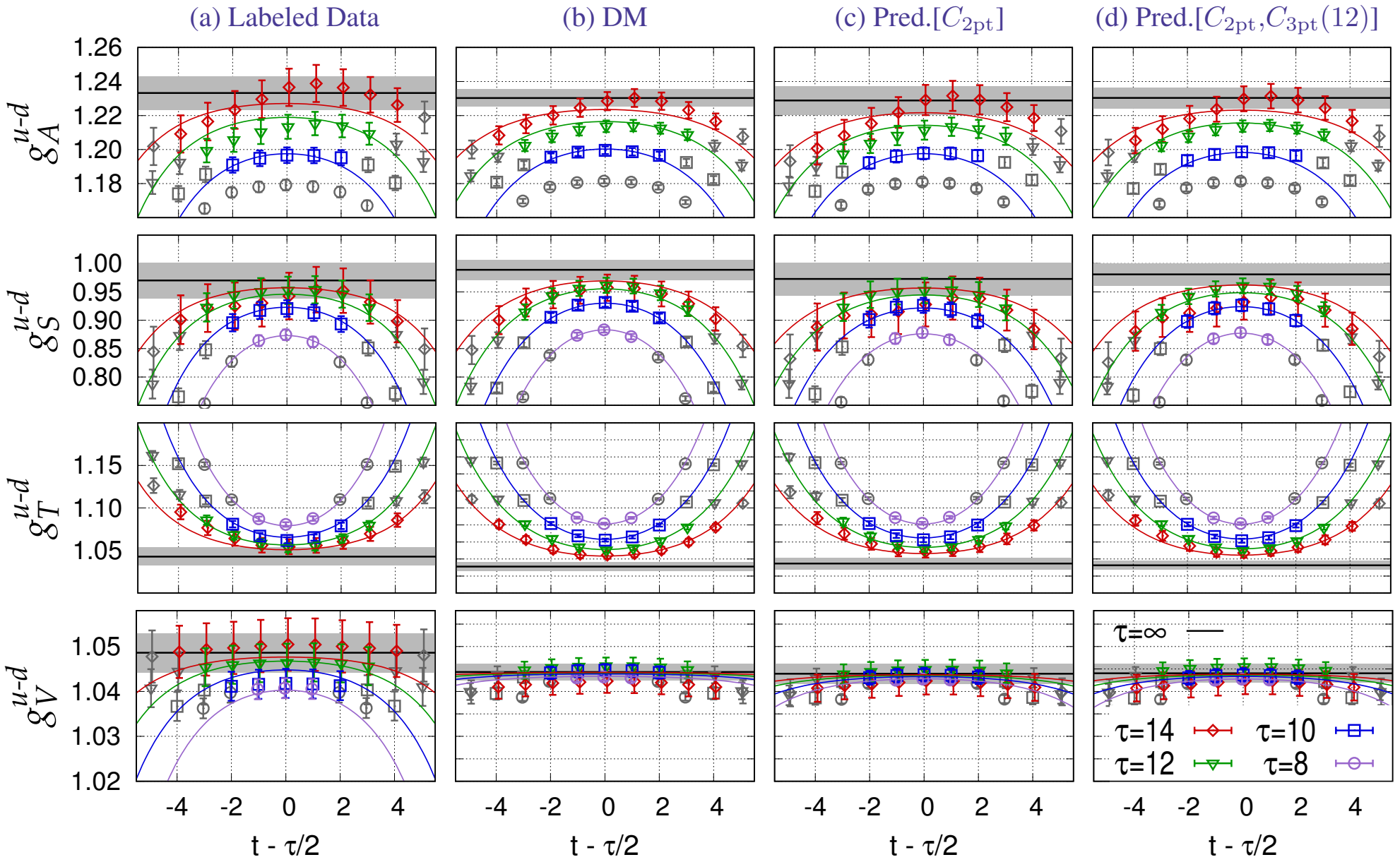
- We need $\boldsymbol{C_{3pt}}$ at four values of source-sink separations ($\tau = 8,10,12,14$) for analysis
- $\boldsymbol{C_{3pt}}(8,10,14)$ can be predicted from $\boldsymbol{C_{2pt}}$ and $\boldsymbol{C_{3pt}}(12)$ data
- Prediction quality $C_{3pt}^{\Gamma}(10,5)$

$$\frac{\sigma_{PE}}{\sigma_{DM}} = 0.53\ (S), 0.35\ (A), 0.33\ (T), 0.10\ (V)$$

(c.f.) only from C_{2pt}: $0.79\ (S), 0.49\ (A), 0.44\ (T), 0.12\ (V)$



Prediction of C_{3pt} from C_{2pt} and more



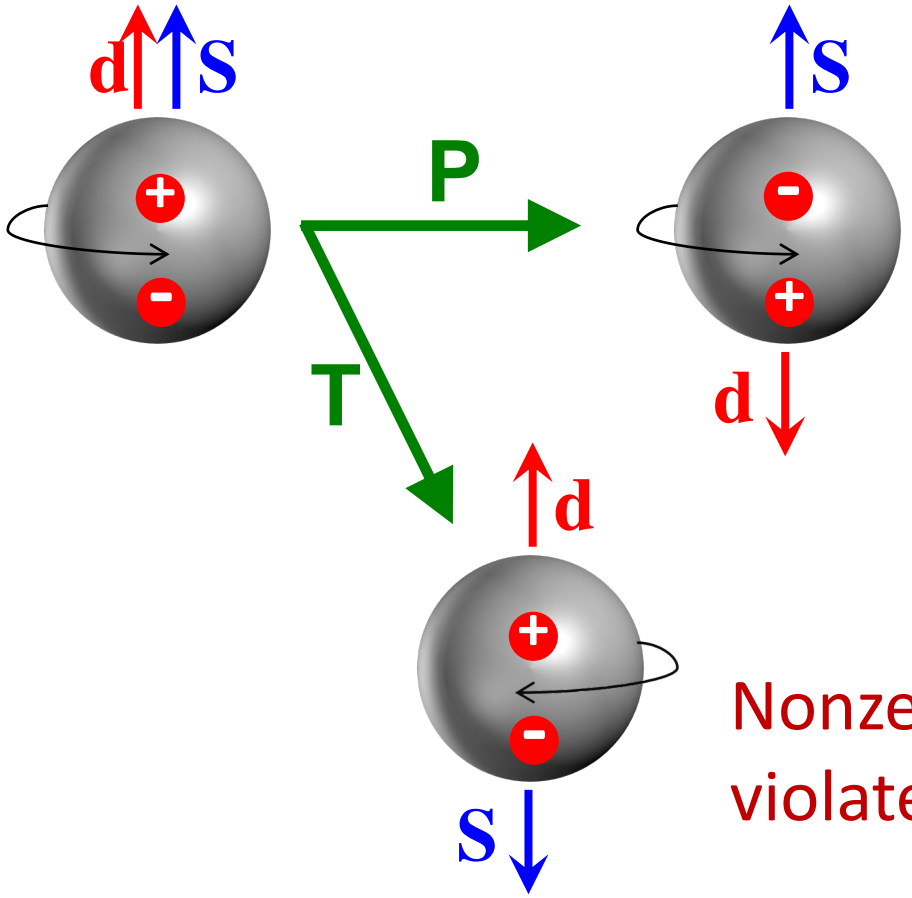
Prediction of C_{3pt} from C_{2pt}

- Results extrapolated to $\tau \to \infty$

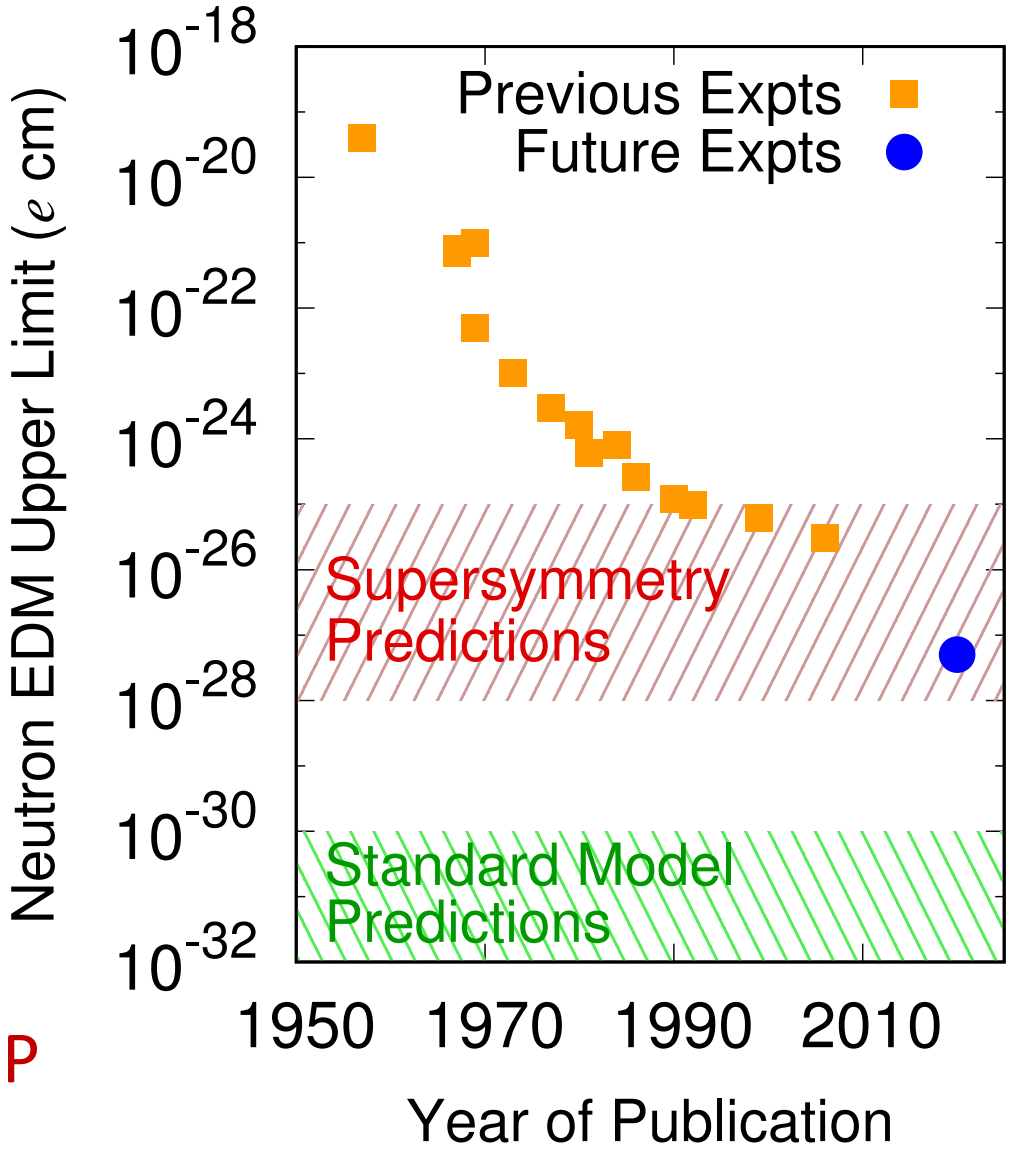
	DM	Pred.$[C_{2\mathrm{pt}}]$	Pred.$[C_{2\mathrm{pt}}, C_{3\mathrm{pt}}(12)]$
g_S	0.989(18)	0.973(29)	0.981(20)
g_A	1.2303(51)	1.2289(83)	1.2304(61)
g_T	1.0311(51)	1.0347(68)	1.0326(54)
g_V	1.0443(19)	1.0439(22)	1.0440(21)
	2263 DM (Direct Meas.)	680 DM + 1583 Pred.	680 DM + 1583 Pred.

Neutron EDM and CP Violation

- Measures separation between centers of (+) and (-) charges



Nonzero nEDM violates P and T, so CP



Effective CPV Lagrangian

$$\mathcal{L}_{\mathrm{CPV}}^{d\le 6} = -\frac{g_s^2}{32\pi^2}\bar{\theta} G\tilde{G}$$ dim=4 QCD θ-term

$$-\frac{i}{2}\sum_{q=u,d,s} d_q \bar{q}(\sigma\cdot F)\gamma_5 q$$ dim=5 Quark EDM (qEDM)

$$-\frac{i}{2}\sum_{q=u,d,s} \tilde{d}_q g_s \bar{q}(\sigma\cdot G)\gamma_5 q$$ dim=5 Quark Chromo EDM (CEDM)

$$+ d_w \frac{g_s}{6} G\tilde{G}G$$ dim=6 Weinberg 3g operator

$$+\sum_i C_i^{(4q)} O_i^{(4q)}$$ dim=6 Four-quark operators

Quark Chromo EDM (cEDM)

- Simulation in presence of CPV cEDM interaction

$$S = S_{QCD} + S_{cEDM}$$

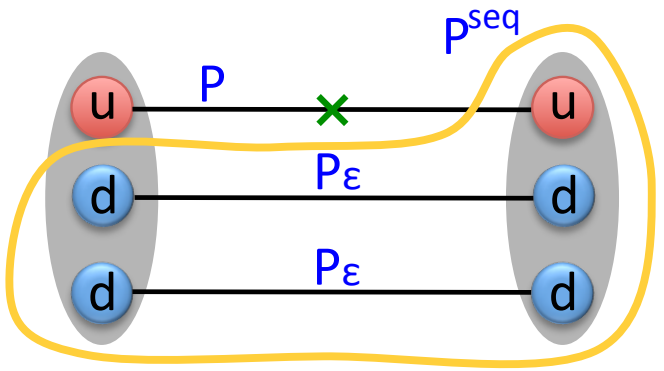
$$S_{cEDM} = -\frac{i}{2}\int d^4x \;\; \tilde{d}_q g_s \bar{q}(\sigma \cdot G)\gamma_5 q$$

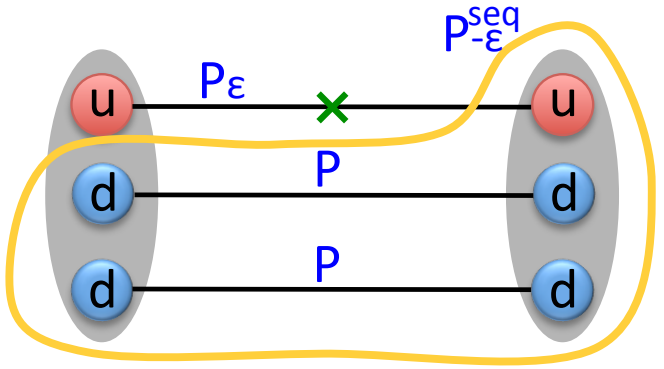
- Schwinger source method

  Include cEDM term in valence quark propagators by modifying Dirac operator

$$\boxed{D_{\text{clov}} \rightarrow D_{\text{clov}} + i\varepsilon\sigma^{\mu\nu}\gamma_5 G_{\mu\nu}}$$

- cEDM contribution to nEDM can be obtained by calculating vector form-factor F_3 with propagators including cEDM & $O_{\gamma_5} = \bar{q}\gamma_5 q$





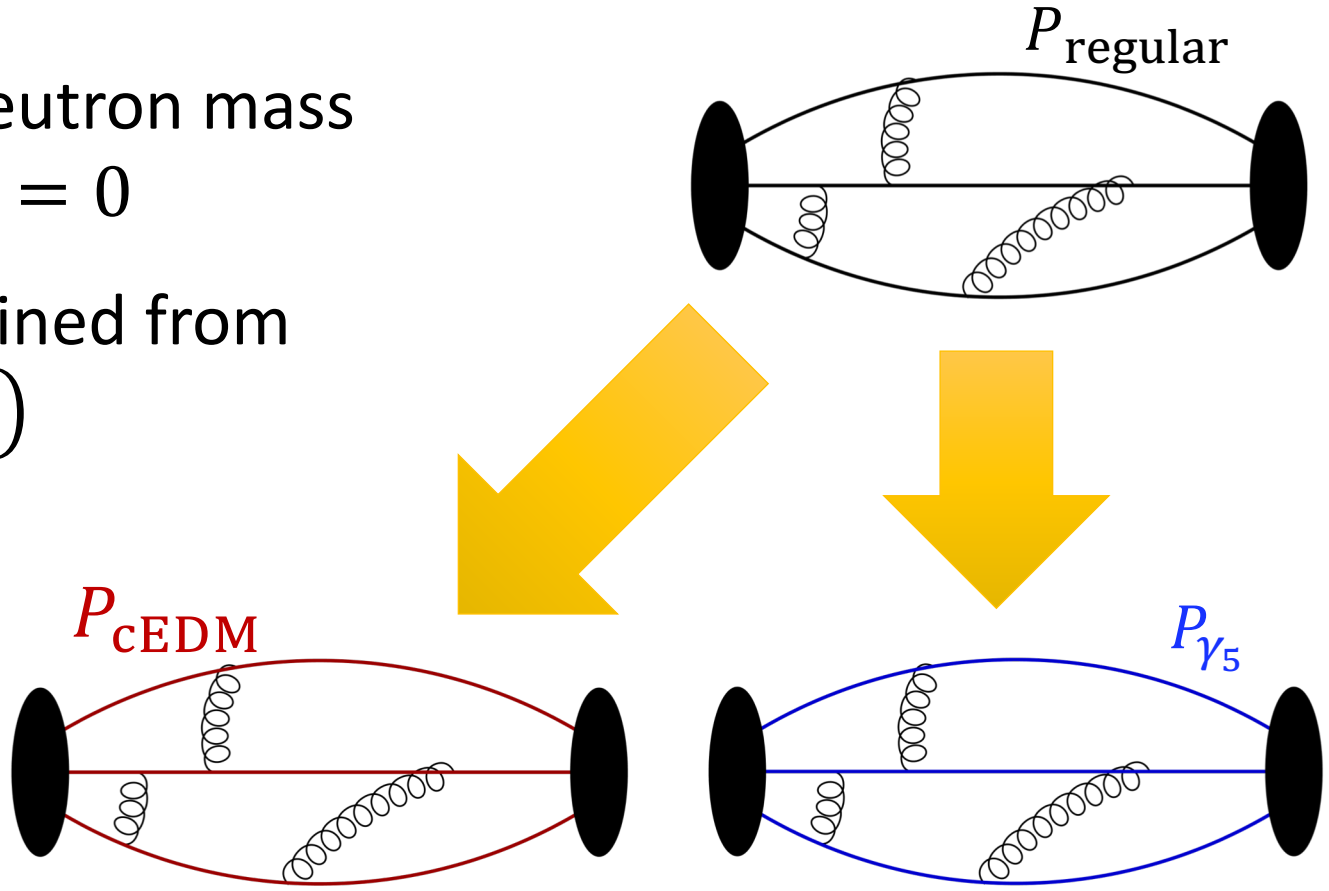
Prediction of C_{2pt}^{CPV} from C_{2pt}

- Predict C_{2pt} for cEDM and γ_5 insertions from C_{2pt} without CPV
- CPV interactions ➔ phase in neutron mass

$$\left(ip_\mu\gamma_\mu + me^{-2i\alpha\gamma_5}\right)u_N = 0$$

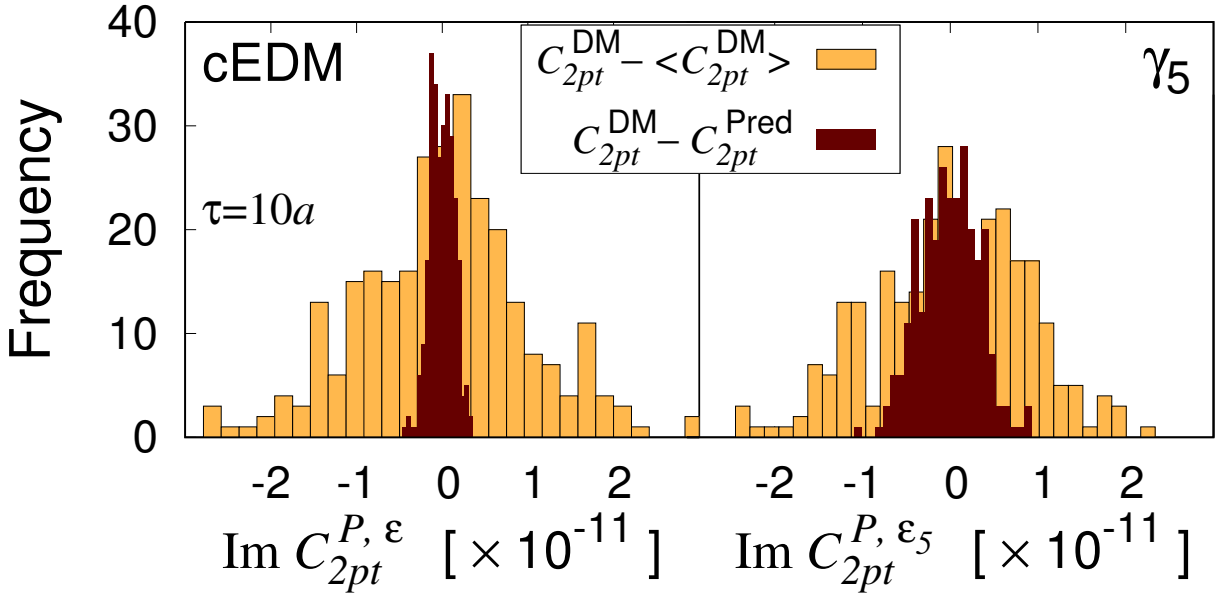
- At leading order, α can be obtained from

$$C_{2pt}^{P} \equiv \mathrm{Tr}\left(\gamma_5\langle NN^\dagger\rangle\right)$$



Prediction of C_{2pt}^{CPV} from C_{2pt}

- Training and Test performed for
  - $a = 0.12$ fm, $M_\pi = 305$ MeV
  - Measurements: 400 confs × 64 srcs
- # of training data: 70 confs
  # of BC data: 50 confs
  # of unlabeled data: 280 confs



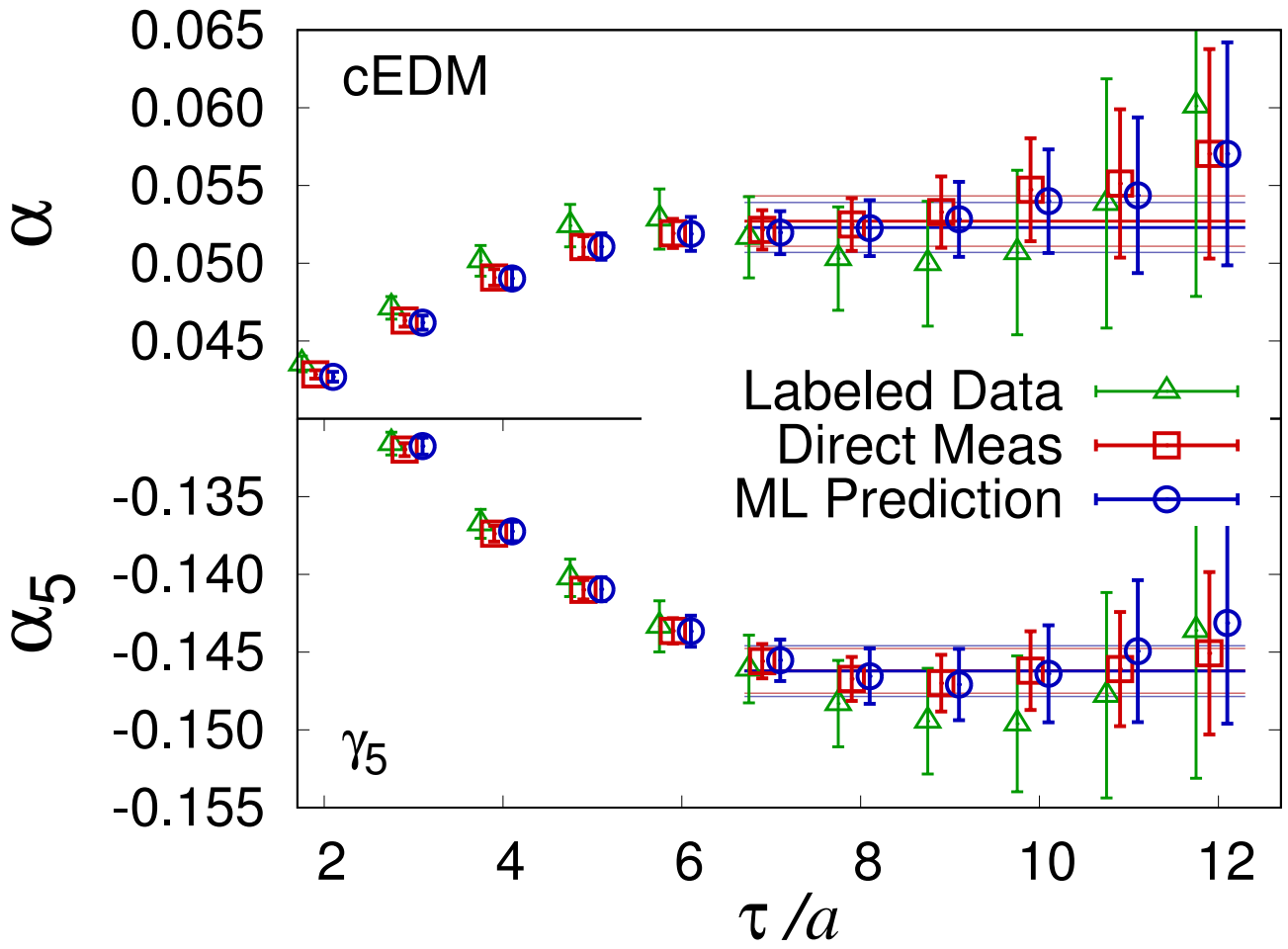
Input:

$$\boldsymbol{X}_i = \{\mathrm{Re}, \mathrm{Im}[C_{2pt}^{S,P}(0 \le \tau/a \le 16)]\}$$

Boosted Decision Tree Regression

Output: $\mathrm{Im}\left[C_{2pt}^{P\,(\mathrm{cEDM},\gamma_5)}(\tau)\right]$

Prediction of C_{2pt}^{CPV} from C_{2pt}



- α $(\mathbf{cEDM})$

  DM: 0.0527(17)

  Prediction: 0.0525(18)

- α_5 (γ_5)

  DM: -0.1463(14)

  Prediction: -0.1460(17)

➢ DM: DM on 400 confs

➢ Prediction: DM on 120 confs
+ ML prediction on 280 confs

Comparison of Regression Models

	Linear Regression	BDT	Neural Network
Speed	Fastest	Fast	Slow
Performance	Bad for nonlinear	Okay	Possibly better
Tuning Parameters	None or a few	Few; not sensitive	Many; sensitive
Overfitting Risk	Very Low	Low	High
Training Data Requirement	Small	Medium	Large
Interpretability	Yes	Somewhat	Not likely

BDT with scikit-learn Python ML Library

```
>>> import numpy
>>> from sklearn.ensemble import GradientBoostingRegressor
>>>
>>> X = numpy.random.uniform(size=(100,2))*10  # 100 random samples
>>> y = [x[0]**2 + 2*x[1] for x in X]
>>>
>>> gbr = GradientBoostingRegressor()
>>> gbr.fit(X,y)   # Training
>>>
>>> gbr.predict([[3,4]])     # 3²+2×4 = 17
array([15.20630936])

>>> gbr.predict([[6,3]])     # 6²+2×3 = 42
array([42.77231812])

>>> gbr.predict([[8,5]])     # 8²+2×5 = 74
array([74.14274825])
```

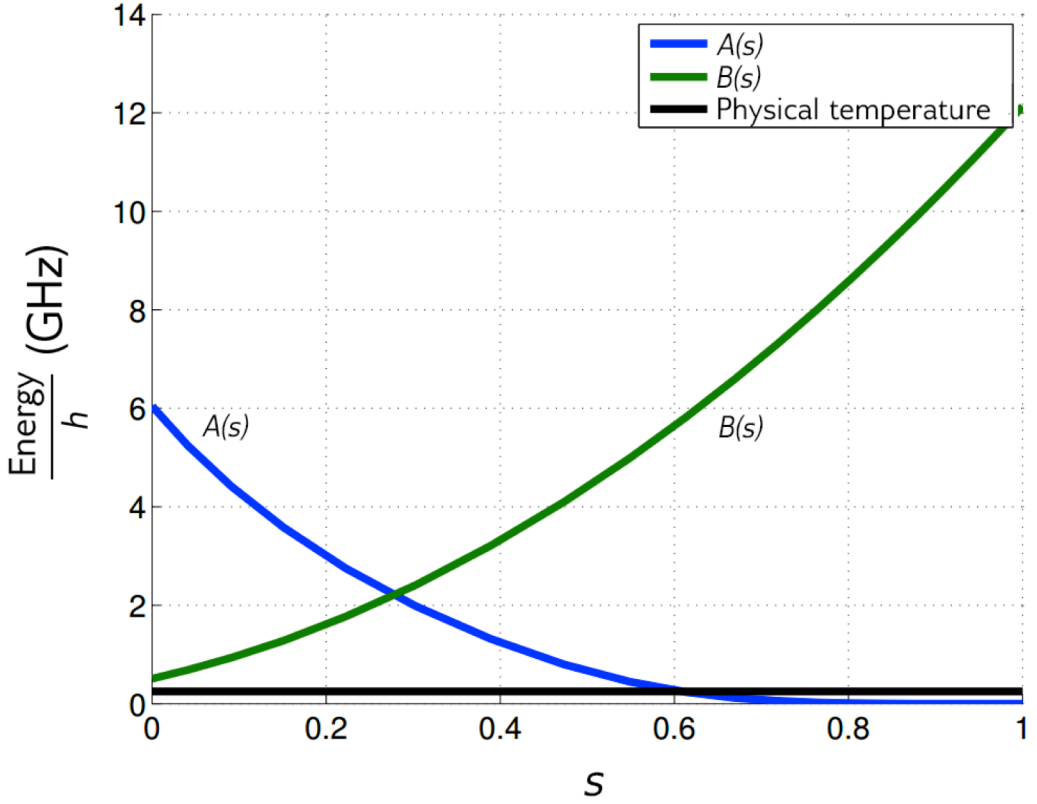
$$X = [[a_1, b_1], [a_2, b_2], \dots]$$
$$y = [a_1^2 + 2b_1, a_2^2 + 2b_2, \dots]$$

Machine Learning Regression on D-Wave Quantum Annealer

D-Wave Quantum Computer

$$\mathcal{H}_{ising} = \underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2}\left(\sum_i h_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}}$$

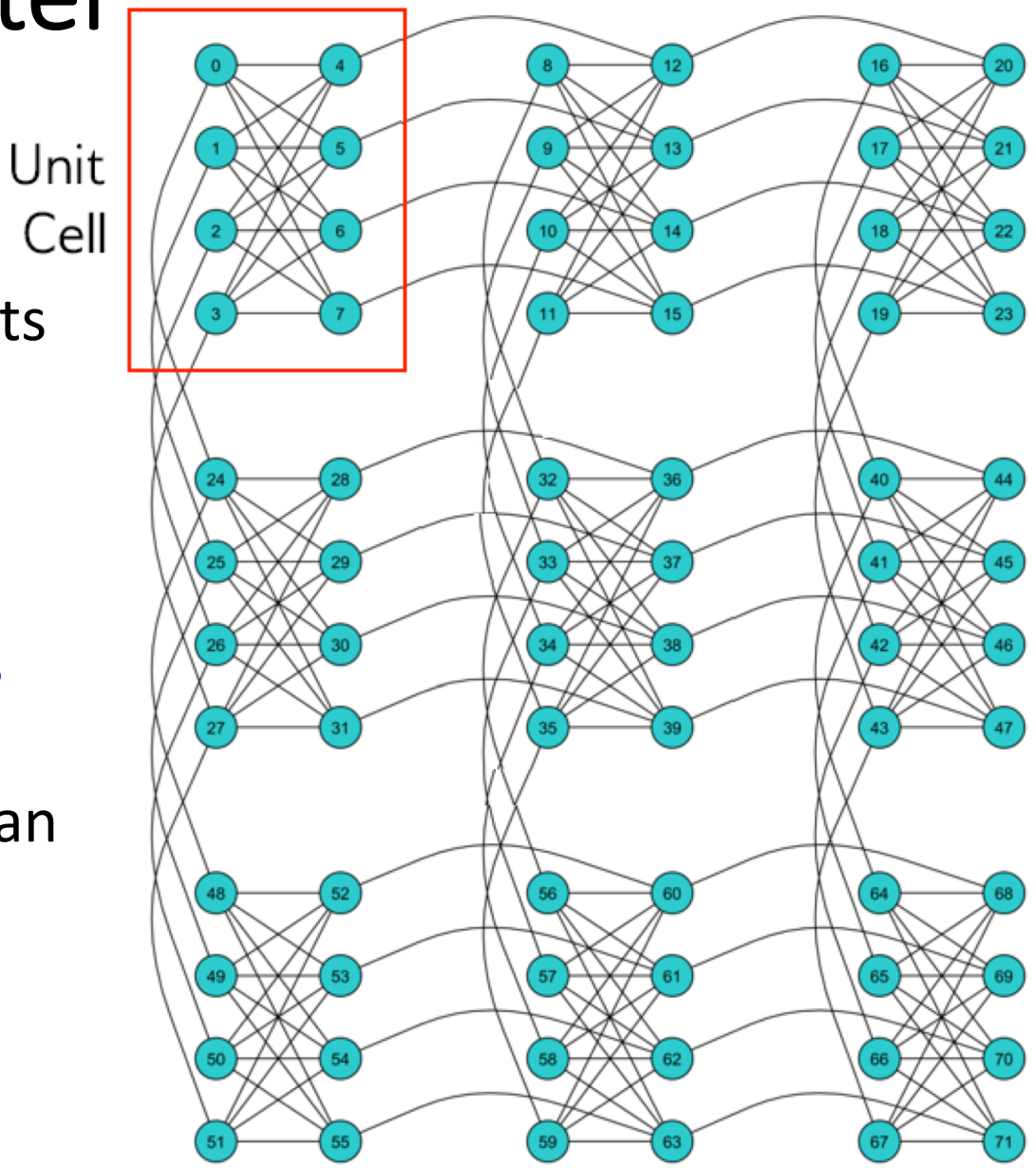
- $\hat{\sigma}_{x,z}^{(i)}$: Pauli matrices operating on a qubit q_i
- h_i, $J_{i,j}$: qubit biases and coupling strengths; set by user
- Qubits collapse to classical states (0 or 1), the lowest-energy state of the final H



D-Wave Quantum Computer

- The D-Wave QPU
  - Lattice of interconnected (Chimera) qubits
  - Not fully connected

- Minor Embedding
  - Mapping logical qubits to physical qubits
  - On D-Wave 2000Q (~2048 qubits), about 65 fully connected logical qubits can be mapped via Embedding



Sparse Coding

$$\min_{\Phi} \sum_{k=1}^{K} \min_{\vec{a}^{(k)}} \left[\frac{1}{2} \left\| \vec{I}^{(k)} - \mathbf{\Phi} \vec{a}^{(k)} \right\|_2 + \lambda \left\| \vec{a}^{(k)} \right\|_0 \right]$$

- Unsupervised ML algorithm
- Find dictionary $\mathbf{\Phi}$ and sparse representation $\vec{a}^{(k)}$ from which input data can be reconstructed by

$$\vec{I}^{(k)} \approx \mathbf{\Phi} \vec{a}^{(k)}$$

- The representation is sparse because the λ-term enforces a minimal set of dictionary elements for the reconstruction of a given input data

Sparse coding on D-Wave quantum annealer

- The sparse coding problem can be mapped onto D-Wave by

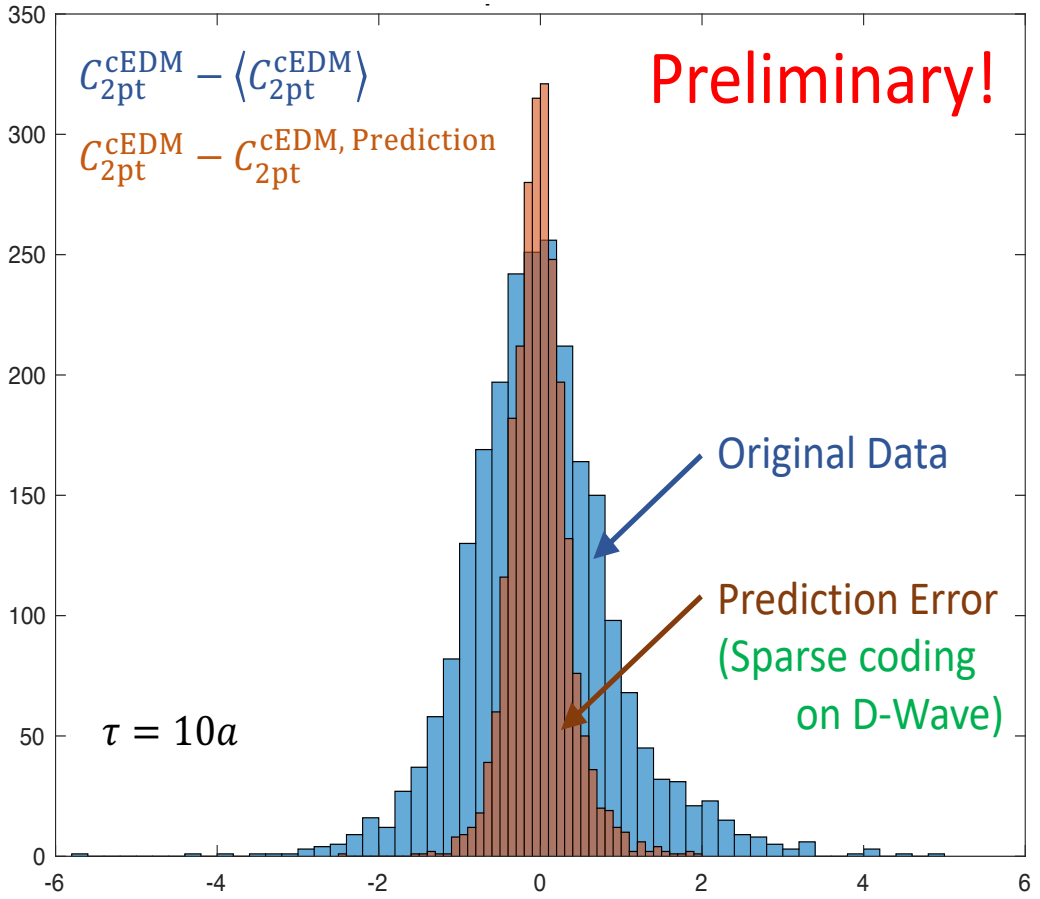
$$H(\vec{h}, \boldsymbol{Q}, \vec{a}) = \sum_i a_i h_i + \sum_{\langle i,j \rangle} Q_{ij} a_i a_j$$

$$\vec{h} = -\boldsymbol{\Phi}^T \vec{I} + \left(\lambda + \frac{1}{2}\right), \qquad \boldsymbol{Q} = \frac{1}{2}\Phi^T \Phi$$

- D-Wave finds $\vec{a}^{(k)}$ minimizing H (Restriction: $a_i = 0$ or 1)
- Optimization for Φ is performed offline (on classical computers)

Regression on D-Wave

- Predictions on C_{2pt}^{CPV}, using only C_{2pt} calculated without CPV, obtained on D-Wave 2000Q
- After trained with labeled data, reconstruction of an input sample with unknown target observable gives prediction
- Fully connected 64 qubits by embedding
- Promising result:
  the narrower spread of the prediction error
  compared to the distribution of original data



Distribution of CPV correlators and ML prediction error

Summary

- Machine learning (ML) is employed to predict unmeasured observables from measured observables
- Bias correction and bootstrap error estimation are used
- Demonstrated for two lattice QCD calculations
  1) Prediction of C_{3pt} from C_{2pt}
  2) Prediction of C_{2pt}^{CPV} from C_{2pt}
- A preliminary study performed on D-Wave 2000Q shows promising results for a regression algorithm.

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