Quantum Integration Network for Efficient Monte Carlo in High Energy Physics

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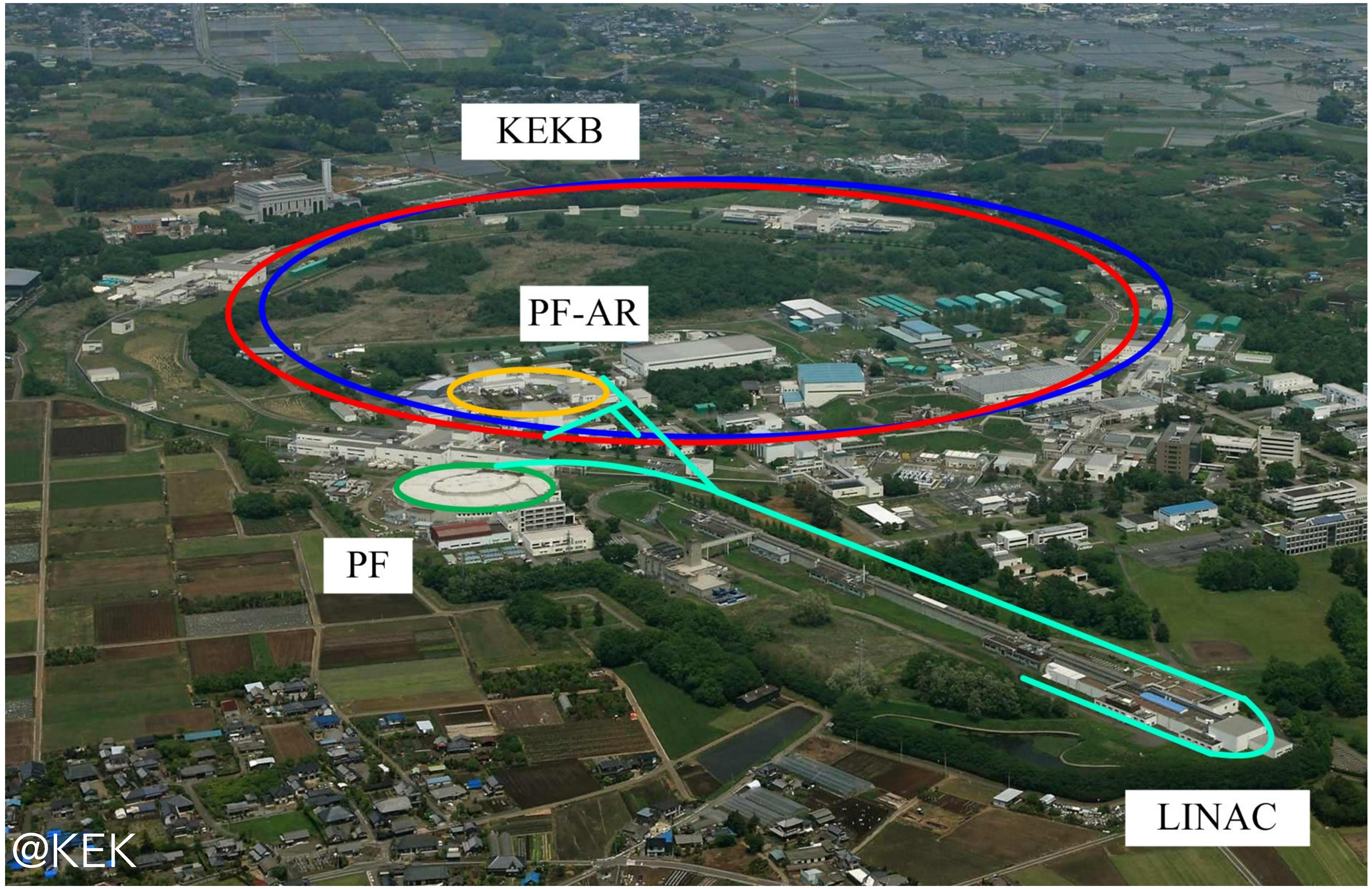
1. Motivation

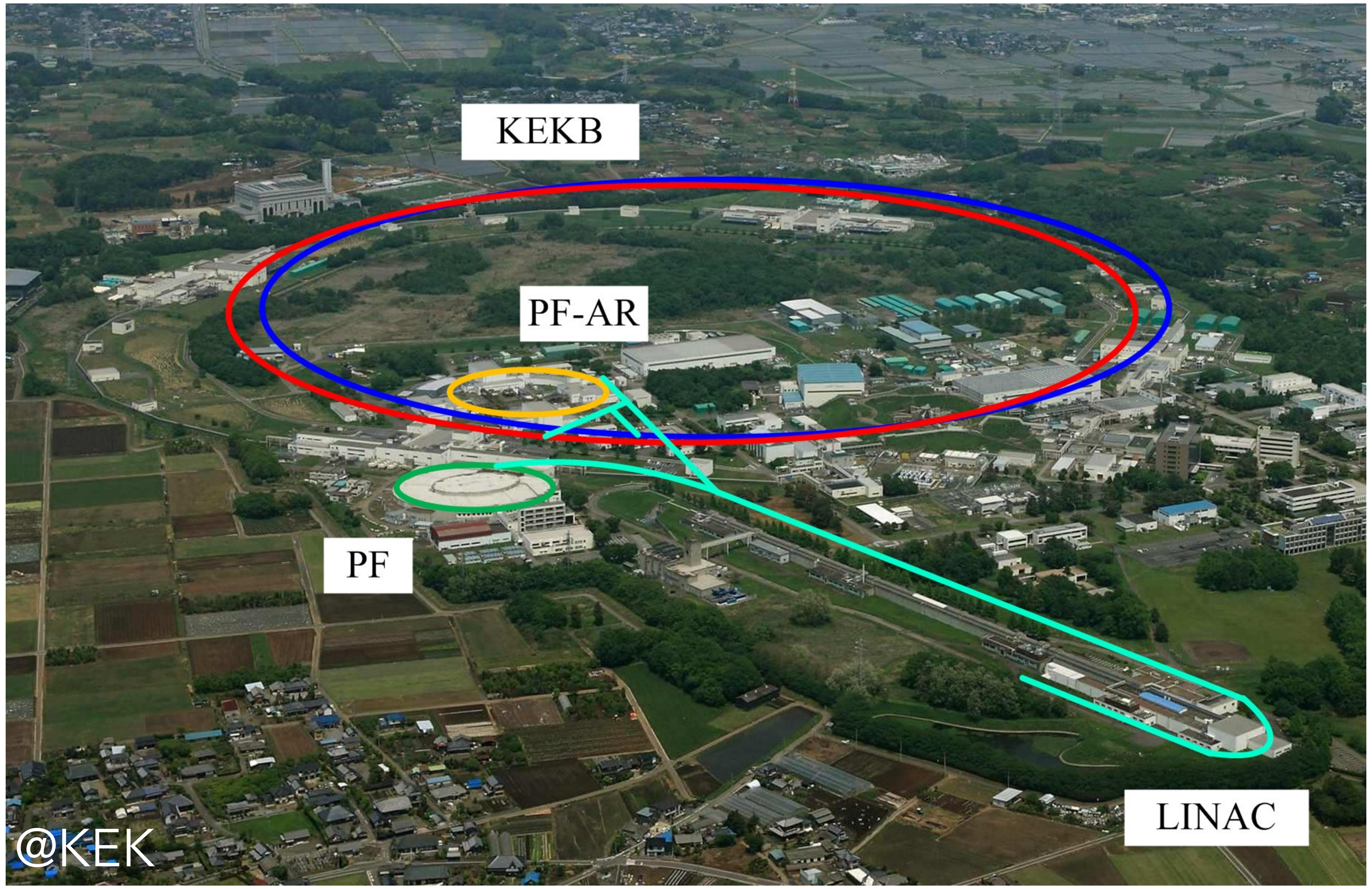
2. Methodology

3. Result

4. Summary & Outlook



Motivation



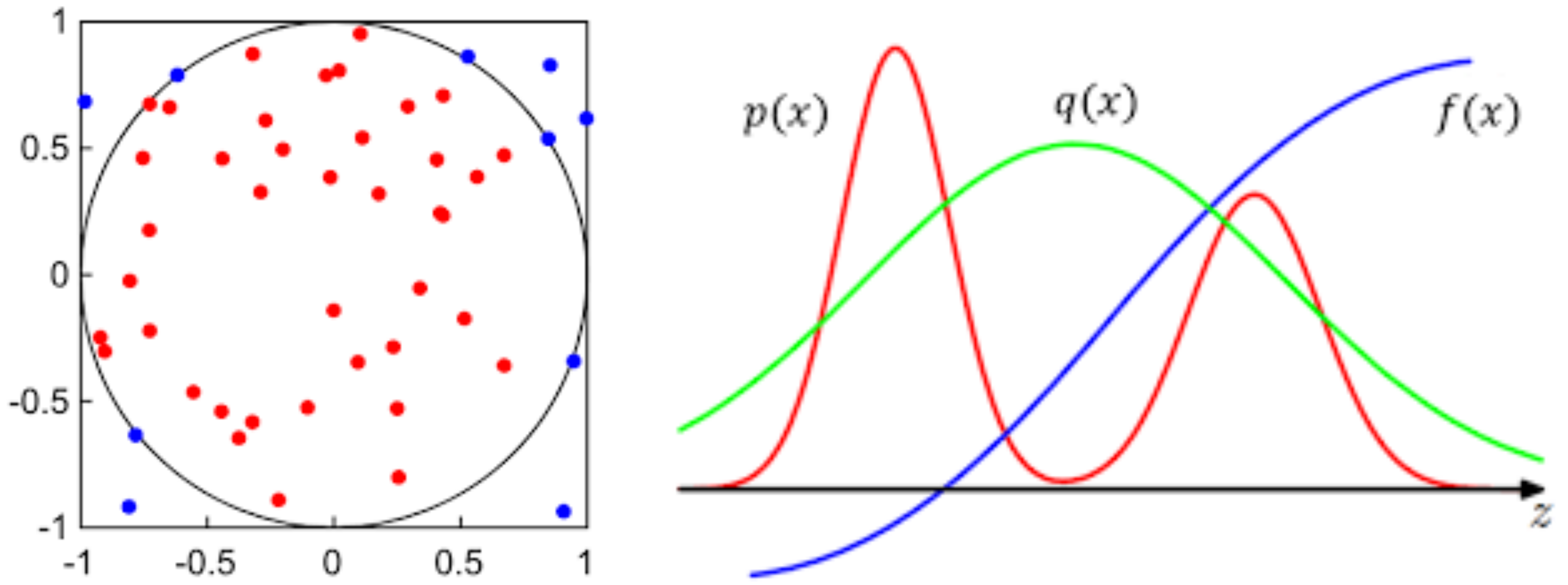
$$\frac{d\sigma}{dX} = \frac{1}{2s}\int \prod_{i=1}^{n} \frac{d^3p_i}{(2\pi)^3 E_i}\delta(k_1 + k_2 - \sum_{i=1}^{n} k_i)$$
$$\times |M_{fi}|^2 \theta_{\rm cut}(p_1, \ldots, p_n)\delta(X - X(p_1, \ldots, p_n))$$

For more accurate calculation,

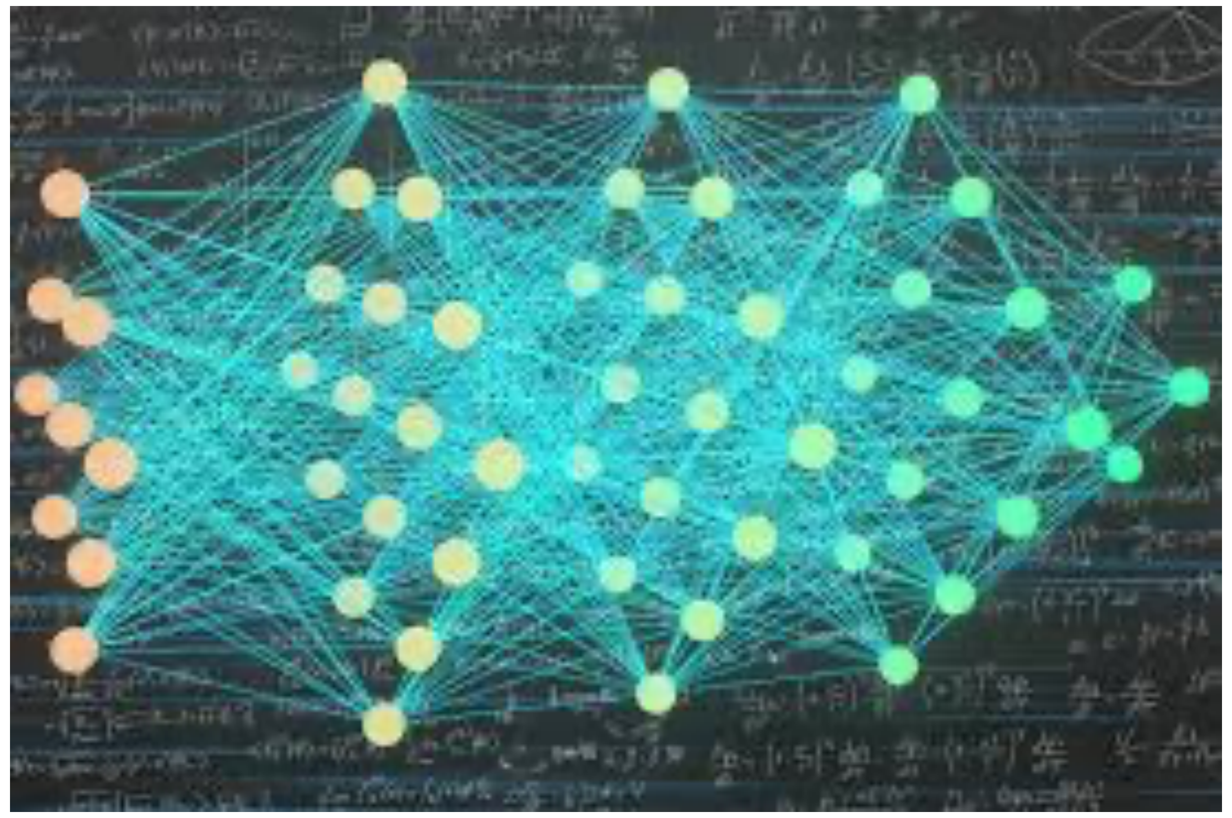
- Higher-order loops corrections
- Complex behaviors like singularities

→ Hard to evaluate !!!

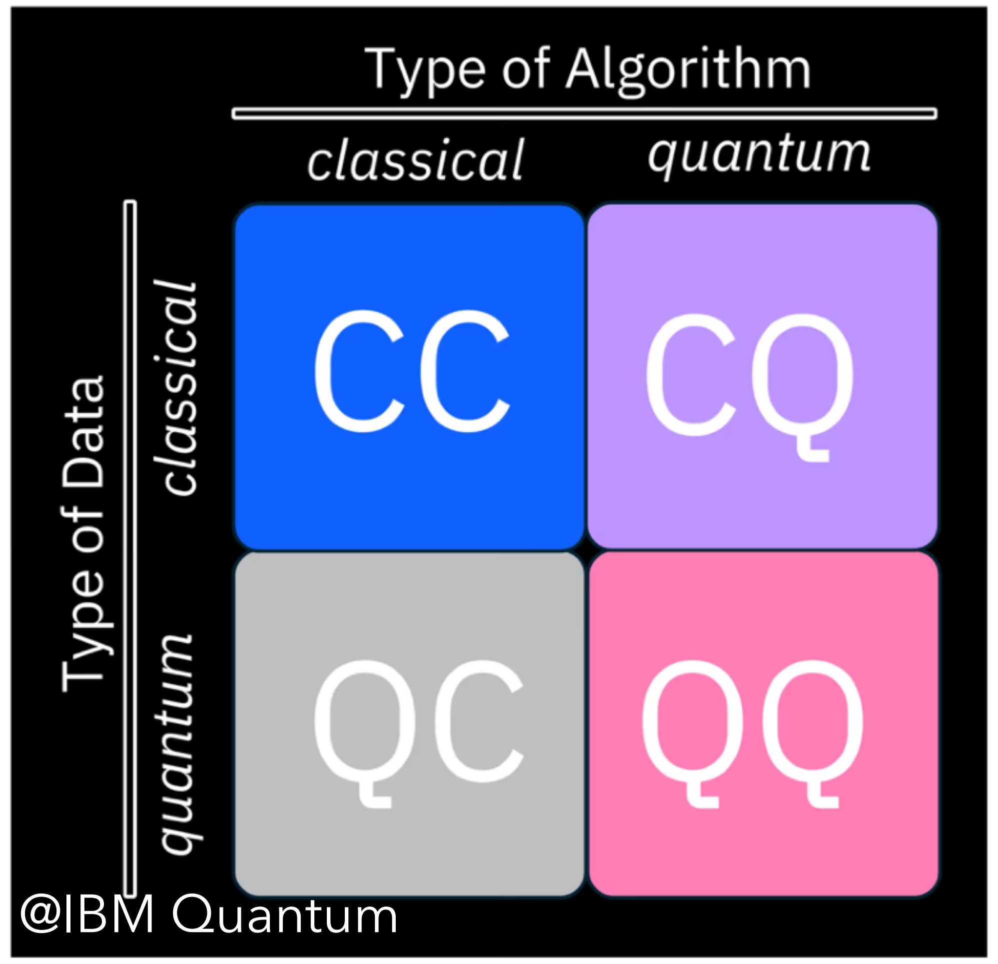
Motivation

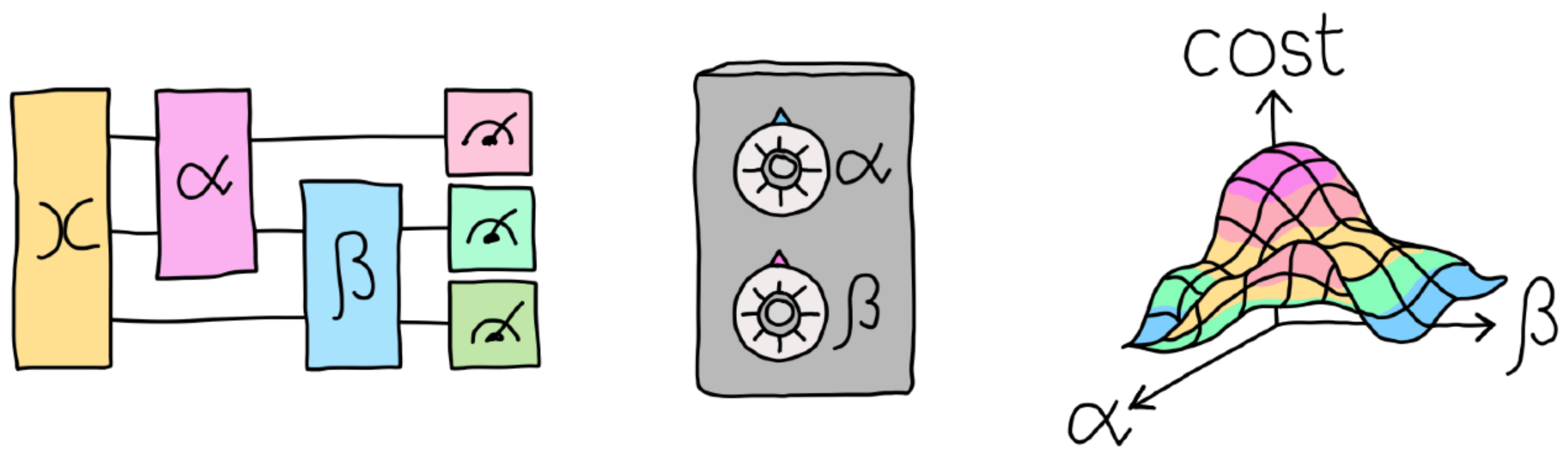


Monte-Carlo Integration


Machine Learning

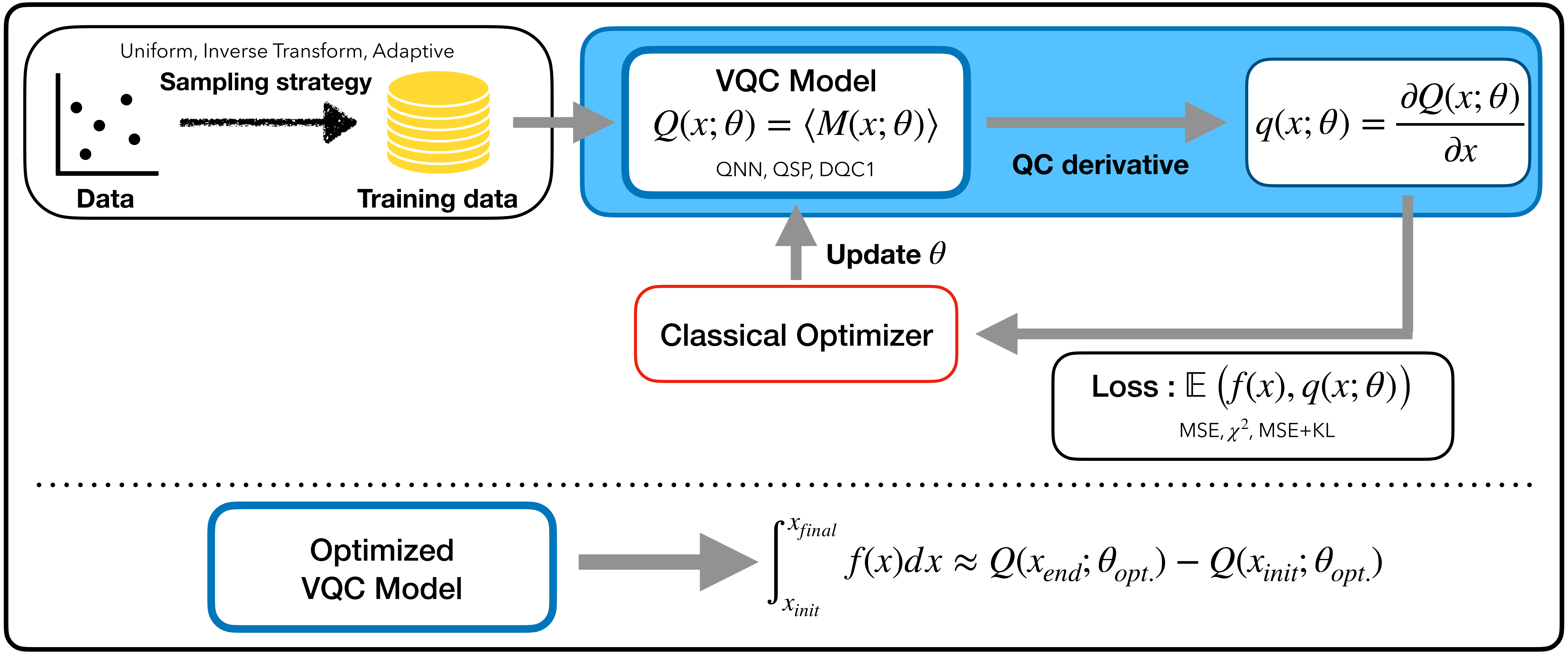
Quantum phenomenon





@Pennylane

Methodology (QuInt-Net)



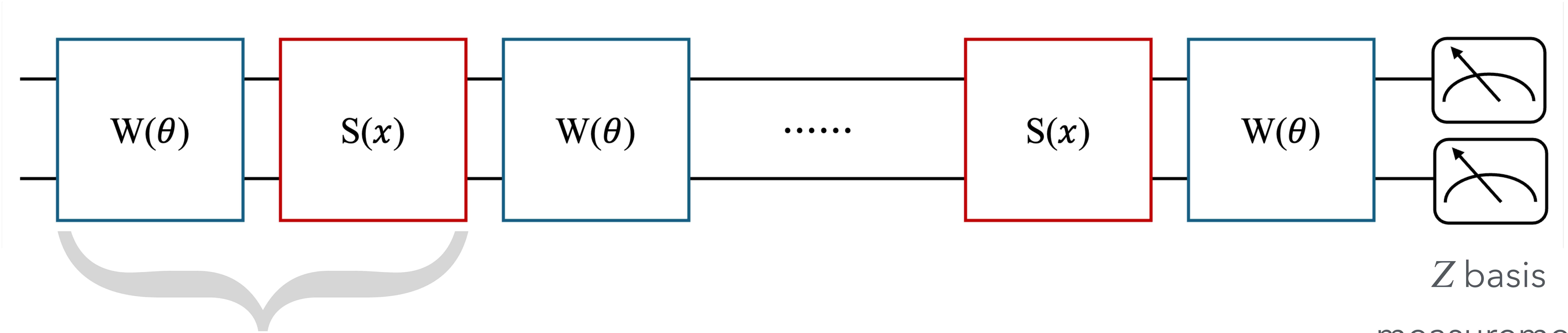
[Quantum Sci.Technol. 9 (2024) 3, 035053] Multi-variable integration with a variational quantum circuit
[arXiv:2510.10501] Quantum Integration Network for Efficient Monte Carlo in High Energy Physics

Methodology (Variational Quantum Circuit)

Basic QNN model

Data Re-uploading method

→ Gives finite Fourier series



Z basis measurement

$R_X(\theta_0)R_Z(\theta_1 \cdot x)R_Y(\theta_2)$ + CZ gate

θ : the trainable parameters

Methodology (Data construction)

Uniform Sampling

- a standard baseline for comparison.
- Samples are generated from a uniform distribution over the domain
- Inefficient for functions with singular features (e.g., resonances) due to slow convergence.

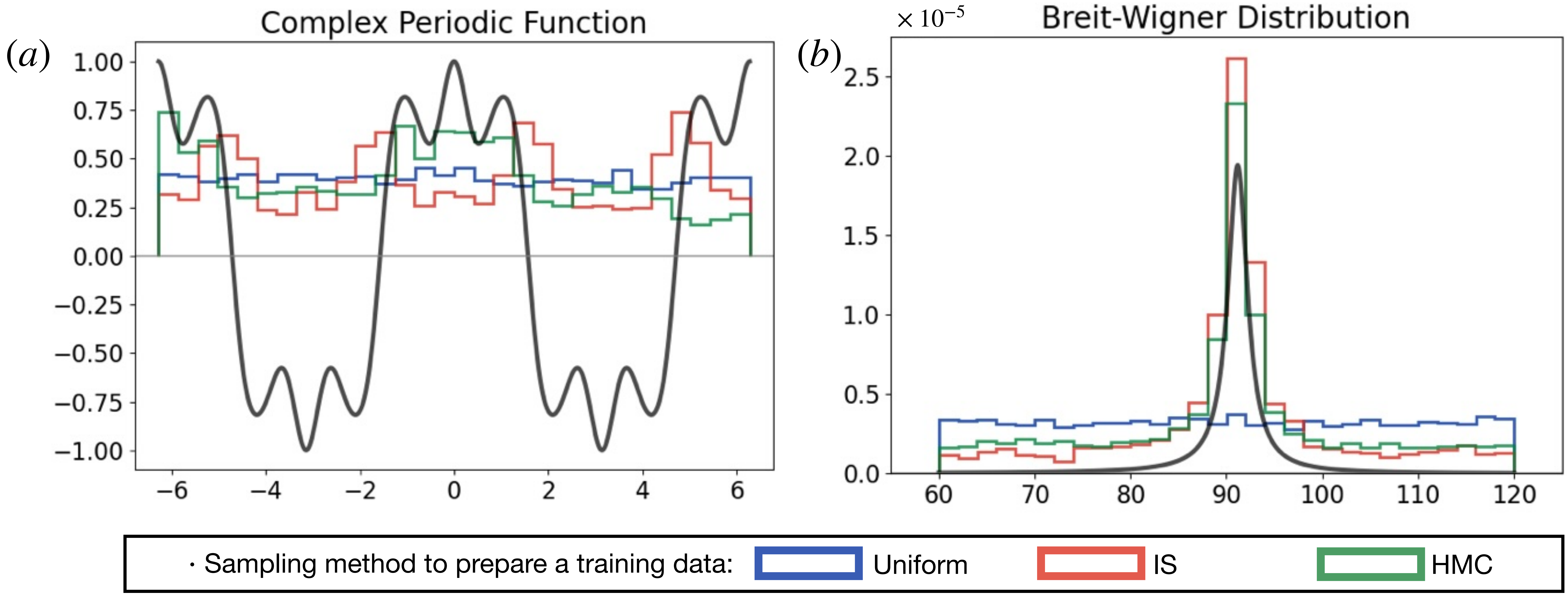
Importance Sampling

- Adopts a variance reduction technique to prioritize "important" regions
- Generates samples based on the derivative of the integrand: $q_{target}(x) \propto (f'(x))^2$.
- **Effectively captures sharp variations and discontinuities.**

HMC sampling

- Adapts Hamiltonian Monte Carlo (MCMC) to navigate complex probability distributions.
- Treats the integrand as a potential field: $H(x, p) = U(x) + K(p)$ where $U(x) = -\log|f(x)|$
- **Allows for large-scale movements to escape local minima and explore peaks**

Methodology (Data construction)



Methodology (Loss function)

Mean-Squared Error (MSE)

- $\mathbb{E}_{\mathrm{MSE}} = \frac{1}{N}\sum_{i=1}^{N}(q(x_i;\theta) - f(x_i))^2$
- Standard metric for regression

χ^2 -weighted loss

- $\mathbb{E}_{\chi^2} = \frac{1}{N}\sum_{i=1}^{N}\frac{(q(x_i;\theta) - f(x_i))^2}{|f(x_i)|}$
- Inspired by the χ^2 statistic to re-weight residuals
- Enhances sensitivity to **lower-magnitude regions** (tails of distributions)

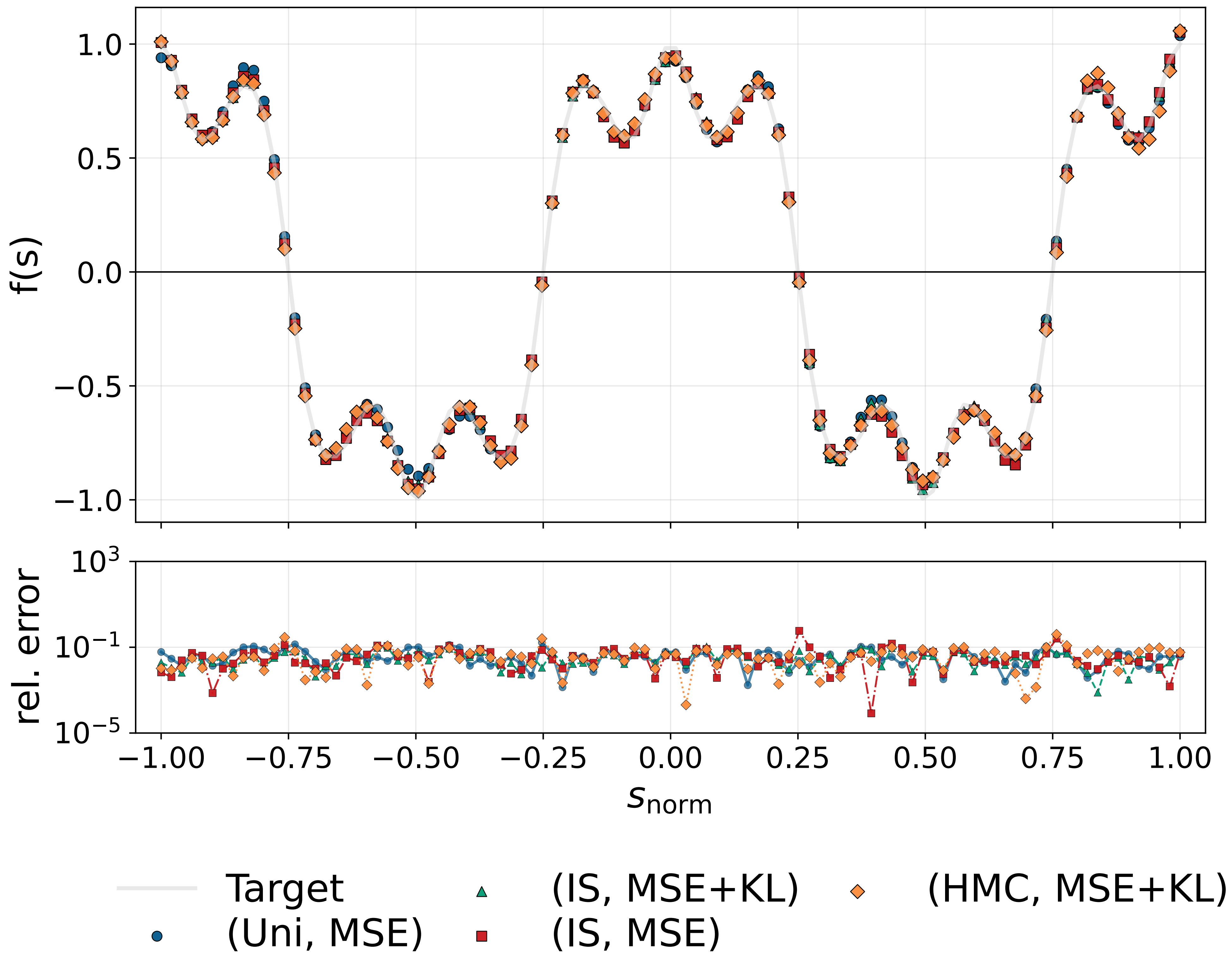
Log-Cosh loss

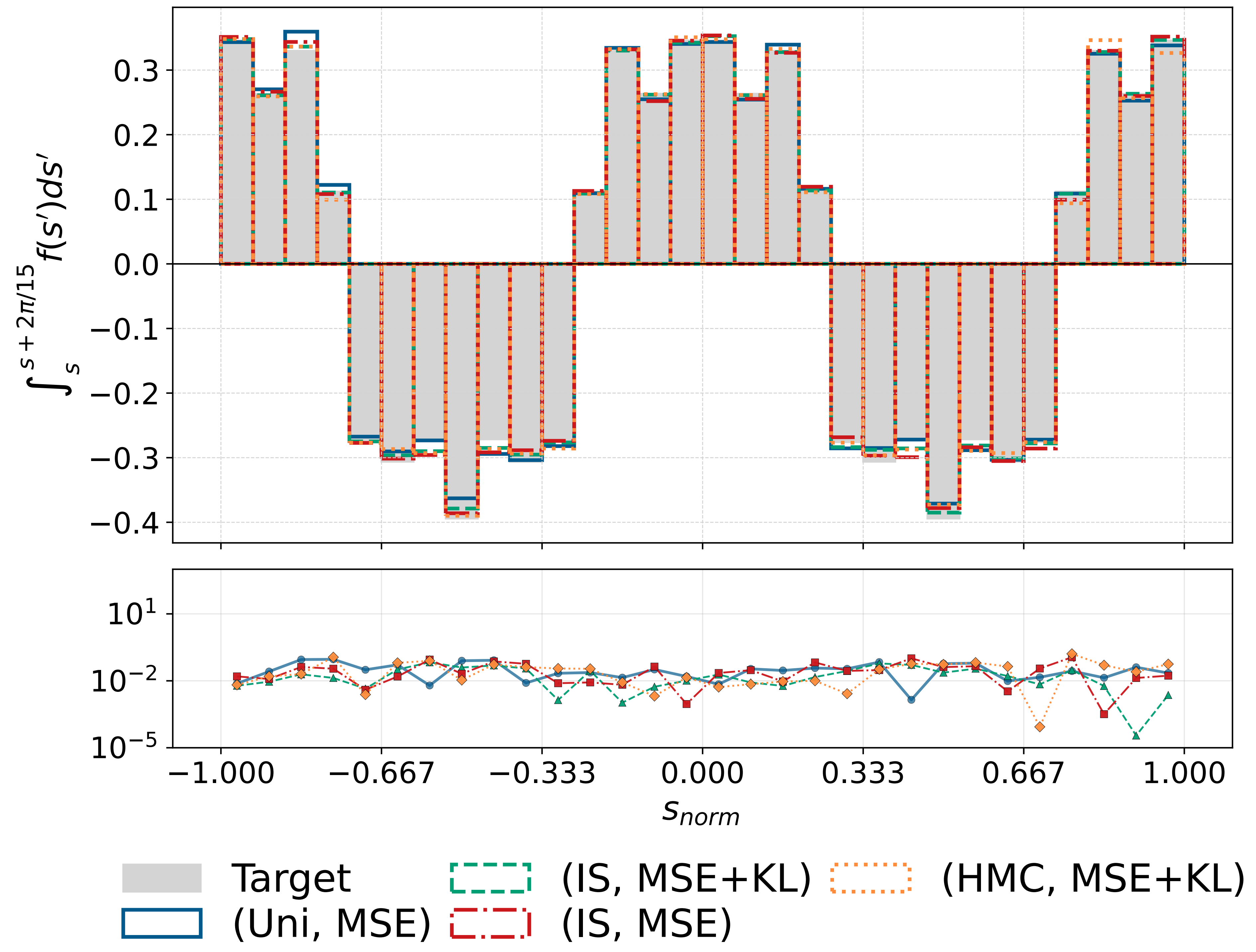
- $\mathbb{E}_{\mathrm{Log-Cosh}} = \frac{1}{N}\sum_{i=1}^{N}\log(\cosh(q(x_i;\theta) - f(x_i)))$
- Smooth interpolation between MSE and Mean Absolute Error (MAE)
- Acts linearly for large errors, making it **less sensitive to outliers**

MSE+KL loss

- $\mathbb{E}_{\mathrm{MSE+KL}} = \mathbb{E}_{\mathrm{MSE}} + \sum_{i=1}^{N}\mathrm{KL}(\sigma(\mathbf{f})\,|\,\sigma(\mathbf{q}_\theta))$
- Applies Softmax (σ) to treat outputs as probability distributions
- Captures the **global structure (shape)** of the integrand, not just point-wise accuracy.

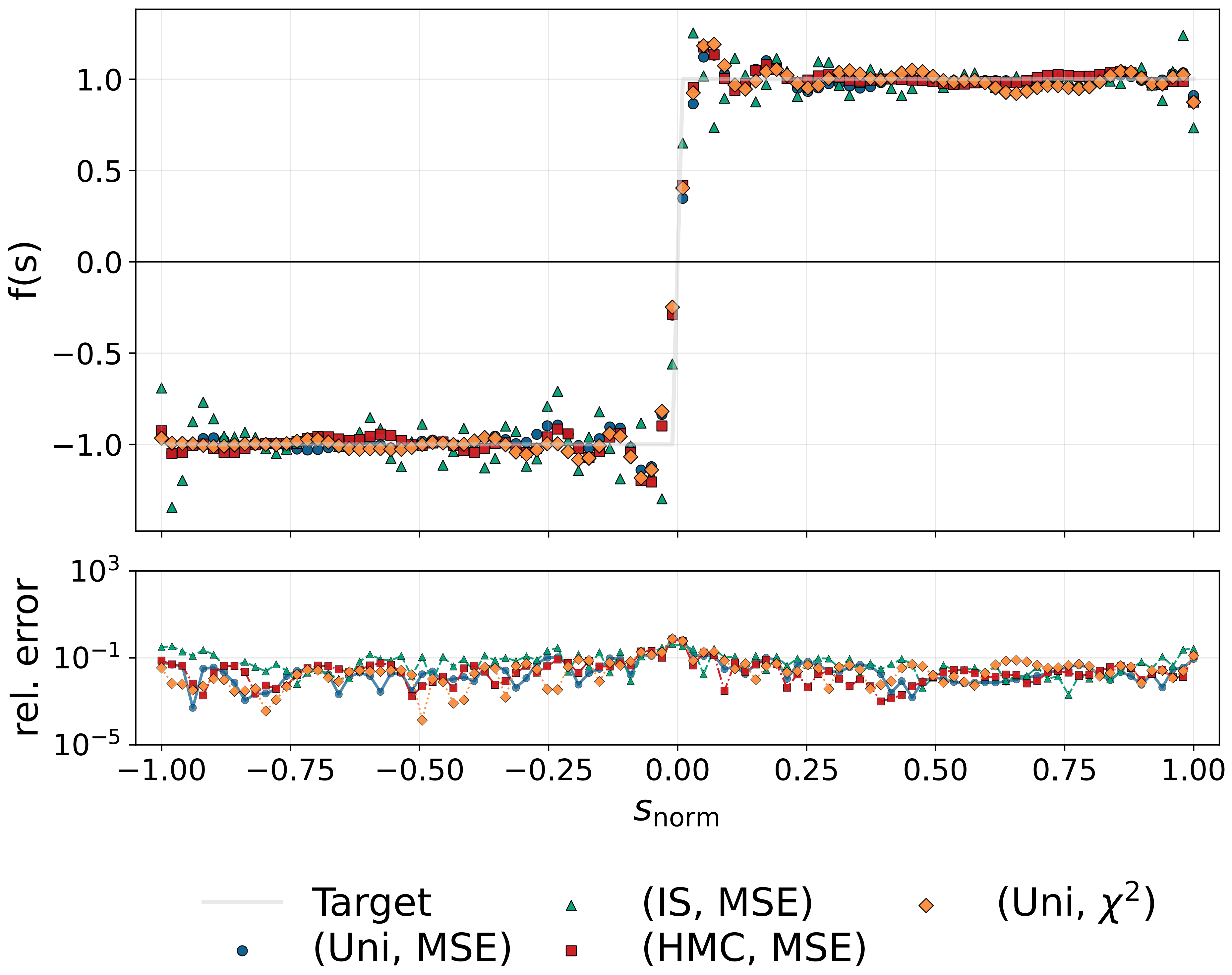
Results (Complex Periodic Function)

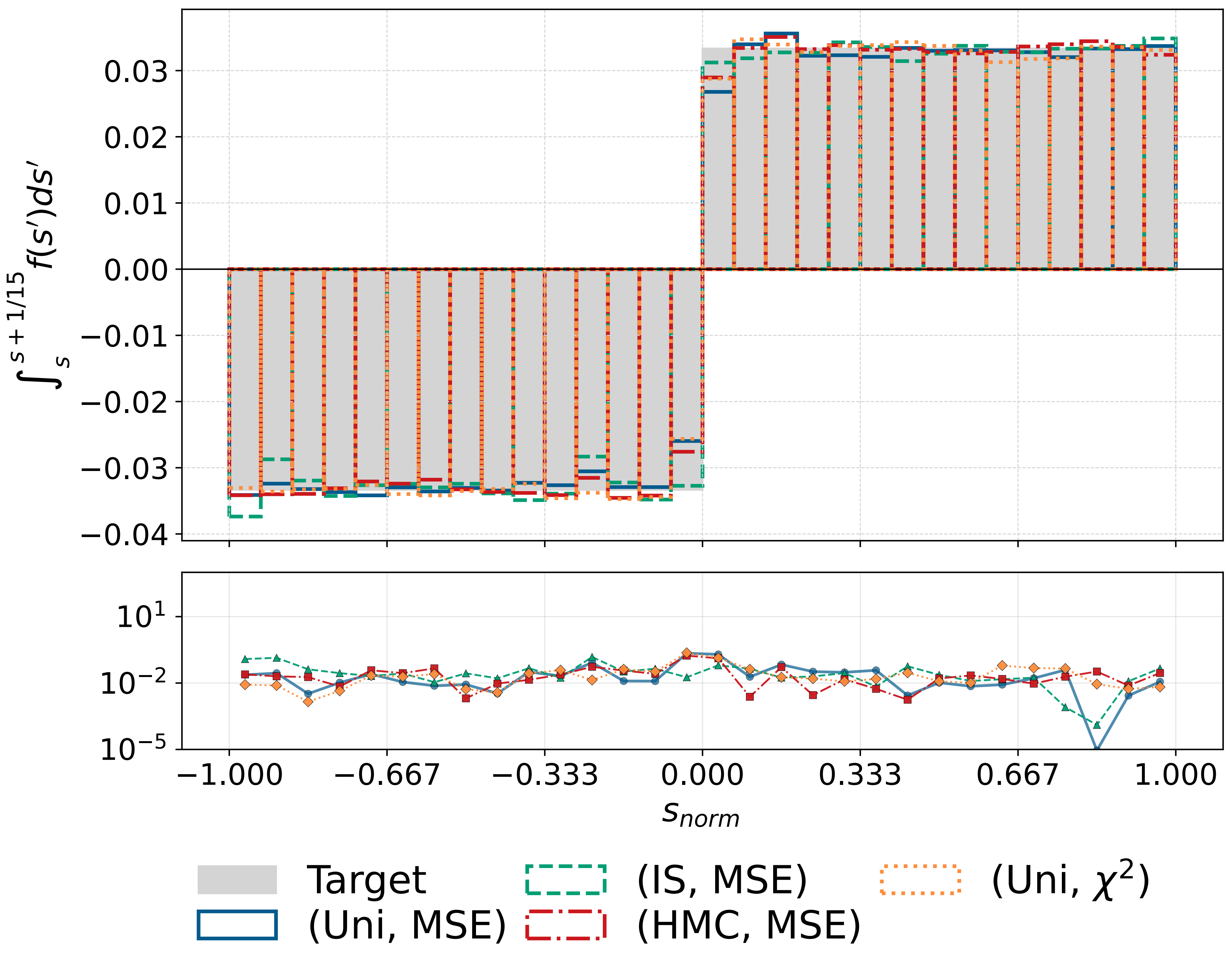




Training Strategy	R^2 (Deriv.)	W_1 (Int.)	$[0, \pi/2]$	$[-\pi/2, \pi/2]$	$[-\pi, \pi]$
(Uni., MSE)	0.9972	0.0635	1.0695 (0.22%)	2.1251 (0.42%)	0.0009
(IS, MSE + KL)	0.9982	0.0062	1.0707 (0.33%)	2.1293 (0.22%)	0.0015
(IS, MSE)	0.9977	0.0100	1.0679 (0.07%)	2.1256 (0.40%)	-0.0055
(HMC, MSE + KL)	0.9975	0.0123	1.0684 (0.12%)	2.1397 (0.25%)	0.0005

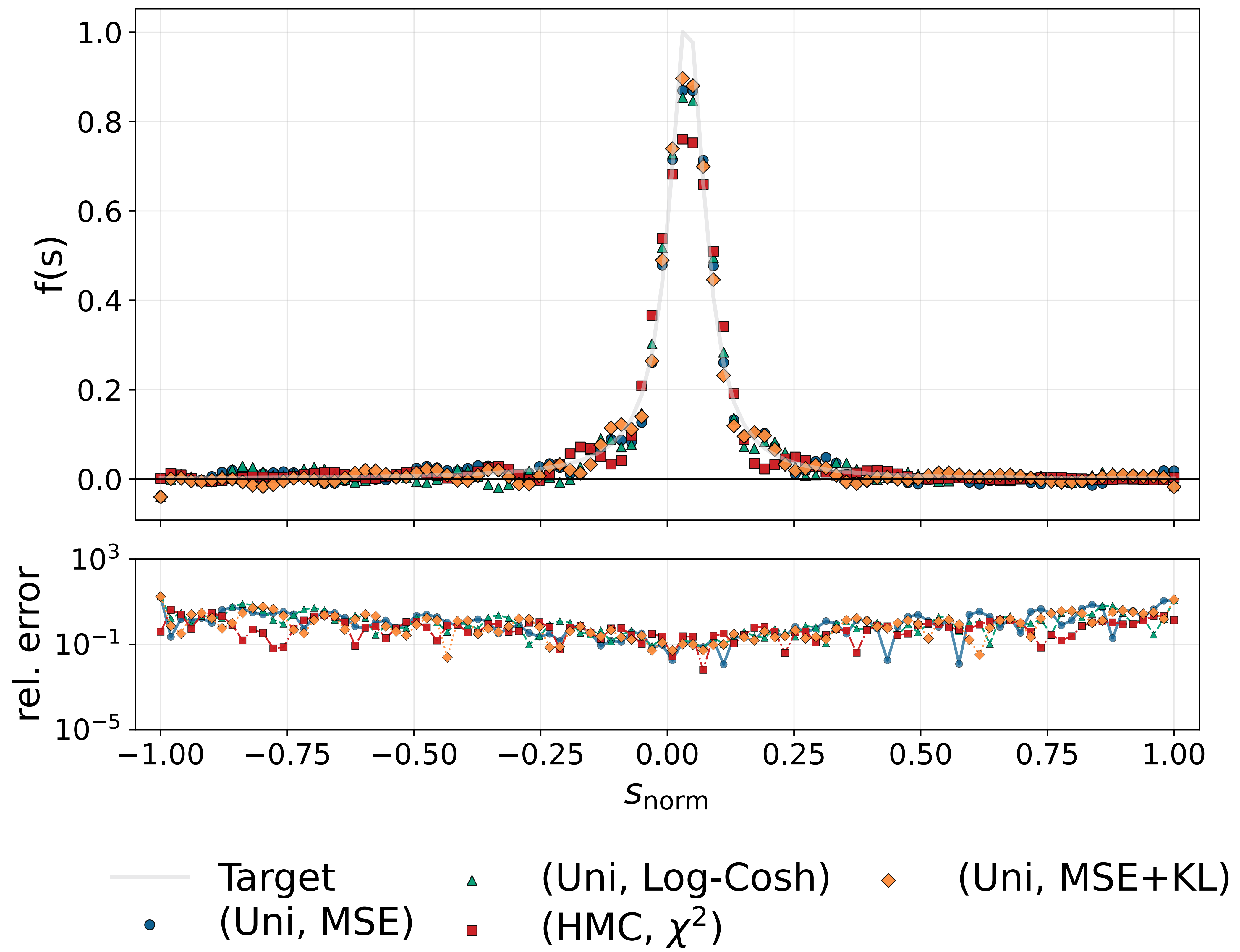
Results (Step Function)

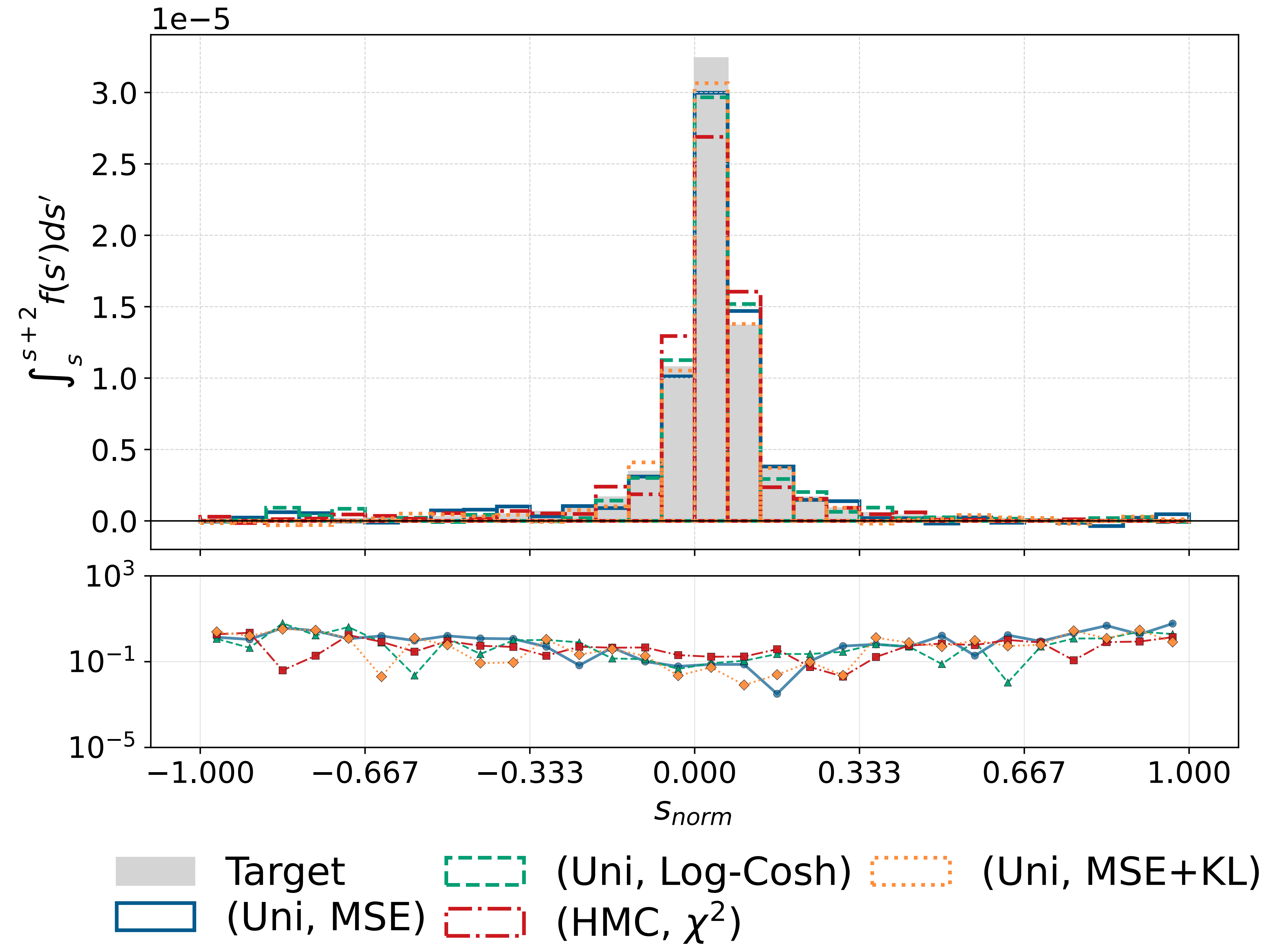




Training Strategy	R^2 (Deriv.)	W_1 (Int.)	$[0, 0.5]$	$[-0.5, 0]$	$[-0.5, 0.5]$
(Uni., MSE)	0.9882	0.0067	0.2429 (2.83%)	-0.2370 (5.19%)	0.0058
(IS, MSE)	0.9856	0.0031	0.2443 (2.28%)	-0.2464 (1.40%)	-0.0021
(HMC, MSE)	0.9890	0.0040	0.2474 (1.03%)	-0.2460 (1.60%)	0.0013
(Uni., χ^2 Loss)	0.9879	0.0043	0.2492 (0.32%)	-0.2453 (1.88%)	0.0039

Results (HEP application)





Training Strategy	R^2 (Deriv.)	W_1 (Int.)	$[M_Z \pm 3\Gamma]$	$[M_Z \pm 5\Gamma]$	$[M_Z \pm 10\Gamma]$
(Uni., MSE)	0.9804	0.0084	6.4476 (5.07%)	6.7863 (4.57%)	6.9471 (5.58%)
(Uni., Log-Cosh)	0.9732	0.0074	6.5534 (3.51%)	6.7091 (5.65%)	6.9818 (5.11%)
(HMC, χ^2 Loss)	0.9472	0.0076	6.4752 (4.66%)	6.7543 (5.02%)	6.9806 (5.13%)
(Uni., MSE+KL)	0.9848	0.0106	6.5748 (3.20%)	6.7207 (5.49%)	6.9180 (5.98%)

Results (HEP application)

Sampling	Loss	Gate Error	Bit Flip	Depolarizing
Uni	MSE	6.9125(±0.0755)(6.05%)	7.1493(2.83%)	7.0412(4.30%)
	Chisqr	5.8253(±0.0561)(20.83%)	5.7385(22.01%)	5.7283(22.15%)
	Log-Cosh	7.1272(±0.0598)(3.13%)	7.0292(4.47%)	7.0305(4.45%)
	MSE+KL	**7.2659**(±**0.0711**)(**1.25**%)	6.8596(6.77%)	**7.3366**(**0.29**%)
IS	MSE	6.7596(±0.760)(8.13%)	7.1136(3.32%)	7.0138(4.68%)
	Chisqr	6.6463(±0.0483)(9.67%)	6.8816(6.47%)	6.9516(5.52%)
	Log-Cosh	6.6472(±0.0947)(9.66%)	7.2050(2.08%)	6.7378(8.43%)
	MSE+KL	6.6799(±0.1151)(9.21%)	6.9450(5.61%)	6.9068(6.13%)
HMC	MSE	6.9905(±0.0817)(4.99%)	6.9769(5.18%)	7.0133(4.68%)
	Chisqr	6.8548(±0.0507)(6.84%)	6.8018(7.56%)	6.7859(7.77%)
	Log-Cosh	6.8899(±0.0933)(6.36%)	**7.2212**(**1.86**%)	6.7862(7.77%)
	MSE+KL	7.5085(±0.1215)(2.04%)	6.7414(8.38%)	7.0583(4.07%)

Calculate the BW distribution across $[M_Z \pm 10\Gamma]$ with noise 0.1% environment

Summary

VQC-based Integration Framework (QuInt-Net)

- Developed QuInt-Net, a VQC framework incorporating adaptive sampling and tailored loss functions to handle singular structures.

Flexible Evaluation of Integrals

- Approximates the antiderivative globally, enabling efficient evaluation over any arbitrary sub-interval without retraining.

Robustness against Hardware Noise

- Demonstrates robustness against NISQ noise (Gate, Bit-flip, Depolarizing)

Future Work

1. **QuInt-Net as a Starting point**
    - QuInt-Net serves as a benchmark model for QML-based numerical integration.
    - Establishes the feasibility of handling singular structures using variational quantum circuits.
2. **Technical Extension**
    - High-Dimensionality: Scaling the framework to multi-dimensional phase-space integrals
    - Real Hardware Implementation: Validating noise robustness on physical quantum processors (e.g., IonQ, IBM) beyond simulation
3. **Evolution to Quantum Integral Calculation**
    - Extending the current supervised learning approach to Quantum Monte Carlo Integral.
    - Utilizing quantum advantages (e.g., superposition, entanglement) not just for function approximation, but for direct, efficient sampling of the phase space.