

Unlocking Multi-Dimensional Integration with Quantum Adaptive Importance Sampling

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Paper



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Theoretical Predictions in HEP

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- Computational Bottleneck: Prediction beyond LO requires numerical integration of multi-dimensional integrals with complicated structures.

$$\hat{\sigma}_{ab \rightarrow 1 \dots n} = \frac{1}{2\sqrt{\lambda((p_a + p_b)^2, m_a^2, m_b^2)}} \int \prod_{j=1}^n \frac{d^3 \mathbf{p}_j}{(2\pi)^3 2\sqrt{\mathbf{p}_j^2 + m_j^2}} (2\pi)^4 \delta^{(4)}\left(p_a + p_b - \sum_{j=1}^n p_j\right) \int \prod_{k=1}^L d^4 l_k \left| \mathcal{M}_{ab \rightarrow 1 \dots n}(\{p\}, \{l\}) \right|^2$$

Phase space integrals

Multi-loop Feynman diagrams
Integrals over loop momenta

Monte Carlo and Importance Sampling

Standard Monte Carlo: By drawing N i.i.d. random samples $\{\mathbf{x}_i\}_{i=1}^N$, the integral is estimated by:

$$I = \int_{\Omega} f(\mathbf{x}) d\mathbf{x} , \quad \hat{I}_N^{(\text{MC})} = \frac{|\Omega|}{N} \sum_{i=1}^N f(\mathbf{x}_i) = |\Omega| \langle f \rangle , \quad \left(\hat{\sigma}_N^{(\text{MC})} \right)^2 = \frac{|\Omega|^2}{N-1} \left(\frac{1}{N} \sum_{i=1}^N f(\mathbf{x}_i)^2 - \langle f \rangle^2 \right) .$$

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Importance Sampling: **Variance reduction Technique.** Using a $q(\mathbf{x})$ as the proposal Probability Density Function (PDF) that is **computationally efficient** to sample from and **resembles** $f(\mathbf{x})$.

the integral is reformulated as:

$$I = \int_{\Omega} \frac{f(\mathbf{x})}{q(\mathbf{x})} q(\mathbf{x}) d\mathbf{x}, \quad \hat{I}_N^{(\text{IS})} = \frac{1}{N} \sum_{i=1}^N \frac{f(\mathbf{x}_i)}{q(\mathbf{x}_i)}. \quad \left(\hat{\sigma}_N^{(\text{IS})} \right)^2 = \frac{1}{N-1} \left(\frac{1}{N} \sum_{i=1}^N \frac{f(\mathbf{x}_i)^2}{q(\mathbf{x}_i)^2} - \left(\hat{I}_N^{(\text{IS})} \right)^2 \right).$$

Adaptive Importance Sampling:

- VEGAS is an Adaptive Importance Sampling Algorithm

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- Generates N uniform samples in $\mathbf{y} \in [0,1]^d$ ($\mathbf{y}$ is discretised) .

- Maps to the original space: $\mathbf{y} \mapsto \mathbf{x}(\mathbf{y})$, through the Jacobian transformation: $J(\mathbf{y}) = \left| \frac{d\mathbf{x}}{d\mathbf{y}} \right|$.

$$\text{1-D grid: } \underbrace{x_0 = a, x_i = x_{i-1} + \Delta x_{i-1}, x_{N_g} = b}_{\text{Interval: } [a,b]}, \quad x(y) = x_i + \Delta x_i(N_g y - i), \quad i = \lfloor N_g y \rfloor, \quad J(y) = N_g \Delta x_i.$$

N_g : Number of Grid cells per dimension/Constant everywhere

- The integral becomes: $I = \int_{[0,1]^d} J(\mathbf{y}) f(\mathbf{x}(\mathbf{y})) d\mathbf{y}$

$$\text{Integral Estimator: } \hat{I}_N^{(\text{VEGAS})} = \frac{1}{N} \sum_{i=1}^N J(\mathbf{y}_i) f(\mathbf{x}(\mathbf{y}_i))$$

$$\text{Variance Estimator: } \left(\hat{\sigma}_N^{(\text{VEGAS})} \right)^2 = \frac{1}{N-1} \left(\frac{1}{N} \sum_{k=1}^N J^2(\mathbf{y}_k) f^2(\mathbf{x}(\mathbf{y}_k)) - \left(\hat{I}_N^{(\text{VEGAS})} \right)^2 \right)$$

VEGAS

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- Efficiently finds important structures but creates **phantom structures** ,
that lead to oversampling of irrelevant parts of the integration domain.

Quantum Monte Carlo

Typical Quantum Computational Approach:

QAE for quadratic advantage in RMSE.

A. Montanaro, Proc. R. Soc. A 471, 20150301 (2015).

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Our approach:

Parenthesis Factor: Gets smaller as $q(\mathbf{x}) \rightarrow f(\mathbf{x}) \longrightarrow$ Precision critically relies on the proposal PDF

Starting Point: In HEP, that standard is the **VEGAS** algorithm

Conceptual basis:

- **Quantum Adaptive Importance Sampling (QAIS):**

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- IS targets small, high-impact regions.
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○ Objective:

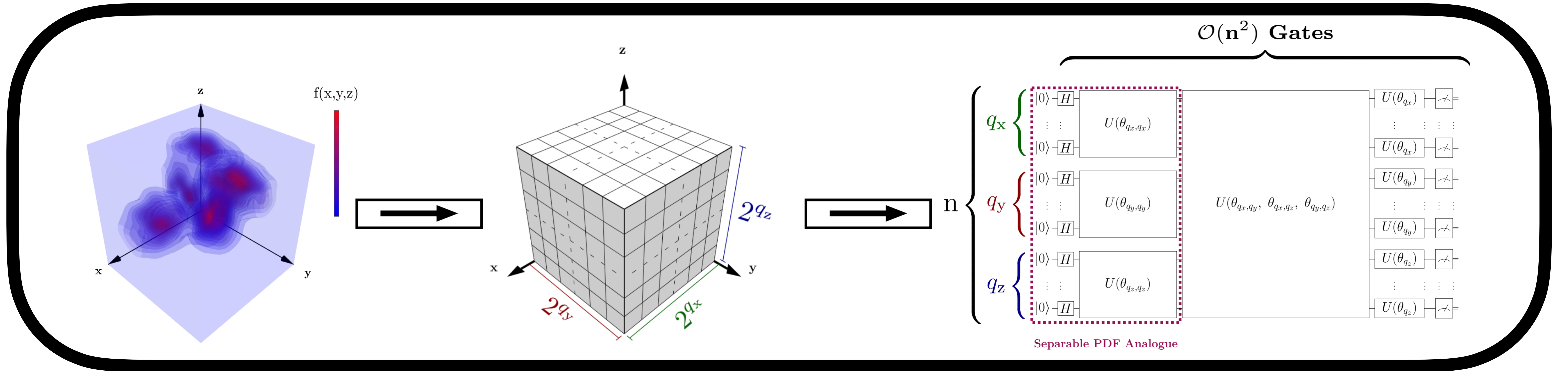
1. Reach target accuracy with fewer samples (function evaluations).

or

2. For a certain samples budget, reach better accuracy.

Quantum Adaptive Importance Sampling

Encoding:

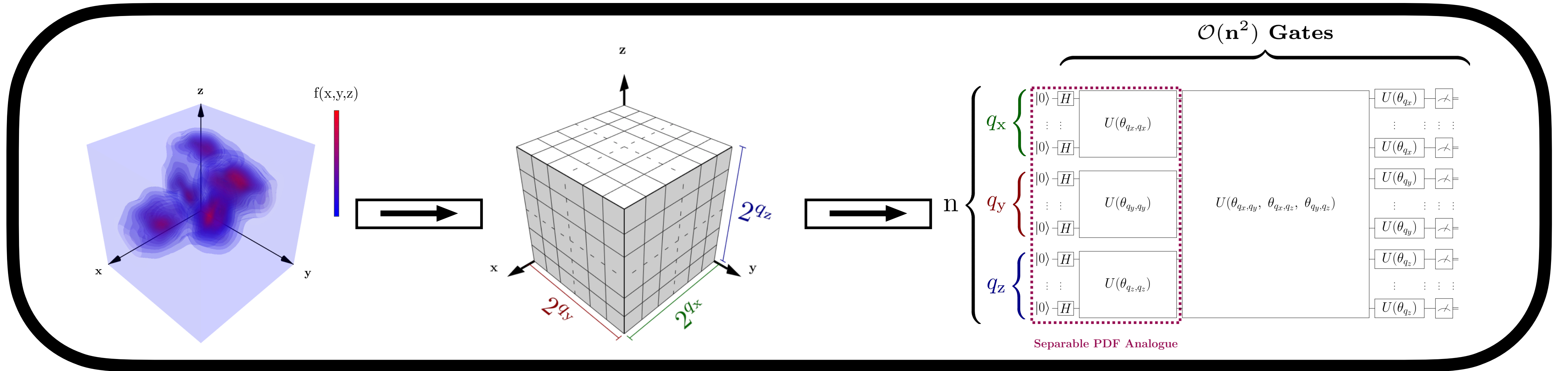


- Domain $\Omega = \prod_{i=1}^d [a_i, b_i]$. Per dimension $i : q_i$ qubits $\rightarrow 2^{q_i}$ grid cells .

$$\text{Total qubits : } n = \sum_{i=1}^d q_i \xrightarrow{\text{Generating}} 2^n \text{ Grid Cells . Cell Width per dimension } i : \Omega_i = \frac{b_i - a_i}{2^{q_i}}.$$

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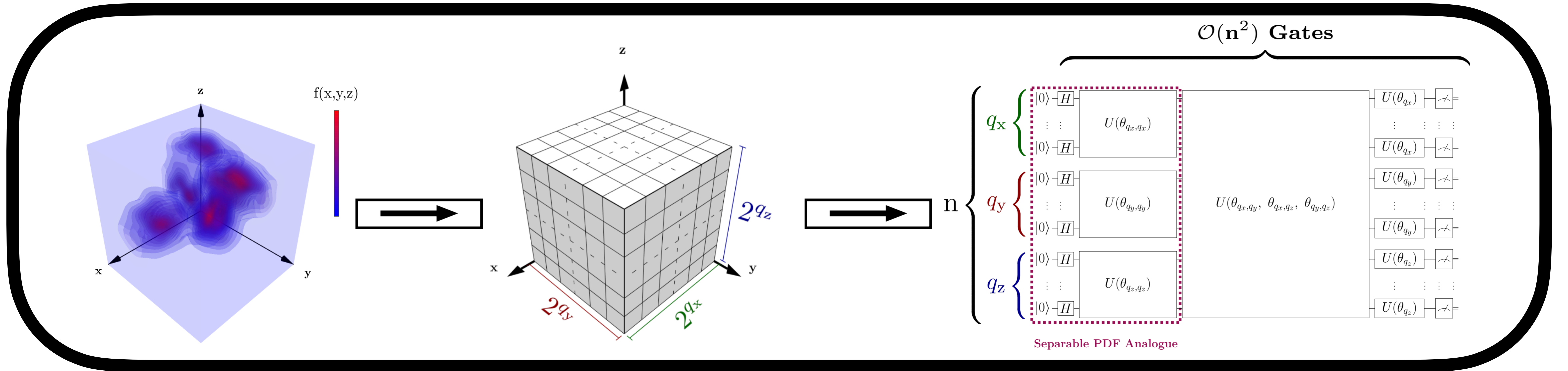
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- 1-1 map between grid cells and basis states:

$$\text{State with index (Big Endian Encoding) } |j\rangle = |j_1\rangle \dots |j_d\rangle = (j_1, \dots, j_d) \text{ maps to the cell: } \Omega^{(j)} = \prod_{i=1}^d [a_i + j_i \Omega_i, a_i + (j_i + 1) \Omega_i]$$

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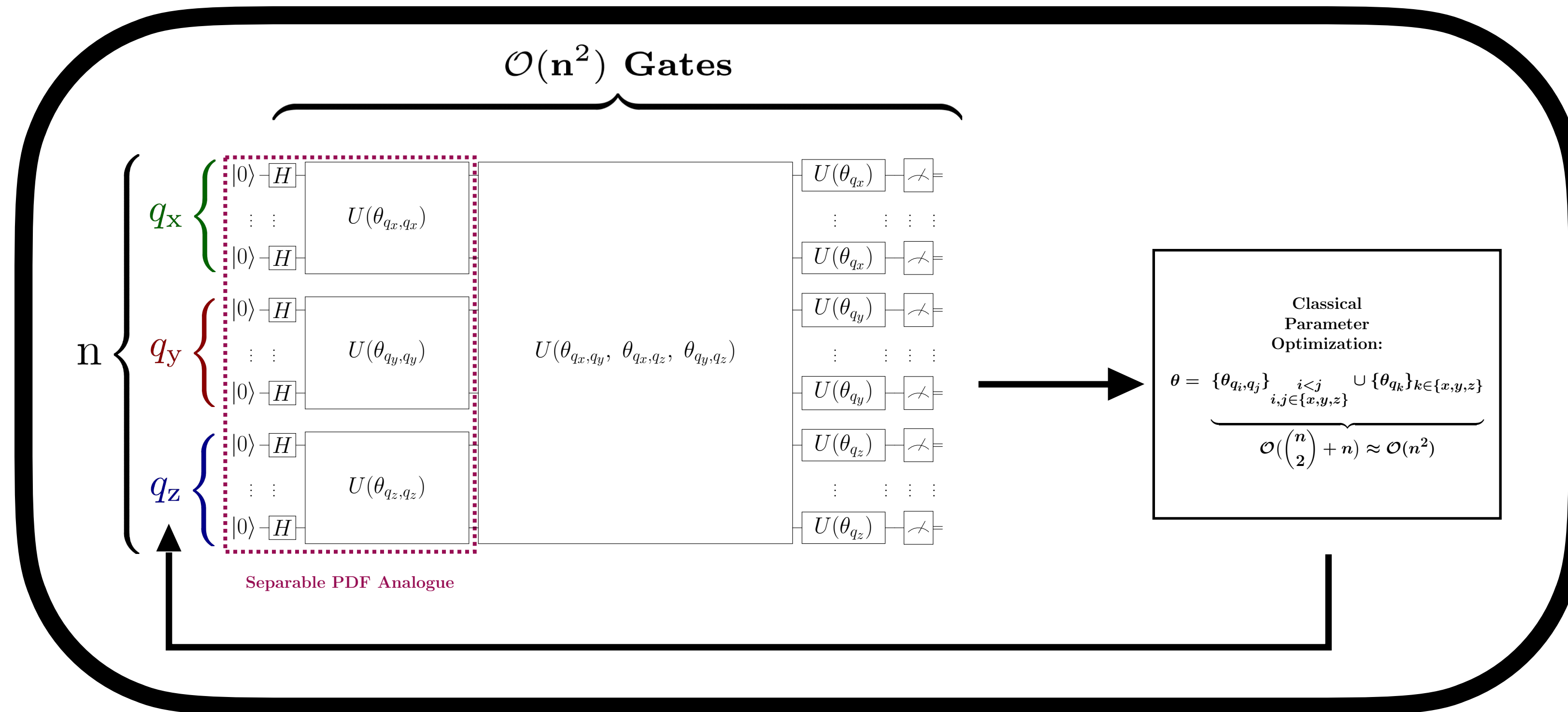
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- Proposal PDF:** $q(\mathbf{x}) = \sum_{j_1, \dots, j_d} |c_{(j_1, \dots, j_d)}|^2 \prod_{i=1}^d \frac{1}{\Omega_i} \left[\Theta(x_i - (a_i + j_i \Omega_i)) - \Theta(x_i - (a_i + (j_i + 1) \Omega_i)) \right]$ (Generally Non-Separable)

Quantum Adaptive Importance Sampling

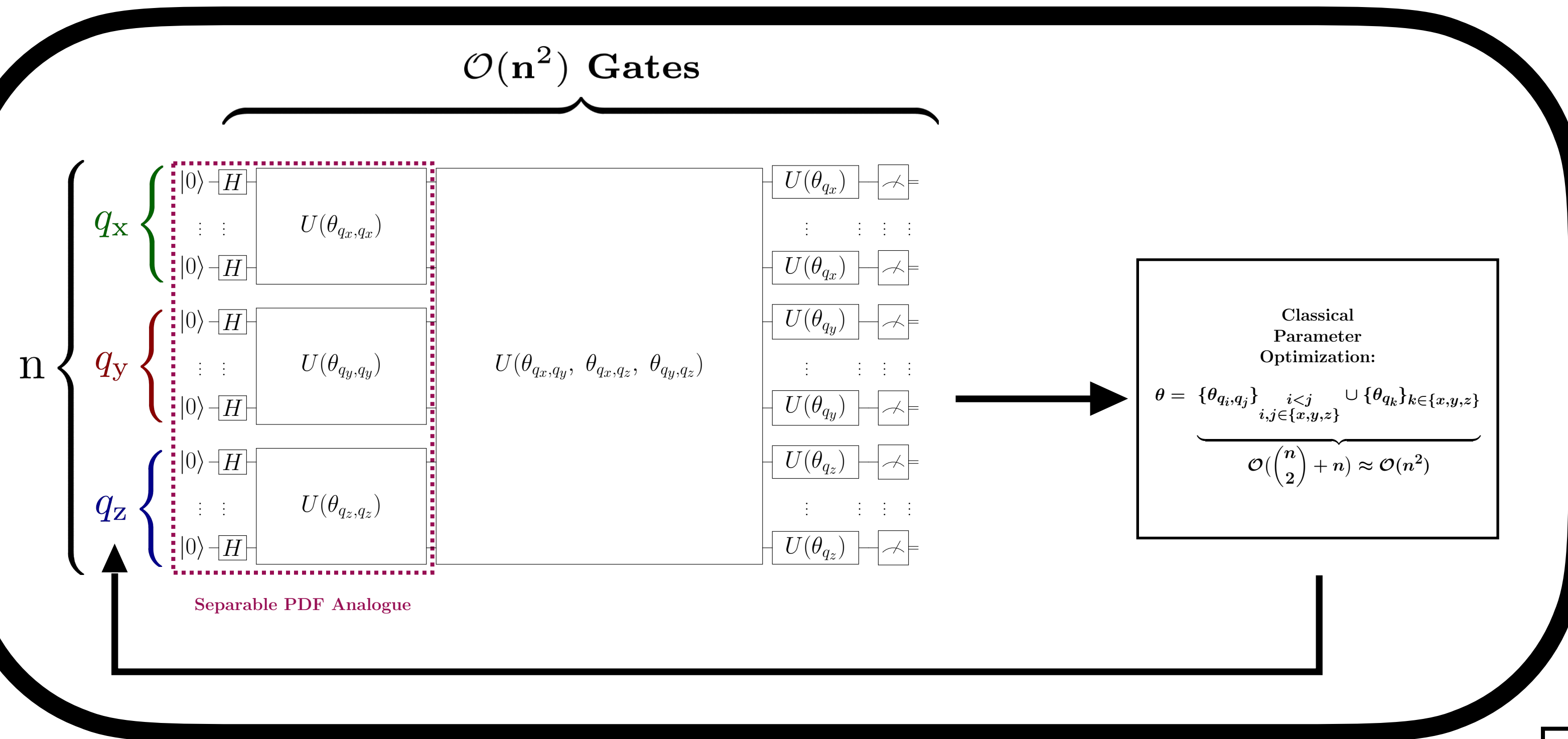
State Preparation:



- Quantum Generative Modelling for State preparation.
- SV Quantum Simulation
- Cost Function: Discretized KL-Divergence
- Optimiser: COBYLA

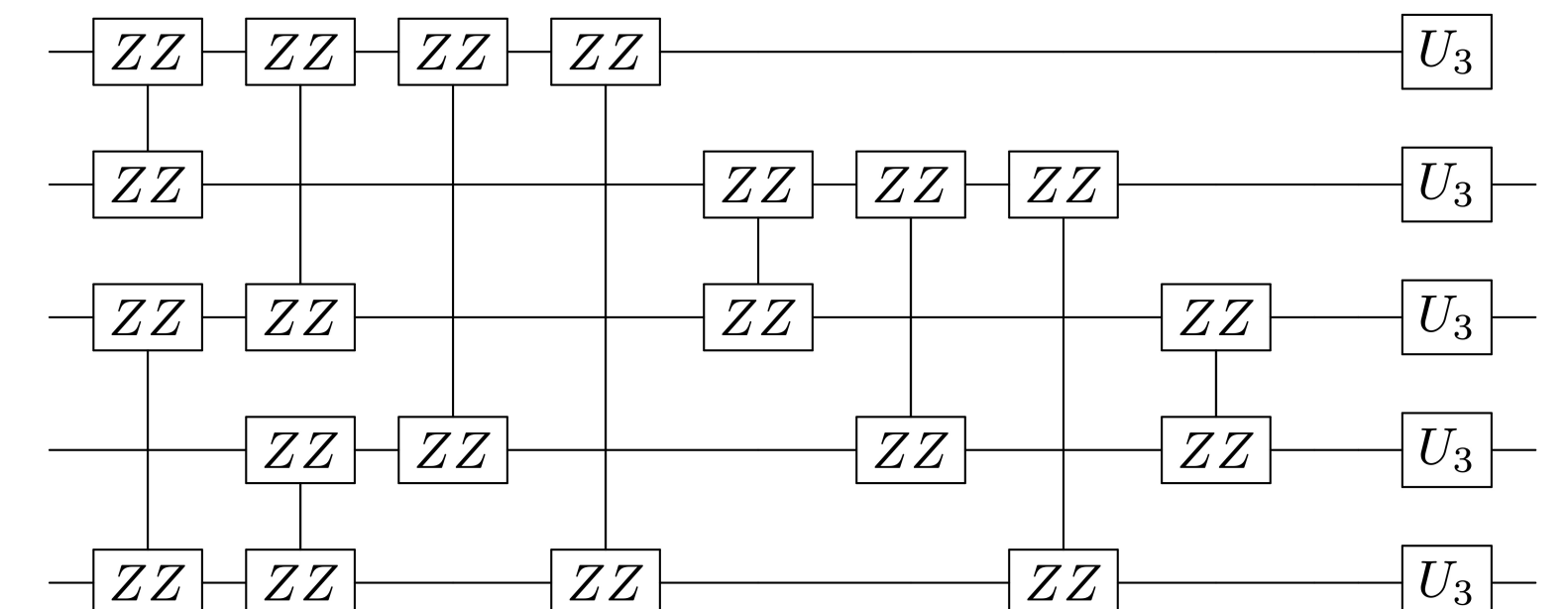
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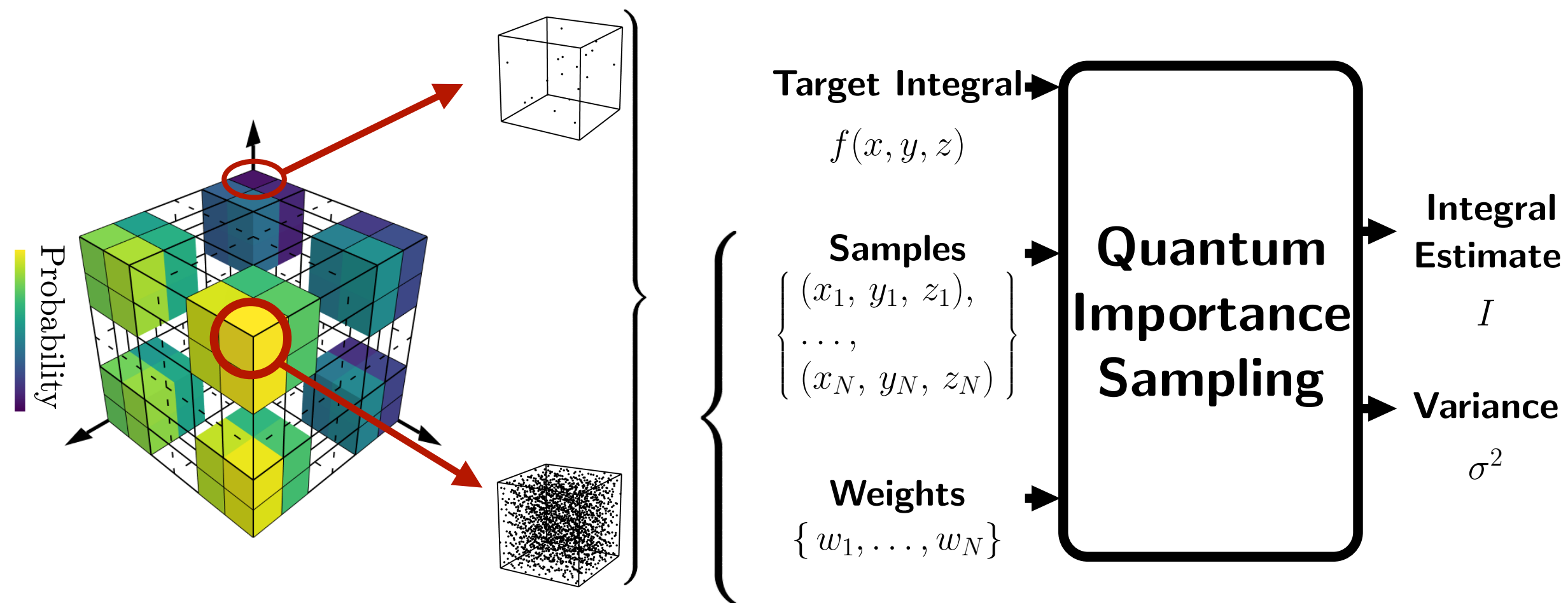
5-Qubit Example



- PQC: all-to-all connectivity 2-qubit gates (QAOA-inspired):
- Number of gates and parameters: $\mathcal{O}(n^2)$:

Quantum Adaptive Importance Sampling

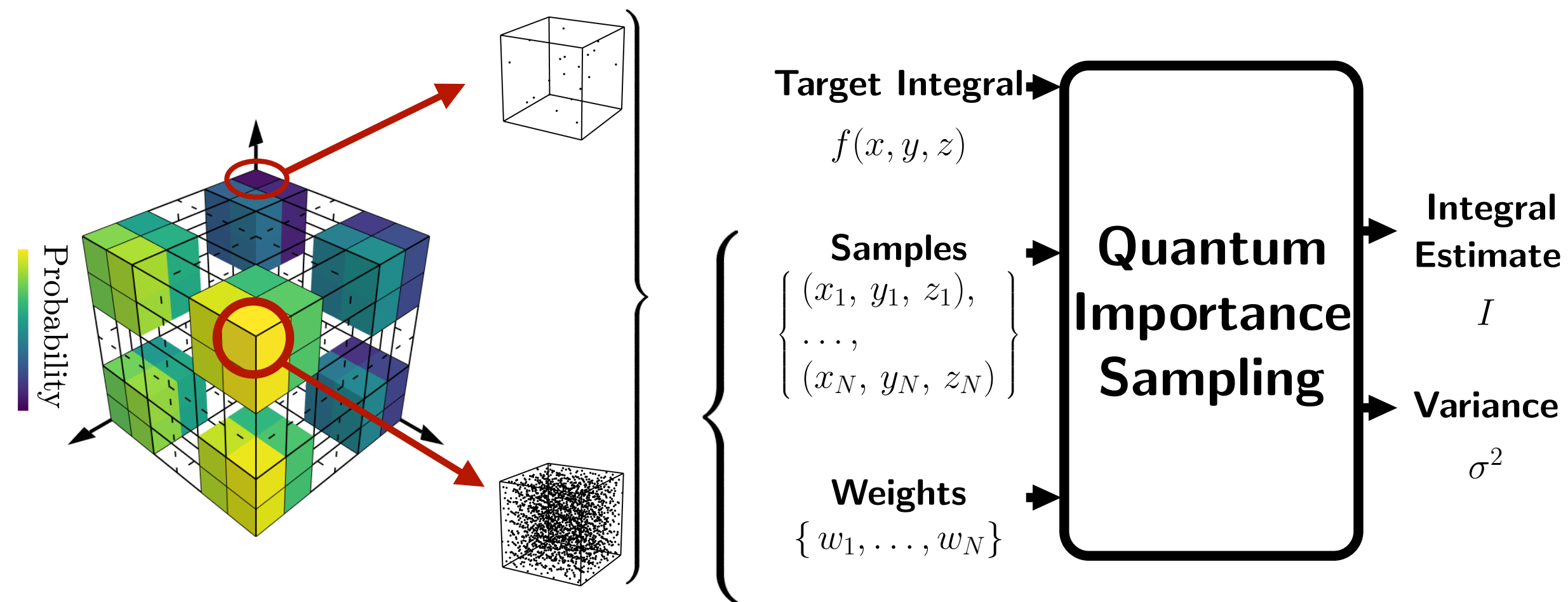
Integral Estimation:



- Direct Sampling:
 N measurements.
 N_j counts per state $|j\rangle$ or cell $\Omega^{(j)}$.
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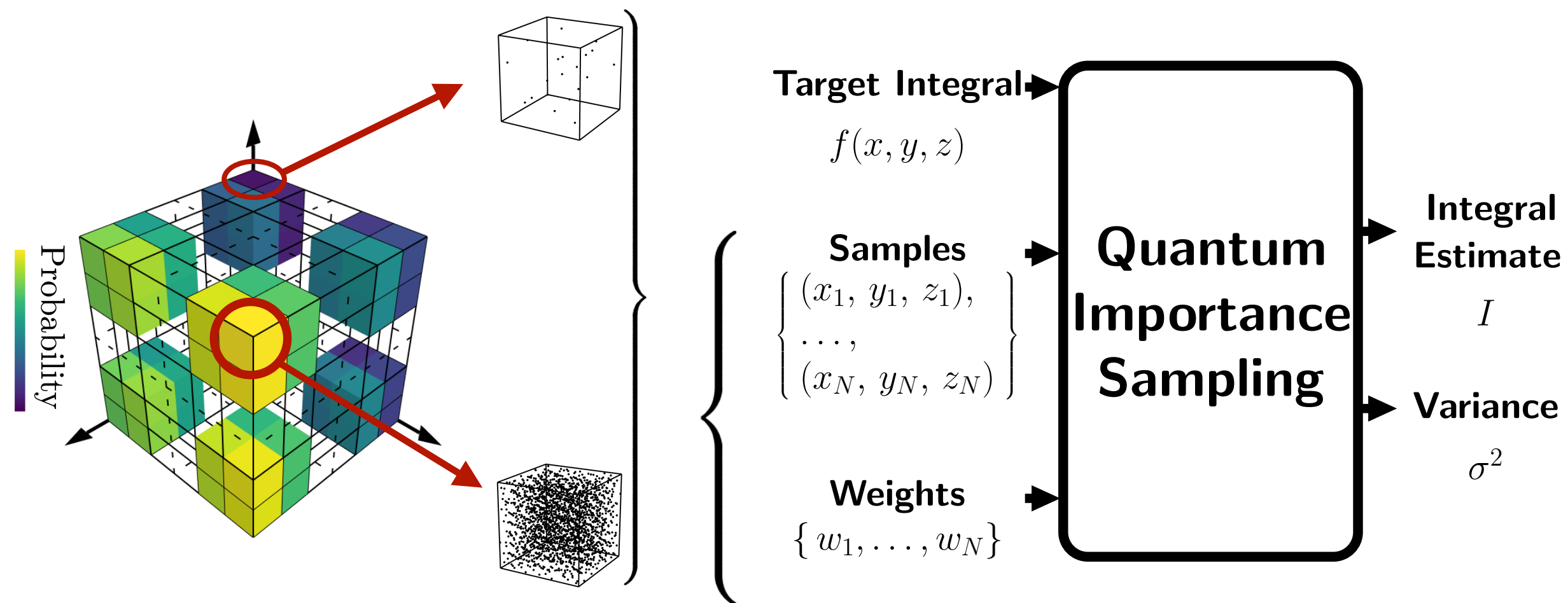
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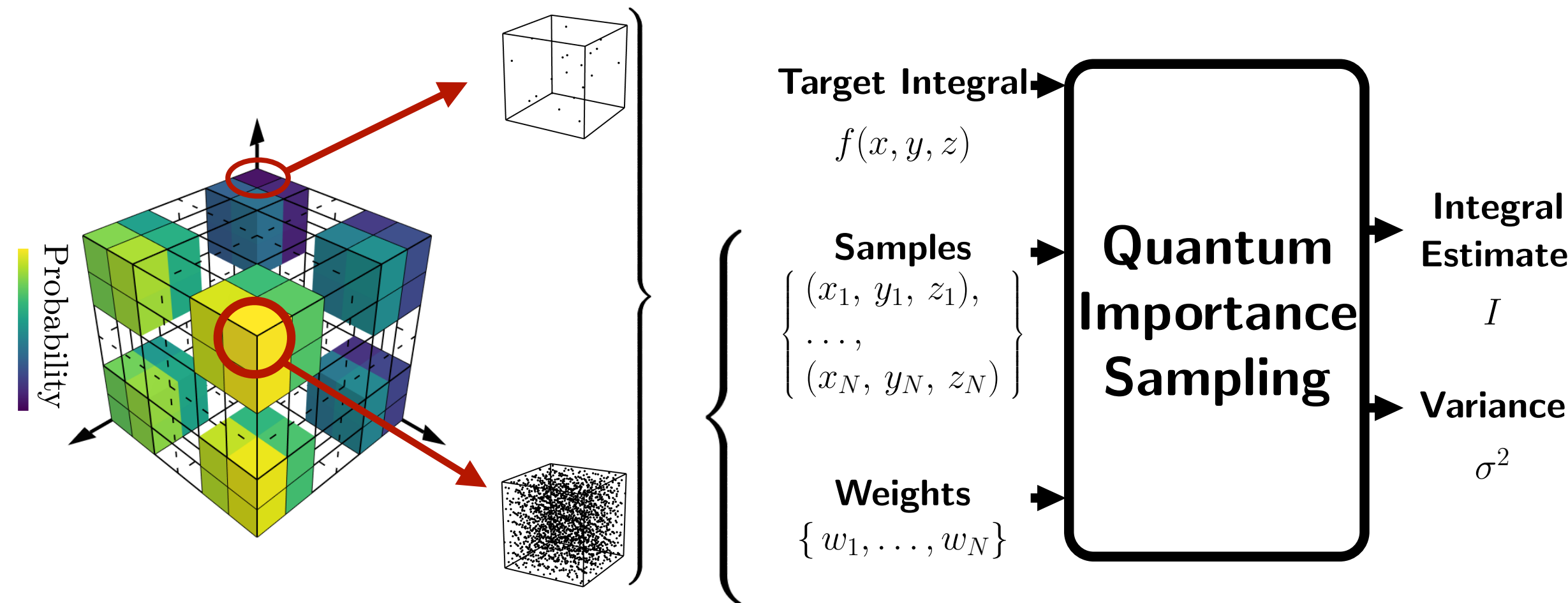
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- Naive Integral estimator and variance:

$$\hat{I}_N^{(\text{QAIS})} = \frac{1}{N} \sum_{i=1}^N w^{(j)} f(\mathbf{x}_i^{(j)}), \quad w^{(j)} = \frac{|\Omega^{(j)}|}{p_j}.$$

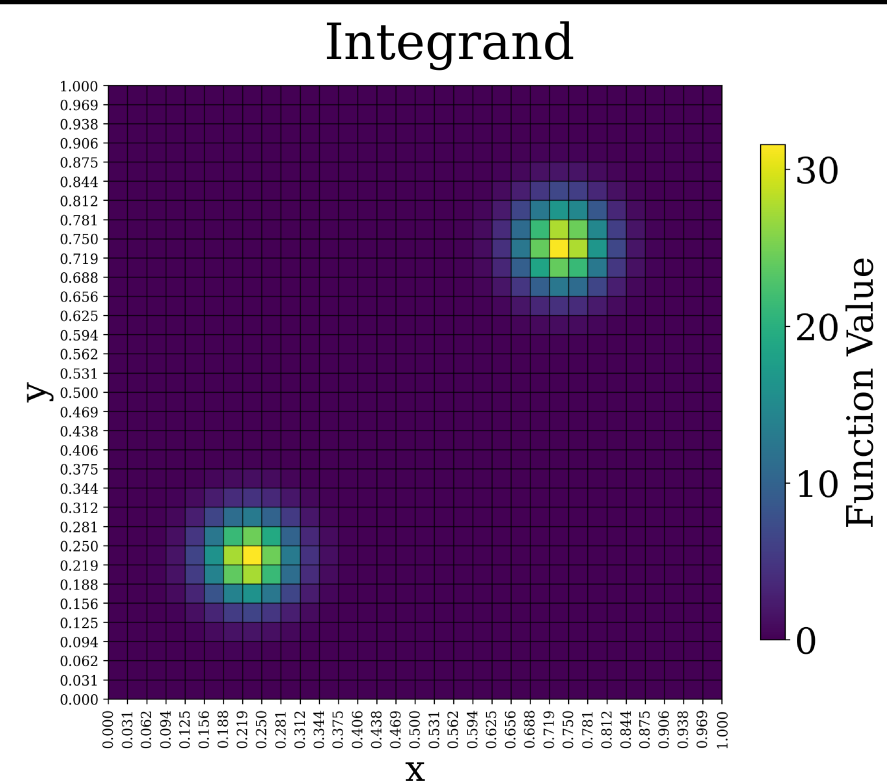
$$\left(\hat{\sigma}_N^{(\text{QAIS})}\right)^2 = \frac{1}{N-1} \left(\frac{1}{N} \sum_{i=1}^N \left[w^{(j)} f(\mathbf{x}_i^{(j)}) \right]^2 - \left(\hat{I}_N^{(\text{QAIS})} \right)^2 \right)$$

$\Omega^{(j)}$: j -th grid cell $\equiv j$ -th quantum state
 $\mathbf{x}_i^{(j)}$: i -th random point at grid cell j
 N : Number of shots
 N_j : Number of times state j was measured

Quantum Adaptive Importance Sampling

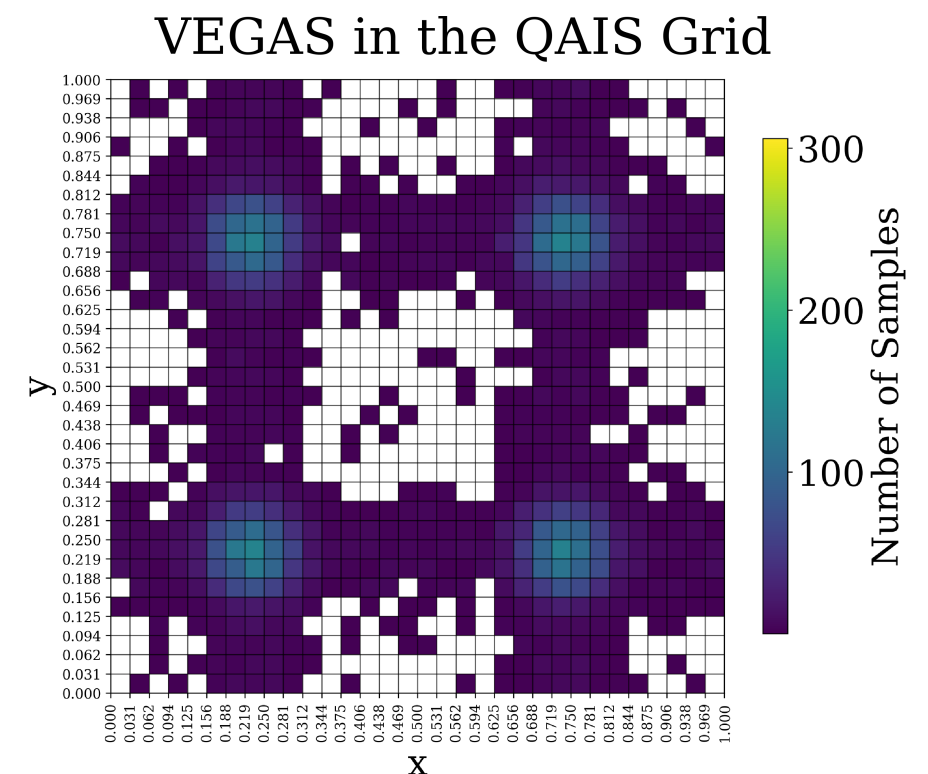
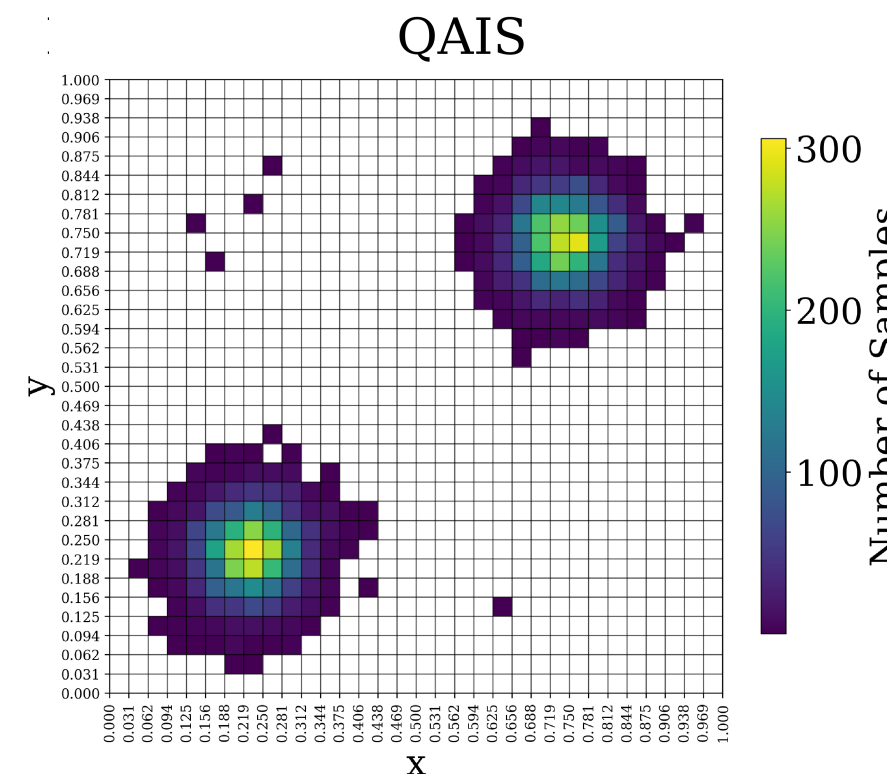
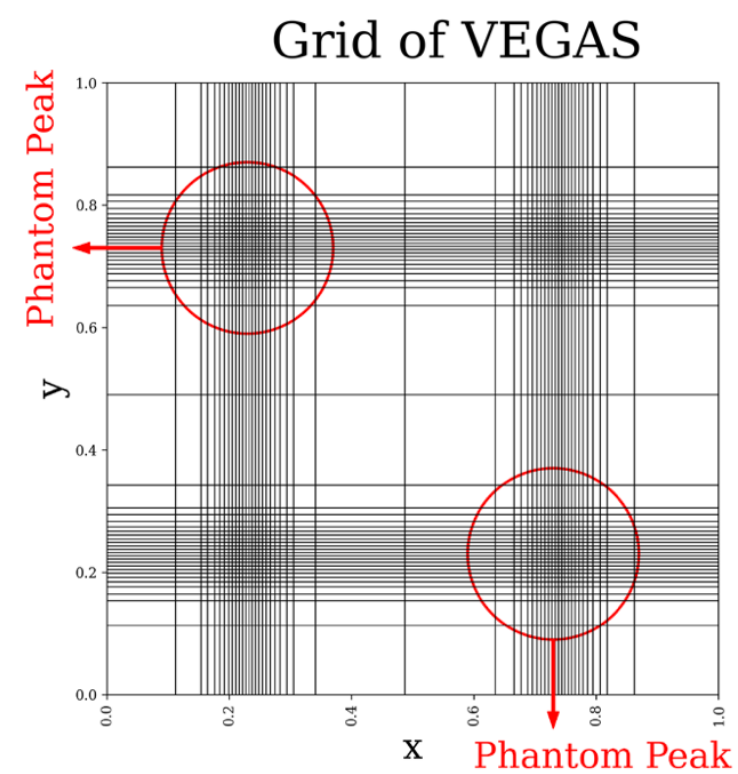
Two-Dimensional Gaussian Case:

$$\int_{[0,0]}^{[1,1]} f(\mathbf{x}) d\mathbf{x} = \int_{[0,0]}^{[1,1]} \left(\sum_{i=0}^1 e^{-200|\mathbf{x}-\mathbf{r}_i|^2} \right) d\mathbf{x}, \quad \mathbf{r}_0 = (0.23, 0.23), \quad \mathbf{r}_1 = (0.74, 0.74)$$



Number of Qubits: $n = 10$

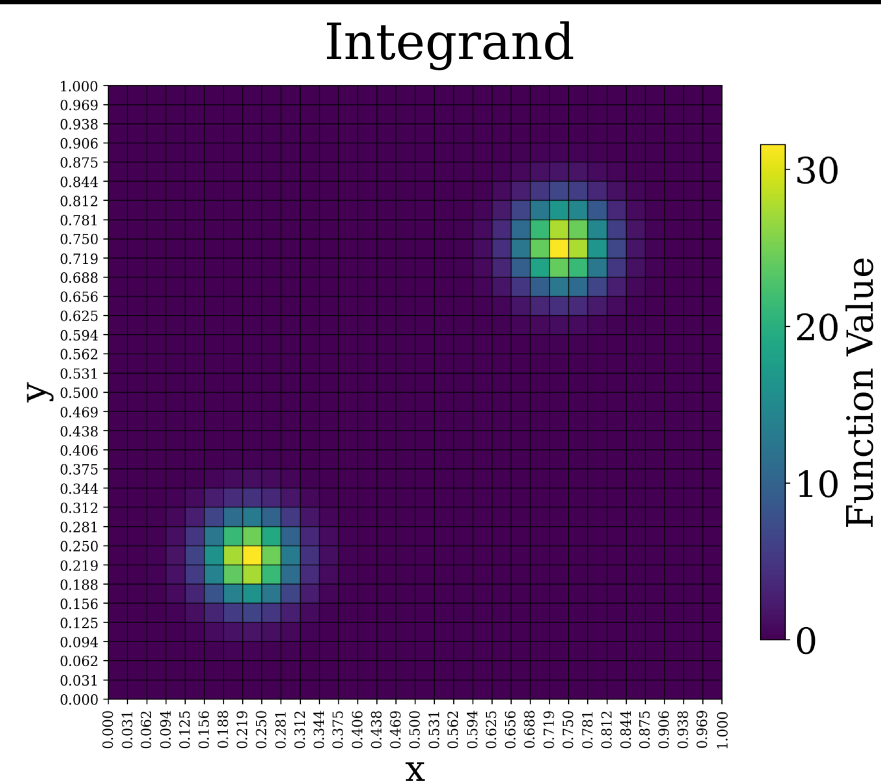
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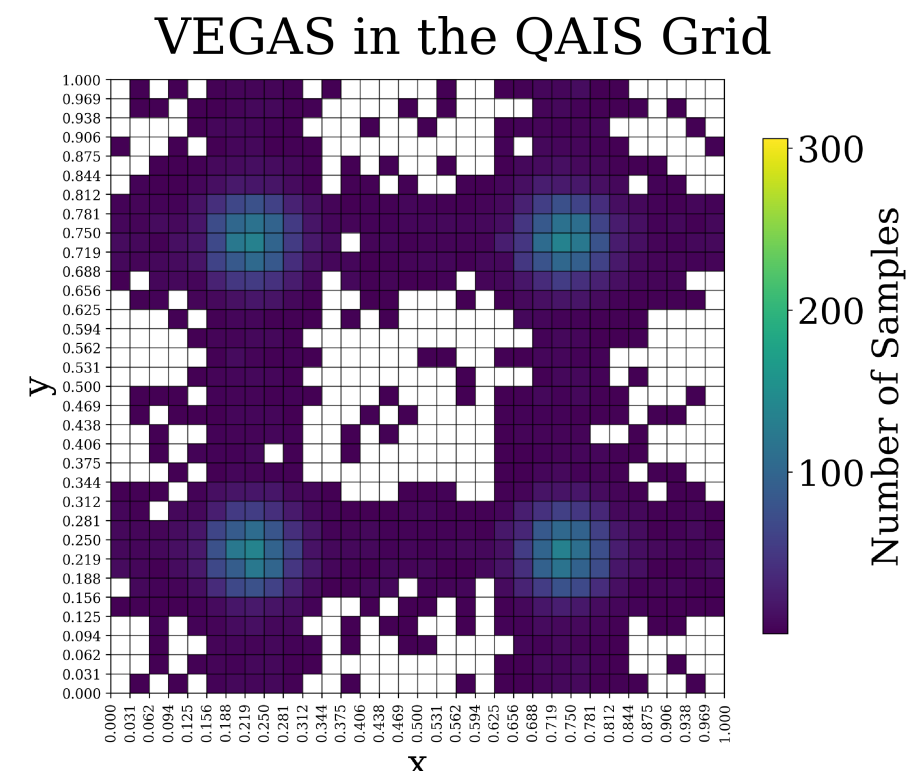
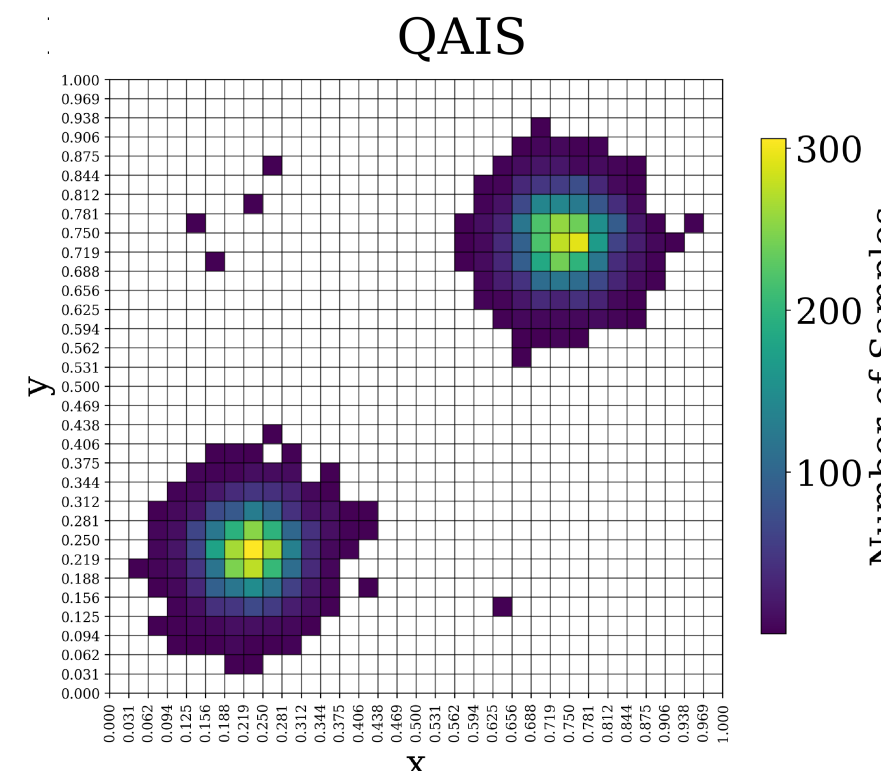
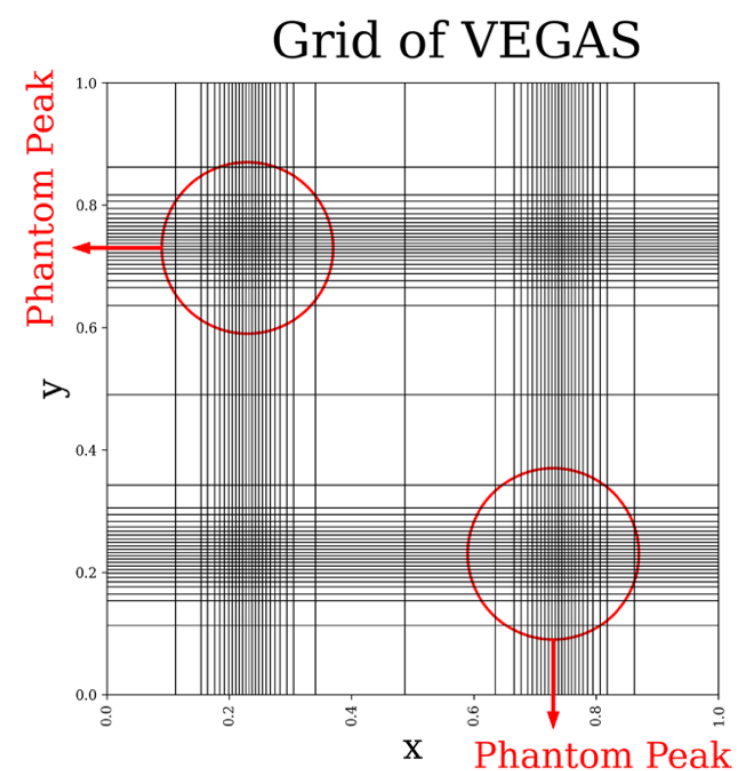
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- Given M observed states out of 2^n :

These correspond to a region $\Omega^- \subset \Omega$

Using the j -th cell estimator: $\hat{I}_j = \frac{|\Omega^{(j)}|}{N_j} \sum_{i=1}^{N_j} f(\mathbf{x}_i^{(j)})$

- We observe a systematic bias:

$$\text{Bias} = - \sum_{j \in \Omega \setminus \Omega^-} I_j$$

Quantum Adaptive Importance Sampling

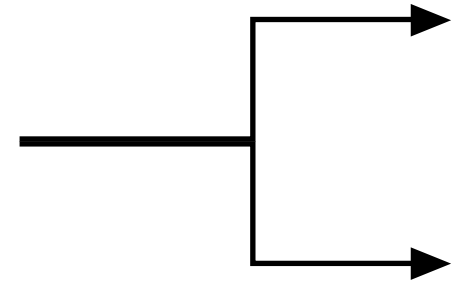
Systematic Bias Solution: Tiling Algorithm

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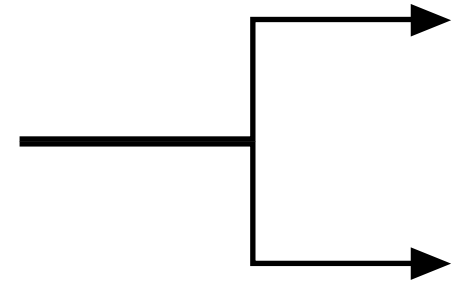
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Target at few states

Unbiasedness:
Evaluate every grid cell

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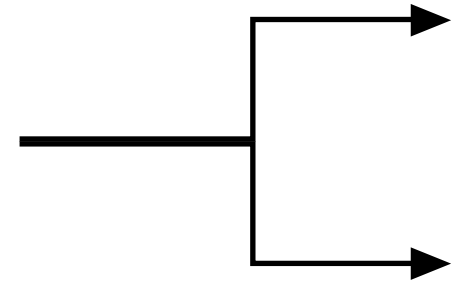
3. **Solution:** **Tiling Algorithm** to reconstruct PDF
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$$\mathcal{O}\left(\underbrace{n M \log M}_{\text{Sorting}} + \overbrace{M d^3 n^2}^{\text{Greedy Expansions}}\right)$$

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I) Detailed sampling in Important Regions

II) Sparse uniform sampling in the Non-Important Region

QAIS estimator:

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Contains Formerly Missing Contribution

Quantum Adaptive Importance Sampling

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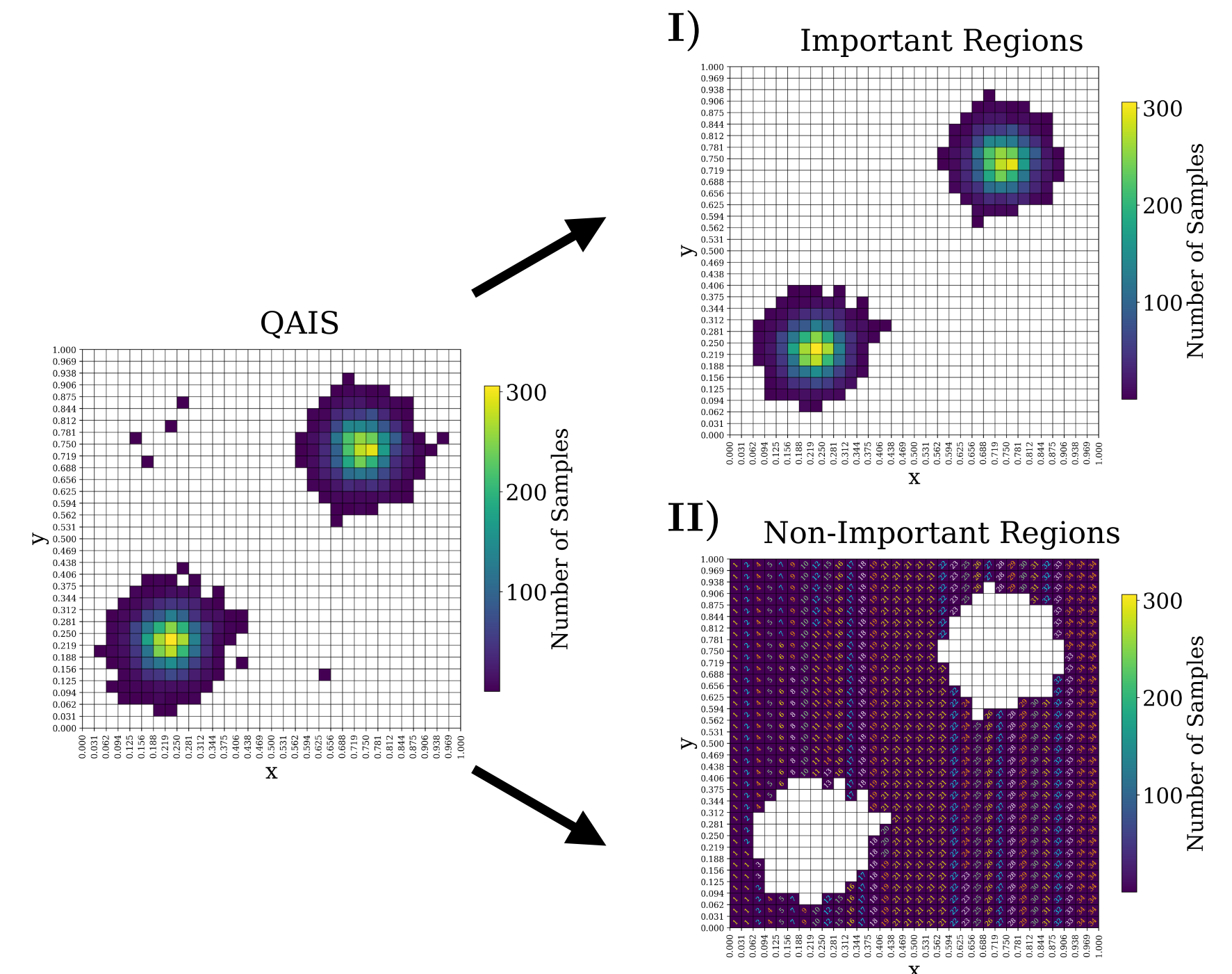
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Practical Demonstration



Quantum Adaptive Importance Sampling

More Two-Dimensional Examples:

- Sampling efficiency of QAIS compared to VEGAS depends heavily on the target integrand's structure.

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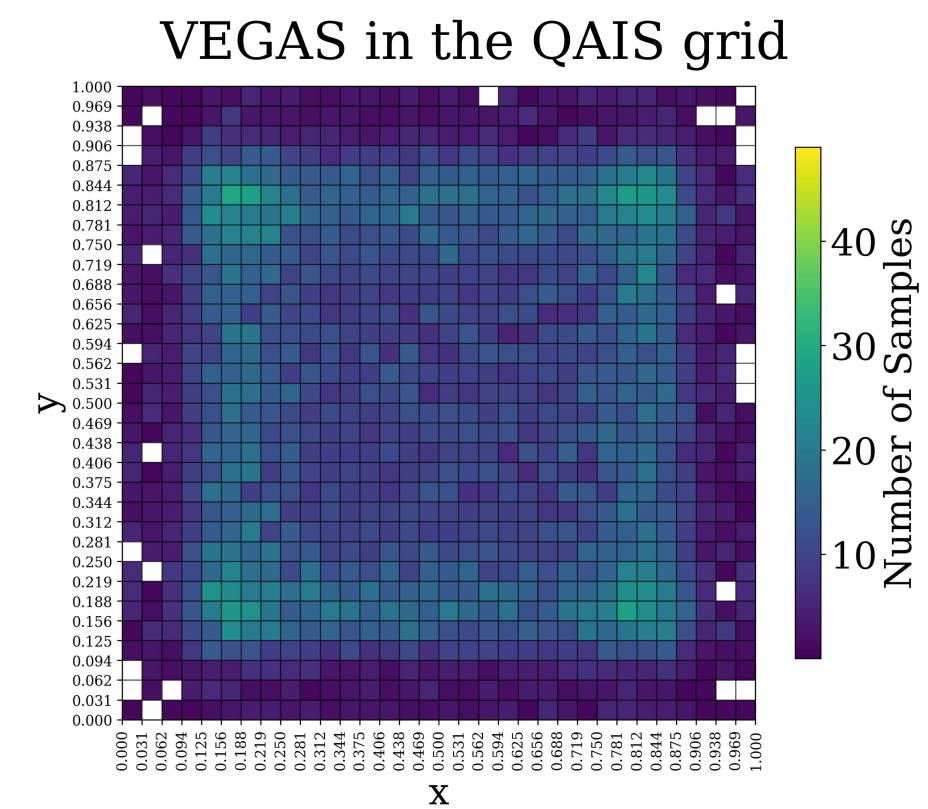
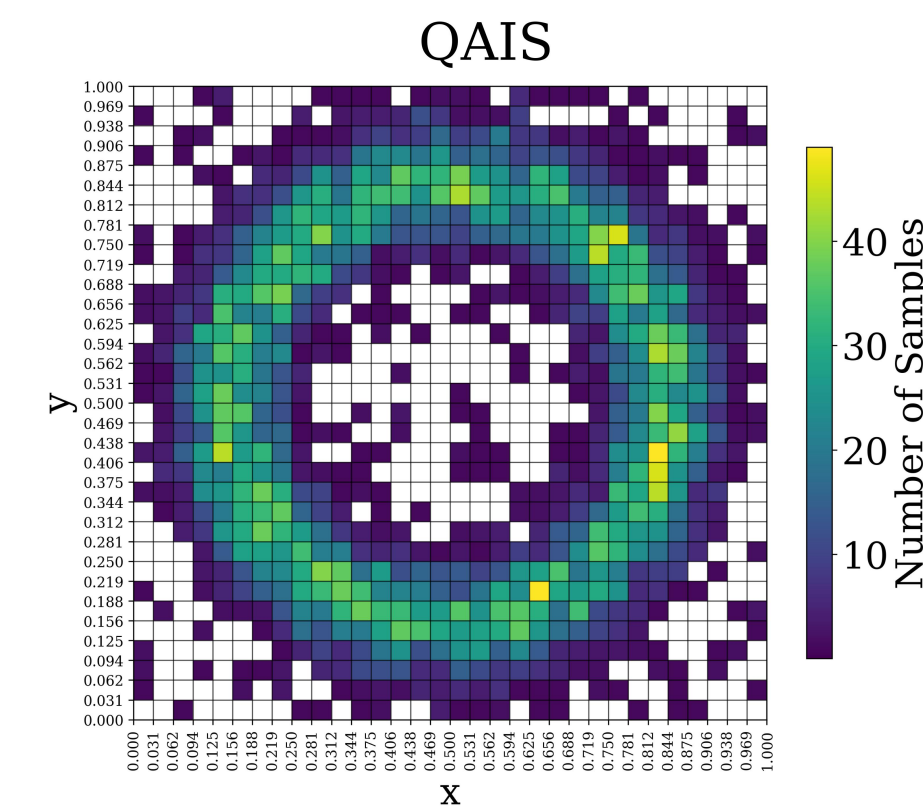
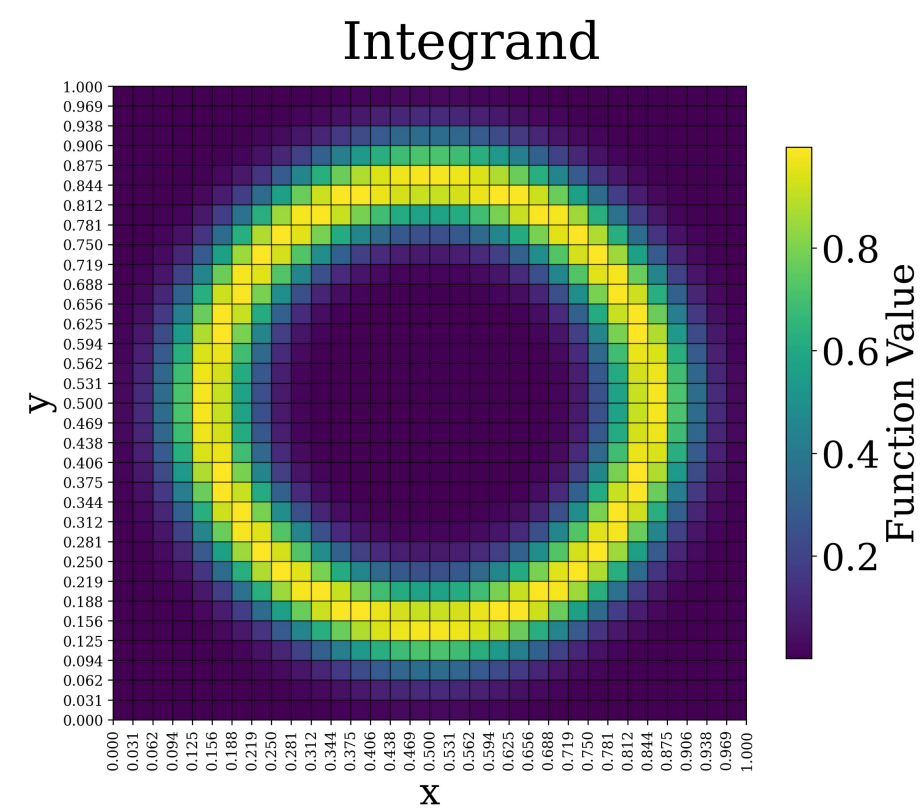
Number of Qubits: $n = 10$

Number of Shots: $N = 10^4$

Ring-Shaped Structure:

$$f_R(x, y) = e^{-k(\sqrt{(x-c_x)^2 + (y-c_y)^2} - \rho)^2}$$

With: $c_x = \frac{1}{2}, \quad c_y = \frac{1}{2}, \quad \rho = 0.35, \quad k = 200$



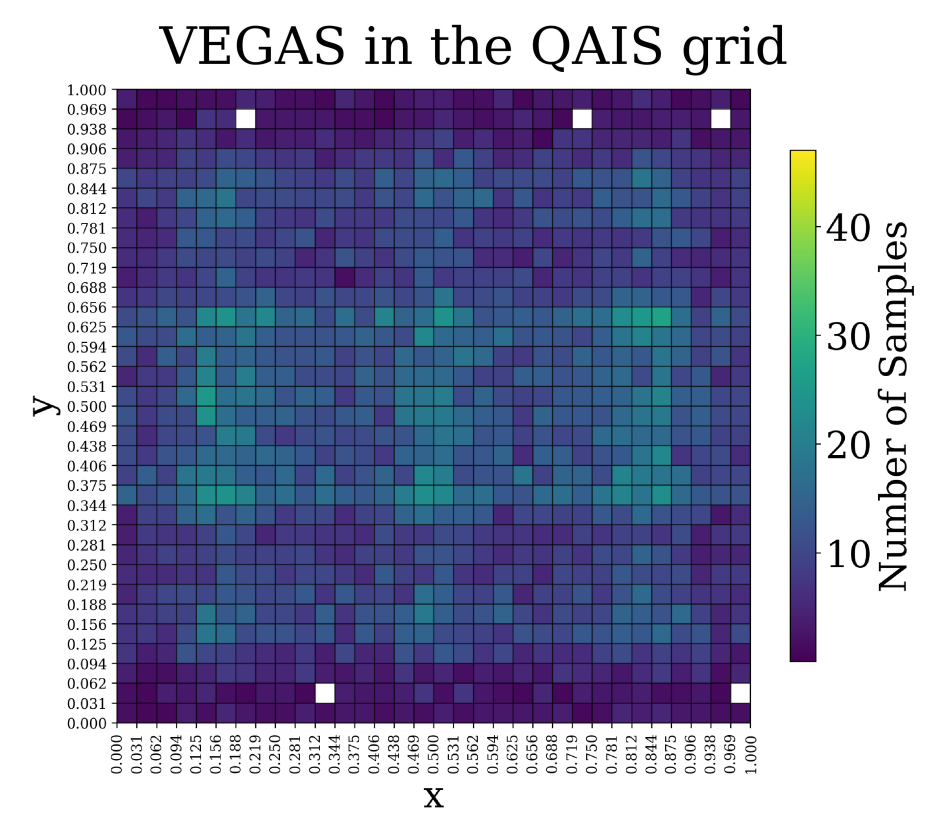
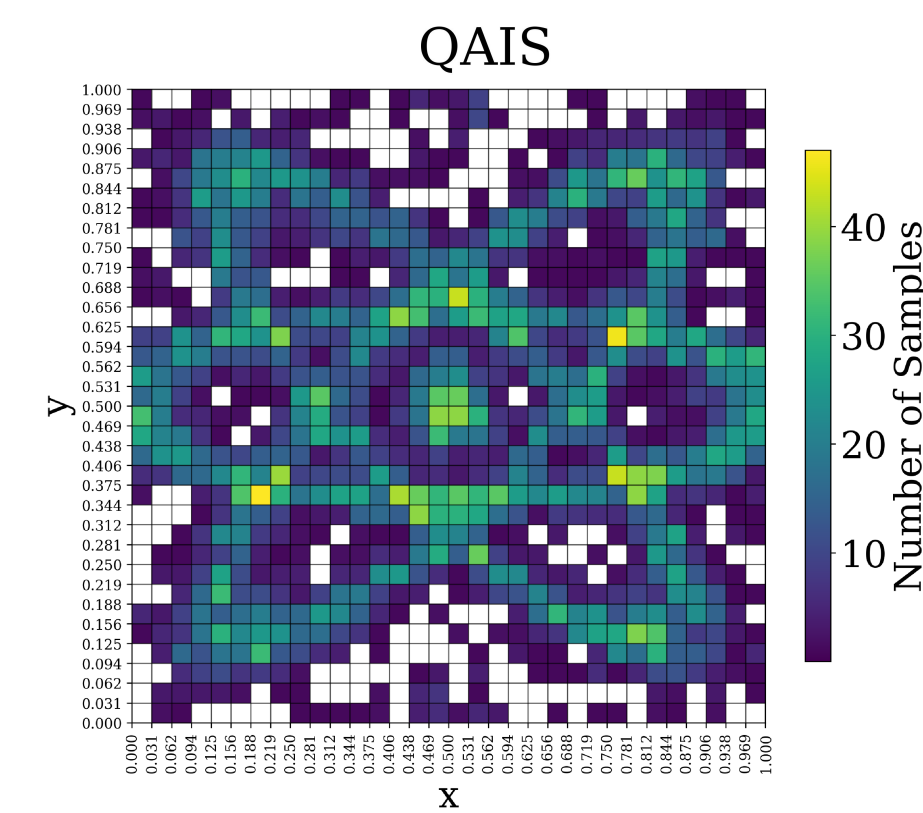
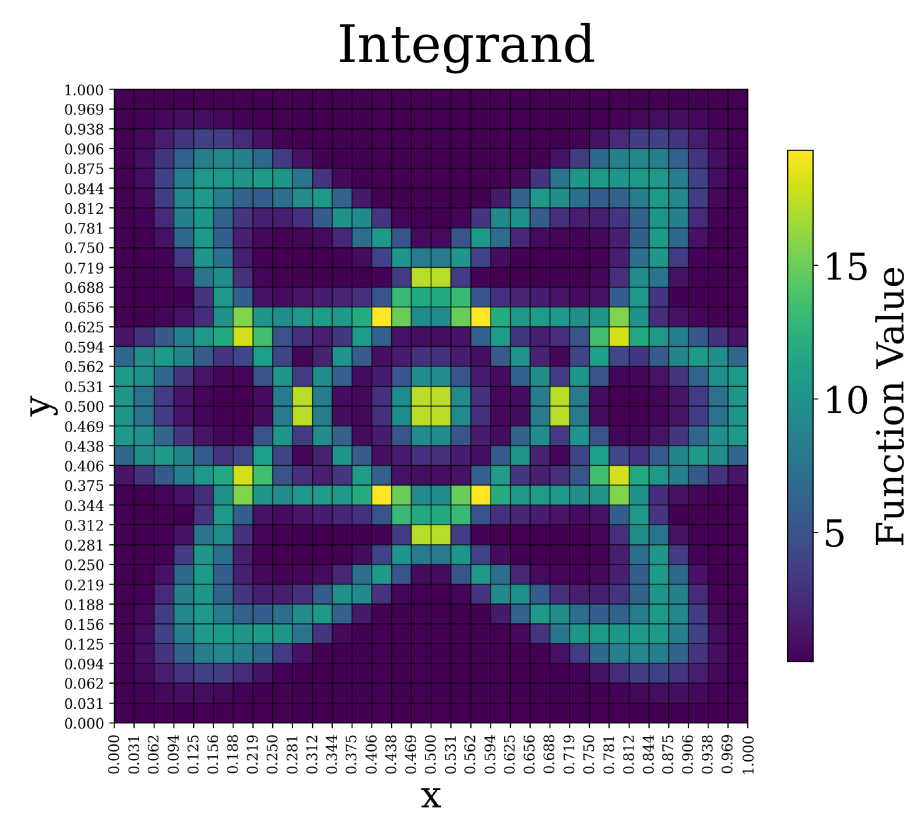
Atom-Shaped Structure:

$$f_A(x, y) = c_g e^{-(u(x)^2 + v(y)^2)/(2s_g^2)} + \sum_{\theta \in \{0, \pi/4, -\pi/4\}} \left[c_0 + c_\theta e^{-(r_e(x, y, \theta) - 1)^2/(2s_r^2)} \right]$$

With: $u(x) = x - \frac{1}{2}, \quad v(y) = y - \frac{1}{2},$

$$r_e(x, y, \theta) = \sqrt{(U(x, y, \theta)/a)^2 + (V(x, y, \theta)/b)^2}$$

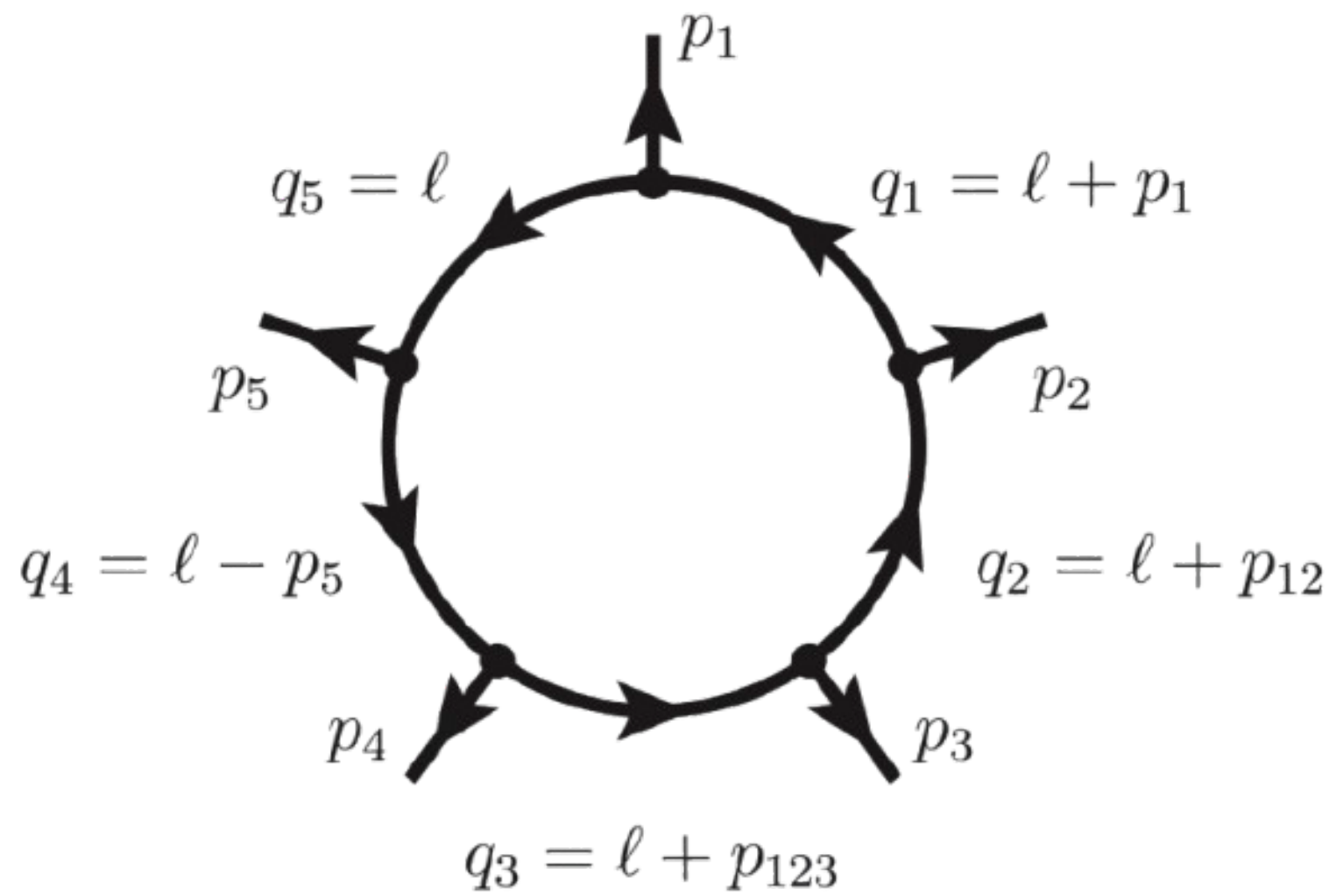
$U(x, y, \theta) = \cos \theta u(x) + \sin \theta v(y), \quad V(x, y, \theta) = -\sin \theta u(x) + \cos \theta v(y), \quad a = \frac{1}{2}, \quad b = 0.15, \quad s_r = 0.1, \quad s_g = 0.04, \quad c_g = 20, \quad c_0 = 0.05, \quad c_\theta = 10.5$



Quantum Adaptive Importance Sampling

HEP example: One-loop Pentagon

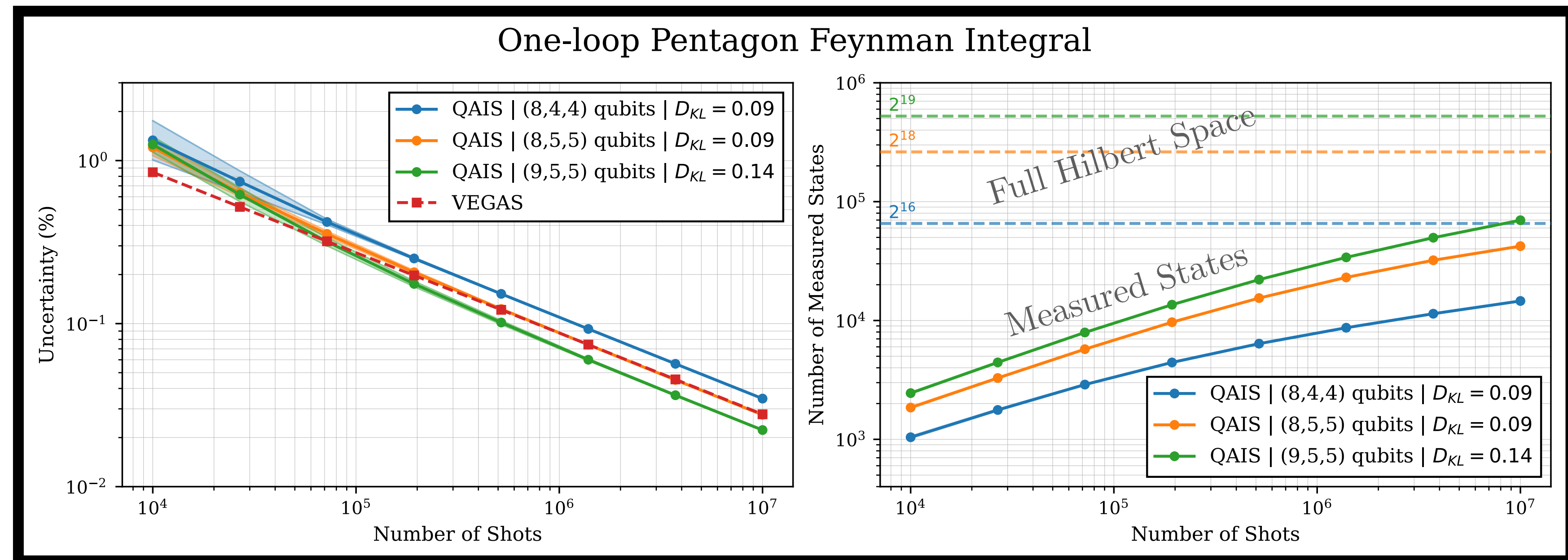
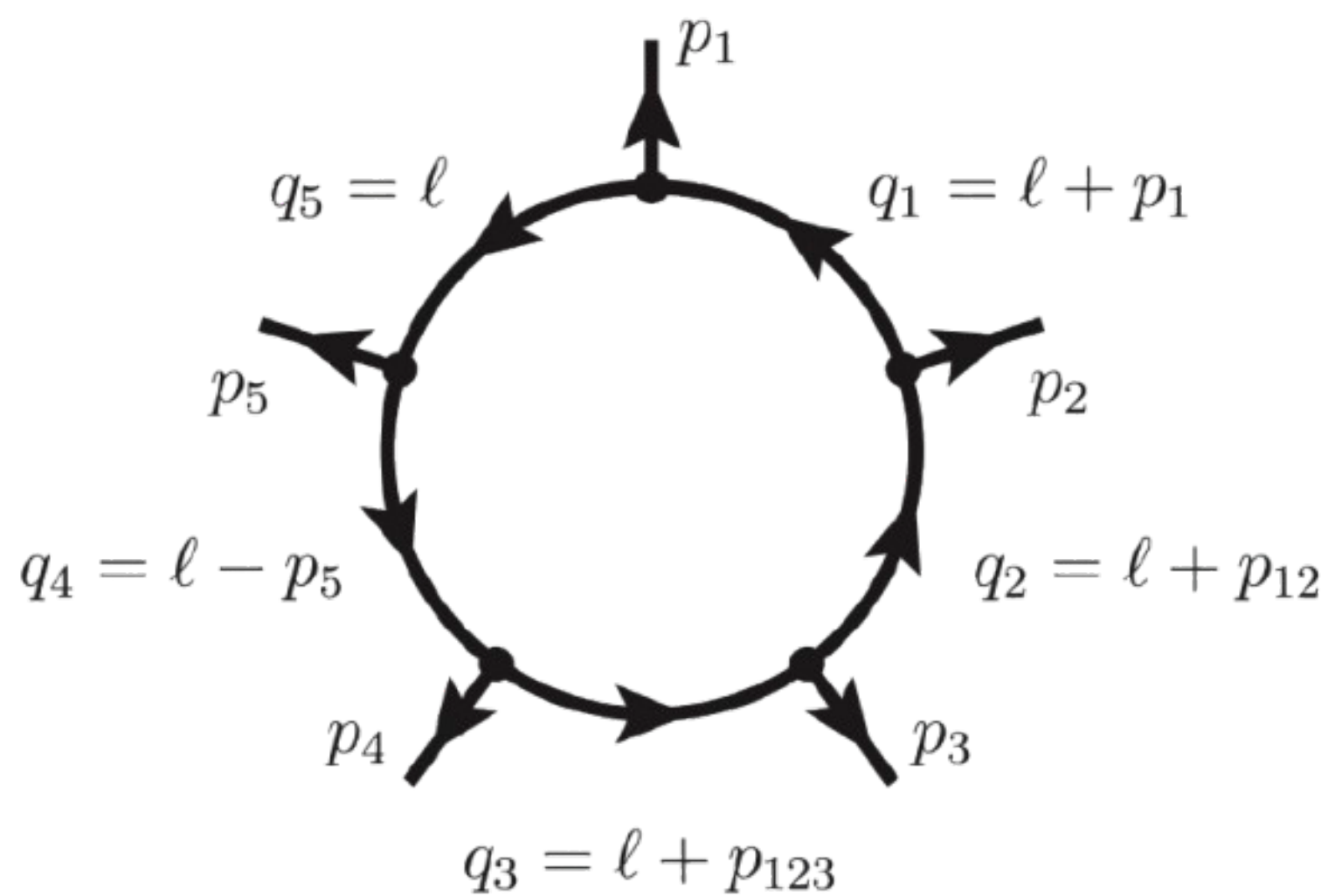
One-Loop Pentagon Diagram :
(Loop-Tree Duality)



Quantum Adaptive Importance Sampling

HEP example: One-loop Pentagon

One-Loop Pentagon Diagram : (Loop-Tree Duality)



- Uncertainty: σ/I
- Discretization: 16-19 qubits
- Comparison made on best VEGAS proposal against best QAIS proposal
- Error bands coming from 100 independent integrations, with the same proposal PDF

Quantum Adaptive Importance Sampling

Cross-Dimensional Results:

- Integrate the same multi-peak structure in different dimension.
- Analytic Expression:

$$\int_{[0,1]^d} f(\mathbf{x}) d\mathbf{x} = \int_{[0,1]^d} \left(\sum_{i=0}^2 e^{-50|\mathbf{x}-\mathbf{r}_i|} \right) d\mathbf{x}$$

$$\mathbf{r}_0 = (0.23, \dots, 0.23), \quad \mathbf{r}_1 = (0.39, \dots, 0.39), \quad \mathbf{r}_2 = (0.74, \dots, 0.74)$$

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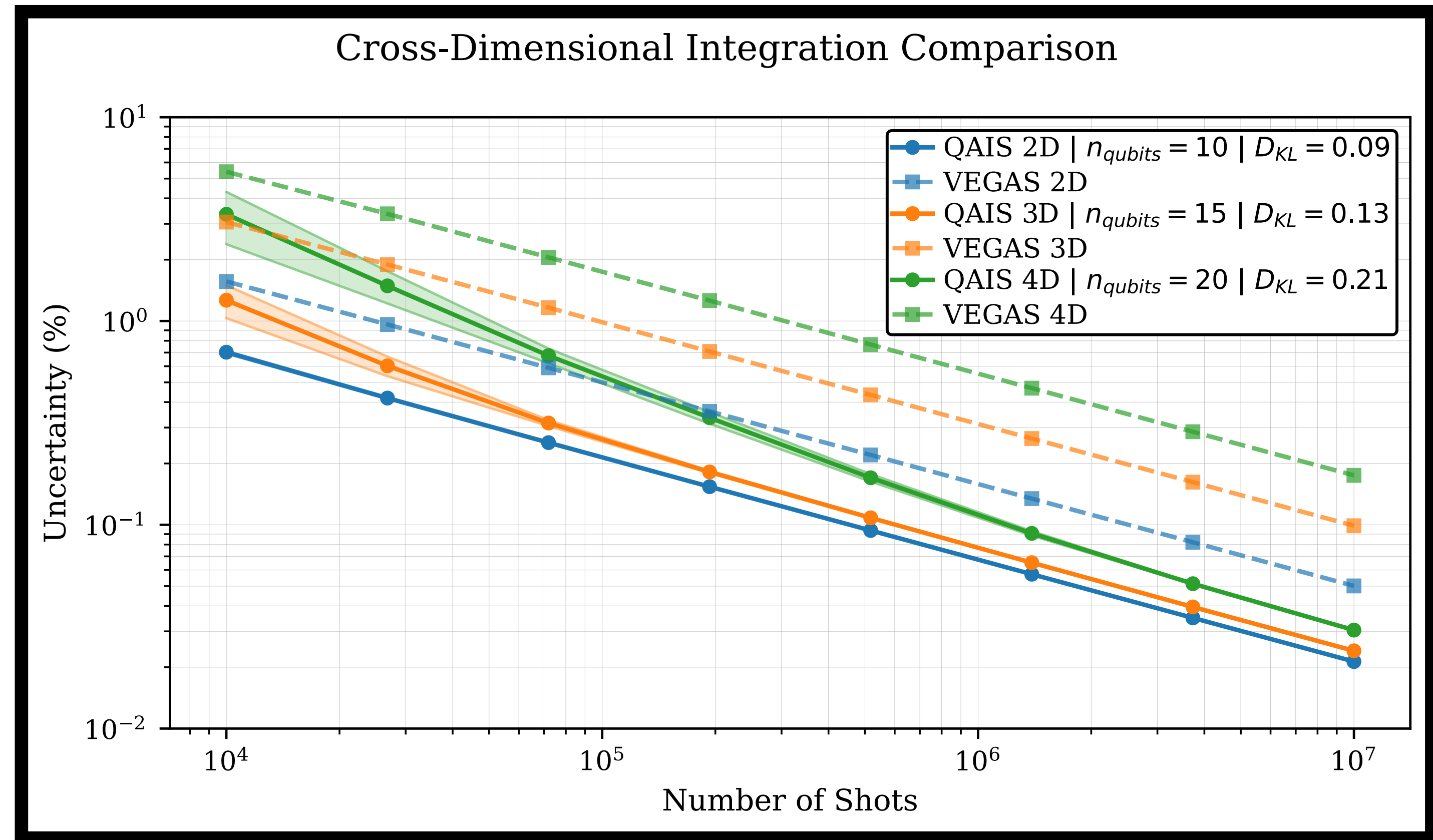
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Integrand Dimension: 2-4 dimensions

Discretisation: 5 qubits/dimension

Approx. : 100 COBYLA iters / parameter



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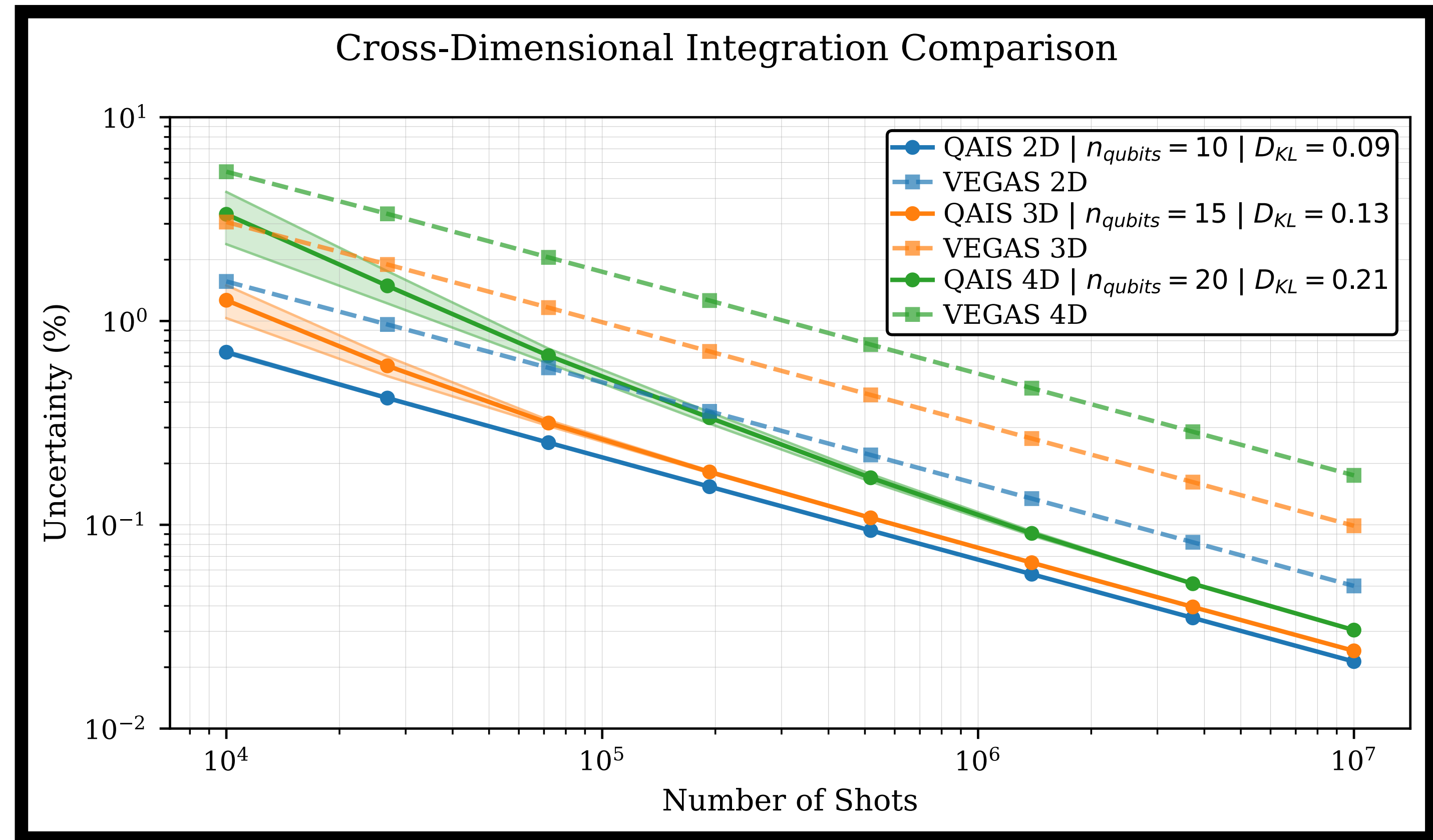
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- We expect the precision to be governed by how well the proposal fits the target
- The main driving force should be the KL divergence
- We see that as the dimension rises , VEGAS' best grid falls behind , while QAIS is able to keep uncertainty low, particularly in the region above

Summary

○ **VEGAS:** Uses a separable proposal $q_{\text{VEGAS}} = \prod_{i=1}^d q_i$. Reduces the grid handling DoF $N_g^d \rightarrow dN_g$.

Captures the important regions, but generates phantom structures, reducing performance.

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In a comparison between best proposals:

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- **Limitations and Future work:** Limitations on arbitrary quantum state preparation. Particularly considering ongoing limitations in Quantum Machine Learning. Plan to formalise the optimisation process.

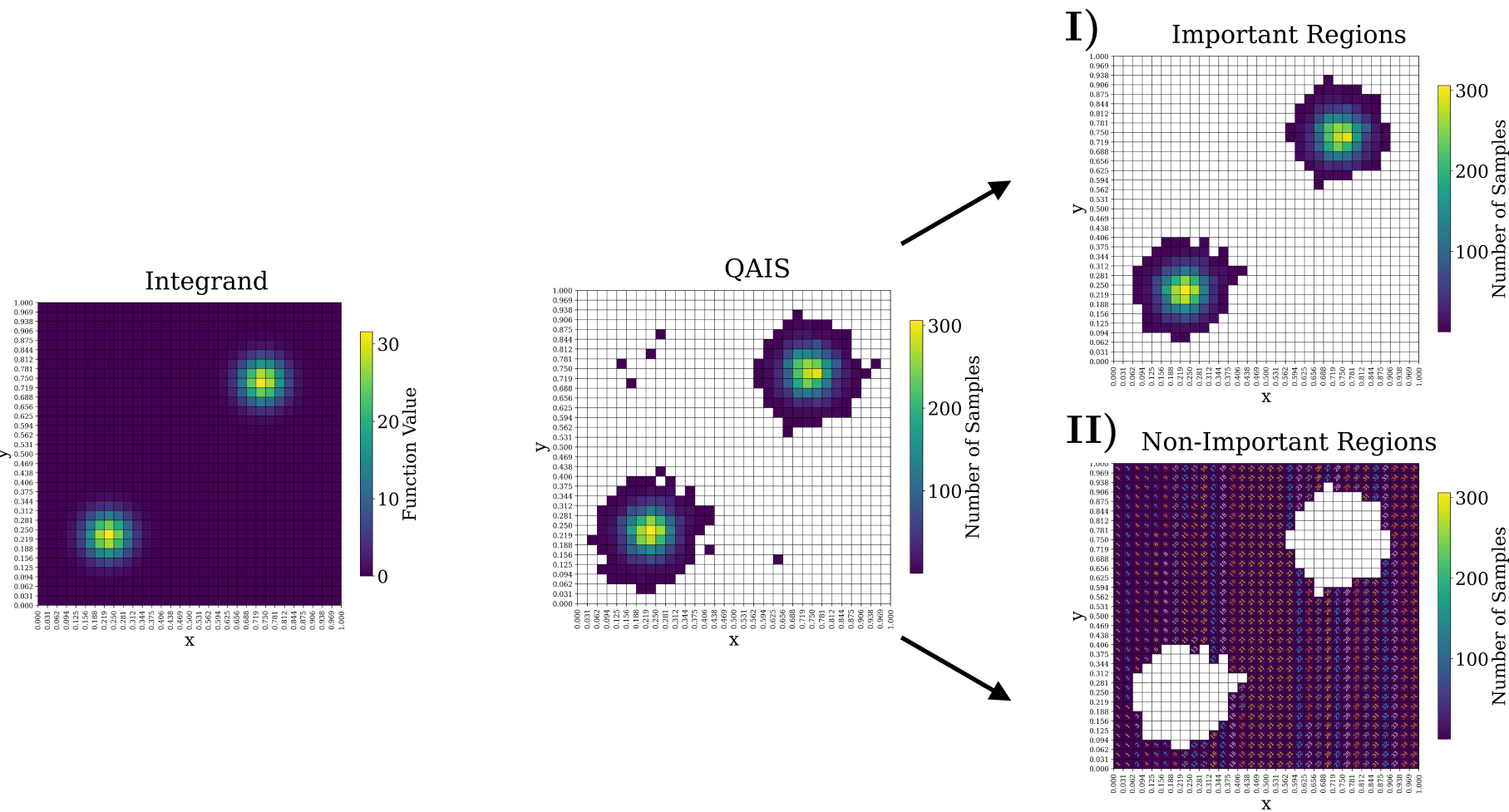
Supplementary Material

Quantum Adaptive Importance Sampling

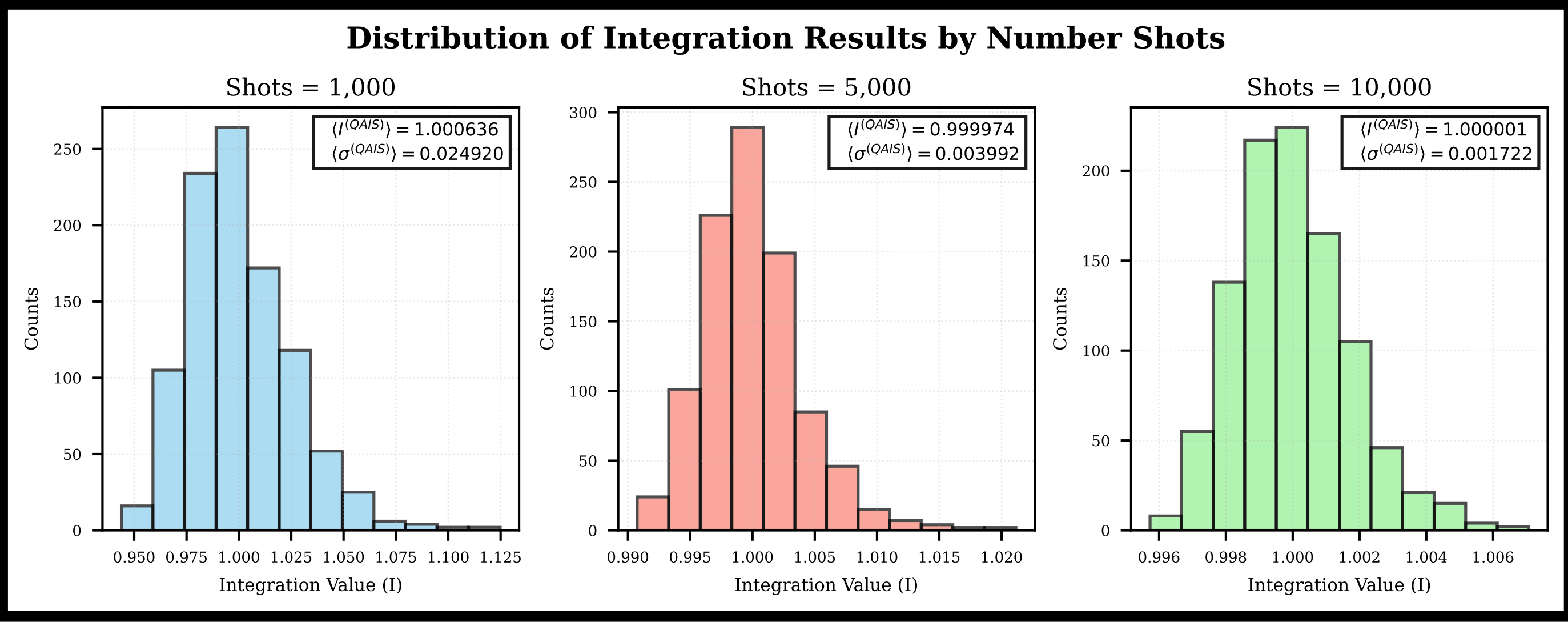
Two-Dimensional Gaussian Case: Bias check

$$\int_{[0,0]}^{[1,1]} f(\mathbf{x}) d\mathbf{x} = \int_{[0,0]}^{[1,1]} \left(\sum_{i=0}^1 e^{(-200|\mathbf{x}-\mathbf{r}_i|^2)} \right) d\mathbf{x}, \quad \mathbf{r}_0 = (0.23, 0.23), \quad \mathbf{r}_1 = (0.74, 0.74)$$

Number of Qubits: $n = 10$



1000 Integrations with the same proposal

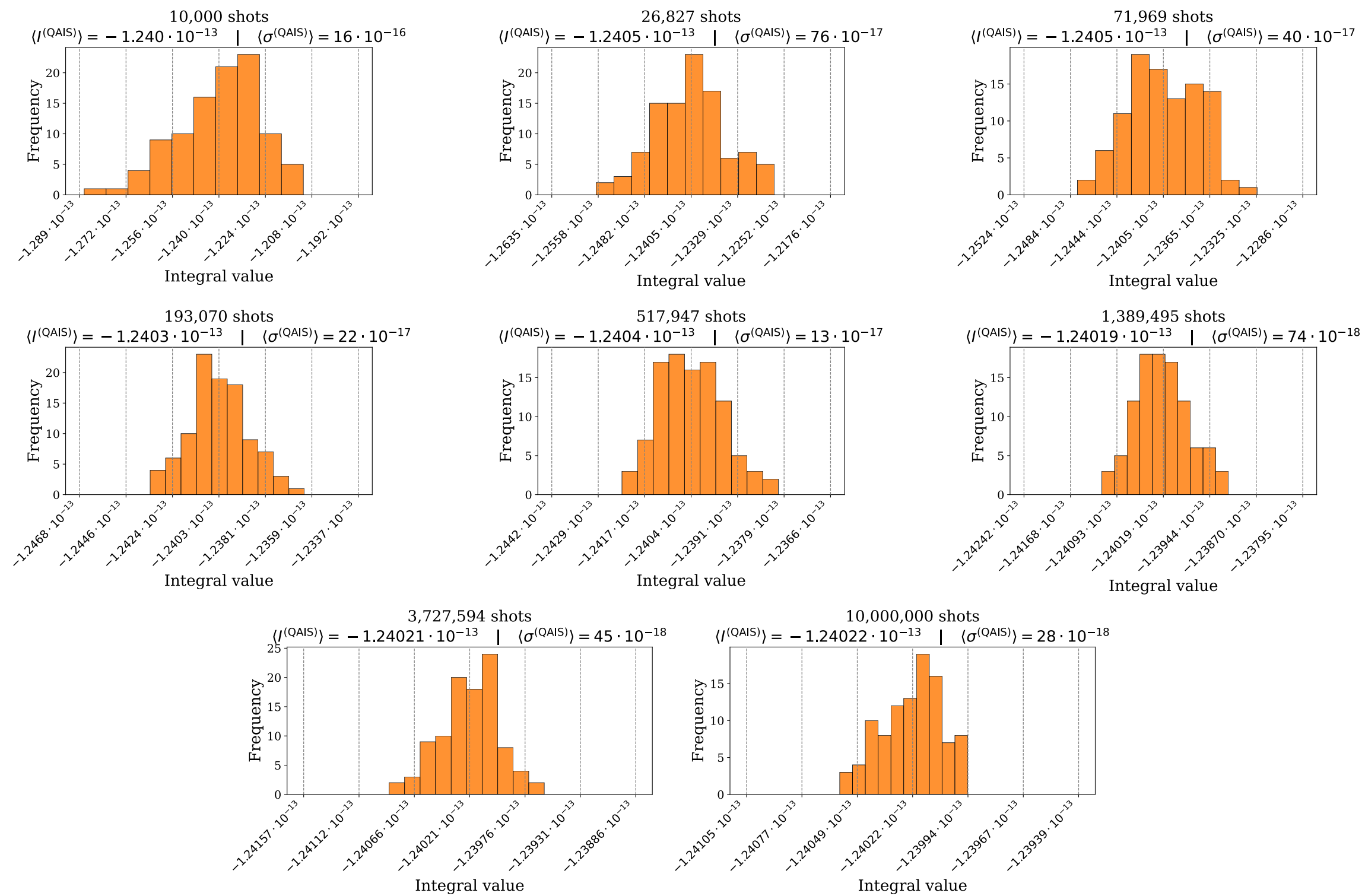


Quantum Adaptive Importance Sampling

Impact of Quasi-Random Sequences

Pseudo-Random (Marsenne Twister)

Histograms of Integral Values | Pentagon Feynman Diagram | (9,5,5) qubits



Quasi-Random (Sobol Sequence)

Histograms of Integral Values | Pentagon Feynman Diagram | (9,5,5) qubits

