University of Mannheim

Master Thesis

Quasi-Monte Carlo Methods and Neural Networks

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A thesis submitted in fulfillment of the requirements for the degree of Master of Science

in the

Research Group Name
Department or School Name

July 2, 2025

Declaration of Authorship

I, Janik V. HRUBANT, declare that this thesis titled, “Quasi-Monte Carlo Methods and Neural Networks” and the work presented in it are my own. I confirm that:

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Abstract

This thesis explores the application of quasi-Monte Carlo (QMC) methods for generating training data for neural networks, with a particular emphasis on convergence behavior in both deterministic and stochastic settings. In contrast to classical Monte Carlo (MC) approaches, which rely on pseudorandom sampling, QMC methods use low-discrepancy sequences to achieve more uniform coverage of the input space, which can lead to improved approximation performance, especially in high-dimensional problems.

In the first part of the thesis, QMC methods are applied to sample training inputs from a bounded domain. The corresponding function values are computed, and the resulting dataset is used to train neural networks. The convergence of the network output with respect to the number of training points is analyzed and compared against networks trained on MC-sampled data. The goal is to quantify the advantage of QMC-based training in terms of learning efficiency and approximation accuracy.

The second part extends this investigation to stochastic functions. Here, the randomness in the system—such as in photon transport models—is explicitly modeled, and both QMC and MC sampling are used to sample from the stochastic variables. The focus is on physically motivated functions that simulate scattered photon radiation, a key challenge in medical imaging applications such as x-ray or CT simulations. Neural networks are trained on data generated from these stochastic models, and their convergence behavior is evaluated under QMC and MC sampling regimes.

Through these experiments, the thesis demonstrates how QMC-based sampling can enhance neural network training, particularly when approximating complex physical processes. The results provide both theoretical insights and empirical evidence that QMC methods offer significant advantages over standard MC approaches in terms of convergence speed and generalization quality in high-dimensional learning problems.

Contents

RITA Rational Inverse Transform with Aliasing

Part I

QMC for training of Neural Networks

Chapter 1

Quasi-Monte Carlo Methods for Deep Learning: Motivation and Objectives

1.1 Challenges in Neural Network Training

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1.2 Limitations of Monte Carlo Sampling

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1.3 Objectives and Scope of the Thesis

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1.4 Outline of the Thesis

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Chapter 2

Theoretical Foundations

2.1 Function Approximation with Neural Networks

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2.2 Sampling-Based Learning: MC vs. QMC

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2.2.1 Monte Carlo Sampling in High Dimensions

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2.2.2 Low-Discrepancy Sequences and QMC Theory

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2.3 Convergence in Deterministic and Stochastic Learning

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2.4 Stochastic Functions and Photon Transport Models

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Chapter 3

Neural Network Training with QMC in Deterministic Settings

3.1 Problem Setup and Input Space Design

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3.2 Generation of Training Sets via QMC and MC

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3.3 Network Architecture and Training Protocols

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3.4 Convergence Evaluation and Error Metrics

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3.5 Comparative Results

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Chapter 4

Neural Network Training for Stochastic Functions

4.1 Modeling Randomness in Physical Simulations

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4.2 Sampling Stochastic Variables with QMC and MC

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4.3 Data Generation: Simulating Photon Scatter

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4.4 Learning Setup and Experimental Design

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4.5 Convergence and Performance Comparison

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Part II

X-ray Simulation using QMC Methods

Chapter 5

X-Ray Simulation using QMC methods

5.1 Algorithm

The following pseudoalgorithm outlines the process of simulating X-ray photon transport using Quasi-Monte Carlo (QMC) methods. The algorithm generates a sequence of QMC samples to determine the initial positions and directions of photons, simulates their transport through a defined geometry, and records the results of interactions with materials. By that many other algorithms are used such als the Rational Inverse Transform with Aliasing (RITA) algorithm.

Algorithm 1 gQMCFFD: X-ray Scatter Simulation using QMC Methods and Forced Fixed Detection

Input: Max. scatter order N, phantom geometry $\mathcal{P}$, energy spectrum ϕ, beam angle α, set of detector pixels $\mathcal{G} = \{G_1, ..., G_s\}$, QMC point $u^j \in [0,1]^{4N}$

Initialize photon using u_1^j, u_2^j, u_3^j:

- energy $E_0 \sim \phi(E)$ by inverse transform sampling with u_1^j
- direction $\vec{\omega}_0$ within cone angle α using u_2^j, u_3^j
- weight $W_0 = I_0(\vec{\omega}_0) = 1$
- escape probability $p_0 = 0$ TODO: ist das richtig initialisiert?

Compute entry point: find smallest t_0 s.t. $A_0 = S + t_0 \cdot \vec{\omega}_0 \in \partial\mathcal{P}$

Initialize: $f_{n,k} = 0$ for all $D_k \in \mathcal{G}$

for $i = 1$ to N **do**

  Sample free path length t_i using u_{4i}^j and update position:

$$\int_0^{t_i} \mu_{\text{tot}}(A_{i-1} + s\vec{\omega}_{i-1}, E_{i-1})ds = -\ln\left(1 - (1 - p_{i-1}) \cdot u_{4i}^j\right)$$

$$A_i = A_{i-1} + t_i \cdot \vec{\omega}_{i-1}$$

  if $A_i \notin \mathcal{P}$ **then**

    break (photon exits phantom) TODO: ist das richtig initialisiert?

  end if

  if $\mu_{\text{tot}}(A_i, E_i) \cdot u_{4i+3}^j < \mu_{\text{comp}}(A_i, E_i)$ **then**

    $\delta^i = 0 \rightarrow$ **Compton Scattering**

    p_{y_0} gemäß Gleichung (5)

  else if $\mu_{\text{comp}}(A_i, E_i) \le \mu_{\text{tot}}(A_i, E_i) \cdot u_{4i+3}^j < \mu_{\text{comp}}(A_i, E_i) + \mu_{\text{ray}}(A_i, E_i)$ **then**

    $\delta^i = 1 \rightarrow$ **Rayleigh Scattering**

    p_{y_1} gemäß Gleichung (6)

  else

    Photoelectric Absorption $\rightarrow$ **break**

  end if

  Sample new direction $\vec{\omega}_i$ using RITA using randoms u_{4i+1}^j, u_{4i+2}^j

  TODO: herausfinden, wie neue Energie berechnet wird

  Compute escape probability along $\vec{\omega}_{i-1}$:

$$p_{i-1} = \exp\left(-\int_0^{c_{i-1}} \mu_{\text{tot}}(A_{i-1} + s\vec{\omega}_{i-1}, E_{i-1})ds\right)$$

  Update weight: $W_i = W_{i-1} \cdot (1 - p_{i-1})$

  for each detector pixel $D_j \in \mathcal{G}$ **do**

    Determine forced direction $\vec{\omega}_{i,j}$ from $A_i \rightarrow D_j$

    Compute transmission factor:

$$T_{i,j} = \exp\left(-\int_0^{b_{i,j}} \mu_{\text{tot}}(A_i + s\vec{\omega}_{i,j}, E_i)ds\right)$$

    Compute directional scatter PDF: $p^y(A_i, E_{i-1} \rightarrow E_i, \vec{\omega}_{i-1} \rightarrow \vec{\omega}_{i,j})$

    Update scatter contribution:

$$f_{n,j} \mathrel{+}= W_i \cdot p^y \cdot T_{i,j}$$

  end for

end for

Primary intensity (if unscattered):

for each detector pixel $D_j \in \mathcal{G}$ **do**

Chapter 6

Synthesis and Discussion

6.1 Summary of Results Across Experiments

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6.2 Strengths and Limitations of QMC-Based Learning

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6.3 Implications for Simulation and Medical Imaging

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Chapter 7

Conclusion and Future Work

7.1 Main Contributions

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7.2 Directions for Future Research

The **poc!** (**poc!**) was successfully implemented to demonstrate the feasibility of the proposed approach.

Appendix A

Frequently Asked Questions

A.1 How do I change the colors of links?

The color of links can be changed to your liking using:

`\hypersetup{urlcolor=red}`, or

`\hypersetup{citecolor=green}`, or

`\hypersetup{allcolor=blue}`.

If you want to completely hide the links, you can use:

`\hypersetup{allcolors=.}`, or even better:

`\hypersetup{hidelinks}`.

If you want to have obvious links in the PDF but not the printed text, use:

`\hypersetup{colorlinks=false}`.