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im Bachelor-Studiengang Physik

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1. Gutachter: Prof. Dr. Walter Strunz
2. Gutachter: Prof. Dr. Oscar Dahlsten

Summary

Abstract
English:
Aufmerksamkeit große Fragen? unsere Frage unsere Antwort

Abstract
Deutsch

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1. Introduction

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1.1. Intro

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2. Background

2.1. Supervised Machine Learning

Machine learning is a subfield of artificial intelligence, 'concerned with the question of how to construct computer programs that automatically improve with experience.' [7] Supervised machine learning is one of the three machine learning disciplines, besides unsupervised and reinforcement learning. The goal is to find a mapping between an input and an output, in our case an excitation and its respective optimal harvesting policy. Multiple algorithms to find such a mapping exist, however for high dimensional problems artificial neural networks (ANNs) are usually used. In this section we review ANNs, following the exposition given in [5].

Let $\mathfrak{R}$ be a fully-connected feedforward ANN, meaning there are no loops in the neuron connections and all neurons in a layer are connected to every neuron of the next layer, $\mathfrak{R} : \mathbb{R}^{n_1} \to \mathbb{R}^{n_L}$. n_1 and n_L denote the dimensionality of the input and output respectively. $\mathfrak{R}$ has L layers, or columns of neurons. The network architecture is given by the amount of neurons n_l in each hidden layer $l \in [2, L-1]$ (see figure 2.1). The neurons in layer l are represented by their activations $\vec{a}_l \in \mathbb{R}^{n_l}$, which represent the matrix multiplication output. Additionally each layer includes trainable parameters $W_l \in \mathbb{R}^{n_{l+1} \times n_l}$ and $\vec{b}_l \in \mathbb{R}^{n_l}$ called weights and biases. The activations can then be calculated using the following formulae [11]:

$$\begin{aligned} \vec{a}_2 &= W_1 \vec{a}_1 + \vec{b}_1, \\ \vec{a}_l &= W_{l-1} \xi(\vec{a}_{l-1}) + \vec{b}_{l-1}, \ l \in [3, L], \end{aligned}$$

where $\xi(x)$ is a function called the activation function applied elementwise. Historically, functions such as *tanh* and sigmoid have been used. However, it has been shown [6, 2] that the rectified linear unit $\mathrm{ReLU}(x) = \max(0, x)$ often provides better results and is used here.

To train an ANN a cost function is defined, often the mean squared error

$$\mathrm{MSE} = \frac{1}{N} \sum_{i=1}^{N} (\vec{a}_{L,i} - \vec{y}_i)^2,$$

where the summation is performed over the training data $\{(\vec{x}_i, \vec{y}_i)\}$ with N samples, where $\{\vec{x}_i\}$ is the input and $\{\vec{y}_i\}$ the output data, and $\vec{a}_{L,i} = \mathfrak{R}(\vec{x}_i)$ is the output of the neural network. The so-called backpropagation algorithm is used to calculate the gradient of the cost function with respect to the trainable parameters and improve the performance of the ANN [9, 8].

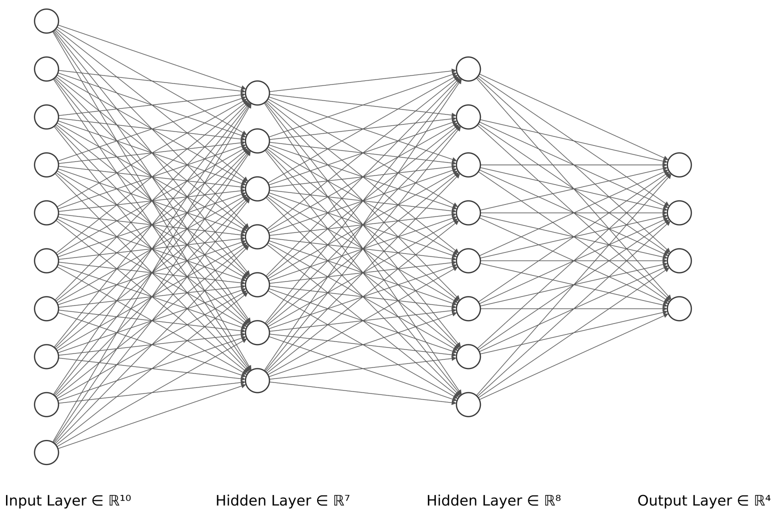

Figure 2.1.: Example fully-connected feedforward ANN with four layers, including input, output and two hidden layers [4]

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2.2. Collision model dynamics

2.3. Setting

Our setting consists of three qubits: the Drive, System and Transducer qubits. The Drive and Transducer qubits can be set by the experimenter in N discrete steps modelled as piecewise constant functions (PWC) of (θ_D, ϕ_D) and (θ_T, ϕ_T) respectively (see figure 2.2), the system qubit is initialised in a pure state. In general, unitary evolution of a multipartite system will lead to entanglement, meaning Drive and Transducer bits are no longer pure states. This is at odds with the assumption of piecewise constant control functions. We therefore model Drive and Transducer qubits as series of ancilla qubits (figure 2.3) which interact with the system such that the state does not entangle and can afterwards be measured [1]. In the remainder of this work we use the interaction Hamiltonian on the three qubit Hilbert space

$$H_{DST} = H_I \otimes \mathbb{1}_T + \mathbb{1}_D \otimes H_I, \qquad H_I = \sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+$$

unless otherwise noted. The time evolution and work extraction is then calculated as follows, where Δt is time span between qubit switching:

$$H_S^i = \langle \psi_D^i | \langle \psi_T^i | H_{DST} | \psi_D^i \rangle | \psi_T^i \rangle \tag{2.1}$$

$$\rho_S^{i+1} = U^i \rho_S^i U^{i\dagger}, \; U^i = e^{-iH_S^i \Delta t} \tag{2.2}$$

$$W = -\Sigma_i \mathrm{Tr}\; \rho_S^i \; dH_S^i \tag{2.3}$$

$$dH_S^i = \langle \psi_D^i | \langle \psi_T^{i+1} | H_{DST} | \psi_D^i \rangle | \psi_T^{i+1} \rangle - \langle \psi_D^i | \langle \psi_T^i | H_{DST} | \psi_D^i \rangle | \psi_T^i \rangle . \tag{2.4}$$

Here we use the partial Hamiltonian H_S^i on S at time step $i \in [1, N-1]$, as well as corresponding system density matrix ρ_S^i.

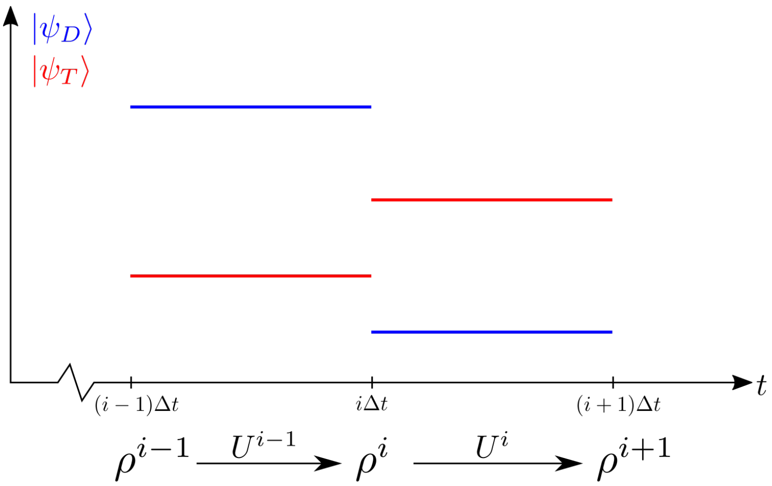

Figure 2.2.: Piecewise constant implementation of Drive and Transducer qubits: the vertical axis shows qubit state in arbitrary units. The qubit states are switched instantaneously and then kept constant for Δt while ρ_S evolves unitarily.

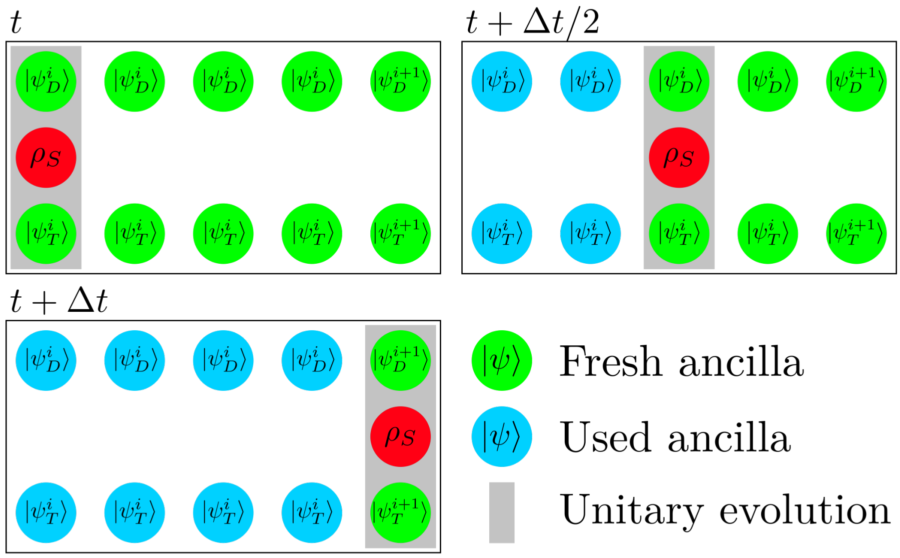

Figure 2.3.: Collision model used in this work: Drive and Transducer are series of qubits interact once with the system and evolve the reduced density operator ρ_S. The qubit configuration can be changed in intervals of Δt.

3. Experimental Results

The training data is created using a minimisation algorithm [10], which finds the optimal Transducer protocol $\{|\psi_T^i\rangle\}$ given a Drive sequence $\{|\psi_D^i\rangle\}$. The networks are trained to learn the mapping $\{|\psi_D^i\rangle\} \to \{|\psi_T^i\rangle\}$. Both the input (Drive) and output (Transducer) are transformed by the embedding

$$\left\{\begin{pmatrix}\theta^i & \phi^i\end{pmatrix}\right\} \to \left\{\begin{pmatrix}sin(\theta^i) & cos(\theta^i) & sin(\phi^i) & cos(\phi^i)\end{pmatrix}\right\}.$$

The reasons for this operation are twofold: it normalises the data to the interval $[-1, 1]$, which is beneficial to learning [3]. Additionally it adds information regarding the periodicity of the qubit angle representation.

To compare the accuracy of different models a performance indicator is required. Naturally one might use the MSE as introduced in section 2.1. Instead we define the *efficiency* of a model $\mathfrak{R}$ on a dataset $\{(\vec{x}_i, \vec{y}_i)\}$ as

$$\eta = \frac{1}{N}\sum_{i=1}^{N}\frac{W(\vec{x}_i, \mathfrak{R}(\vec{x}_i))}{W(\vec{x}_i, \vec{y}_i)}, \tag{3.1}$$

i.e. the arithmetic mean of the ratios of work output predicted by the model to optimal work output. The function $W(\vec{x}_i, \vec{y}_i) = W(\{|\psi_D\rangle\}_i, \{|\psi_T\rangle\}_i)$ returns the work given a Drive and Transducer protocol.

3.1. Dependence of Δt on Work Output

We start our investigation by determining the work output W when varying the time between qubit switching Δt. If the System qubit is initialised in the pure state $\rho_S = |0\rangle\langle 0|$, the work output for a single jump is given by (see appendix A.1 for a derivation)

$$W = \frac{1}{|\alpha|} sin(2|\alpha|\Delta t)\, \mathrm{Im}\{(\tau' - \tau)\alpha^*\} \tag{3.2}$$

$$\alpha = \frac{1}{2}\left[sin(\theta_D^1)e^{i\phi_D^1} + sin(\theta_T^1)e^{i\phi_T^1}\right], \qquad \tau' - \tau = \frac{1}{2}\left[sin(\theta_T^2)e^{i\phi_T^2} - sin(\theta_T^1)e^{i\phi_T^1}\right].$$

From equation 3.2 it becomes evident that for $\Delta t \to 0, W \to 0$. This is confirmed by the following where, for multiple values of N, we simulate 500 random Drive functions for each Δt and find their optimal Transducer policy. The average work output over the 500 runs scaled by the amount of PWC steps $\overline{W}/N$ for 20 values of Δt is shown in figure 3.1.

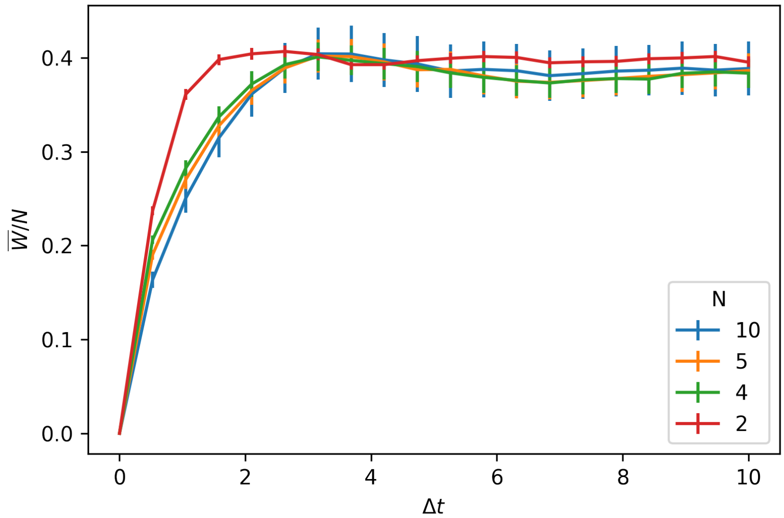

Figure 3.1.: We plot the average work $\overline{W}$ over 500 runs for random excitations divided by amount of PWC steps N, for all of which we use $\rho_0 = |0\rangle\langle 0|$. The error bars correspond to the standard deviation $\sigma_{\overline{W}}$.

3.2. $N = 2$: Learning Single Jump Optimal Control Sequences

For the simplest case of $N = 2$, we generate a data set of size $N_{data} = 50000$ with $\rho_0 = |0\rangle\langle 0|$, which we then separate into train and test data.

4. Summary and Outlook

A. Derivations

A.1. Single jump work output

$$
\begin{aligned}
H_S(\theta_D(t), \phi_D(t), \theta_T(t), \phi_T(t)) &= \frac{1}{2}\left[\sin(\theta_D(t))e^{i\phi_D(t)} + \sin(\theta_T(t))e^{i\phi_T(t)}\right]\sigma_+ + h.c. \\
&= \alpha\sigma_+ + h.c. \\
dH &= H_S(\theta_D(t), \phi_D(t), \theta_T(t+1), \phi_T(t+1)) - H_S(\theta_D(t), \phi_D(t), \theta_T(t), \phi_T(t)) \\
&= \frac{1}{2}(\sin(\theta_T(t+1))e^{i\phi_T(t+1)} - \sin(\theta_T(t))e^{i\phi_T(t)})\sigma_+ + h.c. =: (\tau' - \tau)\sigma_+ + h.c. \\
U = e^{-iH_S\Delta\mathrm{T}} &= exp\begin{pmatrix} 0 & -i\alpha^*\Delta\mathrm{T} \\ -i\alpha\Delta\mathrm{T} & 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \frac{\alpha^*}{|\alpha|} & -\frac{\alpha^*}{|\alpha|} \\ 1 & 1 \end{pmatrix}\begin{pmatrix} e^{-i|\alpha|\Delta\mathrm{T}} & 0 \\ 0 & e^{i|\alpha|\Delta\mathrm{T}} \end{pmatrix}\begin{pmatrix} \frac{|\alpha|}{\alpha^*} & 1 \\ -\frac{|\alpha|}{\alpha^*} & 1 \end{pmatrix} \\
&= \begin{pmatrix} \cos(|\alpha|\Delta\mathrm{T}) & -i\frac{\alpha^*}{|\alpha|}\sin(|\alpha|\Delta\mathrm{T}) \\ -i\frac{|\alpha|}{\alpha^*}\sin(|\alpha|\Delta\mathrm{T}) & \cos(|\alpha|\Delta\mathrm{T}) \end{pmatrix} \\
\text{With } \left|\psi_0\right\rangle &= a\left|0\right\rangle + b\left|1\right\rangle, |a|^2 + |b|^2 = 1, \text{ we have} \\
\rho_0 &= \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix},\ \rho = U\rho_0U^\dagger =
\end{aligned}
$$

$$
\begin{pmatrix} |a|^2\ \cos^2(|\alpha|\Delta\mathrm{T}) + |b|^2\ \sin^2(|\alpha|\Delta\mathrm{T}) - \frac{1}{|\alpha|}\sin(2|\alpha|\Delta\mathrm{T})\,\mathrm{Im}\{ab^*\alpha\} & \frac{\alpha^*}{2|\alpha|}i\ \sin(2|\alpha|\Delta\mathrm{T})(|a|^2 - |b|^2) + \frac{\alpha^*}{\alpha}a^*b\sin^2(|\alpha|\Delta\mathrm{T}) + ab^*\ \cos^2(|\alpha|\Delta\mathrm{T}) \\ \frac{|\alpha|}{2\alpha^*}i\ \sin(2|\alpha|\Delta\mathrm{T})(|b|^2 - |a|^2) + \frac{\alpha}{\alpha^*}ab^*\ \sin^2(|\alpha|\Delta\mathrm{T}) + a^*b\ \cos^2(|\alpha|\Delta\mathrm{T}) & |a|^2\ \sin^2(|\alpha|\Delta\mathrm{T}) + |b|^2\ \cos^2(|\alpha|\Delta\mathrm{T}) + \frac{1}{|\alpha|}\sin(2|\alpha|\Delta\mathrm{T})\,\mathrm{Im}\{ab^*\alpha\} \end{pmatrix}
$$

$$
\begin{aligned}
\mathrm{dW} = -\mathrm{Tr}\ \rho\ \mathrm{dH} &= \frac{|a|^2 - |b|^2}{|\alpha|}\sin(2|\alpha|\Delta\mathrm{T})\,\mathrm{Im}\{(\tau' - \tau)\alpha^*\} \\
&-2\ [\cos^2(|\alpha|\Delta\mathrm{T})\,\mathrm{Re}\{(\tau' - \tau)ab^*\} + \sin^2(|\alpha|\Delta\mathrm{T})\,\mathrm{Re}\left\{(\tau' - \tau)a^*b\frac{\alpha^*}{\alpha}\right\}]
\end{aligned}
$$

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Erklärung

Hiermit erkläre ich, dass ich diese Arbeit im Rahmen der Betreuung am Institut für Theoretische Physik ohne unzulässige Hilfe Dritter verfasst und alle Quellen als solche gekennzeichnet habe.

Felix Soest
Dresden, Monat 2021