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A Quantum-Inspired Approach to Predicting Geometric Changes in Head and Neck Cancer

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INTRODUCTION

Modern radiotherapy stands to benefit from the ability to efficiently adapt plans during-treatment in response to geometric variations such as those caused by organs deformation and tumor shrinkage.

A promising strategy is to develop a robust framework which, given an initial state defined by relevant patient-attributes, can predict future states based on pre-learnt patterns from a well-defined patient population. *This is reminiscent of the time-evolution of a stationary state in quantum mechanics.*

Here, we investigate the feasibility of predicting patient changes across a fractionated treatment schedule using a joint framework employing quantum mechanics in combination with deep recurrent neural networks (RNNs).

The expected benefit of a quantum-based framework are: (i) efficient solutions; and (ii) increased robustness against stochastic uncertainties.

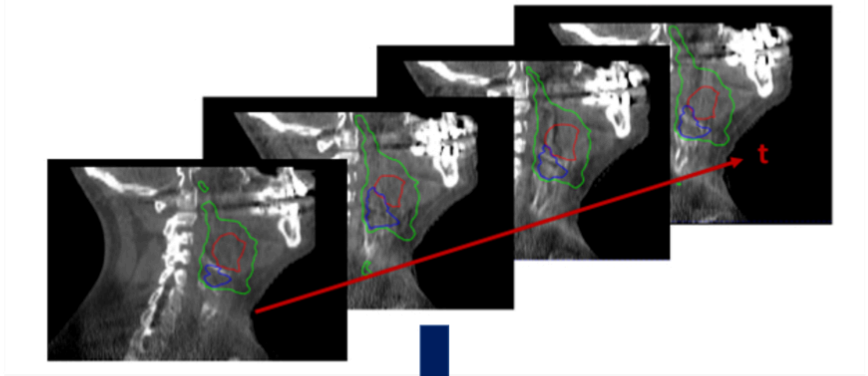
AIMS

1. Develop a predictive model for inter-fractional geometric changes in head and neck cancer patients which treats the conditions of interest as a stationary quantum state.
2. Benchmark the performance of this quantum-inspired model against a classical Markov model.

DATA ACQUISITION

Volume data for primary clinical target volume (CTV) structures were obtained from daily cone beam CT (CBCT) images from 104 head and neck cancer patients who received fractionated radiotherapy at one institution.

The percent change of the primary CTV volumes (with respect to the first treatment fraction) were converted into unitary state vectors by: (i) mapping them to discrete state values using Lloyd-Max quantization and (ii) encoding these states as one-hot vectors.



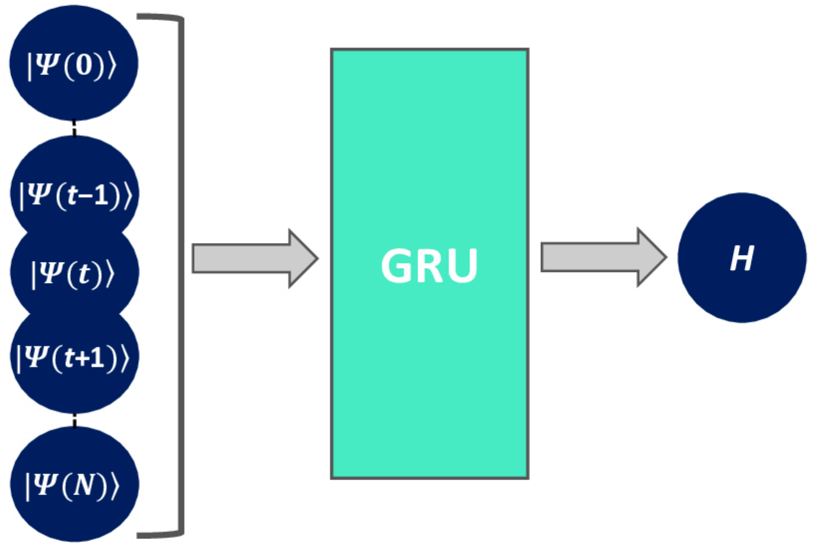
$$|v\rangle \in |1000\rangle, |0100\rangle, |0010\rangle, |0001\rangle$$

GEOMETRIC VARIATION MODELING

Quantum and Markov models of tumor volume change were both trained on a 2-layer gated recurrent unit (GRU) neural network to find the parameters which defined their respective transition matrices. Predictions were made for N-1 out of N fractions using the fraction immediately preceding as input; loss was defined as the negative log likelihood error.

Quantum Model	
System State	$\|\Psi(t)\rangle = a_1\|v_1\rangle + a_2\|v_2\rangle + a_3\|v_3\rangle + \cdots + a_L\|v_L\rangle$ a_i is the probability amplitude of state $\|v_i\rangle$: $\|a_i\|^2 = p_i$
Time Evolution	Governed by the time-independent Schrödinger equation: $\|\Psi(t+1)\rangle = \mathrm{U}(t+1)\|\Psi(t)\rangle$
Transition Matrix	$U(t) = e^{-\frac{itH}{\hbar}}$, is a doubly stochastic transition matrix H, the Hamiltonian, is a symmetric matrix
Loss Function	$QLoss = \frac{1}{N}\sum_{t=2}^{N} \log(\|\Psi(t)\rangle\|^2) - \log(\|U(1)\|\Psi(t-1)\rangle\|^2)$

Markov Model	
System State	$\Phi(t) = p_1\|v_1\rangle + p_2\|v_2\rangle + p_3\|v_3\rangle + \cdots + p_L\|v_L\rangle$ p_i is the probability of being in state v_i
Time Evolution	Governed by the forward Kolmogorov equation $\Phi(t+1) = \mathrm{A}(t)\Phi(\mathrm{T})$
Transition Matrix	$\mathrm{A}(t) = e^{Qt}$, is a stochastic transition matrix Q, the intensity matrix, has positive off-diagonals and sums to 0 within columns.
Loss Function	$MLoss = \frac{1}{N}\sum_{t=2}^{N} \log(\Phi(t)) - \log(A(t)\Phi(t-1))$



Flow of information through the RNN for the quantum model. States were fed into a Gated Recurrent Unit (GRU) neural network to predict the parameters of H.

RESULTS

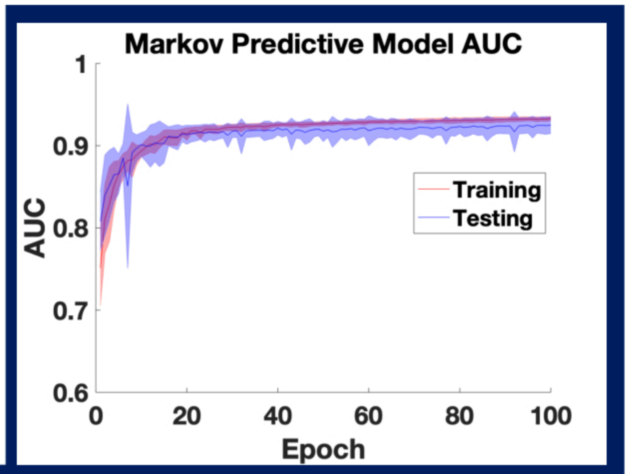
100 epochs of 5-fold cross-validation were performed for both the Quantum and Markov models.

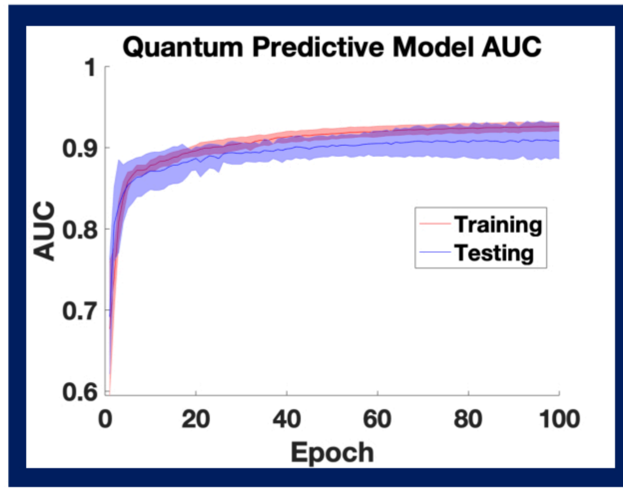
Quantum Results

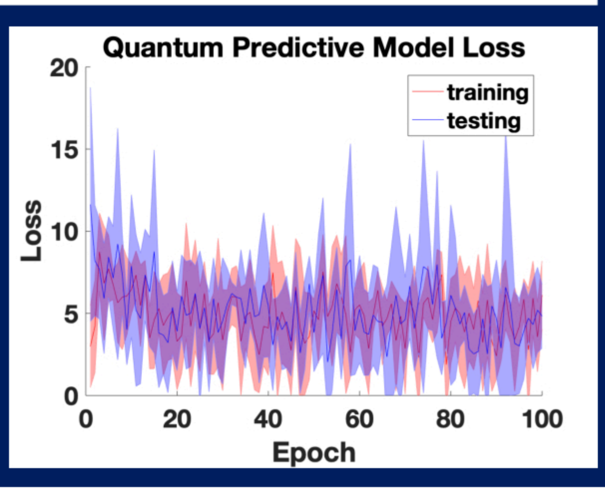
For the quantum model, the final are under the curve (AUC) averaged across the 5 folds was 0.9180 ± 0.0039 and 0.8884 ± 0.0177 for training and testing, respectively.

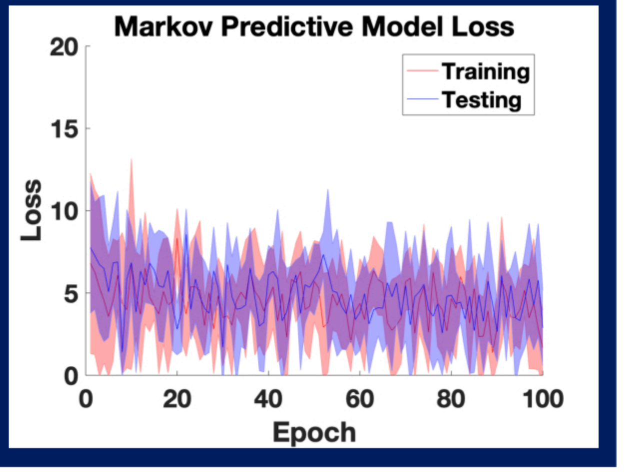
Markov Results

For the Markov model, the final AUC averaged across the 5 folds was 0.9330 ± 0.0025 and 0.9248 ± 0.0100 for training and testing, respectfully.









Average AUC scores (solid) with standard deviations (shaded) from 5-fold cross validation over 100 epochs.

CONCLUSIONS

This study investigated the feasibility of a novel framework for predicting changes in patient geometry over time by combining quantum mechanics with RNN techniques to improve robustness. We then benchmarked this framework against a classical Markov model.

Our results indicate that predictive information of primary tumor volume can be learnt from sequential patient data mapped to a discrete unitary state.

There were no substantial differences between the Quantum and Markov models; however, we acknowledge that the current objective may be too easy of a problem to exploit the full power of the quantum-based approach.

Future studies will investigate model performance on more challenging predictive problems including changes in tumor position and predictions farther into the future.

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