

Robust and High Performance Quantum Machine Learning for Single-Base-Resolution Prediction of Mammalian Transcription Factor Bindings and Chromatin Accessibility in Immune Cells

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Bindings and Chromatin Accessibility in Immune Cells (哺乳類の転写因子結
合および免疫細胞におけるクロマチンアクセス性を単一塩基解像度で予測する
ための頑健かつ高性能な量子機械学習)

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論 文 内 容 の 要 旨

This thesis presents the development and validation of quantum-classical hybrid deep learning methods for genomic regulatory element prediction. The central hypothesis is that quantum convolutional layers, through their capacity to explore exponentially large feature spaces and capture complex nonlinear relationships, can enhance the prediction of transcription factor binding and chromatin accessibility from DNA sequences. To test this hypothesis, two models are introduced: QTFPred for base-resolution transcription factor binding site prediction, and Qhromformer for simultaneous multi-cell-type chromatin accessibility prediction across the mammalian immune system.

QTFPred represents the first integration of parameterized quantum circuits into deep learning architectures for genomic sequence analysis. Comprehensive evaluation across 49 transcription factors from three human cell lines demonstrated state-of-the-art performance in 92% of binary classification tasks and 98% of quantitative signal prediction tasks. The performance advantage was particularly pronounced in data-limited scenarios: for transcription factors with fewer than 10,000 binding peaks, QTFPred substantially outperformed classical baselines, and in extreme downsampling experiments with only 250 training peaks, maintained a Pearson correlation of 0.56 compared with 0.24 for classical approaches. Beyond predictive accuracy, the quantum convolutional filters exhibited interpretable motif learning capabilities, successfully recovering known binding motifs and revealing cooperative binding relationships between transcription factor pairs, including characteristic distance constraints between E2F6 and MAX motifs.

Qhromformer extends the quantum-classical framework by incorporating Transformer layers with rotary position embedding and cell-type-specific prediction heads. Applied to the ImmGen ATAC-seq atlas, Qhromformer simultaneously predicts base-resolution chromatin accessibility signals for 92 distinct mouse immune cell types. Systematic comparison demonstrated that multi-cell-type learning significantly outperforms single-cell-type learning in 9 of 11

representative cell types, validating the multi-task learning approach. Cross-species transfer learning experiments revealed that for four of six immune lineages, models trained on mouse data achieved prediction performance on human sequences comparable to models trained directly on human data, indicating that Qhromformer captures evolutionarily conserved cis-regulatory grammar rather than species-specific artifacts.