Doctorate of Philosophy

Schrödinger's Catwalk

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Appendix

LIST OF TABLES

LIST OF FIGURES

LISTINGS

ACRONYMS

^{13}C	carbon-13. 118, 122
^{14}N	nitrogen-14. 118, 120–122
AI	artificial intelligence. 15
AIC	Akaike information criterion. 103, 104
AICC	Akaike information criterion corrected. 103
BF	Bayes factor. 49–51, 57, 59, 72, 76, 80, 82, 87–89, 96, 98, 99, 104–109, 112, 113, 126, 127, 132
BFEER	Bayes factor enhanced Elo ratings. 98, 99, 111, 112
BIC	Bayesian information criterion. 104
CLE	classical likelihood estimation. 37, 123
CPU	central processing unit. 15, 22
EDH	experiment design heuristic. 42–45, 47, 50, 59, 69, 80, 81, 101, 128, 129
ES	exploration strategy. 51–55, 57–59, 64, 67, 69, 73, 74, 76, 87, 90, 92, 97, 118, 121, 123, 125–129, 132, 138
ET	exploration tree. 52, 53, 55, 57–59, 71, 92, 126, 127, 132
FH	Fermi-Hubbard. 83
FN	false negatives. 95
FP	false positives. 19, 95
GA	genetic algorithm. v–vii, 22, 23, 27, 29, 30, 58, 92, 93, 98, 100, 101, 106, 108, 111, 114, 115, 138, 140, 141
GES	genetic exploration strategy. 92, 96, 111, 112, 116
GPU	graphics processing unit. 15, 22
HPD	high particle density. 42
IQLE	interactive quantum likelihood estimation. 37, 38, 111, 112

LTL log total likelihood. 40

ML machine learning. 15–17, 19, 21, 22, 50, 51, 95
MS model search. 51–53, 55, 59, 67, 69
MVEE minimum volume enclosing ellipsoid. 42

NV nitrogen-vacancy. 33, 118
NVC nitrogen-vacancy centre. v, vii, 38, 118–122, 124–128, 132, 133, 136, 138–141

OF objective function. vi, 17, 23, 26, 30, 92, 93, 96, 99, 101, 103, 106, 109–111

PGH particle guess heuristic. 43, 44, 69, 128, 129
PL photoluminescence. 120, 125, 130

QC quantum computer. 7, 13–15, 22
QHL quantum Hamiltonian learning. vi, 32–38, 40, 42, 44–46, 49–51, 55–59, 64, 67, 72, 80, 81, 92, 93, 111, 112, 125, 128
QL quadratic loss. 41
QLE quantum likelihood estimation. 37, 56, 120
QM quantum mechanics. 4, 6, 8, 9, 145, 155
QML quantum machine learning. 15, 21, 22
QMLA Quantum Model Learning Agent. v–vii, 32, 37, 48, 49, 51–55, 58, 59, 64, 67–74, 76, 77, 85–90, 92–95, 98, 101, 104–106, 108, 109, 111, 112, 114–116, 118, 121–123, 125–141

SMC sequential monte carlo. 35–37, 39, 42, 43, 47, 55
SVM support vector machine. 16

TLTL total log total likelihood. 40, 49–51, 59, 101, 103, 109
TN true negatives. 95
TP true positives. 19, 95

GLOSSARY

Jordan Wigner transformation (JWT)	Jordan Wigner transformation . 85, 86, 89
Loschmidt echo (LE)	Quantum chaotic effect described. . 38
chromosome	A single candidate in the space of valid solutions to the posed problem in a genetic algorithm. . 23, 25
expectation value	Average outcome expected by measuring an observable of a quantum system many times, **??**.. i, 12
gene	Individual element within a chromosome. . 23, 25
hyperparameter	Variable within an algorithm that determines how the algorithm itself proceeds.. 35
instance	a single implementation of the QMLA algorithm. vi, 72, 112, 114, 115, 132
likelihood	Value that represents how likely a hypothesis is.. 12, 34, 37, 39, 42, 55, 57, 58, 60, 105, 120, 125
model	The mathematical description of some quantum system. 48
model space	Abstract space containing all descriptions (within defined constraints such as dimension) of the system as models. 53, 138
probe	Input probe state, $\|\psi\rangle$, which the target system is initialised to, before unitary evolution. plural. 37, 39, 42–46, 79
results directory	Directory to which the data and analysis for a given run of QMLA are stored. . 73

run	collection of QMLA instances. iii, vi, vii, 72, 73, 89, 90, 112, 115, 116, 129, 132, 139, 140
spawn	Process by which new models are generated by combining previously considered models.. 53
success rate	. 73
term	Individual constituent of a model, e.g. a single operator within a sum of operators, which in total describe a Hamiltonian. . 48
volume	Volume of a parameter distribution's credible region.. 42, 80, 81, 88, 129
win rate	. 73

APPENDIX

A

FIGURE REPRODUCTION

Most of the figures presented in the main text are generated directly by the QMLA framework. Here we list the implementation details of each figure so they may be reproduced by ensuring the configuration in Table A.1 are set in the launch script. The default behaviour of QMLA is to generate a results folder uniquely identified by the date and time the run was launched, e.g. results can be found at the *results directory* qmla/Launch/Jan_01/12_34. Given the large number of plots available, ranging from high-level run perspective down to the training of individual models, we introduce a plot_level $\in \{1, ..., 6\}$ for each run of QMLA: higher plot_level informs QMLA to generate more plots.

Within the results directory, the outcome of the run's instances are stored, with analysis plots broadly grouped as

1. evaluation: plots of probes and times used as the evaluation dataset.
2. single_instance_plots: outcomes of an individual QMLA instance, grouped by the instance ID. Includes results of training of individual models (in model_training), as well as sub-directories for anlaysis at the branch level (in branches) and comparisons.
3. combined_datasets: pandas dataframes containing most of the data used during analysis of the run. Note that data on the individual model/instance level may be discarded so some minor analyses can not be performed offline.
4. exploration_strategy_plots plots specifically required by the exploration strategy (ES) at the run level.
5. champion_models: analysis of the models deemed champions by at least one instance in the run, e.g. average parameter estimation for a model which wins multiple instances.
6. performance: evaluation of the QMLA run, e.g. the win rate of each model and the number of times each term is found in champion models.
7. meta analysis of the algorithm' implementation, e.g. timing of jobs on each process in a cluster; generally users need not be concerned with these.

In order to produce the results presented in this thesis, the configurations listed in Table A.1 were input to the launch script. The launch scripts in the QMLA codebase consist of many configuration settings for running QMLA; only the lines in snippet in Listing A.1 need to be set according to altered to retrieve the corresponding figures. Note that the runtime of QMLA grows quite quickly with N_E, N_P (except for the AnalyticalLikelihood ES), especially for the entire QMLA algorithm; running quantum Hamiltonian learning (QHL) is feasible on a personal computer in < 30 minutes for $N_e = 1000; N_p = 3000$.

```
#!/bin/bash
```

```
###############
# QMLA run configuration
###############
num_instances=1
run_qhl=1 # perform QHL on known (true) model
run_qhl_mulit_model=0 # perform QHL for defined list of models.
exp=200 # number of experiments
prt=1000 # number of particles

###############
# QMLA settings
###############
plot_level=6
debug_mode=0

###############
# Choose an exploration strategy
###############

exploration_strategy='AnalyticalLikelihood'
```

Listing A.1: "QMLA Launch scipt"

Figure	Exploration Strategy	N_E	N_P	Data
??	DemoHeuristicPGH	1000	3000	Nov_27/19_39
	DemoHeuristicNineEighths	1000	3000	Nov_27/19_40
	DemoHeuristicTimeList	1000	3000	Nov_27/19_42
	DemoHeuristicRandom	1000	3000	Nov_27/19_47
??	DemoProbesPlus	1000	3000	Nov_27/14_43
	DemoProbesZero	1000	3000	Nov_27/14_45
	DemoProbesTomographic	1000	3000	Nov_27/14_46
	DemoProbes	1000	3000	Nov_27/14_47
??	DemoProbesPlus	1000	3000	Nov_27/14_43
	DemoProbesZero	1000	3000	Nov_27/14_45
	DemoProbesTomographic	1000	3000	Nov_27/14_46
	DemoProbes	1000	3000	Nov_27/14_47
??	AnalyticalLikelihood	500	2000	Nov_16/14_28
??	DemoIsing	500	5000	Nov_18/13_56
??	DemoIsing	1000	5000	Nov_18/13_56
??	DemoIsing	1000	5000	Nov_18/13_56
??	IsingLatticeSet	1000	4000	Nov_19/12_04
	IsingLatticeSet	1000	4000	Nov_19/12_04
	IsingLatticeSet	1000	4000	Nov_19/12_04
??	IsingLatticeSet	1000	4000	Sep_30/22_40
	HeisenbergLatticeSet	1000	4000	Oct_22/20_45
	FermiHubbardLatticeSet	1000	4000	Oct_02/00_09

Table A.1: Implementation details for figures used in the main text.

Figure	Exploration Strategy	N_E	N_P	Data
??	DemoBayesFactorsByFscore	500	2500	Dec_09/12_29
	DemoFractionalResourcesBayesFactorsByFscore	500	2500	Dec_09/12_31
	DemoBayesFactorsByFscore	1000	5000	Dec_09/12_33
	DemoBayesFactorsByFscoreEloGraphs	500	2500	Dec_09/12_32
??	HeisenbergGeneticXYZ	500	2500	Dec_10/14_40
??	HeisenbergGeneticXYZ	500	2500	Dec_10/14_40
	HeisenbergGeneticXYZ	500	2500	Dec_10/14_40
??	HeisenbergGeneticXYZ	500	2500	Dec_10/16_12
	HeisenbergGeneticXYZ	500	2500	Dec_10/16_12
??	NVCentreExperimentalData	1000	3000	2019/Oct_02/18_01
	SimulatedExperimentNVCentre	1000	3000	2019/Oct_02/18_16
??	NVCentreExperimentalData	1000	3000	2019/Oct_02/18_01
??	SimulatedExperimentNVCentre	1000	3000	2019/Oct_02/18_16
??	SimulatedExperimentNVCentre	1000	3000	2019/Oct_02/18_16
	NVCentreExperimentalData	1000	3000	2019/Oct_02/18_01
??	NVCentreGenticAlgorithmPrelearnedParameters	2	5	Sep_09/12_00
	NVCentreGenticAlgorithmPrelearnedParameters	2	5	Sep_09/12_00
??	NVCentreGenticAlgorithmPrelearnedParameters	2	5	Sep_09/12_00
	NVCentreGenticAlgorithmPrelearnedParameters	2	5	Sep_09/12_00

Table A.2: [Continued from Table A.1] Implementation details for figures used in the main text.

B

FUNDAMENTALS

There are a number of concepts which are fundamental to any discussion of quantum mechanics (QM), but are likely to be known to most readers, and are therefore cumbersome to include in the main body of the thesis. We include them here for completeness[1].

B.1 LINEAR ALGEBRA

Here we review the language of linear algebra and summarise the basic mathematical techniques used throughout this thesis. We will briefly recall some definitions for reference.

- Notation

Definition of	Representation
Vector (or *ket*)	$\|\psi\rangle$
Dual Vector (or *bra*)	$\langle\psi\|$
Tensor Product	$\|\psi\rangle \otimes \|\phi\rangle$
Complex conjugate	$\|\psi^*\rangle$
Transpose	$\|\psi\rangle^T$
Adjoint	$\|\psi\rangle^\dagger = (\|\psi\rangle^*)^T$

Table B.1: Linear algebra definitions.

The dual vector of a vector (ket) $|\psi\rangle$ is given by $\langle\psi| = |\psi\rangle^\dagger$.

The *adjoint* of a matrix replaces each matrix element with its own complex conjugate, and then switches its columns with rows.

$$M^\dagger = \begin{pmatrix} M_{0,0} & M_{0,1} \\ M_{1,0} & M_{1,1} \end{pmatrix}^\dagger = \begin{pmatrix} M^*_{0,0} & M^*_{0,1} \\ M^*_{1,0} & M^*_{1,1} \end{pmatrix}^T = \begin{pmatrix} M^*_{0,0} & M^*_{1,0} \\ M^*_{0,1} & M^*_{1,1} \end{pmatrix} \tag{B.1}$$

1 Much of this description is reproduced from my undergraduate thesis [1].

The *inner product* of two vectors, $|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix}$ and $|\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{pmatrix}$ is given by

$$\langle\phi|\psi\rangle = (|\phi\rangle^\dagger)\,|\psi\rangle = (\phi_1^* \ \phi_2^* \ \dots \ \phi_n^*) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} = \phi_1^*\psi_1 + \phi_2^*\psi_2 + \cdots + \phi_n^*\psi_n \tag{B.2}$$

$|\psi\rangle_i, |\phi\rangle_i$ are complex numbers, and therefore the above is simply a sum of products of complex numbers. The inner product is often called the *scalar product*, which is in general complex.

B.2 POSTULATES OF QUANTUM MECHANICS

There are numerous statements of the postulates of quantum mechanics. Each version of the statements aims to achieve the same foundation, so we endeavour to explain them in the simplest terms.

1 Every moving particle in a conservative force field has an associated wave-function, $|\psi\rangle$. From this wave-function, it is possible to determine all physical information about the system.

2 All particles have physical properties called observables (denoted q). In order to determine a value, q, for a particular observable, there is an associated *operator* $\hat{Q}$, which, when acting on the particles wavefunction, yields the value times the wavefunction. The observable q is then the eigenvalue of the operator $\hat{Q}$.

$$\hat{Q}\,|\psi\rangle = q|\psi\rangle \tag{B.3}$$

3 Any such operator $\hat{Q}$ is Hermitian

$$\hat{Q}^\dagger = \hat{Q} \tag{B.4}$$

4 The set of eigenfunctions for any operator $\hat{Q}$ forms a complete set of linearly independent functions.

5 For a system with wavefunction $|\psi\rangle$, the expectation value of an observable q with respect to an operator $\hat{Q}$ is denoted by $\langle q\rangle$ and is given by

$$\langle q\rangle = \langle\psi|\hat{Q}|\psi\rangle \tag{B.5}$$

6 The time evolution of $|\psi\rangle$ is given by the time dependent *Schrodinger Equation*

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi, \tag{B.6}$$

where $\hat{H}$ is the system's Hamiltonian.

Using these building blocks, we can begin to construct a language to describe quantum systems.

B.3 STATES

An orhthonormal basis consists of vectors of unit length which do not overlap, e.g. $|x_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, |x_2\rangle = \begin{pmatrix}0\\1\end{pmatrix} \Rightarrow \langle x_1|x_2\rangle = 0$. In general, if $\{|x\rangle\}$ are the eigenstates of a system, then the system can be written as some state vector, $|\psi\rangle$, in general a superposition over the basis-vectors:

$$|\psi\rangle = \sum_x a_x|x\rangle \tag{B.7a}$$

$$\text{subject to} \quad \sum_x |a_x|^2 = 1, \quad a_x \in \mathbb{C} \tag{B.7b}$$

The *state space* of a physical system (classical or quantum) is then the set of all possible states the system can exist in, i.e the set of all possible values for $|\psi\rangle$ such that Eq. (B.7b) are satisfied.

For example, photons can be polarised horizontally ($\leftrightarrow$) or vertically ($\updownarrow$); take those two conditions as observable states to define the eigenstates of a two-level system, so we can designate the photon as a qubit. Then we can map the two states to a 2-dimensional, x-y plane: a general vector on such a plane can be represented by a vector with coordinates $\begin{pmatrix}x\\y\end{pmatrix}$. These polarisations can then be thought of as standard basis vectors in linear algebra. Denote $\leftrightarrow$ as the eigenstate $|0\rangle$ and $\updownarrow$ as $|1\rangle$

$$|\leftrightarrow\rangle = |0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad \text{A unit vector along x-axis} \tag{B.8a}$$

$$|\updownarrow\rangle = |1\rangle = \begin{pmatrix}0\\1\end{pmatrix} \qquad \text{A unit vector along y-axis} \tag{B.8b}$$

Now, in relation to the concept of superposition, we can consider, for example, a photon in an even superposition of the vertical and horizontal polarisations, evenly splitting the two basis vectors. As such, we would require that, upon measurement, it is equally likely that the

photon will *collapse* into the polarised state along x as it is to collapse along y. That is, we want $\Pr(\updownarrow) = \Pr(\leftrightarrow)$ so assign equal modulus amplitudes to the two possibilities:

$$|\psi\rangle = a\,|\leftrightarrow\rangle + b\,|\updownarrow\rangle\,, \quad \text{with} \quad \Pr(\updownarrow) = \Pr(\leftrightarrow) \Rightarrow |a|^2 = |b|^2 \tag{B.9}$$

We consider here a particular case, due to the significance of the resultant basis, where $\leftrightarrow$-polarisation and $\updownarrow$-polarisation have real amplitudes $a, b \in \mathbb{R}$.

$$\begin{aligned} &\Rightarrow a = \pm b \quad \text{but also} \quad |a|^2 + |b|^2 = 1 \\ \Rightarrow \quad &a = \frac{1}{\sqrt{2}} \quad ; \quad b = \pm\frac{1}{\sqrt{2}} \\ &\Rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}\,|\leftrightarrow\rangle \pm \frac{1}{\sqrt{2}}\,|\updownarrow\rangle \\ &\Rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}\,|0\rangle \pm \frac{1}{\sqrt{2}}\,|1\rangle \end{aligned} \tag{B.10}$$

These particular superpositions are of significance:

$$|+\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle + |1\rangle) \tag{B.11a}$$

$$|-\rangle = \frac{1}{\sqrt{2}}\,(|0\rangle - |1\rangle) \tag{B.11b}$$

This is called the Hadamard basis: it is an equally valid vector space as the standard basis which is spanned by $\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}$, as it is simply a rotation of the standard basis.

B.3.1 *Mulitpartite systems*

In reality, we often deal with systems of multiple particles, represented by multiple qubits. Mathematically, we consider the state vector of a system containing n qubits as being the tensor product of the n qubits' individual state vectors[2]. For instance, suppose a 2-qubit system, $|\psi\rangle$ consisting of two independent qubits $|\psi_A\rangle$ and $|\psi_B\rangle$:

$$|\psi\rangle = |\psi_A\rangle\,|\psi_B\rangle = |\psi_A\psi_B\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \tag{B.12}$$

Consider first a simple system of 2 qubits. Measuring in the standard basis, these qubits will have to collapse in to one of the basis states $|0,0\rangle, |0,1\rangle, |1,0\rangle, |1,1\rangle$. Thus, for such a 2-qubit system, we have the general superposition

$$|\psi\rangle = \alpha_{0,0}|0,0\rangle + \alpha_{0,1}|0,1\rangle + \alpha_{1,0}|1,0\rangle + \alpha_{1,1}|1,1\rangle$$

2 We will later discuss entangled states, which can not be described thus.

where $\alpha_{i,j}$ is the amplitude for measuring the system as the state $|i,j\rangle$. This is perfectly analogous to a classical 2-bit system necessarily occupying one of the four possibilities $\{(0,0),(0,1),(1,0),(1,1)\}$.

Hence, for example, if we wanted to concoct a two-qubit system composed of one qubit in the state $|+\rangle$ and one in $|-\rangle$

$$\begin{aligned}
|\psi\rangle &= |+\rangle \otimes |-\rangle \\
|\psi\rangle &= \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) \\
&= \frac{1}{2}\left[|00\rangle - |01\rangle + |10\rangle - |11\rangle\right] \\
&= \frac{1}{2}\left[\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} - \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}\right] \\
&= \frac{1}{2}\left[\begin{pmatrix}1\\0\\0\\0\end{pmatrix} - \begin{pmatrix}0\\1\\0\\0\end{pmatrix} + \begin{pmatrix}0\\0\\1\\0\end{pmatrix} - \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right]. \\
\Rightarrow |\psi\rangle &= \frac{1}{2}\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}
\end{aligned} \tag{B.13}$$

That is, the two qubit system – and indeed any two qubit system – is given by a linear combination of the four basis vectors

$$\{|00\rangle, |0,1\rangle, |10\rangle, |11\rangle\} = \left\{\begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\1\end{pmatrix}\right\}. \tag{B.14}$$

We can notice that a single qubit system can be described by a linear combination of two basis vectors, and that a two qubit system requires four basis vectors to describe it. In general we can say that an n-qubit system is represented by a linear combination of 2^n basis vectors.

B.3.2 *Registers*

A *register* is generally the name given to an array of controllable quantum systems; here we invoke it to mean a system of multiple qubits, specifically a subset of the total number of

available qubits. For example, a register of ten qubits can be denoted $|x[10]\rangle$, and we can think of the system as a register of six qubits together with a register of three and another register of one qubit.

$$|x[10]\rangle = |x_1[6]\rangle \otimes |x_2[3]\rangle \otimes |x_3[1]\rangle$$

B.4 ENTANGLEMENT

Another unique property of quantum systems is that of *entanglement*: when two or more particles interact in such a way that their individual quantum states can not be described independent of the other particles. A quantum state then exists for the system as a whole instead. Mathematically, we consider such entangled states as those whose state can not be expressed as a tensor product of the states of the individual qubits it's composed of: they are dependent upon the other.

To understand what we mean by this dependence, consider a counter-example. Consider the Bell state,

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right), \tag{B.15}$$

if we measure this state, we expect that it will be observed in either eigenstate $|00\rangle$ or $|11\rangle$, with equal probability due to their amplitudes' equal magnitudes. The bases for this state are simply the standard bases, $|0\rangle$ and $|1\rangle$. Thus, according to our previous definition of systems of multiple qubits, we would say this state can be given as a combination of two states, like Eq. (B.12),

$$\begin{aligned} |\Phi^+\rangle &= |\psi_1\rangle \otimes |\psi_2\rangle \\ &= (a_1|0\rangle + b_1|1\rangle) \otimes (a_2|0\rangle + b_2|1\rangle) \\ &= a_1a_2|00\rangle + a_1b_2|01\rangle + b_1a_2|10\rangle + b_1b_2|11\rangle \end{aligned} \tag{B.16}$$

However we require $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, which would imply $a_1b_2 = 0$ and $b_1a_2 = 0$. These imply that either $a_1 = 0$ or $b_2 = 0$, and also that $b_1 = 0$ or a_2=0, which are obviously invalid since we require that $a_1a_2 = b_1b_2 = \frac{1}{\sqrt{2}}$. Thus, we cannot express $|\Phi^+\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$; this inability to separate the first and second qubits is what we term *entanglement*.

B.5 UNITARY TRANSFORMATIONS

A fundamental concept in quantum mechanics is that of performing transformations on states. *Quantum transformations*, or *quantum operators*, map a quantum state into a new state within the same Hilbert space. There are certain restrictions on a physically possible quantum transformation: in order that U is a valid transformation acting on some superposition $|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle + \ldots a_k|\psi_k\rangle$, U must be linear

$$U(a_1|\psi_1\rangle + a_2|\psi_2\rangle + \ldots a_k|\psi_k\rangle) = a_1(U|\psi_1\rangle) + a_2(U|\psi_2\rangle) + \cdots + a_k(U|\psi_k\rangle). \tag{B.17}$$

To fulfil these properties, we require that U *preserve the inner product*:

$$\langle \psi_0 | U^\dagger U | \psi \rangle = \langle \psi_0 | \psi \rangle$$

That is, we require that any such transformation be *unitary*:

$$UU^\dagger = I \Rightarrow U^\dagger = U^{-1} \tag{B.18}$$

Unitarity is a sufficient condition to describe any valid quantum operation: any quantum transformation can be described by a unitary transformation, and any unitary transformation corresponds to a physically implementable quantum transformation.

Then, if U_1 is a unitary transformation that acts on the space $\mathcal{H}_1$ and U_2 acts on $\mathcal{H}_2$, the product of the two unitary transformations is also unitary. The tensor product $U_1 \otimes U_2$ acts on the space $\mathcal{H}_1 \otimes \mathcal{H}_2$. So, then, supposing a system of two separable qubits, $|\psi_1\rangle$ and $|\psi_2\rangle$ where we wish to act on $|\psi_1\rangle$ with operator U_1 and on $|\psi_2\rangle$ with U_2, we perform it as

$$(U_1 \otimes U_2)(|\psi_1\rangle \otimes |\psi_2\rangle) = (U_1 |\psi_1\rangle) \otimes (U_2 |\psi_2\rangle) \tag{B.19}$$

B.6 DIRAC NOTATION

In keeping with standard practice, we employ *Dirac notation* throughout this thesis. Vectors are denoted by *kets* of the form $|a\rangle$. For example, the standard basis is represented by,

$$\begin{aligned} |x\rangle = |0\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |y\rangle = |1\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \tag{B.20}$$

We saw in Table B.1 that for every such ket, $|\psi\rangle$, there exists a *dual vector*: its complex conjugate transpose, called the *bra* of such a vector, denoted $\langle \psi |$. That is,

$$\begin{aligned} \langle \psi |^\dagger &= |\psi\rangle \\ |\psi\rangle^\dagger &= \langle \psi | \end{aligned} \tag{B.21}$$

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \Rightarrow \langle \psi | = \begin{pmatrix} \psi_1^* & \psi_2^* & \dots & \psi_n^* \end{pmatrix} \tag{B.22}$$

Then if we have two vectors $|\psi\rangle$ and $|\phi\rangle$, their *inner product* is given as $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle$.

$$\begin{aligned} |\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_n \end{pmatrix} \quad ; \quad |\phi\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \vdots \\ \phi_n \end{pmatrix} \\ \Rightarrow \langle\phi| = \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & \dots & \phi_n^* \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & \dots & \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_n \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \phi_1^*\psi_1 + \phi_2^*\psi_2 + \phi_3^*\psi_3 + \cdots + \phi_n^*\psi_n \end{aligned} \tag{B.23}$$

Example B.6.1.

$$\begin{aligned} |\psi\rangle = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad ; \quad |\phi\rangle = \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} \\ \Rightarrow \langle\phi|\,|\psi\rangle = \begin{pmatrix} 4 & 5 & 6 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \\ = (4)(1) + (5)(2) + (6)(3) = 32 \end{aligned} \tag{B.24}$$

Similarly, their *outer product* is given as $|\phi\rangle\langle\psi|$. Multiplying a column vector by a row vector thus gives a matrix. Matrices generated by a outer products then define operators:

Example B.6.2.

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \begin{pmatrix} 3 & 4 \end{pmatrix} = \begin{pmatrix} 3 & 4 \\ 6 & 8 \end{pmatrix} \tag{B.25}$$

Then we can say, for $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$$|0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{B.26a}$$

$$|0\rangle\langle 1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{B.26b}$$

$$|1\rangle\langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{B.26c}$$

$$|1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{B.26d}$$

And so any 2-dimensional linear transformation in the standard basis $|0\rangle, |1\rangle$ can be given as a sum

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = a|0\rangle\langle 0| + b|0\rangle\langle 1| + c|1\rangle\langle 0| + d|1\rangle\langle 1| \tag{B.27}$$

This is a common method of representing operators as outer products of vectors. A transformation that *exchanges* a particle between two states, say $|0\rangle \leftrightarrow |1\rangle$ is given by the operation

$$\hat{Q} : \begin{cases} |0\rangle \to |1\rangle \\ |1\rangle \to |0\rangle \end{cases}$$

Which is equivalent to the outer product representation

$$\hat{Q} = |0\rangle\langle 1| + |1\rangle\langle 0|$$

For clarity, here we will prove this operation

Example B.6.3.

$$\begin{aligned} \hat{Q} &= |0\rangle\langle 1| + |1\rangle\langle 0| \\ &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

So then, acting on $|0\rangle$ *and* $|1\rangle$ *gives*

$$\hat{Q}|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle$$

$$\hat{Q}\left|1\right\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left|0\right\rangle$$

To demonstrate how Dirac notation simplifies this:

$$\begin{aligned} \hat{Q}\left|0\right\rangle &= \left(\left|0\right\rangle\left\langle 1\right| + \left|1\right\rangle\left\langle 0\right|\right)\left|0\right\rangle \\ &= \left|0\right\rangle\left\langle 1\right|\left|0\right\rangle + \left|1\right\rangle\left\langle 0|0\right\rangle \\ &= \left|0\right\rangle\left\langle 1|0\right\rangle + \left|1\right\rangle\left\langle 0|0\right\rangle \end{aligned}$$

Then, since $\left|0\right\rangle$ and $\left|1\right\rangle$ are orthogonal basis, their inner product is 0 and the inner product of a vector with itself is 1, ($\left\langle 1|1\right\rangle = \left\langle 0|0\right\rangle = 1, \left\langle 0|1\right\rangle = \left\langle 1|0\right\rangle = 0$). So,

$$\begin{aligned} \hat{Q}\left|0\right\rangle &= \left|0\right\rangle(0) + \left|1\right\rangle(1) \\ \Rightarrow \hat{Q}\left|0\right\rangle &= \left|1\right\rangle \end{aligned} \tag{B.28}$$

And similarly for $\hat{Q}\left|1\right\rangle$. This simple example then shows why Dirac notation can significantly simplify calculations across quantum mechanics, compared to standard matrix and vector notation. To see this more clearly, we will examine a simple 2-qubit state under such operations. The method generalises to operating on two or more qubits generically: we can define any operator which acts on two qubits as a sum of outer products of the basis vectors $\left|00\right\rangle, \left|01\right\rangle, \left|10\right\rangle$ and $\left|11\right\rangle$. We can similarly define any operator which acts on an n qubit state as a linear combination of the 2^n basis states generated by the n qubits.

Example B.6.4. *To define a transformation that will exchange basis vectors $\left|00\right\rangle$ and $\left|11\right\rangle$, while leaving $\left|01\right\rangle$ and $\left|10\right\rangle$ unchanged (ie exchanging $\left|01\right\rangle \leftrightarrow \left|01\right\rangle, \left|10\right\rangle \leftrightarrow \left|10\right\rangle$) we define an operator*

$$\hat{Q} = \left|00\right\rangle\left\langle 11\right| + \left|11\right\rangle\left\langle 00\right| + \left|10\right\rangle\left\langle 10\right| + \left|01\right\rangle\left\langle 01\right| \tag{B.29}$$

Then, using matrix calculations this would require separately calculating the four outer products in the above sum and adding them to find a 4×4 matrix to represent $\hat{Q}$, which then acts on a state $\left|\psi\right\rangle$. Instead, consider first that $\left|\psi\right\rangle = \left|00\right\rangle$, ie one of the basis vectors our transformation is to change:

$$\hat{Q}\left|00\right\rangle = \left(\left|00\right\rangle\left\langle 11\right| + \left|11\right\rangle\left\langle 00\right| + \left|10\right\rangle\left\langle 10\right| + \left|01\right\rangle\left\langle 01\right|\right)\ \left|00\right\rangle \tag{B.30}$$

And as before, only the inner products of a vector with itself remains:

$$\begin{aligned} &= \left|00\right\rangle\left\langle 11\,|00\right\rangle + \left|11\right\rangle\left\langle 00\,|00\right\rangle + \left|10\right\rangle\left\langle 10\,|00\right\rangle + \left|01\right\rangle\left\langle 01\,|00\right\rangle \\ &= \left|00\right\rangle(0) + \left|11\right\rangle(1) + \left|10\right\rangle(0) + \left|01\right\rangle(0) \\ \Rightarrow &\hat{Q}\left|00\right\rangle = \left|11\right\rangle \end{aligned} \tag{B.31}$$

i.e the transformation has performed $\hat{Q} : |00\rangle \rightarrow |11\rangle$ *as expected. Then, if we apply the same transformation to a state which does not depend on one of the target states, eg,*

$$\begin{aligned} |\psi\rangle =& a\,|10\rangle + b\,|01\rangle \\ \hat{Q}\,|\psi\rangle =& \Big(|00\rangle\langle 11| + |11\rangle\langle 00| + |10\rangle\langle 10| + |01\rangle\langle 01| \Big)\Big(a\,|10\rangle + b\,|01\rangle \Big) \\ =& a\Big(|00\rangle\langle 11|10\rangle + |11\rangle\langle 00|10\rangle + |10\rangle\langle 10|10\rangle + |01\rangle\langle 01|10\rangle \Big) \\ &+ b\Big(|00\rangle\langle 11|01\rangle + |11\rangle\langle 00|01\rangle + |10\rangle\langle 10|01\rangle + |01\rangle\langle 01|01\rangle \Big) \end{aligned} \tag{B.32}$$

And since the inner product is a scalar, we can factor terms such as $\langle 11|10\rangle$ *to the beginning of expressions, eg* $|00\rangle\langle 11|\,|10\rangle = \langle 11\,|10\rangle\,|00\rangle$*, and we also know*

$$\begin{aligned} \langle 11|10\rangle = \langle 00|10\rangle = \langle 01|10\rangle = \langle 11|01\rangle = \langle 00|01\rangle = \langle 10|01\rangle = 0 \\ \langle 10|10\rangle = \langle 01|01\rangle = 1 \end{aligned} \tag{B.33}$$

We can express the above as

$$\begin{aligned} \hat{Q}\,|\psi\rangle =& a\Big((0)\,|00\rangle + (0)\,|11\rangle + (1)\,|10\rangle + (0)\,|01\rangle \Big) \\ &+ b\Big((0)\,|00\rangle + (0)\,|11\rangle + (0)\,|10\rangle + (1)|01\rangle \Big) \\ =& a\,|10\rangle\,| + b|01\rangle \\ =& |\psi\rangle \end{aligned} \tag{B.34}$$

Then it is clear that, when $|\psi\rangle$ *is a superposition of states unaffected by transformation* $\hat{Q}$*, then* $\hat{Q}\,|\psi\rangle = |\psi\rangle$*.*

This method generalises to systems with greater numbers of particles (qubits). If we briefly consider a 3 qubit system - and initialise all qubits in the standard basis state $|0\rangle$ - then the system is represented by $|000\rangle = |0\rangle \otimes |0\rangle \otimes |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. This quantity is an 8-row vector. To calculate the outer product $\langle 000|000\rangle$, we would be multiplying an 8-column bra $\langle 000|$ by an 8-row ket $|000\rangle$. Clearly then we will be working with 8×8 matrices, which will become quite difficult to maintain effectively and efficiently quite fast. As we move to systems of larger size, standard matrix multiplication becomes impractical for hand-written analysis, although of course remains tractable computationally up to $n \sim 10$ qubits. It is obvious that Dirac's bra/ket notation is a helpful, pathematically precise tool for QM.

C

EXAMPLE EXPLORATION STRATEGY RUN

Here we provide a complete example of how to run the Quantum Model Learning Agent (QMLA) framework, including how to implement a custom exploration strategy (ES), and generate/interpret analysis.

First, *fork* the QMLA codebase from [2] to a Github user account (referred to as username in Listing C.1). Now, we must download the code base and ensure it runs properly; these instructions are implemented via the command line[1].

```
# Install redis (database broker)
sudo apt update
sudo apt install redis-server

# make directory for QMLA
cd
mkdir qmla_test
cd qmla_test

# make Python virtual environment for QMLA
# note: change Python3.6 to desired version
sudo apt-get install python3.6-venv
python3.6 -m venv qmla-env
source qmla-env/bin/activate

# Download QMLA
git clone --depth 1 https://github.com/username/QMLA.git #
   REPLACE username

# Install dependencies
cd QMLA
pip install -r requirements.txt
```

1 Note: these instructions are tested for Linux and presumed to work on Mac, but untested on Windows. It is likely some of the underlying software (redis servers) can not be installed on Windows, so running on *Windows Subsystem for Linux* is advised.

Listing C.1: QMLA codebase setup. (i) install redis; (ii) creaet a virtual Python environment for installing QMLA dependencies without damaging other parts of the user's environment; (iii) download the QMLA codebase from the forked Github repository; (iv) install packages upon which QMLA depends.

Note there may be a problem with some packages in the requirements.txt arising from the attempt to install them all through a single call to pip install. Ensure these are all installed before proceeding.

When all of the requirements are installed, test that the framework runs. QMLA uses redis databases to store intermittent data: we must manually initialise the database. Run the following (note: here we list redis-4.0.8, but this must be corrected to reflect the version installed on the user's machine in the above setup section):

```
~/redis-4.0.8/src/redis-server
```

Listing C.2: Launch redis database

which should give something like Fig. C.1.

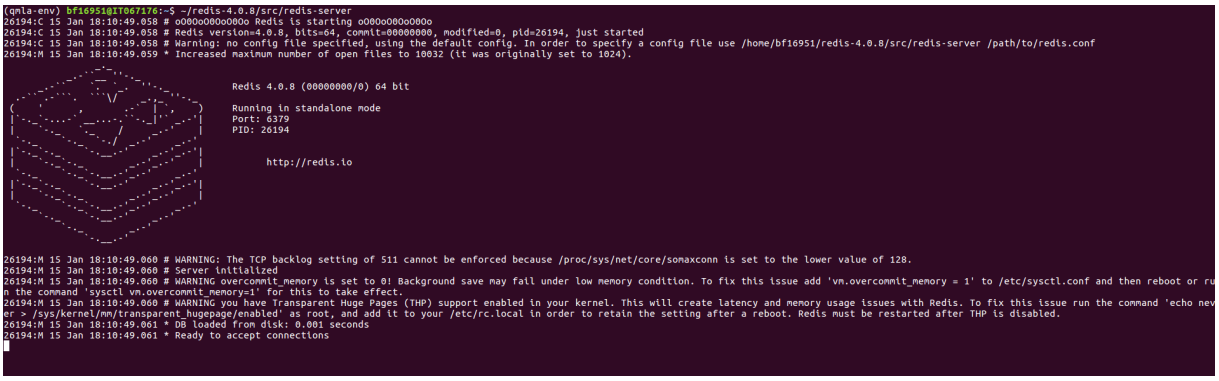


Figure C.1: Terminal running redis-server.

In a text editor, open qmla_test/QMLA/launch/local_launch.sh; here we will ensure that we are running the QHL algorithm, with 5 experiments and 20 particles, on the ES named TestInstall. Ensure the first few lines of local_launch.sh read:

```
#!/bin/bash

##### ---------------------------------------------------- #####
# QMLA run configuration
##### ---------------------------------------------------- #####
num_instances=2 # number of instances in run
```

```
run_qhl=0 # perform QHL on known (true) model
run_qhl_multi_model=0 # perform QHL for defined list of models
experiments=2 # number of experiments
particles=10 # number of particles
plot_level=5


##### ---------------------------------------------- #####
# Choose an exploration strategy
# This will determine how QMLA proceeds.
##### ---------------------------------------------- #####
exploration_strategy="TestInstall"
```

Listing C.3: local_launch script

Now we can run Ensure the terminal running redis is kept active, and open a separate terminal window. We must activate the Python virtual environment configured for QMLA, which we set up in Listing C.1. Then, we navigate to the QMLA directory, and launch:

```
# activate the QMLA Python virtual environment
source qmla_test/qmla-env/bin/activate

# move to the QMLA directory
cd qmla_test/QMLA
# Run QMLA
cd launch
./local_launch.sh
```

Listing C.4: Launch QMLA

There may be numerous warnings, but they should not affect whether QMLA has succeeded; QMLA will raise any significant error. Assuming the run has completed successfully, QMLA stores the run's results in a subdirectory named by the date and time it was started. For example, if the run was initialised on January 1st at 01:23, navigate to the corresponding directory by

```
cd results/Jan_01/01_23
```

Listing C.5: QMLA results directory

For now it is sufficient to notice that the code has run successfully: it should have generated (in results/Jan_01/01_23) files like storage_001.p and results_001.p.

C.1 CUSTOM EXPLORATION STRATEGY

Next, we design a basic ES, for the purpose of demonstrating how to run the algorithm. ESs are placed in the directory qmla/exploration_strategies. To make a new one, navigate to the exploration strategies directory, make a new subdirectory, and copy the template file.

```
cd ~/qmla_test/QMLA/exploration_strategies/
mkdir custom_es

# Copy template file into example
cp template.py custom_es/example.py
cd custom_es
```

Listing C.6: QMLA codebase setup

Ensure QMLA will know where to find the ES by importing everything from the custom ES directory into to the main exploration_strategy module. Then, in the custom_es directory, make a file called __init__.py which imports the new ES from the example.py file. To add any further ESs inside the directory custom_es, include them in the custom __init__.py, and they will automatically be available to QMLA.

```
# inside qmla/exploration_strategies/custom_es
#   __init__.py
from qmla.exploration_strategies.custom_es.example import *

# inside qmla/exploration_strategies , add to the existing
# __init__.py
from qmla.exploration_strategies.custom_es import *
```

Listing C.7: Providing custom exploration strategy to QMLA

Now, change the structure (and name) of the ES inside custom_es/example.py. Say we wish to target the true model

$$\begin{aligned} \vec{\alpha} &= (\alpha_{1,2} \quad \alpha_{2,3} \quad \alpha_{3,4}) \\ \vec{T} &= \begin{pmatrix} \hat{\sigma}_z^1 \otimes \hat{\sigma}_z^2 \\ \hat{\sigma}_z^2 \otimes \hat{\sigma}_z^3 \\ \hat{\sigma}_z^3 \otimes \hat{\sigma}_z^4 \end{pmatrix} \\ \implies \hat{H}_0 &= \hat{\sigma}_z^{(1,2)} \hat{\sigma}_z^{(2,3)} \hat{\sigma}_z^{(3,4)} \end{aligned} \tag{C.1}$$

QMLA interprets models as strings, where terms are separated by +, and parameters are implicit. So the target model in Eq. (C.1) will be given by

pauliSet_1J2_zJz_d4+pauliSet_2J3_zJz_d4+pauliSet_3J4_zJz_d4.

Adapting the template ES slightly, we can define a model generation strategy with a small number of hard coded candidate models introduced at the first branch of the exploration tree. We will also set the parameters of the terms which are present in $\hat{H}_0$, as well as the range in which to search parameters. Keeping the imports at the top of the example.py, rewrite the ES as:

```
class ExampleBasic(
    exploration_strategy.ExplorationStrategy
):

    def __init__(
        self,
        exploration_rules,
        true_model=None,
        **kwargs
    ):
        self.true_model = 'pauliSet_1J2_zJz_d4+
            pauliSet_2J3_zJz_d4+pauliSet_3J4_zJz_d4'
        super().__init__(
            exploration_rules=exploration_rules,
            true_model=self.true_model,
            **kwargs
        )

        self.initial_models = None
        self.true_model_terms_params = {
            'pauliSet_1J2_zJz_d4' : 2.5,
            'pauliSet_2J3_zJz_d4' : 7.5,
            'pauliSet_3J4_zJz_d4' : 3.5,
        }
        self.tree_completed_initially = True
        self.min_param = 0
        self.max_param = 10

    def generate_models(self, **kwargs):

        self.log_print(["Generating models; spawn step {}".format
            (self.spawn_step)])
```

```
        if self.spawn_step == 0:
            # chains up to 4 sites
            new_models = [
                'pauliSet_1J2_zJz_d4',
                'pauliSet_1J2_zJz_d4+pauliSet_2J3_zJz_d4',
                'pauliSet_1J2_zJz_d4+pauliSet_2J3_zJz_d4+
                   pauliSet_3J4_zJz_d4',
            ]
            self.spawn_stage.append('Complete')

        return new_models
```

Listing C.8: ExampleBasic exploration strategy.

To run[2] the example ES for a meaningful tests, return to the local_launch of Listing C.3, but change some of the settings:

```
prt=2000
exp=500
run_qhl=1
exploration_strategy=ExampleBasic
```

Listing C.9: local_launch configuration for QHL.

Run locally again as in Listing C.4; then move to the results directory as in Listing C.5.

C.2 ANALYSIS

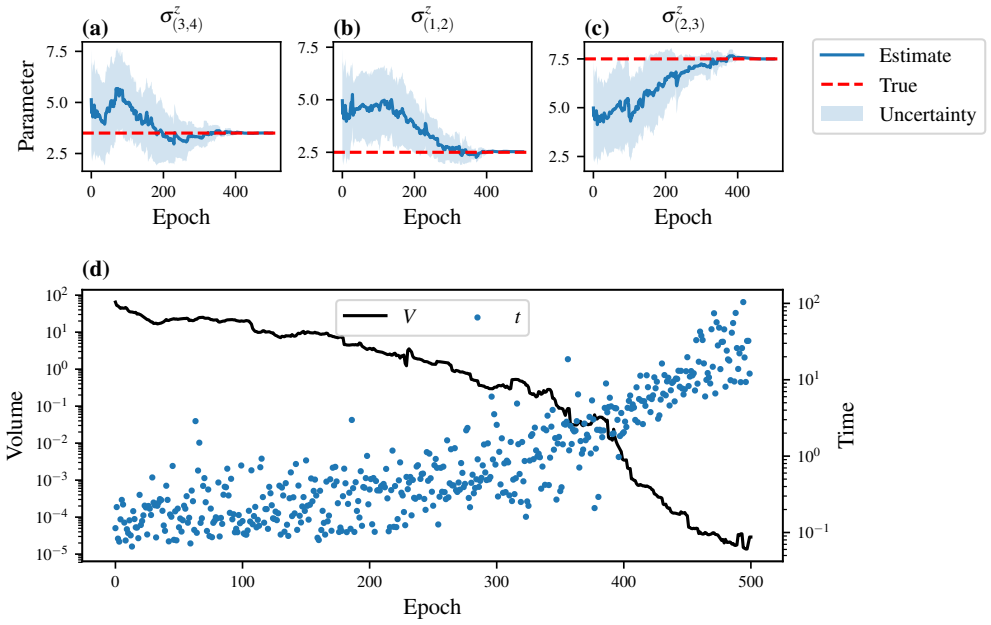
QMLA stores results and generates plots over the entire range of the algorithm[3], i.e. the run, instance and models. The depth of analysis performed automatically is set by the user control plot_level in local_launch.sh; for plot_level=1, only the most crucial figures are generated, while _level=6 generates plots for every individual model considered. For model searches across large model spaces and/or considering many candidates, excessive plotting can cause considerable slow-down, so users should be careful to generate plots only to the degree they will be useful. Next we show some examples of the available plots.

2 Note this will take up to 15 minutes to run. This can be reduced by lowering the values of prt, exp, which is sufficient for testing but note that the outcomes will be less effective than those presented in the figures of this section.

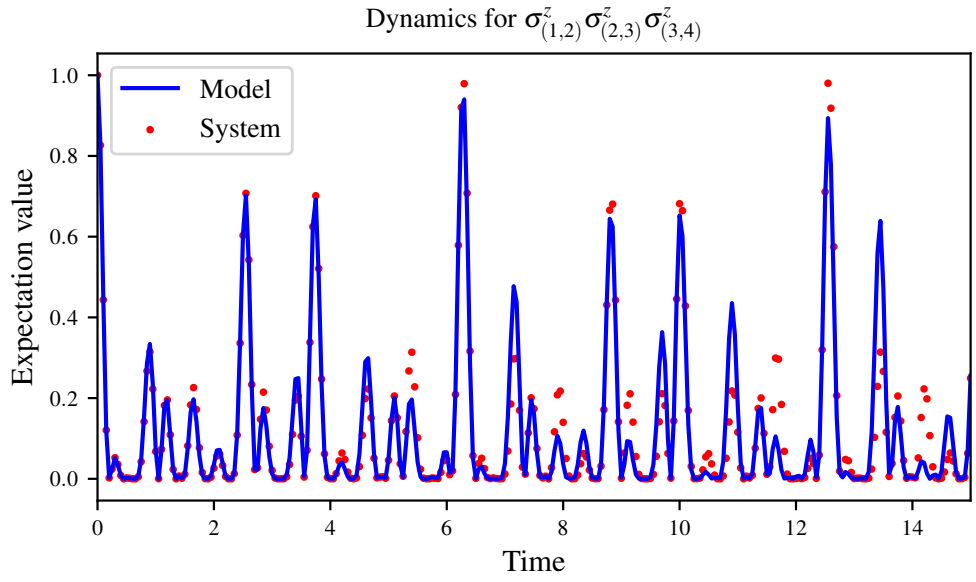
3 Recall that a single implementation of QMLA is called an instance, while a series of instances – which share the same target model – is called the run.

C.2.1 *Model analysis*

We have just run quantum Hamiltonian learning (QHL) for the model in Eq. (C.1) for a single instance, using a reasonable number of particles and experiments, so we expect to have trained the model well. Instance-level results are stored (e.g. for the instance with qmla_id=1) in Jan_01/01_23/instances/qmla_1. Individual models' insights can be found in model_training, e.g. the model's learning_summary Fig. C.2a, and dynamics in Fig. C.2b.



(a)



(b)

Figure C.2: Model analysis plots, stored in (for example) Jan_01/01_23/instances/qmla_1/model_training. **a** learning_summary_1. Displays the outcome of QHL for the given model: Subfigures (a)-(c) show the estimates of the parameters; (d) shows the total parameterisation volume against experiments trained upon, along with the evolution times used for those experiments. **(b)** dynamics_1 The model's attempt at reproducing dynamics from $\hat{H}_0$.

C.2.2 *Instance analysis*

Now we can run the full QMLA algorithm, i.e. train several models and determine the most suitable. QMLA will call the generate_models method of the ExampleBasic ES, set in Listing C.8, which tells QMLA to construct three models on the first branch, then terminate the search. Here we need to train and compare all models so it takes considerably longer to run: the purpose of testing, we reduce the resources so the entire algorithm runs in about 15 minutes. Some applications will require significantly more resources to learn effectively. In realistic cases, these processes are run in parallel, as we will cover in **??**.

Reconfigure a subset of the settings in the local_launch.sh script (Listing C.3) and run it again:

```
exp=250
prt=1000
run_qhl=0
exploration_strategy=ExampleBasic
```

Listing C.10: local_launch configuration for QMLA.

In the corresponding results directory, navigate to instances/qmla_1, where instance level analysis are available.

```
cd results/Jan_01/01_23/instances/qmla_1
```

Listing C.11: Navigating to instance results.

Figures of interest here show the composition of the models (Fig. C.3a), as well as the Bayes factors between candidates (Fig. C.3b). Individual model comparisons – i.e. Bayes factor (BF) – are shown in Fig. C.3c, with the dynamics of all candidates shown in Fig. C.4c. The probes used during the training of all candidates are also plotted (Fig. C.3e).

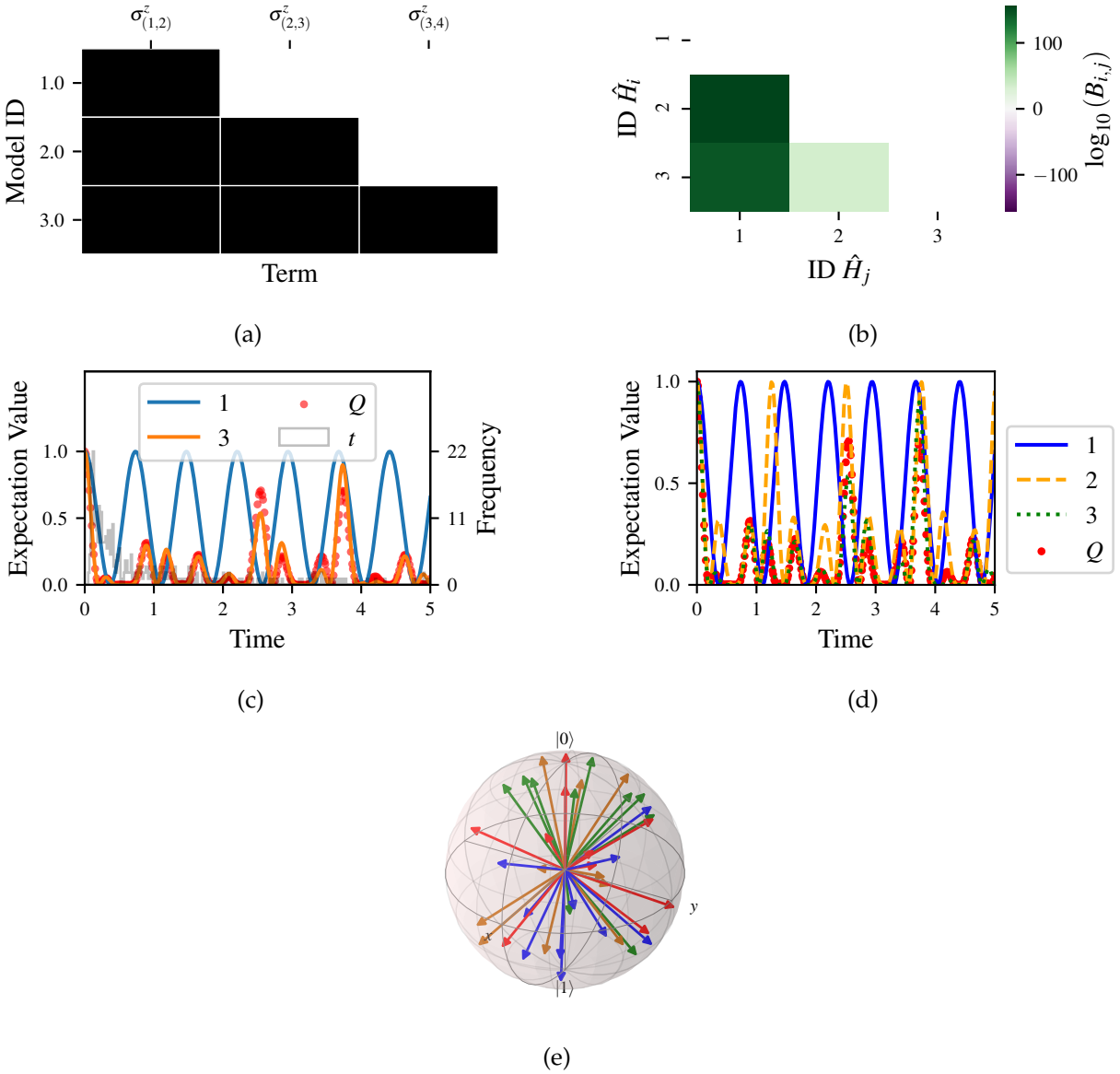


Figure C.3: QMLA plots; found within instance directory e.g. Jan_01/01_23/instances/qmla_1, and its subdirectories. **(a)** composition_of_models: constituent terms of all considered models, indexed by their model IDs. Here model 3 is $\hat{H}_0$. **(b)** bayes_factors: Bayes factor (BF) comparisons between all models. Bayes factors (BFs) are read as $B_{i,j}$ where i is the model with lower ID, e.g. $B_{1,2}$ rather than $B_{2,1}$. Thus $B_{ij} > 0$ (< 0) indicates $\hat{H}_i$ ($\hat{H}_j$), i.e. the model on the y-axis (x-axis) is the stronger model. **(c)** comparisons/BF_1_3: direct comparison between models with IDs 1 and 3, showing their reproduction of the system dynamics (red dots, Q), as well as the times (experiments) against which the BF was calculated. **(d)** branches/dynamics_branch_1: dynamics of all models considered on the branch compared with system dynamics (red dots, Q). **(e)** probes_bloch_sphere: probes used for training models in this instance (only showing 1-qubit versions).

C.2.3 *Run analysis*

Considering a number of instances together is a *run*. In general, this is the level of analysis of most interest: an individual instance is liable to errors due to the probabilistic nature of the model training and generation subroutines. On average, however, we expect those elements to perform well, so across a significant number of instances, we expect the average outcomes to be meaningful.

Each results directory has an analyse.sh script to generate plots at the run level.

```
cd results/Jan_01/01_23
./analyse.sh
```

Listing C.12: Analysing QMLA run.

Run level analysis are held in the main results directory and several sub-directories created by the analyse script. Here, we recommend running a number of instances with very few resources so that the test finishes quickly[4]. The results will therefore be meaningless, but allow fo elucidation of the resultant plots. First, reconfigure some settings of Listing C.3 and launch again.

```
num_instances=10
exp=20
prt=100
run_qhl=0
exploration_strategy=ExampleBasic
```

Listing C.13: local_launch configuration for QMLA run.

Some of the generated analysis are shown in Figs. C.4 to C.5. The number of instances for each model, i.e. their *win rates* are given in Fig. C.4a. The *top models*, i.e. those with highest win rates, analysed further: the average parameter estimation progression for $\hat{H}_0$ – including only the instances where $\hat{H}_0$ was deemed champion – are shown in Fig. C.4b. Irrespecitve of the champion models, the rate with which each term is found in the champion model ($\hat{t} \in \hat{H}'$) indicates the likelihood that the term is really present; these rates – along with the parameter values learned – are shown in Fig. C.4c. The champion model from each instance can attempt to reproduce system dynamics: we group together these reproductions for each model in Fig. C.5.

4 This run will take about ten minutes

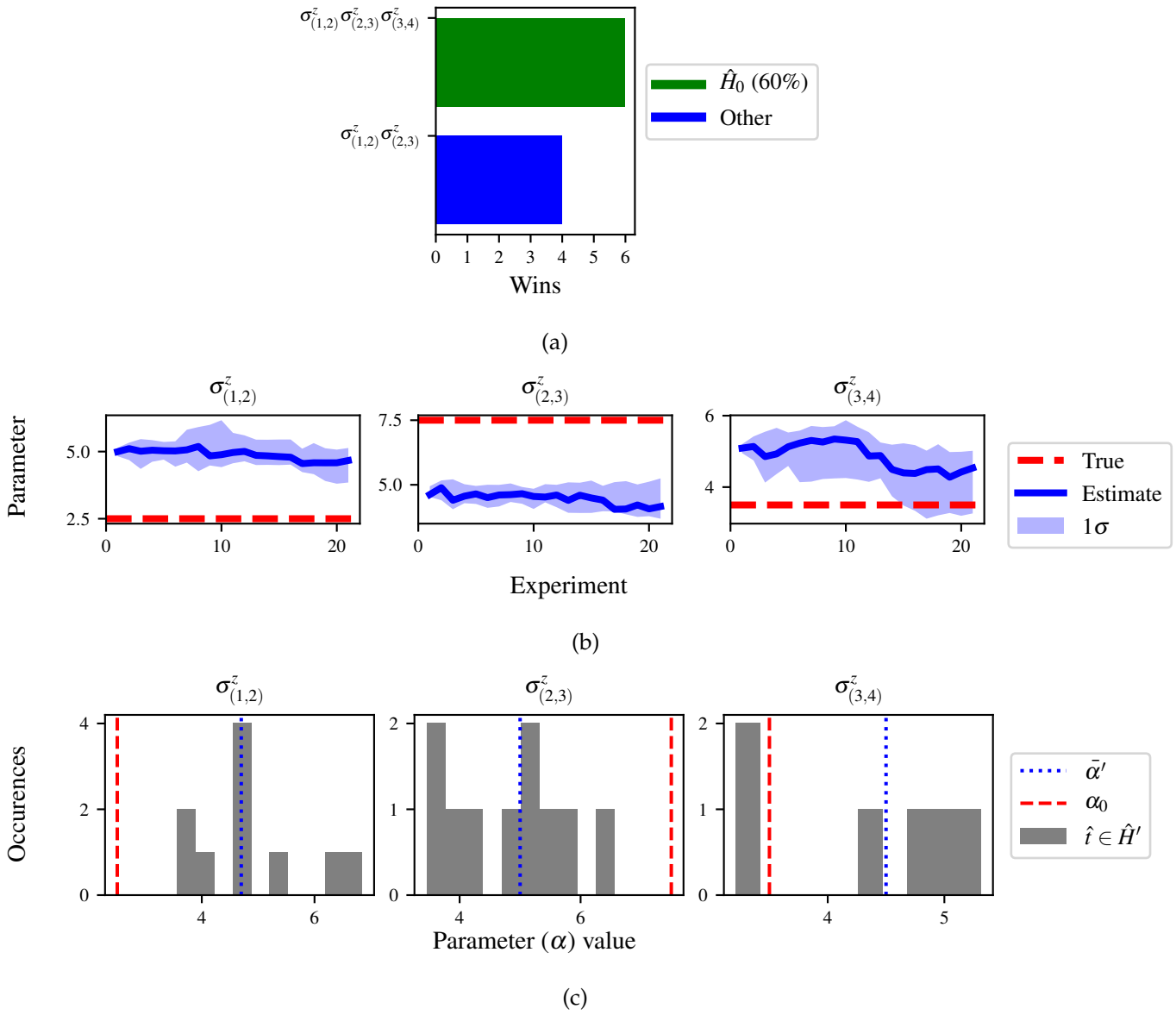


Figure C.4: QMLA run plots; found within run directory e.g. Jan_01/01_23/. **(a)** performace/model_wins: number of instance wins achieved by each model. **(b)** champion_models/params_params_pauliSet_1J2_zJz_d4+pauliSet_2J3_zJz_d4+pauliSet_3J4_zJz_d4: parameter estimation progression for the true model, only for the instances where it was deemed champion. **(c)** champion_models/terms_and_params: histogram of parameter values found for each term which appears in any champion model, with the true parameter (α_0) in red and the median learned parameter ($\bar{\alpha}'$) in blue.

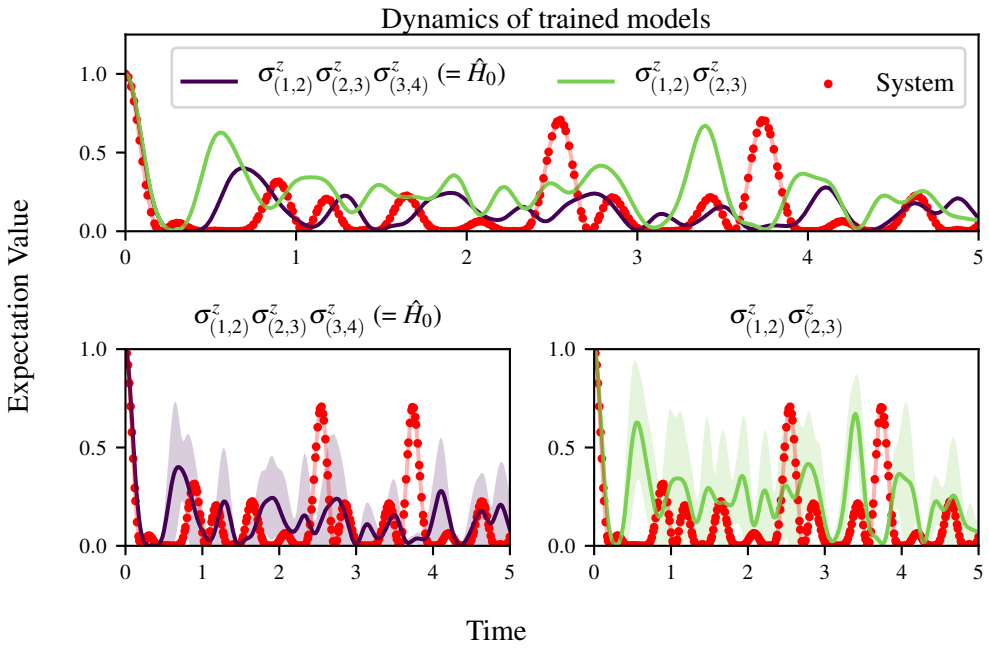


Figure C.5: Run plot performace/dynamics: median dynamics of the champion models. The models which won most instances are shown together in the top panel, and individually in the lower panels. The median dynamics from the models' learnings in its winning instances are shown, with the shaded region indicating the 66% confidence region.

C.3 PARALLEL IMPLEMENTATION

We provide utility to run QMLA on parallel processes. Individual models' training can run in parallel, as well as the calculation of BF between models. The provided script is designed for portable batch system (PBS) job scheduler running on a compute cluster. It will require a few adjustments to match the system being used. Overall, though, it has mostly a similar structure as the local_launch.sh script used above.

QMLA must be downloaded on the compute cluster as in Listing C.1; this can be a new fork of the repository, though it is sensible to test installation locally as described in this chapter so far, then *push* that version, including the new ES, to Github, and cloning the latest version. It is again advisable to create a Python virtual environment in order to isolate QMLA and its dependencies[5]. Open the parallel launch script, QMLA/launch/parallel_launch.sh, and prepare the first few lines as

```
#!/bin/bash
```

5 Indeed it is sensible to do this for any Python development project.

```
##### ---------------------------------------------- #####
# QMLA run configuration
##### ---------------------------------------------- #####
num_instances=10 # number of instances in run
run_qhl=0 # perform QHL on known (true) model
run_qhl_multi_model=0 # perform QHL for defined list of models
experiments=250
particles=1000
plot_level=5


##### ---------------------------------------------- #####
# Choose an exploration strategy
# This will determine how QMLA proceeds.
##### ---------------------------------------------- #####
exploration_strategy="ExampleBasic"
```

Listing C.14: parallel_launch script

When submitting jobs to schedulers like PBS, we must specify the time required, so that it can determine a fair distribution of resources among users. We must therefore *estimate* the time it will take for an instance to complete: clearly this is strongly dependent on the numbers of experiments (N_e) and particles (N_p), and the number of models which must be trained. QMLA attempts to determine a reasonable time to request based on the max_num_models_by_shape attribute of the ES, by calling QMLA/scripts/time_required_calculation.py. In practice, this can be difficult to set perfectly, so the timing_insurance_factor attribute of the ES can be used to correct for heavily over- or under-estimated time requests. Instances are run in parallel, and each instance trains/compares models in parallel. The number of processes to request, N_c for each instance is set as num_processes_to_parallelise_over in the ES. Then, if there are N_r instances in the run, we will be requesting the job scheduler to admit N_r distinct jobs, each requiring N_c processes, for the time specified.

The parallel_launch script works together with launch/run_single_qmla_instance.sh, though note a number of steps in the latter are configured to the cluster and may need to be adapted. In particular, the first command is used to load the redis utility, and later lines are used to initialise a redis server. These commands will probably not work with most machines, so must be configured to achieve those steps.

```
module load tools/redis-4.0.8

...
```

```
SERVER_HOST=$(head -1 "$PBS_NODEFILE")
let REDIS_PORT="6300 + $QMLA_ID"

cd $LIBRARY_DIR
redis-server RedisDatabaseConfig.conf --protected-mode no --port
    $REDIS_PORT &
redis-cli -p $REDIS_PORT flushall
```

Listing C.15: run_single_qmla_instance script

When the modifications are finished, QMLA can be launched in parallel similarly to the local version:

```
source qmla_test/qmla-env/bin/activate

cd qmla_test/QMLA/launch
./parallel_launch.sh
```

Listing C.16: run_single_qmla_instance script

Jobs are likely to queue for some time, depending on the demands on the job scheduler. When all jobs have finished, results are stored as in the local case, in QMLA/launch/results/-Jan_01/01_23, where analyse.sh can be used to generate a series of automatic analyses.

C.4 CUSTOMISING EXPLORATION STRATEGYS

User interaction with the QMLA codebase should be achieveable primarily through the exploration strategy (ES) framework. Throughout the algorithm(s) available, QMLA calls upon the ES before determining how to proceed. The usual mechanism through which the actions of QMLA are directed, is to set attributes of the ES class: the complete set of influential attributes are available at [3].

QMLA directly uses several methods of the ES class, all of which can be overwritten in the course of customising an ES. Most such methods need not be replaced, however, with the exception of generate_models, which is the most important aspect of any ES: it determines which models are built and tested by QMLA. This method allows the user to impose any logic desired in constructing models; it is called after the completion of every branch of the exploration tree on the ES.

C.4.1 *Greedy search*

sec:greedy$_s$*earch*

A first non-trivial ES is to build models greedily from a set of *primitive* terms, $\mathcal{T} = \{\hat{t}\}$. New models are constructed by combining the previous branch champion with each of the remaining, unused terms. The process is repeated until no terms remain.

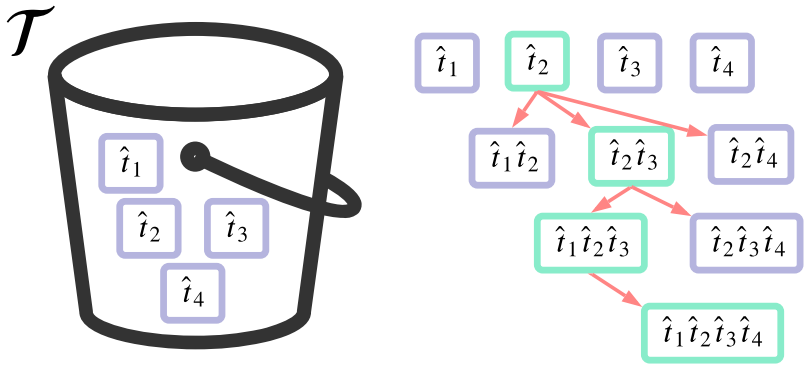


Figure C.6: Greedy exploration strategy. **Left**, a set of primitive terms, $\mathcal{T}$, are defined in advance. **Right**, models are constructed from $\mathcal{T}$. On the first branch, the primitve terms alone constitute models. Thereafter, the strongest model (marked in green) from the previous branch is combined with all the unused terms.

We can compose an ES using these rules, say for

$$\mathcal{T} = \left\{\hat{\sigma}_x^1, \hat{\sigma}_y^1, \hat{\sigma}_x^1 \otimes \hat{\sigma}_x^2, \hat{\sigma}_y^1 \otimes \hat{\sigma}_y^2\right\}$$

as follows. Note the termination criteria must work in conjunction with the model generation routine. Users can overwrite the method check_tree_completed for custom logic, although a straightforward mechanism is to use the spawn_stage attribute of the ES class: when the final element of this list is Complete, QMLA will terminate the search by default. Also note that the default termination test checks whether the number of branches (spawn_step) exceeds the limit max_spawn_depth, which must be set artifically high to avoid ceasing the search too early, if relying solely on spawn_stage. Here we demonstrate how to impose custom logic to terminate the seach also.

```
class ExampleGreedySearch(
    exploration_strategy.ExplorationStrategy
):
    r"""
```

```
    From a fixed set of terms, construct models iteratively,
    greedily adding all unused terms to separate models at each
       call to the generate_models.

    """

    def __init__(
        self,
        exploration_rules,
        **kwargs
    ):

        super().__init__(
            exploration_rules=exploration_rules,
            **kwargs
        )
        self.true_model = 'pauliSet_1_x_d3+pauliSet_1J2_yJy_d3+
           pauliSet_1J2J3_zJzJz_d3'
        self.initial_models = None
        self.available_terms = [
            'pauliSet_1_x_d3', 'pauliSet_1_y_d3',
            'pauliSet_1J2_xJx_d3', 'pauliSet_1J2_yJy_d3'
        ]
        self.branch_champions = []
        self.prune_completed_initially = True
        self.check_champion_reducibility = False

    def generate_models(
        self,
        model_list,
        **kwargs
    ):
        self.log_print([
            "Generating models in tiered greedy search at spawn
               step {}.".format(
                 self.spawn_step,
            )
        ])
        try:
            previous_branch_champ = model_list[0]
```

```
            self.branch_champions.append(previous_branch_champ)
        except:
            previous_branch_champ = ""

        if self.spawn_step == 0 :
            new_models = self.available_terms
        else:
            new_models = greedy_add(
                current_model = previous_branch_champ,
                terms = self.available_terms
            )

        if len(new_models) == 0:
            # Greedy search has exhausted the available models;
            # send back the list of branch champions and
               terminate search.
            new_models = self.branch_champions
            self.spawn_stage.append('Complete')

        return new_models

    def check_tree_completed(
        self,
        spawn_step,
        **kwargs
    ):
        r"""
        QMLA asks the exploration tree whether it has finished
           growing;
        the exploration tree queries the exploration strategy
           through this method
        """
        if self.tree_completed_initially:
            return True
        elif self.spawn_stage[-1] == "Complete":
            return True
        else:
            return False
def greedy_add(
    current_model,
```

```
    terms,
):
    r"""
    Combines given model with all terms from a set.

    Determines which terms are not yet present in the model,
    and adds them each separately to the current model.

    :param str current_model: base model
    :param list terms: list of strings of terms which are to be
       added greedily.
    """

    try:
        present_terms = current_model.split('+')
    except:
        present_terms = []
    nonpresent_terms = list(set(terms) - set(present_terms))

    term_sets = [
        present_terms+[t] for t in nonpresent_terms
    ]

    new_models = ["+".join(term_set) for term_set in term_sets]

    return new_models
```

Listing C.17: ExampleGreedySearch exploration stategy

This run can be implemented locally or in parallel as described above[6], and analysed as in Listing C.12, generating figures in accordance with the plot_level set by the user in the launch script. We advise reducing plot_level to 3 to avoid excessive/slow figure generation. Outputs can again be found in the instances subdirectory, including a map of the models generated, as well as the branches they reside on, and the BFs between candidates.

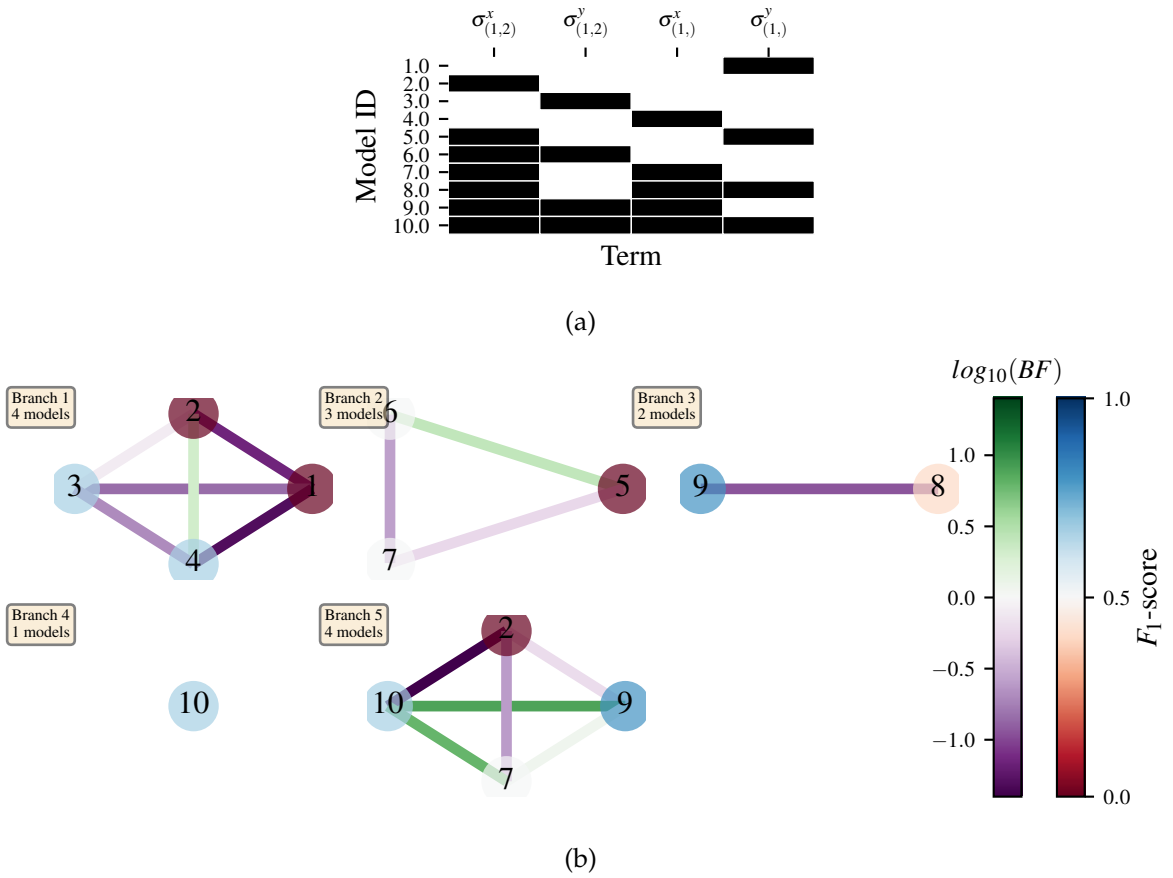


Figure C.7: Greedy exploration strategy. **(a)**, model compostion. **b**, graph of branches on the exploration tree. Models are coloured by their F_1-score, and edges represent the BF between models. The first four branches are equivalent to those in Fig. C.6 , while the final branch considers the set of branch champions, in order to determine the overall champion.

C.4.2 *Tiered greedy search*

We provide one final example of a non-trivial ES: tiered greedy search. Similar to the idea of **??**, except terms are introduced hierarchically: sets of terms $\mathcal{T}_1, \mathcal{T}_2, \ldots \mathcal{T}_n$ are each examined greedily, where the overall strongest model of one tier forms the seed model for the subsequent tier. This is depicted in the main text in **??**. A corresponding ES is given as follows.

```
class ExampleGreedySearchTiered(
    exploration_strategy.ExplorationStrategy
):
    r"""
```

```
    Greedy search in tiers.

    Terms are batched together in tiers;
    tiers are searched greedily;
    a single tier champion is elevated to the subsequent tier.

    """

    def __init__(
        self,
        exploration_rules,
        **kwargs
    ):
        super().__init__(
            exploration_rules=exploration_rules,
            **kwargs
        )
        self.true_model = 'pauliSet_1_x_d3+pauliSet_1J2_yJy_d3+
           pauliSet_1J2J3_zJzJz_d3'
        self.initial_models = None
        self.term_tiers = {
            1 : ['pauliSet_1_x_d3', 'pauliSet_1_y_d3', '
               pauliSet_1_z_d3' ],
            2 : ['pauliSet_1J2_xJx_d3', 'pauliSet_1J2_yJy_d3', '
               pauliSet_1J2_zJz_d3'],
            3 : ['pauliSet_1J2J3_xJxJx_d3', '
               pauliSet_1J2J3_yJyJy_d3', 'pauliSet_1J2J3_zJzJz_d3
               '],
        }
        self.tier = 1
        self.max_tier = max(self.term_tiers)
        self.tier_branch_champs = {k : [] for k in self.
           term_tiers}
        self.tier_champs = {}
        self.prune_completed_initially = True
        self.check_champion_reducibility = True

    def generate_models(
        self,
        model_list,
```

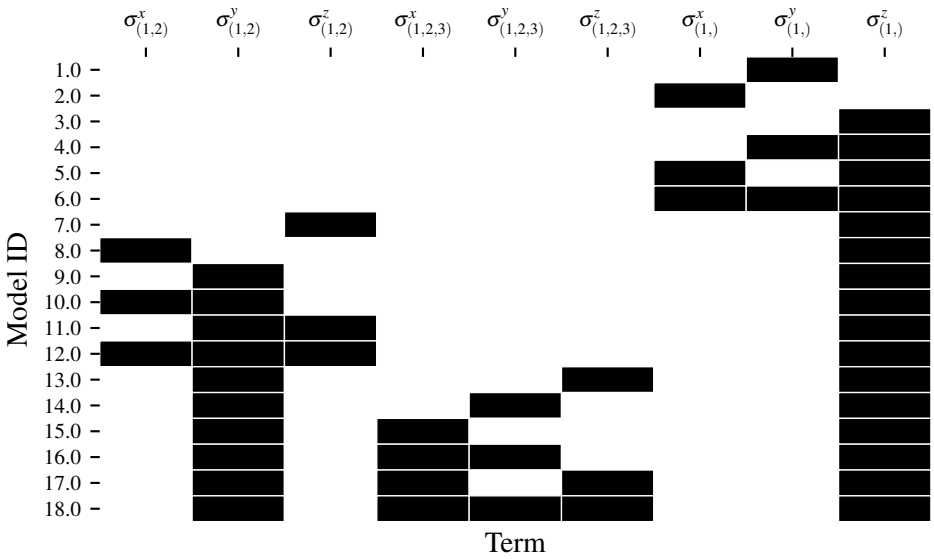
```
        **kwargs
    ):
        self.log_print([
            "Generating models in tiered greedy search at spawn
               step {}.".format(
                self.spawn_step,
            )
        ])

        if self.spawn_stage[-1] is None:
            try:
                previous_branch_champ = model_list[0]
                self.tier_branch_champs[self.tier].append(
                   previous_branch_champ)
            except:
                previous_branch_champ = None

        elif "getting_tier_champ" in self.spawn_stage[-1]:
            previous_branch_champ = model_list[0]
            self.log_print([
                "Tier champ for {} is {}".format(self.tier,
                   model_list[0])
            ])
            self.tier_champs[self.tier] = model_list[0]
            self.tier += 1
            self.log_print(["Tier now = ", self.tier])
            self.spawn_stage.append(None) # normal processing

            if self.tier > self.max_tier:
                self.log_print(["Completed tree for ES"])
                self.spawn_stage.append('Complete')
                return list(self.tier_champs.values())
        else:
            self.log_print([
                "Spawn stage:", self.spawn_stage
            ])

        new_models = greedy_add(
            current_model = previous_branch_champ,
            terms = self.term_tiers[self.tier]
```

```
        )
        self.log_print([
            "tiered search new_models=", new_models
        ])

        if len(new_models) == 0:
            # no models left to find - get champions of branches
              from this tier
            new_models = self.tier_branch_champs[self.tier]
            self.log_print([
                "tier champions: {}".format(new_models)
            ])
            self.spawn_stage.append("getting_tier_champ_{}".
              format(self.tier))
        return new_models

def greedy_add(
    current_model,
    terms,
):
    r"""
    Combines given model with all terms from a set.

    Determines which terms are not yet present in the model,
    and adds them each separately to the current model.

    :param str current_model: base model
    :param list terms: list of strings of terms which are to be
      added greedily.
    """


    try:
        present_terms = current_model.split('+')
    except:
        present_terms = []
    nonpresent_terms = list(set(terms) - set(present_terms))

    term_sets = [
        present_terms+[t] for t in nonpresent_terms
    ]
```

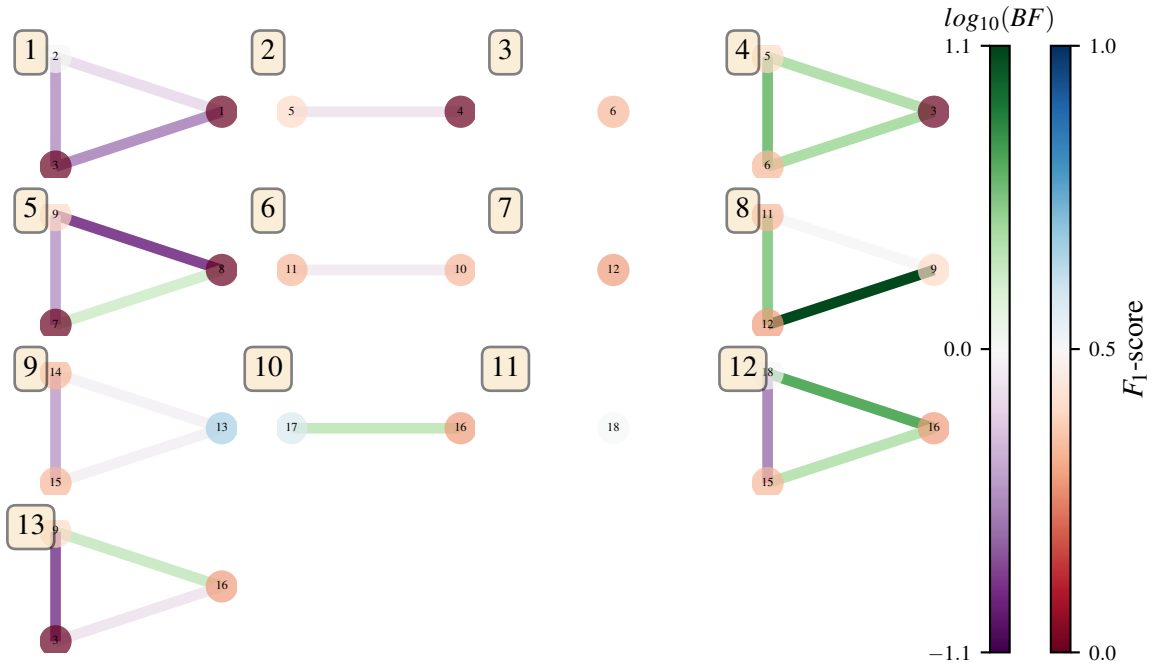
```
        new_models = ["+".join(term_set) for term_set in term_sets]

        return new_models
```

Listing C.18: ExampleGreedySearchTiered exploration stategy

with corresponding results



(a)



(b)

Figure C.8: Tiered greedy exploration strategy. **(a)**, composition$_o f_m odels$.b,

BIBLIOGRAPHY

[1] Brian Flynn. Mathematical introduction to quantum computation, 2015. Undergraduate thesis.

[2] Brian Flynn. Quantum model learning agent. https://github.com/flynnbr11/QMLA, 2021.

[3] Quantum model learning agent documentation. https://quantum-model-learning-agent.readthedocs.io/en/latest/, Jan 2021. [Online; accessed 12. Jan. 2021].