Doctorate of Philosophy

Schrödinger's Catwalk

Brian Flynn

University of Bristol

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ACRONYMS

C	carbon
^{14}N	nitrogen-14
AI	artificial intelligence
AIC	Akaike information criterion
AICC	Akaike information criterion corrected
BF	Bayes factor
BFEER	Bayes factor enhanced Elo ratings
BIC	Bayesian information criterion
CLE	classical likelihood estimation
CPU	central processing unit
DAG	directed acyclic graph
EDH	experiment design heuristic
ES	exploration strategy
ET	exploration tree
FH	Fermi-Hubbard
FN	false negatives
FP	false positives
GA	genetic algorithm
GES	genetic exploration strategy
GPU	graphics processing unit
HPD	high particle density
IQLE	interactive quantum likelihood estimation
JWT	Jordan Wigner transformation
LE	Loschmidt echo

LTL log total likelihood

ML machine learning

MVEE minimum volume enclosing ellipsoid
MW microwave

NN neural network
NV nitrogen-vacancy
NVC nitrogen-vacancy centre

OF objective function

PBS portable batch system
PGH particle guess heuristic
PL photoluminescence

QC quantum computer
QHL quantum Hamiltonian learning
QL quadratic loss
QLE quantum likelihood estimation
QM quantum mechanics
QML quantum machine learning
QMLA Quantum Model Learning Agent

SMC sequential monte carlo
SVM support vector machine

TLTL total log total likelihood
TN true negatives
TP true positives

VQE variational quantum eigensolver

GLOSSARY

Q	Quantum system which is the target of Quantum Model Learning Agent, i.e. the system to be characterised
champion model	The model deemed by Quantum Model Learning Agent (QMLA) as the most suitable for describing the target system
chromosome	A single candidate, in the space of valid solutions to the posed problem in a genetic algorithm
expectation value	Average outcome expected by measuring an observable of a quantum system many times, **??**
gene	Individual element within a chromosome
hyperparameter	Variable within an algorithm that determines how the algorithm itself proceeds
instance	A single implementation of the QMLA algorithm, resulting in a nominated champion model
likelihood	Value that represents how likely a hypothesis is. Usually used in the context of likelihood estiamation, **??**
model	The mathematical description of some quantum system, Section 1.1
model space	Abstract space containing all descriptions (within defined constraints such as dimension) of the system as models
probe	Input probe state, $\|\psi\rangle$, which the target system is initialised to, before unitary evolution
results directory	Directory to which the data and analysis for a given run of QMLA are stored
run	Collection of QMLA instances, usually targeting the same system with the same initial conditions

spawn Process by which new models are generated, ususally by combining previously considered models

success rate Fraction of instances within a run where QMLA nominates the true model as champion

term Individual constituent of a model, e.g. a single operator within a sum of operators, which in total describe a Hamiltonian.

volume Volume of a parameter distribution's credible region, **??**

win rate For a given candidate model, the fraction of instances within a run which nominated it as champion

Part I

ALGORITHMS

1

QUANTUM MODEL LEARNING AGENT

A *model* is the mathematical description of a quantum system of interest, Q. In **??**, we discussed a number of systems in terms of their Hamiltonian descriptions, although in general the description of a quantum system need not be Hamiltonian, e.g. Lindbladian models describe open quantum systems, so we will generically refer to the *model* of Q throughout.

Quantum Model Learning Agent (QMLA) is an algorithm that extends the concept of applying machine learning to the characterisation of Hamiltonians we've seen in **??**. The extension, and central question of QMLA is: if we do not know the structure of the model which describes a target quantum system, can we still learn about the physics of the system? That is, we remove the assumption about the form of the Hamiltonian model, and attempt to uncover which *terms* constitute the Hamiltonian, and in so doing, learn the interactions the system is subject to.

For the remainder of this thesis, our objective is to learn the model underlying a series of target quantum systems. We will first introduce some concepts which will prove useful when discussing QMLA, before describing the protocol in detail in Section 1.3.

1.1 MODELS

Models are simply the mathematical objects which can be used to predict the behaviour of a system. In this thesis, models are synonymous with Hamiltonians, composed of a set of *terms*, $\mathcal{T} = \{\hat{t}\}$, where each $\hat{t}$ is a matrix. Each term is assosiated with a multiplicative scalar, which may be referred to as that term's *parameter*: we impose order on the terms and parameters such that we can succinctly summarise any model as

$$\hat{H} = \begin{pmatrix} \alpha_0 & \dots & \alpha_n \end{pmatrix} \begin{pmatrix} \hat{t}_1 \\ \vdots \\ \hat{t}_n \end{pmatrix} = \vec{\alpha} \cdot \vec{T} \tag{1.1}$$

where $\vec{\alpha}, \vec{T}$ are the model's parameters and terms, respectively.

For example, a model which is the sum of the (non-identity) Pauli operators is given by

$$\begin{aligned} \hat{H} &= \begin{pmatrix} \alpha_x & \alpha_y & \alpha_z \end{pmatrix} \cdot \begin{pmatrix} \hat{\sigma}_x \\ \hat{\sigma}_y \\ \hat{\sigma}_z \end{pmatrix} \\ &= \alpha_x \hat{\sigma}_x + \alpha_y \hat{\sigma}_y + \alpha_z \hat{\sigma}_z \\ &= \begin{pmatrix} \alpha_z & \alpha_x - i\alpha_y \\ \alpha_x + i\alpha_y & \alpha_z \end{pmatrix}. \end{aligned} \tag{1.2}$$

Through this formalism, we can say that the sole task of quantum Hamiltonian learning (QHL) was to optimise $\vec{\alpha}$, given $\vec{T}$. The principle task of QMLA is to identify the terms $\vec{T}$ which are supported by the most statistical evidence as describing the target system Q. In short, QMLA proposes *candidate models* $\hat{H}_i$ as hypotheses to explain Q; we *train* each model independently through a parameter learning routine, and finally nominate the model with the best performance after training. In particular, QMLA uses QHL as the parameter learning *subroutine*, but in principle this step can be performed by any algorithm which learns $\vec{\alpha}$ for given $\vec{T}$, [**?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**]. While discussing a model $\hat{H}_i$, their *training* then simply means the implementation of QHL[1], where $\hat{H}_i$ is *assumed* to represent Q, such that $\vec{\alpha}_i$ is optimised as well as it can be, even if $\hat{H}_i$ is entirely inaccurate.

1.2 BAYES FACTORS

We can use the tools introduced in **??** to *compare* candidate models. Of course it is first necessary to ensure that each model has been adequately trained: while inaccurate models are unlikely to strongly capture the system dynamics, they should first train on the system to determine their best attempt at doing so, i.e. they should undergo the process in **??**. It is statistically meaningful to compare models via their total log total likelihood (TLTL), $\mathcal{L}_i$, if and only if they have considered the same data, i.e. if models have each attempted to account for the same set of experiments, $\mathcal{E}$ [**?**].

We can then exploit direct pairwise comparisons between models, by imposing that both models' TLTL are computed based on *any* shared set of experiments $\mathcal{E}$, with corresponding measurements $\mathcal{D} = \{d_e\}_{e \in \mathcal{E}}$. Pairwise comparisons can then be quantified by the Bayes factor (BF),

$$B_{ij} = \frac{\Pr(\mathcal{D}|\hat{H}_i; \mathcal{E})}{\Pr(\mathcal{D}|\hat{H}_j; \mathcal{E})}. \tag{1.3}$$

Intuitively, we see that the BF is the ratio of the likelihood, i.e. the performance, of model $\hat{H}_i$'s attempt to account for the data set $\mathcal{D}$ observed following the experiment set $\mathcal{E}$, against the same likelihood for model $\hat{H}_j$. BFs are known to be statistically signicative of the stronger model from a pair, at explaining observed data, while favouring models of low cardinality, thereby supressing overfitting models.

We have that, for independent experiments, and recalling **??**,

$$\begin{aligned} \Pr(\mathcal{D}|\hat{H}_i; \mathcal{E}) &= \Pr(d_n|\hat{H}_i; e_n) \times \Pr(d_{n-1}|\hat{H}_i; e_{n-1}) \times \cdots \times \Pr(d_0|\hat{H}_i; e_0) \\ &= \prod_{e \in \mathcal{E}} \Pr(d_e|\hat{H}_i; e) \\ &= \prod_{e \in \mathcal{E}} (l_e)_i. \end{aligned} \tag{1.4}$$

1 Or the chosen parameter learning subroutine.

We also have, from **??**

$$\begin{aligned} \mathcal{L}_i &= \sum_{e\in\mathcal{E}} ln\left((l_e)_i\right) \\ \implies e^{\mathcal{L}_i} &= \exp\left(\sum_{e\in\mathcal{E}} ln\left[(l_e)_i\right]\right) = \prod_{e\in\mathcal{E}} \exp\left(ln\left[(l_e)_i\right]\right) = \prod_{e\in\mathcal{E}} (l_e)_i. \end{aligned} \tag{1.5}$$

So we can write

$$B_{ij} = \frac{\Pr(\mathcal{D}|\hat{H}_i;\mathcal{E})}{\Pr(\mathcal{D}|\hat{H}_j;\mathcal{E})} = \frac{\prod_{e\in\mathcal{E}}(l_e)_i}{\prod_{e\in\mathcal{E}}(l_e)_j} = \frac{e^{\mathcal{L}_i}}{e^{\mathcal{L}_j}} \tag{1.6}$$

$$\implies B_{ij} = e^{\mathcal{L}_i - \mathcal{L}_j} \tag{1.7}$$

This is simply the exponential of the difference between two models' total log-likelihoods when presented the same set of experiments. Intuitively, if $\hat{H}_i$ performs well, and therefore has a high TLTL, $\mathcal{L}_i = -10$, and $\hat{H}_j$ performs worse with $\mathcal{L}_j = -100$, then $B_{ij} = e^{-10-(-100)} = e^{90} \gg 1$. Conversely for $\mathcal{L}_i = -100, \mathcal{L}_j = -10$, then $B_{ij} = e^{-90} \ll 1$. Therfore $\left|B_{ij}\right|$ is the strength of the statistical evidence in favour of the interpretation

$$\begin{cases} B_{ij} > 1 & \Rightarrow \hat{H}_i \text{ favoured over } \hat{H}_j \\ B_{ij} < 1 & \Rightarrow \hat{H}_j \text{ favoured than } \hat{H}_i \\ B_{ij} = 1 & \Rightarrow \hat{H}_i \text{ equally favoured as } \hat{H}_j. \end{cases} \tag{1.8}$$

1.2.1 *Experiment sets*

As mentioned it is necessary for the TLTL of both models in a BF calculation to refer to the same set of experiments, $\mathcal{E}$. There are a number of ways to achieve this, which we briefly summarise here for reference later.

During training (the QHL subroutine), candidate model $\hat{H}_i$ is trained against $\mathcal{E}_i$, designed by an experiment design heuristic (EDH) to optimise parameter learning specifically for $\hat{H}_i$; likewise $\hat{H}_j$ is trained on $\mathcal{E}_j$. The simplest method to compute the BF is to enforce $\mathcal{E} = \mathcal{E}_i \cup \mathcal{E}_j$ in Eq. (1.3), i.e. to cross-train $\hat{H}_i$ using the data designed specifically for training $\hat{H}_j$, and vice versa. This is a valid approach because it challenges each model to attempt to explain experiments designed explicitly for its competitor, at which only truly accurate models are likely to succeed.

A second approach builds on the first, but incorporates *burn–in* time in the training regime: this is a standard technique in the evaluation of machine learning (ML) models whereby its earliest iterations are discounted for evaluation so as not to skew its metrics, ensuring the evaluation reflects the strength of the model. In BF, we achieve this by basing the TLTL only on a subset of the training experiments. For example, the latter half of experiments designed

during the training of $\hat{H}_i$, $\mathcal{E}_i'$. This does not result in less predictive BF, since we are merely removing the noisy segments of the training for each model, e.g. the first half of experiments in **??**. Moreover it provides a benefit in reducing the computation requirements: updating each model to ensure the TLTL is based on $\mathcal{E}' = \mathcal{E}_i' \cup \mathcal{E}_j'$ requires only half the computation time, which can be further reduced by lowering the number of particles used during the update, N_p', which will give a similar result as using N_p, assuming the posterior has converged. We will verify this claim later in **??**, in the context of real examples.

A final option is to design a set of *evaluation* experiments, $\mathcal{E}_v$, that are valid for a broad variety of models, and so will not favour any particular model. Again, this is a common technique in ML: to use one set of data for training models, and a second, unseen dataset for evaluation. This is clearly a favourable approach: provided for each model we compute **??** using $\mathcal{E}_v$, we can automatically select the strongest model based solely on their TLTLs, meaning we do not have to perform further computationally-expensive updates, as required to cross-train on opponents' experiments during BF calculation. However, it does impose on the user to design a *fair* $\mathcal{E}_v$, requiring unbiased probe states $\{|\psi\rangle\}$ and times $\{t\}$ on a timescale which is meaningful to the system under consideration. For example, experiments with $t > T_2$, the decoherence time of the system, would result in measurements which offer little information, and hence it would be difficult to extract evidence in favour of any model from experiments in this domain. It is difficult to know, or even estimate, such meaningful time scales a priori, so it is difficult for a user to design $\mathcal{E}_v$. Additionally, the training regime each model undergoes during QHL is designed to provide adaptive experiments that take into account the specific model entertained, to choose an optimal set of evolution times, so it is likely that the set of times in $\mathcal{E}_i$ is *reasonable* by default. This approach would be favoured in principle, in the case where such constraints can be accounted for, e.g. an experiment repeated in a laboratory where the available probe states are limited and the timescale achievable is understood.

1.3 QUANTUM MODEL LEARNING AGENT PROTOCOL

Given a target quantum system, Q, described by some *true* Hamiltonian model, $\hat{H}_0$, QMLA distills a model $\hat{H}' \approx \hat{H}_0$. We can think of QMLA as a forest search algorithm[2]: consisting of a number of trees, each of which can have an arbitrary number of branches, where each leaf on each branch is an individual model, QMLA is the search for the leaf in the forest with the strongest statistical evidence of representing Q. Each tree in the QMLA forest corresponds to an independent *model search* , structured according to a bespoke exploration strategy (ES), which we detail in Section 1.4.

In short, the components of the iterative model search for a given ES, depicted in Fig. 1.1**(a-d)**, are

2 Note QMLA is not a random forest, where decision trees are added at random, because in QMLA trees are highly structured and included manually.

BRANCHES A set of candidate models, $\{\hat{H}_i\}$, are held together on a branch, μ.

TRAINING Each model $\hat{H}_i \in \mu$ is trained according to a parameter learning subroutine.

CONSOLIDATION The performance of candidates in μ are ranked relative to each other, such that some models are favoured over others, for instance through selection of a *branch champion*, $\hat{H}^{\mu}_{C}$. Consolidation can rely on any statistical test, with BFs providing a robust platform to disinguish any pair of candidates.

SPAWN A set of new models are constructed, accounting for the immediately prior consolidation stage, i.e. leveraging the best-yet-known models to construct similar hypotheses.

Following the iterative model generation procedure, the model selects the strongest considered candidate, for instance by consolidating the set of branch champions, $\{\hat{H}^{\mu}_{C}\}$, resulting in the nomination of a single *champion model*, $\hat{H}'_{S}$, Fig. 1.1**(e)**. Multiple model searches can proceed in parallel, and they are each assigned an independent exploration tree (ET), S. The final step of QMLA is then to consolidate the set of champion models from all ETs, $\{\hat{H}'_{S}\}$, in order to delcare a *global* champion model, $\hat{H}'$, Fig. 1.1**(f)**.

1.4 EXPLORATION STRATEGIES

QMLA is implemented by running N_t ETs concurrently, where each ET corresponds to a unique model search and ultimately nominates a single model as its favoured approximation of $\hat{H}_0$. An ES is the set of rules which guide a single ET throughout its model search . We elucidate the responsibilities of ESs in the remainder of this section, but in short they can be summarised as:

i. model generation: combining the knowledge progressively acquired on the ET to construct new candidate models;
ii. decision criteria for the model search phase: instructions for how QMLA should respond at predefined junctions, e.g. whether to cease the model search after a branch has completed;
iii. true model specification: detailing the terms and parameters which constitute $\hat{H}_0$ (in the case where Q is simulated);
iv. modular functionality: subroutines called throughout QMLA are interchangeable such that each ES specifies the set of functions to achieve its goals.

QMLA acts in tandem with one or more ESs, through the process depicted in Fig. 1.2. In summary: QMLA sends a request to the ES for a set of models; ES designs models and places them as leaves on a new branch on its ET, and returns the set $\mathbb{H}$; QMLA places $\mathbb{H}$ on a unique layer; QMLA trains the models in $\mathbb{H}$; QMLA consolidates $\mathbb{H}$; QMLA informs the ES of the results of training/consolidation of $\mathbb{H}$; ES decides whether to continue the search, and informs QMLA.

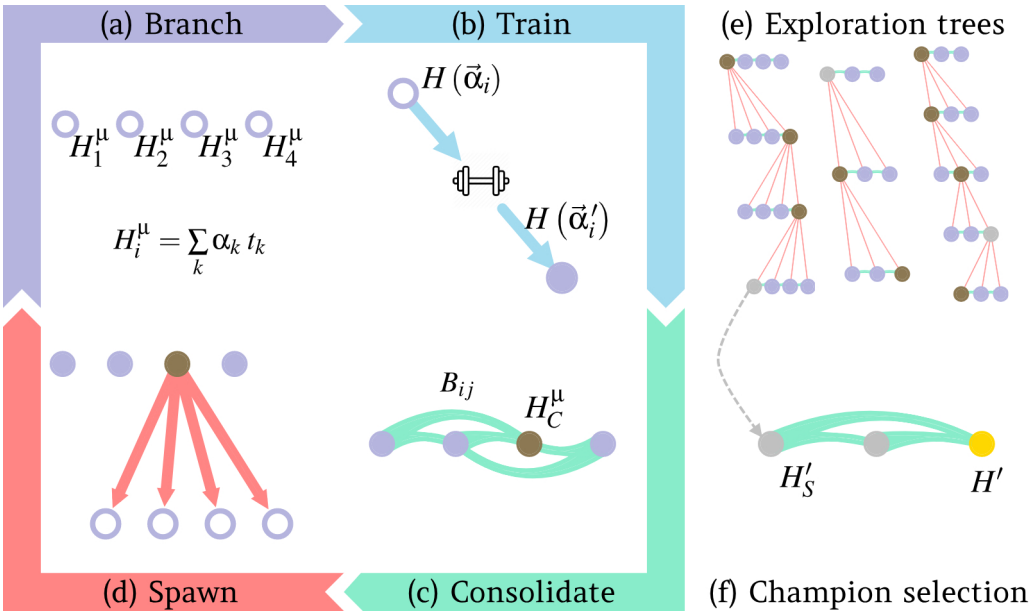


Figure 1.1: Schematic of Quantum Model Learning Agent (QMLA). **(a-d)** Model search phase within an Exploration strategy (ES). **(a)** Models are placed as (empty, purple) nodes on the *active branch* μ, where each model is a sum of terms $\hat{t}_k$ multiplied by corrresponding scalar parameters α_k. **(b)** Each active model is trained according to a subroutine such as quantum Hamiltonian learning to optimise $\vec{\alpha}_i$, resulting in the trained $\hat{H}(\vec{\alpha}_i')$ (filled purple node). **(c)** μ is consolidated, i.e. models are evaluated relative to other models on μ, according to the consolidation mechanism specificed by the ES. In this example, pairwise Bayes factors, B_{ij}, between $\hat{H}_i, \hat{H}_j$ are computed, resulting in the election of a single branch champion $\hat{H}_C^\mu$ (bronze). **(d)** A new set of models are *spawned* according to the chosen ES's model generation strategy. In this example, models are spawned from a single parent. The newly spawned models are placed on the next layer, $\mu + 1$, iterating back to **(a)**. **(e-f)** Higher level of entire QMLA procedure. **(e)** The model search phase for a unique ES is presented on an *exploration tree*. Multiple ES can operate in parallel, e.g. assuming different underlying physics, so the overall QMLA procedure involves a *forest search* across multiple exploration trees. Each ES nominates a champion, $\hat{H}_S'$ (silver), after consolidating its branch champions (bronze). **(f)** $\hat{H}_S'$ from each of the above exploration trees are gathered on a single layer, which is consolidated to give the final champion model, $\hat{H}'$ (gold).

1.4.1 *Model generation*

The main role of any ES is to design candidate models to test against $\hat{H}_0$. This can be done through any means deemed appropriate, although in general it is sensible to exploit the information gleaned so far in the ET, such as the performance of previous candidates and their comparisons, so that successfel models are seen to *spawn* new models, e.g. by combining

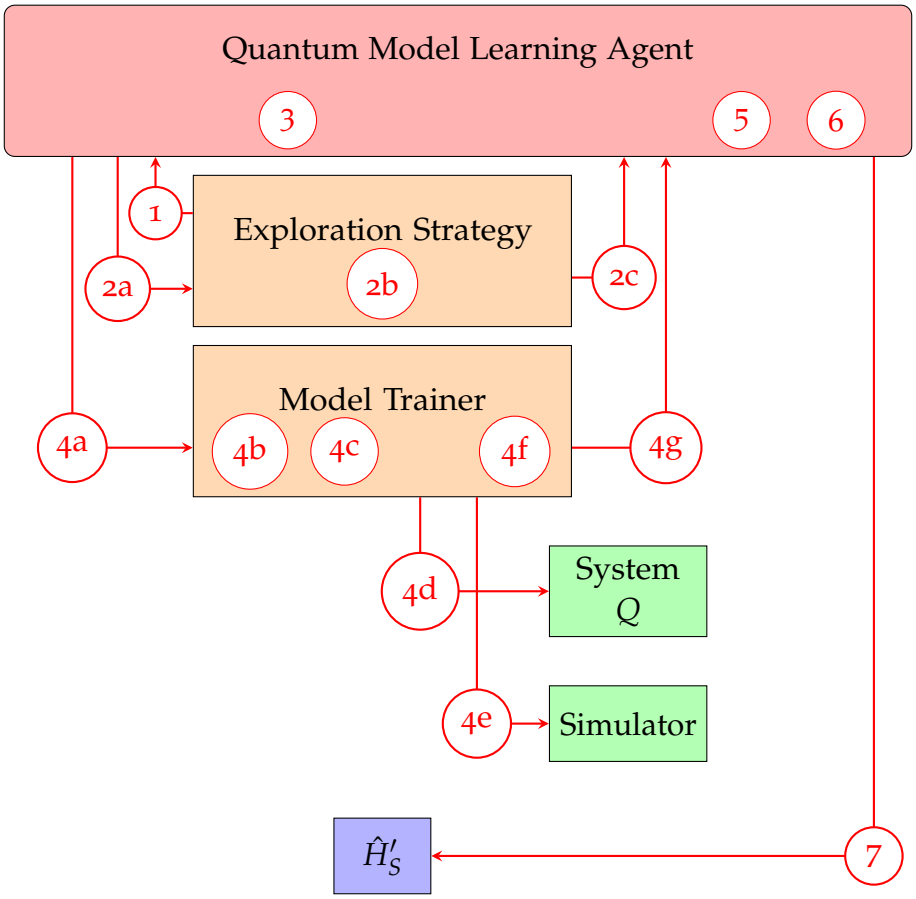


Figure 1.2: Interface between Quantum Model Learning Agent (QMLA) and a single exploration strategy (ES) The main components are the ES, model training subroutine, target quantum system (i.e. black box, Q), and (quantum) simulator. The main steps of the algorithm, shown in red with arrows denoting data transferred during that step, are as follows. **1**, QMLA retrieves decision infrastructure from ES, such as the consolidation mechanism and termination criteria. **2**, models are designed/spawned; **2a**, QMLA signals to ES requesting a set of models, passing the results of the previous layers' models if appropriate. **2b**, ES spawns new models, $\mathbb{H}$; **2c**, ES passes $\mathbb{H}$ to QMLA. **3**, QMLA assigns a new layer $(\mu \leftarrow \mu + 1)$ and places the newly proposed models upon it. **4**, Model training subroutine (here quantum Hamiltonian learning), performed independently for each model $\hat{H}_i \in \mu$; **4a**, QMLA passes $\hat{H}_i$ to the model trainer; **4b**, construct a prior distribution P_i describing the model's parameterisation $\vec{\alpha}_i$; **4c**, design experiment e to perform on Q to optimise $\vec{\alpha}_i$; **4d**, perform e on Q to retrieve a datum d; **4e**, simulate e for particles $\{\vec{\alpha}_1, \ldots, \vec{\alpha}_N\}$ sampled from P_i to retrieve a *likelihood* l_e; **4e**, update the prior P_i based on (d, l_e). **5**, Evaluate and rank $\hat{H}_i \in \mu$ according to the ES's consolidation mechanism. **6**, Check ES's termination criteria; if reached, proceed to **(7)**, otherwise return to **(2)**. **7**, Nominate champion model, $\hat{H}'_S$.

previously successful models, or by building upon them. Conversely, model generation can be completely determined in advance or entirely random. This alludes to the central design choice in composing an ES: how broad and deep should the searchable *model space* be, considering that adequately training each model is expensive, and that model comparisons are similarly expensive. The model search occurs within some *model space*, the size of which can usually be easily found by assuming that terms are binary – either the interaction they represent is present or not. If all possible terms are accounted for, and the total set of terms is $\mathcal{T}$, then there are $2^{|\mathcal{T}|}$ available candidates in the model space. The model space encompasses the closed[3] set of models construable by the set of terms considered by an ES. Because training models is slow in general, a central aim of QMLA is to search this space efficiently, i.e. to minimise the number of models considered, while retaining high quality models and providing a reasonable prospect of uncovering the true model, or a strong approximation thereof.

1.4.2 *Decision criteria for the model search phase*

Further control parameters, which direct the growth of the ET, are set within the ES. At several junctions within Algorithm 1, Algorithm 2, QMLA queries the ES in order to decide what happens next. Here we list the important cases of this behaviour.

PARAMETER-LEARNING SETTINGS

- such as the prior distribution to assign each parameter during QHL, and the parameters needed to run sequential monte carlo (SMC).
- the time scale on which to examine Q.
- the input probes to train upon, Ψ, described in **??**.

BRANCH COMPARISON STRATEGY

- How to consolidate models within a branch. Some examples used in this work are

* a points-ranking, where all candidates are compared via BF and points are assigned to the favoured model according to Eq. (1.8);
* ranking reflecting each model's log-likelihood (Eq. (1.5)) after training;
* models are ranked according to some objective function, as in the case of genetic algorithms (GAs) which we detail in **??**.

3 It is feasible to define an ES which uses an open model space, that is, there is no pre-defined $\mathcal{T}$, but rather the ES determines models through some other heuristic mechanism. In this thesis, we do not propose any such ES, but note that the QMLA framework facilitates the concept, see **??**.

MODEL SEARCH TERMINATION CRITERIA

– e.g. instruction to stop after a fixed number of iterations, or when a certain fitness has been reached.

CHAMPION NOMINATION

– when a single ET is explored, identify a single champion from the branch champions, $\{\hat{H}_C^\mu\}$;

– if multiple ETs are explored, the mechanism to compare champions across trees.

1.4.3 *True model specification*

It is necessary also to specify details about the true model, $\hat{H}_0$, at least in the case where QMLA acts on simulated data. Within the ES, we can set $\vec{T}_0$ as well as $\vec{\alpha}_0$. For example where the target system is an untrusted quantum simulator to be characterised, S_u, by interfacing with a trusted (quantum) simulator S_t, we decide some $\hat{H}_0$ in advance: the model training subroutine calls for likelihoods, those corresponding to $\hat{H}_0$ are computed S_u, while particles' likelihood are computed on S_t.

1.4.4 *Modular functionality*

Finally, there are a number of fundamenetal subroutines which are called upon throughout the QMLA algorithm. These are written independently such that each subroutine has a number of available implementations. These can be chosen to match the requirements of the user, and are set via the ES.

MODEL TRAINING PROCEDURE

– i.e. whether to use QHL or quantum process tomography, etc.

– In this work we always used QHL.

LIKELIHOOD FUNCTION the method used to estimate the likelihood for use during quantum likelihood estimation (QLE) within QHL, which ultimately depends on the measurement scheme.

– The role of these functions is to compute the probability of measuring each experimental outcome.

– These functions compute the *expectation value* of the unitary operator, $e^{-i\hat{H}t}$, corresponding to the dynamics of either Q or the hypothesis model.

- By default, here we use projective measurement back onto the input probe state, $\left|\langle\psi| e^{-i\hat{H}t} |\psi\rangle\right|^2$.
- In the usual case where Q has binary outcomes, we label one outcome – say, measurement in the state $|+\rangle$– as $d = 0$ and compute $\Pr(0)$ so that the likelihood, expectation value and $\Pr(0)$ refer to the same quantity, see **??**.
- It is possible instead to implement any measurement procedure, for example an experimental procedure where the environment is traced out, as we address in **??**.

PROBE defining the input probes to be used during training, Ψ, see **??**.

- In general it is preferable to use numerous probes in order to avoid biasing particular terms.
- In some cases we are restricted to a small number available input probes, e.g. to match experimental constraints.

EXPERIMENT DESIGN HEURISTIC bespoke experiments to maximise the information on which models are individually trained, described in **??**.

- In particular, in this work the experimental controls consist solely of $\{|\psi\rangle, t\}$.
- Currently, probes are generated offline, but in principle it is feasible to choose optimal probes based on available or hypothetical information. For example, probes can be chosen as a normalised sum of the candidate model's eigenvectors.
- Choice of t has a large effect on how well the model can train. By default, times are chosen proportional to the inverse of the current uncertainty in $\vec{\alpha}$ to maximise Fischer information, through the multi-particle guess heuristic described in sec:pgh [**?**].
- ∗ Alternatively, evolution times may be chosen from a fixed set in order to force QHL to reproduce the dynamics within those times' scale. For instance, if a small amount of experimental data is available offline, it is sensible to train all candidate models against the entire dataset.

MODEL TRAINING PRIOR specify the structure of the prior distribution, e.g. Fig. **??**(a)

- Set the initial mean and width of each parameter separately to define the prior multi-dimensional $\Pr(\vec{\alpha})$.

1.4.5 *Exploration strategy examples*

To solidifiy the concept of ESs, and how they affect the overall reach and runtime of a given ET, consider the following examples, where each strategy specifies how models are generated, as

well as how trained models are compared within a branch. Recall that all of these strategies rely on QHL as the model training strategy, so that the run time for training, is $t_{\text{QHL}} \sim N_e N_p t_{U(n)}$, where $t_U(n)$ is the time to compute the unitary evolution via the matrix exponential for an n-qubit model All models are trained using the default likelihood in **??**. Assume the conditions

- all models considered are represented by 4-qubit models;
  - $t_{U(4)} \sim 10^{-3}$sec.
- each model undergoes a reasonable training regime;
  - $N_e = 1000, N_p = 3000$;
  - $\implies t_{\text{QHL}} = N_e \times N_p \times t_{U(4)} = 3000s \sim$ 1h;
- Bayes factor calculations use
  - $N_e = 500, N_p = 3000$
  - $\implies t_{\text{BF}} \sim 2 \times 500 \times 3000 \times 10^{-3} \sim$ 1h;
- there are 12 available terms
  - allowing any combination of terms, this admits a model space of size $2^{12} = 4096$
- access to 16 computer cores to parallelise calculations over
  - i.e. we can train 16 models or perform 16 BF comparisons in 1h.

Then, consider the following model generation/comparison strategies.

a. Predefined set of 16 models, comparing every pair of models
   (i) Training takes 1h, and there are $\binom{16}{2} = 120$ comparisons spread across 16 processes, requiring 8h
   (ii) total time is 9h.

b. Generative procedure for model design, comparing every pair of models, running for 12 branches
   (i) One branch takes 9h $\implies$ total time is $12 \times 9 = 108$h;
   (ii) total number of models considered is $16 \times 12 = 192$.

c. Generative procedure for model design, where less model comparisons are needed (say one third of all model pairs are compared), running for 12 branches
   (i) Training time is still 1h
   (ii) One third of comparisons, i.e. 40 BF to compute, requires 3h
   (iii) One branch takes $4h \implies$ total time is 36h
   (iv) total number of models considered is also 192.

These examples illustrate some of the design decisions involved in ESs, namely whether timing considerations are more important than thoroughly exploring the model space. They also show considerable time–savings in cases where it is acceptable to forego all model comparisons. The approch in (a) is clearly limited in its applicability, mainly in that there is a heavy requirement

for prior knowledge, and it is only useful in cases where we either know $\hat{H}_0 \in \mathbb{H}$, or would be satisfied with approximating $\hat{H}_0$ as the closest available $\hat{H}_j \in \mathbb{H}$. On the opposite end of this spectrum, (c) is an excellent approach with respect to minimising prior knowledge required by the algorithm, although at the significant expense of testing a much larger number of candidate models. There is no optimal strategy for all use–cases: specific quantum systems of study demand particular considerations, and the amount of prior information available informs how wide the model search should reach.

1.5 GENERALITY

Several aspects of QMLA are deliberately vague in order to facilitate generality.

MODEL can mean any description of a quantum system which captures the interactions it is subject to.

- Here we exclusively consider Hamiltonian models, but Lindbladian models can also be considered as generators of quantum dynamics.

MODEL TRAINING is any subroutine which can train a given model, i.e. optimise a given parameterisation under the assumption that it represents the target system.

- Currently only QHL has been implemented, although for example tomography is valid in principle, with its own advantages and disadvantages. Overall QHL is found to fulfil the remit of model training with a balance of efficiency and rigour [**?**].
- QHL relies on the calculation of a characteristic likelihood function; this too is not restricted to the generic form of **??** and can be replaced by any form which represents the likelihood that experimental conditions e result in measurement datum d. We will see examples of this in **??** where we trace out part of the system in order to represent open systems.

MODEL SELECTION or *consolidation* can be as rigourous as desired by the user.

- Consolidation occurs at the branch level of each ET, but also in finding the tree champion, and ultimately the global champion.
- In practice, we use either BF or a related concept such as TLTL which are statistically signicative. However, in **??** we will consider a number of alternative schemes for discerning the strongest models.

1.5.1 *Agency*

While the concept of *agency* is contentious [**?**], we can view our overall protocol as a multi-agent system [**?**], or even an agent based evolutionary algorithm [**?**], because any given ES satisfies the definition, *the population of individuals can be considered as a population of agents*, where we mean

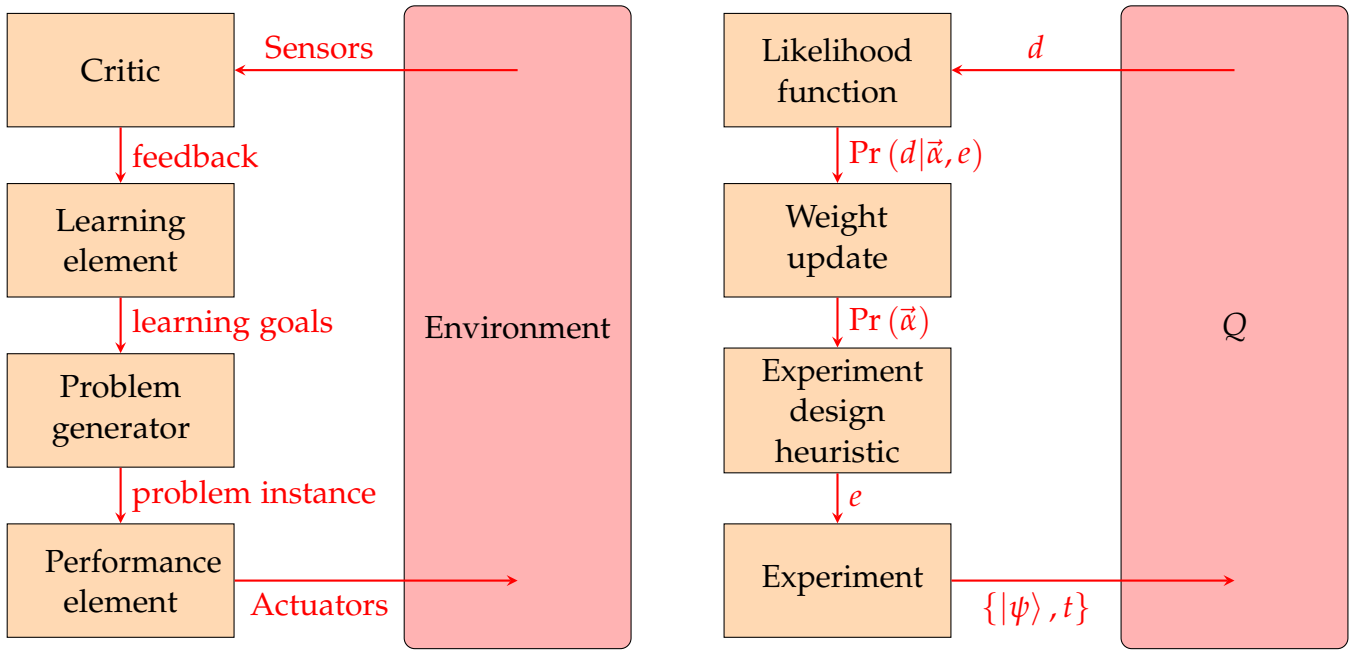


Figure 1.3: Learning agents. **Left**: definition of a learning agent, where an *environment* is affected by *actuators* which realise a *problem instance*, designed by a *problem generator*, through some *performance element*. The result of the agent's action is detected by *sensors*, which the *critic* interprets with respect to the agent's *learning goals*, by providing *feedback* to the *learning element*. *Right*: mapping of the concept of a learning agent on to an individual model. A target quantum system, Q, is queried by performing some experiment e, designed by an experiment design heuristic, and implemented by evolving a probe state $|\psi\rangle$ for time t. The systems is measured, and the datum d is sent to the likelihood function, which sends the likelihood $\Pr(d|\vec{\alpha}, t)$ to the weight update (and the parameter distribution update), before designing another experiment.

the population of models present on a given ET. More precisely, we can view individual models as *learning agents* according to the criteria of [**?**], i.e. that a learning agent has

- a *problem generator*: designs actions in an attempt to learn about the system – this is precisely the role of the EDH;
- a *performance element*: implements the the designed actions and measures the outcome – the measurement of a datum following the experiment chosen by the EDH;
- a *critic*: the likleihood function informs whether the designed action (experiment) was successful;
- a *learning element*: the updates to the weights and overall parameter distribution improve the model's performance over time.

We depict this analogy in Fig. 1.3. Finally, the model design strategy encoded in the ES *can* allow agency, by permitting the spawn rules autonomy, so we label the entire procedure as the quantum model learning agent.

1.6 ALGORITHMS

We conclude this chapter by listing the algorithms used most frequently, in order to clarify each of their roles, and how they interact. Algorithm 1 shows the overall QMLA algorithm, which is simplified greatly to a loop over the model search of each ES. The model search iteself is listed in Algorithm 2, which contains calls to subroutines for model learning (QHL, Algorithm 5), branch evaluation (which can be based upon BF, Algorithm 6) and centers on the generation of new models, an example of which – based on a *greedy search* prerogative – is given in Algorithm 4.

Algorithm 1: Quantum Model Learning Agent

Input: Q // some physically measurable or simulateable quantum system
Input: $\mathbb{S}$ // set of exploration strategies

Output: $\hat{H}'$ // champion model

$\mathbb{H}_c \leftarrow \{\}$
for $S \in \mathbb{S}$ **do**
  $\hat{H}'_S \leftarrow$ model_search(Q, S) // Run model search for this ES
  $\mathbb{H}_c \leftarrow \mathbb{H}_c \cup \{\hat{H}'_S\}$ // add ES champion to collection
end
$\hat{H}' \leftarrow$ final_champion($\mathbb{H}_c$)
return $\hat{H}'$

Algorithm 2: ES subroutine: model_search

Input: Q // some physically measurable or simulateable quantum system
Input: S // Exploration strategy: collection of rules/subroutines

Output: $\hat{H}'_S$ // Exploration strategy's nominated champion model

$\nu \leftarrow \{\}$
$\mathbb{H}_c \leftarrow \{\}$
while !S.terminate() **do**
  $\mu \leftarrow$ S.generate_models(ν) // e.g. Algorithm 4
  for $\hat{H}_i \in \mu$ **do**
    $\hat{H}'_i \leftarrow$ S.train($\hat{H}_i$) // e.g. Algorithm 5
  end
  $\nu \leftarrow$ S.consolidate(μ) // e.g. pairwise via Algorithm 3
  $\hat{H}^{\mu}_c \leftarrow$ S.branch_champion(ν) // use ν to select a branch champion
  $\mathbb{H}_c \leftarrow \mathbb{H}_c \cup \{\hat{H}^{\mu}_c\}$ // add branch champion to collection
end
$\hat{H}'_S \leftarrow$ S.nominate_champion($\mathbb{H}_c$)
return $\hat{H}'_S$

Algorithm 3: ES subroutine: consolidate (example: points per Bayes factor win)

Input: μ // information about models considered to date
Input: b // threshold for sufficient evidence that one model is stronger
Input: BF() // callable function to compute the Bayes factor between $\hat{H}_j$ and $\hat{H}_k$, Algorithm 6
Output: ν // information about models' relative performance

$\mathbb{H} \leftarrow$ extract_models(μ)
for $\hat{H}_j \in \mathbb{H}$ **do**
  $s_j = 0$ // Initialise score for each model
end
for $\hat{H}_j, \hat{H}_k \in \mathbb{H}$ // pairwise Bayes factor between all models in the set **do**
  $B \leftarrow \mathrm{BF}(\hat{H}_j, \hat{H}_k)$
  if $B \gg b$ // Increase score of winning model **then**
    $s_j \leftarrow s_j + 1$
  else if $B \ll 1/b$ **then**
    $s_k \leftarrow s_k + 1$
end
$k' \leftarrow \max_k\{s_k\}$ // Find which model has most points
return $\hat{H}_{k'}$

Algorithm 4: ES subroutine: generate_models (example: greedy spawn)

Input: ν // information about models considered to date

return $\mathbb{H}$

Algorithm 5: Quantum Hamiltonian Learning

Input: Q // some physically measurable or simulatable quantum system, described by $\hat{H}_0$
Input: $\hat{H}_i$ // Hamiltonian model attempting to reproduce data from $\hat{H}_0$
Input: $\Pr(\vec{\alpha})$ // probability distribution for $\vec{\alpha} = \vec{\alpha}_0$
Input: N_e // number of experiments to iterate learning procedure for
Input: N_p // number of particles to draw from $\Pr(\vec{\alpha})$
Input: $\Lambda(\Pr(\vec{\alpha}))$ // Heuristic algorithm which designs experiments
Input: $\mathrm{RS}(\Pr(\vec{\alpha}))$ // Resampling algorithm for redrawing particles
Output: $\vec{\alpha}'$ // estimate of Hamiltonian parameters

Sample N_p times from $\Pr(\vec{\alpha}) \leftarrow \mathcal{P}$ // particles

for $p \in \mathcal{P}$ **do**
  $w_p \leftarrow 1/N_p$ // set weights for each particle
end

for $e \in \{1 \rightarrow N_e\}$ **do**
  $t, |\psi\rangle \leftarrow \Lambda(\Pr(\vec{\alpha}))$ // design an experiment
  for $p \in \mathcal{P}$ **do**
    Retrieve particle $p \leftarrow \vec{\alpha}_p$
    Prepare Q in $|\psi\rangle$, evolve and measure after $t \leftarrow d$ // datum
    $|\langle d| e^{-iH(\vec{\alpha}_p)t} |\psi\rangle|^2 \leftarrow \Pr(d|\vec{\alpha}_p; t)$ // likelihood
    $w_p \leftarrow w_p \times \Pr(d|\vec{\alpha}_p; t)$ // weight update
  end
  if $1/\sum_p w_p^2 < N_p/2$ // check whether to resample (are weights too small?)
  then
    $\mathrm{RS}(\Pr(\vec{\alpha})) \leftarrow \mathcal{P}$ // Redraw particles via resampling algorithm
    for $p \in \mathcal{P}$ **do**
      $w_p \leftarrow 1/N_p$ // set weights for each particle
    end
  end
end
$\mathrm{mean}(\Pr(\vec{\alpha})) \leftarrow \vec{\alpha}'$
return $\vec{\alpha}'$

Algorithm 6: Bayes Factor calculation

Input: Q // some physically measurable or simulateable quantum system.
Input: $\hat{H}'_j, \hat{H}'_k$ // Hamiltonian models after training (i.e. $\vec{\alpha}_j, \vec{\alpha}_k$ already optimised), on which to compare performance.
Input: $\mathcal{E}_j, \mathcal{E}_k$ // experiments on which $\hat{H}'_j$ and $\hat{H}'_k$ were trained during QHL.
Output: B_{jk} // Bayes factor between two candidate Hamiltonians

$\mathcal{E} = \{\mathcal{E}_j \cup \mathcal{E}_k\}$ // common experiments for fair comparison

for $\hat{H}'_i \in \{\hat{H}'_j, \hat{H}'_k\}$ **do**
  $\mathcal{L}_i = 0$ // total log-likelihood of $\hat{H}_i$
  for $e \in \mathcal{E}$ **do**
    $e \leftarrow t, |\psi\rangle$ // assign time and probe from experiment control set
    Prepare Q in $|\psi\rangle$, evolve and measure after $t \leftarrow d$ // datum
    $\left|\langle d| e^{-i\hat{H}'_i t} |\psi\rangle\right|^2 \leftarrow \Pr(d|\hat{H}_i, t)$ // total likelihood for $\hat{H}'_i$ on e
    $log\left(\Pr(d|\hat{H}_i, t)\right) \leftarrow l_e$ // log total likelihood for $\hat{H}'_i$ on e
    $\mathcal{L}_i + l_e \leftarrow \mathcal{L}_i$ // add l_e to total log total likelihood
  end
end
$\exp\left(\mathcal{L}_j - \mathcal{L}_k\right) \leftarrow B_{jk}$ // Bayes factor between models

return B_{jk}

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

- evaluation: plots of probes and times used as the evaluation dataset.
- 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.
- 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.
- exploration_strategy_plots plots specifically required by the ES at the run level.
- 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.
- 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.
- 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 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. Continued in Table A.2.

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
??	NVCentreGenticAlgorithmPrelearnedParameters	2	5	Sep_08/23_58
??	NVCentreGenticAlgorithmPrelearnedParameters	2	5	Sep_08/23_58

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 [?].

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:

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

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. Note: these examples are included in the QMLA documentation in a format that may be easier to follow – where possible, we recommend readers follow the Tutorial section of [**?**].

First, *fork* the QMLA codebase from [**?**] 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].

The steps of preparing the codebase are

1. install redis;
2. create a virtual Python environment for installing QMLA dependencies without damaging other parts of the user's environment;
3. download the QMLA codebase from the forked Github repository;
4. install packages upon which QMLA depends.

```
# 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
```

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.

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

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

Listing C.1: QMLA codebase setup language

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

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 test, return to the local_launch of Listing C.3, but change some of the settings:

```
particles=2000
experiments=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.

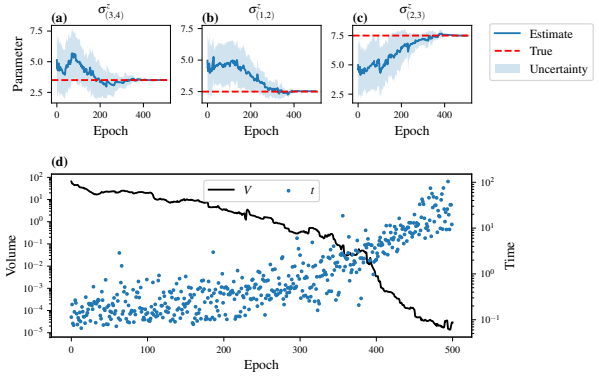
2 Note this will take up to 15 minutes to run. This can be reduced by lowering the values of particles, experiments, which is sufficient for testing but note that the outcomes will be less effective than those presented in the figures of this section.

C.2 ANALYSIS

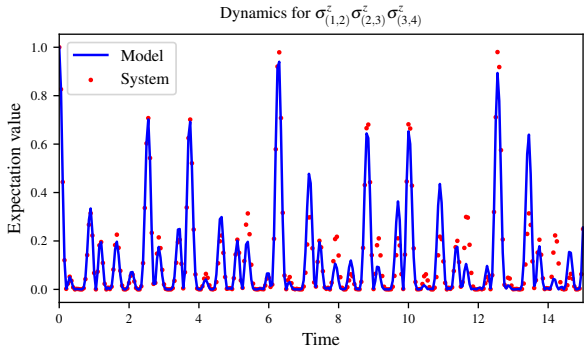
QMLA stores results and generates plots over the entire range of the algorithm[3], i.e. the run, instance and models. The depth of analysis performed automatically is set by the user control plot_level in local_launch.sh; for plot_level=1, only the most crucial figures are generated, while plot_level=6 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.

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 $\hat{H}_0$.

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.2.2 *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: for 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 Appendix C.3.

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

```
experiments=250
particles=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).

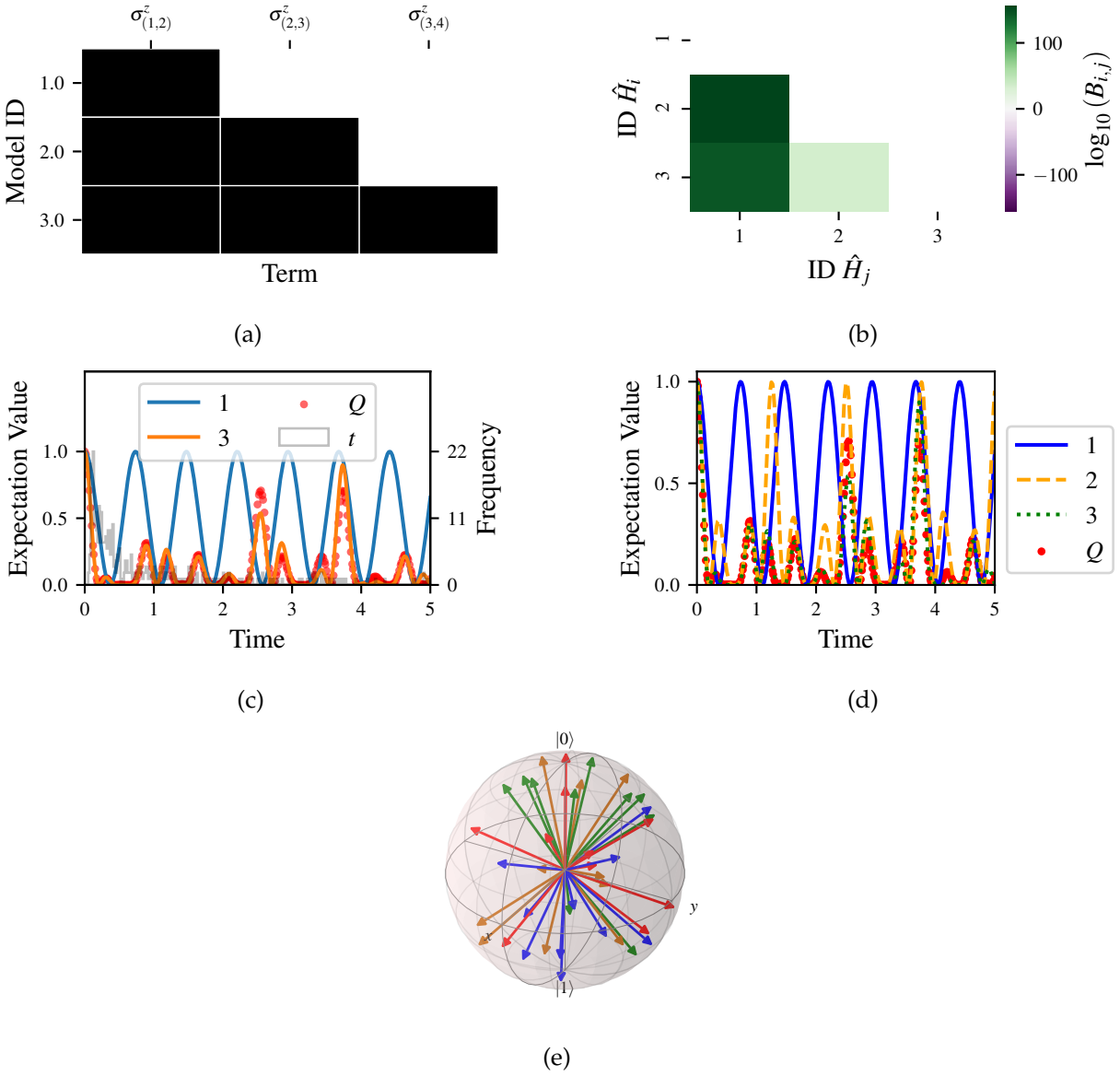


Figure C.3: QMLA plots; found within instance directory e.g. Jan_01/01_23/instances/qmla_1, and its subdirectories. **(a)** composition_of_models: constituent terms of all considered models, indexed by their model IDs. Here model 3 is $\hat{H}_0$. **(b)** bayes_factors: Bayes factor (BF) comparisons between all models. 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
experiments=20
particles=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 which each model was deemed champion, 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

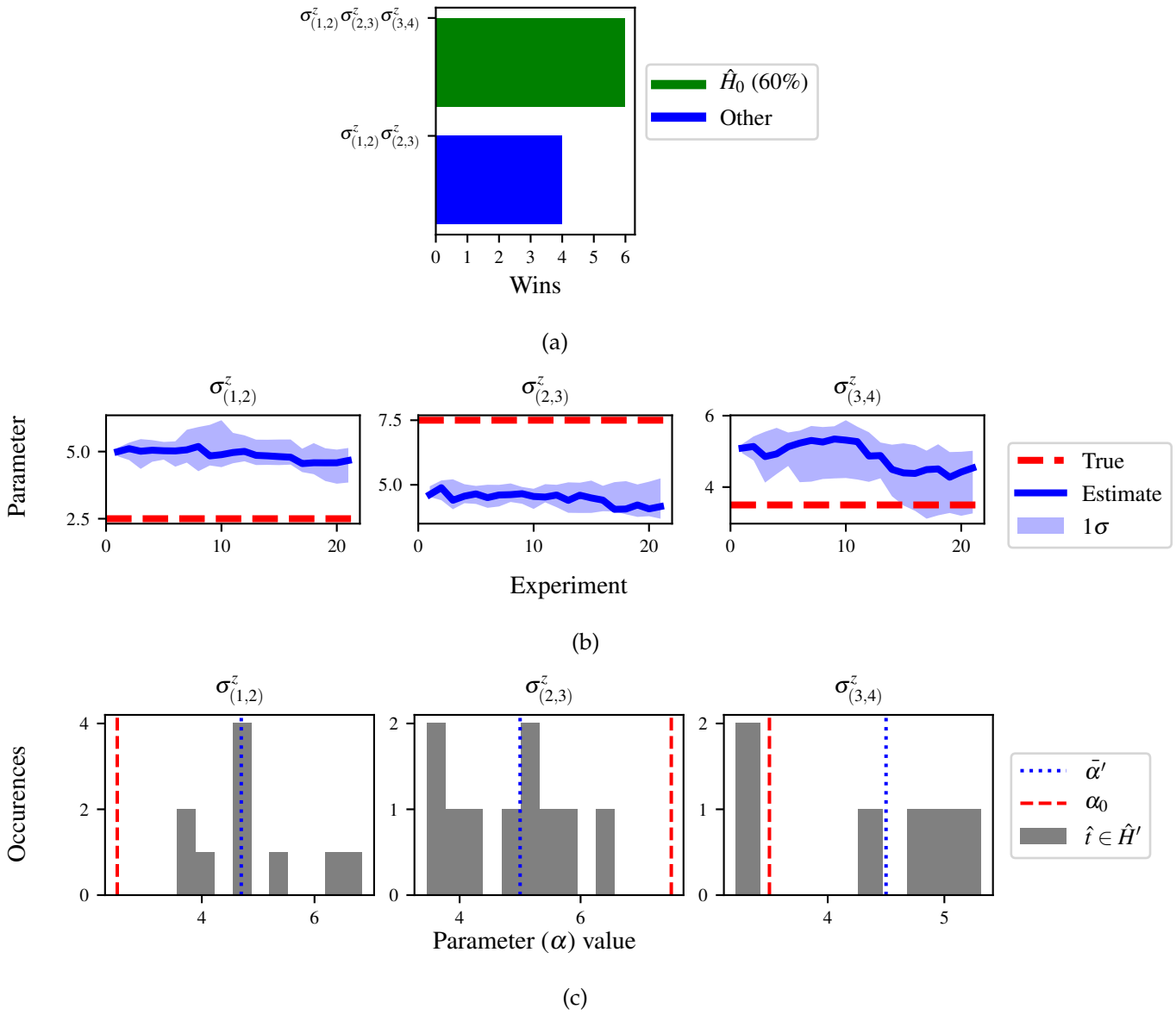


Figure C.4: QMLA run plots; found within run directory e.g. Jan_01/01_23/. **(a)** performance/model_wins: number of instance wins achieved by each model. **(b)** champion_models/params_params_pauliSet_1J2_zJz_d4+pauliSet_2J3_zJz_d4+pauliSet_3J4_zJz_d4: parameter estimation progression for the true model , 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.

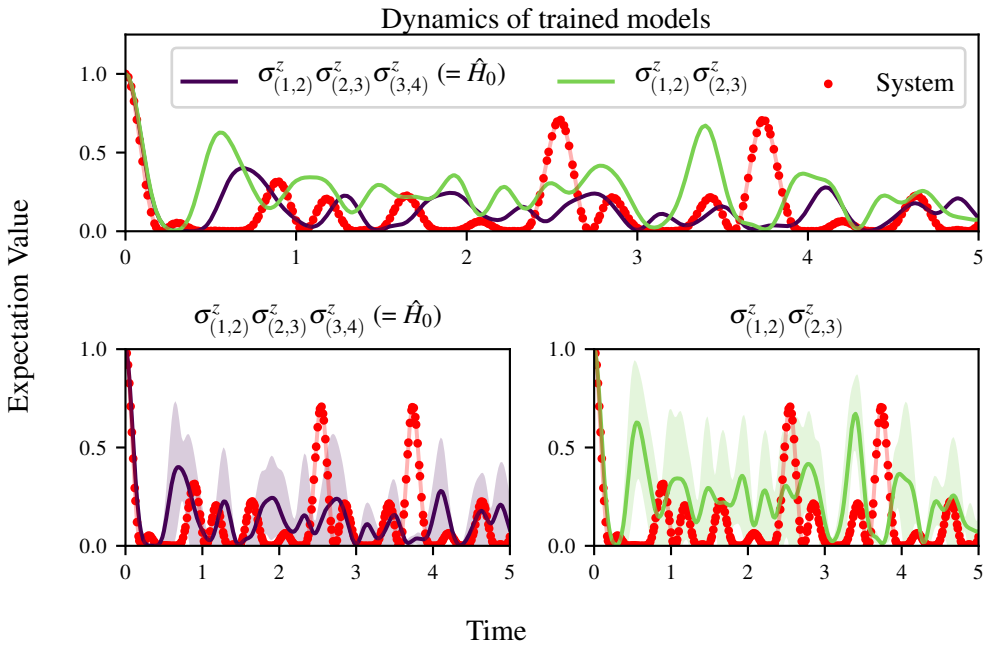


Figure C.5: Run plot performace/dynamics: median dynamics of the champion models. The models which won most instances are shown together in the top panel, and individually in the lower panels. The median dynamics from the models' learnings in its winning instances are shown, with the shaded region indicating 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 \glspl{instance} 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 [**?**].

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*

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.

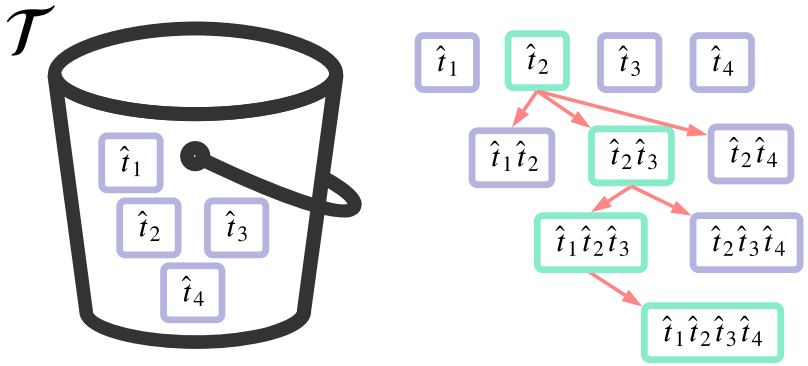


Figure C.6: Greedy search mechanism. **Left**, a set of primitive terms, $\mathcal{T}$, are defined in advance. **Right**, models are constructed from $\mathcal{T}$. On the first branch, the primitve terms alone constitute models. Thereafter, the strongest model (marked in green) from the previous branch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

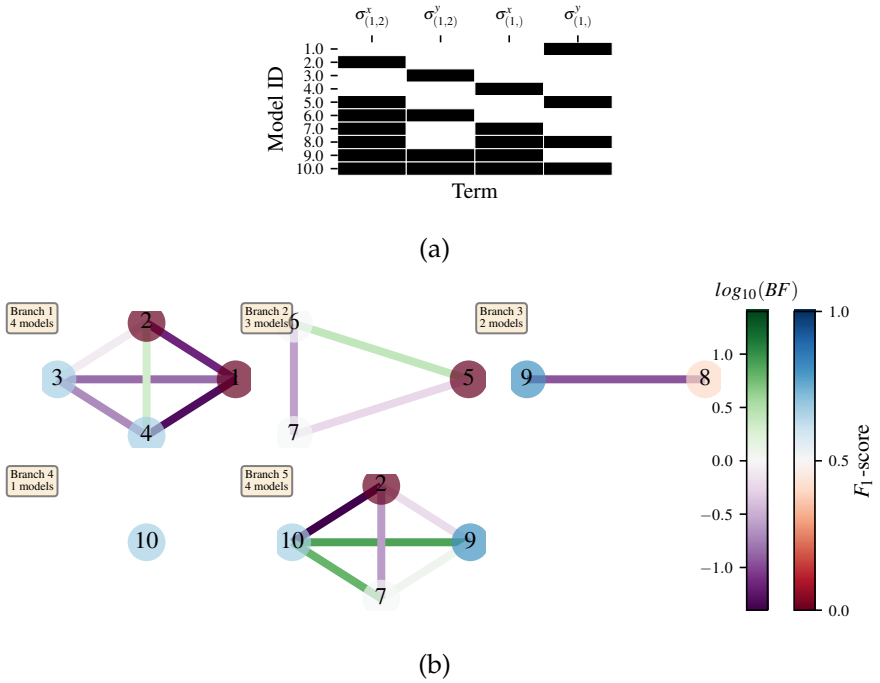
```
    greedily adding all unused terms to separate models at each
       call to the generate_models.

    """

    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 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. 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, Fig. C.7.



(a)

(b)

Figure C.7: Greedy exploration strategy. **(a)**, composition_of_models. **b**, graphs_of_branches_ExampleGreedySearch: shows which models reside on each branches of 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.

6 We advise reducing plot_level to 3 to avoid excessive/slow figure generation.

C.4.2 *Tiered greedy search*

We provide one final example of a non-trivial ES: tiered greedy search. Similar to the idea of Appendix C.4.1, 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
               '],
```

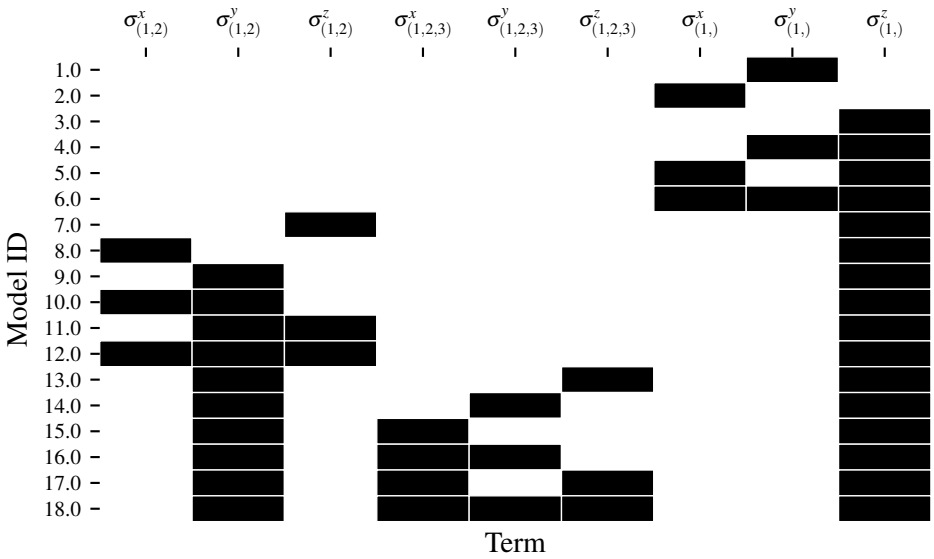
```
        }
        self.tier = 1
        self.max_tier = max(self.term_tiers)
        self.tier_branch_champs = {k : [] for k in self.
            term_tiers}
        self.tier_champs = {}
        self.prune_completed_initially = True
        self.check_champion_reducibility = True

    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 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:
```

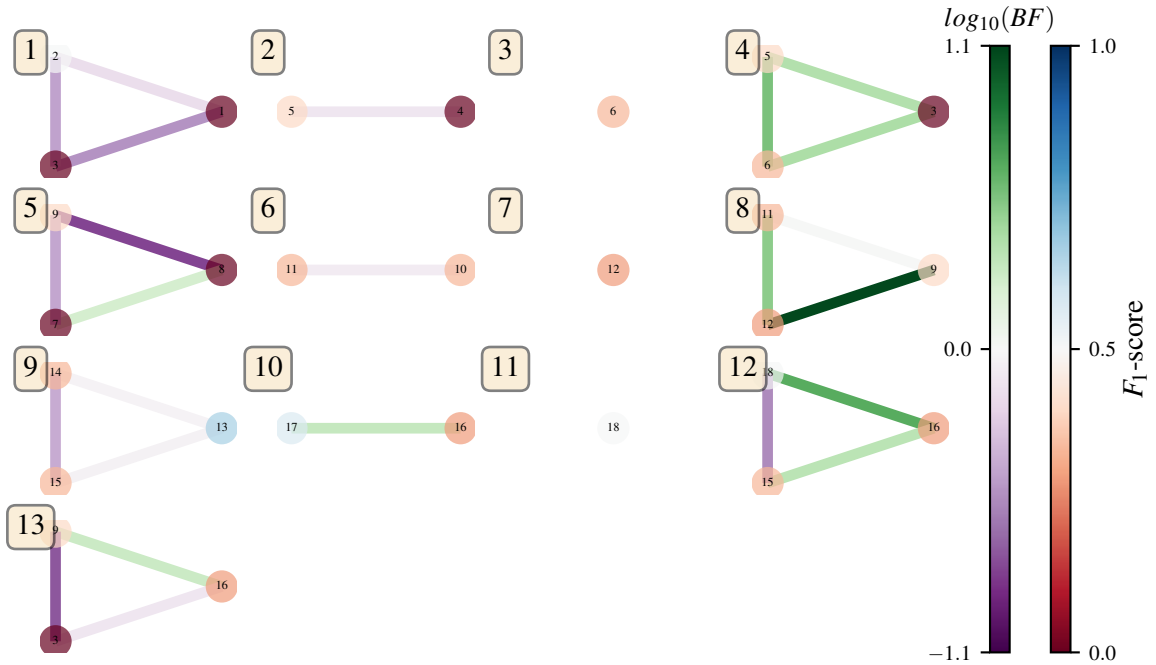
```
            return True
        elif self.spawn_stage[-1] == "Complete":
            return True
        else:
            return False


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.18: ExampleGreedySearchTiered exploration stategy

with corresponding results in Fig. C.8.



(a)



(b)

Figure C.8: Tiered greedy exploration strategy. **(a)**, composition_of_models. **b**, graphs_of_branches_ExampleGreedySearchTiered: shows which models reside on each branches of the exploration tree. Models are coloured by their F_1-score, and edges represent the BF between models. In each tier, three branches greedily add terms, and a fourth branch considers the champions of the first three branches in order to nominate a tier champion. The final branch consists only of the tier champions, to nominate the global champion, $\hat{H}'$.

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