Doctorate of Philosophy

Schrödinger's Catwalk

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LISTINGS

ACRONYMS

BF	Bayes factor. 24–26, 32–34, 47, 50, 54, 56, 61–63
CLE	classical likelihood estimation. 13
EDH	experiment design heuristic. 18–20, 22, 25, 34, 44, 54, 55
ES	exploration strategy. 26–34, 39, 42, 44, 48, 50, 61, 64, 73, 76
ET	exploration tree. 27, 28, 30, 31, 33, 34, 44, 46
FH	Fermi-Hubbard. 57
GA	genetic algorithm. 33
HPD	high particle density. 17
IQLE	interactive quantum likelihood estimation. 13, 14
LTL	log total likelihood. 15
ML	machine learning. 6, 25, 26
MS	model search. 26–28, 30, 34, 42, 44
MVEE	minimum volume enclosing ellipsoid. 17
NV	nitrogen-vacancy. 9
NVC	nitrogen-vacancy centre. 14
PGH	particle guess heuristic. 18–20, 44
QHL	quantum Hamiltonian learning. v, 8–14, 16, 18, 20, 21, 24–26, 30, 31, 33, 34, 39, 42, 47, 54, 55, 73
QL	quadratic loss. 16
QLE	quantum likelihood estimation. 13
QMLA	Quantum Model Learning Agent. v, viii, 8, 13, 23, 24, 26–30, 33, 34, 39, 42–48, 50, 51, 59–64, 73

SMC sequential monte carlo. 11–13, 15, 18, 19, 22, 30

TLTL total log total likelihood. 16, 24–26, 33

GLOSSARY

Jordan Wigner transformation (JWT)	Jordan Wigner transformation . 59, 60, 63
Loschmidt echo (LE)	Quantum chaotic effect described. . 13, 14
hyperparameter	Variable within an algorithm that determines how the algorithm itself proceeds.. 11
instance	a single implementation of the Quantum Model Learning Agent (QMLA) algorithm. 47, 73
model	The mathematical description of some quantum system. 23
probe	Input probe state, $\|\psi\rangle$, which the target system is initialised to, before unitary evolution. plural. 13, 14, 18, 20, 21, 53
results directory	Directory to which the data and analysis for a given run of QMLA are stored. . 48
run	collection of QMLA instances. ii, viii, 47, 48, 63, 64, 73
spawn	Process by which new models are generated by combining previously considered models.. 28
success rate	. 47, 48
term	Individual constituent of a model, e.g. a single operator within a sum of operators, which in total describe a Hamiltonian. . 23
volume	Volume of a parameter distribution's credible region.. 16, 17, 54, 55, 62
win rate	. 47, 48

Part I

THEORETICAL STUDY

1

GENETIC ALGORITHMS

The QMLA framework lends itself easily to the family of optimsation techniques called *evolutionary algorithms*, where individuals, sampled from a population of candidates, are considered, in generations, as solutions to the given problem, and iterative generations aim to efficiently search the available population, by mimicing biological evolutionary mechanisms [**?**]. In particular, we develop a exploration strategy (ES) which incorporates an genetic algorithm (GA) in the generation of models; GAs are a subset of evolutionary algorithms where candidate solutions are expressed as strings of numbers representing some configuration of the system of interest [**?**]. Here we will first introduce the concept of a GA, before describing the adaptations which allow us to build a genetic exploration strategy (GES).

1.1 GENETIC ALGORITHM DEFINITION

GAs work by assuming a given problem can be optimised, if not solved, by a single candidate among a fixed, closed space of candidates, called the population, $\mathcal{P}$. A number of candidates are sampled at random from $\mathcal{P}$ into a single *generation*, and evaluated through some objective function (OF), which assesses the fitness of the candidates at solving the problem of interest. Candidates from the generation are then mixed together to produce the next generation's candidates: this *crossover* process aims to combine only relatively strong candidates, such that the average candidates' fitness improve at each successive generation, mimicing the biological mechanism whereby the genetic makeup of offspring is an even mixture of both parents. The selection of strong candidates as parents for future generations is therefore imperative; in general parents are chosen according to their fitness as determined by the OF. Buidling on this biological motivation, much of the power of GAs comes from the concept of *mutation*: while offspring retain most of the genetic expressions of their parents, some elements are mutated at random. Mutation is crucial in avoiding local optima of the OF landscape by maintaining diversity in the examined subspace of the population.

Pseudocode for a generic GA is given in Algorithm 1, but we can also informally define the procedure as follows. Given access to the population, $\mathcal{P}$,

1. Sample N_m candidates from the population at random
   (a) call this group of candidates the first generation, μ.
2. Evaluate each candidate $\gamma_j \in \mu$.
   (a) each γ_j is assigned a fitness, g_j
   (b) the fitness is computed through an objective function acting on the candidate, $g(\gamma_j)$.
3. Map the fitnesses of each candidate, $\{g_j\}$, to selection probabilities for each model, $\{s_j\}$

   (a) e.g. by normalising the fitnesses, or by removing some poorly-performing candidates and then normalising.
4. Generate the next generation of candidates, μ'
   (a) $\mu = \{\}$
   (b) Select pairs of parents, p_1, p_2, from μ
      i. Each candidate's probability of being chosen is given by their s_j
   (c) Cross over p_1, p_2 to produce children candidates, c_1, c_2.
      i. mutate c_1, c_2 according to some random probabilistic process
      ii. keep c_i only if it is not already in μ', to ensure N_m unique models are tested at each generation.
   (d) until $|\mu'| = N_m$, iterate to step (b).
5. Until the N_g^{th} generation is reached, iterate to step 2..
6. The strongest candidate on the final generation is deemed the solution to the posed problem.

Candidates are manifested as *chromosomes*, i.e. strings of fixed length, whose entries, called *genes*, each represent some element of the system. In general, genes can have continuous values, although usually, and for all purposes in this thesis, genes are binary, capturing simply whether or not the gene's corresponding feature is present in the chromosome.

1.1.1 *Example: knapsack problem*

One commonly referenced combinatorial optimisation problem is the *knacksack problem*: given a set of objects, where each object has a defined mass and also a defined value, determine the set of objects to pack in a knapsack which can support a limited weight, such that the value of the packed objects is maximised. Say there are n objects, we can write the vector containing the values of those objects as $\vec{v}$, and the vector of their weights as $\vec{w}$. We can then represent configurations of object sets as candidate vectors $\vec{\gamma}_j$, whose genes are binary, and simply indicate whether or not the associated object is included in the set. For example, with $n = 6$,

$$\gamma_j = 100001 \Longrightarrow \vec{\gamma}_j = (1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1), \tag{1.1}$$

indicates a set of objects consisting only of those indexed first and last, with none of the intermediate objects included.

The fitness of any candidate is then given by the total value of that configuration of objects, $v_j = \vec{v} \cdot \vec{\gamma}_j$, but candidates are only admitted[1] if the weight of the corresponding set of objects is less than the capacity of the knapsack, i.e. $\vec{w}_j \cdot \vec{\gamma}_j \leq w_{max}$.

1 Note there are alternative strategies to dealing with candidates who violate the weight condition, such as to impose a penalty within the OF, but for our purposes let us assume we simply disregard violators.

Algorithm 1: Genetic algorithm

Input: $\mathcal{P}$ // Population of candidate models
Input: $g()$ // objective funtion
Input: map_g_to_s() // function to map fitness to selection probability
Input: select_parents() // function to select parents among generation
Input: crossover() // function to cross over two parents to produce offspring
Input: N_g // number of generations
Input: N_m // number of candidates per generation

Output: γ' // strongest candidate

$\mu \leftarrow \text{sample}\,(\mathcal{P}, N_m)$
for $i \in 1, ..., N_g$ **do**
  for $\gamma_j \in \mu$ **do**
    $g_j \leftarrow g(\gamma_j)$ // assess fitness of candidate
  end
  $\{s_j\} \leftarrow$ map_g_to_s($\{g_j\}$) // map fitnesses to normalised selection probability
  $\mu_c = \arg\max_{s_j}\{\gamma_j\}$ // record champion of this generation

  $\mu \leftarrow \{\}$ // empty set for next generation
  while $|\mu| < N_m$ **do**
    $p_1, p_2 \leftarrow$ select_parents($\{s_j\}$) // choose parents based on candidates' s_j
    $c_1, c_2 \leftarrow$ crossover(p_1, p_2) // generate offspring candidates based on parents
    for $c \in \{c_1, c_2\}$ **do**
      if $c \notin \mu$ **then**
        $\mu \leftarrow \mu \cup \{c\}$ // keep if child is new
      end
    end
  end
end
$\gamma' \leftarrow \arg\max_{s_j}\{\gamma_j \in \mu\}$ // strongest candidate on final generation

return γ'

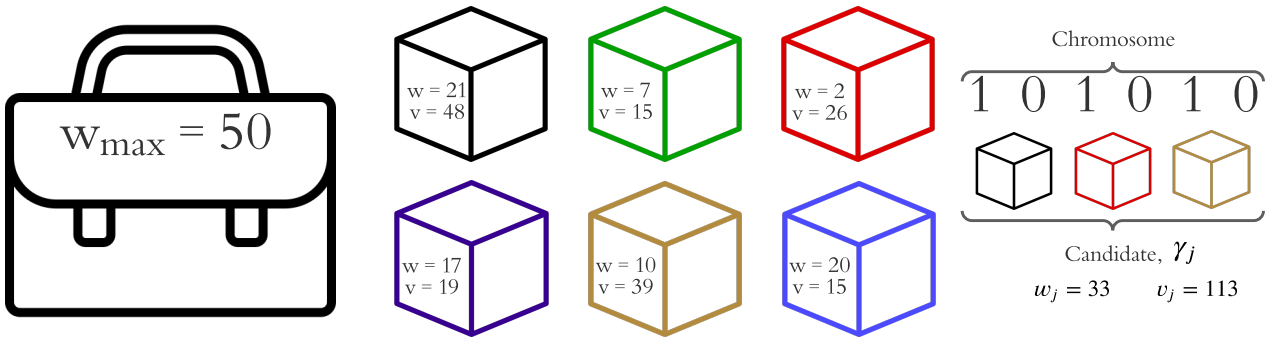

Figure 1.1: Depiction of the knapsack problem. **Left**, A knapsack which can hold any number of objects but is constrained by the total weight it can support, $w_{max} = 50$. **Centre**, A set of objects are available, each with associated weight, w, and value v. The objective is to find the subset of objects which maximise the total value, while not exceeding the capacity of the knapsack. **Right**, An example chromosome, i.e. candidate γ_j, where the bits of the chromosome indicate whether the corresponding object is included, allowing for calculation of the total weight and value of the candidate, w_j, v_j.

For example where each individual object has value < 50 and weight < 25 and $w_{max} = 50$, recalling $\gamma_j = 100001$, say,

$$\vec{v} = (48 \quad 15 \quad 26 \quad 19 \quad 39 \quad 15) \implies v_j = \vec{\gamma}_j \cdot \vec{v} = 48 + 15 = 63; \tag{1.2a}$$

$$\vec{w} = (21 \quad 7 \quad 2 \quad 17 \quad 10 \quad 20) \implies w_j = \vec{\gamma}_j \cdot \vec{w} = 21 + 20 = 41. \tag{1.2b}$$

We can hence assess the fitness of γ_j as 63 and deem it a valid candidate since it does not exceed the weight threshold. We can likewise compute the total weight and value of a series of randomly generated candidates, and deem them valid or not.

Name	Candidate	Value	Weight	Valid
γ_1	110011	117	58	No
γ_2	101010	113	33	Yes
γ_3	011110	99	36	Yes
γ_4	011011	95	39	Yes
γ_5	111000	89	30	Yes
γ_6	010111	88	54	No
γ_7	100010	87	31	Yes
γ_8	110001	78	48	Yes
γ_9	011101	75	46	Yes
γ_{10}	110000	63	28	Yes
γ_{11}	000011	54	30	Yes
γ_{12}	000101	34	37	Yes

Table 1.1: Candidate solutions to the knapsack problem.

The strongest (valid) candidates from Table 1.1 are 101010, 011110. By spawning from these candidates through a one-point crossover at the midpoint, we get $\gamma_{c_1} = 101110, \gamma_{c_2} = 011010$, from which we can see $v_{c_1} = 132, w_{c_1} = 50$, i.e. by combining two strong candidates we produce the strongest-yet-seen valid candidate.

By repeating this procedure, it is expected to uncover candidates which optimise v_j while maintining $w_j \leq w_{max}$, or at least to produce near-optimal solutions, using far less time/resources than brute-force evaluation of all candidates, which is usually sufficient. For instance, with $n = 100$ objects to consider, there are $2^{100} \approx 10^{30}$ candidates to consider; the most powerful supercomputers in the world currently claim on the order of Exa-FLOPs, i.e. 10^{18} operations per second, of which say ~ 1000 operations are required to test each candidate, meaning 10^{15} candidates can be checked per second in a generous example. This would still require 10^{12} seconds to solve absolutely, so it is reasonable in cases like this to accept *approximately optimal* solutions[2].

1.1.2 *Selection mechanism*

A key subroutine of every GA is the mechanism through which it nominates candidates from generation μ as parents to offsping candidates in $\mu + 1$ [**?**]. All mechanisms have in common that they act on a set of candidates from the previous generation, where each candidate, γ_j, has

2 Simply put: in machine learning, *good enough* is good enough. We will adopt this philosophy for the remainder of this thesis and life.

been evaluated and has fitness value, g_j. Among the viable schemes for selecting individual parents from the set of candidates, μ are

- Rank selection: candidates are selected with probabilty proportional to their ranking relative to the fitness of contemporary candidates in the same generation.
- Tournament selection: a subset of k candidates are chosen at random from μ, of which the candidate with the highest fitness is taken as the parent.
- Stochastic universal sampling: candidates are sampled proportional to their fitness, but the sampling algorithm is biased to ensure high-fitness candidates are chosen at least once within the generation.

We will only detail the mechanism used later within QMLA, the common fitness proportional selection, known as *roulette selection* [**?**]. This is a straightforward strategy where we directly map candidates' fitness, g_i to a selection probability, s_i, simply by normalising $\{g_i\}$, allowing us to visualise a roulette wheel of uneven wedges, eachh of which correspond to a candidate. Then we need only conceptually spin the roulette wheel to select the first parent, γ_{p_1}. We then remove γ_{p_1} from the set of potential parents, renormalise the remaining $\{s_i\}$, and spin the wheel again to choose the second parent, γ_{p_2}.

Practically, we repeat the process outlined until the next generation is filled, usually we have $|\mu| = N_m$, and desire that every generation should contain the same N_m candidates, so we repeat the roulette selection $N_m/2$ times per generation, since every pair of parents yield two offspring. It is important that meaningful differences in fitness are reflected by the selection probability, which is difficult to ensure for large N_m, e.g. with ten models, the strongest candidate is only a marginally more probable parent than the worst – this effect is amplified for larger N_m. We therefore wish to reduce the set of potential parents to ensure high quality offspring: we truncate μ and retain only the highest-fitness $\frac{N_m}{2}$ models as selectable parents. The roulette selection is shown in Fig. 1.2.

1.1.3 *Offspring production*

When a pair of parents have been nominated by the selection mechanism above, it remains to use those parents to spawn offsprint, which should inherit the properties of their parents. Here we use a *one point crossover*, whereby the two parent chromosomes are mixed together to form two offspring, about a single point, κ: for candidates of n genes, the first κ genes of γ_{p_1} are conjoined with the latter $n - \kappa$ genes of γ_{p_2}. Often κ is restricted to the midpoint of the chromosomes, although in general we need not impose this: we will instead consider $\kappa \in \left(\frac{n}{4}, \frac{3n}{4}\right)$, e.g. with $n = 12$, $\kappa \in (3, 9)$. The one-point crossover is shown for $n = 6$ with $\kappa = 3$ in Fig. 1.3, recalling the chromosome structure from Section 1.1.1.

By allowing κ other than the midpoint, we drastically increase the number of combinations of parents available for reproduction. Finally, then, parent selection is done by constructing a database of pairs of potentital parents with all available crossover points, with selection

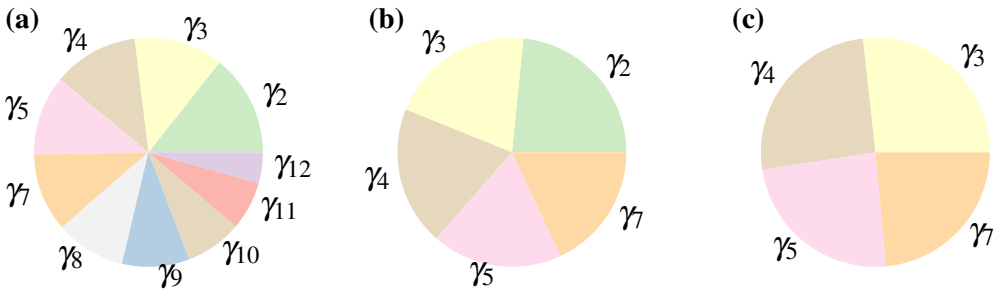

Figure 1.2: Roulette wheels showing selection probability s_i for corresponding candidates γ_i. Colours here only distinguish candidates, they do not encode any information. **b**, The set of potential parents is truncated to include only the strongest five candidates. **a**, All valid candidates are assigned selection probability based on their value in Table 1.1. **c**, After one parent (γ_2) has been chosen, it is removed from the roulette wheel and the remaining candidates' probabilities are renormalised for the selection of the second parent.

probability given by the product of their individual fitnesses. This is conceptually equivalent to selection via roulette wheel as above. Recalling the fitnesses (values) of 1.1, for example:

Parent 1	Parent 2	κ	Selection probability
γ_2	γ_3	2	$11,187\ (= 113 \times 99)$
γ_2	γ_3	3	$11,187$
γ_2	γ_3	4	$11,187$
γ_2	γ_4	2	$10,735\ (= 113 \times 95)$
γ_2	γ_4	3	$10,735$
γ_2	γ_4	4	$10,735$

Table 1.2: Example of parent selection database.

The GA maintains diversity in the subspace of $\mathcal{P}$ it studies, by *mutating* some of the newly proposed offspring candidates. Again, there are a multitude of approaches for this step **[?]**, but for brevity we only describe those used in this thesis. For each proposed child candidate, γ_c, we probabilistically mutate each gene with some mutation rate r_m.

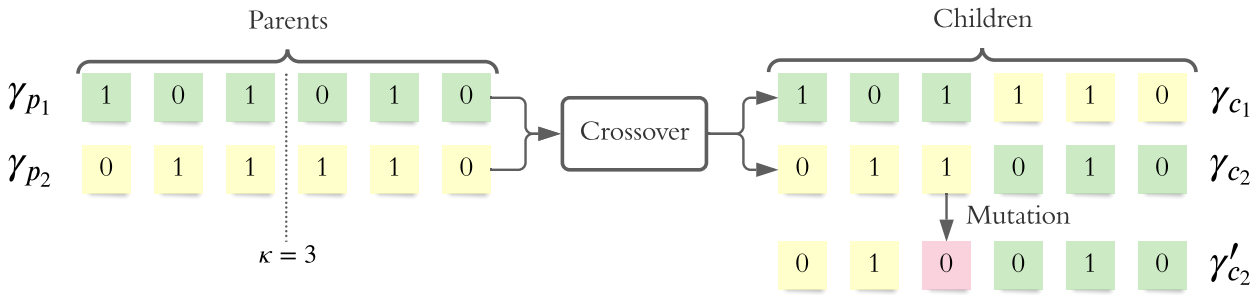

Figure 1.3: Crossover and mutation of chromosomes. Two parents, $\gamma_{p_1}, \gamma_{p_2}$, are nominated from the process in Fig. 1.2. They are then crossed-over via a one-point crossover with crossing point $\kappa = 3$, resulting in children candidates $\gamma_{c_1}, \gamma_{c_2}$. One child chromosome is mutated to yield a new candidate, γ'_{c_2}. The candidates added to the next generation are then $\{\gamma_{c_1}, \gamma'_{c_2}\}$.

1.1.4 *Candidate evaluation*

1.2 ADAPTATION TO QMLA FRAMEWORK

1.3 OBJECTIVE FUNCTIONS

1.4 APPLICATION

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 quantum Hamiltonian learning (QHL) is feasible on a personal computer in < 30 minutes for $N_e = 1000; N_p = 3000$.

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

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

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

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

exploration_strategy='AnalyticalLikelihood'
```

Listing A.1: "QMLA Launch scipt"

Figure	Exploration Strategy	Algorithm	N_E	N_P	Data
??	AnalyticalLikelihood	QHL	500	2000	Nov_16/14_28
??	DemoIsing	QHL	500	5000	Nov_18/13_56
??	DemoIsing	QHL	1000	5000	Nov_18/13_56
??	DemoIsing	QHL	1000	5000	Nov_18/13_56
??	IsingLatticeSet	QMLA	1000	4000	Nov_19/12_04
3***??**	IsingLatticeSet	QMLA	1000	4000	Sep_30/22_40
	HeisenbergLatticeSet	QMLA	1000	4000	Oct_22/20_45
	FermiHubbardLatticeSet	QMLA	1000	4000	Oct_02/00_09

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

B

EXAMPLE EXPLORATION STRATEGY RUN

A complete example of how to run the ;sqmla framework, including how to implement a custom ES, and generate/interpret analysis, is given.

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