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The Markov network fitness model

Alexander E.I. Brownlee, John A.W. McCall and Siddhartha K. Shakya

Abstract Fitness modelling is an area of research which has recently received much interest among the evolutionary computing community. Fitness models can improve the efficiency of optimisation through direct sampling to generate new solutions, guiding of traditional genetic operators or as surrogates for a noisy or long-running fitness functions. In this chapter we discuss the application of Markov networks to fitness modelling of black-box functions within evolutionary computation, accompanied by discussion on the relationship between Markov networks and Walsh analysis of fitness functions. We review alternative fitness modelling and approximation techniques and draw comparisons with the Markov network approach. We discuss the applicability of Markov networks as fitness surrogates which may be used for constructing guided operators or more general hybrid algorithms. We conclude with some observations and issues which arise from work conducted in this area so far.

1 Introduction, motivation and alternatives

The end-goal of an evolutionary algorithm is usually efficient optimisation. Fitness modelling [20] is one of the many techniques which can support this goal, by reducing overall run-time or by simplifying the problem in some way.

Previous work including [4, 51, 52, 50] has described a number of approaches using undirected probabilistic graphical models (Markov networks) within a framework called Distribution Estimation Using Markov networks (DEUM), an Estimation of Distribution algorithm [24]. With the Markov network approach model-

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building overhead is significant, particularly as the number of variables and interactions increases. While the number of function evaluations to reach an optimum were significantly fewer than with other algorithms in our earlier work the time taken to build and sample the probabilistic model was large. However, it has been found that the Markov network at the heart of DEUM represents a good model of fitness [5, 7], and this has been exploited in recent work [8] as well as providing an explanation for the previous good results.

The broader concepts of fitness modelling, approximation and surrogates [20, 26] have attracted much interest among the evolutionary computing community. A motivation for using fitness modelling within an evolutionary algorithm is to improve the efficiency of optimisation; this can be achieved in several ways. If evaluating the model is cheaper than evaluating the fitness function, it can be used to reduce overall run-time [21, 41, 57, 62, 31]. A model may be used where no explicit fitness function exists such as in evolutionary art and music [22]. Further, a fitness model may be employed to simplify the search by reducing noise [42, 58, 10] or smoothing a multimodal landscape [63].

Many approaches to fitness modelling exist. One common approach is artificial neural networks [21], with more recent examples including [57] and [14]. In [33] an algorithm groups individuals of similar fitness into classes that are then passed to Bayesian classifiers which can be sampled to generate individuals of high fitness. Schmidt and Lipson [48] use co-evolution to generate fitness predictors. In [12], an archive of already-evaluated solutions are fuzzily matched to new solutions, with fitness taken from the archive if matches are found. The Learnable Evolution Model (LEM) [32] incorporates machine learning to identify features distinguishing high and low fitness individuals. In [13], the authors report the use of a Gaussian random field meta-model as a surrogate in a $(\mu+\lambda)$ ES for single and multi-objective continuous problems with good results on a number of benchmarks.

Fitness inheritance (passing of fitness values from parents to offspring) to reduce the number of fitness evaluations [11, 56] is arguably a form of fitness modelling. A fitness model may also be used to guide standard genetic operators such as crossover and mutation as in [27, 1, 21, 40, 60]. Other hybrid approaches combine probabilistic models with different algorithms such as that described by [61, 36, 47]. In contrast to the use of undirected models in this chapter there has also been some work done using directed probabilistic graphical models for fitness modelling, such as that described as a variant of fitness inheritance in [38].

Polynomial regression or the fitting of a response surface has also been used to construct a model of fitness [64]. The Markov fitness model described in this chapter bears some similarity to this, in effect being a response surface for the fitness function.

Much of the above work concentrates on continuous fitness functions. The Markov fitness model described here models discrete functions and there are a number of related works with such functions. One of the earliest is [35], where the authors use a neural network to classify low and high fitness solutions with a bit-string encoding. In [65], the authors use a meta-model built using machine learning techniques (one example is genetic programming), also to classify high and low fitness

solutions having a bit-string encoding. Some approaches map the discrete function onto a continuous space: in [25], a radial basis function network is used as a surrogate for a mixed-integer search space. The model is used as a filter; too many offspring are created each generation and the model is used to choose promising ones which are evaluated with the true fitness function and retained. Similar to this, [59] proposes candidate over sampling in EBCOA [33]; generating too many solutions and trimming back to the number required. The authors found that picking the solutions predicted by the model to be less fit worked best. Their work looked at bit-string encoded functions and used machine learning approaches to infer rules distinguishing high and low fitness solutions.

Han and Yang [18] describe mapping discrete variables onto continuous ones to allow multiple linear regression for screening variables prior to optimisation. In [30], Gaussian processes are used for learning discrete fitness landscapes, demonstrated on Multidimensional Gaussian Landscapes and NK landscapes. Takahashi et al [58] use fitness estimation from a statistical model of the history of solutions to deal with noisy fitness functions; the example given is on a weight vector with discrete values. This builds on the earlier work with continuous functions in [42]. Finally, in [34] the author builds a surrogate from a Gibbs model which is derived from the distribution learnt by an EDA. This is demonstrated with both discrete and continuous benchmark functions.

Jin’s comprehensive 2005 review [20] presents a wider survey of existing work in this area, and further recent developments can be found in [55].

2 Defining the model

Previous publications on DEUM including [54, 5] describe how a Markov network is used to model the distribution of energy across the set of variables in a bit-string encoded problem. In this section we summarise how the model is derived.

A Markov Network is a pair (G, Ψ) , where G is the structure and the Ψ is the parameter set of the network. G is an undirected graph where each node corresponds to a random variable in the modelled data set and each edge corresponds to a probabilistic joint dependency between variables. We say that two nodes connected by an edge are *neighbouring nodes*. A subset $K = \{X_{i1}, \dots, X_{ik}\}$ of k mutually-neighbouring nodes is termed a *k-clique*. Note that we include the empty set $\emptyset$ as a 0-clique and each singleton 1-clique $\{x_i\}$ in our definition of clique.

The Hammersley-Clifford Theorem states that the joint probability distribution of a Markov Network factorises as a Gibbs Distribution, completely determined by a set Ψ of parameters, each of which is a real number α_k that defines the energy contribution from clique k .

The precise form of the Gibbs Distribution is given in equation (1):

$$p(x) = \frac{e^{-U(x)/T}}{Z} \quad (1)$$

where,

$$Z = \sum_{y \in \Omega} e^{-U(y)/T} \quad (2)$$

Here, the numerator, $e^{-U(x)/T}$, represents the likelihood of a particular configuration x of the variables. The denominator, Z , is the normalising constant computed by summing over the set Ω of all possible configurations (note Z is never computed in practice). $U(x)$ is an *energy function* computed by summing contributions calculated from the values that x takes on each clique. Thus this exponentiated sum gives a factorisation of the distribution based on the structure G . We will consider the energy function in more detail shortly. T is a temperature constant which controls the ruggedness of the probability distribution.

The key idea of the DEUM EDA is to model solution fitness as a mass distribution that equates to the Gibbs distribution as shown in equation (3):

$$p(x) = \frac{f(x)}{\sum_{y \in \Omega} f(y)} = \frac{e^{-U(x)/T}}{Z} \quad (3)$$

Sampling this distribution will generate high fitness individuals with high probability. We now explain how the DEUM algorithm estimates this distribution.

Identifying corresponding terms in the numerator and denominator gives, for each solution $x = \{x_1, x_2, \dots, x_n\}$, the following negative log relationship between $f(x)$ and $U(x)$:

$$-\ln(f(x)) = U(x) \quad (4)$$

Let structure G contain a set of cliques $K = \{K_1, \dots, K_m\}$. Then, for any solution $x = \{x_1, x_2, \dots, x_n\}$, $U(x)$ has the form:

$$U(x) = \sum_i \alpha_i V_{K_i}(x) \quad (5)$$

The V_k are the characteristic functions of a Walsh decomposition of the fitness function. Walsh functions [3, 15, 16, 17] are a set of rectangular waveforms taking two amplitude values, +1 and -1. Similar to the use of Fourier transforms representing for analogue waveforms, Walsh functions may be combined linearly to represent any fitness function based on a bit-string representation.

The $V_K(x)$ for each clique K are defined in (6) to (8).

$$K = \emptyset \quad V_{\emptyset}(x) \equiv 1 \quad \forall x \quad (6)$$

$$K = \{i\} \quad V_i(x) = \begin{cases} 1 & x_i = 1 \\ -1 & x_i = 0 \end{cases} \quad (7)$$

$$\text{For } K \subseteq \{1, \dots, n\}, \quad |K| \geq 2, \quad V_K(x) = \prod_{i \in K} V_i(x) \quad (8)$$

Thus the energy function, and hence the fitness, is completely determined by the parameters α_i . The α_i are non-zero only for cliques present in the structure G . Given a sufficiently-sized population of solutions and their fitnesses, equations (4) and (5) yield a system of equations in the parameters that can be solved using a least-squares approximation to estimate the distribution. [50] describes how singular value decomposition [39] is used for this.

Of principle interest here is that, once the parameters are determined, we can combine (4) and (5) to obtain a model of the fitness function:

$$-\ln(f(x)) = \sum_i \alpha_i V_{K_i}(x) \quad (9)$$

We call this the *Markov Fitness Model* (MFM) of f . We now proceed to discuss how the quality of the model may be measured before moving on to applications.

2.1 Model quality and the fitness prediction correlation

Given the relationship in (9), it is possible to extrapolate information about the fitness function and in particular the optimal solution by looking at the values given to the model parameters α_i . Minimising the energy of a solution is equivalent to maximising fitness. For the univariate terms this means that a positive α_i will require a negative value for $V(x_i)$ to minimise the energy contribution from that term. This equates to x_i (the i th bit) being set to 0. Likewise, a negative α_i value indicates the i th bit should be set to 1 to minimise the contribution from that term. For bivariate terms, a positive α_{ij} value indicates that the two bits x_i and x_j associated with it should be opposite in value, to minimise the contribution from the term involving $V(x_{ij})$. Similarly, a negative α_{ij} indicates that they should take the same value. This principle can be further extended to multivariate terms.

In [9] such analysis of MFM coefficients revealed a clear relationship with properties underlying the fitness function. This was despite having used a very small number (120) of function evaluations. Fitness was modelled for a bio-control problem, where bits set to 1 indicated times that nematode worms should be applied to a mushroom crop for control of the pest sciarid fly. The coefficients pointed towards application of the nematodes at points which matched the lifecycle of the fly larvae. Analysis of univariate and bivariate model coefficients for a number of further fitness functions was conducted in [4] and reinforced this finding.

The relationship between model coefficients and the global optimum is further illustrated here for the Checkerboard problem [2, 24]. The objective for this is to realise a grid with a checkerboard pattern of alternating 1s and 0s; each 1 should be surrounded by 0s and vice versa, not including corners. Interactions occur between neighbours on the lattice without wrapping around at the edges. The 2D lattice structure for a 25-bit instance of the problem is illustrated in Figure 2. We constructed the MFM using the perfect structure for the problem (that is, *univariate* terms for each variable X_i and *bivariate* terms for each neighbouring pair of variables $X_i X_j$

Fig. 1a Univariate alpha coefficients for 2D checkerboard

Fig. 1b Bivariate alpha coefficients for 2D checkerboard

on the lattice) and the model parameters were estimated using the fittest 220 solutions from a randomly generated starting population of 300 solutions. This process was repeated for 100 random starting populations, and the mean and standard deviation for each coefficient value over the 30 runs was computed. The coefficient values for the univariate and bivariate terms are illustrated in Figures 1a and 1b respectively. The univariate alphas are all close to zero: this is because there are two global optima which have complementary bits set to 1 and 0, so the model does not bias individual variables towards one value. The bivariate alphas are all positive, indicating that neighbouring variables should be opposite in value. Of particular interest is that several of the bivariate alpha values are approximately double the magnitude of the others. The higher alpha values correspond to the interactions in the middle of the lattice (that is, neither of the variables they are associated with is on the edge of the checkerboard); these are dashed in Figure 2. These have a greater

Fig. 2 Model structure for 25 bit 2D Checkerboard Problem - numbers beside interactions correspond to those on the horizontal axis in Figure 1b. Note that the dashed interactions match the coefficients with a higher magnitude.

Algorithm 1 Calculation of fitness prediction correlations

```

1: Generate random initial population  $p$ 
2: Evaluate  $p$  using the fitness function and select a subset  $\sigma_1$  of  $p$ 
3: Use  $\sigma_1$  to estimate MFM parameters
4: for all individuals in  $\sigma_1$  do
5:   Mutate one bit in the individual
6:   Use MFM to predict fitness of individual
7:   Use fitness function to determine true fitness
8: end for
9: Calculate the correlation coefficient between the predicted and true fitnesses ( $C_m$ )
10: Generate random population  $\sigma_2$  equal in size to  $\sigma_1$ 
11: for all individuals in  $\sigma_2$  do
12:   Use MFM to predict fitnesses
13:   Use fitness function to determine true fitness
14:   Calculate the correlation coefficient between the predicted and true fitnesses ( $C_r$ )
15: end for

```

influence on fitness than those near the edge because if they break the constraint of neighbours not matching, their neighbours will also be affected. Thus we can see that the model places greater importance on these alphas. This shows that the MFM provides us with more information about the fitness function than simply pointing us in the direction of the global optimum.

A quantitative measure of model quality is also useful and the *Fitness prediction correlation* (FPC) [5] serves this purpose. This measures the MFM's ability to predict the fitness of unseen solutions. It is the Spearman's rank correlation [28] between the set of true fitnesses and fitnesses predicted by the model of an unseen population. Rank correlation is used because for discrete optimisation, it is only necessary to rank individuals in order of relative fitness. Predicting fitness is simply a reversal of the process used to estimate the α_K ; the variable values for a solution being substituted into (9).

[7] defines two variants of FPC – C_m and C_r . C_r measures fitness prediction capability for randomly generated individuals; it follows that if this high then the MFM closely models the general fitness function. C_m measures fitness prediction capability for solutions neighbouring the current population, which is important for using the model to guide operators such as mutation. C_m and C_r are calculated by following Algorithm 1.

Given the right conditions (particularly when the model structure closely matches the non-zero components of the Walsh expansion of the fitness function, and large population), FPC values for the MFM can be close to 1 [5, 7, 6, 4]. This indicates a strong correlation between predicted and true fitnesses for complex problems such as Ising and MAXSAT. This explains the success of the optimisation approaches using the MFM described in the next section.

3 Applications

There are several ways to exploit the model of fitness in the MFM. Within DEUM, direct sampling is used to generate new solutions with a high probability of being high in fitness [54, 53, 5]. This direct sampling of the fitness model rather than the fitness function has the benefit that the model can make the problem easier for the search part of the algorithm – the smoothing effect described in [63]. For example, in [54], it was found that directly sampling solutions from the MFM rather than the true fitness function for 2D Ising increased the success rate of a bitwise Gibbs sampler from 87% to 99%. It was concluded that by using a real-valued search space within the MFM rather than the discrete values within the fitness function, the fitness landscape was altered to allow the algorithm to escape being trapped within plateaux, leading to more efficient searching of the landscape.

3.1 MFM-GA

[8] proposes MFM-GA, applying the MFM as a surrogate in a genetic algorithm. The model is constructed at the start of the run, then the GA samples evaluations exclusively from the model. A number of benchmark functions were used as a proof-of-concept, then the algorithm was applied to a computationally expensive fitness function – feature selection for case-based reasoning. Promising results were reported, with a significant reduction in overall run-time over a GA. A major issue with the approach is that the model is only constructed once, making MFM-GA sensitive to modelling errors, with the result that the optimisation could not find solutions as fit as the GA. However, the solutions found were fitter than those found using a CBR-specific optimiser and represent something of a compromise between finding the fittest solution and a short run time.

3.2 Guided local search

A previously unpublished approach is to use the MFM as a fitness surrogate for a local search; allowing the local search many iterations without consuming many fitness evaluations. The MFM is used to filter solutions for evaluation by the true fitness function; this is similar to the approaches in [25, 13, 59].

This was applied with some success to the Huygens probe problem [29], part of a competition at the 2006 Congress on Evolutionary Computation (CEC). The objective of the problem is to find the lowest point on each of a series of 20 “moons” – fractal landscapes that are wrapped in both x and y dimensions. For each moon an algorithm is restricted to 1000 probes (fitness evaluations).

A bit-string encoding of the coordinate values was used. The algorithm rebuilds the model around progressively smaller areas of the lunar surface, suited to the frac-

tal nature of the landscape (equal levels of detail at different zoom levels). Only univariate terms were included in the model; given that it is looking at neighbouring solutions to those used to build the model (those a short Hamming distance away), the results in Chapter 4 of [4] indicate that this should be enough to provide a reasonable fitness prediction capability. The workflow of the guided local search for this problem is given in Algorithm 2.

Algorithm 2 Guided Local Search

```

1: Generate random initial population  $p$  of size  $M$ 
2: while chosen proportion of the available fitness evaluations not completely used do
3:   Build univariate MFM modelling  $p$ 
4:   Truncation selection: select a subset  $\sigma$ , the fittest  $s$  individuals in  $p$ 
5:   for all individuals in  $\sigma$  do
6:     Generate  $m$  neighbours  $\mu$ :
7:     Convert bit-string into real valued coordinates
8:     Mutate values by up to a fixed amount (which decreases with each generation)
9:     Convert numbers back to bit-string
10:  end for
11:  Use MFM to predict fitnesses of  $\mu$ 
12:  Select predicted best  $l$  individuals  $\varsigma$  from  $\mu$ , calculate true fitnesses
13:  Take best  $M$  from combined pool of  $p$  and  $\varsigma$  and replace  $p$ 
14: end while

```

Once the algorithm terminated with a single best solution x , the remainder of the 1000 evaluations were used for an exhaustive search of the neighbours to x . The proportion of evaluations allocated to each stage fixed per run; in the first instance the guided local search was given 2/3 of the total, in the second it was given 3/4.

Results for this algorithm were compared with the others taking part in the CEC competition. Each algorithm was run on the same set of 100 randomly generated moons, with a central server providing fitness evaluations and performing comparisons between algorithms via a SOAP interface. The algorithm performed comparably with a number of well-known problem solvers such as evolutionary strategies (ES), memetic algorithms (MA) and simulated annealing (SA), coming in 9th and 11th out of 16 with the two configurations. Unfortunately no more data is available on the specific implementations of these algorithms; however, these results do show that the approach is competitive with a wide range of others on this black-box problem.

4 Issues affecting modelling capability

There are a number of factors which affect the quality of the fitness model, which also provide the grounding for future study.

4.1 Model building time

Of particular note is that the singular value decomposition used to estimate model parameters is $O(N^2m)$ complexity in the number of model coefficients N and the population size m , meaning that building the model becomes expensive for increasing problem sizes and complexities. In much of our work, the population has had to be large enough to be slightly over-specified ($m > N$), so the overall model building complexity is $O(N^3)$. This is comparable to other EDAs – for example hBOA is dominated by Bayesian network structure learning complexity of $O(kn^2m)$ [37], for problems of n variables which can be decomposed into subproblems of order k . Note however that for the MFM, the number of model coefficients N typically includes terms for each problem variable and for each interaction, so N is usually greater than the number of variables n in the problem, particularly for problems with many high-order interactions. A method of building the model incrementally or with multiple threads would help to mitigate this issue.

4.2 Model structure

The structure of the MFM strongly influences its fitness modelling capability; in [7, 4] we observed the impact on fitness prediction capability of removing different cliques from the model. It is known that not all interactions which are present in a problem will necessarily be required in the model for the algorithm to rank individuals by fitness and find a global optimum. This observation is related to the concepts of necessary and unnecessary interactions [19] and benign and malign interactions [23]. This is also related to spurious correlations [45], false relationships in the model resulting from selection. Much of our previous work with the MFM has used a fixed structure derived from the problem definition, but for black-box problems in particular, the structure is unknown and must be inferred by sampling the fitness function. Works describing structure learning techniques for Markov networks include [43, 44, 46, 49]; the issue of structure learning specifically for the MFM in DEUM is explored in [6] and [51]. Approaches have typically involved conducting dependency tests such as Chi-Square on pairs of variables, either using existing members of the population or generating new solutions by mutating specific variables. A deterministic clique-finding algorithm can then be run on the resulting graph to find higher order cliques.

We further explore the issue of model and problem structure in relation to fitness modelling in [7, 4]. There we introduce the terms *perfect* and *imperfect*; perfect referring to the ideal structure with exactly the same interactions as present in the fitness function and imperfect referring any other structure.

4.3 Population size and selection

There is a clear and quantifiable relationship between the number of solutions present in the population used to estimate model parameters and the fitness modelling capability. In [7] and more extensively in [4], a number of experiments show the effect of structure, population size and selection on the fitness prediction correlation. As population size reaches, then exceeds, the number of parameters in the model, there is a sharp transition from near zero to strong positive correlation between model and fitness function, for a number of fitness functions including one-max, Ising, MAXSAT and Trap-k. An example is given in Figure 3. With imperfect structures the model can typically predict fitnesses of solutions neighbouring those in the training population, but not those of randomly generated solutions.

The MFM is a probabilistic distribution over the fitness function, so sampling the model produces solutions with a high probability of being high in fitness. This means that explicit selection is not required for building the model; however selection still plays a crucial role in improving the fitness modelling capability [7, 4]. This is particularly the case where the population is too small or the model structure is imperfect, where selection sharpens the information about fitness already present in the population.

5 Conclusion and future work

In this chapter we have explained how the MFM applies Markov networks to fitness modelling of discrete problems. This may be exploited by directly sampling the model to generate new solutions, or by using the model as a surrogate, predicting fitness of solutions and filtering out promising ones for evaluation. Population size, model structure and selection are important factors in establishing a good model of fitness. Further exploration of these factors will help us to build better and more

Fig. 3 FPC with increasing population size for 1000 bit onemax. Note the rapid increase in both FPC figures at the point where the population size exceeds 1001; the number of coefficients in the model for this problem (1000 univariate terms plus the constant).

useful models of fitness, and also provide better understanding of how fitness is distributed within a population, which will be of use to the wider EA community. Further, the MFM is currently limited to fitness functions having a binary representation. Extension to higher cardinality or continuous representations would result in a more generally applicable model of fitness; this could entail adding additional terms to the model for each possible value. Finally, improving the efficiency of the model building process will increase the number of situations where it offers an overall performance improvement.

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