Abstract

Heuristic optimisers which search for an optimal configuration of variables relative to an objective function often get stuck in local optima where the algorithm is unable to find further improvement. The standard approach to circumvent this problem involves periodically restarting the algorithm from random initial configurations when no further improvement can be found. We propose a method of partial reinitialization, whereby, in an attempt to find a better solution, only sub-sets of variables are re-initialised rather than the whole configuration. Much of the information gained from previous runs is hence retained. This leads to significant improvements in the quality of the solution found in a given time for a variety of optimisation problems in machine learning.

1. Introduction

Multivariate optimisation is of central importance in industry and is used for a range of problems from finding solutions which satisfy a set of constraints to training classifiers in machine learning. Despite the wide range of applications, nearly all of them involve finding an optimal assignment of a set of variables with respect to a cost function. An exact global optimum is, however, rarely required and is in general significantly more costly to find than a very good local optimum. Heuristic optimisers are therefore ubiquitous for many industrial application problems (Zhang et al., 2001; Likas et al., 2003; Burges et al., 2011).

A heuristic optimiser generally starts from a random configuration of variables and optimises this configuration until a local optimum is found. For a convex optimisation problem this optimum is also the global optimum and no further effort is required. However, problems which are considered NP-hard have in general exponentially many such local optima and hence the probability that a particular local optimum is also the global one is exponentially suppressed. Nevertheless, such problems often contain some amount of structure which makes their solution useful. This structure can be used to obtain configurations of a given cost much faster than random guessing. As such, each subsequent query to the cost function makes use of preceding queries to make a more informed guess of an optimal configuration.
Partial Reinitialisation for Optimisers

Figure 1. An illustration of the partial reinitialisation algorithm. On each level $l$, sub-sets of $k_l$ variables are reinitialised (black circles) such that $(k_m = N) > k_{m-1} > \ldots > k_0$. On the bottom level the $k_0$-optimal optimiser is called (yellow circles). Each level starts with the most optimal configuration of its parent and reinitialises a sub-set of $k_l$ variables before calling the optimiser on the next level (green arrows). Checkpoints of the most optimal configuration found are kept on each level with a flow from left to right (blue arrows).

A strategy that is frequently used to escape a local optimum is to restart the optimisation process from a new random initial configuration. Repeating this process multiple times, the local optimum with the lowest cost is then returned, which is with high probability better and with certainty no worse than the initial configuration. Although such restarts allow the optimiser to get out of local optima, different restarts are also completely decoupled from each other. That is, information which was learned about the structure of the problem in one restart is not passed on to the next and has to be relearned from scratch. Hence, this way of running an optimiser is effectively coarse grained random guessing, but where each guess is further improved towards a local optimum.

Here we introduce a general approach to address this problem which allows an optimiser to find the global optimum with high probability in a single run.

2. Algorithm

Let assume we have a heuristic which picks sub-sets of variables. Also, let us define $k_0$-optimality of an optimiser such that for any configuration it returns, reinitialising the variables in a typical sub-set smaller than $k_0$ found by this heuristic does not get the configuration out of the local optimum. That is, the optimiser would just return the same configuration again. However, reinitialising sub-sets of $k_1 > k_0$ variables may allow the optimiser to find a set of new local optima, some of which may be worse or better than the current one. Starting from $k_1 = k_0$, let increase $k_1$ until a better local optimum is reachable for a typical sub-set picked by our heuristic. If the current local optimum is good, that is, the number of better local optima is negligible, increasing $k_1$ further would only reduce the chance of finding a better local optimum. Hence, except in the very beginning of the optimisation process, the optimiser has a higher chance of finding a better local optimum after reinitialising sub-sets of only $k_1$ rather than $N$ variables, where $k_0 < k_1 \ll N$.

As sub-sets of $k_1$ variables are reinitialised and the optimiser called after each re-initialisation, the configuration becomes $k_1$-optimal with high probability and the chance of finding a better local optimum decreases. To prevent the optimiser from getting stuck in the $k_1$-optimum, sub-sets of $k_2 > k_1$ variables can be re-initialised. In turn, to get out of $k_2$-local optima, sub-set of $k_3 > k_2$ variables can be re-initialised and so on. Repeating this process iteratively, each time increasing the size of the sub-set until $(k_m = N)$, the configuration becomes $N$-optimal, which is the global optimum with high probability. This process can hence refine a local optimizer into a global optimizer. We call this approach partial re-initialisation with the following algorithm (see also Fig. 1).

Algorithm 1 Partial reinitialisation

- **Input:** current level $l$, number of reinitialisations $M_l$ and number of variables for each reinitialisation $k_l$

  - if $l = 0$ then
    - call heuristic optimiser on $x$
  - else
    - $x_0 \leftarrow x$
    - reinitialize sub-set of $k_l$ variables in $x$
    - for $i \in \{1 \ldots M_l\}$ do
      - call partial reinitialisation on level $l - 1$
    - end for
    - if $\text{cost}(x) > \text{cost}(x_0)$ then
      - $x \leftarrow x_0$
    - end if
  - end if

With $m$ levels in the hierarchy, the algorithm is started from the $m^{th}$ level. The configuration is denoted by $x$ and the checkpoints by $x_0$; the checkpoints are optimal configurations found thus far, to which the algorithm reverts if no improved configuration is found by partial reinitialization. At each level $l$, $M_l$ reinitialisations of $k_l$ variables are performed and $(k_m = N) > k_{m-1} > \ldots > k_0$. The complexity of a single run of the algorithm is hence $O(\prod M_l)$.

Not only the number of variables, but also the heuristic which picks the variables in a sub-set is important. The simplest approach is to pick variables at random. However,
if variables are chosen according to a problem-specific heuristic, the probability that re-initialising a sub-set of a given size leads to a more optimal configuration can be maximised. One approach is to pick sub-sets such that the optimality of variables within the set depends on the values of the other variables in the set as much as possible. This could increase the chance of getting out of a local optimum by reducing the number of constraints on the sub-set from the rest of the system.

If the outcome of the heuristic optimiser does not directly depend on the initial configuration, but also on a random seed, it could be used to optimise only the variables within a sub-set, while the other variables in the problem are kept fixed. Such an approach was employed in (Zintchenko et al., 2015) for finding ground states of Ising spin glasses with simulated annealing and showed significant speedup relative to conventional global restarts.

If the optimisation problem is over the space of continuous variables, the concept of partial reinitialisation can be extended to partially reinitialising each variable in addition to sub-sets of variables. That is, rather than setting a variable to a random value within a pre-defined domain, it can be perturbed by, for example, adding noise with some standard deviation \( \sigma \), that is

\[
x = \alpha x + (1 - \alpha)N(\mu, \sigma)
\]

where \( \mu \) is the mean and \( \sigma \) is the standard deviation of the distribution \( N \). Hence, we can either fully reinitialise sub-sets of variables, add small perturbations to all variables, or combine the two and partially perturb sub-sets of variables, which could further improve performance. For simplicity we use \( \alpha = 0 \) in the benchmarks below.

### 2.1. Choosing \( M_\ell \)

Although \( M_\ell \) can be chosen empirically to optimise the performance of an optimiser over a set of randomly chosen optimization problems, there is also a theoretical basis behind the choice. \( M_\ell \) should be chosen such that the probability of being in a local optima (with respect to reinitialisation of \( k_\ell \) variables from the input) is maximised. We call such a configuration probabilistically \( k_\ell \)-optimal.

If we require that the probability that a reinitialization of \( k_\ell \) variables does not improve the optimum is less than \( 1 - \delta \) and assert that the probability that a given reinitialisation improves the objective function is \( P \geq \epsilon \) then it suffices to take (Donmez et al., 2009)

\[
M_\ell \geq \lceil \ln(\delta) / \ln(1 - \epsilon) \rceil .
\]

Thus the values of \( \delta \) and \( \epsilon \) specify the value of \( M_\ell \) needed to conclude that the local optimum is probabilistically \( k_\ell \)-optimal within a margin of error. Furthermore, if we consider \( 1 - \epsilon \) to be a constant then only a logarithmic number of samples are needed to conclude with high probability that the value is \( k_\ell \)-optimal. If \( \epsilon \) is small on the other hand, such as in unstructured search, then the number of requisite reinitialisations can be exponential in the number of variables. Thus the value of \( \epsilon \) taken makes an implicit assumption about the structure and complexity of the problem.

### 3. Benchmarks

On a set of machine learning problems we study the advantage of partial reinitialisation compared to the standard full reinitialisation for finding optimum model parameters. These problems are picked from the ones with which we have most experience. The size of each problem was chosen to be large enough such that finding the optimal configuration is non-trivial using the respective standard algorithms.

It is worth noting that in machine learning, the local optimum is sometimes sufficient or even more desired than a global optimum due to overtraining (LeCun et al., 2015). However, as we show below, partial reinitialisation improves not only the quality of the final solution, but also the speed at which a local optimum of a given quality is obtained. Also, although in general more expensive, overtraining can be reduced by using the classification accuracy on random sub-sets of the training data as a cost function.

For simplicity we use only one level in the hierarchy between a full reinitialisation and calling the heuristic optimiser. That is, for each full reinitialisation, multiple reinitialisations of sub-sets of variables are performed. To maintain generality, we choose sub-sets at random for all benchmark problems.

The parameters in the benchmarks, such as the size of each subset (denoted by \( k_1 \)) and the number of partial reinitialisations (denoted by \( M_1 \)) which are done within each full reinitialisation, were manually optimised and are not the true optima for the respective performance metrics.

As a performance measure for each benchmark we use the most optimal cost obtained after a given elapsed time or number of iterations averaged over multiple runs with different random initial states. Elapsed time was measured on Intel Xeon E5-2660 v2 processors.

#### 3.1. Training hidden Markov models

Learning temporal patterns in a signal is of central importance in a wide range of fields including speech recognition, finance and bioinformatics. A classic method to model such systems is hidden Markov models (HMM), which are based on the assumption that the signal follows a Markov process. That is, the future state of the system depends solely on the present state without any memory of the past.
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This assumption turns out to be surprisingly accurate for many applications.

In discrete HMMs, which we will consider here, the system can be in one of $N$ possible states hidden from the observer. Starting from a discrete probability distribution over these states, as time evolves the system can transition between states according to an $N \times N$ probability matrix $A$. Each hidden state can emit one of $M$ possible visible states. The model is hence composed of three parts: the initial probability distribution of length $N$ over the hidden states; the $N \times N$ transition matrix between hidden states; the $N \times M$ emission matrix from each hidden state into $M$ possible visible states. During training on a given input sequence, these matrices are optimised such as to maximise the likelihood for this sequence to be observed.

The standard algorithm for training HMMs is the Baum-Welch algorithm (Rabiner, 1989). It is based on the forward-backward procedure, which computes the posterior marginal distributions using a dynamic programming approach. The model is commonly initialised with random values and optimised to maximise the expectation of the input sequence until convergence to a local optimum. To improve accuracy, multiple restarts are usually performed. Over the sequence of restarts, we will investigate if partial reinitialisation can improve the convergence rate towards a global optimum.

As a benchmark we choose learning a random 128-bit string. Although artificial, this problem is very simple and has few free parameters. At the same time, finding a model which accurately represents the sequence is non-trivial starting from random transition and emission matrices. If the number of hidden states is at least as large as the length of the bit-string, the model can be trained until that bit-string is observed with certainty within the model. Here we will use two visible states and the same number of hidden states as bits in the input. For generality we do not impose any restrictions on the transition matrix.

Each full reinitialisation starts with random emission and transition matrices. In a partial reinitialisation only the elements in the matrices corresponding to a sub-set of hidden states are reinitialised. We found about 8000 reinitialisations of 8 variables within each global restart to be optimal and leads to a much more rapid increase in accuracy with training time than with full reinitialisations (see Fig. 2).

3.2. Clustering with k-means

Dividing objects into clusters according to a similarity metric is of central importance in data analysis and is employed ubiquitously in machine learning. Given a set of points in a finite-dimensional space, the idea is to assign points to clusters in such a way as to maximise the similarities within a cluster and minimise the similarities between clusters. Similarity can be defined in many ways, depending on the particular needs of the application. Here we use the Euclidean distance.

One of the most widely used algorithm for finding such clusters is the k-means algorithm (MacQueen, 1967). K-means searches for an assignment of points to clusters such as to minimise the within-cluster sum of square distances to the center. That is, it seeks to minimise the following

$$\sum_{i=1}^{K} \sum_{x \in C_i} (x - \mu_i)^2$$

where $K$ is the number of clusters, $C_i$ is the set of points assigned to cluster $i$, and $\mu_i$ is the mean of the points in cluster $i$.
cost function

\[ \sum_{i=1}^{k} \sum_{j \in C_i} \| x_j - \mu_i \|^2 \]

Starting from a random initialisation of centers, each iteration proceeds in two stages. First all points are assigned to the nearest cluster center. In the second part each center is picked to be the Euclidean center of its cluster. This is repeated until convergence to a local optimum. As the cost is never increased, convergence is guaranteed. It has been shown that there exists problems on which k-means converges in exponentially many iterations in the number of points (Vattani, 2011). The smoothed running time is, however, polynomial (Arthur et al., 2009) and it typically converges very quickly. Similar to the Baum-Welch algorithm, multiple global reinitialisations of centers are often performed to improve the quality of the clusters.

Our benchmark problem is set A3 in a standard clustering data set (clu, 2015). The clusters have points sampled from Gaussian distributions. There are 7500 points around 50 uniformly placed centres. Each full reinitialisation starts with an initial assignment of all centers to random points using Forgy’s method (Forgy, 1965). In a partial reinitialisation only a single cluster center is reinitialised. We found about 100 partial reinitialisations for each global restart to be optimal.

Except in the very beginning, a given quality of clusters is obtained significantly quicker with partial rather than full reinitialisation (see Fig. 3). The reason full reinitialisation is here more efficient at finding low quality clusters is because in the regime where the cost is high, larger strides in reducing the cost can be made by just random guessing than optimising a bad global restart with partial reinitialisations. However, as the cost threshold becomes harder to reach, partial reinitialisation quickly becomes more efficient.

### 3.3. Clustering with k-medoids

An often more robust approach, called k-medoids, for clustering data is to pick the best cluster center to be one of the points in the cluster rather than the Euclidean center. The standard algorithm for finding such clusters is partitioning around medoids (PAM) (Theodoridis & Koutrombas, 2006). Similar to the k-means algorithm, PAM iterates between assigning points to their closest center and finding the best center of each cluster until convergence.

As the centers are constrained to the positions of the points and no cluster assignment can occur twice during a run, the trivial upper bound on the number of iterations until convergence is \( \binom{N}{k} \) for \( N \) points and \( k \) clusters. Similar to k-means, however, it typically converges very quickly.

The benchmark problem we use here is clustering 900 images of faces from the Olivetti database (fac, 2015a). This dataset has been used previously to benchmark a novel method, called affinity propagation (Frey & Dueck, 2007), for finding k-medoids clusters against PAM. Here we repeat this benchmark, but also compare to PAM with partial reinitialisations.

We chose to find 121 clusters as this was roughly the regime where affinity propagation had the largest advantage over k-medoids (Frey & Dueck, 2007). Within each global restart, we found that about \( 0.5 \cdot 10^3 \) reinitialisations of only a single randomly chosen cluster center is optimal. We use a pre-computed similarity matrix, available from (fac, 2015b), the entries of which are the pixel-wise squared distances between the images after some pre-processing.

Affinity propagation indeed quickly finds much better clusters than PAM with full reinitialisations. However, after some time PAM with partial reinitialisations finds even better clusters which keep improving even further with time (see Fig. 4). Full reinitialisation finds better clusters in the beginning for similar reasons as in k-means.

### 3.4. Training Boltzmann machines

Boltzmann machines are a class of highly generalizable models, related to feed-forward neural networks, that are have proven to be very useful for modeling data sets in many areas including speech and vision (Bengio, 2009; Hinton, 2002; Salakhutdinov & Hinton, 2009). The goal in Boltzmann machine training is not to replicate the prob-
ability distribution of some set of training data, but rather to identify patterns in the data set and generalize them to cases that have not yet been observed.

The Boltzmann machine takes the following form: Let us define two layers of units, which we call the visible layer and the hidden layer. The visible units comprise the input and output of the Boltzmann machine and the hidden units are latent variables that are marginalized over in order to generate the correlations present in the data. We call the vector of visible units \( v \) and the vector of hidden units \( h \). These units are typically taken to be binary and the joint probability of a configuration of visible and hidden units is

\[
P(v, h) = \frac{\exp(-E(v, h))}{Z},
\]

where \( Z \) is a normalization factor known as the partition function and

\[
E(v, h) = -v \cdot a - h \cdot b - v^T W h,
\]

is the energy. Here \( W \) is a matrix of weights that models the interaction between pairs of hidden and visible units, \( a \) and \( b \) are vectors of biases for each of the units. This model can be viewed as an Ising model on a complete bipartite graph that is in thermal equilibrium.

This model is commonly known as a Restricted Boltzmann Machine (RBM). Such RBMs can be stacked to form layered Boltzmann machines which are sometimes called deep Boltzmann machines. For simplicity we will focus on training RBMs since training deep Boltzmann machines using popular methods, such as contrastive divergence training, involves optimising the weights and biases for each layered RBM independently.

The training process involves optimising the maximum likelihood training objective, \( O_{ML} \), which is

\[
O_{ML} = \mathbb{E}_{v \in x_{train}} \left( \ln \left[ \mathbb{E}_h P(v, h) \right] \right) - \frac{\lambda \sum_{ij} W_{ij}^2}{2}, \tag{5}
\]

where \( \lambda \) is a regularization term introduced to prevent over-fitting. The exact computation of the training objective function is \#P hard, which means that its computation is expected to be intractable for large RBMs under reasonable complexity theoretic assumptions.

Although \( O_{ML} \) cannot be efficiently computed, its derivatives can be efficiently estimated using a method known as contrastive divergence. The algorithm, described in detail in (Hinton, 2002), uses a Markov chain algorithm that estimates the expectation values of the hidden and visible units which are needed to compute the derivatives of \( O_{ML} \).

Specifically,

\[
\frac{\partial O_{ML}}{\partial W_{ij}} = \langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_{model} - \lambda W_{ij}, \tag{6}
\]

Here \( \langle \cdot \rangle_{data} \) denotes an expectation value over the Gibbs distribution of (3) with the visible units clamped to the training data and the \( \langle \cdot \rangle_{model} \) denotes the unconstrained expectation value. The derivative with respect to the biases is similar. Locally optimal configurations of the weights and biases can then be calculated by stochastic gradient ascent using these approximate gradients.

As a benchmark we will examine small synthetic examples of Boltzmann machines where the training objective function can be calculated exactly. Although this differs from the task based estimates of the performance of a Boltzmann machine, we focus on it because the contrastive divergence

Figure 5. Training of Restricted Boltzmann Machine (RBM) with \( \lambda = 0 \) (left) absolute values of objective functions and (right) relative difference between mean \( O_{ML} \) and the “approximate global optima” found by maximizing \( O_{ML} \) over all experimental runs.

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training algorithm formally seeks to approximate the gradients of this objective function. As such the value of the training objective function is a more natural metric of comparison for our purposes than classification accuracy for an appropriate data set.

The training set consists of four distinct functions:

\[
x_1 = \begin{cases} 1 & j = 1, \ldots, [n_v/2] \\ 0 & \text{otherwise} \end{cases}
\]

\[
x_2 = j \mod 2, \quad \text{(7)}
\]

and their bitwise negations. In order to make the data set more challenging to learn, we add 10% Bernoulli noise to each of the training examples. One hundred training examples were used in each instance with a learning rate of 0.01 and $10^5$ epochs per reinitialization. We take the model to be an RBM consisting of 8 visible units and 10 hidden units. Finally, rather than reinitialising a fixed number of weights at each iteration we update each weight with a fixed probability. This formally differs from previous approaches, but performs similarly to reinitialising a constant fraction. Upon initialisation, each variable is drawn from a zero-mean Gaussian distribution.

We see in Figure 5 that partial reinitialization accelerates the process of estimating the global optima for contrastive divergence training. We find that the optimal probability of reinitializing a weight or bias in the BM is roughly 10%. We find that the optimal probability of the process of estimating the global optima for contrastive divergences training and the fact that it takes fewer epoches at each stage then it only takes 58 resets on average to obtain the same training objective function as the strategy that resets every variable attains with 1000 resets. Furthermore, we see evidence that suggests a possible polynomial advantage of the 10% strategy over the traditional random resetting strategy.

Strong regularization is expected to lead to a much simpler landscape for the optimisation since as $\lambda \to \infty$ the optimisation problem becomes convex. We find that for $\lambda = 0.01$ that the difference between the partial and total reinitialisation strategies becomes on the order of 0.01%. Although partial reinitialising 10% of the variables continues to be the superior method, these small differences could also arise solely from the stochastic nature of contrastive divergence training and the fact that it takes fewer epoches for the partial reinitialization to approach the local optima. It is evident from these benchmarks that partial reinitialization can substantially reduce the complexity of finding an approximate global optimum for Boltzmann machines. Consequently, we expect that this approach will also work for optimising Boltzmann training for large task-based problems such as MNIST digit classification. Similarly, these improvements should be able to be leveraged in other forms of neural net training, such as feedforward convolutional neural nets.

4. Conclusion

We introduced a general purpose approach, which we termed partial re-initialisation, to significantly improve the performance of an optimiser. We numerically explored comparisons to state of the art algorithms on a range of optimisation problems in machine learning and although we only used the most basic version of our algorithm, with a single additional level in the hierarchy and picking sub-sets of variables at random, the advantage over the standard full reinitialisation is substantial. We expect a hierarchy with multiple levels and with sub-sets picked according to more advanced problem-specific heuristics to lead to even further improvements.

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