

Experiments in Developing Discrete Particle Swarm Optimisers

Martin Gate

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Contents

I	Algorithms	3
1	Overview and Introduction	4
1.1	Setting the Scene	4
1.2	Architecture	5
1.2.1	More on the Direction of Interest	6
1.2.2	Implementation and Development	7
2	Set Particle Swarm Optimiser	8
2.1	Introduction	8
2.1.1	Continuous Case model	8
2.2	Set PSO	9
2.2.1	The Importance of Satisfying Constraint on Solutions	9
2.2.2	Generalised Link Between COP and SPSO	9
2.2.3	Heuristics	10
2.2.4	Reading Across from the Continuous Case	10
2.2.5	Completing the Particle Update	13
2.2.6	Grouping Swarm Particles	14
2.2.7	Finding the Global Best Particle	14
2.3	PSO types	15
2.3.1	CLPso	15
2.3.2	GPso	16
3	Cost Function Factory	17
3.1	Cost Function interface with SPSO	17
3.1.1	Catering for Changing a Set Item	18
3.2	Try Interface and Internals	18
3.2.1	Providing a Meaningful Interpretation of Parameters	19
3.2.2	Try Data and its Interface	19
3.3	Try Data Centric Cost Function and the Use of Stubs	19
3.4	Standard Cost Representation Cases for a Try	20
3.4.1	SFloatFun	20
3.4.2	FloatFun	22
3.4.3	IntFun	23

<i>CONTENTS</i>	2
II Miscellaneous Ideas	24
4 Statistics	25
4.1 Recursive formula for calculating expected values	25
4.2 Cost-function Value Representation	29
4.2.1 SFloatCostValue implementaation of CostValue . . .	29
4.3 Multi-linear functions and binary data probabilities	33
4.3.1 bivariate binary table polynomial representation	34
5 Parking Place	36

Part I

Algorithm Description and Justification

Chapter 1

Overview and Introduction

1.1 Setting the Scene

In many cases a complex organism in nature has a goal to survive well in a changing environment it does this by actuating various limbs or change of internal perception, exploring possible outcomes or revoking memories under the control of a nervous system to get a desired outcome. The degree of effort and lack of a expected result can be regarded as a *cost* that depends on the environment and sequence of actions/perceptions that it evokes. By analogy with robots, the current algorithm and computers the system can be regarded as finding *program* fragments to give good results most of the time so that it can respond effortlessly to changes of environment. Sometimes the program gives an unexpected costly outcome and the organism must modify the program. I believe such tweaking is done by directed random choice anything else such as deductive reasoning is really part of the program. Such choice is directed in the sense that it will be biased towards cases that worked in the past. As such the specific program-to-outcome cost is like a *cost function* but with some random fluctuation since the same program may produce different outcomes depending on unknown-to-the-system influence in the environment. The *program* in this context can be regarded in general as decoded *input* to the function that gives a cost, the input being a string of bits while the directed random choice is to be regarded as an *optimiser*; by its nature the optimiser cannot see into the workings of this function otherwise it would be part of the cost function; all it has is the cost associated with the input as a string of bits and the constraint that chosen input indeed gives a working program.¹

By its nature the input generated by the optimiser is discrete so the optimiser is strictly a combinatorial one, but is continuous to the extent that a small change in the string of bits *often* gives a moderate change in the associated cost or a jump to an alternative working solution.² This is an important requirement to ensure it works properly and puts a significant burden on the

¹in the algorithm a cost function tries to convert an arbitrary binary string to a meaningful input and gives it back to the optimiser.

²This leads to a thought that encoding should be mutable with an additional transformation by the optimiser which is independently tuned to find a better total encoding that reflects this requirement.

design of a cost function. In a sense the optimiser both innovates and finds solutions by flipping bits in the input string and can be quite competitive by effectively carrying out an *evidence based probabilistic binary search*.

The rest of this book will explore the relation between function and the above optimiser type, describing algorithms to implement them and hopefully eventually apply them to interesting cases that are models of systems that reflect real world behaviour.

1.2 Architecture

I think it helps to have a visual over view that is a cartoon of the software so far. Figure 1.2.1 gives my attempt to give this.

The examples are stored in the directory `github.com/mathrgo/setpso/examples` and consist of short code snippets that can be edited to change parameters. SPSO or SPO stands for Set-based Particle Swarm Optimiser loosely based on [KE95], although the current algorithms have been extended to deal with combinatorial problems, include shotgun randomisation to improve convergence and deals with noisy cost functions.

The PSOKit is a tool kit that runs the chosen optimiser or cost function, generating diagnostic output in the form of *Actions* where the environment is for the moment desk-top computer running the example. There are several optimisers, cost functions and Actions which are *always* referred in the toolkit by name. The user can generate new named versions as and when needed. Using names opens the door to future cost functions being able to refer additional components at run time although implementation at this moment is too restrictive. Code for the toolkit is in directory `github.com/mathrgo/setpso/psokit`.

The Cost Function receives a string of bits to convert into a bundle of components referred to as a *Try*, which can be a complex object containing a program. A Try is used and generated by the Cost Function, represented as a factory, which also carry out relative cost function comparisons of Try pairs, using a function call `CMP()`, represented by balancing scale, when required by the optimiser. There are two types of comparison one that compares cost represented by the \$ sign and a comparison of how frequently the try gives a better cost when compared with other tries and is represented by the rosette badge, which symbolises historic success of a try that is needed to deal with noisy costing.

A Try has a wrapper that provides an interface to the optimiser; examples are given in the directory `github.com/mathrgo/setpso/fun/futil` for different cost types. The wrapper also reduces the overhead of generating a new Cost Function and corresponding Try from scratch, such wrapped functions are given in the directory `github.com/mathrgo/setpso/fun`.

The optimiser is represented by a lightbulb and base; signifying that it is like an ideas generator; this is bourn out by the way in which the optimiser jumps to significantly better solutions in the matter of a few cycles preceded by a period of comparative smooth progress. The base SPSO provides most of the interface and search algorithms; it contains a list of interacting Particles, represented by Pac-Man figures. Each Particle maintains a list of Tries that compete to be the personal best for the Particle. If Cost Function is de-

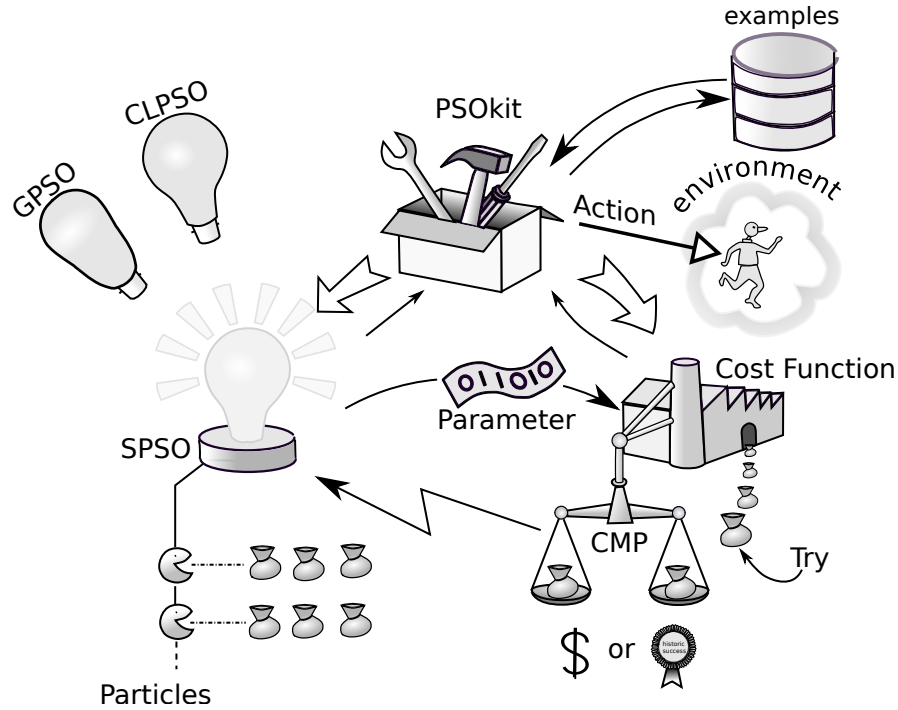


Figure 1.2.1: This provides a cartoon of the SPSO software giving an image of intended behaviour of system parts.

terministic then the list contains just one Try which is the current personal best. As depicted there is more than one optimiser represented by a different bulb shape. At the moment they differ only in the way Particles interact: GP50 stands for Global PSO where the Particles learn from the global best one; CLP50 stands for Comprehensive Learning PSO where a Particle learns from other Particle's best Try in a structured way to encourage more exploration. Alternative strategies can be easily coded using a few lines of code. At the moment optimisers are in github.com/mathrgo/setps0/setps0.go.

1.2.1 More on the Direction of Interest

The main interest is developing an optimiser for Machine Learning that bridges the gap between neural nets and more structure determining optimisers such as genetic algorithms. To do this the current work looks at combinatorial optimisation problems (COP) using discrete tuning parameters in the form of binary strings (BS) for particle state with a range of cost-function value types. Such a PSO will be called a Set PSO (abbreviated to SPSO) to emphasise that it interprets BS as sub sets to represent the parameters of SPSO.

the binary representation can be regarded as an encoding of algorithms or anything representable in a computer. For instance, by reinterpreting the

string as an encoding of a vector value the SPSO can be used to deal with (possibly low precision) continuous vector states as will be shown later on. It is hoped that the SPSO is powerful enough to be used as a general optimiser in this sense without knowing how the cost function is constructed. The idea is that because of its general nature it may take a lot of iterations to find a useful optimisation so general solutions in the form of learnt programs will need to be fed back into a list of things to try and thus accelerate finding optimisation of related cost functions using this bootstrap approach. Each solution with parameters could be encoded using a short binary string. How this is to be done in detail is intended to be part of SPSO use to be explored here.

Machine Learning Extensions

For Machine Learning there is a need to extend the basic SPSO to cope with:

1. noisy data mainly due to a restricted amount of available data when evaluating a cost-function.
2. represent continuous state such as design or neural net parameters by a set of discrete values some what similar to the way genetic algorithms deal with this by digitizing the continuous case.
3. treat random strings of bits as a way of generating useful programs to find optimising solutions which in turn can be used as a way of tuning meta parameters.
4. Acknowledge need to avoid over fitting and that only approximate solutions are needed.

1.2.2 Implementation and Development

The SPSO is developed mainly through biased intuitive analogy with other systems. As such it needs a programming language to explore empirically its properties and implement it. The language chosen is Golang. The treatment of SPSO here attempts to make the description language agnostic, however sometimes golang constructs such as interface are directly used to simplify the description of algorithms and help the user understand what the code is trying to do.

Chapter 2

Set Particle Swarm Optimiser

2.1 Introduction

2.1.1 Continuous Case model

Particle Swarm Optimisers (PSO) introduced in [KE95] have been developed to optimise problems with continuous tuning parameters. The PSO consists of a finite collection (called a swarm) of particles with current state (often called *Parameters*) x_t^i , personal best state p_t^i and velocity V_t^i ; where i is the particle index and t is the iteration index. These three properties of each particle are updated at every iteration using

$$V_{t+1}^i = \mu \left(x_t^i, V_t^i, N_t^i \right) \quad (2.1.1)$$

$$x_{t+1}^i = \xi \left(x_t^i, V_t^i \right) \quad (2.1.2)$$

$$p_{t+1}^i = \begin{cases} p_t^i & \text{if } x_{t+1}^i \notin \Omega \text{ or } F(p_t^i) < F(x_{t+1}^i) \\ x_t^i & \text{otherwise} \end{cases} \quad (2.1.3)$$

where $F(x)$ is the cost of the state x ; N_t^i is the collection of particles who's personal best states are targeted by the i th particle to update its velocity from iteration t to $t + 1$ and $i \in N_t^i$; Ω is a feasible subset of states usually characterised as satisfying a collection of constraints.

The PSO has several variants and the above description is a general summary where for continuous parameters the state is a d dimensional vector space of real numbers \mathbb{R}^d . Typically the velocity is made up from random multiples of the vector difference between x_t^i and personal best of members of N_t^i giving the swarms directions to go to look for improved $F(x)$ values. Also μ and ξ are not true functions since they depend on hidden random variables that are crucial for ensuring the ability to find a low cost near optimal personal best after sufficient iteration, but are otherwise processes that depend on the variables given as their arguments and personal best of members in N_t^i .

2.2 Set PSO

2.2.1 The Importance of Satisfying Constraint on Solutions

COP problems such as the Travelling Sales Person(TSP) have constraints defining Ω that must be satisfied if to be of any use so one must continuously ensure the candidate solution is in Ω before evaluating its cost ¹. Often feasible points Ω do not form an open subset of the space of states so a raw update of x_t^i will not give a feasible state most of the time. To cope with this ξ computes a raw update \tilde{x}_{t+1}^i which it then attempts to convert into a feasible one before being returned as a update. Sometimes this may not be possible and the returned x_t^i is not in Ω . As indicated in the update equation this results in no change to the personal best thus ensuring that personal bests are updated to only feasible states. To achieve a working alternative in Ω the cost function does this.

2.2.2 Generalised Link Between COP and SPSO

The link between COP and SPSO is forged by using binary strings to represent candidate algorithms which are obtained by decoding the string. I use the term algorithm to represent any method for finding approximate solutions to a COP problem including just providing an approximate solution with no use of an algorithm. I think decoding to an algorithm rather than just a solution gives the PSO significantly more expressive power to find approximate solutions. The structure of candidate solutions may not be the same as binary strings so several binary strings may map to the same solution. The resulting solution is then evaluated by the cost-function to give its cost value indicating how well the algorithm fits; this could include some cost regularising component such as the complexity of used algorithm; lower values being preferred to higher values as determined by `Cmp()` ². This procedure gives a mapping from a binary string to relative cost value of the binary string. The SPSO is used to learn a low cost global solution by using a swarm of proposed solutions to iteratively search for a low cost one.

Even in the case of a deterministic function it may be expedient to cut down on the evaluation time by only partially evaluating it thus introducing uncertainty. For instance the solution string may represent a *program* that has to be tested on a ridiculously large number of cases to give a perfect cost value in this case the cases are randomly chosen to test the solution and thus introducing uncertainty which is traded against speed of evaluation. The cost-function must determine to what extent two try solutions can be compared and feed this back to the SPSO via `Cmp()`. How this is done is mainly implemented by using convenience functions associated with the `Try` type being used.

For the moment we restrict the SPSO state to be at most N bits³. Each

¹Such a feasible states are in the code referred to as a `Try`, which embodies variables to help the Cost Function calculate cost of the `Try`.

²Note the optimiser has no visibility of the cost only relative cost provided by a general comparator `Cmp()` to be described later on.

³Internally `Try` parameter is represented as a positive `*big.Int` so most of the code does not need the restriction to a fixed number of bits. N is used mainly when initialising with random parameters.

binary string x can thus be regarded as a subset of integers in the range $1 \cdots N$ where $j \in x$ when $x[j] = 1$. To this extent each non zero bit represents the inclusion of some element with a feature and as such encodings that favour this interpretation is expected to do better using the following algorithms.

2.2.3 Heuristics

SPSO has a collection of heuristics for tuning the optimiser they are :

Name	Type	Value	Comment
Phi	float64	1.0	target shooting probability range.
Omega	float64	0.73	probability velocity factoring after target blur.
Lfactor	float64	0.15	target shotgun blurring factor.
Loffset	float64	2.0	target residual blur.
TryGap	in	100	used by the SPSO CLP _{so} to give minimum number of tries before doing something different.
Threshold	float64	0.99	threshold for acting on a comparison.
NTries	int	250	maximum number of un committed competing Tries stored in a particle.

At this point the heuristics will not mean much, but will be described in detail when they are first used. The table just gives a list of heuristics in one place together with their variable name.

2.2.4 Reading Across from the Continuous Case

In the following let $rand$ be a random number generator that produces a number in the range $0 \leq rand < 1$ for each use of it. Also let \neg be the logical negation and \leftarrow the assignment of left side to the right side of the arrow.

Semantic Reinterpretation of Notation

The notation for the continuous case can be now used where x_t^i is just a subset rather than a vector. The velocity is interpreted as a vector of probabilities where the j th component $V_t^i[j]$ is just the probability that $x_t^i[j]$ will flip during the update going from 0 to 1 or *vice versa*.

Adding up velocity contributions

The velocity is built up from several contributions, which will be described in detail below, so there is a need for a way of adding up the contributions. the velocity is an array of probabilities each component being regarded as independent so one is interested in how to add probabilities. direct adding of probabilities does not work because this can give values greater than 1; multiplying probabilities just leads to a value smaller than the probabilities being combined. A possible compromise is to combine the probabilities p_1 and p_2 as follows:

$$p_1 \dot{+} p_2 = p_1 + p_2 - p_1 p_2 \quad (2.2.1)$$

and for two velocities we define

$$(V_1 \dot{+} V_2)[j] = V_1[j] \dot{+} V_2[j] \quad \forall j \quad (2.2.2)$$

this is the method adopted although not the only one that could have been used. For instance taking the maximum value of the probabilities is popular and could be an alternative. the chosen operation (2.2.1) is called *pseudo-addition* since it has most properties of addition. This can be seen by putting

$$p_i = 1 - e^{-\xi_i} \quad (2.2.3)$$

and then noting that

$$p_1 \dot{+} p_2 = (1 - e^{-\xi_1}) + (1 - e^{-\xi_2}) - (1 - e^{-\xi_1})(1 - e^{-\xi_2}) \quad (2.2.4)$$

$$= 1 - e^{-\xi_1} e^{-\xi_2} \quad (2.2.5)$$

$$= 1 - e^{-(\xi_1 + \xi_2)} \quad (2.2.6)$$

so the mapping $p_1 \mapsto \xi_i$ is a homomorphism between $\dot{+}$ and $+$. In particular the pseudo-sum is commutative and associative.

Velocity Components for Directing Towards N_t^i

As for continuous case the velocity, as an indicator of the direction to go to find better solutions, is roughly increased along the difference between x_t^i and p_t^k for each $k \in N_t^i$. For the SPSO the difference is represented by the exclusive or of the corresponding subsets giving the difference:

$$del_t^{(i,k)} = x_t^i \oplus p_t^k$$

From this a velocity increment can be produced as $Vdel_t^{(i,k)}$ where

$$r(i, k) \leftarrow \phi rand \quad (2.2.7)$$

$$r_t^{(i,k)} \leftarrow \begin{cases} r(i, k) & \text{if } r(i, k) < 1 \\ 2 - r(i, k) & \text{otherwise} \end{cases} \quad (2.2.8)$$

$$Vdel_t^{(i,k)}[j] = \begin{cases} r_t^{(i,k)} & \text{if } j \in del_t^{(i,k)} \\ 0 & \text{otherwise} \end{cases} \quad (2.2.9)$$

the ϕ is a heuristic Phi for tuning how aggressively the velocity points towards the target particle k and here takes on a predetermined heuristic value between 0 and 2 (following tradition of continuous case). However, the velocity is limited to be in the range 0 to 1 since it is a probability of flipping, so values above 1 are reflected back. This doubles the density of $Vdel_t^{(i,k)}$ near 1 when $\phi > 1$. The treatment of how to cope with $r(i, k) > 1$ case is not well derived and alternatives such as limiting all such cases to 1 may be better. The velocity increment encourages movement to the target p_t^k by only contributing to the difference between x_t^i and p_t^k .

Shotgun Blurring of Targets

Typically there are a large number of elements (corresponding to dimensions in the continuous case) while the number of particles is kept to just a few say at most 30. This means the use of just the velocity contributions directed to targets will explore only a small subset of changes. In the continuous case this has been solved in [BM14] by adding a noise component to the velocity proportional to distance of particle from corresponding target, which effectively gives a *shotgun* effect. Further more this simple device makes the PSO converge to a local optimal solution.

For SPSO the distance is the Hamming distance between the particle and target given by

$$d_H(i, k) = |del_t^{(i,k)}| \quad (2.2.10)$$

where $|z|$ is just the number of elements in z . This gives a blurring velocity

$$b = rand(L_{factor}d_H(i, k) + L_{offset})/N \quad (2.2.11)$$

$$Vblur_t^{(i,k)}[j] = b \quad \forall j \quad (2.2.12)$$

where L_{factor} and L_{offset} are heuristics L_{factor} and L_{offset} used to tune the shotgun effect.

Inertia Term

A heuristic ω borrowed from the continuous case is an inertia term Ω that multiplies the velocity probability by a reducing factor to slow down the progress of a particle and stop the velocity terms from over saturation.

Using the multiplying operation is crude and simple, which may not be the best; mapping from pseudo-addition to addition given in Equation 2.2.3 suggests a more complex operation involving raising the probability of not flipping to some power. However, for the moment, simpler operation of multiplying which has the desired reduction of velocity is used here.

Combining the Velocity Contributions

these various contributions are combined to give

$$V_{t+1}^i = \omega \left(V_t^i + \sum_{k \in N_t^i} Vblur_t^{(i,k)} \right) + \sum_{k \in N_t^i} Vdel_t^{(i,k)} \quad (2.2.13)$$

where multiplying by ω multiply each component of the velocity by ω . In the continuous case ω just multiplies V_t^i ; in the discrete case blurring tends to saturate and mask the update that moves the solution in direction of targets, so ω is applied to this as well.

Updating to the Next Frame Using the Probabilistic Velocity

In the continuous case the raw update is given by adding the velocity component to the current state. For the SPSO case by analogy we use flipping to

give a raw update from the velocity, thus put for each component:

$$(V_{t+1}^i[j], \check{x}_{t+1}^i[j]) \leftarrow \begin{cases} (0, -x_t^i[j]) & \text{if } V_{t+1}^i[j] > rand \\ (V_{t+1}^i[j], x_t^i[j]) & \text{otherwise} \end{cases} \quad (2.2.14)$$

2.2.5 Completing the Particle Update

Once the raw state has been found each particle is reevaluated to find its personal best candidate. This starts by first reevaluating cost of personal best $F(p_t^i)$ since the cost function may have changed or further evaluations improve the cost estimate.

At this stage the raw state \check{x}_{t+1}^i may not satisfy the constraint so to keep things general a function `ToConstraint()`⁴ supplied by the cost-function interface is applied to attempt to make the raw state satisfy the constraint based on the raw state as a starting hint and the old state, x_t^i to facilitate this attempt. If it fails then revert back to the old state and nothing changes; thus:

$$\check{x}_{t+1}^i \leftarrow \text{ToConstraint}(x_t^i, \check{x}_{t+1}^i) \quad (2.2.15)$$

$$x_{t+1}^i \leftarrow \begin{cases} \check{x}_{t+1}^i & \text{if } \check{x}_{t+1}^i \in \Omega \\ x_t^i & \text{otherwise} \end{cases} \quad (2.2.16)$$

this gives an update that satisfies the constraints, Ω ⁵.

if the update x_{t+1}^i is \check{x}_{t+1}^i then it is a candidate for personal best; to describe how this is done we need to look at the comparison function `Cmp()` in more detail.

`Cmp()` always returns a real number and has two modes represented here by the two binary operators, \triangleright and \trianglerighteq . Given two Tries x and y $x \triangleright y$ gives a value between -1 and 1. $x \triangleright y = 1$ means that the cost of x is definitely greater than y while $x \triangleright y = -1$ means that x is definitely less than or equal to y in cost. Values between these extremes represent some uncertainty in the relative cost. $x \trianglerighteq y$ represents the credentials of y in the form of how likely y costs less than x . If $x \trianglerighteq y \geq 1$ then it is safe to replace x by y . If on the other hand $x \trianglerighteq y \leq -1$ it is safe to ignore y as a contender for a lower cost than x .

Each particle i maintains a set \mathcal{B}_t^i of personal best candidates, that does not include the current personal best Try of the particle; before carrying out any comparisons the members' costs are updated; then the SPSO looks for a better try in \mathcal{B}_t^i if it is not empty as follows:

$$z_*^i = \arg \max_{z \in \mathcal{B}_t^i} p_t^i \trianglerighteq z \quad (2.2.17)$$

$$\check{p}_t^i = \begin{cases} z_*^i & \text{if } \mathcal{B}_t^i \neq \emptyset \wedge p_t^i \trianglerighteq z_*^i > 1 \\ p_t^i & \text{otherwise} \end{cases} \quad (2.2.18)$$

$$\check{\mathcal{B}}_t^i = \begin{cases} \mathcal{B}_t^i - \{z_*^i\} & \text{if } \mathcal{B}_t^i \neq \emptyset \wedge p_t^i \trianglerighteq z_*^i > 1 \\ \mathcal{B}_t^i & \text{otherwise} \end{cases} \quad (2.2.19)$$

⁴in the code this function has a different interface to minimise the API but is used to achieve the same thing.

⁵where the initialisation of the state x_0^i is chosen to ensure it also satisfies the constraint. this is done by random selection until the application of `ToConstraint()` gives something that satisfies the constraint. Note during this operation the first argument will be the empty set and should be treated as a special case by the cost function.

Let θ be the Threshold heuristic, then

$$p_{t+1}^i \leftarrow \begin{cases} x_{t+1}^i & \text{if } \check{p}_t^i \triangleright x_{t+1}^i > \theta \\ \check{p}_t^i & \text{otherwise} \end{cases} \quad (2.2.20)$$

$$\mathcal{B}_{t+1}^i \leftarrow \begin{cases} \check{\mathcal{B}}_t^i \cup \{x_{t+1}^i\} & \text{if } \theta \geq \check{p}_{t+1}^i \triangleright x_{t+1}^i > -\theta \\ \mathcal{B}_t^i & \text{otherwise} \end{cases} \quad (2.2.21)$$

Finally if ν_{Try} is the heuristic NTries for the maximum number of elements in \mathcal{B}_{t+1}^i the Tries set is pruned by removing the worst case:

$$y_*^i = \arg \min_{y \in \mathcal{B}_{t+1}^i} p_{t+1}^i \triangleright y \quad (2.2.22)$$

$$\mathcal{B}_{t+1}^i \leftarrow \begin{cases} \mathcal{B}_{t+1}^i - \{y_*^i\} & \text{if } |\mathcal{B}_{t+1}^i| > \nu_{Try} \\ \mathcal{B}_{t+1}^i & \text{otherwise} \end{cases} \quad (2.2.23)$$

2.2.6 Grouping Swarm Particles

It is anticipated that the main things that improve the SPSO performance is change in heuristics and the method used to choose the target sets N_t^i . Further more it is expected that particles in the swarm will adopt specialist behaviour by belonging to a group of particles. To support this the swarm is partitioned into groups where each group of swarm particles has the same set of targets and heuristics. Groups are each given a name ⁶ to aid describing a group. To begin with there is one group called "root" which contains all particles. When a new group is formed the group's heuristics point to the "root" group so all group heuristics can be updated just by changing heuristics for "root" group. New groups are initially empty and are populated by moving swarm particles from other groups thus maintaining a partition of particle swarm. By default the heuristics are chosen to have useful values and need not be explicitly given. A future update will facilitate changing heuristic values.

2.2.7 Finding the Global Best Particle

After completing the personal best of each Particle one with the best scoring Personal Best is found by comparing using the cost operator \triangleright rather than \trianglerighteq since the personal best cost usually has been evaluated several times in the non deterministic case and so the cost value will have stabilised usually by internally taking an average cost value; where Try p_t^j is taken to be better than p_t^k if $p_t^j \triangleright p_t^k > 0$. This is done in two stages. First by finding the Group with best particle and then by finding the best Group and selecting the best particle from this group. This two stage process is done to support finding the best Group which may be of use when managing the targets N_t^i .

⁶Referring to groups by name is only used to set up a group and such a costly reference to a group is internally replaced by links from a particle to its group and indexing of group members by a group to be used during iterative updates

2.3 PSO types

everything in Section 2.2 is carried out each iteration with `PUpdate()` in `github.com/mathrgo/setpso/setpso.go` all that remains to have a working SPSO is a code snippet before calling this that determines N_t^i . At the moment there are two types. GPso and CLPso. Both cases are given in the above source code.

2.3.1 CLPso

CLPso is at the moment the preferred implementation it is a comprehensive learning SPSO that targets other personal best rather than just the global best Particle. As such it takes longer to converge but encourages searching for optional solutions.

Each i th particle has its own unique group and a probability $P_c(i)$ of looking for an alternative particles' personal best to target when given the opportunity. Where

$$P_c(i) = 0.5 + 0.45 \frac{e^{10i/(N-1)} - 1}{e^{10} - 1} \quad (2.3.1)$$

this equation is a copy from the continuous case given in [LQSB06]. Let ν_{MAX} be the heuristic TryGap. The idea is to stay with a fixed target for at least ν_{MAX} updates without improvement giving the particle a chance to find good solutions between where it's current best is and the current best of the chosen target particle. To do this the particle maintains a counter ν_t^i and last best try b_t^i . At the beginning $\nu_0^i > \nu_{MAX}$ forcing the target to be defined.

The target choice is calculated before invoking `PUpdate()` from SPSO which does the main update given the choice of target. Determining the Target is stateful, Figure 2.3.1 gives a diagram of the states. On entry to the update transitions are calculated and executed before executing the state related code.

Search-for-Better-Try state

The transitions are dealt with in order given by the exit number. It acts as the main arbiter and it executes $\nu_{t+1}^i = \nu_t^i + 1$ thus incrementing the count of number of contiguous cases where nothing significant has been found to give better cost. It also sets $b_{t+1}^i = b_t^i$ and $N_{t+1}^i = N_t^i$.

Record-Best-Try state

This records that a significant improvement has been found and sets the ν counter to zero thus making CLPSO continue with the same target:

$$b_{t+1}^i = x_t^i \quad (2.3.2)$$

$$\nu_{t+1}^i = 0 \quad (2.3.3)$$

$$N_{t+1}^i = N_t^i \quad (2.3.4)$$

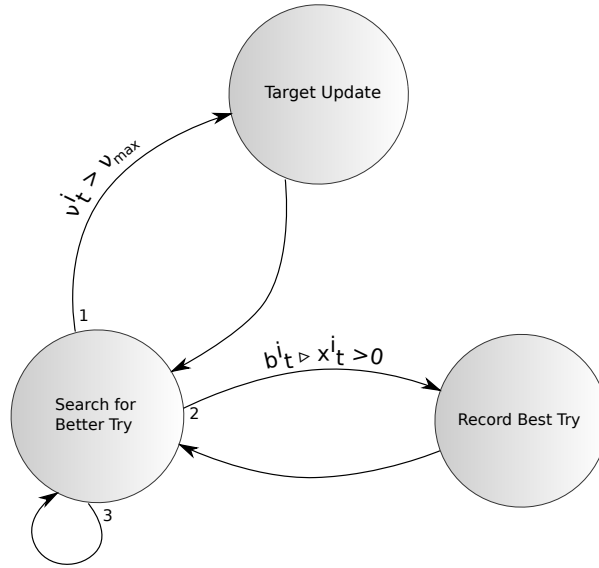


Figure 2.3.1: CLPSO Target determining state diagram. The Target is only changed when the chosen target fails to give improvement in v_{MAX} iterations.

Target-Update state

This decides on the next target and resets the search:

$$b_{t+1}^i = x_t^i \quad (2.3.5)$$

$$v_{t+1}^i = 0 \quad (2.3.6)$$

$$N_{t+1}^i = \begin{cases} \{P_s(i), i\} & \text{if } P_c(i) > rand \\ \{i\} & \text{otherwise} \end{cases} \quad (2.3.7)$$

where $P_s(i)$ is a randomised function based on a random choice of two particles k_1 and k_2 for each Particle as follows:

$$P_s(i) = \begin{cases} k_1 & \text{if } p_t^{k_2} \triangleright p_t^{k_1} > 0 \\ k_2 & \text{otherwise} \end{cases} \quad (2.3.8)$$

So $P_s(i)$ chooses the particle with personal best that gives a better cost result.

2.3.2 GPso

GPso was the first complete SPSO coded up where all particles belong to one Group and Group target is the particle with best personal best. This is the same choice of target as proposed for the original continuous PSO in [KE95]; it often gives more rapid convergence but is more easily stuck at a local minimum which is far from optimal.

Chapter 3

Cost Function Factory

3.1 Cost Function interface with SPSO

Cost function links up with a SPSO through a *golang interface* called `Fun` in github.com/mathrigo/setpso/setpso.go. The interface is as follows:

NewTry() *t Try* creates a new Try which is a pointer to a structure with a Try interface. A pointer is used so that as an argument in a function it can be modified by the function. As far as SPSO is concerned *t* is opaque apart from having a Try interface to be described later. *t* is ready to be used as a try with default Parameters that satisfy prevailing constraints. As such a try is a container of data that matches its Parameter.

SetTry() *t Try, z *big.Int* sets up *t* from Parameter *z*, where *z* is a Parameter assumed to satisfy constraints Ω and it also computes dependants such as cost etc. Note that a parameter is represented by a positive big integer and as such has the potential to have an arbitrary number of set elements.

Copy() *dest, src Try* sets the *dest* by copying *src* to *dest*. The copy is a deep copy and is independent of changes to *src* once the copy is done.

UpdateCost() *x Try* updates internal cost evaluation of a Try where a lower cost is better. this is needed when the cost changes or where a repeated cost evaluation is used to improve a cost estimate.

Cmp() *x, y Try, mode futil.CmpMode* float64 checks to see if *y* is better than *x* where it has the following modes:

futil.CostMode: `Cmp()` compares two tries returning a value that is $x \triangleright y$ with a spread of uncertainty from -1.0 to 1.0. It returns -1.0 for definitely $F(x) < F(y)$ and 1.0 for definitely $F(x) > F(y)$. A deterministic cost should always return -1.0 or 1.0 with a value of -1.0 if the costs are equal.

futil.TriesMode (used only when cost is not deterministic) `Cmp()` compares how successful *y* has been in being better than an *x*, updates

y 's success stats leaving x unchanged and returns $x \geq y$. While being compared a value > 1.0 indicates y should replace x ; a value < -1.0 indicates y should be removed as a candidate.

MaxLen() (*maxlen* int) maximum number of bits in the parameter big integer which is the maximum number of elements in the subset. At the moment this is fixed during a run but in the future could vary possibly to incorporate some form of subroutine use where subroutines are added to the list of items represented by the Try Parameter.

About() (*s* string) string giving a description of the cost function.

ToConstraint(*pre* Try, *hint* *big.Int) bool this attempts to give a constraint satisfying Try in *pre* that matches the Parameter, *hint*. On success **ToConstraint()** returns true otherwise it returns false and should leave *pre* unchanged. This function enables the SPSO to pass a Try Parameter to the cost-function factory in a form of a request to update *pre* if possible.

By convention *pre* always is a Try (apart from when it is the default one at the beginning) that was a personal best and thus satisfies the constraints required by the function to give a meaningful solution. The function should be able to find a constraint satisfying version for *hint* that approximates to *hint* most of the time so that the SPSO can frequently change the Particle's Parameter during an update.

Delete(*i* int) bool this hints to the function to replace the i^{th} particle-item. If it returns True the function has replaced the item with a new meaning thus modifying the decoder.

3.1.1 Catering for Changing a Set Item

This is an advanced feature for cost functions. Certain set items will after a while not be used to give personal best at which point a cost function can be hinted to remove this item through **Delete()** which returns true if the cost function does so. if the cost function returns true it is then up to the cost function to either replace this by a new item with its own contribution to cost or set the corresponding item in a hint to zero during a successful **ToConstraint()** call. in this way the cost function can try out alternative items that may result in an improved cost. Typically this feature is not used and a call to **Delete()** returns false.

3.2 Try Interface and Internals

Try is data associated with a Try Parameter that comprises a copy of the parameter, internal representation of a decoded version as TryData and a cost structure for recording cost related data. The following is the Try interface given in github.com/mathrigo/setpsso/fun/futil/futil.go:

Fbits() float64 returns floating point representation of cost as signed number of bits needed to represent cost as if an integer. This is used in plotting a cost with a logarithmic scale that works for positive and negative

values returning zero if the cost is zero. for a continuous cost $c = F()$ we have

$$fbits(c) = \text{sign}(c) \log_2(|c| + 1) \quad (3.2.1)$$

It must be remembered that, At least for the moment, `Fbits()` is never used by the SPSO optimiser and is only used for graphical output.

Parameter() `*big.Int` subset parameter used by Try.

Decode() `string` this gives a human readable interpretation of Try based on the internal decoding of the Parameter.

Cost() `string` this gives human readable cost details such as variance or mean value depending on the cost type.

Data() `TryData` decoded data part.

3.2.1 Providing a Meaningful Interpretation of Parameters

Representing a particle's Parameters as a binary string or subset may not be easily interpreted as a meaningful representation of a solution to a combinatorial optimization so the cost function must provide an easily understood description of a Parameter as a string supplied by the `Decode()` function.

3.2.2 Try Data and its Interface

Try Data with interface `TryData` is used to store useful variables value produced during decoding to the Try Parameter and is typically only visible to the Cost Function. Try Data effectively acts as a cache so that the Parameter does not have to be decoded every time the decoded representation is used often many times while evaluating cost. For instance if the decoded Parameter is a program it is evaluated several times on test data to give a cost. The `TryData` interface has just one public method:

Decode() `string` this gives a human readable description of the data.

As will be shown in Section 3.3 the main interface that has to be coded up for each Cost Function only needs to explicitly deal with the Try Data part of a Try and choice of standard stub to represent the type of cost being used by the Cost Function thus reducing the overhead of writing one.

3.3 Try Data Centric Cost Function and the Use of Stubs

the Cost Function interface given in operates at the level of Tries. Implementing this interface results in a lot of common code that only depends on the type of cost used by the Cost Function, while most of the operations specific to a Cost Function implementation involves manipulating Try Data; because of this the software supplies Cost Function stubs for each cost type that takes a Try Data manipulation cost function with the following interface in github.com/mathrgo/setpsso/fun/futil/futil.go :

CreateData() TryData creates an empty try data store for the decoded part of the try.

DefaultParam() *big.Int returns a default parameter which should satisfy constraints.

CopyData(dest,src TryData) copies try data from *src* to *dest*.

MaxLen() int maximum number of bits used in the try parameter.

About() string description of the function.

Constraint(pre TryData, hint *big.Int) (valid bool) attempts to update *hint* to give a constraint satisfying try parameter possibly with the help of *pre* which is assumed to be constraint satisfying. Note it is rare that *pre* is needed and *pre* should be not modified by this function.

Delete(i int) bool hints to the function to remove/replace the i^{th} item. Return true if the function decides to do this otherwise it returns false and does nothing.

IDecode(data TryData,z *big.Int) decodes the parameter *z* and stores the result in *data*.

Each Try Data manipulation cost function must have a specific **Cost()** method for calculating a cost based on Try Data. Under the heading of each cost type this will be referred to as the *cost interface*.

3.4 Standard Cost Representation Cases for a Try

Here is a description of each cost representation.

3.4.1 SFloatFun

This Try Data manipulation cost function is used when the underlying cost is float64 and has noise that can be removed by repeated evaluation of a cost and averaging the result with a forgetting time constant T_c to allow for a slow change in cost, possibly due to a change in the environment. Time is measured as the number of iterations. The cost interface and function stub creation are:

Cost(data TryData) float64 calculates the raw cost of the try using the decoded data, returning the cost.

NewSFloatFunStub(f SFloatFun, T_c , σ_M float64) *SFloatFunStub creates an instance of the SFloatFunStub ready for use as the interface setpso.Fun. T_c is the initial try cost update time constant; σ_M is a acceptance margin used in the assessment of a Tries comparison using \supseteq .

code is in github.com/mathrigo/setpso/fun/futil/sfloat.go, and corresponding Try type is SFloatTry.

Each Try *x* maintains cost related variables. In the following we will refer to these variables without referring to *x* unless there is a need to do so. A Try

has a forgetting factor α so if one take measurements a_i, a_{i+1}, \dots the sum of these measurements up to n using the forgetting factor is

$$S_n(a) = \sum_{k=i}^n a_k \alpha^{n-k} \quad (3.4.1)$$

$$= \alpha S_{n-1}(a) + a_n \quad (3.4.2)$$

where we take $a_{i-1} = 0$. The influence from the past decays as α^{n-k} so the decay is exponential with time constant T_c if

$$\alpha^{n-k} = e^{-(n-k)/T_c} \quad (3.4.3)$$

so

$$\alpha = e^{-1/T_c} \quad (3.4.4)$$

$$\cong 1 - 1/T_c \quad (3.4.5)$$

in the algorithm time constant is large so we adopt the approximate version (3.4.5) to avoid taking exponential. for notational convenience put

$$S_n = \sum_{k=i}^n \alpha^{n-k} \quad (3.4.6)$$

$$= \alpha S_{n-1} + 1 \quad (3.4.7)$$

then we see that if we have sequence of independent measurements of raw cost c we get

$$mean = \frac{S_n(c)}{S_n} \quad (3.4.8)$$

is an unbiased estimate of the mean cost when the statistics is fixed, this is used to compare with other tries as an ongoing value for the cost $F()$. When the Try is initialised with a Parameter, *mean* is set to the raw cost and uses above recursion when updated with additional raw costs. this gives an estimate of cost that improves after each update up to a point limited by the time constant T_c .

For comparison $x \triangleright y$ returns 0.5 if $F(x) > F(y)$ otherwise it returns -0.5. This indicates to SPSO that the comparison is uncertain and forces SPSO to look at $x \triangleright y$ to compare two costs. when this happens x is usually a personal best and the Try y starts to record the success sequence \mathbf{k} and the comparison sequence \mathbf{n} . where $\mathbf{k}_t = 1$ when a comparison gives $F(x_t) > F(y_t)$ for some x and is zero for other comparisons. Similarly $\mathbf{n}_t = 1$ for each such comparison. Allowing for the forgetting factor we get the frequency counts:

$$k_t = S_t(\mathbf{k}) \quad (3.4.9)$$

$$n_t = S_t(\mathbf{n}) \quad (3.4.10)$$

This is then used to calculate an estimate of the probability that $F(x) > F(y)$ as PT .

$$PT_t = \frac{k_t + 1}{n_t + 2} \quad (3.4.11)$$

this is the Bayesian estimate with a probability prior uniformly distributed used to avoid misplacing the estimate when there is only a few measurements. $x \succeq y$ is meant to be a score of how likely $F(x) > F(y)$ is based on PT . Let σ_M be the confidence that a random sequence giving PT would be within σ_M standard deviations of $1/2$ we get using Wald's approximation such a random sequence would be within

$$PT_t \pm \sigma_M \sqrt{\frac{PT_t(1 - PT_t)}{n_t}} \quad (3.4.12)$$

so to ensure y is better than x to within σ_M certainty we need

$$PT_t - \sigma_M \sqrt{\frac{PT_t(1 - PT_t)}{n_t}} > 1/2 \quad (3.4.13)$$

this is equivalent to

$$s_t = \frac{n_t r_t}{\sigma_M^2} > 1 \wedge PT_t > 1/2 \quad (3.4.14)$$

$$r_t = \frac{(PT_t - 1/2)^2}{PT_t(1 - PT_t)} \quad (3.4.15)$$

this in turn is equivalent to

$$\epsilon_t = PT_t - 1/2 \quad (3.4.16)$$

$$r_t = \frac{\epsilon_t^2}{1/4 - \epsilon_t^2} \quad (3.4.17)$$

$$s_t = \frac{n_t r_t}{\sigma_M^2} > 1 \wedge \epsilon_t > 0 \quad (3.4.18)$$

from this we get an appropriate score

$$x \succeq y = \begin{cases} s_t & \text{if } \epsilon_t > 0 \\ -s_t & \text{otherwise} \end{cases} \quad (3.4.19)$$

which is used by the algorithm to give a credentials score.

3.4.2 FloatFun

This Try Data manipulation cost function is used when the underlying cost is `float64` and the computed cost is a deterministic function of the Try Parameter. The cost interface and function stub creation are:

Cost(*data* TryData) float64 calculates the raw cost of the try using the decoded data, returning the cost as $F()$.

NewFloatFunStub(*f* FloatFun) *FloatFunStub creates an instance of the FloatFunStub ready for use as the interface `setpso.Fun`.

code is in `github.com/mathrigo/setpso/fun/futil/float.go`, and corresponding Try type is `FloatTry`.

3.4.3 IntFun

This Try Data manipulation cost function is used when the underlying cost is `*big.Int` and the computed cost is a deterministic function of the Try Parameter. The cost interface and function stub creation are:

Cost(*data* TryData, **cost** *big.Int) calculates the raw cost of the try using the decoded data, returning the result in cost as $F()$.

NewIntFunStub(*f* IntFun) *IntFunStub creates an instance of the IntFunStub ready for use as the interface setpso.Fun.

code is in `github.com/mathrigo/setpso/fun/futil/int.go`, and corresponding Try type is IntTry.

Using Big Integer

Big integer cost values are used to include some of the difficult cases in combinatorial optimisation, although the chance of finding global best solutions to these problems is minimal; however, The algorithms are expected to produce good useful approximations to these hard problems; I would like to suggest that main area of application is *machine learning where one is interested in good approximate minimisation solutions of difficult problems*.

Part II

Miscellaneous Ideas

Chapter 4

Statistics

4.1 Recursive formula for calculating expected values

Let S be a finite set and $P : 2^S \rightarrow [0, 1]$ be the probability of subsets of S . Let b_i be a sequence of independent samples of subsets of S representing P .

For a subset $A \subset S$ and a map $g : 2^A \rightarrow \mathbb{R}$ we can get a sequence of estimates of expected values

$$\mathbb{E}_n[g \parallel A] = \frac{1}{n} \sum_{i=1}^n g(b_i \cap A)$$

of

$$\mathbb{E}[g \parallel A] = \sum_{B \subset S} P(B)g(B \cap A)$$

which just calculates the expected value of g acting on subsets of A . The double bar notation \parallel is used to indicate that we are looking on to the probability distribution through the sub set window A . Now for $n > 1$

$$\mathbb{E}_n[g \parallel A] = \left(1 - \frac{1}{n}\right) \mathbb{E}_{n-1}[g \parallel A] + \frac{1}{n}g(b_n \cap A)$$

we can generalise this to the sequence

$$\check{\mathbb{E}}_n[g \parallel A] = (1 - \lambda_n) \check{\mathbb{E}}_{n-1}[g \parallel A] + \lambda_n g(b_n \cap A)$$

with

$$\check{\mathbb{E}}_1[g \parallel A] = g(b_1 \cap A)$$

taking expected values and putting $\check{\mathbb{E}}_n[g \parallel A] = \mathbb{E}[\check{\mathbb{E}}_n[g \parallel A]]$ we get

$$\check{\mathbb{E}}_n[g \parallel A] = (1 - \lambda_n) \check{\mathbb{E}}_{n-1}[g \parallel A] + \lambda_n \mathbb{E}[g \parallel A] \quad (4.1.1)$$

$$= (1 - \lambda_n) \mathbb{E}[g \parallel A] + \lambda_n \mathbb{E}[g \parallel A] \quad (4.1.2)$$

$$= \mathbb{E}[g \parallel A] \quad (4.1.3)$$

by induction on n . So even this sequence is an unbiased estimate of the expected value. The important thing is to check for variance. We have

$$\begin{aligned}
 \mathbb{E} \left[\left(\check{\mathbb{E}}_n[g \parallel A] - \mathbb{E}[g \parallel A] \right)^2 \right] &= \mathbb{E} \left[\left(\check{\mathbb{E}}_n[g \parallel A] \right)^2 \right] - 2\mathbb{E} \left[\check{\mathbb{E}}_n[g \parallel A] \right] \mathbb{E}[g \parallel A] + \mathbb{E}[g \parallel A]^2 \\
 &= \mathbb{E} \left[\left(\check{\mathbb{E}}_n[g \parallel A] \right)^2 \right] - \mathbb{E}[g \parallel A]^2 \\
 &= (1 - \lambda_n)^2 \mathbb{E} \left[\left(\check{\mathbb{E}}_{n-1}[g \parallel A] \right)^2 \right] + \lambda_n^2 \mathbb{E} \left[g(b_n \cap A)^2 \right] + (2\lambda_n(1 - \lambda_n) - 1) \mathbb{E}[g \parallel A] \mathbb{E}[g(b_n \cap A)] \\
 &= (1 - \lambda_n)^2 \mathbb{E} \left[\left(\check{\mathbb{E}}_{n-1}[g \parallel A] \right)^2 \right] + \lambda_n^2 \mathbb{E} \left[g(b_n \cap A)^2 \right] - ((1 - \lambda_n)^2 + \lambda_n^2) \mathbb{E}[g \parallel A]^2 \\
 &= (1 - \lambda_n)^2 \mathbb{E} \left[\left(\check{\mathbb{E}}_{n-1}[g \parallel A] - \mathbb{E}[g \parallel A] \right)^2 \right] + \lambda_n^2 \mathbb{E} \left[(g(b_n \cap A) - \mathbb{E}[g \parallel A])^2 \right]
 \end{aligned}$$

where we have used the independence of the b_i 's to give

$$\begin{aligned}
 \mathbb{E} \left[\check{\mathbb{E}}_{n-1}[g \parallel A] g(b_n \cap A) \right] &= \mathbb{E} \left[\check{\mathbb{E}}_{n-1}[g \parallel A] \right] \mathbb{E} [g(b_n \cap A)] \\
 &= \mathbb{E}[g \parallel A]^2
 \end{aligned}$$

put

$$\begin{aligned}
 \sigma^2 &= \mathbb{E} \left[(g(b_n \cap A) - \mathbb{E}[g \parallel A])^2 \right] \\
 \alpha_n &= \mathbb{E} \left[\left(\check{\mathbb{E}}_n[g \parallel A] - \mathbb{E}[g \parallel A] \right)^2 \right] / \sigma^2
 \end{aligned}$$

then we have

$$\alpha_n = (1 - \lambda_n)^2 \alpha_{n-1} + \lambda_n^2$$

as a formulae that gives the change in variance of the estimates $\check{\mathbb{E}}_n[g \parallel A]$.

As one can see there are several ways of combining measured means to give unbiased estimates of a noisy function's mean that gives a trade off on variance.

To directly calculate the expected cost at each iteration would be too expensive an operation especially if the parameters are way off optimal. Let $C(X)$ be the random variable representing the cost function for a given parameter vector X . for a given particle the current parameter changes rapidly while when it matters the personal best parameter, X_b varies comparatively slowly so when the X_b is not updated one can take the opportunity to update the estimated expected cost function value $\hat{C}(X_b)$ of $\mathbb{E}[C(X_b)]$ in this case. This reduces the variance of the expected value compared to its raw value $C(X_b)$.

Lets look at some ways in which the estimate in principle can be updated iteratively. Given samples C_1, \dots, C_i and a forgetting gain α we could produce an unbiased estimate

$$\hat{C}(X_b)_i = \frac{\sum_{j=1}^i \alpha^{j-1} C_{i-j+1}}{\sum_{j=1}^i \alpha^{j-1}} \quad (4.1.4)$$

Put

$$A_i = \sum_{j=1}^i \alpha^{j-1} \quad (4.1.5)$$

$$= \frac{1 - \alpha^i}{1 - \alpha} \quad (4.1.6)$$

then using (4.1.4) we get

$$A_i \hat{C}(X_b)_i - \alpha A_{i-1} \hat{C}(X_b)_{i-1} = C_i \quad (4.1.7)$$

rearranging and using (4.1.6) we get

$$\hat{C}(X_b)_i = \frac{\alpha A_{i-1} \hat{C}(X_b)_{i-1} + C_i}{A_i} \quad (4.1.8)$$

$$= \frac{\alpha(1 - \alpha^{i-1}) \hat{C}(X_b)_{i-1} + (1 - \alpha) C_i}{1 - \alpha^i} \quad (4.1.9)$$

now if we put

$$\lambda_i = \frac{1 - \alpha}{1 - \alpha^i} \quad (4.1.10)$$

we get substituting into (4.1.9) the iterative update

$$\hat{C}(X_b)_i = (1 - \lambda_i) \hat{C}(X_b)_{i-1} + \lambda_i C_i \quad (4.1.11)$$

In fact any update of the form given in (4.1.11) always gives an unbiased estimate for arbitrary λ_i . So we can use this as a generalised update. the choice of parameter is tuned to cater for how rapidly one wants to converge and the required variance of the result.

Looking at the variance update assuming independent samples. Put σ_i^2 as the variance of $\hat{C}(X_b)_i$ and σ^2 as the variance of C_i then we get

$$\sigma_i^2 = (1 - \lambda_i)^2 \sigma_{i-1}^2 + \lambda_i^2 \sigma^2 \quad (4.1.12)$$

The minimum value of the update variance as a function of λ_i occurs at the point of inflexion given by

$$0 = \frac{\partial \sigma_i^2}{\partial \lambda_i} \quad (4.1.13)$$

$$= -2(1 - \lambda_i) \sigma_{i-1}^2 + 2\lambda_i \sigma^2 \quad (4.1.14)$$

$$= 2\{\lambda_i(\sigma_{i-1}^2 + \sigma^2) - \sigma_{i-1}^2\} \quad (4.1.15)$$

This gives the smallest variance λ_i as

$$\lambda_i^* = \frac{\sigma^2}{\sigma_{i-1}^2 + \sigma^2} \quad (4.1.16)$$

$$= \frac{1}{1 + (\frac{\sigma^2}{\sigma_{i-1}^2})} \quad (4.1.17)$$

$$= \frac{\sigma^{-2}}{\sigma_{i-1}^{-2} + \sigma^{-2}} \quad (4.1.18)$$

From (4.1.18) we get

$$1 - \lambda_i^* = \frac{\sigma_{i-1}^{-2}}{\sigma_{i-1}^{-2} + \sigma^{-2}} \quad (4.1.19)$$

(4.1.17) show that the result depends only on the ratio of variances while (4.1.18) gives the result in form of inverse variance. using this gives easy to use

results as will shortly be seen. Based in this remark substitute (4.1.18),(4.1.19) into (4.1.12) and calculate the updated inverse variance as

$$\sigma_i^{*-2} = ((1 - \lambda_i^*)^2 \sigma_{i-1}^{-2} + \lambda_i^{*2} \sigma^2)^{-1} \quad (4.1.20)$$

$$= \frac{\sigma_{i-1}^{-2} \sigma^{-2}}{(1 - \lambda_i^*)^2 \sigma^{-2} + \lambda_i^{*2} \sigma_{i-1}^{-2}} \quad (4.1.21)$$

$$= \frac{\sigma_{i-1}^{-2} \sigma^{-2} (\sigma_{i-1}^{-2} + \sigma^{-2})^2}{\sigma_{i-1}^{-4} \sigma^{-2} + \sigma_{i-1}^{-2} \sigma^{-4}} \quad (4.1.22)$$

$$= \sigma_{i-1}^{-2} + \sigma^{-2} \quad (4.1.23)$$

This shows the inverse variance using the optimal λ is additive and the expression is particularly simple so it can be calculated first and then λ_i^* is evaluated from

$$\lambda_i^* = \sigma^{-2} / \sigma_i^{*-2} \quad (4.1.24)$$

This gives the minimum variance update. However in the long run as it repeats the λ_i becomes so small that it ignores the current measurement and any change in the underlying statistics is ignored. We can avoid this by deliberately choosing a λ_i which is larger than the optimal given by (4.1.24). To this end put

$$\lambda_i = (1 + \delta) \lambda_i^* \quad (4.1.25)$$

then evaluate the updated inverse variance by substituting into (4.1.12) the expression (4.1.25) and simplifying using (4.1.23),(4.1.18) and (4.1.19)

$$\sigma_i^{-2} = \frac{\sigma^{-2} \sigma_{i-1}^{-2}}{[(1 - \lambda_i^*) - \delta \lambda_i^*]^2 \sigma^{-2} + \lambda_i^{*2} (1 + \delta)^2 \sigma_{i-1}^{-2}} \quad (4.1.26)$$

$$= \frac{\sigma^{-2} \sigma_{i-1}^{-2}}{(1 - \lambda_i^*)^2 \sigma^{-2} + \lambda_i^{*2} \sigma_{i-1}^{-2} - 2(1 - \lambda_i^*) \sigma^{-2} + 2 \lambda_i^* \sigma_{i-1}^{-2} + \lambda_i^{*2} \delta^2 (\sigma^{-2} + \sigma_{i-1}^{-2})} \quad (4.1.27)$$

$$= \frac{\sigma^{-2} \sigma_{i-1}^{-2} \sigma_i^{*-4}}{\sigma^{-2} \sigma_{i-1}^{-2} \sigma_i^{*-2} + \sigma^{-4} \sigma_i^{*-2} \delta^2} \quad (4.1.28)$$

$$= \frac{\sigma_i^{*-2}}{1 + \sigma^{-2} / \sigma_{i-1}^{-2} \delta^2} \quad (4.1.29)$$

Equation (4.1.29) is a particularly simple expression that shows how the inverse variance depends on δ .

Most models of probability distribution start with combining pairs of variables to give more elaborate models of the probability function. Often in the case of neural nets the pairs are combined linearly to give a single linear function which is then threshold before being passed onto an output or hidden layer. Unfortunately this in the case of neural nets gives rise to difficult to interpret models with with often pathological behaviour. The aim here is to use

the multilinear approach that encourages more unique representation of the data which can also be interpreted. However multi-linear functions are only linear on each variable in isolation and are in general non linear, hopefully in a useful way. When combining pairs of variables we will combine to produce a result for a hidden variable (or output from this) and not threshold it. This section gives results for combining pairs of variables.

4.2 Cost-function Value Representation

Here is a cost function value representation that has been superseded but contains an interesting iterative method for calculating mean and variance subject to including a history forgetting process. The code for it is at

github.com/mathrigo/setps0/fun/futil/s0float.go.

4.2.1 S0FloatCostValue implementaation of CostValue

In the targeted application of Machine Learning the cost-function value $F(x)$ is not a direct mathematical function of x and has a random component so it has to be evaluated several times before comparing the fitness of x . S0FloatCostValue was used in this case if the underlying mean value is the cost to minimise. Even if the cost function is deterministic, The evaluation of a cost value may include a very large number of tests to evaluate the cost. for instance the cost may be a measure of a program output miss match for all possible inputs. faced with this a small set of randomly selected test cases is used instead. Each time there is a need to calculate another value a fresh set of random samples is used to generate another approximate cost. To keep things simple assume that each cost sample is independent for a given x and that the statistics of $F(x)$ for a given x is slowly varying with a time constant of at least T_C . The idea is that S0FloatCostValue maintains a mean and variance running value subject to the time constant constraint.

Let x, y be two parameters for comparison that has the corresponding estimated mean C_x, C_y and estimated variance $\sigma^2 C_x, \sigma^2 C_y$ of these respective means . The noisy raw cost signal is replaced by the mean estimates for comparison. Put

$$\Delta = (C_x - C_y)^2 - (\sigma_{thres})^2(\sigma^2 C_x + \sigma^2 C_y)$$

the difference is regarded as significant if

$$\Delta > 0$$

for some comparison threshold σ_{thres} used as a heuristic.¹ As more measurements are included the variance of estimates reduces. As will be shown the time constant constraint stops this variance reduction beyond a certain point at which the variance is time constant limited. We get the following cases:

$$\begin{aligned} F(x) &< F(y) \text{ when } \Delta > 0 \text{ and } C_x < C_y \\ F(x) &> F(y) \text{ when } \Delta > 0 \text{ and } C_x > C_y \end{aligned}$$

¹normally σ_{thres} is independent of the cost value but in the code is stored by $F(x)$; in the code x, y is used as in $F(x).Cmp(F(y))$ so there is a slight lack of symmetry in the treatment of (x, y)

$F(x) \succ F(y)$ when $\Delta \leq 0$ and $\sigma^2 C_x > \sigma^2 C_y$ with $\sigma^2 C_x, \sigma^2 C_y$ not time constant limited.

$F(x) \succ F(y)$ when $\Delta \leq 0$ and $\sigma^2 C_y$ is time constant limited but $\sigma^2 C_x$ is not.

$F(x) \prec F(y)$ when $\Delta \leq 0$ and $\sigma^2 C_x \leq \sigma^2 C_y$ with $\sigma^2 C_x, \sigma^2 C_y$ not time constant limited.

$F(x) \prec F(y)$ when $\Delta \leq 0$ and $\sigma^2 C_x$ is time constant limited but $\sigma^2 C_y$ is not.

$F(x) = F(y)$ for all other cases.

The idea is to carry on asking for cost function updates until the difference in the estimated means are significant, always asking for further evaluations that are likely to achieve this and failing this regard the cost values to be effectively equal.

evaluating running mean and its variance

This leads to how the C and $\sigma^2 C$ are evaluated. Let $(x_0, \dots, x_j \dots)$ be a sequence of raw cost values produced by the cost function for a parameter x then intuitively an estimate of the mean C_j minimises

$$J_j = \frac{1}{2} \sum_{i=0}^j \alpha_{ji} (x_i - C_j)^2 \quad (4.2.1)$$

where the α_{ji} are chosen to be of the form

$$\alpha_{ji} = \prod_{k=i+1}^j b_k \text{ for } j > i; \alpha_{jj} = 1 \quad (4.2.2)$$

The b_k can be regarded as forgetting weights and for the moment has a value between 0 and 1. the form of α_{ji} has been chosen to give incremental updates. Choose C_j to minimise J_j so the derivative with respect to C_j will be zero giving

$$0 = \frac{\partial J_j}{\partial C_j} = - \sum_{i=0}^j (x_i - C_j) \alpha_{ji} \quad (4.2.3)$$

which gives

$$C_j = D_j \lambda_j \quad (4.2.4)$$

where

$$D_j = \sum_{i=0}^j x_i \alpha_{ji} \quad (4.2.5)$$

$$\lambda_j = \beta_j^{-1}; \beta_j = \sum_{i=0}^j \alpha_{ji} \quad (4.2.6)$$

Later on we will need

$$\delta_j = \sum_{i=0}^j \alpha_{ji}^2 \quad (4.2.7)$$

$$I_j = \lambda_j \sum_{i=0}^j \alpha_{ji} x_i^2 \quad (4.2.8)$$

using 4.2.2 we get the following iterative evaluations for $j > i \geq 0$

$$\alpha_{ji} = b_j \alpha_{j-1,i} \quad (4.2.9)$$

$$\beta_j = b_j \beta_{j-1} + 1; \beta_0 = 1 \quad (4.2.10)$$

$$\lambda_j = \frac{\lambda_{j-1}}{\lambda_{j-1} + b_j}; \lambda_0 = 1 \quad (4.2.11)$$

$$D_j = b_j D_{j-1} + x_j; D_0 = x_0 \quad (4.2.12)$$

$$\delta_j = b_j^2 \delta_{j-1} + 1 \quad (4.2.13)$$

from this we get an iteration rule for C_j

$$C_j = (b_j D_{j-1} + x_j) \lambda_j \quad (4.2.14)$$

$$= \frac{b_j D_{j-1} \lambda_j}{\lambda_j + b_j} + x_j \lambda_j \quad (4.2.15)$$

$$= (1 - \lambda_j) C_{j-1} + x_j \lambda_j; C_0 = x_0 \quad (4.2.16)$$

Similarly we get the iteration

$$I_j = (1 - \lambda_j) I_{j-1} + \lambda_j x_j^2; I_0 = x_0^2 \quad (4.2.17)$$

To get a handle on the statistics assume that it is effectively constant with the samples of x_j being independent with mean μ and variance σ^2 then taking expected values we get

$$\mathbb{E}(C_j) = (1 - \lambda_j) \mathbb{E}(C_{j-1}) + \mathbb{E}(x_j) \lambda_j \quad (4.2.18)$$

$$= (1 - \lambda_j) \mu + \lambda_j \mu \quad (4.2.19)$$

$$= \mu \quad (4.2.20)$$

by induction, so C_j is an unbiased estimate of the mean as expected. To calculate the variance of C_j first calculate

$$\mathbb{E}(C_j^2) = \lambda_j^2 \mathbb{E} \left\{ \left(\sum_{i=0}^j x_i \alpha_{ji} \right) \left(\sum_{k=0}^j x_k \alpha_{jk} \right) \right\} \quad (4.2.21)$$

$$= \lambda_j^2 \left\{ \sum_{i=0}^j \mathbb{E}(x_i^2) \alpha_{ji}^2 + \sum_{i \neq k} \mathbb{E}(x_i) \alpha_{ji} \mathbb{E}(x_k) \alpha_{jk} \right\} \quad (4.2.22)$$

$$= \lambda_j^2 \{ (\sigma^2 + \mu^2) \delta_j + \mu^2 \beta_j^2 - \mu^2 \delta_j \} \quad (4.2.23)$$

$$= \sigma^2 \delta_j \lambda_j^2 + \mu^2 \quad (4.2.24)$$

so the variance of C_j is given by

$$\sigma^2 C_j = \sigma^2 \delta_j \lambda_j^2 \quad (4.2.25)$$

Now

$$\mathbb{E}(I_j) = \lambda_j \sum_{i=0}^j \alpha_{ji} \mathbb{E}(x_i^2) \quad (4.2.26)$$

$$= \lambda_j \beta_j (\sigma^2 + \mu^2) \quad (4.2.27)$$

$$= \sigma^2 + \mu^2 \quad (4.2.28)$$

from this we get for

$$\gamma_j = \frac{\delta_j \lambda_j^2}{1 - \delta_j \lambda_j^2} \quad (4.2.29)$$

$$K_j = \gamma_j (I_j - C_j^2) \quad (4.2.30)$$

$$\mathbb{E}(K_j) = \gamma_j \{ \mathbb{E}(I_j) - \mathbb{E}(C_j^2) \} \quad (4.2.31)$$

$$= \gamma_j \{ \sigma^2 + \mu^2 - \sigma^2 \delta_j \lambda_j^2 - \mu^2 \} \quad (4.2.32)$$

$$= \frac{\delta_j \lambda_j^2}{1 - \delta_j \lambda_j^2} (1 - \delta_j \lambda_j^2) \sigma^2 \quad (4.2.33)$$

$$= \sigma^2 \delta_j \lambda_j^2 \quad (4.2.34)$$

so K_j is an unbiased estimate of $\sigma^2 C_j$, so we can use C_j as the running estimate of mean and K_j as estimate of C_j variance.

choosing values for b_j

All that remains is to choose the b_j which is limited to be in the range $[0, 1]$. by Equations 4.2.25, 4.2.13, 4.2.13 we can see that

$$\frac{\partial \sigma^2 C_j}{\partial b_j} = \frac{\partial}{\partial b_j} \left[\sigma^2 \frac{\lambda_{j-1}^2 (b_j^2 \delta_{j-1} + 1)}{(\lambda_{j-1} + b_j)^2} \right] \quad (4.2.35)$$

$$= -2\sigma^2 \lambda_{j-1}^2 \frac{\delta_j b_j^2 + 1 - b_j \delta_{j-1} (\lambda_{j-1} + b_j)}{(\lambda_{j-1} + b_j)^3} \quad (4.2.36)$$

$$= -2\sigma^2 \lambda_{j-1}^2 \frac{(1 - b_j \delta_{j-1} \lambda_{j-1})}{(\lambda_{j-1} + b_j)^3} \quad (4.2.37)$$

$$(4.2.38)$$

Now by using the restricted range for b_j and Equations 4.2.6, 4.2.10, 4.2.10 and the fact that $b_j^2 \leq b_j$ we get by induction that

$$0 \leq b_j \lambda_j \delta_j \leq 1 \quad (4.2.39)$$

so plugging this into Equation 4.2.37 gives

$$\frac{\partial \sigma^2 C_j}{\partial b_j} \leq 0 \quad (4.2.40)$$

so the largest b_j gives the best decrease in the variance of C_j . also if we put $b_j = 0$ we get no change in the variance from the previous variance so we also have

$$\sigma^2 C_j \leq \sigma^2 C_{j-1} \quad (4.2.41)$$

as well as this we get a decrease in λ_j at each stage. However, if λ_j gets too small the estimates start to ignore any changes in the statistics so we need to restrict λ_j to ensure it has a time constant of not more than T_C this means that

$$1 - \lambda_j \leq e^{-1/T_C} \quad (4.2.42)$$

since the time constant is large we can use the approximation

$$\lambda_j \geq 1/T_C \quad (4.2.43)$$

So to get the best reduction of $\sigma^2 C_j$ we keep $b_j = 1$ until λ_j hits the time constant limit and set

$$\lambda_j = 1/T_C \quad (4.2.44)$$

$$b_j = 1 - \lambda_j \quad (4.2.45)$$

to stop any further increase in the time constant of the iterative update.

4.3 Multi-linear functions and binary data probabilities

Multi-linear expressions are a natural way of generating functions of binary data. Let S be a finite ordered set of size n containing the elements x_1, x_2, \dots, x_n then we can for each binary sequence $a : S \rightarrow \{0, 1\}$ of n 0 and 1's associate a subset $\varphi(a) \subset S$ given as the elements x_i of S such that the sequence a maps $a(i)$ to 1. Put for $A \subset S$

$$Q(A)[x_1, x_2, \dots, x_n] = \prod_{x_i \in A} x_i \prod_{x_j \notin A} (1 - x_j)$$

Let $A, B \subset S$ such that $A \neq B$ then there exists an k such that either $x_k \in A$ and $x_k \notin B$ or $x_k \in B$ and $x_k \notin A$. assuming the former and let b be the associated binary sequence of B . Evaluating $Q(A)$ with b we get that $b(k) = 0$ so

$$Q(A)(b) \triangleq Q(A)(b(1), b(2), \dots, b(n)) = \prod_{x_i \in A} b(i) \prod_{x_j \notin A} (1 - b(j)) = 0$$

similarly for the other case. Also $Q(B)(b) = 1$ by inspection. This also shows that the $Q(A)[x_1, x_2, \dots, x_n]$ are linearly independent since if

$$\sum_{A \subset S} c(A) Q(A)[x_1, x_2, \dots, x_n] = 0$$

for coefficients $c(A) \in \mathbb{R}$ by substituting $a = \varphi^{-1}(A)$ we get

$$c(A) = c(A) Q(A)(a) = 0$$

If we put for $A \subset S$

$$\tilde{Q}(A)[x_1, x_2, \dots, x_n] = \prod_{x_i \in A} x_i$$

then by induction on n we can show that $Q(A)$ is a linear combination of $\tilde{Q}(A)$. Also by definition the $\tilde{Q}(A)$ are independent and have the same number of dimensions 2^n so span the same subspace of polynomials. Because of this the $Q(A)$ for $A \subset S$ span the space of *multilinear polynomials*.

Further for each map $f : 2^S \rightarrow \mathbb{R}$ we can associate a polynomial $Q(f)$ over the elements of S given by

$$Q(f)[x_1, x_2, \dots, x_n] = \sum_{A \subset S} f(A)Q(A)$$

and we get

$$Q(f)(b) = f(\varphi(b))$$

This multi-linear or polynomial representation of the map f is in one to one correspondence so there is nothing added by using the more complex polynomial representation of the map from subsets of S other than providing a smooth continuous representation of such functions that can be easily approximated by simple combination of polynomials that can be used to provide a more compact approximation of f . In the general case $Q(f)$ is a large expression to evaluate or store in a computer since it has 2^n terms. Also the coefficients by themselves do not convey any useful structure or pattern without further analysis. The question is can one introduce more restrictive polynomial expressions that approximate $Q(f)$ and give easy interpretations of the underlying patterns of sequences that generate significant values of f without significant loss of information.

In particular if $P(a)$ is the probability of the sequence a then $Q(P \circ \varphi^{-1})$ is a polynomial that maps binary sequences to their respective probability. Call this the *probability polynomial* and Use the notation $Q_P[x_1, x_2, \dots, x_n]$ for this. The φ map is an equivalence between subsets and binary sequences so when not ambiguous leave it out. For instance $P(A) \triangleq P(\varphi^{-1}(A))$ for a subset A .

As a general rule low order polynomial representations avoid over fitting so polynomials involving a small number of variables (that is elements of S) are useful. in particular combining variables in pairs is useful especially if we create intermediate variables called hidden that represent linear polynomials of variables and hidden variables.

4.3.1 bivariate binary table polynomial representation

let x and y be binary valued variables. let $a : \{0,1\} \times \{0,1\} \rightarrow \{0,1\}$ be a function. this is represented by a polynomial

$$Q(a)[x, y] = a(0,0)(1-x)(1-y) + a(0,1)(1-x)y + a(1,0)x(1-y) + a(1,1)xy \quad (4.3.1)$$

$$= a(00) + [a(1,0) - a(0,0)]x + [a(0,1) - a(0,0)]y + [a(0,0) + a(1,1) - a(0,1) - a(1,0)]xy \quad (4.3.2)$$

that agrees with the binary function a for binary values. we can get a clean uncluttered parametrisation by putting

$$X_0 = a(0,0) \quad (4.3.3)$$

$$X_1 = a(1,0) - a(0,0) \quad (4.3.4)$$

$$X_2 = a(0,1) - a(0,0) \quad (4.3.5)$$

$$x_3 = a(1,1) - a(0,0) \quad (4.3.6)$$

$$(4.3.7)$$

to give

$$Q(a)[x,y] = X_0 + X_1x + X_2y + (X_3 - X_1 - X_2)xy \quad (4.3.8)$$

Chapter 5

Parking Place

This provides a place to put text snippets while rearranging the document.

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