Penalty Functions

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C 5.2.1 Introduction to Constraints

Most optimization problems have constraints. The solution or set of solutions which are obtained as the final result of an evolutionary search must necessarily be feasible, that is, satisfy all constraints. A taxonomy of constraints can be considered and composed of (a) number, (b) metric, (c) criticality and (d) difficulty. A first aspect is number of constraints, ranging upwards from one. Sometimes problems with multiple objectives are reformulated with some of the objectives acting as constraints. Difficulty in satisfying constraints will increase (generally more than linearly) with the number of constraints. A second aspect of constraints is their metric, either continuous or discrete, so that a violation of the constraint can be assessed in distance from satisfaction using that metric. A third consideration is the criticality of the constraint, in terms of absolute satisfaction. A constraint is generally formulated as hard (absolute) when in fact, it is often somewhat soft. That is, small violations would be considered for the final solution if the solution is otherwise superior to other solutions. Evolutionary algorithms are especially capable of handling soft constraints since a population of solutions is returned at each point in the search. This allows the user to select a solution which violates a soft constraint (technically infeasible) over a solution which would be the best, technically feasible solution found. A final aspect of constraints to be considered is the difficulty of satisfying the constraints. This difficulty can be characterized by the size of the feasible region (F) compared to the size of the sample space (S). The difficulty may not be known *a priori*, but can be gauged in two ways. The first way is how simple it is to change a solution which violates the constraint to a solution which does not violate the constraint. The second way is the probability of violating the constraint during search. For example, a constraint may be frequently violated but the solution can be easily made feasible. Conversely, a constraint violation may be very difficult to resolve, but occur rarely in the search.

C 5.2.2 Methods of Handling Constraints

As originally conceived, evolutionary methods produce new solutions by recombining and / or perturbing existing solutions. In certain instances, an encoding, a reproduction (e.g. crossover) operator and a perturbation (e.g. mutation) operator can be devised such that feasible existing solutions (parents) will always produce feasible new solutions (children). An example using binary integers illustrates this: exchanging bits between two *k*-bit integers will always produce a *k*-bit integer. If a one-to-one correspondence between *k*-bit integers and feasible solutions is established, every newly-produced encoding will correspond to a feasible solution to the original problem. This is an example of a constraint which is easily handled through encoding and operators, so all solutions examined during evolution are feasible, as was demonstrated effectively in Esbensen (1995).

In other cases, it is not clear how an encoding and operators can be defined to preserve feasibility. One approach is to increase the complexity of the evolution operators by adding repair operators, so that they are guaranteed to produce feasible encodings. For problems such as TSP, compensatory conflict-resolution operators (repair operators) could be implemented, so that the resulting child encoding is itself a valid permutation. Several researchers have taken this approach to problems (Liepins et al. 1990, Liepins and Potter 1991, Orvosh and Davis 1994, Tate and Smith 1995A), and it works well without restrictive computational cost. Interestingly, the first three papers repaired the infeasible solution to calculate the fitness, but left the solution unrepaired in the population (with some probability). When an infeasible solution can be readily modified to yield a feasible solution which maintains most or all of the structure of the parent solutions, repair mechanisms can be efficient and effective. However, some repair mechanisms can introduce systematic bias into the search.

Unfortunately, many optimization problems involve constraints for which it is not easy to repair an infeasible solution in order to make it feasible. The repair operators may be prohibitively computationally expensive or they may severely disturb the superior aspects of the parent solutions carried in the children, defeating the fundamental strength of evolution. A method to consider in this case is to allow only feasible solutions to be maintained during

evolution. Solutions which violate constraints are immediately discarded upon creation, and not considered further. If constraint violations are encountered relatively infrequently during evolution (that is, a fairly loosely constrained problem), then discarding infeasible solutions can be an efficient method.

However, in many cases the problem of finding any feasible solution is itself NP-hard (Garey and Johnson 1979). A number of methods have been proposed in the evolutionary computation literature for such highly constrained problems. DeJong and Spears (1989) suggest polynomially reducing other NP-Complete problems to the Boolean Satisfiability problem, for which effective (and compact) GA implementations are known. This method has the drawback that the polynomial reduction involved may be extremely complex, and may greatly increase the size of the problem. Michalewicz (1992) and Michalewicz and Janikow (1991) suggest eliminating the equalities in constraints and formulating special genetic operators which guarantee feasibility. This approach works efficiently for linear constraints and continuous variable domains. A more generic approach borrowed from the mathematical programming literature is that of exterior penalty methods.

C 5.2.3 Introduction to Penalty Functions

Penalty functions have been a part of the literature on constrained optimization for decades. Three degrees of penalty functions exist: barrier methods in which no infeasible solution is considered, partial penalty functions in which a penalty is applied near the feasibility boundary, and global penalty functions which are applied throughout the infeasible region (Schwefel 1995). In the area of combinatorial optimization, the popular Lagrangian relaxation method (Avriel 1976, Fisher 1981, Reeves 1993) is a variation on the same theme: temporarily relax the problem's most difficult constraints, using a modified objective function to avoid straying too far from the feasible region. In general, a penalty function approach is as follows. Given an optimization problem,

$$\begin{aligned} \min \quad & f(\mathbf{x}) \qquad (P) \\ \text{s.t.} \quad & \mathbf{x} \in A \end{aligned}$$

$$\mathbf{x} \in \mathrm{B}$$

where **x** is a vector of decision variables, the constraints "**x** ∈ A" are relatively easy to satisfy, and the constraints "**x** ∈ B" are relatively difficult to satisfy, the problem can be reformulated as

$$\begin{aligned} \min \quad & f(\mathbf{x}) + p(d(\mathbf{x}, \mathrm{B})) \qquad (\mathrm{R}) \\ \text{s.t.} \quad & \mathbf{x} \in \mathrm{A} \end{aligned}$$

where $d(\mathbf{x}, \mathrm{B})$ is a metric function describing the distance of the solution vector **x** from the region B, and $p(\cdot)$ is a monotonically non-decreasing penalty function such that $p(0) = 0$. If the exterior penalty function, $p(\cdot)$, grows quickly enough outside of B, the optimal solution of (P) will also be optimal for (R). Furthermore, any optimal solution of (R) will provide an upper bound on the optimum for (P), and this bound will in general be tighter than that obtained by simply optimizing $f(\mathbf{x})$ over A.

In practice, the constraints "**x** ∈ B" are expressed as inequality and equality constraints in the form of

$$g_i(\mathbf{x}) \le 0 \text{ for } i = 1, \ldots, q$$

$$h_i(\mathbf{x}) = 0 \text{ for } i = q + 1, \ldots, m$$

where q = number of inequality constraints

$m - q$ = number of equality constraints

Various families of functions $p(\cdot)$ and $d(\cdot)$ have been studied for evolutionary optimization to dualize constraints. Different possible distance metrics, $d(\cdot)$, include a count of the number of violated constraints, the Euclidean distance between **x** and B as suggested by Richardson et al. (1989), a linear sum of the individual constraint violations or a sum of the individual constraint violations raised to an exponent, κ. Variations of these approaches have been attempted with different levels of success. Some of the more notable examples are described in the following sections.

It can be difficult to find a penalty function which is an effective and efficient surrogate for the missing constraints. The effort required to tune the penalty function to a given problem instance or repeatedly calculate it during search may negate any gains in eventual solution

quality. As noted by Siedlecki and Sklansky (1989), much of the difficulty arises because the optimal solution will frequently lie on the boundary of the feasible region. Many of the solutions most similar to the genotype of the optimum solution will be infeasible. Therefore, restricting the search to only feasible solutions or imposing very severe penalties makes it difficult to find the schemata that will drive the population toward the optimum as shown in the research of (Smith and Tate 1993, Anderson and Ferris 1994, Coit et al. 1995, Michalewicz 1995). Conversely, if the penalty is not severe enough, then too large a region is searched and much of the search time will be used to explore regions far from the feasible region. Then, the search will tend to stall outside the feasible region. A good comparison of six penalty function strategies applied to continuous optimization problems is given in Michalewicz (1995). These strategies include both static and dynamic approaches, as discussed below, as well as some less generic approaches such as sequential constraint handling (Schoenauer and Xanthakis 1993) and forcing all infeasible solutions to be dominated by all feasible solutions in a given generation (Powell and Skolnick 1993).

C 5.2.4 Static Penalty Functions

A simple method to penalize infeasible solutions is to apply a constant penalty to those solutions which violate feasibility in any way. The penalized objective function would then be the unpenalized objective function plus a penalty (for a minimization problem). A variation on this simple penalty function is to add a metric based on number of constraints violated, where there are multiple constraints. The penalty function for a problem with m constraints would then be as below (for a minimization problem):

$$f_p(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{m} C_i \delta_i \qquad (1)$$

$$\text{where } \begin{cases} \delta_i = 1, \text{ if constraint } i \text{ is violated} \\ \delta_i = 0, \text{ if constraint } i \text{ is satisfied} \end{cases}$$

$f_p(\mathbf{x})$ is the penalized objective function, $f(\mathbf{x})$ is the unpenalized objective function, and C_i is a constant imposed for violation of constraint i. This penalty function is based only on the number

of constraints violated, and is generally inferior to the second approach based on some distance metric from the feasible region (Goldberg 1989, Richardson et al. 1989).

More common and more effective is to penalize according of distance to feasibility, or the "cost to completion" as termed by Richardson et al. (1989). This was done crudely in the constant penalty functions of the preceding paragraph by assuming distance can be stated solely by number of constraints violated. A more sophisticated and more effective penalty includes a distance metric for each constraint, and adds a penalty which becomes more severe with distance from feasibility. Complicating this approach is the assumption that the distance metric chosen appropriately provides information concerning the nearness of the solution to feasibility, and the further implicit assumption that this nearness to feasibility is relevant in the same magnitude to the fitness of the solution. Distance metrics can be continuous (see for example, Juliff 1993) or discrete (see for example, Patton et al. 1995), and could be linear or non-linear (see for example, Le Riche et al. 1995).

A general formulation is as follows for a minimization problem:

$$f_p(\mathbf{x}) = f(\mathbf{x}) + \sum_{i=1}^{m} C_i d_i^{\kappa} \qquad (2)$$

$$\text{where} \quad d_i = \begin{cases} \delta_i g_i(\mathbf{x}), & \text{for } i = 1, \ldots, q \\ |h_i(\mathbf{x})|, & \text{for } i = q+1, \ldots, m \end{cases}$$

d_i is the distance metric of constraint i applied to solution $\mathbf{x}$ and κ is user defined exponent, with values of κ of 1 or 2 often used. Selection of C_i is more difficult. The advice from Richardson et al. (1989) is to base C_i on the expected or maximum cost to repair the solution (i.e. alter the solution so it is feasible). For most problems, however, it is not possible to determine C_i using this rationale. Instead, it must be estimated based on the relative scaling of the distance metrics of multiple constraints, the difficulty of satisfying a constraint, and the seriousness of a constraint violation, or be determined experimentally.

Many researchers in evolutionary computation have explored variations of distance based static penalty functions (e.g., Baeck and Khuri 1994, Goldberg 1989, Huang et al. 1994, Olsen

1994, Richardson et al. 1989). One example (Thangiah 1995) uses a linear combination of three constant distance based penalties for the three constraints of the vehicle routing with time windows problem. Another novel example is from (Le Riche et al. 1995) where two separate distance based penalty functions are used for each constraint in two GA segregated subpopulations. This "double penalty" somewhat improved robustness to penalty function parameters since the feasible optimum is approached with both a severe and a lenient penalty. Homaifar et al. (1994) developed a unique static penalty function with multiple violation levels established for each constraint. Each interval is defined by the relative degree of constraint violation. For each interval *l*, a unique constant, C_{il} is then used as a penalty function coefficient.

C 5.2.5 Dynamic Penalty Functions

The primary deficiency with static penalty functions is the inability of the user to determine criteria for the C_i coefficients. Also, there are conflicting objectives involved with allowing exploration of the infeasible region, yet still requiring that the final solution be feasible. A variation of distance based penalty functions, which alleviates much of these difficulties, is to incorporate a dynamic aspect which (generally) increases the severity of the penalty for a given distance as the search progresses. This has the property of allowing highly infeasible solutions early in the search, while continually increasing the penalty imposed to eventually move the final solution to the feasible region. A general form of a distance based penalty method incorporating a dynamic aspect based on length of search, *t*, is as follows for a minimization problem:

$$f_p(\mathbf{x},t) = f(\mathbf{x}) + \sum_{i=1}^{m} s_i(t) d_i^{\kappa} \qquad (3)$$

where $s_i(t)$ is a monotonically non-decreasing in value with *t*. Metrics for *t* include number of generations or the number of solutions searched. Recent uses of this approach include Joines and Houck (1994) for continuous function optimization and Olsen (1994), who compares several penalty functions, all of which consider distance, but some also consider evolution time. A

common concern of these dynamic penalty formulations is that they result in feasible solutions at the end of evolution. If $s_i(t)$ is too lenient, final infeasible solutions may result, and if $s_i(t)$ is too severe, the search may converge to non-optimal feasible solutions. Therefore, these penalty functions typically require problem specific tuning to perform well. One explicit example of $s_i(t)$ is as follows, from Joines and Houck (1994),

$$s_i(t) = (C_i\, t)^{\alpha}$$

where α is constant equal to 1 or 2, as defined by Joines and Houck.

C 5.2.6 Adaptive Penalty Functions

While incorporating distance together with the length of the search into the penalty function has been generally effective, these penalties ignore any other aspects of the search. In this respect, they are not adaptive to the ongoing success (or lack thereof) of the search and cannot guide the search to particularly attractive regions or away from unattractive regions based on what has already been observed. A few authors have proposed making use of such search specific information. Siedlecki and Sklansky (1989) discuss the possibility of self-adapting penalty functions, but their method is restricted to binary-string encodings with a single constraint, and involves considerable computational overhead.

Bean and Hadj-Alouane (1992) and Hadj-Alouane and Bean (1992) propose penalty functions which are revised based on the feasibility or infeasibility of the best, penalized solution during recent generations. Their penalty function allows either an increase or a decrease of the imposed penalty during evolution as shown below, and was demonstrated on multiple choice integer programming problems with one constraint. This involves the selection of two constants, β_1 and β_2 ($\beta_1>\beta_2>1$), to adaptively update the penalty function multiplier, and the evaluation of the feasibility of the best solution over successive intervals of N_f generations. As the search progresses, every N_f generations the penalty function multiplier is updated based on whether the best solution was feasible during that interval. Specifically, the penalty function is as follows,

$$f_p(\mathbf{x}, k) = f(\mathbf{x}) + \sum_{i=1}^{m} \lambda_k d_i^{\kappa} \qquad (4)$$

$$\lambda_{k+1} = \begin{cases} \lambda_k \beta_1, & \text{if previous } N_f \text{ generations have infeasible best solution} \\ \lambda_k / \beta_2, & \text{if previous } N_f \text{ generations have feasible best solution} \\ \lambda_k, & \text{otherwise} \end{cases}$$

Smith and Tate (1993) and Tate and Smith (1995B) used both search length and constraint severity feedback in their penalty function which was enhanced by the work of Coit et al. (1995). This penalty function involves the estimation of a near-feasible threshold (*NFT*) for each constraint. Conceptually, the *NFT* is the threshold distance from the feasible region at which the user would consider the search as "getting warm." The penalty function encourages the evolutionary algorithm to explore within the feasible region and the *NFT*-neighborhood of the feasible region, and discourage search beyond that threshold. This formulation is below:

$$f_p(\mathbf{x}, t) = f(\mathbf{x}) + (F_{feas}(t) - F_{all}(t)) \sum_{i=1}^{m} \left(\frac{d_i}{NFT_i} \right)^{\kappa} \qquad (5)$$

where $F_{all}(t)$ denotes the unpenalized value of the best solution yet found, and $F_{feas}(t)$ denotes the value of the best feasible solution yet found. The $F_{all}(t)$ and $F_{feas}(t)$ terms serve several purposes. First, they provide adaptive scaling of the penalty based on the results of the search. Second, they combine with the NFT_i term to provide a search specific and constraint specific penalty.

The general form of *NFT* is:

$$NFT = \frac{NFT_o}{1 + \Lambda} \qquad (6)$$

where NFT_o is an upper bound for *NFT*. Λ is a dynamic search parameter used to adjust *NFT* based on the search history. In the simplest case, Λ can be set to zero and a static *NFT* results. Λ can also be defined as a function of the search, for example, a function of the generation number (t), i.e., $\Lambda = f(t) = \lambda t$. A positive value of λ results in a monotonically decreasing *NFT* (and thus, a larger penalty) and a larger λ more quickly decreases *NFT* as the search progresses, incorporating both adaptive and dynamic elements.

If *NFT* is ill defined *a priori*, it can be set at a large value initially with a positive constant λ used to iteratively guide the search to the feasible region. With problem specific information, a more efficient search can take place by defining a tighter region or even static values of *NFT*.

C 5.2.7 Future Directions in Penalty Functions

Two areas requiring further research are the development of completely adaptive penalty functions which require no user specified constants and the development of improved adaptive operators to exploit characteristics of the search as they are found. The notion of adaptiveness is to leverage the information gained during evolution to improve both the effectiveness and the efficiency of the penalty function used. Another area of interest is to explore the assumption that multiple constraints can be linearly combined to yield an appropriate penalty function. This implicit assumption of all penalty function used in the literature assumes that constraint violations incur independent penalties and therefore, there is no interaction between constraints. Intuitively, this seems to be a possibly erroneous assumption, and one could make a case for a penalty which increases more than linearly with the number of constraints violated.

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