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Service: IRIDIA

CONDOR USER'S GUIDE

Constrained, Non-linear, Derivative-free, parallel,
Multi-Objective Optimization of continuous, high
computing load, noisy objective functions.

document v1.05



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Chapter 1

Introduction

This article is a user's guide for CONDOR “*C*Onstrained, *N*on-linear, *D*irect, parallel, multi-objective Optimization using trust Region method for high-computing load, noisy objective functions”. The aim of the CONDOR optimizer is to find the minimum $x^* \in \mathfrak{R}^n$ of an objective function $\mathcal{F}(x) \in \mathfrak{R}$ using the least number of function evaluations. It is assumed that the dominant computing cost of the optimization process is the time needed to evaluate the objective function $\mathcal{F}(x)$ (One evaluation can range from 2 minutes to 2 days). The algorithm will try to minimize the number of evaluations of $\mathcal{F}(x)$, at the cost of a huge amount of routine work.

CONDOR is mostly useful when used in combination with big software simulators that simulate industrial processes. These kind of simulators are often encountered in the chemical industry (simulators of huge chemical reactors), in the compressor and jet- engine industry (simulators of huge radial turbo-compressors), in the space industry (simulators of the path of a satellite in low orbit around earth),... These simulators were written to allow the design engineer to correctly estimate the consequences of the adjustment of one (or many) design variables (or parameters of the problem). Such softwares very often demands a great deal of computing power. One run of the simulator can take as much as one or two hours to finish. Some extreme simulations take a day to complete.

These kind of codes can be used to optimize “in batch” the design variables: The research engineer can aggregate the results of the simulation in one unique number that represents the “goodness” of the current design (The aggregation process is handled by CONDOR in a specific way that allows to easily do multi-objective optimization). This final number y can be seen as the result of the evaluation of an objective function $y = \mathcal{F}(x)$ where x is the vector of design variables and \mathcal{F} is the simulator. We can run an optimization program that finds x^* : the optimum design: the optimum of $\mathcal{F}(x)$.

Here are the assumptions needed to use CONDOR:

- The dimension n of the search space (the number of design variables) must be lower than 100. For larger dimension the time consumed by this algorithm will be so long and the number of function evaluations will be so great that I advice you to use another algorithm.
- CONDOR is a *direct* optimization tool (i.e., that the derivatives of \mathcal{F} are not required). The only information needed about the objective function is a simple method (written in Fortran, C++,...) or a program (a Unix, Windows, Solaris,... executable) that can evaluate the objective function $\mathcal{F}(x)$ at a given point x . In particular, no derivatives of

$\mathcal{F}(x)$ are required. However, the algorithm assumes that they exist. If the function is not continuous, the algorithm can still converge but in a greater time.

- If the objective function is an external executable, it should be possible to run it “in batch” (without user-interaction). If it’s not the case, you can use tools like “Winbatch” to transform your executable into a “batch” process.
- Some evaluations of the objective function can “fail”, returning no value at all. CONDOR simply handles these “failed evaluations” as “virtual constraints” and continues the optimization process without any problem.
- The algorithm tries to minimize the number of evaluations of $\mathcal{F}(x)$, at the cost of a huge amount of routine work that occurs during the decision of the next value of x to try. Therefore, the algorithm is particularly well suited for high computing load objective function.
- The algorithm will only find a local (maybe global) minimum of $\mathcal{F}(x)$.
- There can be a limited noise on the evaluation of $\mathcal{F}(x)$. The algorithm has been specially developed to be very robust against noise inside the evaluation of the objective function $\mathcal{F}(x)$.
- All the design variables must be continuous.
- The non-linear constraints are “cheap” to evaluate.

CONDOR is able to use several CPU’s in a cluster of computers. Different computer architectures can be mixed together and used simultaneously to deliver a huge computing power. The optimizer will make simultaneous evaluations of the objective function $\mathcal{F}(x)$ on the available CPU’s to speed up the optimization process.

You will never lose one evaluation anymore! Why always throwing away the results of costly evaluations of the objective function? CONDOR manages transparently a database of old evaluations. Using this database, CONDOR is able to “hot start” very near the optimum point. This proximity ensures rapid convergence. CONDOR uses the database of old evaluation and a special aggregation process in a way that allows design engineers to easily “play” with the different sub-objectives without losing time. Design engineers can easily customize the objective function, until it finally suits their needs.

The experimental results of CONDOR [VB04] are very encouraging and validate the quality of the approach: CONDOR outperforms many commercial, high-end optimizers and it might be the fastest optimizer in its category (fastest in terms of number of function evaluations). When several CPU’s are used, the performances of CONDOR are unmatched. When performing multi-objective optimization, the possibility to “hot start” near the optimum point allows to converge to the optimum even faster.

The experimental results open wide possibilities in the field of noisy and high-computing-load objective function optimization (from two minutes to several days) like, for instance, industrial shape optimization based on CFD (computation fluid dynamic) codes (see [CAVDB01, PVdB98, Pol00, PMM⁺03]) or PDE (partial differential equations) solvers.

More specifically, in the field of aerodynamic shape optimization, optimizers based on genetic algorithm (GA) and Artificial Neural Networks (ANN) are very often encountered. When used on such problems, CONDOR usually outperforms all the state-of-the-art optimizers based on GA and ANN by a factor of 10 to 100 (see [PPGC04] for classical performances of GA+NN optimizer). In brief, CONDOR will converge to the solution of the optimization problem in a time that is 10 to 100 times shorter than any GA+NN optimizers. When the dimension of the search space increases, the performances of optimizers based on GA and ANN are drastically dropping. When using a GA+NN optimizer, a problem with a search-space dimension greater than three is already nearly unsolvable if the objective function is high-computing-load (All what you can expect is a slight improvement of the value of the objective function compared to the value of the objective function at the starting point). Unlike all GA+ANN optimizers, CONDOR scales very well when the search space dimension increases (at least up to 100 dimensions).

CONDOR has been designed with one application in mind: the METHOD project. (METHOD stands for Achievement Of Maximum Efficiency For Process Centrifugal Compressors THrough New Techniques Of Design). The goal of this project is to optimize the shape of the blades inside a Centrifugal Compressor (see illustration of the compressor's blades in Figure 1.1). The objective function is based on a CFD (computation fluid dynamic) code that simulates the flow of the gas inside the compressor. The shape of the blades in the compressor is described by 31 parameters. CONDOR is currently the only optimizer that can solve this kind of problem (an optimizer based on GA+ANN is useless due to the high number of dimensions and the huge computing time needed at each evaluation of the objective function). We extract from the numerical simulation the outlet pressure, the outlet velocity, the energy transmit to the gas at stationary conditions. We aggregate all these indices in one general overall number representing the quality of the turbine. We are trying to find the optimal set of 31 parameters for which this quality is maximum. The evaluations of the objective function are very noisy and often take more than one hour to complete (the CFD code needs time to “converge”).

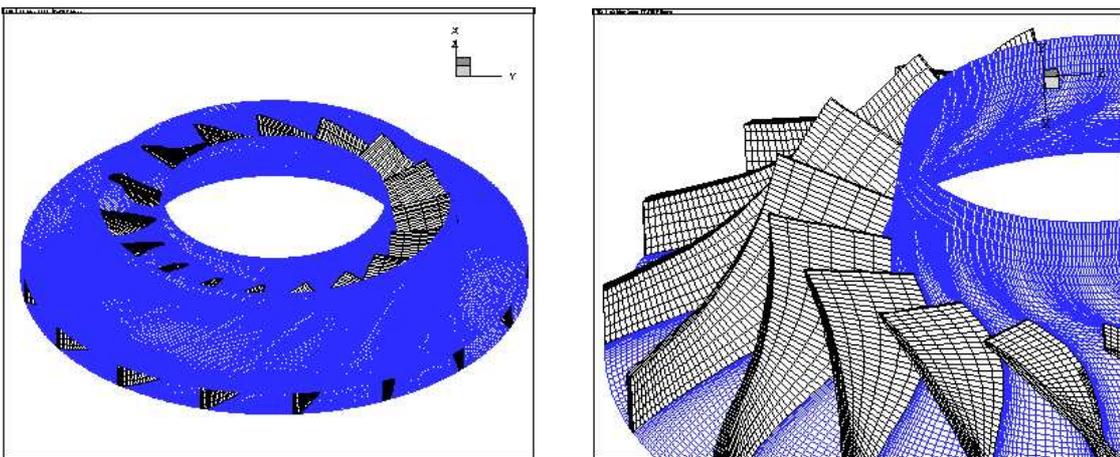


Figure 1.1: Illustration of the blades of the compressor

Finally, The code of CONDOR is completely new, original, easily comprehensible (Object Oriented approach in C++), (partially) free and fully stand-alone. There is no call to fortran, external, unavailable, expensive, copyrighted libraries. You can compile the code under Unix,

Windows, Solaris, etc. The only library needed is the standard TCP/IP network transmission library based on sockets (only in the case of the parallel version of the code).

The algorithms used inside CONDOR are part of the Gradient-Based optimization family. The algorithms implemented are Dennis-Moré Trust Region steps calculation (It's a restricted Newton's Step), Sequential Quadratic Programming (SQP), Quadratic Programming (QP), Second Order Corrections steps (SOC), Constrained Step length computation using L_1 merit function and Wolf condition, Active Set method for active constraints identification, BFGS update, Multivariate Lagrange Polynomial Interpolation, Cholesky factorization, QR factorization and more! For more in depth information about the algorithms used, see my thesis [VB04]

Many ideas implemented inside CONDOR are from Powell's UOBYQA (Unconstrained Optimization BY quadratical approximation) [Pow00] for unconstrained, direct optimization. The main contribution of Powell is equation 1.1 that allows to construct a full quadratical model of the objective function in very few function evaluations (at a *low* price).

$$\text{Powell's heuristic} : \frac{M}{6} \|\mathbf{x}_{(j)} - \mathbf{x}_{(k)}\|^3 \max_d \{|P_j(\mathbf{x}_{(k)} + d)| : \|d\| \leq \rho\} \leq \epsilon \quad j = 1, \dots, N \quad (1.1)$$

See section 3.4.2 (equation 3.37) and section 6.2 (equation 6.6) of [VB04] for a full explanation of this equation. This equation is very successful and having a full quadratical model allows us to reach high convergence speed.

From the user point of view, there are several interfaces to CONDOR available:

1. **XML-Based interface:** This is the main interface of CONDOR. All the options are available. CONDOR will communicate (using standard ASCII text files) with an external executable that will compute all the evaluations of the objective functions. This approach allows to use very easily old evaluations of the objective function via a database that is internally managed by CONDOR. There is no need to compile or code anything. You give to CONDOR a simple, intuitive configuration file based on XML and CONDOR will start and solve directly your problem! See chapter 2 for a detailed explanation of this approach.
2. **MATLAB interface:** You can now optimize in Matlab any objective function you like using the matlab interface of CONDOR. You only need to provide an .m file that can compute the value of the objective function at a given position. This interface is not able to do parallel optimization.
3. **C++ code approach:** CONDOR is programmed using Object Oriented approach. Internally, an objective function is represented by an instance of a child of the super-class "ObjectiveFunction". All you have to do is to create a child of the class "ObjectiveFunction", instantiate it, and give it to CONDOR. That's all folks!

1.1 Formal description

CONDOR is an optimizer for non-linear **continuous** objective functions subject to box, linear and non-linear constraints. We want to find $x^* \in \mathcal{R}^n$ that satisfies:

$$\mathcal{F}(x^*) = \min_x \mathcal{F}(x) \quad \text{Subject to:} \quad \begin{cases} b_l \leq x \leq b_u, & b_l, b_u \in \mathfrak{R}^n \\ Ax \geq b, & A \in \mathfrak{R}^{m \times n}, b \in \mathfrak{R}^m \\ c_i(x) \geq 0, & i = 1, \dots, l \end{cases} \quad (1.2)$$

Conventions

$\mathcal{F}(x) : \mathfrak{R}^n \rightarrow \mathfrak{R}$ n b_l and b_u $Ax \geq b$ $c_i(x)$ x^* k x_k $g(x) = \left(\frac{\partial \mathcal{F}}{\partial x_1}(x), \dots, \frac{\partial \mathcal{F}}{\partial x_n}(x) \right)$ $g_k = g(x_k)$ $H_{i,j} = \frac{\partial^2 \mathcal{F}}{\partial x_i \partial x_j}(x)$ $H_k = H(x_k)$ $B_k = B(x_k)$ $H^* = H(x^*)$ $\mathcal{F}(x_k + \delta) \approx \mathcal{Q}_k(\delta) = \mathcal{F}(x_k) + g_k^t \delta + \frac{1}{2} \delta^t B_k \delta$	<p>The objective function. We search for the minimum of it.</p> <p>the dimension of the search space</p> <p>the box-constraints.</p> <p>the linear constraints.</p> <p>the non-linear constraints.</p> <p>The optimum of $\mathcal{F}(x)$. We search for it.</p> <p>The iteration index of the algorithm</p> <p>The current point (best point found)</p> <p>g is the gradient of \mathcal{F}.</p> <p>g_k is the gradient of \mathcal{F} at x_k</p> <p>$H(x)$ is the Hessian matrix of \mathcal{F}.</p> <p>The Hessian Matrix of \mathcal{F} at point x_k</p> <p>The current approximation of the Hessian Matrix of \mathcal{F} at point x_k</p> <p>If not stated explicitly, we will always assume $B = H$.</p> <p>The Hessian Matrix at the optimum point.</p> <p>$\mathcal{Q}_k(\delta)$ is the quadratical approximation of \mathcal{F} around x_k.</p>
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All vectors are column vectors.

An optimization (minimization) algorithm is nearly always based on this simple principle:

1. Build an approximation (also called “local model”) of the objective function around the current point.
2. Find the minimum of this model and move the current point to this minimum. This is called an “optimization step” or, in short, a “step”.
3. Evaluate the objective function at this new point. Reconstruct the “local model” of the objective function around the new point using the new evaluation. Go back to step 2.

Like most optimization algorithms, CONDOR uses, as local model, a polynomial of degree two. There are several techniques to build this quadratic. CONDOR uses multivariate lagrange interpolation technique to build its model. This technique is particularly well-suited when the dimension of the search space is low ($n < 100$).

Let's rewrite this algorithm, using more standard notations:

1. Build the "local model" $\mathcal{Q}_k(\delta)$ of the objective function around the current point x_k .
2. Find the minimum δ_k of the local model at $\mathcal{Q}_k(\delta_k)$ and move the current point to this minimum: $x_{k+1} = x_k + \delta_k$. δ_k is the step.
3. Compute $y = \mathcal{F}(x_{k+1})$ and use y to build the new "local model" $\mathcal{Q}_{k+1}(\delta)$. Increase k and go back to step 2.

Currently, most of the research in optimization algorithms is oriented to huge dimensional search-space ($n > 1000$). In these algorithms, approximative search directions are computed. CONDOR is one of the very few algorithms that adopts the opposite point of view. CONDOR build the most precise local models of the objective function and computes the most precise steps to reduce at all cost the number of function evaluations.

The material of this chapter is based on the following references: [VB04, Fle87, PT95, BT96, Noc92, CGT99, DS96, CGT00, Pow00].

1.2 A basic overview of the CONDOR algorithm.

A (very) basic explanation of the CONDOR algorithm is:

1. **Initialization** An initial point $x_0 = x_{start}$, an initial trust region radius Δ_0 and an initial sampling distance $\rho_0 = \rho_{start}$ are given. In CONDOR, we have $\Delta_0 := \rho_0$. Let's define k , the iteration index of the algorithm. Set $k = 0$. Let's compute using multivariate interpolation techniques, the initial quadratical approximation of $\mathcal{F}(x)$ around $x_k = x_0 = x_{start}$:

$$\mathcal{Q}_k(\delta) = f(x_k) + g_k^t \delta + \frac{1}{2} \delta^t B_k \delta$$

The initial sampling points (used to build $\mathcal{Q}_k(\delta)$) are separated by a distance of exactly ρ_{start} . Go directly to step 3.

2. **Update the Local Model.** Update $\mathcal{Q}_k(\delta)$. This will require to "sample" the objective function $\mathcal{F}(x)$ around the current position x_k to know what is exactly locally its shape. The sampling points are separated from the current point x_k by a distance of maximum $2\rho_k$. This update is performed only when we detect that $\mathcal{Q}_k(\delta)$ is degenerated and does not represent accurately the real shape of the objective function $\mathcal{F}(x)$ anymore.
3. **Step computation** Compute a step δ_k that goes to the minimum of the local model $\mathcal{Q}_k(\delta)$. The length of the steps must be between $\frac{1}{2}\rho_k$ and Δ_k . In other words:

$$\mathcal{Q}(\delta_k) = \min_{\delta} \mathcal{Q}_k(\delta) \text{ such that } \frac{\rho_k}{2} < \|\delta_k\|_2 < \Delta_k \quad (1.3)$$

4. **Compute the "degree of agreement"** τ_k between \mathcal{F} and \mathcal{Q} :

$$\tau_k = \frac{\mathcal{F}(x_k) - \mathcal{F}(x_k + \delta_k)}{\mathcal{Q}_k(0) - \mathcal{Q}_k(\delta_k)} \quad (1.4)$$

5. **update** x_k and Δ_k , based on τ_k :

$\tau_k < 0.01$ (bad iteration)	$0.01 \leq \tau_k < 0.9$ (good iteration)	$0.9 \leq \tau_k$ (very good iteration)	(1.5)
$x_{k+1} = x_k$ $\Delta_{k+1} = \frac{\Delta_k}{2}$	$x_{k+1} = x_k + \delta_k$ $\Delta_{k+1} = \Delta_k$	$x_{k+1} = x_k + \delta_k$ $\Delta_{k+1} = 2\Delta_k$	

6. **Update of** ρ_k . If $\|\delta_k\|_2 < \rho_k$, the step sizes are becoming small, we are near the optimum, we must increase the precision of $\mathcal{Q}_k(\delta)$: decrease ρ .

7. Increment k . Stop if $\rho_k = \rho_{end}$ otherwise, go to step 2.

The local model \mathcal{Q}_k allows us to compute the steps δ_k that we will follow towards the minimum point x^* of $\mathcal{F}(x)$. To which extend can we “trust” the local model \mathcal{Q}_k ? How “big” can be the steps δ_k ? The answer is: as big as the *Trust Region Radius* Δ_k : We must have $\|\delta_k\| < \Delta_k$. Δ_k is adjusted dynamically at step 5 of the algorithm. The main idea of step 5 is: only increase Δ_k when the local model \mathcal{Q}_k reflects well the real function \mathcal{F} (and gives us good directions).

Under some very weak assumptions, it can be proven that this algorithm (Trust Region algorithm) is globally convergent to a local optimum [CGT00].

To start the unconstrained version of the CONDOR algorithm, we basically need:

- The starting point x_{start}
- The length ρ_{start} that represents, basically, the initial distance between the points where the objective function will be sampled.
- The length ρ_{end} that represents, basically, the final distance between the interpolation points when the algorithm stops.
- **Optional:** Some rescaling factors: r_i , $i = 1, \dots, n$

1.3 “Fine tuning” CONDOR parameters

There are only a few parameters that have some influence on the convergence speed of CONDOR. We will review them here.

1.3.1 ρ_{start}

Most people accustomed with finite-difference gradient-based optimization algorithm are confusing the ρ_{start} or ρ_k parameters with the ϵ parameter used inside the finite difference formula:

$$\overline{\nabla f(\bar{x})}_i = \bar{g}_i(\bar{x}) \approx \frac{f(\bar{x} + \epsilon \bar{e}_i) - f(\bar{x})}{\epsilon}$$

The ρ_{start} or ρ_k parameters are totally different from the ϵ parameter. ϵ must be chosen as small as possible to accurately approximate the gradient. Contrary to ϵ , ρ_{start} should nearly never be taken small.

Recalling from step 1 of the algorithm: “The initial sampling points are separated by a distance of exactly ρ_{start} ”. If ρ_{start} is too small, we will build a local approximation $\mathcal{Q}_k(\delta)$ that will approximate only the noise inside the evaluations of the objective function.

What’s happening if we start from a point that is far away from the optimum? CONDOR will make big steps and move rapidly towards the optimum. At each iteration of the algorithm, we must re-construct $\mathcal{Q}_k(\delta)$, the quadratic approximation of $\mathcal{F}(x)$ around x_k . To re-construct $\mathcal{Q}_k(\delta)$ we will use as interpolating points, old evaluations of the objective function. Recalling from step 2 of the algorithm: “The sampling points are separated from the current point x_k by a distance of maximum $2\rho_k$ ”. Thus, if x_k is moving very fast inside the search space and if ρ_k is small, we will drop many old sampling points because they are “too far away”. A sampling point that has been dropped must be replaced by a new one, requiring a costly evaluation of the objective function. ρ_{start} should thus be chosen big enough to be able to “move” rapidly without requiring many evaluations to update/re-construct $\mathcal{Q}_k(\delta)$.

ρ_k represents the average distance between the sample points at iteration k . Above all it represents the “accuracy” we want to have when constructing $\mathcal{Q}_k(\delta)$. A small ρ_k will give us a local model $\mathcal{Q}_k(\delta)$ that represents at very high accuracy the local shape of the objective function $\mathcal{F}(x)$. Constructing a very accurate approximation of $\mathcal{F}(x)$ is very costly (for the reason explained in the previous paragraph). Thus, at the beginning of the optimization process, most of the time, a small ρ_{start} is a bad idea.

ρ_{start} can be set to a small value only if we start really close to the optimum point x^* . See section 1.3.3 to know more about this subject.

See also the end of section 1.3.4 to have more insight how to choose an appropriate value for ρ_{start} .

1.3.2 ρ_{end}

ρ_{end} is the stopping criterion. You should stop once you have reached the noise level inside the evaluation of the objective function.

1.3.3 Starting point x_{start}

The closer the starting point x_{start} is from the optimum point x^* , the better it is.

If x_{start} is far from x^* , the optimizer may fall into a local minimum of the objective function. The objective function encountered in aero-dynamic shape optimization are in a way “gentle”: they have usually only one minimum. The difficulty is coming from the noise inside the evaluations of the objective function and from the (long) computing time needed for each evaluation.

Equation 1.3 means that the steps sizes must be greater than $\frac{1}{2}\rho_k$. Thus, if you start very close to the optimum point x^* (using for example the hot-start functionality of CONDOR), you should consider to use a very small ρ_{start} otherwise the algorithm will be forced to make big steps at the beginning of the process. This behavior is easy to identify: it gives a spiraling path to the optimum.

1.3.4 Rescaling factors

From equation 1.3:

$$\delta_k = \min_{\delta} \mathcal{Q}_k(\delta) \text{ such that } \frac{\rho_k}{2} < \|\delta_k\|_2 < \Delta_k$$

you can see that the step size is maximum Δ_k in all the directions/axis of the search space (this is linked to the $\|\cdot\|_2 = L_2$ -norm used). This means that the “trust” we have inside $\mathcal{Q}_k(\delta)$ is spanned over the same distance in all the directions of the search space.

Let’s consider the following optimization problem that aims to optimize the shape of the hull of a boat:

$$\mathcal{F}(x^*) = \min_{x \in \mathbb{R}^2} \mathcal{F} \left(\begin{array}{l} x_1 = \text{length of the boat in mm} \\ x_2 = \text{angle between the port side (left)} \\ \quad \text{and the starboard side (right) at} \\ \quad \text{the bow of the boat in radian} \end{array} \right)$$

Clearly, x_1 is of magnitude around 10^4 and x_2 is of magnitude around 10^1 . Intuitively, it means that we can “trust” $\mathcal{Q}_k(\delta)$ over a greater distance along the direction x_1 than along direction x_2 . It means that we can do “big” steps in direction x_1 and “small” steps in direction x_2 . Unfortunately, without any scaling factors, CONDOR will limit the step size independently of the step direction, preventing to do “big” steps in direction x_1 (this is linked to the L_2 -norm which is a simple ball instead of an ellipsoid). The aim of the scaling factors is to have all the variable in the same order of magnitude. Let’s consider the following equivalent re-scaled optimization problem:

$$\mathcal{F}'(y^*) = \min_{y \in \mathbb{R}^2} \mathcal{F}'(y_1; y_2) = \min_{x \in \mathbb{R}^2} \mathcal{F}(x_1 = 10000 y_1 ; x_2 = 10 y_2)$$

CONDOR will find y^* , the optimum of $\mathcal{F}'(y)$ in a shorter time than the time needed to find x^* , the optimum of $\mathcal{F}(x)$ because $\mathcal{F}'(y)$ is well-scaled (or normalized).

In this example the re-scaling factors are $r_1 = 10000$ and $r_2 = 10$.

When automatic re-scaling is used, CONDOR will rescale automatically and transparently the variables to obtain the highest speed. The re-scaling factors r_i are computed in the following way: $r_i = \text{abs}(x_{\text{start},i}) + 1.0$. If some bounds constrained (b_l and b_u) are defined on axis i , then $r_i = b_{u,i} - b_{l,i}$.

To obtain higher convergence speed, you can override the auto-rescaling feature and specify yourself more accurate rescaling factors.

ρ_{start} and ρ_{end} are distances expressed in the rescaled-space. Usually, when using auto-rescaling, a good starting value for ρ_{start} is 0.1. This will make the algorithm very robust against noise. Depending on the noise level and on the experience you have with your objective function, you may, at a later time, decide to reduce ρ_{start} .

1.4 Parallel CONDOR

The different evaluations of $\mathcal{F}(x)$ are used to:

- (a) guide the search to the minimum of $\mathcal{F}(x)$ (see evaluation performed at step 4: computation of the “degree of agreement” τ_k). To guide the search, the information gathered until now and available in $\mathcal{Q}_k(\delta)$ is *exploited*.
- (b) increase the quality of the approximator $\mathcal{Q}_k(\delta)$ (see evaluation performed at step 2). To avoid the degeneration of $\mathcal{Q}_k(s)$, the search space needs to be additionally *explored*.

(a) and (b) are antagonist objectives like it is usually the case in the *exploitation/exploration* paradigm. The main idea of the parallelization of the algorithm is to perform the *exploration* on distributed CPU’s. Consequently, the algorithm will have better models $\mathcal{Q}_k(\delta)$ of $\mathcal{F}(x)$ at its disposal and choose better search directions, leading to a faster convergence.

When the dimension of the search space is low, there is no need to make many samples of $\mathcal{F}(x)$ to obtain a good approximation $\mathcal{Q}_k(\delta)$. Thus, the parallel algorithm is more useful for large dimension of the search space.

Chapter 2

XML-Based interface to CONDOR

The CONDOR optimizer is using as parameter on the command-line the name of a XML file containing all the required information needed to start the optimization process.

2.1 File structure of the XML-based configuration file

Let's start with a simple, rather complete, example. This example will be explained in detail in the following subsections.

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<configCONDOR>
  <!-- name of all design variables (tab separated) -->
  <varNames dimension="4">
    x1 x2 x3 x4
  </varNames>

  <objectiveFunction nIndex="5">

    <!-- name of the outputs that are computed by the
    simulator. If not enough names are given, the same
    names are used many times with a different prefixed
    number (tab separated) -->
    <indexNames>
      indexA indexB
    </indexNames>

    <!-- the aggregation function -->
    <aggregationFunction>

      indexA_1+indexB_1+indexA_2+indexB_2+indexA_3

    <!-- if there are several sub-objective,
    specify them here:
    <subAggregationFunction name="a">
    </subAggregationFunction> -->
```

```

</aggregationFunction>

<!-- blackbox objective function -->
<executableFile>
    OF/testOF
</executableFile>

<!-- objective function: input file -->
<inputObjectiveFile>
    optim.out
</inputObjectiveFile>

<!-- objective function: output file -->
<outputObjectiveFile>
    simulator.out
</outputObjectiveFile>

<!-- optimization of only a part of the variables -->
<variablesToOptimize>
    <!-- 1 2 3 4 -->
        1 1 1 1
</variablesToOptimize>
</objectiveFunction>

<!-- a priori estimated x (starting point) -->
<startingPoint>
<!-- 1 2 3 4 -->
    -1.2 -1.0 -1 3
</startingPoint>

<constraints>
    <!-- lower bounds for x -->
    <lowerBounds>
        <!--
            1 2 3 4 -->
            -10 -10 -10 -10
    </lowerBounds>

    <!-- upper bounds for x -->
    <upperBounds>
        <!--
            1 2 3 4 -->
            10 10 10 10
    </upperBounds>

    <!-- Here would be the matrix for linear
        inequalities definition if they were needed
    <linearInequalities>

```

```

        <eq>
        </eq>
</linearInequalities> -->

<!-- non-Linear Inequalities
<nonLinearInequalities>
        <eq>
        </eq>
</nonLinearInequalities> -->

<!-- non-Linear equalities
<equalities>
        <eq>
        </eq>
</equalities> -->
</constraints>

<!-- scaling factor for the normalization of
        the variables (optional) -->
<scalingFactor auto />

<!-- parameter for optimization:
        *rho_start: initial distance between
                sample sites (in the rescaled space)
        *rho_end: stopping criteria(in the
                rescaled space)
        *timeToSleep: when waiting for the result
                of the evaluation of the objective
                function, we check every xxx seconds
                for an appearance of the file containing
                the results (in second).
        *maxIteration: maximum number of iteration
-->
<optimizationParameters
        rhostart      =".1  "
        rhoend        ="1e-3"
        timeToSleep  =".1  "
        maxIteration ="1000"
/>

<!-- all the datafile are optional:
        *binaryDatabaseFile: the filename of the full
                DB data (WARNING!! BINARY FORMAT!)
        *asciiDatabaseFile: data to add to the full DB
                data file (in ascii format)
        *traceFile: the data of the last run are inside
                a file called? (WARNING!! BINARY FORMAT!) -->
<dataFiles

```

```

        binaryDatabaseFile="dbEvalsQ4N.bin"
        asciiDatabaseFile="dbEvalsQ4N.txt"
        traceFile="traceQ4N.bin"
    />

    <!-- name of the save file containing the end
         result of the optimization process -->
    <resultFile>
        traceQ4N.txt
    </resultFile>

    <!-- the sigma vector is used to compute sensibilities
         of the Obj.Funct. relative to variation of
         amplitude sigma_i on axis i -->
    <sigmaVector>
        1 1 1 1
    </sigmaVector>

    <!-- All the next tags are related to the configuration of the network. -->

    <!-- here would be the user data that will be shared among all
         the computer nodes, if needed:
    <userData> ... </userData> -->

    <!-- here would be information about NET address and configuration
         for each computer node:
    <cluster nMinParallelComputation="1">
        <node address="localhost" file="c:\sifbro1.xml"> ... </node>
        <node address="192.168.1.27" port="1305"> ... </node>
        ...
    </cluster> -->
</configCONDOR>

```

All the extra tags that are not used by CONDOR are simply ignored. You can thus include additional information inside the configuration file without any problem (it's usually better to have one single file that contains everything that is needed to start an optimization run). The full path to the XML file is given as first command-line parameter to the executable that evaluates the objective function.

2.1.1 Design variables and dimension of search space

The `varNames` tag describes the name of the variables we want to optimize. These variables will be referenced thereafter as *design variables*. These are three equivalent definitions of the same design variable names:

```

<varNames dimension="2" />

<varNames> X_01 X_02 </varNames>

```

```
<varNames dimension="2"> X_01 X_02 </varNames>
```

In the last case, the `dimension` attribute and the number of name given inside the `varNames` tag must match. When giving specific name, each name is separated from the next one by either a space, a tabulation or a carriage return (unix,windows). The `varNames` tag also describes what's the dimension of the search space. Let's define n , the dimension of the search space.

2.1.2 Objective function and index variables

The `objectiveFunction` tag describes the objective function. Usually, each evaluation of the objective function is performed by an external executable. The name of this executable is specified in the tag `executableFile`. This executable must read a file that contains the point where the objective function must be evaluated. The name of this file is specified in the tag `inputObjectiveFile`. In return, the executable write the result of the evaluation inside a file specified in the tag `outputObjectiveFile`.

When CONDOR runs the executable, it gives three extra parameters on the command-line: the full path to the XML-configuration file, the `inputObjectiveFile` and the `outputObjectiveFile`. The result file `outputObjectiveFile` contains a vector V_{iv} of numbers called *index variables* (iv). There are 2 ways to specify the dimension of V_{iv} :

1. Use the `nIndex` attribute
2. If the `nIndex` attribute is missing then the dimension of v_{iv} is the number of index variable names given inside the tag `indexNames`

Let's define $nIndex$, the number of *index variables*. We have: $V_{iv} \in \mathfrak{R}^{nIndex}$. The values inside V_{iv} will be saved inside an internal database. They will be used to enable "hot start". Each *index variable* has a name. The following example demonstrates two equivalent definition of the same three index variable names:

```
<objectiveFunction nIndex="3">
  ...

<objectiveFunction>
  <indexNames> Y_001 Y_002 Y_003 </indexNames>
  ...
```

These are two equivalent definition of the same six index variable names:

```
<objectiveFunction nIndex="6">
  <indexNames> U V </indexNames>
  ...

<objectiveFunction>
  <indexNames> U_1 V_1 U_2 V_2 U_3 V_3 </indexNames>
  ...
```

2.1.3 Aggregation of the index variables

Let's assume that you want to optimize a seal design. For a seal optimization, we want to minimize the leakage at low speed and high pressure(1), minimize the efficiency-loss due to friction at high speed(2), maximize the "lift" at low speed and low pressure(3). The overall quality of a specific design of a seal, we will be computed based on 3 different simulations of the same seal design at the following three operating point: low speed and high pressure(1), high speed(2), low speed and low pressure(3). Suppose each run of the simulator gives as result four *index variables*: A,B,C,D. We will have the following XML configuration (the content of the `aggregationFunction` tag will be explained hereafter):

```

...
<objectiveFunction nIndex="12">
  <indexNames> A B C D </indexNames>
  <aggregationFunction>
    <subAggregationFunction name="leakage">
      <!-- compute the leakage based on A_1, B_1, C_1, D_1 -->
      5*(A_1^3)
    </subAggregationFunction>
    <subAggregationFunction name="friction_loss">
      <!-- compute the efficiency loss due to friction
      based on A_2, B_2, C_2, D_2 -->
      2.1*(-B_1^2+C_1^2)
    </subAggregationFunction>
    <subAggregationFunction name="lift">
      <!-- compute the "lift" based on A_3, B_3, C_3, D_3 -->
      0.5*(sqrt(D_3))
    </subAggregationFunction>
  </aggregationFunction>
...

```

All the values of the *index variables*) must be aggregated into one number that will be optimized by CONDOR. The aggregation function is given in the tag `aggregationFunction`. If this tag is missing, CONDOR will use as aggregation function the sum of all the *index variables*.

You can define inside the tag `aggregationFunction`, some sub-objectives. Each sub-objective is defined inside the tag `subAggregationFunction`. The tag `subAggregationFunction` can have an optional parameter `name` that will appear inside the `tracefile`. The global aggregation function is the sum of all the sub-objectives. You can look inside the trace-file of the optimization process to see how the different subobjectives are comparing together and adjust accordingly the equations defining the subobjectives. Typically, this procedure is iterative: you define some approximate sub-objectives functions, you run CONDOR, you observe "where" CONDOR is heading for, you look inside the trace file to see what's the reason of such direction, you adjust the different sub-objectives giving more or less weight to specific sub-objectives and you restart CONDOR, etc.

The `aggregationFunction` tag or the `subAggregationFunction` tag contains simple equations that can have as "input variables" all the *design variables* and all the *index variables*. The mathematical operators that are allowed are: `+`, `-`, `*`, `/`, `^`, `exp`, `log` (base:e), `sqrt`, `sin`, `cos`, `tan`,

ctan, asin, acos, atan, actan, sinh, cosh, tanh, ctanh, asinh, acosh, atanh, actanh, fabs.

In the example above (about seal design), the sub-objectives are the “leakage”, the “efficiency-loss due to friction” and the “lift”. The weights of the different sub-objectives have been adjusted to respectively 5, 2.1 and 0.5 by the design engineer. The values of the *index variables* A_1, B_1, C_1, D_1, A_2, B_2, C_2, D_2, A_3, B_3, C_3, D_3 for all the different computed seal designs have been saved inside the database of CONDOR and can be re-used to “hot-start” CONDOR. The initialization phase of CONDOR is usually time consuming because we need to compute many samples of the objective function $\mathcal{F}(x)$ to build the first $\mathcal{Q}_k(\delta)$. The initialization phase can be strongly shortened using the “hot-start” or using the parallel version of CONDOR.

There is an additional feature that is mainly useful for quick demonstration purposes: If none of the sub-aggregation functions are using any *index variables*, you don’t need any external executable to compute the objective function. You can thus omit the following tags: `indexNames`, `executableFile`, `inputObjectiveFile`, `outputObjectiveFile`. You can also omit the following attributes: the `nIndex` attribute of the `objectiveFunction` tag, the `timeToSleep` attribute of the `optimizationParameters` tag, the `binaryDatabaseFile` attribute and the `asciiDatabaseFile` attribute of the `dataFiles` tag.

2.1.4 Selection of a part of the search space

The `variablesToOptimize` tag defines which design variables CONDOR will optimize. This tag contains a vector O of dimension n ($O \in \mathbb{R}^n$). If O_i equals 0 the design variable of index i will not be optimized.

2.1.5 Starting point

The `startingPoint` tag defines what’s the starting point. It contains a vector x_{start} of dimension n . If this tag is missing, CONDOR will use as starting point the best point found inside its database. If the database is empty, then CONDOR issues an error and stops.

2.1.6 Constraints

The `constraints` tag defines what are the constraints. It’s an optional tag. It contains the tags `lowerBounds` and `upperBounds` which are self explanatory. It also contains the tag `linearInequalities` which describes linear inequalities. If the feasible space is described by the following three linear inequalities:

$$\begin{pmatrix} -1 & -1 \\ 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \geq \begin{pmatrix} -4 \\ 4 \\ 0 \end{pmatrix}$$

then we will have:

```
<constraints>
  <linearInequalities>
    -1 -1 -4
```

```

    1  1  4
   -1  1  0
</linearInequalities>
...

```

or by:

```

<constraints>
  <linearInequalities>
    <eq> -1 -1 -4 </eq>
    <eq>  1  1  4 </eq>
    <eq> -1  1  0 </eq>
  </linearInequalities>
...

```

A carriage return or a `<eq>..</eq>` tag pair is needed to separate each linear inequality. The two notations cannot be mixed. The `constraints` tag also contains the `nonLinearInequalities` tag that describes non linear inequalities $c_i(x)$. The feasible space is described by $c_i(x) \geq 0 \ \forall i$. Each non-linear inequalities $c_i(x)$ must be defined inside a separate `<eq>..</eq>` tag pair. For example the two non-linear constraints $1 - x_0^2 - x_1^2 \geq 0$ and $x_1 - x_0^2 \geq 0$ are defined by:

```

...
<varNames> x0 x1 </varNames>
...
<constraints>
  <nonLinearInequalities>
    <eq> 1-x0*x0-x1*x1 </eq>
    <eq> -x0*x0+x1 </eq>
  </nonLinearInequalities>
...

```

If there is only one non-linear inequality, you can write it directly, without the `eq` tags. CONDOR also handles a primitive form of equality constraints. The equalities must be given in an explicit way. For example:

```

...
<varNames> x0 x1 x2 </varNames>
<constraints>
  <equalities> x2=(1-x0)^2 </equalities>
...

```

(the `<eq>...</eq>` tag pair has been omitted because there is only one equality).

2.1.7 Re-scaling factors

The re-scaling factors r_i , $i = 1, \dots, n$ are defined inside the `scalingFactor` tag. For more information about the re-scaling factors, see section 1.3.4. If the re-scaling factors are missing, CONDOR assumes $r_i = 1 \ \forall i$. To have automatic computation of the re-scaling factors, write:

```

<scalingFactor auto/>

```

2.1.8 Optimization parameters

The `optimizationParameters` tag contains the following attributes:

- **rhostart**: initial distance between sample sites (in the rescaled space). See section 1.3.1 for more information.
- **rhoend**: stopping criteria(in the rescaled space). See section 1.3.2 for more information.
- **timeToSleep**: when waiting for the result of the evaluation of the objective function, we check every *xxx* seconds for an appearance of the file containing the results (in second).
- **maxIteration**: maximum number of iterations of the optimization algorithm.

2.1.9 Data files

The `dataFiles` tag contains the following attributes:

- **binaryDatabaseFile**: the filename of the full DB data (WARNING!! BINARY FORMAT!). If the file is missing, a new one will be created containing the evaluations that are inside the **asciiDatabaseFile** and the evaluations performed during the optimization process.
- **asciiDatabaseFile**: evaluation data (in ascii format) which will be added in memory and on the disk to the full binary DB. No error will be echoed if the file is missing or empty.
- **traceFile**: This tag contains the name of the file that contains the data of the last run of CONDOR (WARNING!! BINARY FORMAT!).

All binary files can be converted to ASCII files using the 'matConvert' utility.

2.1.10 Final output file

The name of the file containing the end result of the optimization process is given inside the `resultFile` tag. This is an ascii file that contains: the dimension of search-space, the total number of function evaluation (total NFE), the number of function evaluation before finding the best point, the value of the objective function at solution, the solution vector x^* , the Hessian matrix at the solution H^* , the gradient vector at the solution g^* (it should be zero if there is no active constraint), the lagrangian Vector at the solution (for lower,upper,linear,non-linear constraints), the sensitivity vector.

2.1.11 Sensitivities of the objective function in regards to small perturbations on the solution point

The sigma vector that is used to compute sensitivities of the Objective Function relatively to variation of amplitude σ_i on axis i is given inside the `sigmaVector` tag.

2.1.12 Network configuration

The parallel/distributed optimization mode of CONDOR is based on a client-server approach. The main computer will use evaluations performed on client computers in order to increase the quality of the local model $\mathcal{Q}_k(\delta)$ of the objective function of $\mathcal{F}(x)$. See section 1.4 for more details about the algorithm.

If n is the dimension of the search space, then CONDOR will never use more than $\frac{1}{2}(n+1)^2$ computers simultaneously.

All the client computers must be waiting to “serve” the master/server computer. This means that, on each of the client computers, the CONDOR optimizer should run in client-mode. To run CONDOR in client mode, simply type:

```
xmlCondor -c [<port_number>]
```

This command will force CONDOR to wait (without consuming any local CPU resources) until the master node asks for an evaluation of the objective function. The client node will be contacted by the master computer via the default port 4320. You can optionally change the default port on the command line. Only values between 1024 and 65535 are accepted.

NOTE: When Condor is run in client-mode, it does NOT check the expiration date of your license. It means that the client computers can be completely disconnected from any internet connection.

If there is a firewall between the master and the node, you should “open” the port on the client, so that the master can contact it. The master is always initiating the connection to the client.

If there is a NAT(Network address translation) system between the master and the node, you should “forward” the port to the client, so that the master can contact it. The master is always initiating the connection to the client.

To perform an evaluation, a client node should know at least some “classical” information: the name of the local `executableFile`, the name of the local `inputObjectiveFile` and the name of the local `outputObjectiveFile`: see subsection 2.1.2 to know more about this subject. These informations for all the nodes are grouped together inside the main XML-configuration file on the master node.

On the other hand, the master needs to know where the client nodes are. What are their IP address and their port number.

Here is a sample XML-file for parallel/distributed optimization that includes all the required information:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<configCONDOR>
  <varNames dimension="2" />
  <objectiveFunction nIndex="1">
    <executableFile> sif0F\xml0FSIF.exe </executableFile>
```

```

        <inputObjectiveFile>    C:\sifcondor.out  </inputObjectiveFile>
        <outputObjectiveFile>   C:\sif.out  </outputObjectiveFile>
    </objectiveFunction>

    ...

<userData> 115 </userData>
<cluster nMinParallelComputation="1">

    <node address="localhost" file="c:\sifbro1.xml">
        <executableFile>    sifOF\xml0FSIF.exe    </executableFile>
        <inputObjectiveFile> C:\sifcondor1.out  </inputObjectiveFile>
        <outputObjectiveFile> C:\sif1.out  </outputObjectiveFile>
    </node>

    <node address="192.168.1.26" port="1305" file="c:\sifbro12.xml">

        <executableFile>    sifOF\xml0FSIF.exe    </executableFile>
        <inputObjectiveFile> C:\sifcondor2.out  </inputObjectiveFile>
        <outputObjectiveFile> C:\sif2.out  </outputObjectiveFile>

        <optionalNodeParameters> coucou2 </optionalNodeParameters>
    </node>
</cluster>
</configCONDOR>

```

This file describes a configuration with 2 client computers located at address "localhost" (default port: 4320) and address 192.168.1.26 (customized port:1305). The tags `executableFile`, `inputObjectiveFile` and `outputObjectiveFile` are self-explanatory: see subsection 2.1.2.

The `nMinParallelComputation` attribute of the `cluster` tag is optional. It means that, at each iteration of the algorithm, the master computer is waiting for at least "nMinParallelComputation" parallel computation to complete before proceeding further. This option could be useful to force CONDOR to wait for completion of remote evaluations. Usually, waiting for such evaluations, is a simple waste of time. I usually recommend to remove the `nMinParallelComputation` attribute.

The aim of the XML configuration-file on the master computer is to group all the information needed to operate all the nodes of the cluster. CONDOR is sending through the network (parts of) the XML file so that all the nodes of the cluster can have access to its content. The "globalization" of the XML configuration-file is controlled via the `userData` tag and `file` attribute of the `node` tag. If the `file` attribute is given, a local XML file will be generated on the client node before running any objective function evaluation. The name of the local distant XML file is given by the `file` attribute. The content of the remote XML-file is illustrated in figure 2.1. The content of the `userData` will be seen by all the nodes. The content of the `node` tag related to client X will be seen only by the client X .

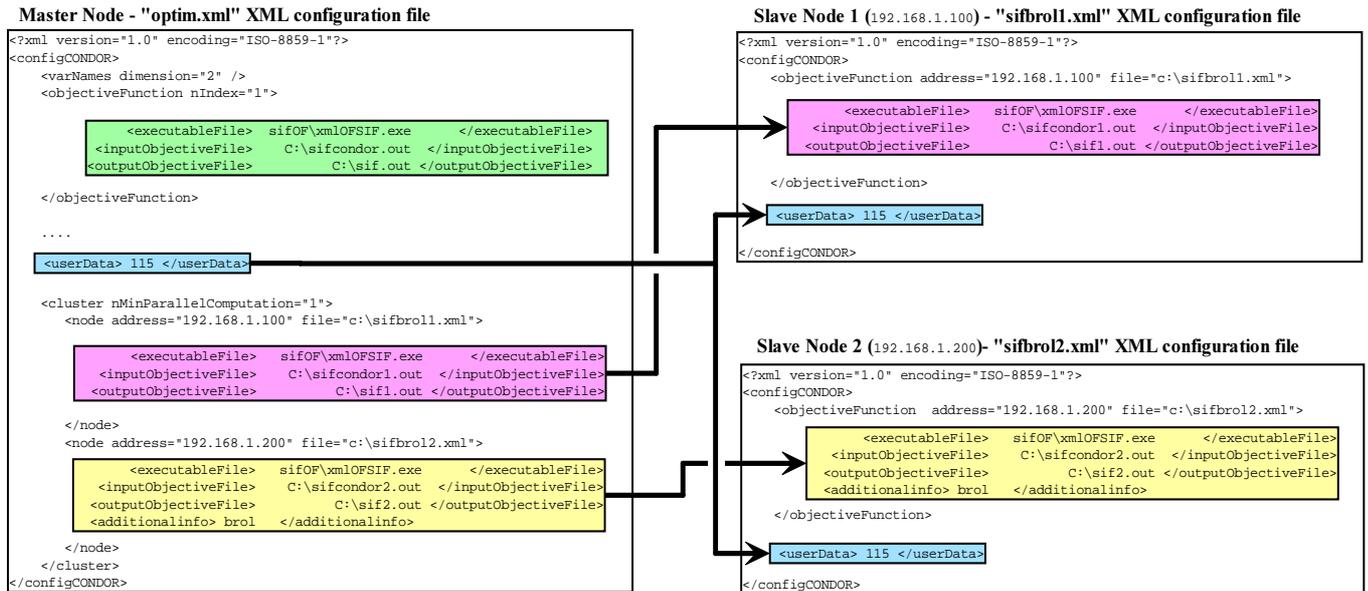


Figure 2.1: “globalization” of the XML configuration-file

2.2 File structure of the inputObjectiveFile

This file contains the point $x \in \mathcal{R}^n$ where the objective function must be evaluated. It's an ascii file containing only one line. This line contains all the component x_i of x separated by a tabulation. The `inputObjectiveFile` is given as second command-line parameter to the executable that evaluates the objective function.

2.3 File structure of the outputObjectiveFile

This file can be ascii or binary. If the first byte of the file is 'A' then the file will be ascii. If the first byte of the file is 'B' then the file will be binary. The `outputObjectiveFile` is given as third command-line parameter to the executable that evaluates the objective function.

2.3.1 ascii structure

The file contains at least 3 lines:

- **First line:** contains only one character: 'A'.
- **Second line:** contains only one number. If this number is 1 then the evaluation of the objective function at the given point has succeeded. If this number is 0, then there has been a failure.
- **Third line and next lines:** contains the value of all the *index variables* separated by a space, a tabulation or a carriage return. If some extra numbers are present inside the file they are ignored. If some *index variables* are NaN or Inf then the evaluation is seen has a failure.

2.3.2 binary structure

The structure is the following:

- **First byte:** the character 'B'.
- **Second byte:** If this byte is '1' then the evaluation of the objective function at the given point has succeeded. If this byte is '0', then there have been a failure.
- **Third byte and next bytes:** contains the value of all the *index variables* in binary format in double precision (floating point numbers in 8 bytes)(The classical 'fread()' C function is used to read the file). There is no carriage return anywhere. If some extra bytes are present inside the file they are ignored. If some *index variables* are NaN or Inf then the evaluation is seen has a failure.

2.4 File structure of the binaryDatabaseFile

The `binaryDatabaseFile` is a simple matrix stored in binary format. Each line corresponds to an evaluation of the objective function. You will find on a line all the *design variables* followed by all the *index variables* ($n + nIndex$ numbers).

The utility 'matConvert.exe' converts a full precision binary matrix file to an easy manipulating matrix ascii files.

The structure of the binary matrix file is the following:

- **Header:** the 13 characters 'CONDORMBv1.0' (this stands for CONDOR/Matrix/Binary/v1.0).
- **Dimensions:** number of lines (integer in 4 bytes, unsigned) followed by number of columns (integer in 4 bytes, unsigned)
- **Column names:** the total sum of all the bytes needed to store in memory the names of all the columns (integer in 4 bytes, signed) (space for null characters are included in the sum). If there is no name, the sum is zero. This is followed by the name of all the columns separated by a null (=0) character.
- **data:** contains all the values of the elements of the matrix stored in binary double precision (floating point numbers in 8 bytes).

2.5 File structure of the asciiDatabaseFile

The `asciiDatabaseFile` is a simple matrix stored in ascii format. Each line of the matrix corresponds to an evaluation of the objective function. You will find on a line all the *design variables* followed by all the *index variables*. ($n + nIndex$ numbers)

The utility 'matConvert.exe' converts a full precision binary matrix file to an easy manipulating matrix ascii files.

The structure of the ascii matrix file is the following:

- **Line 1: Header:** the 13 characters 'CONDORMAv1.0' (this stands for CONDOR/Matrix/ASCII/v1.0).

- **Line 2&3: Dimensions:** the number of lines inside the matrix is stored in line 2. The number of columns inside the matrix is stored in line 3.
- **Line 4: Column names:** The name of all the columns separated by a tabulation character.
- **Line 5 and following: Data:** contains all the values of the elements of the matrix. One line of the ascii file corresponds to one line of the matrix.

2.6 File structure of the traceFile

The `traceFile` is a simple matrix stored in binary format. The utility 'matConvert.exe' converts a full precision binary matrix file to an easy manipulating matrix ascii files. Each line of the matrix corresponds to an evaluation of the objective function. You will find on a line:

1. All the *design variables* (n numbers)
2. All the sensibilities computed using the Sigma vector. (n numbers)
3. The global sensibility (the sum of all the sensibilities). (1 number)
4. If some `subAggregationFunction` are defined, you will find their value here (? numbers)
5. The value of the objective function that is the result of the aggregation process (1 number)
6. A flag that indicates if the evaluation considered on this line has failed. If this flag is 1 then there have been a failure. This flag is normally zero (no failure of the evaluation of the objective function). (1 number)

2.7 Examples

Most of the time, when researchers are confronted to a noisy optimization problem, they are using an algorithm that is a combination of Genetic Algorithm and Neural Network. This algorithm will be referred in the following text under the following abbreviation: (GA+NN). The principle of this algorithm is the following:

1. Sample the objective function at different points of the space to obtain an initial database of evaluation.
2. Use the database of evaluation to build a Neural Network approximation of the real objective function $\mathcal{F}(x)$ that we want to optimize.
3. Use a genetic algorithm to find the minimum X_k of the Neural Network build at the previous step. Evaluate $\mathcal{F}(X_k)$ and add the result of the evaluation to the database of evaluation.
4. if termination criteria is not met go back to step 2.

This approach has no proof of convergence and there is no guarantee that it will find a simple local minimum. In opposition CONDOR is part of a family of optimizers that are always convergent to a local optimum. The (GA+NN) approach can be made globally convergent using a *surrogate* approach [KLT97, BDF⁺99]. The *surrogate* approach has a strong mathematical background and is assured to always converge to a local minimum.

2.7.1 The classical Rosenbrock Objective function

The xml-configuration file for this example is the following:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<configCONDOR>
  <varNames> x_1 x_2 </varNames>
  <objectiveFunction>
    <aggregationFunction>
      100*(x_2-x_1^2)^2+(1-x_1)^2
    </aggregationFunction>
  </objectiveFunction>
  <startingPoint> -1.2 -1.0 </startingPoint>
  <constraints>
    <lowerBounds> -10 -10 </lowerBounds>
    <upperBounds> 10 10 </upperBounds>
  </constraints>
  <optimizationParameters
    rhoStart      =" 1      "
    rhoEnd        =" 1e-2  "
    maxIteration  =" 1000  "
  />
  <dataFiles traceFile="traceRosen.dat" />
  <resultFile> resultsRosen.txt </resultFile>
  <sigmaVector> 1 1 </sigmaVector>
</configCONDOR>
```

You can run this example with the script file named 'testRosen'. In the optimization community this function is a classical test-case. The minimum of the function is at (1,1). To reach it the optimizer must follow the bottom of a narrow "valley". The edge of the valley are very steep and the bottom is nearly flat. It's thus very difficult to find the right direction to follow. Following the slope is even more difficult as the search direction in the valley is changing continuously. See figure 2.2 for an illustration of the Rosenbrock function.

For optimizers that are following the slope (like CONDOR), this function is a real challenge. In opposition, (GA+NN) optimizers are not using the concept of slope and should not have any special difficulties to find the minimum of this function. Beside (GA+NN) are most efficient on small dimensional search space (in opposition to CONDOR). They should thus exhibit very good performances compared to CONDOR on this problem. Using CONDOR we obtain:

- best (lowest) value found: 7.480071e-007
- Number of function Evaluation to reach the optimum: 77
- Number of function Evaluation before stop: 79
- Solution Vector is : [1.000690e+000, 1.001432e+000]

The performances of CONDOR on this problem (compared to the performances of (GA+NN) optimizers) are rather low, as expected (a typical (GA+NN) optimizer requires at least 140 evaluations of the objective function (usually:800 evaluations) for less precision on the minimum). In this example, CONDOR cannot go "directly" to the minimum: it must avoid the

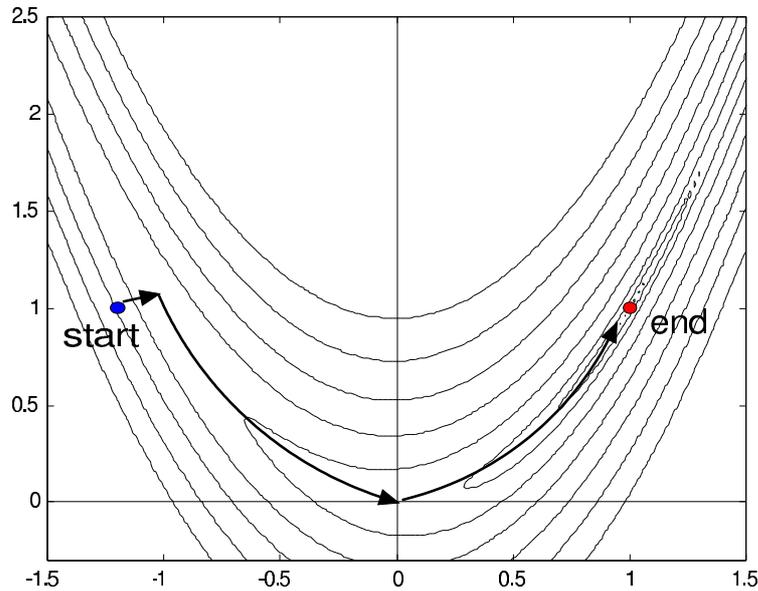


Figure 2.2: The Rosenbrock function

big “bump” in the function and go through the point $(0,0)$ before being allowed to “fall” into the minimum. This explains why the performances of CONDOR are poor. In opposition, a (GA+NN) algorithm starts by sampling all the space. This strategy allows to start from a point that is already on the right side of the barrier (a point that has $x_1 > 0$). Starting from there, there is no “bump” anymore to avoid. A future extension of CONDOR will be able to start simultaneously from different points of the space. It will then exchange information between each trajectory to increase convergence speed. This new strategy should increase the convergence speed substantially on such problems.

2.7.2 A simple quadratic in two dimension

In the previous subsection, we have seen that the performances of CONDOR on the Rosenbrock function are low because the optimizer must avoid a “bump” inside the objective function before it can “home” to the minimum. What happens if we remove this ‘bump’? Let’s consider the following xml-configuration file:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<configCONDOR>
  <varNames> x_0 x_1 </varNames>
  <objectiveFunction>
    <aggregationFunction> (x_1-2)^2+(x_0-2)^2 </aggregationFunction>
  </objectiveFunction>
  <startingPoint> 0 0 </startingPoint>
  <constraints>
    <lowerBounds> -10 -10 </lowerBounds>
    <upperBounds> 10 10 </upperBounds>
  </constraints>
</configCONDOR>
```

```

<scalingFactor auto/>
<optimizationParameters
  rhostart    =" 1    "
  rhoend      =" 9e-1 "
  maxIteration=" 1000 "
/>
<dataFiles traceFile="traceQ2.dat" />
<resultFile> resultsQ2.txt </resultFile>
<sigmaVector> 1 1 </sigmaVector>
</configCONDOR>

```

You can run this example with the script file named 'testQ2'. Using CONDOR we obtain:

- best (lowest) value found: 9.860761e-032
- Number of function Evaluation to reach the optimum: 8
- Number of function Evaluation before stop: 9
- Solution Vector is : [2.000000e+000, 2.000000e+000]

As comparison, a (GA+NN) algorithm requires between 150 and 500 evaluations of the objective function before reaching an approximative optimum point (the value of the objective function is around $1e-12$). Beside, the performances of (GA+NN) optimizers are dropping very rapidly when the search space dimension increases.

2.7.3 Simple standard case (no failure)

A xml-configuration file for the standard case is given in section 2.1. You can run this example with the script file named 'testQ4N'. The objective function is computed in an external executable and is:

$$f(x_1, x_2, x_3, x_4) = \sum_{i=1}^4 (x_i - 2)^2 + rand(1e - 5)$$

where $rand(t)$ is a random number with uniform distribution that is between 0 and t ($0 \leq rand(t) < t$). This random number simulates the noise inside the evaluation of the objective function. An interesting test to perform is to change the `variablesToOptimize` tag and re-run CONDOR. Using the database of old evaluation, CONDOR will build the first quadratical approximation $\mathcal{Q}_k(\delta)$ of $\mathcal{F}(x)$ (see step 1. of the algorithm) without requiring the normal, classical large number of evaluations. CONDOR will start "for free". Figure 2.3 is representing the trace of 100 runs of the optimizer (with a noise of amplitude $1e - 4$). You can see on figure 2.3 that usually after 50 evaluations of the objective function, we find the optimum. Because of the noise, CONDOR continues to sample the objective function and does not stop immediately.

The script-file named 'testQ4N' optimizes the same objective function but, this time, without noise. Using CONDOR we obtain:

- best (lowest) value found: 1.972152e - 031
- Number of function Evaluation to reach the optimum: 17
- Number of function Evaluation before stop: 18

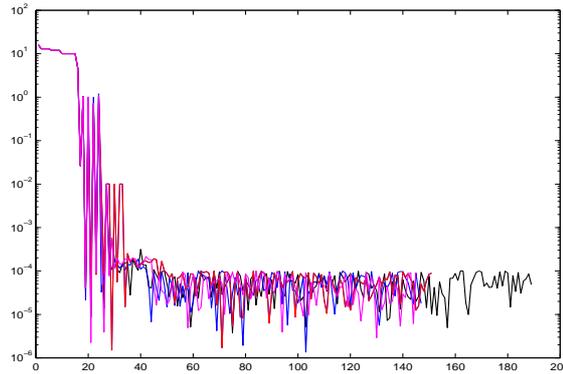


Figure 2.3: the trace of some runs of the optimizers

2.7.4 Simple standard case (with failures)

The xml-configuration file for this example is given in section 2.1. The content of the tag `executableFile` needs to be changed: it must be replaced by `”OF/testOFF”`. You can run this example with the script file named `’testQ4NF’`. The objective function is the same as in the previous subsection: a simple 4 dimensional quadratic centered at $(2, 2, 2, 2)$ and perturbed with a noise of maximum amplitude $1e - 5$. The failures are simulated using a random number:

```
if rand(1.0) > .55 then fail else succeed.
```

The evaluation of the objective function at the given starting point cannot fail. If this happens, CONDOR has no starting point and it stops immediately.

2.7.5 A badly scaled objective function

The xml-configuration file for this example is the following:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<configCONDOR>
  <varNames> x0 x1 </varNames>
  <objectiveFunction>
    <aggregationFunction>
      100*(x1/1000-x0^2)^2+(1-x0)^2
    </aggregationFunction>
  </objectiveFunction>
  <startingPoint> -1.2 -1000 </startingPoint>
  <constraints>
    <lowerBounds> -10 -10000 </lowerBounds>
    <upperBounds> 10 10000 </upperBounds>
  </constraints>
  <scalingFactor auto/>
  <optimizationParameters
    rhostart    =" .1  "
    rhoend      =" 1e-5 "
    maxIteration=" 1000 "
  />
```

```

<dataFiles traceFile="traceScaledRosen.dat" />
<resultFile> resultsScaledRosen.txt </resultFile>
<sigmaVector> 1 1 </sigmaVector>
</configCONDOR>

```

You can run this example with the script file named 'testScaledRosen'. As explained in section 1.3.4, the design variables x_0 and x_1 must be in the same order of magnitude to obtain high convergence speed. This is not the case here: x_1 is 1000 times greater than x_0 . Some appropriate re-scaling factors are computed by CONDOR and applied. Using CONDOR we obtain:

- best (lowest) value found: 2.907483e-012
- Number of function Evaluation to reach the optimum: 39
- Number of function Evaluation before stop: 46
- Solution Vector is : [1.000001e+000, 1.000003e+003]

After removing the line `<scalingFactor auto/>`, we obtain:

- best (lowest) value found: 5.165404e-015
- Number of function Evaluation to reach the optimum: 237
- Number of function Evaluation before stop: 294
- Solution Vector is : [9.999999e-001, 9.999999e+002]

This demonstrates the importance of the scaling factors.

2.7.6 Optimization with linear and box constraints

One technique to deal with linear and box constraints is the "Gradient Projection Methods". In this method, we follow the gradient of the objective function. When we enter the infeasible space, we will simply project the gradient into the feasible space. The convergence speed of this algorithm is, at most, linear, requiring many evaluation of the objective function.

A straightforward (unfortunately false) extension to this technique is the "Newton Step Projection Method". This technique should allow (if it works) a very high (quadratical) speed of convergence. It is illustrated in figure 2.4. This method is the following:

1. Construct a quadratic approximation $Q_k(\delta)$ of $\mathcal{F}(x)$ around the current point x_k .
2. Find the minimum δ_k of $Q_k(\delta)$ and go to $x_k + \delta_k$. δ_k is called the "Newton Step".
3. If $x_k + \delta_k$ is feasible then $x_{k+1} = x_k + \delta_k$.
If $x_k + \delta_k$ is infeasible then project it to the feasible space. This projection is x_{k+1} .
4. If stopping criteria not met, go back to step 1.

In figure 2.4, the current point is $x_k = O$. The Newton step (δ_k) lead us to point P that is infeasible. We project P into the feasible space: we obtain B. Finally, we will thus follow the trajectory OAB, that *seems* good.

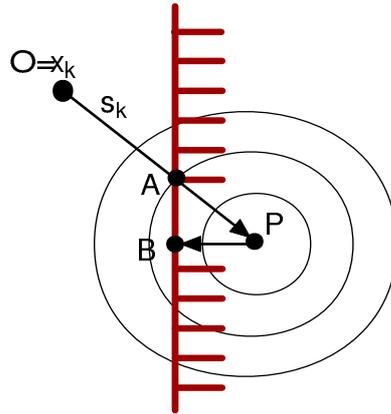


Figure 2.4: "newton's step projection algorithm" seems good.

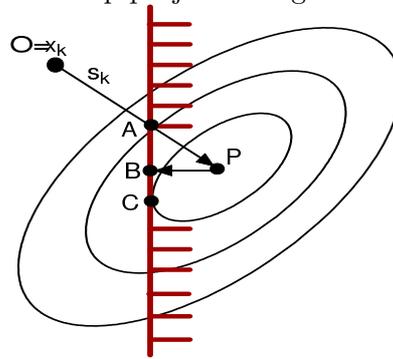


Figure 2.5: "Newton's step projection algorithm" is failing.

In figure 2.5, we can see that the "Newton step projection algorithm" can lead to a false minimum. As before, we will follow the trajectory OAB. Unfortunately, the real minimum of the problem is C.

Despite its wrong foundation, the "Newton Step Projection Method" is very often encountered [BK97, Kel99, SBT⁺92, GK95, CGP⁺01]. CONDOR uses an other technique based on active-set method that allows very high (quadratical) speed on convergence even when "sliding" along a constraint.

Let's have a small example:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<configCONDOR>
  <varNames> x0 x1 </varNames>
  <objectiveFunction>
    <aggregationFunction> (x0-2)^2+(x1-5)^2 </aggregationFunction>
  </objectiveFunction>
  <startingPoint> 0 0 </startingPoint>
  <constraints>
    <lowerBounds> -2 -3 </lowerBounds>
    <upperBounds> 3 3 </upperBounds>
    <linearInequalities>
```

```

        <eq>  -1  -1  -4 </eq>
    </linearInequalities>
</constraints>
<scalingFactor auto/>
<optimizationParameters
    rhoStart    =" 1  "
    rhoEnd     =" 1e-2 "
    maxIteration=" 1000 "
/>
<dataFiles traceFile="traceSuperSimple.dat"  />
<resultFile>  resultsSuperSimple.txt  </resultFile>
<sigmaVector> 1 1 </sigmaVector>
</configCONDOR>

```

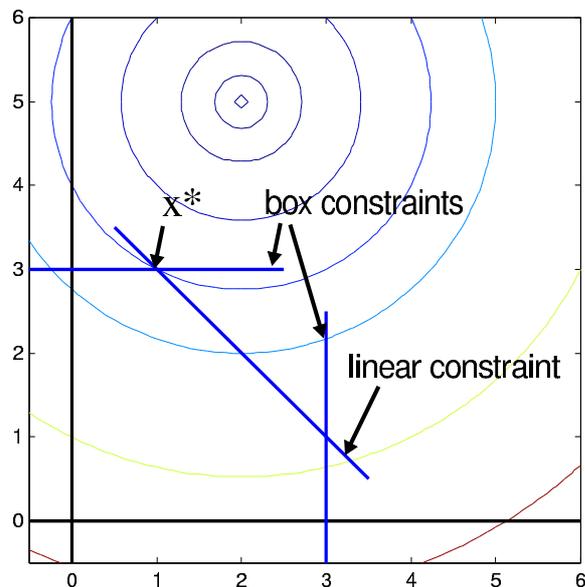


Figure 2.6: Optimization with Linear and Box constraints

You can run this example with the script file named 'testSuperSimple'. This problem is illustrated in figure 2.6. Using CONDOR, we obtain

- best (lowest) value found: 5.0
- Number of function Evaluation to reach the optimum: 8
- Number of function Evaluation before stop: 10
- Solution Vector is : [1.000000e+000, 3.000000e+000]

At the solution, the upper bound on variable x_1 and the first linear constraint are active.

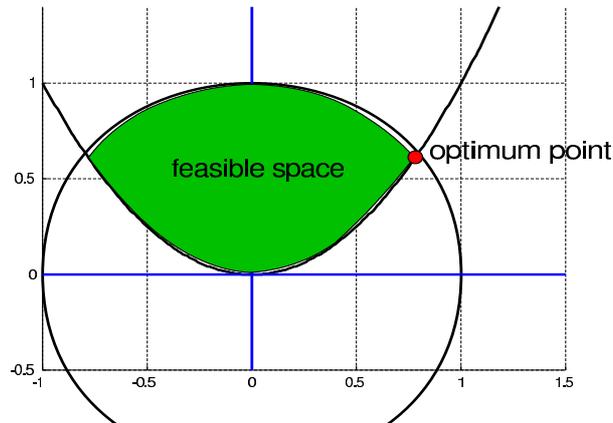


Figure 2.7: Feasible space of Fletcher's problem

2.7.7 Optimization with non-linear constraints

The xml-configuration file for this example is the following:

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<configCONDOR>
  <varNames> v0 v1 </varNames>
  <objectiveFunction>
    <aggregationFunction> -v0 </aggregationFunction>
  </objectiveFunction>
  <startingPoint> 0 0 </startingPoint>
  <constraints>
    <!-- non-Linear Inequalities: v is feasible <=> c_i(v)>=0 -->
    <nonLinearInequalities>
      <eq> 1-v0*v0-v1*v1 </eq> <!-- the circle -->
      <eq> v1-v0*v0 </eq> <!-- the parabola -->
    </nonLinearInequalities>
  </constraints>
  <optimizationParameters
    rhoStart = ".1 "
    rhoEnd = "1e-6 "
    maxIteration=" 1000 "
  />
  <dataFiles traceFile="traceFletcher.dat" />
  <resultFile> resultsFletcher.txt </resultFile>
  <sigmaVector> 1 1 </sigmaVector>
</configCONDOR>
```

You can run this example with the script file named 'testFletcher'. The feasible space is illustrated in figure 2.7. Using CONDOR, we obtain

- best (lowest) value found: -7.861514e-001
- Number of function Evaluation to reach the optimum: 13
- Number of function Evaluation before stop: 16

- Solution Vector is : [7.861514e-001, 6.180340e-001]

2.7.8 Distributed Optimization on several CPU's

The xml-configuration file for this example is the following:

```
<?xml version="1.0" encoding="ISO-8859-1"?> <configCONDOR>
  <varNames dimension="2" />
  <userData>
    <functionIndex> 115 </functionIndex>
  </userData>

  <objectiveFunction nIndex="1">
    <executableFile>   sifOF\xmlOFSIF.exe       </executableFile>
    <inputObjectiveFile> C:\sifcondor.out     </inputObjectiveFile>
    <outputObjectiveFile> C:\sif.out         </outputObjectiveFile>
  </objectiveFunction>

  <startingPoint>    0  -1.0  </startingPoint>
  <optimizationParameters
    rhostart    =".1  "
    rhoend      ="1e-3"
    timeToSleep =".1  "
    maxIteration="1000"
  />

  <resultFile>      resultsSif.txt    </resultFile>

  <cluster nMinParallelComputation="1">
    <node address="127.0.0.1" file="c:\sifbro11.xml">
      <executableFile>   sifOF\xmlOFSIF.exe       </executableFile>
      <inputObjectiveFile> C:\sifcondor1.out     </inputObjectiveFile>
      <outputObjectiveFile> C:\sif1.out         </outputObjectiveFile>
    </node>
  </cluster>
</configCONDOR>
```

In this example, CONDOR will contact a “distant” computer located at network address 127.0.0.1. This address is a little bit special: it’s the loop-back address: it means that CONDOR will try to contact a CONDOR-client that is located on the same computer than the master. It’s very handy for debug purposes.

To run this example, you must first launch CONDOR in client-mode (type in a DOS-prompt “start xmlCondor -c”) and thereafter, on the same computer, launch CONDOR as usual (type in a DOS-prompt “xmlCondor optimNet.xml”). You can also double-click on the “test.NET.bat” script that will execute these 2 commands for you.

NOTE: When Condor is run in client-mode, it does NOT check the expiration date of your license. It means that the client computers can be completely disconnected from any internet

connection.

The objective function "`sifOF/XMLOFSIF.exe`" that is used in this example is a little bit more complex than the objective functions encountered so far. It is, in reality, a collection of many different objective functions (a complete list is given in figure 2.8). When you run "`sifOF/XMLOFSIF.exe`", it first loads the XML-file that is given as the first parameter on the command-line. Thereafter it search for the `functionIndex` tag inside the XML file. This tag is selecting the objective functions that will be used. A complete list of the different values that this tag can have is given in figure 2.8.

Index	Function Name	Index	Function Name	Index	Function Name
104	akiva	118	hatfde	130	power
105	allinitu	119	schmvett	131	morebv
107	heart	120	growthls	132	brybnd
108	osborneb	121	gulf	133	brownal
109	vibrbeam	122	brownden	134	dqdrtic
110	kowosb	123	eigenals	135	watson
111	helix	124	heart6ls	136	dixmaank
112	rosenbrock	125	biggs6	137	fminsurf
113	snail	126	hart6	138	tointgor
114	sisser	127	cragglvy	139	tointpsp
115	cliff	128	vardim	140	3pk
116	hairy	129	mancino	141	deconvu
117	pfit1ls	130	power		

Figure 2.8: Index of Objective functions

These are standard test objective functions available in the literature. In the example, the objective function 115 is optimized. This corresponds to the standard "cliff" objective function.

If you want to change the objective function, you must change:

1. the value of the `functionIndex` tag.
2. the starting point (you should use the standard one from the literature).
3. the dimension of the search space.

Before running any evaluation on a remote computer, the CONDOR-client creates a local XML-file (`c:\sifbro11.xml`) based on the global XML file (`optimNet.xml`). This local XML-file contains the `functionIndex` tag. This tag is needed by the "`sifOF/XMLOFSIF.exe`" objective function. CONDOR has transferred through the network the required XML data so that the full process runs transparently.

If you have some difficulties to handle XML files, you suggest you to use the small and simple C++ XML-parser library that is available freely at:

<http://iridia.ulb.ac.be/~fvandenb/tools/xmlParser.html>

Chapter 3

MATLAB interface.

3.1 Usage

You can obtain anytime a short description of all the parameters of CONDOR for MATLAB. To display the short help, run CONDOR without any arguments.

The functionalities of the MATLAB interface of CONDOR compared to the XML interface are reduced: There is no MATLAB equivalence for the following XML tags: `variablesToOptimize`, `<dataFiles binaryDatabaseFile>`, `<dataFiles asciiDatabaseFile>`. There is no Hot-Start, no Database of old evaluations.

The usage of CONDOR for Matlab is the following:

```
[xopt,vopt,lambdapt,trace]=  
    matlabCondor(rhostart,rhoend,maxIteration,params,optionalParam);
```

The input parameters are:

- **rhostart**: initial distance between sample sites (in the rescaled space). See section 1.3.1 for more information.
- **rhoend**: stopping criteria(in the rescaled space). See section 1.3.2 for more information.
- **maxIteration**: maximum number of iterations of the optimization algorithm.
- **optionalParam**: A variable that is passed to the .m files that are computing the objective functions and the constraints. You can put inside this variable whatever is needed to perform the required computations.
- **params**: a variable with the following fields:
 - **params.xstart** (required)
The starting point of the optimization process. See section 1.3.3 for more information.
 - **params.f** (required)
This field contains a string that is the name of an .m file used to evaluate the objective function. The prototype of this function is:

```
function [output,error] = ObjFunct(px)
```

The output parameter **error** is optional. If the evaluation has failed then the function must return **error=1**. **output** is a scalar that contains the value of the objective function $f(x)$ evaluated at position **px**.

- **params.lb** and **params.ub** (optional)
These two vectors containing the lower and upper bounds on variables
(no lower bound on axis i is **p.bl(i)=-1.7E308**)
(no upper bound on axis i is **p.bu(i)= 1.7E308**)
- **params.a** and **params.b** (optional):
These 2 parameters are describing the linear constraints:

$$x \text{ is feasible} \Leftrightarrow Ax \geq b \Leftrightarrow \text{params.a } x \geq \text{params.b}$$

- **params.scalingFactor** (optional)
The re-scaling factors. For more information about the re-scaling factors, see section 1.3.4. If this parameter is omitted then automatic rescaling will be used.
p.scalingFactor=[] is equivalent (but faster) to
p.scalingFactor=ones(size(p.xstart)).
- **params.nNLConstraints** (optional)
Number of non-linear constraints
- **params.c** (required if **params.nNLConstraints<>0**)
This field contains a string that is the name of an .m file used to compute the value and the gradient of the non-linear constraints at a given point x . The prototype of this function is:

```
function [output,error] = NLConstr(isGradNeeded,J,px)
```

$$x \text{ is feasible} \Leftrightarrow \text{NLConstr}(x) \geq 0$$

The output parameter **error** is optional. If **isGradNeeded=0**, then **output** must be a scalar that contains the value of the J^{th} non-linear constraint evaluated at position **px**. If **isGradNeeded=1**, then **output** must be a vector that contains the gradient of the J^{th} non-linear constraint evaluated at position **px**.

The output parameters are:

- **xopt** (required)
xopt is a vector containing the optimum x^* of the objective function $f(x)$.
- **vopt** (optional)
The value $f(x^*)$ of the objective function $f(x)$ at the optimum.
- **lambdaopt** (optional)
The vector of the Lagrange or dual variables λ^* associated with the constraints (see section 5.5.2 for more information). The order in the constraints is the following: lower bound constraints, upper bound constraints, linear constraints, non-linear constraints.
- **trace** (optional)
The matrix **trace** contains the trace of execution (or in other words: the path of execution) followed by CONDOR towards the optimum x^* . Each line of this matrix represents an evaluation of the objective function. The content of line i is the following:

$$- x_i$$

- $f(x_i)$
- error in evaluation of $f(x_i)$ (0 if no error; 1 if error)

3.2 Examples

The examples available under MATLAB are the following:

- **Noisy optimization of a quadratic in four dimension (no failure)**
A complete description of this problem is given in section 2.7.3. The .m files used in this examples are 'test_Q4N.m' and 'OF_Q4N.m'.
- **Noisy optimization of a quadratic in four dimension (with failure)**
A complete description of this problem is given in section 2.7.4. The .m files used in this examples are 'test_Q4NF.m' and 'OF_Q4NF.m'.
- **The classical Rosenbrock Objective function**
The parameters for this problem are:

```
pRosen.xstart=[-1.2 -1.0];
pRosen.f = 'OF_Rosen';
pRosen.lb=[-10-10];
pRosen.ub=[ 10 10];
pRosen.scalingFactor= [];
rhoStart=1;
rhoend=.01;
niter=1000;
```

The function OF_Rosen is the following:

```
function [out,error] = OF_Rosen(x)
out= 100*(x(2)-x(1)^2)^2+(1-x(1))^2;
error=0;
```

A complete description of this problem is given in section 2.7.1. The .m files used in this examples are 'test_Rosen.m' and 'OF_Rosen.m'.

- **A simple quadratic in two dimension**
A complete description of this problem is given in section 2.7.2. The .m files used in this examples are 'test_Q2.m' and 'OF_Q2.m'.
- **A badly scaled objective function**
A complete description of this problem is given in section 2.7.5. The .m files used in this examples are 'test_ScaledRosen.m' and 'OF_ScaledRosen.m'.
- **Optimization with linear and box constraints**
A complete description of this problem is given in section 2.7.6. The .m files used in this examples are 'test_SuperSimple.m' and 'OF_SuperSimple.m'.
- **Optimization with non-linear constraints**
A complete description of this problem is given in section 2.7.7. The .m files used in this examples are 'test_Fletcher.m', 'OF_Fletcher.m' and 'NLConstr_Fletcher.m'.

Chapter 4

C++ code interface.

In preparation.

Chapter 5

Some useful remarks and tricks.

5.1 Typical behavior of CONDOR

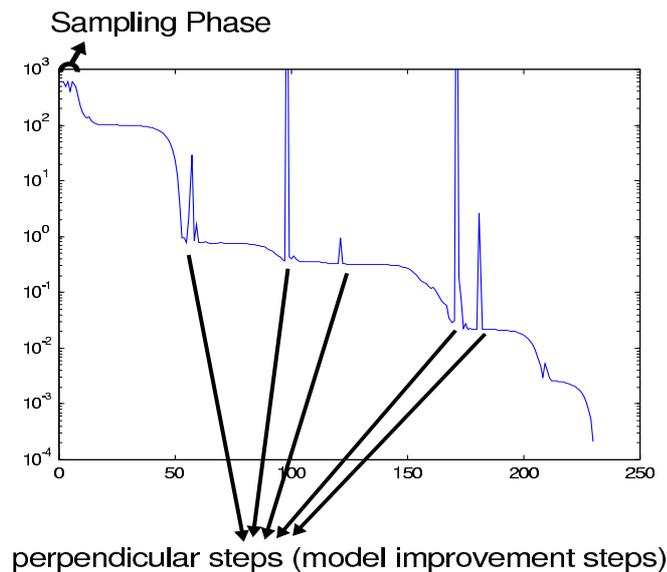


Figure 5.1: Optimization trace

You can see in figure 5.1 a trace of an optimization run of CONDOR. On the x-axis, you have the time t . On the y-axis you have the value of the objective function that has been computed at time t .

CONDOR always starts by sampling the objective function to build the initial quadratical approximation $\mathcal{Q}_0(\delta)$ of $\mathcal{F}(x)$ around x_{start} (see section 1.2 - step 1: **Initialization**). This is called the sampling/initial construction phase. During this phase the optimizer will not follow the slope towards the optimum. Therefore the values of the objective function remains more or less the same during all the sampling phase (as you can see in figure 5.1). Once this phase is finished, CONDOR has enough information to be able to follow the slope towards the minimum. The information gathered up to now during the sampling phase are finally used. This is why, usually, just after the end of the sampling phase, there is a significant drop inside the value of the objective function (see figure 2.3).

This first construction phase requires $\frac{1}{2}(n+1)(n+2)$ evaluations of the objective function (n is the dimension of the search space). This phase is thus very lengthy. Furthermore, during this phase, the objective function is usually not “reduced”. The computation time can be strongly reduced if you use “hot start”. Another possibility to reduce the computation time is to use the parallel version of CONDOR. This phase can be parallelized very easily and without efficiency-loss. If you use $N = \frac{1}{2}(n+1)^2$ computers in parallel the computation time of the sampling phase will be reduced by N .

From time to time CONDOR is making a “perpendicular” or “model improvement” step. The aim of this step is to avoid the degeneration of the quadratical approximation $Q_k(\delta)$ of $\mathcal{F}(x)$. Thus, when performing a “model improvement” step, CONDOR will not try to follow the slope of the objective function and will produce (most of the time) a very bad values of $\mathcal{F}(x)$.

5.2 Help! I don’t have any more CPU’s available!

The parallel/distributed version of CONDOR can use as many as $\frac{1}{2}(n+1)^2$ computers in parallel (n is the dimension of the search space). CONDOR can fully exploit all these resources during the first sampling phase (see section 5.1 about sampling phase).

However, the parallel efficiency of CONDOR during the later research phase is limited. Especially when the dimension of the search space is low, there is no need to make many samples of the objective function $\mathcal{F}(x)$ to obtain a good approximation $Q_k(\delta)$ of $\mathcal{F}(x)$.

Thus, if you need to perform several optimization tasks with a limited number of CPU’s, I suggest you to use the maximum number of CPU’s for the initialization phase (because the parallel efficiency is very high during this phase) and, as soon as the initialization phase is finished, disconnect the client-computers and use them all to perform the initialization phase of the next optimization task.

You can disconnect a CONDOR-client connected to a master in a very simple way: just press CTRL-C (or kill it any other way). The master computer will be notified of the interruption and handle it gracefully.

5.3 Shape optimization: parametrization trick.

Let’s assume you want to optimize a shape. A shape can be parameterized using different tools:

- Discrete approach (fictious load)
- Bezier & B-Spline curves
- Uniform B-Spline (NURBS)
- Feature-based solid modeling (in CAD)

Let's assume we have parameterized the shape of a blade using "Bezier curves". An illustration of the parametrization of an airfoil blade using Bezier curves is given in figures 5.2 and 5.3.

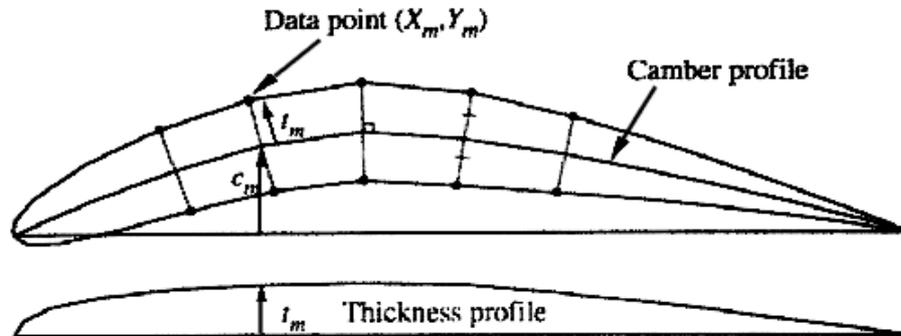


Figure 5.2: Superposition of thickness normal to camber to generate an airfoil shape

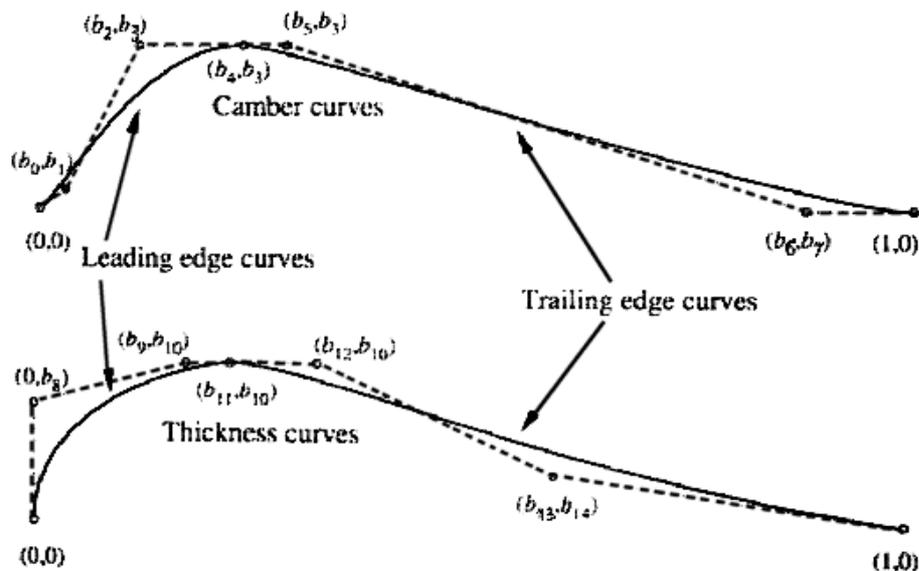


Figure 5.3: Bezier control variable required to form an airfoil shape

Some set of shape parameters generates infeasible geometries. The "feasible space" of the constrained optimization problem is defined by the set of parameters that generates feasible geometries. A good parametrization of the shape to optimize should only involve box or linear constraints. Non-linear constraints should be avoided.

In the airfoil example, if we want to express that the thickness of the airfoil must be non-null, we can simply write $b_8 > 0, b_{10} > 0, b_{14} > 0$ (3 box constraints) (see Figure 5.3 about b_8, b_{10} and b_{14}). Expressing the same constraint (non-null thickness) in an other, simpler, parametrization of the airfoil shape (direct description of the upper and lower part of the airfoil using 2 bezier curves) can lead to non-linear constraints. The parametrization of the airfoil proposed here is thus very good and can easily be optimized.

5.4 A note about the `variablesToOptimize` tag

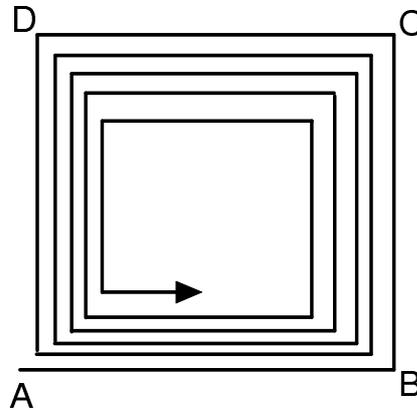


Figure 5.4: Illustration of the slow linear convergence when performing consecutive optimization runs with some variables deactivated.

If you want, for example, to optimize $n + m$ variables, never do the following:

- Activate the first n variables, let the other m variables fixed, and run CONDOR (Choose as starting point the best point known so far)
- Activate the second set of m variables, let the first set of n variables fixed, and run CONDOR (Choose as starting point the best point known so far).
- If the stopping criteria is met then stop, otherwise go back to step 1.

This algorithm will result in a very slow linear speed of convergence as illustrated in Figure 5.4. The config-file-parameter `variablesToOptimize` allows you to activate/deactivate some variables, it's sometime a useful tool but don't abuse from it! Use with care!

5.5 Sensibilities

5.5.1 Sigma vector ($\sigma \in \mathbb{R}^n$)

Let's apply a small perturbation σ_i to the optimum point \bar{x}^* in the direction \bar{e}_i . Let's assume that the objective function is minimum at \bar{x}^* . How much does this perturbation increase the value of the objective function?

$$\begin{array}{l} \text{sensibility} \\ \text{along} \\ \text{axis } i \end{array} = \begin{array}{l} \text{increase due to} \\ \text{perturbation of length} \\ \sigma_i \text{ in direction } \bar{e}_i \end{array} = \mathcal{F}(\bar{x}^* + \sigma_i \bar{e}_i) - \mathcal{F}(\bar{x}^*) = (H^*)_{i,i} \sigma_i^2 \quad (5.1)$$

The sigma vector is used to check the sensibilities of the objective function relative to small perturbation on the coordinates of x^* . If x^* represents the optimal design for a shape, the sigma vector help us to see the impact on the objective function of the manufacturing tolerances of the optimal shape.

The same result can be obtained when convoluting the objective function with a gaussian function that has as variances the σ_i 's.

5.5.2 Lagrangian vector

One of the output CONDOR is giving at the end of the optimization process is the lagrangian Vector λ^* at the solution. What's useful about this lagrangian vector?

We define the classical Lagrangian function \mathcal{L} as:

$$\mathcal{L}(x, \lambda) = f(x) - \sum_i \lambda_i c_i(x). \tag{5.2}$$

where the λ_i are the Lagrangian variables or Lagrangian multipliers associated with the constraints. In constrained optimization, we find an optimum point (x^*, λ^*) , called a KKT point (Karush-Kuhn-Tucker point) when:

$$(x^*, \lambda^*) \text{ is a KKT point} \iff \nabla \mathcal{L}(x^*, \lambda^*) = 0 \iff \begin{cases} \nabla_x \mathcal{L}(x^*, \lambda^*) = 0 \\ \lambda_i^* c_i(x^*) = 0 \end{cases} \tag{5.3}$$

where $\nabla = \begin{pmatrix} \nabla_x \\ \nabla_\lambda \end{pmatrix}$

The second equation of 5.3 is called the *complementarity condition*. It states that both λ^* and c_i^* cannot be non-zero, or equivalently that inactive constraints have a zero multiplier. An illustration is given in figure 5.5.

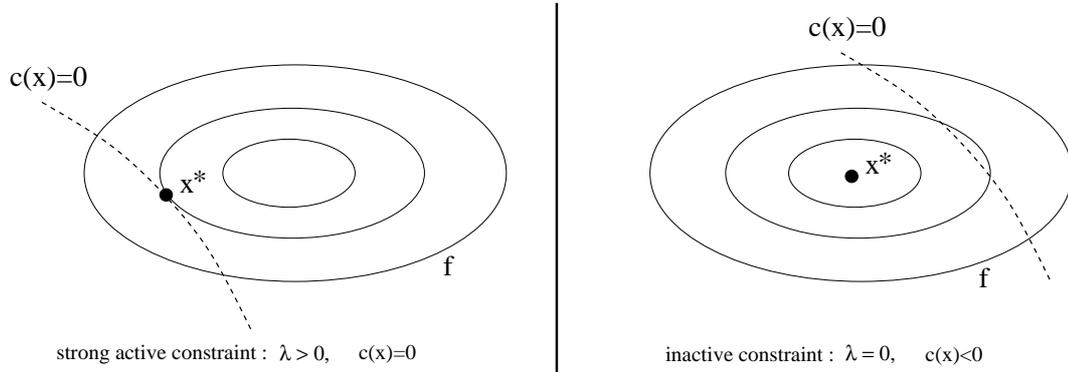


Figure 5.5: complementarity condition

To have some insight into the meaning of Lagrange Multipliers λ , consider what happens if the right-hand sides of the constraints are perturbed, so that

$$c_i(x) = \epsilon_i, \quad i \in E \quad (E \text{ is the set of the active constraints at the solution}) \tag{5.4}$$

Let $x(\epsilon)$, $\lambda(\epsilon)$ denote how the solution and lagrangian multipliers are changing as ϵ changes. The Lagrangian for this problem is:

$$\mathcal{L}(x, \lambda, \epsilon) = f(x) - \sum_{i \in E} \lambda_i (c_i(x) - \epsilon_i) \tag{5.5}$$

From 5.4, $f(x(\epsilon)) = \mathcal{L}(x(\epsilon), \lambda(\epsilon), \epsilon)$, so using the chain rule, we have

$$\frac{df}{d\epsilon_i} = \frac{d\mathcal{L}}{d\epsilon_i} = \frac{dx^t}{d\epsilon_i} \nabla_x \mathcal{L} + \frac{d\lambda^t}{d\epsilon_i} \nabla_\lambda \mathcal{L} + \frac{d\mathcal{L}}{d\epsilon_i} \tag{5.6}$$

Using Equation 5.3, we see that the terms $\nabla_x \mathcal{L}$ and $\nabla_\lambda \mathcal{L}$ are null in the previous equation. It follows that:

$$\frac{df}{d\epsilon_i} = \frac{d\mathcal{L}}{d\epsilon_i} = \lambda_i \quad (5.7)$$

Thus the Lagrange multiplier of any constraint measures the rate of change in the objective function, consequent upon changes in that constraint function. This information can be valuable in that it indicates how sensitive the objective function is to changes in the different constraints.

5.6 About virtual constraints and failed evaluations

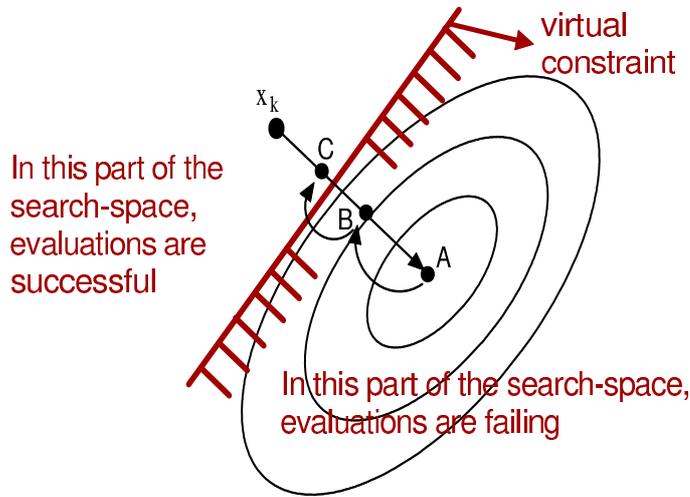


Figure 5.6: two consecutive failures

Let's consider figure 5.6 that is illustrating two consecutive failure (points A and B) inside the evaluation of the objective function. The part of the search-space where the evaluations are successful is defined by a "virtual constraint" (the red line in figure 5.6). We don't have the equation of this "virtual constraint". Thus it's not possible to "slide" along it. The strategy that is used is simply to "step back". Each time an evaluation fails, the trust region radius Δ_k is reduced and δ_k is re-computed. This indirectly decreases the step size $\|\delta_k\|$ since δ_k is the solution of:

$$\mathcal{Q}(\delta_k) = \min_{\delta} \mathcal{Q}_k(\delta) \text{ such that } \frac{\rho_k}{2} < \|\delta_k\| < \Delta_k \quad (5.8)$$

Inside figure 5.6, the three points A,B,C are aligned. In general, these three points will NOT be aligned since their position is given by equation 5.8 with different values of Δ_k .

The simple strategy described above has strong limitations. In the example illustrated in figure 5.7, Condor will find as optimal solution the point A. If the same constraint is specified using a box or a linear constraint, Condor will be able to "slide" along it and to find the real optimum point, the point B.

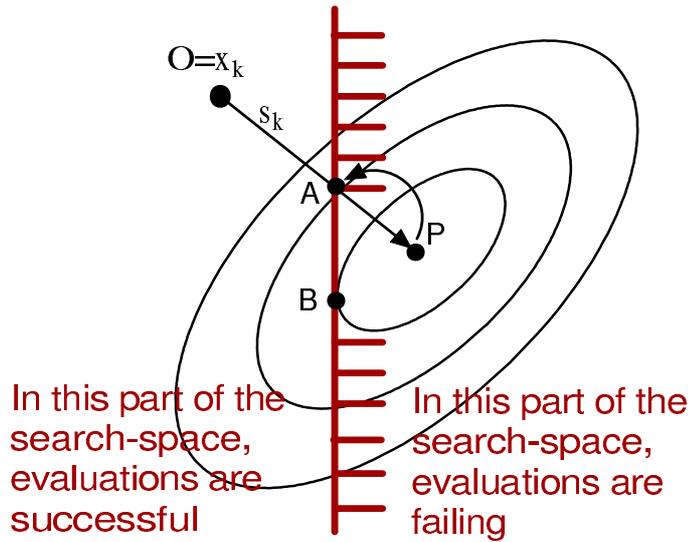


Figure 5.7: Limitations of virtual constraints

5.7 About linked evaluations of the objective function and constraints

In some cases you obtain as a result of an evaluation of the objective function not only the value of the objective function itself but also the value of a constraint that must be respected. For such constraint (that is linked to the evaluation of the objective function), the strategy to use is the following: use a penalty function.

What's a penalty function? Suppose you want to find:

$$\min_x f(x) \text{ subject to } \begin{cases} c_1(x) \leq 0 \\ c_2(x) = 0 \end{cases}$$

The associated penalty function is:

$$\min_x f(x) + \mu_1 \max(c_1(x), 0) + \mu_2 \text{abs}(c_2(x)) \quad (5.9)$$

or you can also use:

$$\min_x f(x) + \mu_1 (\max(c_1(x), 0))^2 + \mu_2 (c_2(x))^2 \quad (5.10)$$

with μ_1 and μ_2 some constants chosen big enough to "push back" the optimizer in the feasible space.

Let's assume that you have a small violation of the constraints. In this case, the equation 5.9 will directly penalizes strongly the objective function. Equation 5.9 should be used if you don't want any violation at all at the end, optimal point found by Condor. This is an advantage of equation 5.9. A disadvantage appears when you choose too high values for μ_1 and μ_2 . This will produce strong non-linearities in the derivatives of the new objective function 5.9 in the part of the search space that is along the constraint (this is known as the Maratos Effect). This

will lead to a longer running time for the optimizer. For some extreme values of μ_1 and μ_2 the optimizer can fail to find the optimum point of the objective function.

In opposition, the equation 5.10 does not produce any non-linearity in the derivative, even for high values of μ_1 and μ_2 . This will lead to a short running time for the optimizer. However, small violations of the constraints could be obtained at the end of the optimization process.

When using penalty functions, Condor can enter during the optimization process in the infeasible space. However, if appropriate values are given to μ_1 and μ_2 , the optimal point found by Condor will be feasible (or, at least, nearly feasible, when using equation 5.10).

You can easily define any penalty function inside Condor. All you have to do is to define a `subAggregationFunction` for each constraints. For example:

```
<aggregationFunction>
  <subAggregationFunction name="main_function">
    ... computation of f(x) ...
  </subAggregationFunction>
  <subAggregationFunction name="constraint_1">
    100 * ... computation of max(c_1(x),0) ...
  </subAggregationFunction>
  <subAggregationFunction name="constraint_2">
    50 * ... computation of abs(c_2(x)) ...
  </subAggregationFunction>
</aggregationFunction>
```

In this example, $\mu_1 = 100$ and $\mu_2 = 50$. If you use this facility, Condor will be able to hot-start at every change of μ_1 and μ_2 . This will lead to a very short optimization time. You will thus be able to precisely adjust μ_1 and μ_2 .

The extension to multiple linked-constraints is straight forward.

When possible, penalty functions should be avoided. In particular, if you have simple box, linear or non-linear constraints, you should encode them inside the XML file as standard constraints. Condor is using advanced techniques that are (a lot) faster and are more robust in these cases.

Let's assume that you have an objective function that is computing some efficiency measure ($0 < Efficiency \leq 1$) that you want to maximize. You will have something like:

```
<varNames dimension="2">
  x1 x2
</varNames>
<objectiveFunction nIndex="1">
  <indexNames> Efficiency </indexNames>
  <aggregationFunction>
    <subAggregationFunction name="good_main_function">
      -1.0 * Efficiency
    </subAggregationFunction>
    ... linked-constrained if any ...
```

```

    </aggregationFunction>
    <executableFile>
        ComputeEfficiency.exe
    </executableFile>
    ...
</objectiveFunction>

```

You will never define:

```

...
<aggregationFunction>
    <subAggregationFunction name="bad_main_function">
        (Efficiency-1)^2
    </subAggregationFunction>
    ...

```

Let's assume that the objective function $Efficiency(x_1, x_2)$ has a shape that is close to a quadratic. If you use the `good_main_function`, CONDOR will “see” an objective function that can easily be approximated by a quadratic. CONDOR is using a quadratical approximation $Q_k(\delta)$ of the objective function to compute the search directions. CONDOR will thus generate good search direction and it will converge very rapidly to the solution of the optimization problem. If you use the `bad_main_function`, CONDOR will “see” an objective function that is of degree 4. It will be difficult to approximate this function with a quadratic. The search direction will thus be of poor quality. The convergence to the optimum will be a lot slower.

A general rule of thumb is: If your objective function “looks like” a quadratic, CONDOR will be faster.

In future extension of the optimizer, the variables μ_1 and μ_2 will be adjusted automatically.

5.8 About constraints violations

Some optimizers that are working with constraints sometimes require to evaluate the objective function in the infeasible space. This is for example the case for the dual-simplex algorithm encountered in linear programming where all the evaluations are in the infeasible space and only the last point of the optimization process (the optimum point) is feasible.

Condor is a 99% feasible optimizer. It means that 99% of the evaluations are feasible. Basically, the Condor algorithm moves a cloud of points in the search space towards the optimum point. The center of this cloud is x_k and is always feasible. See illustration in figure 5.8. The other points (the sampling point) are used to build (using Lagrange interpolation technique) $Q_k(\delta)$, the local approximation of the objective function $f(x)$ around x_k . These last points can be in the infeasible space. They are separated from the center point x_k (that is feasible) by a distance that is at most ρ_k (see section 1.2 for a complete explanation of these variables). Thus, the length of the violation is at most ρ_k .

You can see in figure 5.8 an illustration of these concepts. The green point is x_k , the center of the cloud, the best point found so far. The blue and red points are sampling points used to build $Q_k(\delta)$. Some of these sampling points (the red ones) are in the infeasible space. The length of

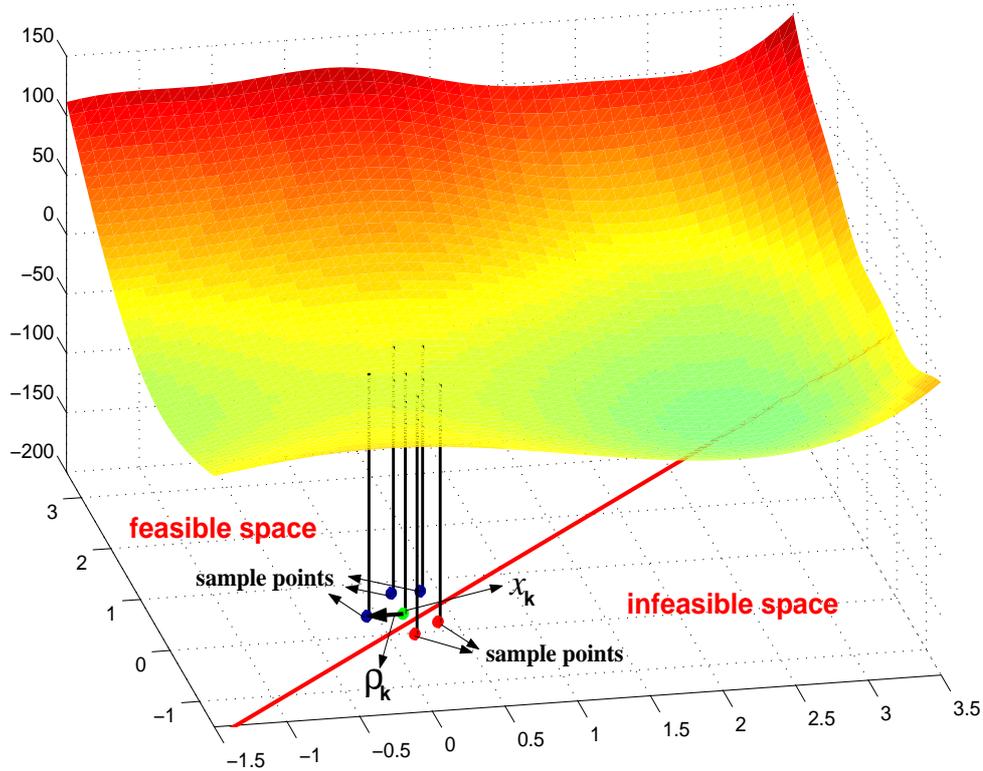


Figure 5.8: Feasibility of the evaluations

the violation is at most ρ_k .

The external code that computes the objective function should always try to give a correct evaluation of the objective function, even when an evaluation is performed in the infeasible space. It should report a failure (see section 5.6 about failure in computation of the objective function) in the least number of cases.

When using a penalty function (see section 5.7), Condor can enter deeply into the infeasible space. However, at the end of the optimization process, Condor will report the optimal feasible point (only for appropriate values of μ_1 and μ_2 : see section 5.7 to know more about these variables).

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