Lévy flights as an underlying mechanism for global optimization algorithms

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Abstract

In this paper we propose and advocate the use of the so called Lévy flights as a driving mechanism for a class of stochastic optimization computations. This proposal, for some reasons overlooked until now, is – in author’s opinion – very appropriate to satisfy the need for an algorithm, which is capable of generating trial steps of very different length in the search space. The required balance between short and long steps can be easily and fully controlled. A simple example of approximated Lévy distribution, implemented in FORTRAN 77, is given. We also discuss the physical grounds of presented methods.

Keywords

Lévy flights, diffusive processes, Brownian motion, quantum tunneling, evolutionary computations, evolutionary algorithms, Lévy distributions, random number generators

I. Optimization algorithms and physics

More and more global optimization tasks are completed today using algorithms originating from mimicking the way the Nature solves them. We have two branches of science, which describe the world around us, namely biology (for living things) and physics (for the rest of it). The problem of global optimization (either minimization or maximization, with or without constraints) of the objective function of many variables still remains a challenge for practitioners. There is no single, universal and deterministic algorithm capable of solving all kinds of optimization problems: those involving smooth as well as non-smooth objective functions, mixed integer-real-boolean valued unknowns, etc.

Classical mathematical analysis was long the only tool for finding extrema of functions of many variables. Unfortunately it is of very limited use in many practical applications, especially when the objective function is not differentiable at least once. On the other hand, we are ready to accept the solutions, which are not perfect in the mathematical sense (often called "ε-optimal"), but are sufficiently close to them.

To overcome such difficulties, researchers in various fields of science and engineering turned to stochastic algorithms. There are several kinds of arguments for doing so. The first, and certainly not the most important one, is increasing availability of the computing power. We are able to examine, usually in a fraction of a second, many trial solutions of the optimization problem under study. Loosely speaking, this is the base of a rich family of Monte-Carlo-type optimization algorithms. Trying to mimic Nature’s actions is another justification for rich variety of optimization algorithms, just because Nature seems very successful. Let’s put aside algorithms of genetic type, grown on biological grounds, and concentrate instead on those, which are based on behavior of purely physical systems. Various physical phenomena were taken into account, mostly from classical mechanics of a single particle (deterministic algorithms of "gradient type") and thermodynamics (simulated annealing) as models for optimization procedures.

In this paper we propose the diffusion processes and quantum tunneling as a base for a class of stochastic optimization routines.
II. Diffusive processes as a model for optimization procedure

Consider the simplest version of familiar Monte-Carlo optimization procedure. Its operation may be summarized as a random walk in the search space (bounded or not) and sampling the values of objective function in visited points. The trajectory of such a random walker is very similar to the trajectory of physical particle subjected to Brownian motion. If we consider many random walkers at the same time (multiple start point Monte-Carlo optimization algorithm), then emerging set of trajectories resembles closely the diffusion process. In the derivation of the law of Brownian motion one assumes that the lengths of individual "jumps" are not equal to each other but are distributed normally, as a result of a huge number (estimated as $10^5$—$10^6$) of independent "kicks" from surrounding molecules. This is practical manifestation of the law of large numbers, known also as the Central Limit Theorem. Under those assumptions it may be shown (Einstein, Smoluchowski) that the average distance, $R$, of a random walker from starting point is a function of time, $t$, and can be expressed as

$$\langle R^2(t) \rangle = D t^\nu, \quad \text{with } \nu = 1$$

(1)

where $D$ is the diffusion constant.

The formula (1) was later confirmed experimentally for small particles suspended in liquids. This, in turn, made possible to estimate the value of very important physical constant, the Avogadro’s number, $N_A$, thus finally confirming the atomic structure of matter. It is worth noting that the early value of $N_A$, obtained this way, differs less than 1% from the one known today, almost 100 years later.

Extensive investigations of diffusion processes revealed, that at least some of them must be governed by other mechanisms, different from familiar Brownian motion. They were classified as subdiffusion ($\nu < 1$, see Eq. 1) and enhanced diffusion ($\nu > 1$). It is often said that the enhanced diffusion is governed by Lévy flights, which will be explained below.

Lévy flights

Paul Lévy (1886—1971), the French mathematician, considered in thirties (XX century) the following problem [1]:

*What, if any, should be the probability density of $N$ independent, identically distributed random variables ($\text{iid}$) $X_1, X_2, \ldots, X_N$ to satisfy the requirement that the probability density of their sum $X_1 + X_2 + \ldots + X_N$ has the same functional form?*

Today we could say, that Lévy tried to find a class of self-similar objects, known as fractals since Benoit Mandelbrot had invented them, much later, in 1968.

Well known answer to Lévy’s problem was based on famous Central Limit Theorem, which, in most widely known version, states that the sum of iid random variables has normal probability density. We can even drop the requirement of identical distributions (but *not* the independence!) and still have the same result. There is a catch, however: the individual distributions have to be narrow, i.e. their first and second moment (Lindberg), and in Lyapunov version also the third moment, have to be finite.

Taking into considerations also other, non-gaussian distributions, Lévy obtained the following condition for the Fourier transform of probability density of the sum of $N$ iid random variables:

$$\tilde{p}_N(k) \sim \exp\left(-N|k|^\beta\right)$$

(2)

In Lyapunov version we need even stronger condition, which may be, not quite precisely, expressed as *no random variable dominates others in the sum*. Finiteness of third moments is necessary but not enough for that.
where the normalization constant was dropped, and $0 < \beta < 2$.

Going back to the searched distribution, not its Fourier transform, is not trivial, and the analytical form of the result is known only for few special cases. Generally it may be expressed as [2]

$$L(x) = \frac{1}{\pi} \int_{0}^{\infty} \exp \left( -\gamma q^\beta \right) \cos qx \, dq$$

and is known as *symmetrical Lévy stable distribution of index* $\beta$ ($0 < \beta \leq 2$) and *scale factor* $\gamma$ ($\gamma > 0$). For simplicity one usually sets $\gamma = 1$.

The special cases mentioned earlier are:

- Cauchy distribution (among physicists known also as Lorentzian shape):
  $$p_N(x) = \frac{1}{\pi N} \frac{1}{1 + \left( \frac{x}{N} \right)^2} = \frac{1}{N} \, p_1 \left( \frac{x}{N} \right) \quad \text{for} \quad \beta = 1,$$

- Gauss normal distribution, when $\beta = 2$.

The integral (3) can be written in a form of (truncated) power series [3]

$$L(x) = -\frac{1}{\pi} \sum_{k=1}^{m} \frac{(-1)^k \Gamma(\beta k + 1)}{k! \pi} \sin \left( \frac{k \pi \beta}{2} \right) + R_m(x)$$

with $R_m(x)$ of order $x^{-(\beta+1)-1}$ and the leading term is proportional to $x^{-1-\beta}$. Looking at the above series and original Lévy’s result (2), one can see that the searched probability density should behave as

$$L(x) \sim |x|^{-1-\beta} \quad \text{as} \quad |x| \to \infty$$

Now we understand, why the index $\beta$ must belong to the interval $]0, 2[$: for $\beta \leq 0$ integral (3) does not exist (is unbounded), while for $\beta \geq 2$ ordinary Central Limit Theorem holds. It is also clear, that there are some Lévy distributions, those with index $0 < \beta < 1$, for which even the first moment, i.e. expectation value, does not exist (second moment, i.e. the variance, is always infinite). This poses a serious problem for physicists, since the ordinary procedure of repeated measurements makes no sense in such cases, and if used nevertheless – leads to strange, confusing and incorrect results.

**III. Diffusive processes, continued**

Allowing the random walker to make steps of length $l$ distributed as

$$P(l) = \frac{C}{(1 + l)^{1+\beta}}$$

with appropriate normalization constant $C$, one can show that the interesting quantity $\langle R^2(t) \rangle$ follows the law

$$\langle R^2(t) \rangle \sim \begin{cases} \frac{t^2}{2} & 0 < \beta < 1 \\ \frac{t^2}{\ln t} & \beta = 1 \\ t^3 & 1 < \beta < 2 \\ t \ln t & \beta = 2 \\ t & \beta > 2 \end{cases}$$

*To be precise: we should write $l/l_0$ here, instead of just $l$, where $l_0$ denotes unit length, in order to operate with dimensionless quantities only. The reason for not doing so is following: we don’t want to create the impression that any particular length scale is better than others; indeed any unit ranging from femtometers to astronomical unit is equally good. That is why the behavior described by power law is often called ‘scale free’ – no length unit is preferred, except for practical reasons.*
assuming that \( l = vt \), and \( v = \text{const} > 0 \) during every jump.

The distribution (7) approximates very well the Lévy distribution for large arguments, see relation (6). Some authors prefer to use another approximation for Lévy distribution: \( P(l) \sim l^{-\left(1+\mu\right)} \) (for large \( l \)), inferring then that \( \langle R^2(t) \rangle \sim t^{2/\mu} \). They use \( P(l) = \text{const} \) for small \( l \). We prefer our form, since it never produces infinite densities of probability, while retaining desired asymptotic properties.

It is interesting, that in such a vigorous movement as the turbulence, the squared average distance from start point, for any particle observed in a coordinate system moving with the fluid (Lagrange’s coordinates), may be characterized by \( \beta = 5/3 \). Other physical systems described by Lévy distribution are mentioned in [2], [4]. Especially, many physical quantities in phase transition region behave according to the power law. Among them we can find relaxing sand piles, magnetic systems, etc. The lengths of flights made by albatrosses are also distributed according to power law. Other examples from everyday life include stock market price fluctuations, www network connectivity (number of computers connected to the given node), compacting the granular systems and ... the number of goals per soccer game.
Why Lévy distribution may be useful for stochastic optimization?

In global stochastic optimization we need two essential ingredients, in some sense acting against each other. One of them is the routine, which finds efficiently the local extremum when the search process happens to be nearby, and the other – a way to escape from local extremum, since it may be not the global one. It is common to observe during evolutionary optimization the prolonged periods of relatively small improvements followed by sudden, rapid transitions to another local extremum. The process may take long time simply because the random walkers move and explore the search space too slowly, i.e. they make too small and hence too cautious steps. Using step size generated accordingly to one of Lévy distributions instead of uniform or gaussian distribution should therefore be advantageous. The population of random walkers will be always concentrated around recently found extremum, as it should in evolutionary algorithms, and in the same time always few population members will explore more distant regions of search space. This happens with normally distributed walkers only very rarely. The ratio between two classes of random walkers may be easily controlled, in a smooth way, by appropriate choice of index $\beta$. This is illustrated in Figs. 1–3.

Fig. 2
Lévy flight with index $\beta = 1.67 \approx 5/3$ (turbulent case, upper curve shifted 400 units up) and $\beta = 1.50$ (lower curve).

True Lévy distribution is hard to implement in computer code, but the approximate form, like the one given by Eq. (7), is easy (see the next section). The optimal choice of index $\beta$ may be problem-dependent, but should not be critical. Further investigations (experiments?) are necessary to address this question. We suppose, that this choice should be concentrated mainly in the range $(0, 1]$, as largely unexplored until now. Values $\beta > 1$ result in slower spreading of random walkers in search space, what may very significantly affect their ability to find desired extremum, when the problem is defined
on unbounded domain. On the other hand, the case $0 < \beta < 1$ may be considered as a computer imitation of the phenomenon known from quantum mechanics, namely \textbf{quantum tunneling}, see Fig. 3. It is interesting to note, that we have obtained this behavior without even mentioning the quantum mechanical methods.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{Lévy flight with index $\beta = 0.67 < 1$. Note the dramatic scale change ($\sim 1000 \times$) comparing to previous figures. Contrary to earlier presented cases, the average position does not exist, so this walker has capability to explore unbounded domains. Recall that this trajectory also consists of 500 sections.}
\end{figure}

One may wonder, whether such an optimization procedure can still be classified as an evolutionary algorithm. Our answer is \textit{yes}, because one can always identify long jumps in search space with \textit{mutations}, but remember that some researchers are simply ruling out mutations from algorithms regarded as evolutionary, reserving them instead for — as they call it — genetic-type routines.

We have to mention here, that similar behavior, i.e. occasional long jumps, was introduced earlier, rather heuristically, by Galar [5] and Kopciuch under the amusing name of \textit{impatience operator} and interpreted there mainly in context of social sciences.

\section{Example FORTRAN 77 procedure for generating Lévy flights}

Here we present the random number generator, implemented in FORTRAN 77, which produces sequences of numbers distributed according to Eq. (7). It is intentionally not optimized and works by inverting the distributive function, which is given by

$$D^{-1}(\xi) = 1/(1 - \xi)^{1/\beta} - 1,$$

where $\xi$ is uniformly distributed on $[0, 1]$. The above form may be safely simplified to

$$D^{-1}(\xi) = \xi^{-1/\beta} - 1$$

by replacement $1 - \xi \leftrightarrow \xi$. 
DOUBLE PRECISION FUNCTION LEVY1 (X, BETA)
DOUBLE PRECISION X, BETA, R, RANF
R = RANF(X)
LEVY1 = 1.D0/R**(1.D0/BETA) - 1.D0
RETURN
END

RANF is the name of any available standard, i.e. uniformly distributed on \([0, 1]\), random number generator taking \(X\) (of type DOUBLE PRECISION) as a dummy argument.

There is no check, whether \(\beta \in [0, 2]\). The subroutine will work even for \(\beta \geq 2\), however one should not expect to obtain normally distributed random numbers in such case.

V. Summary and discussion

In this paper we have described two distinct, but closely related classes of stochastic optimization algorithms, based on a single mathematical model and being the computer counterparts of two different physical effects: classical diffusion and quantum tunneling. They received unified mathematical background and may be distinguished according to the properties of random walkers, as summarized below:

| properties        | Lévy index     | physical effect                                      |
|-------------------|----------------|------------------------------------------------------|
| no moment exists  | \(0 < \beta \leq 1\) | quantum tunneling                                    |
| only first moment | \(1 < \beta < 2\) | superdiffusion, including turbulence                 |
| gaussian distribution | \(\beta = 2\) | diffusion (Brownian motion)                          |
| unknown with \(\sigma^2 < \infty\) | \(\beta > 2\) | subdiffusion                                         |
| or not applicable |                |                                                      |

The unexpected similarities between classical diffusion processes and quantum tunneling have their roots probably in properties (similarities) of the corresponding partial differential equations describing them. Both equations, i.e. the diffusion equation (Fick’s law) and Schrödinger equation relate first partial derivatives of the unknown function with respect to time with its second spatial derivatives. The important difference is the explicit presence of imaginary unit, \(i\), in Schrödinger’s equation. The algorithm we describe here is able to mimic the properties of both types of solutions. It can be easily switched from one type of behavior to another one by merely changing the value of a single control parameter, i.e. Lévy index.

The question arises, whether the familiar evolutionary algorithms should be immediately thrown away in favor of Lévy flights based ones. Even, if we stick to the orthodox definition of evolutionary algorithms as the ones, which accept only small, gradual changes in position within the searched domain – then the answer is no. The main problem with evolutionary algorithms is their poor ability to escape from unwanted, suboptimal extrema. Indeed, if evolutionary random walkers make steps with lengths distributed uniformly on \([0, l_{max}]\), then they are unable to escape from extremum, which is wider than \(\sim 2l_{max}\). Using normally distributed numbers as step lengths – good in theory – doesn’t help much in practice. And here is why: gaussian generators of poor quality never produce random numbers exceeding few (say \(\sim 3\)) \(\sigma\) in magnitude. On the other hand, even perfect normal generators produce very rarely steps longer than that. So it is a pure illusion, that it is possible to find the global optimum in reasonable time with one of such algorithms – even if the appropriate theorem states so. This may only happen, when our first approximation to the solution is already quite good. Quite different situation
occurs, when our goal is to keep track and adapt to the varying environment, i.e. when objective function changes smoothly and slowly enough while the optimization procedure is in progress (for example satellite or missile tracking). In such cases, providing the starting point is already well known – i.e. is located closer to the global optimum than to any other one – the evolutionary algorithm, without any mutations, is indispensable.

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REFERENCES

[1] Joseph Klafter, Michael F. Shlesinger, Gert Zumofen Beyond Brownian Motion, Physics Today, p. 33—39, February 1996
[2] Exact form of Lévy distribution is rarely quoted in literature, we have found it in: Rosario N. Mantegna and H. Eugene Stanley Stochastic Process with Ultraslow Convergence to a Gaussian: The Truncated Lévy Flight, Phys. Rev. Lett. 73(22), 2946—2947, 1994
[3] H. Bergstrom, Arkiv. för Matematik, 2, 375, 1952
[4] François Bardou Cooling gases with Lévy flights: using the generalized central limit theorem in physics, in mini proceedings of Conference on Lévy processes: theory and applications, Aarhus, January 18–22, 1999, MaPhySto Publication (Miscellanea No. 11, ISSN 1398-5957), O. Barndorff-Nielsen, S.E. Craversen and T. Mikosch (eds.), also available at URL: http://arxiv.org/abs/physics/0012049
[5] Roman Galar, Ryszard Kopciuch Zniecierpliwienie i polaryzacja w procesach ewolucyjnych II Krajowa Konferencja Algorytmy Ewolucyjne i Optymalizacja Globalna, Potok Złoty, 25—28 maja 1999, str. 115—122 (Impatience and polarization in evolutionary processes, II Domestic Conference Evolutionary Algorithms and Global Optimization, Potok Złoty (Poland), May 25–28, 1999, conference materials, page 115-122, in polish).