

The Complete-Basis-Functions Parameterization in ES and its Application to Laser Pulse Shaping

Ofer M. Shir
LIACS, Universiteit Leiden
Niels Bohrweg 1, Leiden
The Netherlands
oshir@liacs.nl

Christian Siedschlag
FOM-Instituut AMOLF
Kruislaan 407, Amsterdam
The Netherlands
siedschlag@amolf.nl

Thomas Bäck^{*}
LIACS, Universiteit Leiden
Niels Bohrweg 1, Leiden
The Netherlands
baeck@liacs.nl

Marc J.J. Vrakking
FOM-Instituut AMOLF
Kruislaan 407, Amsterdam
The Netherlands
vrakking@amolf.nl

ABSTRACT

This paper presents a new *parameterization* method for the Evolution Strategies (ES) field, and its application to a challenging real-life high-dimensional Physics optimization problem, namely *Femtosecond Laser Pulse Shaping*. The so-called *Complete-Basis-Functions Parameterization method* (CBFP), to be introduced here for the first time, is developed for tackling efficiently the given laser optimization task, but nevertheless is a general method that can be used for learning any n -variables functions. The emphasis is on dimensionality reduction of the search space and the speeding-up of the convergence process respectively. This is achieved by learning the target function by using complete-basis functions as building blocks in an evolutionary search. The method is shown to boost the learning process of the given laser problem, and to yield highly satisfying results.

Categories and Subject Descriptors

I.2.8 [Computing Methodologies]: ARTIFICIAL INTELLIGENCE—*Problem Solving, Control Methods, and Search*

General Terms

Algorithms, Experimentation, Performance

^{*}NuTech Solutions
Martin-Schmeisser-Weg 15
44227 Dortmund, Germany.

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. To copy otherwise, to republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee.

GECCO '06, July 8–12, 2006, Seattle, Washington, USA.
Copyright 2006 ACM 1-59593-186-4/06/0007 ...\$5.00.

Keywords

Parameterization, Evolution Strategies, Laser Pulse Shaping

1. INTRODUCTION

Evolutionary Algorithms (EAs) are a set of general purpose probabilistic search methods, which are based upon the theory of natural evolution. Inspired by the genetic concepts and motivated by the "survival of the fittest" principle, the basic idea in EAs is to generate an artificial environment which encodes a search problem into biology-like terms. By defining the appropriate artificial genetic operators, EAs imitate the natural evolution process, and let the artificial environment evolve towards discovering near-optimal solutions. EAs have three main streams [2]: *Genetic Algorithms* (GAs), developed by J. Holland in the U.S. [8], *Evolution Strategies* (ES), developed in Germany by I. Rechenberg [11] and H.P. Schwefel [13], and *Evolutionary Programming* (EP), developed by L.J. Fogel et al. in the U.S. [4]. Whereas ES and EP are close and share many basic characteristics [3], the principal difference between them and GAs is the encoding of the genetic information - the traditional GAs use discrete values (similar to the DNA code in nature) versus continuous real values used typically in ES and in EP. Another significant difference has to do with the concept of *self-adaptation*, which is typical only in ES, and in some variants of EP. Evolution Strategies are a *canonical way for real-valued function optimizations*, and obviously have the most natural environment among all the branches of EAs in the context of real-valued variables. This is simply due to their straightforward encoding, as well as to their successful performance in this domain in comparison with other methods. The higher the dimensionality of the search space, the more suitable a task becomes for an ES (see, e.g., [2] pp. 149-159).

To investigate, and more importantly, to control the motion of atoms or molecules by irradiating them with laser light, one has to provide laser pulses with durations on the same time scale as the motion of the particles. Recent technological developments have made lasers with pulse lengths on the order of femtoseconds routinely available. Moreover, the

time profile of these pulses can be shaped to a great extent. In our research we focus on the *alignment* of molecules by a laser pulse, and in particular on the optimization of the pulse shape for the purpose of high alignment. From the computer-science point of view, the task is learning a one-variable phase function, which plays the key role in the shaping of the laser pulse.

In this study we apply a new ES-based optimization method to this so-called Femtosecond Laser Pulse Shaping problem. The idea of the proposed method is to learn the target function by means of the coefficients of a complete set of functions which will span it, rather than learning function values to be interpolated. This method reduces the dimensionality of the search space, and achieves the speeding up of the convergence respectively.

The remainder of the paper is organized as follows. Section 2 presents briefly the Physics problem, namely *Femtosecond Laser Pulse Shaping*. Section 3 introduces our proposed method for optimizing the evolutionary search using a parameterization based on a set of complete-basis-functions. A mathematical background is provided, followed by the presentation of the method. In section 4 we briefly introduce the core evolutionary mechanism in use, the Covariance Matrix Adaptation Evolution Strategy (CMA-ES). This is followed by the description of the experimental setup, the preliminary tests and the results of the application of the method to the problem. In section 5 we draw conclusions, summarize our study and propose future directions in the domain of our study.

2. THE PROBLEM: LASER PULSE SHAPING

We provide a short introduction to the given Physics problem, limited to the scope and the framework of this paper.

2.1 General

The advent of modern laser pulse shaping techniques in the femtosecond regime has made it possible to control the motion of nuclei and even electrons by a judicious choice of the pulses shapes. The application to dynamic molecular alignment [15] is of considerable interest in this context because of its many practical consequences: a multitude of chemical and physical processes ranging from bimolecular reactions [5] to high harmonic generation [7] are influenced by the angular distribution of the molecular sample.

Furthermore, in many fundamental molecular dissociation or ionization experiments the interpretation of the collected data becomes much easier when the molecules are known to be aligned with respect to a certain axis. Hence, techniques to generate molecular alignment are much needed.

The goal of our research is thus to optimize the *alignment* of an ensemble of molecules after the interaction with a shaped laser pulse. There is currently a great interest in the atomic and molecular physics community to align molecules with laser pulses, since dealing with an aligned sample of molecules simplifies the interpretation of experimental data. By applying a self-learning loop using an evolutionary mechanism, the interaction between the system under study and the laser field can be steered, and optimal pulse shapes for a given optimization target can be found. In our work, the role of the experimental feedback in the self-learning loop is played by a numerical simulation [12].

2.2 Numerical Modeling

To calculate the time-dependent alignment, the Schrödinger's equation for the angular degrees of freedom of a model diatomic molecule under the influence of the shaped laser field is solved. Explicitly, the time-dependent profile of the pulse, which completely determines the dynamics after the transition to the rotating frame has been performed, is described by:

$$E(t) = \int_{-\infty}^{\infty} A(\omega) \exp(i\phi(\omega)) \exp(i\omega t) d\omega, \quad (1)$$

where $A(\omega)$ is a Gaussian window function describing the contribution of different frequencies to the pulse and $\phi(\omega)$, the *phase function*, equips these frequencies, which are equally distributed across the spectrum of the pulse, with different complex phases. Hence, by changing $\phi(\omega)$, the temporal structure of $E(t)$ can be altered. In a real life pulse shaping experiment, $A(\omega)$ is fixed and $\phi(\omega)$ is used to control the shape of the pulses. We have used the same approach in our numerical simulations, i.e. the search space is in the frequency domain while the fitness evaluation is performed in the time domain. To this end, we interpolated $\phi(\omega)$ at N frequencies ω_N ; the N values $\phi(\omega_N)$ are our decision parameters to be optimized. In order to achieve a good trade-off between high resolution and optimization efficiency, the value of $N = 80$ turned to be a good compromise.

The alignment's quantity, i.e. the success-rate or fitness, is defined as the expectation value of the *cosine-squared* of the angle of the molecular axis with respect to the laser polarization axis. Moreover, since a high degree of alignment with a peak intensity as low as possible was the desired result, an additional constraint was introduced as a *punishment term* for pulses that are too intense.

Explicitly, we have used

$$I_p = \int_0^T E^2(t) \cdot \Theta(E^2(t) - I_{thr}) dt \quad (2)$$

where $\Theta(x)$ is the *Heaviside step function*. Hence, the fitness function assigned to a pulse shape is given by

$$F = \max_{E(t)=0} \langle \cos^2(\theta) \rangle - \lambda I_p. \quad (3)$$

By choosing λ large enough, I_{thr} can be used to effectively operate the evolutionary algorithms only on a subset of pulses whose maximum peak intensity approaches the threshold intensity from below. We have used $\lambda = 1$ and I_{thr} was 0.36.

A typical phase function and a typical laser pulse, obtained by an evolutionary optimization, are given for illustration as Fig. 1 and Fig. 2, respectively.

It should be noted that this *laser pulse shaping problem*, based on numerical simulations, has been tackled at several levels. A recent work has studied the application of *niching methods* to this problem [14].

3. THE COMPLETE-BASIS-FUNCTIONS PARAMETERIZATION METHOD

We hereby propose a new method for learning a function, based on a representation transformation, which can also be referred to as parameterization. The so-called *Complete-Basis-Functions Parameterization Method* was originally constructed for learning the target function of the laser shaping

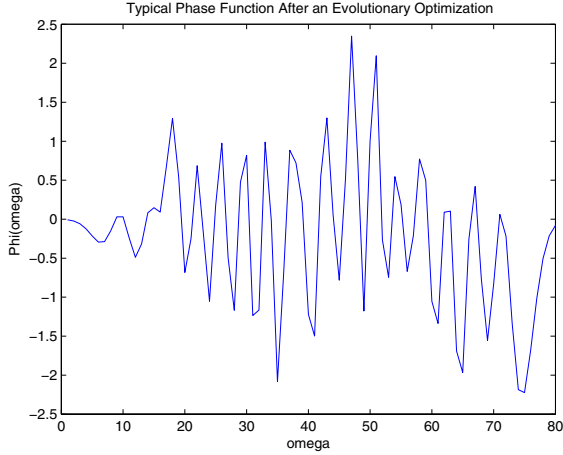


Figure 1: A phase function obtained by an evolutionary search (frequency domain).

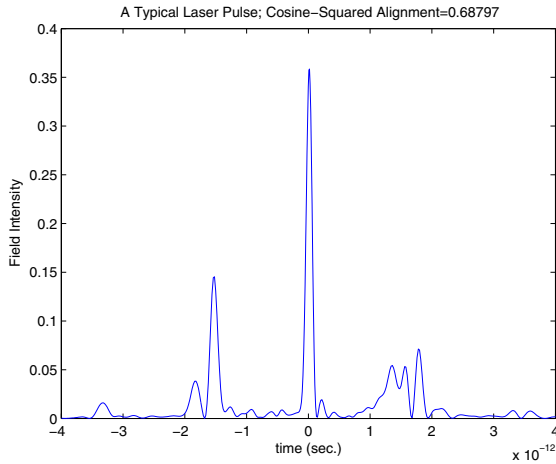


Figure 2: A laser pulse, given an optimized phase function (time domain).

problem, the phase $\phi(\omega)$, but is a general method for learning a generic n -variables function. It reduces the dimensionality of the search space and speeds up the convergence respectively, as will be explained in detail.

3.1 Mathematical Background

Here is a brief summary of the fundamental mathematical concepts which are used for our method. This part is mainly based on Abramowitz [1] and Kaplan [9].

Let $f(x)$ be given in the interval $a \leq x \leq b$, and let

$$\xi_1(x), \xi_2(x), \dots, \xi_k(x), \dots \quad (4)$$

be functions all piecewise continuous in this interval. The set $\{\xi_k(x)\}_{k=1}^{\infty}$ is called *complete* if it can span any piecewise continuous function, in particular $f(x)$:

$$f(x) = \sum_{k=1}^{\infty} c_k \xi_k(x) \quad (5)$$

where the coefficients c_k are given by:

$$c_k = \frac{1}{B_k} \int_a^b f(x) \xi_k(x) dx, \quad B_k = \int_a^b [\xi_k(x)]^2 dx \quad (6)$$

The convergence is guaranteed by the *completeness theorem*. Explicitly, the series

$$R_m = \int_a^b \left(f(x) - \sum_{k=1}^m c_k \xi_k(x) \right)^2 dx \quad (7)$$

converges to 0 for sufficiently large m :

$$\lim_{m \rightarrow \infty} R_m = 0 \quad (8)$$

We note the sequence of *partial sums* as:

$$S_m(x) = \sum_{k=1}^m c_k \xi_k(x) \quad (9)$$

By definition, the convergence of the series of functions is equivalent to the convergence of S_m .

3.1.1 The Fourier (Trigonometric) Series

A *trigonometric series* is the expansion of a periodic function in terms of an infinite sum of *sines* and *cosines*, making use of the orthogonality property of the harmonic functions. Without loss of generality, let us consider from now on the interval $[0, L]$. Given $f(x)$, a single-valued function defined on that interval, its *trigonometric series* or *trigonometric expansion* is given by:

$$\tilde{f}(x) = \frac{1}{2} a_0 + \sum_{k=1}^{\infty} a_k \cos\left(\frac{2\pi k}{L} \cdot x\right) + \sum_{k=1}^{\infty} b_k \sin\left(\frac{2\pi k}{L} \cdot x\right) \quad (10)$$

If the coefficients a_k and b_k satisfy certain conditions, then the series is called a *Fourier series*.

If $f(x)$ is periodic with period L , and has continuous first and second derivatives for all x in the interval, it is guaranteed that the trigonometric series of $f(x)$ will converge uniformly to $f(x)$ for all x (this is known as the *Dirichlet conditions*). We shall refer in this paper to the *trigonometric series* as the *Fourier series*.

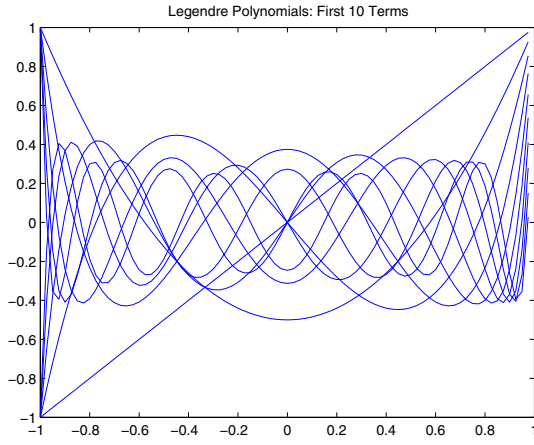


Figure 3: The First 10 *Legendre Polynomials*.

3.1.2 Other Sets of Functions

If one is indeed interested in periodic functions, there is no natural alternative but using the trigonometric series. However, if one is concerned with other representations of a general function over a given interval, a great variety of other sets of functions is available:

- Introduce the *Legendre polynomials*, $P_k(x)$:

$$P_k(x) = \frac{(2k-1)(2k-3)\dots 1}{k!} \left\{ x^k - \frac{k(k-1)}{2(k-1)} x^{k-2} + \frac{k(k-1)(k-2)(k-3)}{2 \cdot 4(2k-1)(2k-3)} x^{k-4} - \dots \right\} \quad (11)$$

which can also be defined via Rodrigues' formula:

$$P_0(x) = 1 \quad P_k(x) = \frac{1}{2^k k!} \frac{d^k}{dx^k} (x^2 - 1)^k, \quad k = 1, 2, \dots \quad (12)$$

If $f(x)$ satisfies the *Dirichlet conditions* mentioned earlier, then there will exist a Legendre series expansion for it in the interval $-1 < x < 1$.

For illustration, the first 10 *Legendre polynomials* are plotted in Fig. 3.

- Introduce the *Bessel Function of the First Kind and of Order l* , $J_l(x)$:

$$J_l(x) = \sum_{k=0}^{\infty} \frac{(-1)^k x^{l+2k}}{2^{l+2k} \cdot k! \cdot \Gamma(l+k+1)} \quad (13)$$

where $\Gamma(\alpha)$ is the *Gamma function*.

Given a fixed $l \geq 0$, the functions $\{\sqrt{x}J_l(\lambda_{lk}x)\}_{k=1}^{\infty}$ form an orthogonal complete system on the interval $0 \leq x \leq 1$.

- Introduce the *Hermite polynomials*, $H_k(x)$:

$$H_k(x) = (-1)^k \exp\{x^2\} \frac{d^k}{dx^k} (\exp\{-x^2\}), \quad k = 0, 1, \dots \quad (14)$$

The *Hermite polynomials* form a complete set of functions over the infinite interval $-\infty < x < \infty$ with respect to the weight function $\exp\{-\frac{1}{2}x^2\}$.

3.1.3 Higher Dimensions

An expansion into a complete set of functions can be generalized for higher dimensions as well. For illustration, let us consider shortly the two-dimensional case for the *trigonometric series*. The functions $\cos(\frac{2\pi k}{L} \cdot x) \cdot \cos(\frac{2\pi l}{L} \cdot y)$, $\sin(\frac{2\pi k}{L} \cdot x) \cdot \cos(\frac{2\pi l}{L} \cdot y)$, $\cos(\frac{2\pi k}{L} \cdot x) \cdot \sin(\frac{2\pi l}{L} \cdot y)$ and $\sin(\frac{2\pi k}{L} \cdot x) \cdot \sin(\frac{2\pi l}{L} \cdot y)$ form an orthonormal complete system of functions in the box $[(0, 0), (0, L), (L, 0), (L, L)]$. Given a function in that domain, $f(x, y)$, its expansion can then be written in the form:

$$f(x, y) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \lambda_{kl} \cdot \{ a_{kl} \cos(\frac{2\pi k}{L} x) \cos(\frac{2\pi l}{L} y) + b_{kl} \sin(\frac{2\pi k}{L} x) \cos(\frac{2\pi l}{L} y) + c_{kl} \cos(\frac{2\pi k}{L} x) \sin(\frac{2\pi l}{L} y) + d_{kl} \sin(\frac{2\pi k}{L} x) \sin(\frac{2\pi l}{L} y) \} \quad (15)$$

3.1.4 Corollary

An infinite series of complete basis functions converges to any "reasonably well behaving" function. Hence, it is straightforward to approximate a given function with a finite series of those functions, i.e. by cutting its tail from a certain point. In principle, the sum S_m can always be found to a desired degree of accuracy by adding up enough terms of the series. For practical applications, the corollary is that every function can be approximated using a series of complete basis functions, to whatever desired or practical accuracy. Moreover, this corollary can be easily generalized to any desired dimension.

3.2 Proposed Method: Learning a Function using a Set of Complete-Basis-Functions

3.2.1 Preliminary: Expansion of a Known Function

As we will demonstrate here, finding the expansion of a known function with respect to a given set of complete basis functions, i.e. finding the coefficients of the functions in this base, is an easy task for a simple evolutionary algorithm, and in particular for the standard ES. For simplicity, and without loss of generality, let us assume that the task is to approximate a one-variable function using a trigonometric series. This task can be generalized to functions of higher dimensions, and by using other expansions.

Consider the *expansion coefficients* of the cosine and sine functions, $\{a_k\}_{k=0}^{\infty}$, $\{b_k\}_{k=1}^{\infty}$, as the decision parameters to be optimized in the evolutionary search. As a preliminary task in this research, we found that the standard ES converged easily and fast to the right coefficients, where this basic fitting problem was simply defined as *minimizing the square error* (fitness was defined respectively as the root-mean-square error function between the original function and its evolving approximation).

Fig. 4 shows the result of learning the *triangle function* with a standard Evolution Strategy, using only the first 20 frequencies ($n = 40$) of a *Fourier series* as building blocks for a given discretization of $N = 100$.

3.2.2 Learning a Function

The idea of spanning a function using a set of complete basis-functions can also be used for the task of learning an n -variables function, and in particular when its profile is unknown apriori, as in our laser pulse shaping problem. The inspiration for this method was the Physicists' intuition to

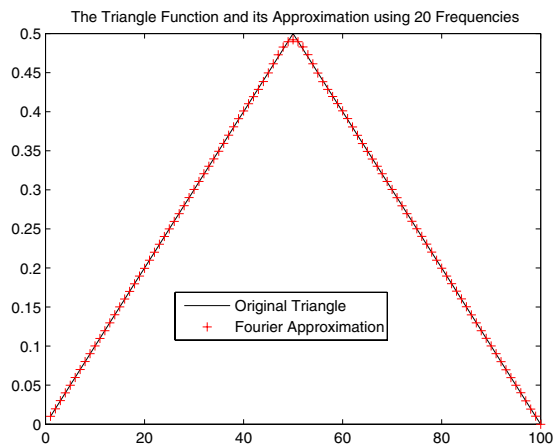


Figure 4: Learning the *triangle function* using the first 20 *Fourier* frequencies. The plot shows the original triangle function and its Fourier approximation.

the laser problem, which claimed that the function to be learned, $\phi(\omega)$, should be periodic. Motivated by this intuition, we started to run experiments in which an Evolution Strategy was trying to learn $\phi(\omega)$ using the *harmonic functions* as building blocks. Rather than learning the values of the target function, in a naive manner so to say, the idea was then to learn the coefficients of the harmonics (Fourier components). Following the success of those experiments, we expanded the method to other sets of complete basis functions, and in particular to the sets of functions which were introduced earlier: the *Legendre Polynomials*, the *Bessel Functions* and the *Hermite Polynomials*.

Assuming that the desired discretization is up to a resolution of N points in the interval, we limit the number of elements in the expansion series to n , where preferably $n \ll N$. By that we can achieve a dramatic dimensionality reduction of the search space, aiming to achieve a speeding-up of the convergence. The idea then is to apply an evolutionary search for the n coefficients of the building functions, where a simple transformation is applied for every fitness evaluation. In practice, the time for additional computation of this transformation is negligible with respect to the time for objective function evaluation in every real-world problem. Since the ES is a natural algorithm to handle the optimization of those real-valued coefficients, we use it here.

An Evolution Strategy using a Fourier auxiliary function has been proposed in the past, known as the FES method [10]. The FES aims to approximate the fitness landscape, in particular its small attraction basins, using the Fourier series.

However, the careful reader should notice that our method is based on a different principle. It uses complete-basis functions for the approximation of the decision parameters themselves, rather than the fitness landscape, which is left untouched. It strongly relies on the fact that these decision parameters represent a continuous function - and this function is due to be approximated.

4. EXPERIMENTAL RESULTS

In this section we provide the reader with the essential information regarding our experimental setup and our experimental results. We begin by giving a brief summary of our evolutionary approach, namely the CMA-ES method, and continue with the description of the set of experiments.

4.1 The Core Mechanism: CMA-ES

The *covariance matrix adaptation evolution strategy* [6], is a variant of ES that has been successful for treating correlations among object variables. This method tackles the critical element of Evolution Strategies, the adaptation of the mutation parameters. We provide here only a short description of the principal elements of the $(1, \lambda)$ -CMA-ES.

The fundamental property of this method is the exploitation of information obtained from previous successful mutation operations. Given an initial search point \mathbf{x}^0 , λ offspring are sampled from it by applying the mutation operator. The best search point out of those λ offspring is chosen to become the parent of the next generation. The action of the *mutation operator* for generating new samples of search points in generation $g + 1$ is defined as follows:

$$\bar{\mathbf{x}}^{g+1} = \bar{\mathbf{x}}^g + \delta \cdot \mathbf{B} \cdot \bar{\mathbf{z}} \quad (16)$$

where δ is the global step size, which is adaptive with respect to the optimization process, and \mathbf{z} is a vector of random variables drawn from the *multivariate normal distribution*. The matrix \mathbf{B} , the crucial element of this process, is composed of the eigenvectors of the covariance matrix with the appropriate scaling of the eigenvalues - defining the distribution of a sequence of successful mutation points. It is initialized as the *unity matrix* and is updated according to cumulative data from the evolution process itself.

We omit most of the details due to the framework of this paper, and refer the reader to [6].

4.2 Experimental Setup

We provide some information about the experimental setup of the laser shaping numerical simulation:

- The *cosine-squared alignment* yields a real value in the interval $[0, 1]$, subject to maximization, as was introduced earlier.

A random feasible solution should yield on average a value of 0.333, due to the isotropic 3D space, and the best result known to us in the given temperature is around 0.7.

- The punishment term, which was introduced earlier in Eq. 2 and Eq. 3, can yield negative fitness values. The probability of a randomly generated pulse to obtain this punishment is extremely low.
- Given the default discretization of $N = 80$, we apply our method with $n = 40$ coefficients for each one of the functions. This configuration is fixed.
- Every fitness evaluation call requires approximately 35 seconds of computation time on a Hyper-threaded Pentium-4 of 2.6GHz.
- Due to the heavy computational cost of a single fitness evaluation, in practice we are limited in function evaluations and obliged to apply minimal settings. Therefore, we chose to use the $(3, 12)$ -CMA strategy as our default algorithm in our experiments.

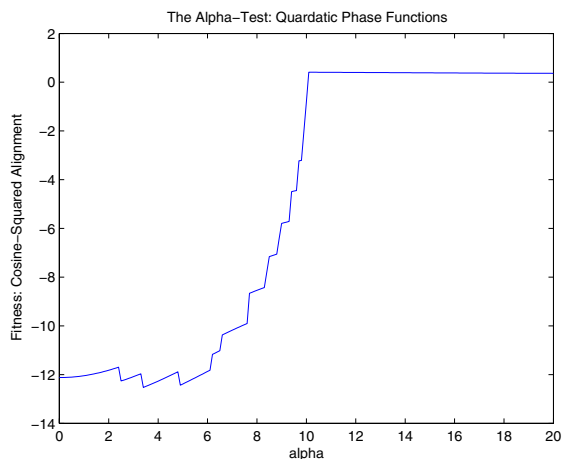


Figure 5: Sampling Quadratic Phase Functions.

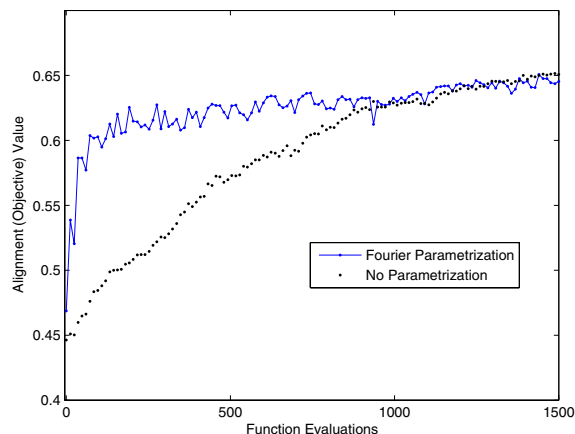


Figure 6: Typical runs of the *Fourier* param. versus the direct param., up to 1500 evaluations.

4.3 Preliminary Experiments

4.3.1 Quadratic Phase Functions: The α -Test

Given representations based on low-order polynomials, we wanted to check whether there exists a trivial local optimum which would become an attractor for such phase functions. Hence, we tested the fitness of quadratic phase functions, centered around the central frequency.

Explicitly, we tested the family of the functions

$$\phi(\omega)_\alpha = \alpha \cdot (\omega - \omega_{central})^2 \quad (17)$$

where the real-valued α is sampled systematically in the interval $[0, 20]$. The results of this so-called α -test are presented in Fig. 5. As can be clearly seen in the given plot, most of the quadratic phase functions get extremely low fitness values, due to large punishment terms, and they never exceed the fitness value of 0.4. This eliminates the existence of a trivial quadratic solution for the problem.

4.3.2 The Initial States Density Test

The following preliminary experiment is meant to compare the natural initial quality of the different parameterizations. We applied a so-called *initial states density test*, a statistical fitness measurement of the initialized phase functions in the different parameterizations. For each parameterization in use, i.e. the direct 80-dimensional random phase vector, or the random 40-dimensional coefficient vector for the various polynomials in use, we initialized 1000 phase functions and calculated the mean fitness and the standard deviation respectively.

4.4 Numerical Results

In this subsection we present the results of the runs of the different parameterization methods - the direct parameterization versus the polynomial-based methods. Our runs were based on the (3, 12)-CMA mechanism, limited to 5,000 function evaluations per run. We performed 20 runs per method. We consider the performance criteria of the various methods as the following:

- The mean and the standard deviation of the fitness values averaged per method over the 20 runs.

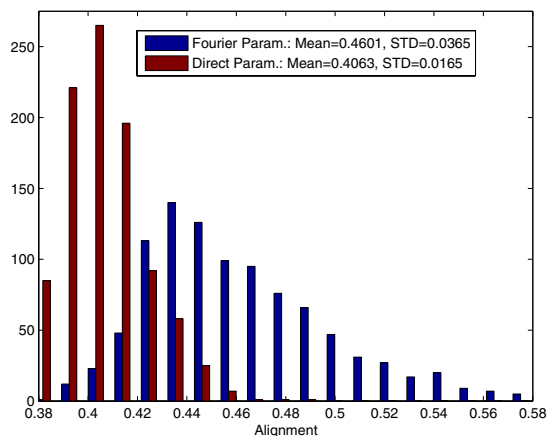


Figure 7: Initial States Density Tests for the *Fourier* Param. versus the Direct Param.

- The averaged number of evaluations per method until the fitness value of 0.6 was reached during the runs, with the standard deviation. We consider the value of 0.6 as the lower bound of the regime of good solutions.
- The results of the *initial states density test*, as was introduced earlier: the averaged initial fitness values per method, with the standard deviation.

We provide a table of results, which consists of the numerical values of the specified performance criteria per method. It is given as table 1.

4.5 Analysis and Discussion

An important result that should be noted is that **all** the runs in the various parameterizations have converged into a highly fit phase function. There was not even a single run of a non-convergence.

Furthermore, we would like to analyze shortly the experi-

Table 1: Parameterizations: Performance Results

Parameterization	Averaged Best-Fitness	Evaluations for 0.6	Initial States Density
Direct-Param	0.6603 ± 0.02	834 ± 476.7	0.4063 ± 0.01
<i>Fourier</i>	0.6595 ± 0.01	255.15 ± 115.5	0.4601 ± 0.03
<i>Legendre</i>	0.6232 ± 0.03	600 ± 517.8	0.4364 ± 0.02
<i>Bessel</i>	0.6167 ± 0.02	1790 ± 1932	0.4633 ± 0.03
<i>Hermite</i>	0.6781 ± 0.01	438.6 ± 188.4	-10.387 ± 0.40

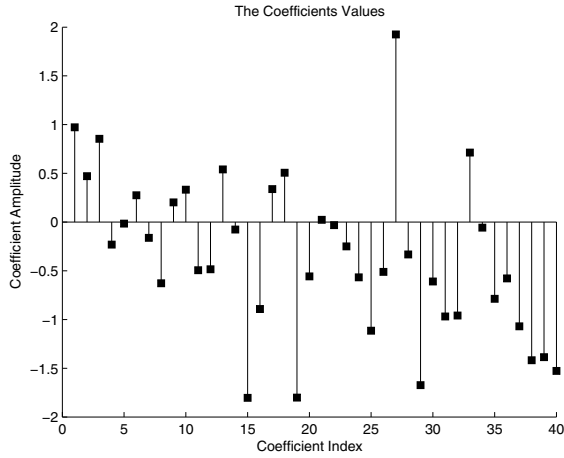


Figure 8: The coefficients values for a solution with cosine-squared alignment of 0.688 in the *Hermite* parameterization.

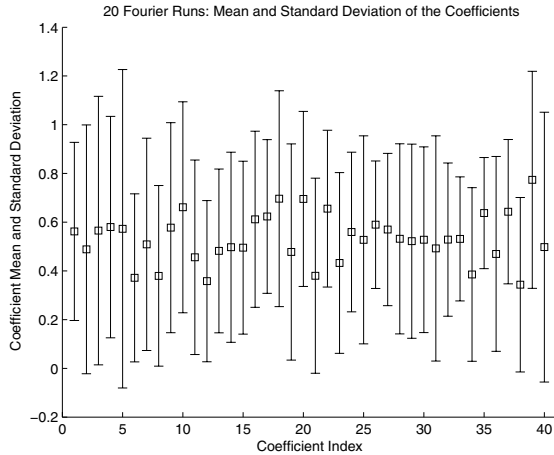


Figure 9: The coefficients' mean and standard deviation values for the *Fourier* parameterization over the 20 runs.

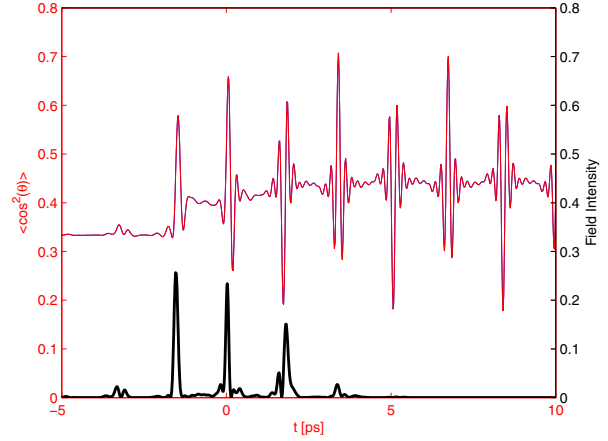


Figure 10: Best solution obtained by the *Hermite* parameterization, with alignment of 0.7038. Thin red line: alignment; thick black line: intensity profile of the optimized laser pulse. The solution consists of three main peaks.

mental results of the various parameterizations with respect to the phase function optimization, as presented in table 1.

1. **Fitness values.** Some of the polynomial-based parameterizations obtained fitness values as high as the direct parameterization method, and in particular the *Hermite* parameterization, which obtained the best results among all the methods. As far as we know, the obtained values are the highest *cosine-squared alignment* values which were ever achieved. Hence, from the optimization perspective, the proposed method is not harmed at all by the transformation and the reduction of dimensionality.
2. **Convergence speeding-up.** An immediate conclusion from the table is that the proposed method achieved a significant speeding-up of the convergence for the *Fourier* as well as for the *Hermite* parameterizations. Fig. 6 provides the typical runs of the *Fourier* parameterization versus the direct parameterization, up to 1500 fitness evaluations.
3. **Initial state.** The *Fourier* and the *Bessel* parameterizations have the most natural **initial** representations for the phase function in our given problem, as reflected from the *initial states density test* results. However, as the other measures show, the *Bessel* parame-

terization fails to obtain satisfying final results, whereas the *Fourier* succeeds dramatically in that. Moreover, the *Hermite* parameterization, due to large punishment values, has a negative initial state, but obtains nonetheless highly satisfying final results. It should be noted that the standard deviations of the different fitness distributions are reasonably low. A comparison between the initial states density of the *Fourier* parameterization versus the density of the direct parameterization, presented in a *histogram*, is given as Fig. 7.

4. **Physics interpretation.** Aiming to get some physics insights into the nature of highly-fit phase functions with respect to the laser shaping problem, we examined the nature of good solutions in the different parameterizations. The idea was to calculate the distributions of the coefficients, and try to identify the dominance of certain components (frequencies in the Fourier case).

Unfortunately, such dominance could not be identified within the results. A typical plot of the coefficients values for a highly-fit solution for the *Hermite* parameterization is given as Fig. 8. Moreover, Fig. 9 provides a visualization of the mean and the standard deviations of the 40 coefficients of the *Fourier* parameterization over the 20 runs.

5. **Best solution.** The highest cosine-squared alignment value ever found was obtained by the *Hermite* parameterization. This best solution has an alignment value of $F = 0.7038$. The time-dependent pulse intensity for the best solution is shown in Fig. 10 together with the time-dependent $\langle \cos^2(\theta) \rangle$.

5. CONCLUSIONS

Being inspired by the physicists' intuition to the given *laser pulse shaping* problem, which suggested a periodic nature of the solutions, we developed a general method for the learning task of any n -variables function.

We have studied and introduced in this paper the mathematical background for this method. Furthermore, we applied a couple of preliminary tests with respect to the application of the method to the given physics problem. The so-called α -test has succeeded in justifying this method and did eliminate the possibility of convergence into a trivial attractor. The *initial states density test* contributed a perspective of the nature of the various parameterizations with respect to the given laser pulse shaping problem. The analysis of its results shows that it does not necessarily reflect the potential of a given parameterization to obtain satisfying final results. By performing a series of numerical simulations, with a fixed number of coefficients $n = 40$, we managed to show that our method qualified as a robust optimization method, and in particular achieved a significant speeding-up the convergence process of the given problem. The obtained solutions were at least as good as any other solutions known to us, but were achieved faster.

Future Research

We would like to outline possible directions for further study with respect to our work. We consider the following main directions:

1. The Complete-Basis-Functions Parameterization method should be applied to other challenging real-world optimization problems. In particular, it may be applied to surface or shaping problems in 2 and 3 dimensional space, where the target surface can be spanned by the appropriate complete basis functions.
2. Further parameterizations should be studied and tested with respect to the laser pulse shaping problem.

6. ACKNOWLEDGMENTS

This work is part of the research programme of the 'Stichting voor Fundamenteel Onderzoek de Materie (FOM)', which is financially supported by the 'Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO)'.

7. REFERENCES

- [1] M. Abramowitz and I. Stegun. *Handbook of Mathematical Functions*. National Bureau of Standards, Applied Math. Series 55, Dover Publications, 1965.
- [2] T. Bäck. *Evolutionary algorithms in theory and practice*. Oxford University Press, New York, NY, USA, 1996.
- [3] T. Bäck, G. Rudolph, and H.-P. Schwefel. Evolutionary programming and evolution strategies: Similarities and differences. In *Proceedings of the second Annual Conference on Evolutionary Programming*, pages 11–22, La Jolla, CA, USA, 1993. Evolutionary Programming Society.
- [4] L. J. Fogel. *Artificial Intelligence through Simulated Evolution*. John Wiley, New York, NY, USA, 1966.
- [5] B. Friedrich and D. Herschbach. *Phys. Chem. Chem. Phys.*, 2(419), 2000.
- [6] N. Hansen and A. Ostermeier. Completely derandomized self-adaptation in evolution strategies. *Evolutionary Computation*, 9(2):159–195, 2001.
- [7] N. Hay. *Phys. Rev.*, A 65(053805), 2000.
- [8] J. H. Holland. *Adaptation in Natural and Artificial Systems: An Introductory Analysis with Applications to Biology, Control and Artificial Intelligence*. MIT Press, Cambridge, MA, USA, 1992.
- [9] W. Kaplan. *Advanced Calculus*. Addison-Wesley, 1983.
- [10] K.-S. Leung and Y. Liang. Evolution strategies with a fourier series auxiliary function for difficult function optimization. In *IDEAL*, volume 2690 of *Lecture Notes in Computer Science*. Springer, 2003.
- [11] I. Rechenberg. *Evolutionstrategien: Optimierung technischer Systeme nach Prinzipien der biologischen Evolution*. Frommann-Holzboog Verlag, Stuttgart, Germany, 1973.
- [12] F. Rosca-Pruna and M. Vrakking. Revival structures in picosecond laser-induced alignment of i2 molecules. *Journal of Chemical Physics*, 116(15):6579–6588, 2002.
- [13] H.-P. Schwefel. *Evolution and Optimum Seeking: The Sixth Generation*. John Wiley & Sons, Inc., New York, NY, USA, 1993.
- [14] O. M. Shir, C. Siedschlag, T. Bäck, and M. J. Vrakking. Niching in evolution strategies and its application to laser pulse shaping. In *Lecture Notes in Computer Science*, volume 3871. Springer, 2006.
- [15] H. Stapelfeldt. *Rev. Mod. Phys.*, 75(543), 2003.