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Nonlinear fitness–space–structure adaptation and principal component analysis in genetic algorithms: an application to x-ray reflectivity analysis

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Abstract

Two novel genetic algorithms implementing principal component analysis and an adaptive nonlinear fitness–space–structure technique are presented and compared with conventional algorithms in x-ray reflectivity analysis. Principal component analysis based on Hessian or interparameter covariance matrices is used to rotate a coordinate frame. The nonlinear adaptation applies nonlinear estimates to reshape the probability distribution of the trial parameters. The simulated x-ray reflectivity of a realistic model of a periodic nanolaminate structure was used as a test case for the fitting algorithms. The novel methods had significantly faster convergence and less stagnation than conventional non-adaptive genetic algorithms. The covariance approach needs no additional curve calculations compared with conventional methods, and it had better convergence properties than the computationally expensive Hessian approach. These new algorithms can also be applied to other fitting problems where tight interparameter dependence is present.

1. Introduction

X-ray reflectivity (XRR) is an efficient metrological tool for thin film characterization. Film thicknesses, surface roughnesses and mass densities are obtained by fitting a theoretical curve, based on Parratt's formalism [1] and the Nevot–Croce surface roughness approximation [2], to a measurement. Due to the nature of the formalism, a slight misprediction of one parameter is balanced by other parameters in nonlinear fashion. This nonlinear interparameter dependence hinders the convergence properties in simple gradient-based optimization methods where a local optimum is typically found instead of the global optimum. Several studies have shown that genetic algorithms (GAs), such as the classical GA (CGA), provide methods to solve these nonlinear inverse XRR problems [3–5]. Recently Ulyanenko and Sobolewski

introduced an algorithm called eXtended GA (XGA), which proved to be an efficient fitting method for x-ray analysis [6].

The XRR fitting capabilities of CGA and XGA are typically limited to models of a few layers since interparameter dependence, called genetic linkage, grows very fast with an increasing number of layers. To reduce genetic linkage efficiently, Wyatt and Lipson introduced a Hessian matrix-based linear transformation technique for real-valued problems, which adapts dynamically to the linear eigenstructure of the fitness space [7]. A major disadvantage of this principal component analysis (PCA) approach relates to the assumption of linearity and to the quadratically increasing number of fits needed for the Hessian matrix computation. Therefore, novel approaches are needed to overcome these issues.

In this paper we introduce two new GAs based on PCA and a nonlinear fitness–space–structure adaptation called

NL-FSSA. The first algorithm, called HGA, utilizes PCA based on a numerically computed Hessian matrix while the second algorithm, CovGA, utilizes PCA based on interparameter covariances. The convergence and stagnation properties of these novel algorithms are studied and compared with CGA and XGA. We show that PCA, NL-FSSA and other modifications together enhance significantly the speed of convergence and reduce stagnation. Finally, PCA can be realized with the computationally efficient covariance method, which has better convergence properties than HGA. In section 2 we describe the implementation of the algorithms studied in this paper. The employed layer model for XRR curve fitting tests and the respective results are shown in section 3.

2. The implementation of the algorithms

Figure 1 shows the flowchart of the algorithms with the exception that CGA and XGA omit NL-FSSA and coordinate rotation. In these methods, the global optimum is approached by minimizing the fitness representing the difference between trial and target XRR curves. The applied fitness function is the scaled sum of the squared difference

$$F = \left[\sum_j (x_j - y_j)^2 \right] \left[\sum_j (x_j^2 + y_j^2) \right]^{-1}$$

$$= 1 - 2 \left(\sum_j x_j y_j \right) \left[\sum_j (x_j^2 + y_j^2) \right]^{-1},$$

where F is the fitness and x_j and y_j are the j th logarithmic values of the respective datapoints. This scaling ensures the upper limit for the fitness. The fitness of each individual is used in parent selection where the conventional elitist strategy is applied.

A nonlinear fitness space estimate model was chosen to be utilized in the movement of parents in parameter space. The model is constructed from separate polynomial fits where each fit describes the individuals' fitnesses as a function of one parameter. A possible divergence of the fits outside the parameter range is removed using cubic splines with reasonable boundary values. The eventual fitness estimate is a linear combination of separate fits, where the mean absolute deviations of the parameters are used to evaluate weighting coefficients. This estimate is used to find the nearest local fitness optimum in a negative gradient direction for each individual. It was found that the eventual step length towards this direction is optimal when the movement is proportional to the difference of the initial fitness and the local optimum estimates divided by the initial fitness estimate. Parents are temporarily moved to the estimated points until the mating is done. This novel movement scheme acts as an adaptive technique which reshapes the probability distribution of the parameters by increasing trials of the next generations in estimated optimal regions.

To reduce linear genetic linkage, new offspring are composed in rotated coordinates. Every even cycle on the new basis is selected to be the set of eigenvectors of the Hessian matrix in the vicinity of the best individual in HGA. The time needed for the Hessian matrix computation is reduced to a reasonable level by taking into account every tenth point of

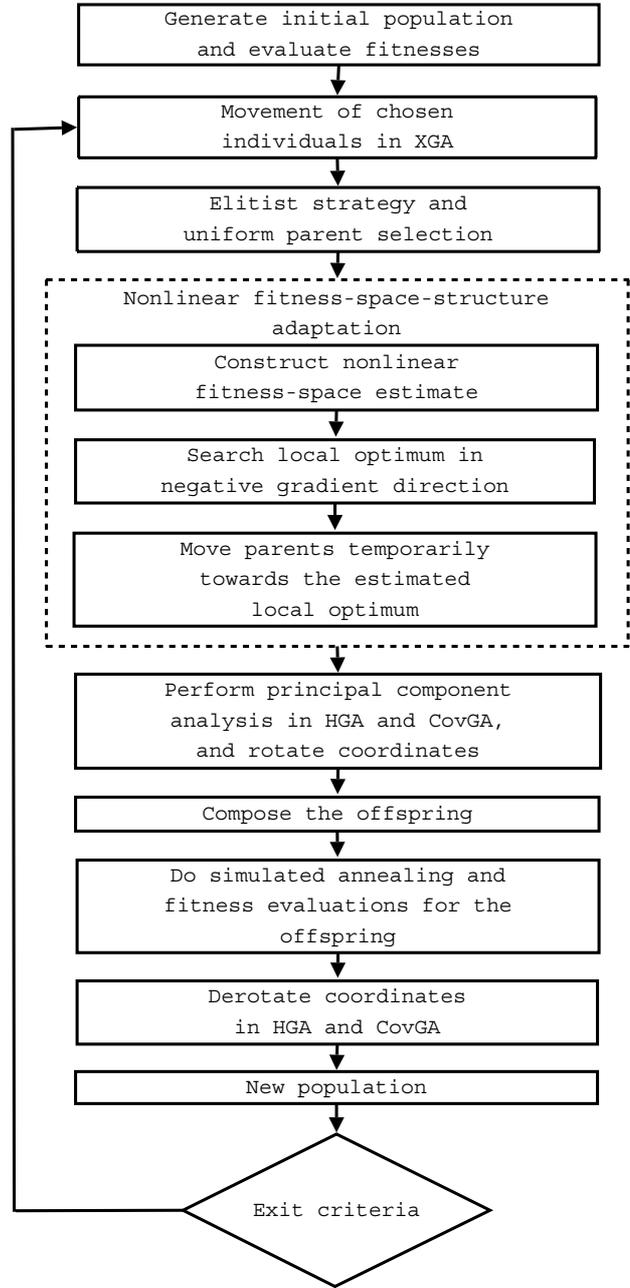


Figure 1. Flowchart of the genetic algorithms.

the XRR curves in the fitness evaluation. Respectively, in CovGA, the eigenvectors calculated from the interparameter covariance matrix of population values are used for the basis selection but computational simplification is not needed as in HGA. The parents are transferred to the new coordinates and the offspring are composed using a fitness weighted crossover operator. The weight is used to move randomly selected genes to the next generation in proportion to the fitness of the parents. If NL-FSSA is applied, a randomly selected child is replaced by the optimal parameter set from the nonlinear fitness space estimate. This was found to give an additional convergence boost by reducing short-term stagnation.

Simulated annealing was selected to be used as a mutation operator in all algorithms to enhance the quality of trials and

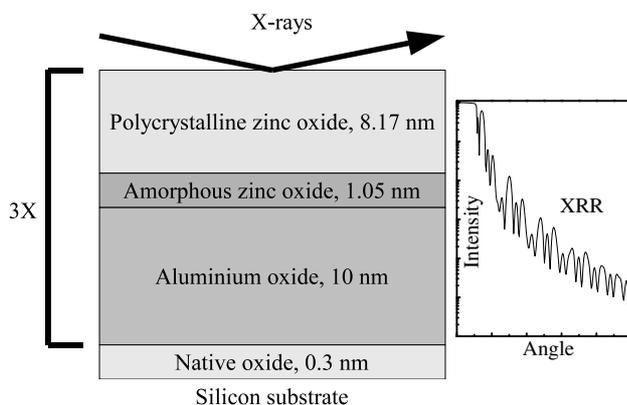


Figure 2. Schematic structure of the modelled nanolaminate and the theoretical x-ray reflectivity curve.

to reduce premature diversity loss of forthcoming populations. HGA and CovGA apply annealing in the new coordinates, and the eigenvalues of respective directions are used to scale space directions to similar resolutions. Finally, a new population is created using the principle of XGA in novel algorithms.

All implementations of the algorithms presented in this paper were based on the code of CGA. The specific features of XGA, HGA and CovGA were to utilize the same code whenever it was possible. This method of implementation preserved the internal parameters between the GAs thus enhancing the reliability of comparison of the algorithms.

3. Results and discussion

Properties of nanolaminates can be analysed from an XRR curve by fitting but the performance of the fitting algorithm can be the bottleneck in the analysis. Therefore, the performance of the algorithms was tested by fitting randomly selected trials to the XRR curve of a realistic model of a three-period ZnO/Al₂O₃ nanolaminate. This type of nanolaminate can be deposited with atomic-layer-deposition (ALD) [8] and typical values of ALD materials were utilized to the model structure shown in figure 2. The 0.3 nm thick native oxide on a HF cleaned silicon substrate typically grows during the deposition of aluminium oxide. The mass density of Al₂O₃ was set to 3.0 g cm⁻³, which is 77% of the sapphire packing density. The amorphous ZnO layer was assumed to have the same proportional packing density as ALD-aluminium oxide and the layer thickness was set at 1.05 nm (7 deposition cycles in ALD, 0.15 nm/cycle). Polycrystalline zinc oxide had a mass density of 5.61 g cm⁻³ (approximately 100% packing density) and the thickness was set to 8.17 nm (43 cycles, 0.19 nm/cycle). Substrate and native oxide roughnesses were set at 0.05 nm and 0.1 nm, respectively. The roughness in the structure was assumed to increase cumulatively by 0.025 nm per amorphous layer and by 0.05 nm per polycrystalline layer.

The robustness of the algorithms was tested with 50 different initial populations, which were used for all the algorithms. The initial parameters were selected to be in the vicinity of the optimal parameters with $\pm 20\%$ deviation using a uniform random distribution. The

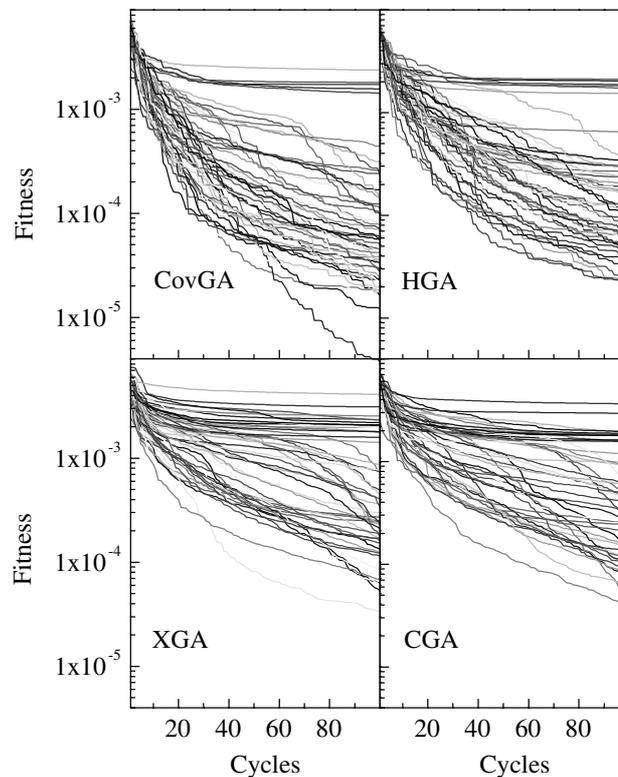


Figure 3. Fitness of the best individual of each population as a function of cycles. Each population has its own line in greyscale. All graphs are shown in the same scale.

populations had 50 individuals and the GA procedures were iterated 100 cycles. XRR curves were fitted without fixed interparameter dependences from 0° to 2.5° using evenly spaced angle points. Figure 3 shows the fitness results of the fitting trials. The convergence lines show that novel algorithms had less stagnated populations than conventional methods. Surprisingly, CovGA has more robust convergence behaviour than HGA. HGA is based on the numerically computed Hessian matrix and it should predict the genetic linkage more precisely than the covariance approach, which is based on semi-arbitrary parameter sets.

Figure 4 shows zoomed plots of the fitted curves based on the parameters of the median fits after the last cycle of the fitting procedures. It can be seen that the fits of the CovGA and HGA follow the theoretical curve very closely but XGA and especially CGA curves exhibit non-matching behaviour.

Figure 5 shows the fraction of solutions (%) below a certain fitness. The fitness representing the median fraction of CovGA is less than 6×10^{-5} , for HGA it is 1.2×10^{-4} , for XGA it is 3×10^{-4} and for CGA it is 5×10^{-4} . Results show that the robustness of convergence is quantitatively better for XGA than for CGA and that the adaptive algorithms exhibit qualitatively better convergence behaviour than non-adaptive methods. The effect of nonlinear adaptation on convergence was studied by switching NL-FSSA off. HGA without NL-FSSA was seen to have clearly better convergence than XGA while HGA with NL-FSSA had a similar convergence fraction as CovGA without NL-FSSA. Thus it can be concluded that the CovGA having nonlinear and linear adaptation mechanisms had the best fitting properties.

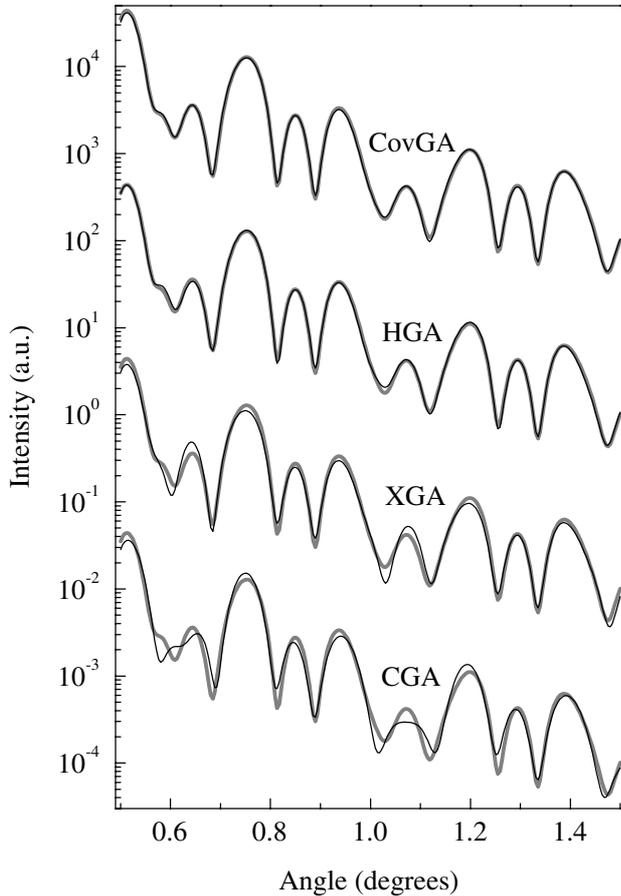


Figure 4. Fitted curves based on the parameters of the median fits. The XRR curves based on the model are plotted with dark grey lines and the median fits with solid black lines. The curves have a vertical offset for clarity.

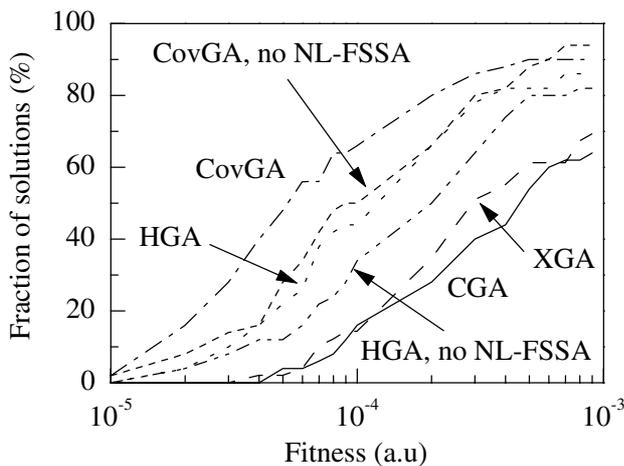


Figure 5. Fraction of solutions (%) below the given fitness. The results of the exclusion of NL-FSSA in CovGA and HGA are also shown.

The applicability of the algorithms with non-ideal data was tested by using the theoretical curve including artificially generated noise. The new algorithms were used for the fitting with and without NL-FSSA. The applied noise was mimicking the typical noise of the x-ray detector of Philip's X'Pert Pro

instrument in a three-minute measurement in the present angle range. As a result, fitnesses were increased similarly between algorithms due to deviations of intensity values in the theoretical curve. Qualitatively the convergence and stagnation properties were unchanged.

4. Conclusion

Genetic algorithms utilizing adaptation techniques have been shown to be more effective and robust fitting algorithms than conventional non-adaptive methods for XRR analysis of a periodic multilayer structure. It was also found that CovGA had better fitting properties than HGA. The interparameter covariance method seemed to predict the genetic linkage better than HGA in the global scale by enhancing convergence properties, although Hessian eigenvectors represent the genetic linkage precisely in the vicinity of the fittest individual. The worse performance of HGA might be due to the inadequate assumption that the local fitness-space-structure can be generalized to a non-periodic fitness landscape. It is also worth mentioning that the sequential use of PCA and identity transformation in both the new algorithms gave the best result by enhancing the robustness of convergence in the first cycles and it was seen to reduce the loss of population diversity in the last steps. This suggests that the genetic linkage in the nonlinear fitness landscape cannot be robustly separated to nearly linearly independent factors. To overcome this issue, a novel NL-FSSA method was introduced. This technique significantly enhanced the speed of convergence and reduced the number of stagnated populations in all of the applied new algorithms. Although only one test case for the periodic nanolaminate structure was shown in this paper, similar differences between conventional and new methods were obtained for a non-periodic multilayer structure. This suggests that the novel algorithms presented in this paper have the potential to be utilized in a wide range of real-valued fitting problems.

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