# Multi-criteria Search and Optimization: an Application to X-ray Plasma Spectroscopy

Igor E. Golovkin
Department of Physics,
University of Nevada Reno,
Reno, NV 89557
golovkin@physics.unr.edu

Roberto C. Mancini
Department of Physics,
University of Nevada Reno,
Reno, NV 89557
rcman@physics.unr.edu

Sushil J. Louis
Department of Computer Science,
University of Nevada Reno,
Reno, NV 89557
sushil@cs.unr.edu

**X-ray spectroscopy diagnostics have been widely used as a standard technique to determine the temperature and density of astrophysical and laboratory plasmas. Traditional techniques have relied on performing an interactive search with a graphical user interface to select theoretical model parameters that best fit the data. We use a Pareto optimal genetic algorithm to drive a search of model parameters that produce high-quality simultaneous fits of spectra and spatially-resolved emissivity profiles. Preliminary results indicate that our Pareto optimal genetic algorithm is able to quickly find physically meaningful solutions.**

## 1 Introduction

X-ray spectroscopic analysis has been widely used as a standard technique to determine temperature and density of astrophysical as well as laboratory plasmas (Griem 1992). Routinely analysis is performed manually, that is, using an interactive graphical user interface to compare experimental and theoretical spectra calculated using a particular set of plasma model parameters. When a good fit to experimental data is achieved, the parameters used to calculate the synthetic spectrum are considered to be representative of the state of the plasma during the formation of the spectrum. A criterion for measuring good fits is the distance between synthetic and experimental spectra defined in a given metric as well as visual similarity. This procedure is simple and convenient as long as the spectral model is not very complex, does not depend on too many parameters, and is relatively inexpensive (can be performed in real time). For many other cases availability of a computer-driven automated analysis procedure is important. In this paper we will make an attempt to estimate plasma temperature and density gradients for high energy density plasmas.

Traditional (as described above) spectroscopic analysis has been used to determine averaged or effective temperatures ($T_e$) and densities ($N_e$). However, the spectroscopic analysis of plasma temperature and density gradients represents a more complicated search problem in parameter space. In this paper we use a genetic algorithm to estimate plasma temperature and density gradients for Inertial Confinement Fusion (ICF) experiments. The goal here is to find temperature and density gradients that produce simultaneous, good fits to time-resolved spatially integrated X-ray line spectra and X-ray monochromatic emissivity profiles. Spatial emissivity profiles can be extracted from Abel inversion of X-ray monochromatic images provided that the plasma is optically thin and spherically symmetric (see Figure 1).

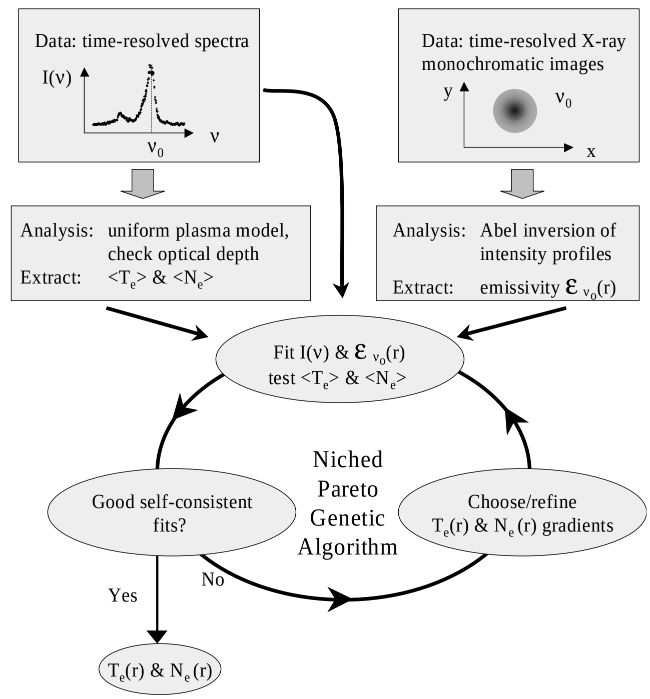


Figure 1. Plasma temperature and density gradients estimation.

Temperature and density spatial gradients as well as other properties of plasmas can be computed using hydrodynamic modeling. Hydro simulations are model calculations that include hydrodynamics, thermal transport, atomic, radiation physics, etc. The models are very complex and it is important to be able to compare simulation results with independent information obtained from the analysis of experimental data. Our work focuses on this subject and to a large degree it is independent from the hydro simulation. Estimating plasma temperature and density gradients based on the analysis of experimental data is a complex inverse problem. This work is one of the first attempts in this direction. The results of the analysis of experimental data can be used to improve characterization of core plasma dynamics and to provide new data for detailed benchmarks of hydrodynamic codes.

Since we need to simultaneously fit both spectra and emissivity the problem involves multi-objective optimization. The multi-objective nature of the problem makes it especially difficult to fit the data by hand. Spectroscopic analysis for non-linear models is also difficult for conventional minimization schemes and exhaustive searches can be prohibitively expensive. We have reported previously (Golovkin 1999) that Genetic Algorithms (GAs) perform very well when applied to spectroscopic diagnostics. In this paper we show that a Pareto optimal Genetic Algorithm is a robust and efficient tool to interpret experimental spectra and monochromatic images.

Genetic Algorithms are search algorithms based on the mechanics of natural selection (Holland 1975, Goldberg 1989). They are capable of finding a solution in a poorly understood search space while exploring only a small fraction of the space and can robustly deal with complex non-linear spaces. A GA's reliability, robustness, ease of use, and speed were our primary motivations to apply it for our purposes. In addition, spectral analysis has a threshold of sensitivity determined by the quality of the experimental data and by the model's sensitivity with respect to parameter changes. Since GA's are especially proficient at finding promising *areas* (corresponding to solutions within our threshold) of the search space, they are well suited for our problem.

We use the principles of Pareto Optimality in designing a Pareto optimal genetic algorithm (Horn 1993). At each generation there is a set of non-dominated solutions that form a surface known as the Pareto optimal front (or Pareto front). The goal of a Pareto optimal GA is to find and maintain a representative sampling of the solutions on the Pareto front. If the criteria are not self-contradictory, there should be a point on the final convex front that satisfies all criteria well. In our case this solution will be considered as the solution to the spectral analysis problem (Figure 2). If there is no such point (concave front), an expert decision has to be made about which (if any) solution on the concave Pareto optimal front represents the most acceptable, physically sound solution. Analysis in this case may not be reliable because a self-consistent high quality spectral model should be able to describe all radiative properties of the plasma. Tracing the Pareto optimal front also helps address the issue of solution uniqueness.

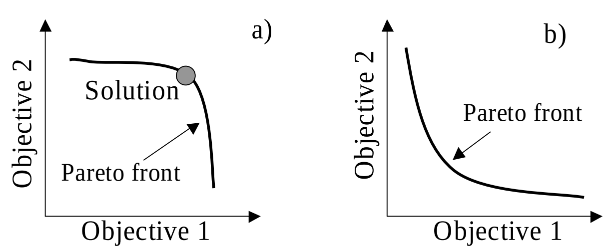


Figure 2. Results of the search a) successful; b) unsuccessful.

In this paper we show that the method we developed is capable of determining correct gradients. To this end we performed numerous calculations based on the analysis of synthetic experimental data. Running our spectral model using known gradients as input produces synthetic data. We add noise to the generated spectra and emissivity profiles to represent experimental uncertainties.

We pursue two main goals: to study how the quality of experimental data affects the diagnostic capability of our method; and to determine whether we can expect to resolve gradients that have complex structure. The first goal can be achieved by analyzing the data with simple gradients and different levels of noise. For the second problem we will try to analyze data produced with gradients obtained from hydro simulations of plasma implosions.

Successful analysis should be able to recover the gradients we used to construct the synthetic data, by fitting emissivities and spectra. We will show, however, that under certain circumstances GA can find alternative gradients that produce good fits to both emissivities and spectra. It is therefore very important to understand the limitations of the method before applying it to the analysis of real experimental data with unknown gradients.

As an application we consider analysis of Ar Heβ and associated Li-like satellites spectral feature observed during the collapse of Ar-doped laser-driven ICF implosions. This feature is widely used for diagnostic purposes. Based on the spectra of this feature effective emissivity-averaged plasma density and temperature can be determined. Combined with the information that can be obtained from monochromatic X-ray images of the plasma (photon energy at the center of Ar Heβ line) the spectra can be used to bracket temperature and density spatial gradients. Our spectral model is a collisional-radiative atomic kinetics steady state model that includes the effects of Stark broadening, line overlapping, and opacity (Golovkin 2000).

Our preliminary results indicate that spectroscopic analysis driven by the Pareto optimal Genetic Algorithm is capable of determining plasma temperature and density gradients. The method is generalizable, and with minor modifications can be used to drive searches in other plasma spectroscopy applications.

The next section describes our implementation of the algorithm that results in good performance. Then we will discuss the results of the computations. Finally we will present the conclusions and some guidelines for future work.

## 2 Implementation

The spectra are fully determined by the spatial distribution of plasma, electron number density and temperature. Both density and temperature should be smooth functions of position and all values must fall within a certain range in order to be physically meaningful. Moreover, the functions must be symmetric with respect to the center of the plasma and the first derivative of temperature should be equal to zero at the center.

There are several plausible gradient choices to satisfy these properties. We enforce these restrictions at the level of our encoding by noting that functions of the form $f(x) = ax^2+b$ or $f(x) = ax^4+bx^2+c$ automatically provide desired properties. A parabolic gradient is the simplest choice, requiring only two parameters to be fully defined, but may not always be flexible enough to approximate all physically possible gradients. The second function is more flexible, but adds a great deal of non-linearity to the encoding (we do not search for the coefficients of the polynomial but rather for extreme points so that the function lies within a given range). Another approach is to characterize each spatial region of the plasma by a density and temperature pair. This type of encoding can approximate any gradient, however special care must be taken to enforce smoothness. This can be done by restricting relative changes between adjacent points at the level of encoding, or to introduce extra terms in the fitness function. In addition, this type of encoding requires many parameters, longer chromosomes, larger population sizes, and therefore greater computing time. Regardless of the type of encoding we use five (5) bits to represent every parameter since five bits provides sufficient precision for diagnostic purposes. Figure 3 illustrates our encoding for the simple case of a parabolic gradient.

Temperature: $T(r) = a_1 r^2 + c_1$ Density: $N(r) = a_2 r^2 + c_2$

| | | | |
|---|---|---|---|
| 1 0 1 0 0 | 1 1 1 0 1 | 1 1 1 0 1 | 1 0 1 0 0 |
| $T(0)$ | $T(R)$ | $N(0)$ | $N(R)$ |

[260 eV - 1500 eV] [$1.00 \times 10^{23}$ $cm^{-3}$ - $1.65 \times 10^{24}$ $cm^{-3}$]

Figure 3. Encoding of temperature and density.

The idea of the analysis is to minimize the difference $\chi^2$ between the experimental and synthetic data; therefore we measure the performance of each candidate as $1/\chi^2$ (the higher the performance, the better the fit). Equation 1 defines a standard method of measuring the difference between the data and the fits for both emissivities and spectra:

$$\chi^2 = \sum_{i \in exp} \omega_i \left( I_i^{exp} - I_i^{theor} \right)^2 , \qquad (1)$$

where $I^{exp}$ and $I^{theor}$ are intensities (emissivities) of experimental and theoretical data respectively and $\omega_i$ is a weight factor. A particular choice of the weight factor may have an impact on the performance of the algorithm, it also may be important for estimation of uncertainty intervals (Coldwell 1991). Since our primary goal was to study the performance of the GA, we have chosen $\omega_i \equiv 1$ for the spectra and $\omega_i \equiv (1/I^{exp})^2$ for the emissivities. This is done to compensate for possible substantial changes in the emissivity profile. The objectives are to find the best possible fits to spectra and emissivities simultaneously.

One approach to solve this problem is to combine the multiple criteria into a single scalar fitness function. Unfortunately, this simple method did not work well on our problem. Instead we turned to multi-objective optimization and used the Niched Pareto Genetic Algorithm (Horn 1993).

The crucial difference between a canonical GA and the Niched Pareto GA is in the implementation of selection. We implemented Pareto domination tournament selection where two candidates are picked at random from the population. A comparison set of individuals is also picked randomly from the population. Each of the candidates is then compared against each individual in the comparison set. If one candidate is dominated by the comparison set, and the other is not, the latter is selected for reproduction. If neither or both are dominated by the comparison set, then we must use sharing to choose a winner. Equivalence class sharing implemented in our model defines the winner as an individual that has the smallest number of the other individuals inside its niche. This technique helps to maintain diversity along the Pareto front. Niche size gets adjusted automatically for each generation based on the average area of the front. We also normalize the objective function for each generation so that the objective function for each criterion ranges from 0 to 1.

In order to increase selection pressure we use an elitist scheme where: 1) members of the current generation and offsprings are combined in a common pool in each generation; 2) the solutions along the Pareto front are selected for the next generation and removed from the pool; 3) the procedure is repeated until the next generation is filled. We have found empirically that elitism combined with uniform crossover provides reliable and rapid convergence.

The size of the comparison set controls selection pressure. However, when using elitist scheme, the algorithm is not very sensitive to size. In our implementation we compare each candidate against 5 individuals.

## 3 Results

In this paper we are addressing two main problems: 1) what is the quality of the data (noise level) that allow for unambiguous determination of the gradients; and 2) can gradients with complex structure be resolved? Here we present the results of our computer runs with the Niched Pareto GA.

### 3.1 Simple Gradients, Different Level of Noise

Level of noise in real experimental data can vary from a few percent (high quality data) to 20 percent (poor data). We performed a series of calculations with the following noise levels: 1, 5, 10, 15, and 20%. For each case we performed 5 runs starting with different initial random seeds. We used simple parabolic gradients to generate the data in all cases and, therefore, parabolic functions to encode solution. Two parameters are required do define a parabola for both temperature and density. We used 5 bit encoding for each parameter, which results in a 20-bit chromosome. With 100 individuals in each generation we achieve rather stable performance.

We will discuss the results of GA runs for 10% noise in more detail. The propagation of the Pareto front in the objective space shows the dynamics of the run. Figure 4 displays propagation of the front for a typical run.

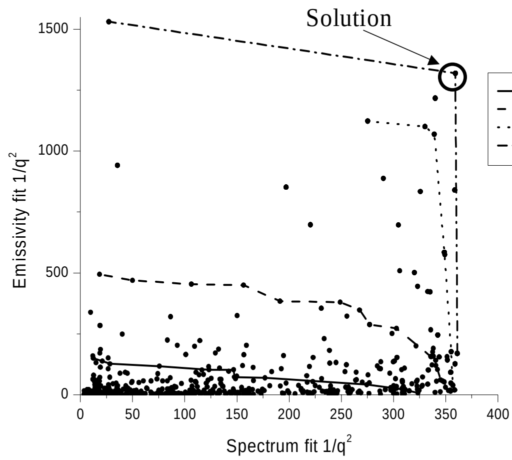


Figure 4. Propagation of Pareto front.

The behavior of the front indicates that GA successfully drives the search towards better solutions. The upper right point represents the solution that has good spectral and emissivity fits (Figures 5 and 6).

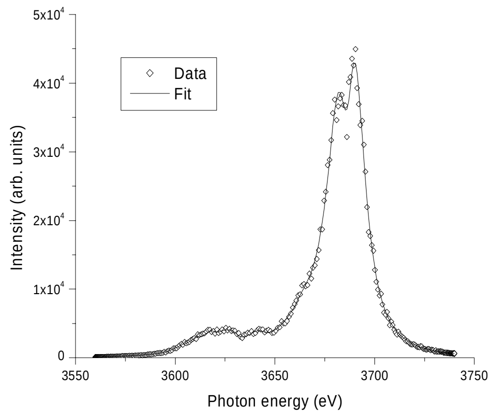


Figure 5. Good spectrum fit (10% noise).

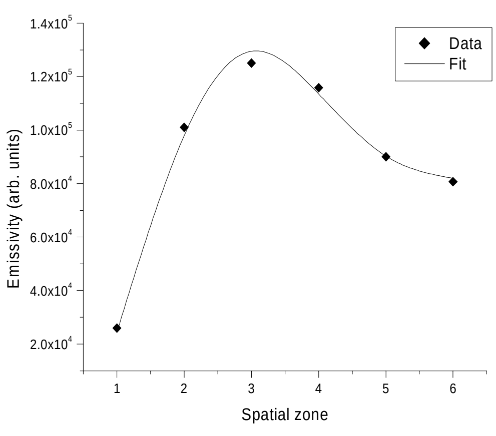


Figure 6. Good emissivity fit (10% noise).

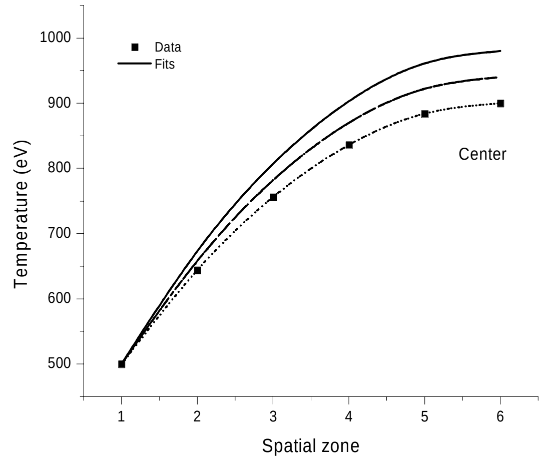


Figure 7. Temperature gradients (10% noise).

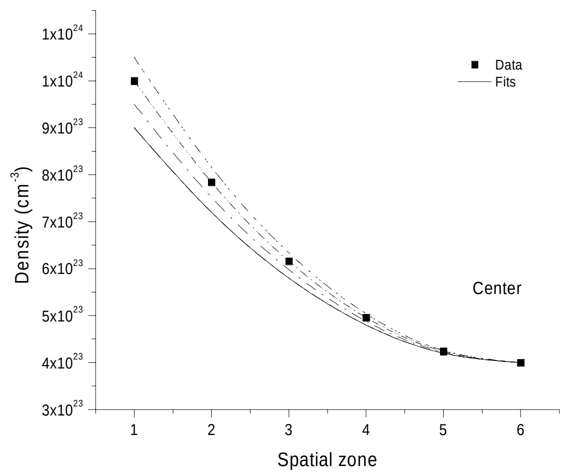


Figure 8. Density gradients (10% noise).

It is important to study the points in the vicinity of the right solution. If the gradients for these points are similar to the one for the correct solution then the analysis is successful. The family of gradients then is indicative of the uncertainty intervals of the analysis. If, on the other hand, there are some points that satisfy all criteria well but nevertheless have different gradients, then we have alternative solutions and the analysis is ambiguous. For the run we discussed above the analysis is successful (Figure 7 and 8). Note that since the plasma is symmetric we display only one half of the gradients.

It is intuitively clear that the higher the level of noise, the more chances there are to find alternative solutions. For 1, 5, and 10% of noise the solution is unique. Starting at 15% noise we see alternative solutions (Figure 9 and 10). Analysis becomes ambiguous since any pair of the gradients produces acceptable fits to spectra and emissivities and no preference can be given to either of the solutions.

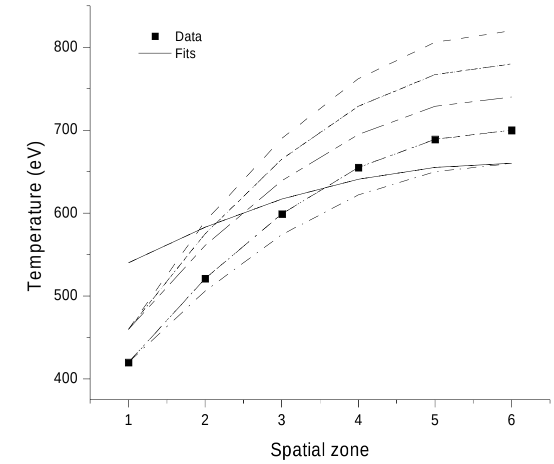


Figure 9. Temperature gradients (20% noise).

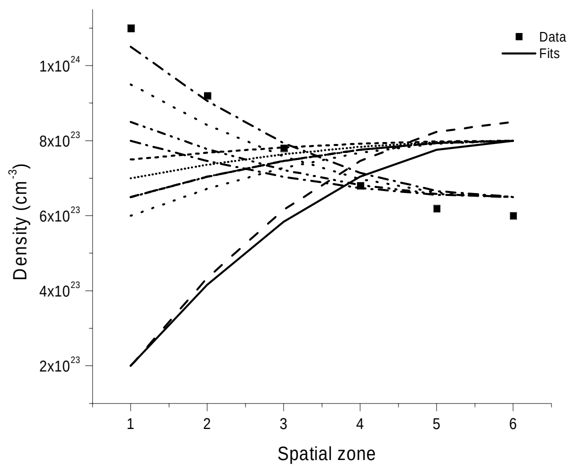


Figure 10. Density gradients (20% noise).

Another interesting aspect is the ability of genetic algorithm to satisfy all objectives. Table 1 summarizes statistics for different levels of noise.

| Noise level | All objectives satisfied |
|---|---|
| 1% | 1 run out of 5 |
| 5% | 3 runs out of 5 |
| 10% | 5 runs out of 5 |
| 15% | 5 runs out of 5 |
| 20% | 5 runs out of 5 |

Table 1. Number of successful runs for different noise level.

It seems that with the same parameters for the genetic algorithm it is easier to fit the noisier data. One possible explanation is that for smaller noise possible candidates are localized in a smaller region of the parameter space and therefore are more difficult to find. Note that objectives can be satisfied with correct as well as alternative solutions.

### 3.2 Complex Gradients

Even though parabolic gradients can be expected to be common for the type of plasmas we are modeling, there might be more complex shapes of the temperature and density spatial profiles. So we applied our method to analyze synthetic data calculated with gradients produced by hydro simulations and 10% noise added.

The problem arises because simple functions may not be capable of reproducing the gradients and will result in poor fits and wrong solutions. We consider several choices to characterize the gradients:

1. parabolic *($f(x) = ax^2+b$)*,
2. bi-quadratic *($f(x) = ax^4+bx^2+c$)*,
3. tabulated (each point in space is represented by a pair of temperature and density that can very within the range of physically acceptable values),
4. tabulated with smoothness restrictions (each point must not be very different from adjacent points)

Other analytical functions (e.g. rational) are difficult to implement due to limitations based on the physical meaningfulness of the gradients.

For each method we performed 5 runs with different initial random seeds. Table 2 summarizes the results for each method used.

| | **1** | **2** | **3** | **4** |
|---|---|---|---|---|
| Real parameters | 4 | 8 | 12 | 12 |
| Chromosome length | 20 | 32 | 60 | 60 |
| Population size | 100 | 150 | 200 | 200 |
| All objectives satisfied | 4/5 | 1/5 | 5/5 | 4/5 |
| Best spectrum fitness | 380 | 380 | 380 | 380 |
| Best emissivity fitness | 1.0 | 4.0 | 6.5 | 6.5 |

Table 2. Summary of the runs.

As can be expected all runs produce good quality fits to spectra. Being space integrated, spectra are not very sensitive to the details of the gradients. Emissivity fitting improves when we use more flexible ways to describe the gradients. The penalty for this flexibility however is having alternative solutions.

Gradients obtained from the best runs for each method are displayed on figures 11 and 12. Results obviously have some room for improvement. Although GA finds fits to spectra and emissivities, the gradients that produce these fits are not necessarily the correct ones. Parabolic function apparently does not have enough flexibility and results in poor performance. Bi-quadratic function is the only one that reproduces correct gradients, by fitting the spectra and emissivities. However there is still some discrepancy with the right solution (thick dashed line on figures 11 and 12). The disadvantage is that it makes the algorithm less reliable due to a highly non-linear nature of the encoding.

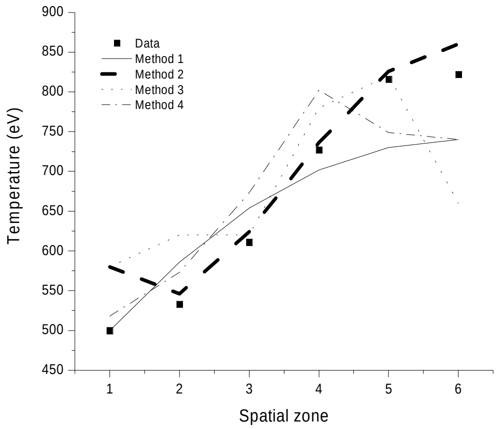


Figure 11. Temperature gradients.

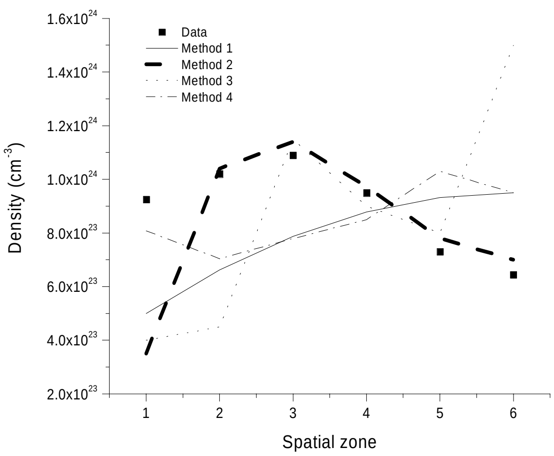


Figure 12. Density gradients.

Methods 3 and 4 produce good quality fits to the spectra and emissivities with gradients that are different from the correct solution. Therefore we may conclude that without imposing restriction to a particular functional dependence the analysis can be ambiguous. It may be possible however to break the ambiguity by specifying additional physical objectives (e.g. another spectral feature to be analyzed simultaneously).

Work is currently in progress to improve performance of our model as well as to understand how much we can expect from the analysis of the data. The goal is to find a method (or a combination of methods) that has high success rate and does not lead to alternative solutions.

## 4 Conclusions and Future Work

We studied the possibility of using Pareto optimal genetic algorithms for the estimation of plasma temperature and density gradients by performing simultaneous analysis of experimental X-ray spectra and monochromatic images. This information may be used to improve characterization of core plasma dynamics and to provide new data for detailed benchmarks of hydrodynamic codes.

The algorithm performs well when we analyze synthetic data produced using simple parabolic gradients. The Genetic Algorithm is capable of finding quality solutions while exploring only a tiny part of the search space. We have shown however that unambiguous determination of the gradients is sensitive to the quality of the experimental data.

Work is currently in progress to improve performance of the method and to perform adequate analysis of the data with more complex gradients. New techniques to parameterize the gradients as well as additional physical constrains may be required.

We are also working on a parallel implementation of the code to be run on our in-house Beowulf machine. This will allow us to increase population sizes (and hopefully improve performance) and perform extensive parameter study. Currently it takes 12 hours to perform a single run with 200 individuals in each generation for 200 iterations on an SGI Power Challenge machine.

This work was supported in part by DOE High Energy Density Science Grant No. DE-FG03-98DP00213.

## Bibliography

Coldwell, R.L. and Bamford, G.J. (1991). *Theory and operation of spectral analysis using ROBFIT*. American Institute of Physics.

Goldberg, D.E. (1989). *Genetic Algorithms in Search, Optimization, and Machine Learning*. Addison-Wesley.

Golovkin, I.E., Mancini, R.C. and Louis, S. (1999). *Plasma X-ray Spectra Analysis Using Genetic Algorithms*. Proceedings of the Genetic and Evolutionary Computation Conference. Pages 1529 – 1534.

Golovkin, I.E. and Mancini, R.C. (2000). *High order satellites and plasma gradients effects on the Ar He$\beta$ line opacity and intensity distribution.* Journal of Quantitative Spectroscopy and Radiative Transfer. **65**, pages 273-286.

Griem, H.R. (1992). Plasma spectroscopy in inertial confinement fusion and soft x-ray laser research. *Plasma Physics*, **4**, pages 2346-2361.

Holland, J. (1975). *Adaptation in natural and artificial systems*. The University of Michigan Press, Ann Arbour.

Horn J. and Nafpliotis, N. (1993). IlliGAL Report No. 93005.