Optimal Dynamic Discrimination of Very Similar Species

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A long standing detection problem in analytical chemistry is distinguishing between the presence of two or more similar species in the same sample. Optimal dynamic detection (ODD) is a technique under development at Princeton that seeks to address this problem by utilizing the subtle quantum mechanical character of the various chemical species in order to maximally differentiate between them. Through closed loop learning control, ODD aims to identify a control field (i.e., a shaped laser pulse) that enhances the signal of a chosen species as well as reduces the signals of the other species present in the sample. The resultant optimal control field can accomplish this task by simultaneous manipulation of the quantum dynamics of all the species, leading to constructive and destructive interferences amongst the relevant wave function components. My research over the summer builds on the early studies of ODD by examining the limits of its behavior and capabilities when the two species being discriminated between are very similar.

A versatile algorithm known as diffeomorphic modulation under observable-response-preserving homotopy (D-MORPH) is being employed to thoroughly stress test ODD. D-MORPH provides the means to rove over the quantum control landscape and return with an optimal control field that provides the best degree of discrimination for the particular mixture of species. D-MORPH's allure is its systematic nature, which allows for a detailed analysis of the control field's evolution as it handles ever more demanding ODD circumstance. Mathematically, D-MORPH operates through a guiding differential equation driven by a so-called homotopy parameter, which is linked to the physical system through the governing Schrodinger equation. D-MORPH was originally formulated with respect to one quantum system, and it allowed for tracking of an observable across the control landscape. In order to explore ODD, the D-MORPH technique is adapted for treating multiple systems. In all cases discussed below, the goal is attainment of the highest level of excitation in species A (therefore producing the strongest signal possible), while minimizing the level of excitiation of species B.

The first extension of D-MORPH for two systems involves tracking the relevant observables for each system. This method requires two tracks be specified: one track increases the degree of excitation of species A to its maximum value while the other track decreases the excitation of B to its minimum value. The control field must fulfill these separate criteria simultaneously. This particular extension of D-MORPH will be simulated later this year.

The next adaptation of D-MORPH that I developed is based on the fact that a linear combination of observables, O^A and O^B, is itself an observable:

$$J = O^A - O^B \tag{1}$$

where the new observable J is the difference between the degree of excitation of species A and that of species B. By specifying a track that maximizes the value of J, both species can be controlled simultaneously. This method is slightly less demanding than the tracking technique above, because tracking the difference of two observables provides more freedom than demanding each observable follow a prescribed path. Preliminary simulations of this adaption of D-MORPH have been successful, with the majority of species pairs reaching maximal discrimination.

A valuable feature of D-MORPH is the homotopy parameter, which provides a means to continously morph the physical systems to become more similar over the course of the discrimination process. This means that a path can be set for the species' Hamiltonians, H_A and H_B, in the same way that a track has been set for observables. By both maximizing J as defined above and prescribing a path such that the Hamiltonian of species A, H_A, approaches H_B, ODD is put in the demanding position of having to improve its performance as its task gets more difficult. This particular adaptation is being implemented in a two step process; first ODD maximizes J, next D-MORPH maintain that final value of J while species A is morphed continuously towards species B. Several simulations of the two step process are complete, and the results have illustrated that as the species become more similar, the control field becomes increasingly complex. The figures on the following page are before and after snapshots of the control field which show its evolution for two separate species pairs. Further analysis of these control fields will offer a clearer picture of the control field's reaction to the high demand of acheiving ODD under the limit as H_A approaches H_B.

The final extension of D-MORPH allows the Hamiltonians of both species to approach each other along paths determined by a gradient based method. In this fashion, the algorithm can explore more of the quantum control landscape, possibly discovering areas where ODD may have less difficulty differentiating between the similar species. This extension is in the early stages of development, but preliminary simulations will be underway in the coming weeks.

While significant progress has been acheived over the summer, there is research left to pursue. More simulations will be run in order to cull enough data for a relevant analysis of the behavior of ODD. In conclusion, the severe tests of ODD enabled by D-MORPH should provide insight into the limits and the strengths of the laser assisted discrimination of similar chemical species.

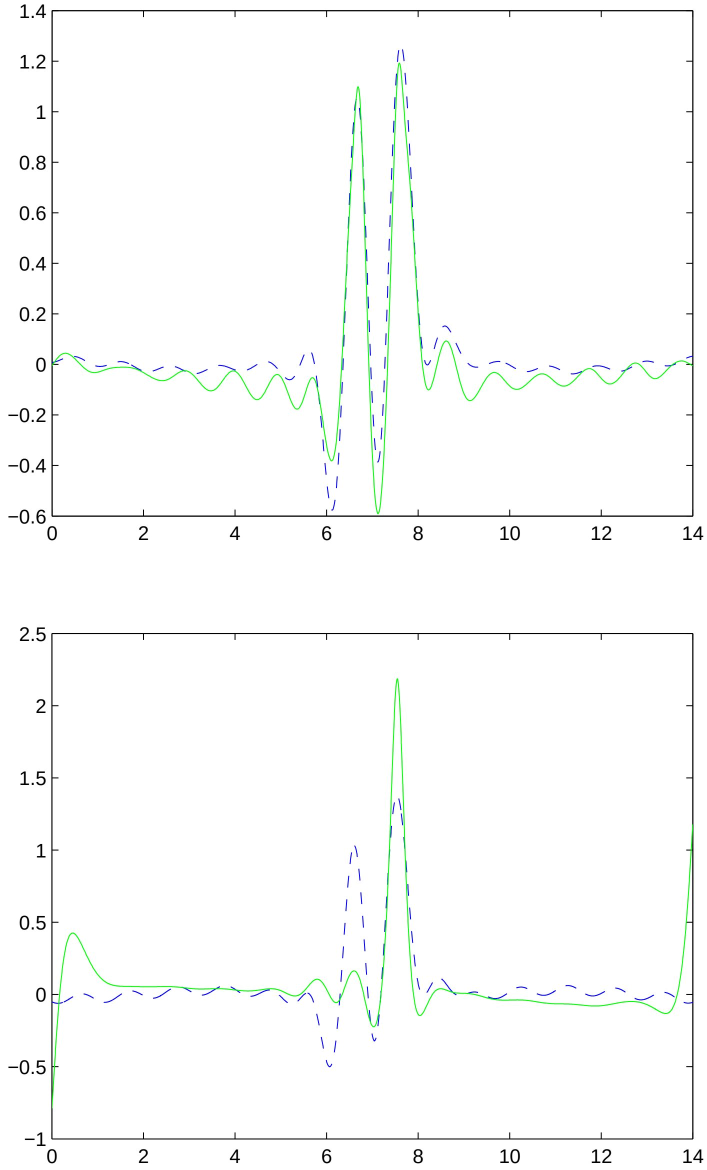

Figure 1: Both of these figures illustrate the evolution of the control field as it maintains maximal discrimination in spite of the fact that the two species are becoming more similar. The blue, dashed control field is the initial field, and the green, solid line is the final control field, that acheives maximal discrimination of two very similar species.