Estimating Parameters in Differential Equations with Application to Laser Data

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Abstract. Many physical problems can be described by systems of ordinary differential equations (ODE) comprising system states and parameters not accessible by direct measurements. The goal is to estimate the unknown parameters and the hidden components from the time series of a single observable and to inspect the compatibility of a model with the data.

INTRODUCTION

For comparing theoretical models for lasers with empirical data, usually simulations of the models are compared with measured time series. Therefore, some parameters in the models had to be chosen. In lack of a systematic adaptation of the parameters of the models, it cannot be decided whether discrepancies between the model predictions and the data stem from wrongly chosen parameters in a sufficient model on the one hand and shortcomings of the model itself on the other. Thus, it would be desirable to base the comparison on best fit parameters for a given model. Various approaches exist to reconstruct the flow vector field from a given time series in order to estimate the parameters of the differential equation [1,2]. For these methods time derivatives must be estimated from the data, which is problematic in the case of noisy time series.

We present a method to deal with this problem by a multiple shooting approach [3,4]. The method is more robust with respect to bad starting guesses of the parameters and noisy data than conventional techniques. The method does neither require an embedding of the time series nor an estimation of time derivatives from the data. Methods for parameter estimation in ODEs that rely on estimation of time derivatives from data are restricted to noise-free data and can not deal with systems of dimension larger than two or three. Our method is demonstrated with

simulated noisy data and applied to measured data from a Q-switched CO_2 laser that is described by a five dimensional ODE.

METHODS

The problem to be considered is described by a set of m nonlinear ODEs

$$\dot{\mathbf{x}} = \mathbf{f}(t, \mathbf{x}, \mathbf{p}), \quad \mathbf{x} \in \mathbf{R}^m, \quad t \in [0, T], \tag{1}$$

depending on a set of parameters $\mathbf{p} \in \mathbf{R}^p$. The initial values $\mathbf{x}_0 = \mathbf{x}(0)$ are treated as additional unknown parameters and included in $\mathbf{p}$. The observed quantity y_i is a function of the system state $\mathbf{x}$, sampled at discrete times t_i and disturbed by white noise of zero mean and variance σ_i^2 which is denoted by $\mathcal{WN}(0, \sigma_i^2)$:

$$y_i = g(\mathbf{x}(t_i, \mathbf{p})) + \eta_i, \quad i = 1..N, \quad \eta_i \sim \mathcal{WN}(0, \sigma_i^2)$$

Let $\hat{\mathbf{x}}(t, \mathbf{p})$ be the solution of Eq. (1) for given parameters $\mathbf{p}$. The objective function is defined as the sum of squared residues between the data and the model, weighted with the inverse variances of the data:

$$\chi^2(\mathbf{p}) = \sum_{i=1}^{N} \left(\frac{y_i - g(\hat{\mathbf{x}}(t_i, \mathbf{p}))}{\sigma_i} \right)^2$$

The initial value approach

If the problem of parameter identification in ODE systems is treated in the same way as other problems of non-linear regression, one is led to the so-called initial value approach: Starting from some initial guess of the parameter vector, the model equations are solved over the whole fitting interval. Then an optimization method is used to minimize $\chi^2(\mathbf{p})$ with respect to $\mathbf{p}$.

The model trajectory $\hat{\mathbf{x}}(t)$ depends sensitively on the parameters, especially in the case of nonlinear dynamical systems. Since $\chi^2(\mathbf{p})$ shows a non-linear dependence on the parameters $\mathbf{p}$, it will usually have several local minima apart from the global one that corresponds to the true parameters. If the parameters are far off from the correct ones, the trial trajectory soon loses contact to the measurements.

Multiple shooting

The technique of multiple shooting was developed in the context of parameter estimation in [3]. One partitions the fitting interval into many subintervals, each having its own initial values. The measurements are used to get starting guesses for them. The parameters of the ODE are the same for all subintervals. This procedure leads to an initially discontinuous trajectory, which is, however, close

to the measurements. In an iterative process, the algorithm minimizes $\chi^2(\mathbf{p})$ on the one hand and enforces the continuity of the full trajectory on the other hand. The freedom of intermediate discontinuity allows the trajectory to stay close to the data. Divergences are avoided and the danger of local minima is reduced.

For the reduction of $\chi^2(\mathbf{p})$, a generalized Gauss-Newton method is employed. The rank-deficient case, e.g. when parameters or combinations of parameters cannot be identified reliably, is treated by an appropriately chosen rank decision criterion. Constraints on the parameters or trajectories, e.g. nonnegativity constraints on rate constants and state variables or bounds for the parameters can be imposed on the update step to further stabilize the fit. At the convergence point, the variance/covariance matrix of the estimated parameters is provided. It is used to compute confidence intervals and to reveal linear combinations of parameters that are not identifiable from the given data.

DEMONSTRATION

To illustrate the behavior of the initial value approach and multiple shooting algorithm we examined the restricted, quasi-Hamiltonian, Lotka-system :

$$\dot{x} = k_1\, x - k_2\, xy$$
$$\dot{y} = k_2\, xy - k_3\, y$$

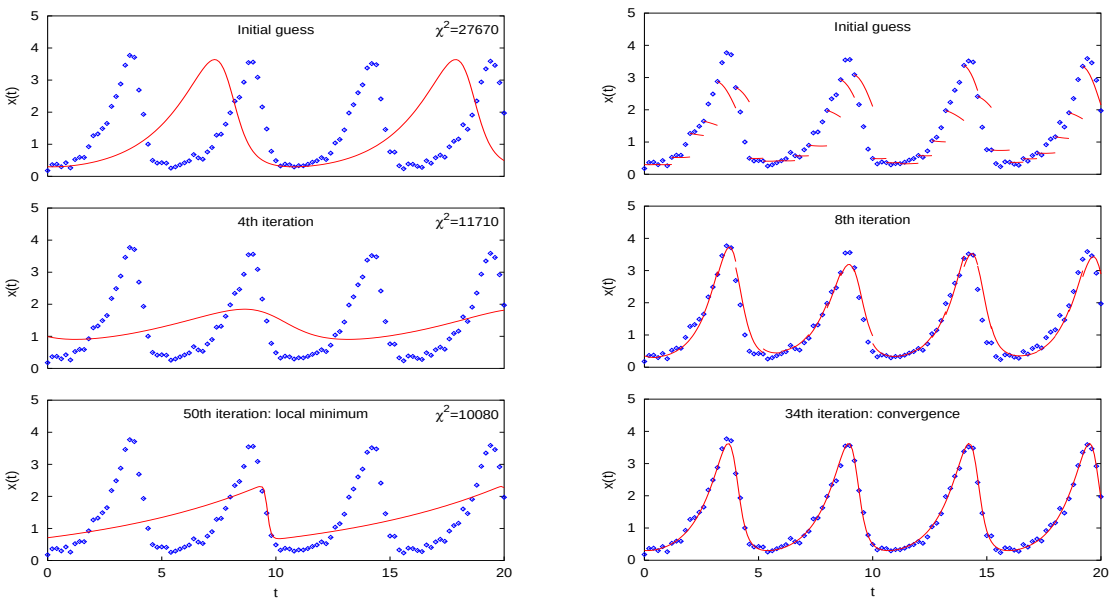

FIGURE 1. Fit of the Lotka-system with the initial value approach (left column) and the multiple shooting approach (right column).

with the parameters $k_1 = 1.0$, $k_2 = 1.5$ and $k_3 = 2.0$ and initial values $x_0 = 0.3$ and $y_0 = 0.8$. This system has often been used to compare algorithms for estimating parameters in ODEs. The system was integrated over $T = 20$ and sampled with $\Delta t = 0.2$. Observational noise with standard deviation of 0.1 was added to the signal, resulting in a signal-to-noise-ratio of 10:1. Only the first components of the data were taken as observations. The initial values of the trial trajectory were fixed to the true values. The starting guesses for the parameters were half the true values.

When trying to estimate the parameters with the initial value approach, the algorithm ran into a local minimum (left column of Fig. 1).

On the other hand, the multiple shooting algorithm converged to the global minimum after 34 iterations (right column of Fig. 1). Thirty starting points were used for the initially discontinuous trial trajectory. All starting points for the second component were set to 0.5. After convergence, the true trajectory is perfectly reproduced. The estimated parameters deviate from the true values by less than 1% in accordance with the estimated confidence intervals. Even for conditions that were much worse than above the parameters could be estimated reliably.

APPLICATION TO Q-SWITCHED CO_2 LASERS

In this section, the methods outlined above are applied to data from a Q-switched CO_2 laser, measured at the Istituto Nazionale di Ottica, Florence. The so-called four level model as described in [5] was used.

The schematic diagram shown in Fig. 2 is represented through the following equations:

$$\begin{aligned}
\dot{n} &= (-2K + G\delta)n, & \delta &= N_2 - N_1 \\
\dot{N}_1 &= -\gamma_R N_1 + \gamma'_R M_1 + G\delta n - \gamma_1 N_1 \\
\dot{N}_2 &= -\gamma_R N_2 + \gamma'_R M_2 - G\delta n - \gamma_2 N_2 + \gamma_2 P \\
\dot{M}_1 &= +\gamma_R N_1 - \gamma'_R M_1 - \gamma_1 M_1 \\
\dot{M}_2 &= +\gamma_R N_2 - \gamma'_R M_2 - \gamma_2 M_2 + \gamma_2 Z P
\end{aligned}$$

The model includes two resonant levels whose populations are denoted by N_1 and N_2 respectively. Each vibrational band contains Z other rotational levels with total populations M_1 and M_2. The pump rate $\gamma_2 P$, acting on the upper levels, generates a population inversion $\delta = N_2 - N_1$. The populations decay with rate constants γ_1, γ_2, γ'_R and $\gamma_R = Z\gamma'_R$.

The photon density n which is the only observable, is amplified by stimulated emission with a field-matter-coupling constant G and damped with a cavity loss parameter $K(t)$. With Q-switched lasers, $K(t)$ is decreased from an initial value $K_1 > \frac{G}{2}\delta$ (laser below threshold) to a final value $K_2 < \frac{G}{2}\delta$ (laser above threshold) with a small time constant t_K:

$$K(t) = K_1 + (K_2 - K_1)e^{-t/t_K}.$$

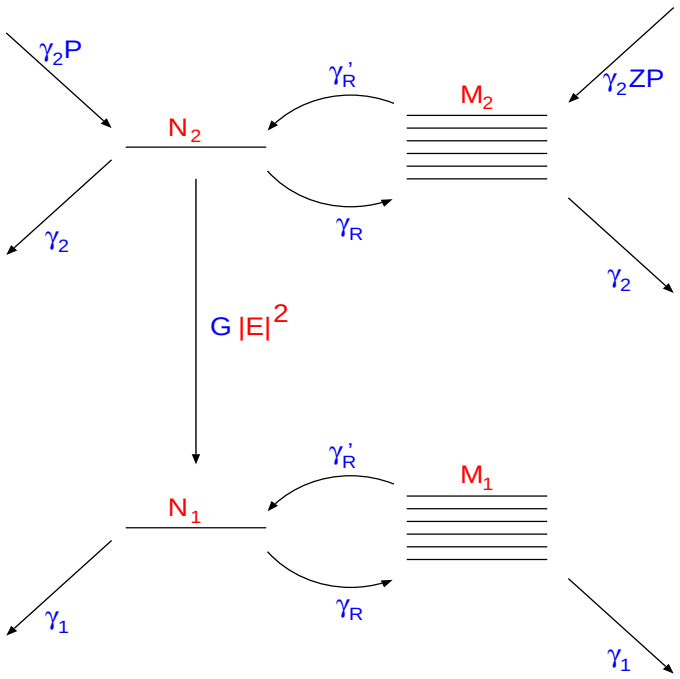

FIGURE 2. Schematic diagram of the four level model.

Results

As usual for Q-switched lasers, the data show a large peak, followed by relaxation oscillations to a steady level. The density of the multiple shooting mesh was adapted to the data. Many shooting points were used for the spike phase and relatively long subintervals in the relaxation phase.

Fig. 3 shows the simultaneous estimation of the parameters in two data sets with different experimental conditions. Three parameters were determined locally for the two experiments while the other three were forced to be the same for both.

The initial guesses for the parameters were taken from [5]. The fit converged after 22 iterations. For the data in the left column of Fig. 3 the model trajectory is in very good agreement with the data. For the right column the fitted trajectory shows systematic discrepancies which suggest a reconsideration of the model.

The minimization algorithm signalled a rank deficiency of 1, i.e. there was one linear combination of parameters to which the objective function was only poorly sensitive. The analysis of the covariance matrix revealed that this direction is nearly identical to the direction of the parameter Z. This means that under the presumption that the model is right, the data does not contain enough information to estimate Z reliably. The confidence intervals of the other parameters are smaller than 2%.

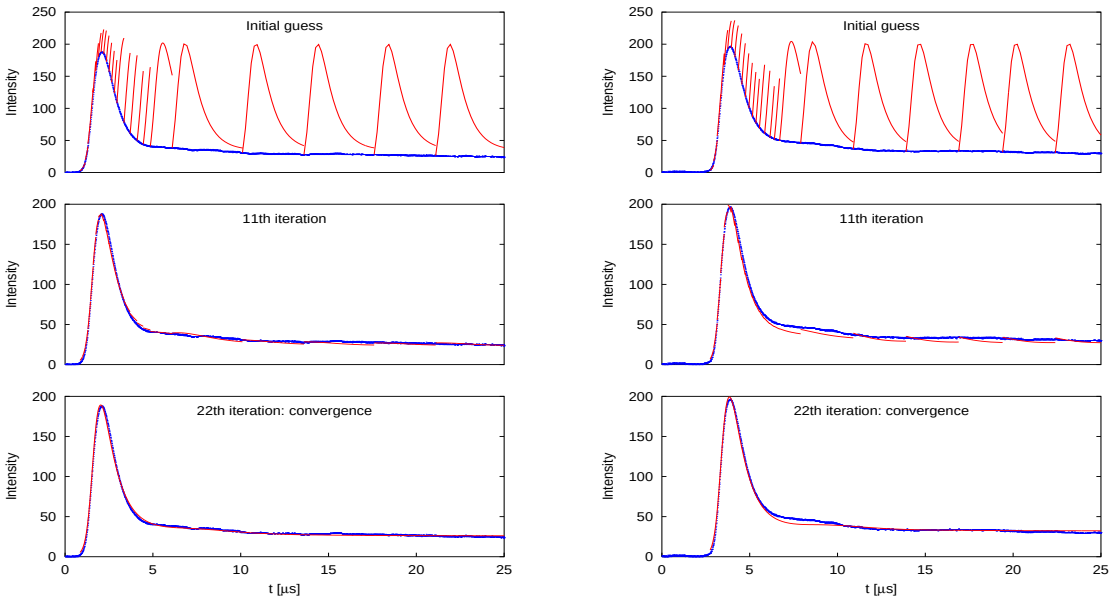

FIGURE 3. Results for fits to two laser time series.

Conclusion

It is possible to estimate parameters from observed time series even in five dimensional ordinary differential equations. Based on these estimates improved comparisons between theoretical models and measured time series can be performed.

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