1 Different tools for Modeling

Two significantly different approaches exist to model a system. One approach is to develop a model that contains equations that make sense physically or equations that are simple empirical relationships that represent the behavior of the system well. Another completely different method uses Neural Networks. Neural Networks are big systems of equations that generally do not have a physical meaning. The degree of freedom in these networks allows the Network to adjust to the specific problem. Neural Networks and relationship models often stand in competition with each other. All approaches have their advantages and disadvantages and it is therefore necessary to know the different characteristics in order to choose the best possible approach to model a system.

1.1 Curve Fits

Curve fitting is a widely used procedure for modeling. Curve fitting adjusts the values of the function coefficients such that the function represents the data as well as possible. The user has to decide what kind of function best fits the data. The judgment can be pretty straight forward for problems with only one independent and one dependent variable, $y=f(x)$, with x being a scalar. As soon as there is more than one independent variable it becomes very difficult, or a lot of experience is needed, to find a functional form that fits the data satisfactorily. If a general mechanistic relationship between the dependent and the independent variable is known, this relationship can also be used.

Curve fitting is very useful for two situations. One is where no physical relationship is known and when the problem is only a function of one dependent variable, $Y=f(x)$. The other is where the general physics of a problem is known but these relationships include physical properties that are not known in advance. The only available information is data from experiments. Using data, the coefficients of either function in the physical relationship or the function not representing physics are chosen such that the function represents the data.

Using an example, the two different approaches for curve fitting are illustrated. One approach will use a function that does not represent a physical relationship, the other approach uses knowledge about the physics represented by a mechanistic model. The problem can be described as follows: An object is mounted to a spring and oscillates around an equilibrium

(Fig. 1.1-1). Neither the mass nor the spring constant nor the damping are known. The available data are measurements of the displacement of the object at certain times.

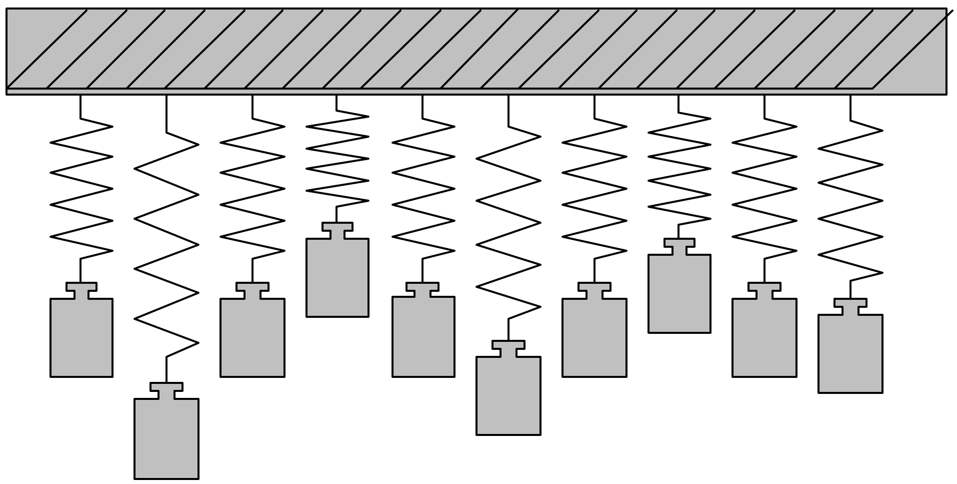

Fig. 1.1-1 Oscillating mass on Spring

For the first approach an equation that appears to have the ability to fit the data adequately has to be chosen. The data in (Fig. 1.1-2) has five local maxima or minima. A polynomial of order six has the ability to have as many as five maxima or minima (Eqn. 1.1-1). This polynomial is therefore used as a fit to the data.

$$\textbf{\textit{Displacement}}(t) = a_0 + a_1 * t + a_2 * t^2 + a_3 * t^3 + a_4 * t^4 + a_5 * t^5 + a_6 * t^6$$

t: time

Eqn. 1.1-1

The result of fitting this polynomial (Eqn. 1.1-1) to the data is shown in (Fig. 1.1-2). The result follows the trend of the data but does not fit it exactly. The other curve in this figure results from a fit of the general relationship (Eqn. 1.1-2) to the data. This relationship is used to model oscillations for a known mass, spring constant and damping coefficient.

$$\boldsymbol{Dispacelment(}t\boldsymbol{)} = C \boldsymbol{*} \boldsymbol{exp}\left(-\boldsymbol{d} \boldsymbol{*} t\right) \boldsymbol{*} \boldsymbol{sin}\left(\boldsymbol{w}_d \boldsymbol{*} t + \boldsymbol{j}_d\right)$$

$$\boldsymbol{d} = \frac{damping}{2 \cdot mass}$$

$$\boldsymbol{w}_d = \sqrt{\boldsymbol{w}_0^2 - \boldsymbol{d}^2}$$

$$\boldsymbol{w}_0 = \sqrt{\frac{springconstant}{mass}}$$

C: Initial maximal Amplitude

$\boldsymbol{j}_d$: Delay past last passing equilibrium

Eqn. 1.1-2

The fit using the physical relationship is better than the polynomial fit. The approach using a polynomial should only be used if no mechanistic model is available. As soon as a mechanistic model is available this should be used.

For the use of a mechanistic model with unknown properties, curve fitting is actually more a tool to fit the physical properties to the data. It rather is a parameter fit than a curve fit.

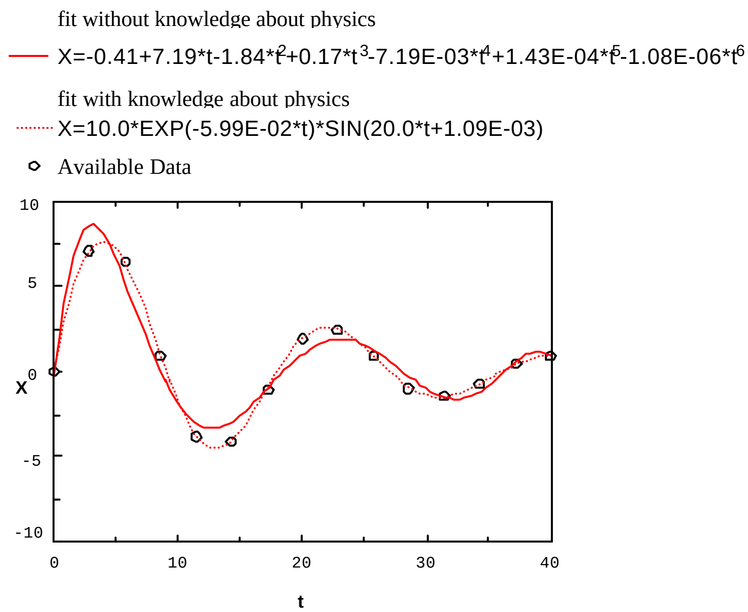

Fig. 1.1-2 Curve Fit for Polynomial and physical relationship

Curve fitting is a procedure that tries to find values for the coefficients in the function such that the function closely approximates the available data. The coefficients can be coefficients of the polynomial or the coefficients in the physical relationship. Then the coefficients of the equation are actually physical properties. These properties are valid not only for the range of the available data, these properties are properties for the system. The approach of using the physical relationships result in a non-linear fit, it is necessary for the non-linear fitting to have initial values for the coefficients. Using these initial values the function generally will not fit the data exactly. A minimization of the error is necessary for a linear and a non-linear fit to get a better fit of the data. As a measure of the error the ***Sum of Squares***

(Eqn. 1.1-3) is most commonly used. The Sum of Squares sums the squared differences between the function values and the data at the points of the available data.

$$\underset{coefficients}{\boldsymbol{min}} \sum_{i=1}^{n} \left(y_i - \boldsymbol{f}(X_i) \right)^2$$

Eqn. 1.1-3

In order to minimize the error, the coefficients have to be changed such that the sum of squares is smallest. By changing the coefficients it is possible for a non-linear fit, that the sum of squares reaches a minimum that is not the global minimum but a local minimum. This means that there is a better selection of the values for the parameters but by changing the coefficients a little the Sum of Squares increases. Good initial guesses of the parameters or ranges of possible values of the parameters help such that the search converges to the global minimum of the sum of squares more easily. Using a physical relationship, where the coefficients have a meaning, it is more easily possible to come up with good initial guesses or with a range of possible values for the coefficients. For the example (Fig. 1.1-1) it is known that the mass of the object cannot be negative and the spring constant and all the other parameters neither. Often it is possible to find ranges of parameters in the literature [CRC]

Extrapolation- Often it is desired to extrapolate over the range of the available data. In the example of the oscillation of the object it can be interesting to determine after what time the maximal amplitude of the displacement would be smaller than a certain maximal bound, and this bound would not be within the range of the available data. For extrapolation purposes like this, using the polynomial is inapproriate. The polynomial only fits the data in the range where the data is available. Outside of this range the function values can be very inaccurate. In (Fig. 1.1-3) the ability of the polynomial to extrapolate is shown. Based on physical reasoning it could be expected that the displacement decreases as time increases. The values for the displacement of the polynomial for times higher than *40* deviate significantly from the expected. Using the physical relationship for extrapolation purposes, with the values for the properties that resulted out of the curve fit, yield the expected result of the displacement depending on time not only for the range of the available data but as well outside of this range (Fig. 1.1-3). The values for the physical properties are properties for the system and therefore as well valid outside of the range of the available data. Using a general mechanistic relationship for the curve fitting yields better results for extrapolation than any other tool for modeling, that are discussed in the following sections of this chapter.

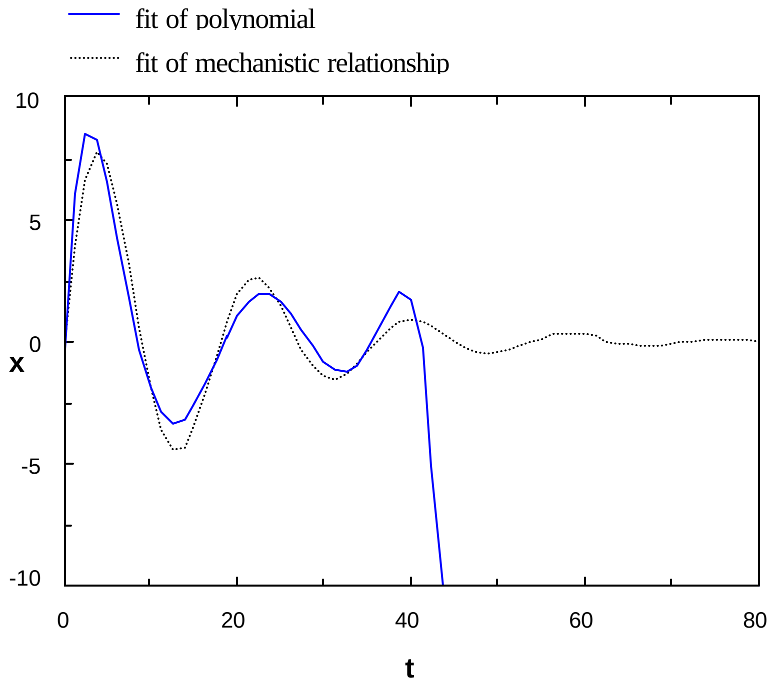

Fig. 1.1-3 Extrapolating abilities of polynomial and mechanistic relationship

Measurement Errors- How to deal with measurement errors in data is a problem for both curve fits of physical models and curve fits of functions that do not represent a physical relationship. The problem can be most significant when no physical relationship is known. In the example of the oscilation of the mass, the decision of what kind of function was chosen, was made based upon the number of maxima and minima. Since the changes in the displacement were so large, it was very clear that these changes were not only measurement errors. For smaller changes in the displacement it could have been that these changes could be regarded only as measurement errors. In other examples it could be that the changes in values that are actually measurement errors are regarded as true oscillations. This mistake can lead to choosing a function that has the ability to follow the trend of each measurement error. It can happen that the function will deviate at certain points from the expected heavily in order fit the data at other points better. The user has to decide whether an oscillation is a measurement error or if it represents the reality.

Some results of several given functions with different abilities to follow each trend of some arbitrary data are shown in (Fig. 1.1-4). The data illustrates effects of noise in measuring the value *Y*. The quadratic function is very smooth and interpolates the data nicely. The polynomial of order six assumes that the changes in the value of *y* are true trends and tries to follow them. The behavior of the polynomial of order four lies in the middle of the other two polynomials. By just looking at the data it cannot be seen whether or not the data includes noise or not. The changes in the values could be true trends or could be measurement errors as well. If these changes are true trends the quadratic polynomial does not represent the data very well. If the changes are measurement errors the polynomial of order six deviates from the expected shape by much. It is therefore necessary to know whether or not the data is biased. Based on this knowledge the choice of the function is easier but still difficult. For the use of a mechanistic relationship, the concern about measurement errors is not that big since the functional form is given.

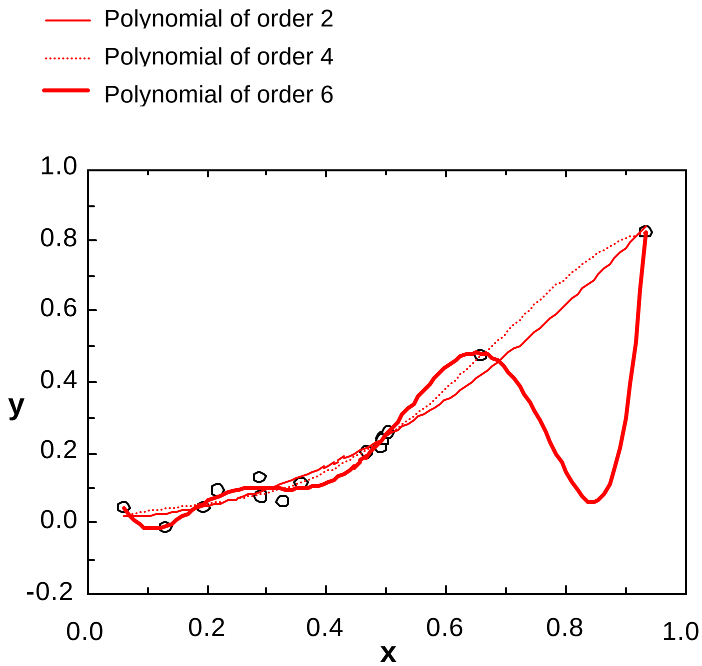

Fig. 1.1-4 Using different functions for curve fit, for biased data