Using Nonlinear Models to Enhance Prediction Performance with Incomplete Data

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Abstract: A great deal of recent methodological research on missing data analysis has focused on model parameter estimation using modern statistical methods such as maximum likelihood and multiple imputation. These approaches are better than traditional methods (for example listwise deletion and mean imputation methods). These modern techniques can lead to unbiased parametric estimation in many particular application cases. However, these methods do not work well in some cases especially for nonlinear systems that have highly nonlinear behaviour. This paper explains the linear parametric estimation in existence of missing data, which includes an overview of biased and unbiased linear parametric estimation with missing data, and provides accessible descriptions of expectation maximization (EM) algorithm and Gauss-Newton method. In particular, this paper proposes a Gauss-Newton iteration method for nonlinear parametric estimation in case of missing data. Since Gauss-Newton method needs initial values that are hard to obtain in the presence of missing data, the EM algorithm is thus used to estimate these initial values. In addition, we present two analysis examples to illustrate the performance of the proposed methods.

1 INTRODUCTION

Missing data problems are closely related to statistical issues because most of missing data analysis and design methods depend on statistical theory. In fact, all predicted values for the missing data are depending on the probability functions. Some researchers have considered missing data analysis problems to be the most significance issue in many real data analyses and applications (Azar, 2002). More than often, missing values are arbitrarily removed or simply replaced by mean values in simple missing data problems. This strategy, however, does not work well for cases where there exist significant missing values (Baraldi and Enders, 2010). Recent research has concentrated on maximum likelihood methods such as the EM (Expectation-Maximization) algorithm to deal with missing data problems, which can produce good results for most applications. Although this approach still has greater interest in the literature, especially in linear missing data analysis, there is no enough knowledge to know if linear missing data analysis methods can still give good result for nonlinear systems. Consequently, the overarching purpose of this paper is to introduce some nonlinear methods for missing data problems and to illustrate the performance of nonlinear parametric estimation by combining maximum likelihood estimation and a Gauss-Newton iteration method. More specifically, this article will present a brief overview of missing data approaches, and provide accessible illustration of expectation-maximization algorithm and the Gauss-Newton optimization method. In some detail, we concentrate on Gauss-Newton iteration estimation and present analysis examples.

2 MISSING DATA MECHANISMS

It is important to classify the mechanisms of missing data because this would determine which missing data handling strategies would be used for specific problems. There are three important patterns of missing data which are MAR (missing at random), MCAR (missing completely at random) and MNAR (missing not at random) (Little and Rubin, 2002). These patterns explain the relationships between the inputs, and outputs of the system and the probability density function of missing values. In more detail, these mechanisms of missing values give the reasons why these values are missing or unobserved. For each pattern, a conceptual explanation will be given

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Y						
Х	Complete	MAR	MCAR	MNAR		
8	0.49	0.49	0.49	0.49		
8	0.49	0.49	0.49	0.49		
10	0.48	0.48	0.48	0.48		
10	0.47	0.47	-	0.47		
10	0.48	0.48	0.48	0.48		
10	0.47	0.47	0.47	0.47		
12	0.46	0.46	-	0.46		
12	0.46	0.46	0.46	0.46	~	
12	0.45	0.45	-	0.45		
12	0.43	0.43	-	0.43		
14	0.45	0.45	0.45	0.45		
14	0.43	0.43	-	0.43		
14	0.43	0.43	0.43	0.43		
16	0.44	0.44	0.44	0.44		
16	0.43	0.43	0.43	0.43		
- 16	0.43	0.43	0.43	0.43		
18	0.46	0.46	0.46	0.46		
18	0.45	0.45	0.45	0.45		
20	0.42	0.42	0.42	0.42		
20	0.43	0.43		0.43	-	
20	0.41	0.41	0.41	0.41		
22	0.41	0.41	0.41	0.41		
22	0.40	0.40	0.4			
22	0.42	0.42	0.42	0.42		
24	0.40	0.40	-	-		
24	0.40	0.40	0.40	-		
24	0.41	0.41	-	0.41		
26	0.40	0.40	0.4	-		
26	0.41	0.41	0.41	0.41		
26	0.41	0.41	0.41	0.41		
28	0.40	0.40	0.40	-		
28	0.40	0.40	0.40	-		
30	0.40	-	-	-		
30	0.38	-	0.38	0.38		
30	0.41	-	0.41	0.41		
32	0.40	-	-	-		
32	0.40	-	0.40	-		
34	0.40	-	0.40	-		
36	0.41	-	0.41	0.41		
36	0.38	-	-	0.38		
38	0.40	-	0.40	-		
38	0.40	-	0.40	-		
40	0.39	-	0.39	0.39		
42	0.39	-	0.39	0.39		
			-			

Table 1: The proportion of chlorine and length of time in weeks with different missing data mechanism (Draper and smith, 1981).

in the next paragraph, and for more details on missing data mechanisms, see (Graham, 2009; Schlomer et al., 2010).

Values are missing at random (MAR) when the probability of a missing value on an output Y (variable Y) is related to the input (or inputs) U in the system but not to the response of the output Y itself. In other words, the probability of the missing values depends on the relation between the output Y and input (or inputs) U, that means there is no direct relationship between the probability of the missing values on Y and the values of Y variable itself. Data are missing completely at random (MCAR) is a mechanism where the probability of a missing value in Y does not depend on the output Y and the input (or inputs) U. Values are missing not at random (MNAR), if the probability of incomplete value on an output Y depends on Y itself but not on the input (or inputs) U. That means the probability of the missing values dont have relation between the output Y and input (or inputs) U (Schafer and Graham, 2002). To give more detail, let have a look at the data given in Table.1, which was taken from (Draper and Smith, 1981). In this example, the dependent variable (Y) is the proportion of available chlorine in a certain quantity of chlorine solution and the independent variable (X) is the length of time in weeks since the product was produced. When the product is produced, the proportion of chlorine is 0.50. During the 8 weeks that it takes to reach the consumer, the proportion declines to 0.49.

The first two columns in Table.1 show the complete values for two variables (input X and output Y). The remaining columns represent the amount of Y, which appear in hypothetical missed data by three mechanisms. In the third column, the probability of missing values has a direct relationship with the variable X where the values started missing after 30 weeks (X > 28), this mechanism is MAR. In the second case, there are 11 measured values randomly selected from those measured in 42 weeks; which means that the probability of each missing data is not affected by the value of X and the values of Y variable itself, that means the mechanism is MCAR but not MAR. In the fifth column, those equal to 0.40 (Y = 0.40) were unobserved, and for these values there is no direct relation between the input variable X and the output Y. In other words, the probability of missing values depends on the variable Y only. This third case represents of MNAR.

3 TRADITIONAL MISSING-DATA TECHNIQUES

Many missing data analysis methods have been presented in the literature. In this paper, we describe a limited selection of these approaches. Readers are referred to (Schafer and Graham, 2002; Enders, 2010) for detailed information on missing data.

3.1 Listwise Deletion

Listwise deletion throws away data whose information is insufficient. Listwise deletion is also known as Filtering Approaches and complete-case analysis (CDS). This method is used in many missing data problems, but its implementation depends on the type of data mechanism (Baraldi and Enders, 2010). That means CDS pays attention to data that have observed values only. For example, if we are calculating a mean and variance for variable Y, CDS discards any cases, which have missing values on the variable Y, those omitted values may lead to biased parametric estimation (Allison, 2002). On the other hand, by omitting the missing values it has a direct dramatic reduction in the complete data. When data missing is completely at random this technique would then generate unbiased estimation but with large number of removed data this is not true (Enders and Bandalos, 2001).



Figure 1: Complete-data scatterplot of the proportion of available chlorine in a certain quantity of chlorine solution.

To explain the principles of deletion approach, the data set in Table.1 for the proportion of available chlorine and length of time in weeks are taken as an example. Fig.1 shows a scatterplot of the complete cases because there are only two variables; the negative correlation between the input X and the output Y (-0.86)means that the low proportion of available chlorine would have acquired high length of time in weeks. Fig.2 shows a scatterplot of the deletion approaches in case of MAR, we will focus on this mechanism to show the effect of the bias on these approaches. Because listwise deletion takes the observed data of the variable Y, it systematically ignores values from 28 weeks. The plot also shows that there is weak nonlinear variation and association between Y and X. In case of complete data set, the estimated value of the variable Y (mean value) is 0.425, whereas the case of omitted data analysis gives an estimated value of 0.435. Similarly, the estimated value of the variable X is 22.27 and 17.56 for the complete-data and listwise deletion, respectively. Even with taking the standard deviation into consideration, the proportion of available chlorine have a standard deviation 0.03053 in the complete case, in contrast the listwise deletion gives a standard deviation 0.02907 that means there is attenuation in the system.



Figure 2: Listwise deletion scatterplot of the proportion of available chlorine in a certain quantity of chlorine solution (MAR).

3.2 Imputation Methods

Imputation points to a group of common traditional missing data methods where the estimator imputes (changes) the missing values with appropriate values (Little and Rubin, 2002). In fact, there are many imputation approaches. This study will concentrate on three of the most common methods: mean substitution imputation, linear regression imputation, and stochastic (random) regression imputation. The simplest one is mean imputation method, which imputes the missing values with the mean of the observed data (Enders, 2006; Allison, 2002). For example for the data in Table.1 for the MAR mechanism case the expected value of the observed output is 0.435, this value can represent the missing values in all cases. Fig.3 shows that the estimated data from mean substitution imputation are in straight line cross the Y-axis at 0.435 and has a zero slope. In this case the correlation between the input X and the output Y is equal to zero and this is because the imputation of the missing data depending only on the output Y. With focusing on more features of mean imputation method, cross correlation between the imputed output and input X is -0.497, in contrast the complete-data correlation is -0.86 (the negative sign represent the opposite relation between the input and the output as the input increase the output decrease). The data variability may not appear when the missing values are replaced by the average of observed data (a constant value). With taking the mean and standard deviation in consideration, the mean imputation produces mean and standard deviation 0.435 and 0.025 respectively, meaning that there is attenuation in the system. Regression imputation is a technique that fills missing values with

expected value by using a regression model (Schafer, 2010). In this method, observed data of the output Y are used to estimate a regression model, which is used to predict the value of missing data. Again, take the data in Table.1 as an example. In MAR mechanism, there are 12 unobserved values and 32 observed cases. The observed data of output Y (variable with missing data) are used with observed data on input X (variable with complete data) to estimate the missing cases on output Y. In this case we have used linear regression model: $\hat{Y} = 0.509 - .0042X$. Applying the input X (complete data) on the regression model yields predicted output (\hat{Y}), and these predicted data represents the missing data of the output Y in the system.



Figure 3: Mean imputation scatterplot of the proportion of available chlorine in a certain quantity of chlorine solution (MAR).

The basic idea of the regression imputation depends on a technique of borrowing information from the observed data from the output variable, this method also leads to biased estimation, as shown in Fig.4. Notice that the estimated missing data represents a straight line with a slope of - 0.0042. This means that the output of the system with imputed data has maximum correlation value (corr=1.0 between the imputed output \hat{Y} and input X). Notice that the linear regression imputation yields a correlation equal to -0.97 between the output Y and input X, in contrast with the correlation of -0.86 for the complete-data. Because the imputed data are generated by a linear function, there are no fluctuations for the estimated values. Consequently, the imputation process will attenuate the variability of the estimation data. For example, the standard deviation of output Y from linear regression estimation is 0.042, whereas it is equal to 0.025 in case of complete data. Although linear imputation gives biased estimation of standard deviation and correlation for the data mechanism MCAR or MAR, it does yield unbiased estimates of the average.

Mean substitution imputation and linear imputation lead to bias estimation, especially in case of correlation and standard deviation of both MAR and MCAR (Allison, 2002; Graham, 2009; Schafer,



Figure 4: Regression model scatterplot of the proportion of available chlorine in a certain quantity of chlorine solution (MAR).

2010). Stochastic linear regression imputation can eliminate these missing values, it is similar to standard regression imputation technique and a regression model estimates for the missing data (Baraldi and Enders, 2010). In some detail, it is a linear regression imputation with each estimated value being added a random error value; this random value is generated randomly from a normal distribution with a variance equal to the residual variance and a mean of zero that is estimated from the linear regression imputation model (Schafer, 2010; Graham, 2009). Recall the data in Table.1, where the regression of the output Y on input X yield a residual variance of 0.000162. Then, the new random error is produced randomly from a normal distribution with a variance of 0.000162 and a mean of zero. These new error terms can then be added to the estimated output \hat{Y} , which is predicted from the linear regression imputation model. Fig.5 shows the scatter plot of the imputed values of available chlorine data obtained from a stochastic linear imputation model. Because there is a random error added to each imputed value the imputed data do not represent a straight line, as that generated from a standard linear regression imputation model.



Figure 5: Stochastic imputation scatterplot of the proportion of available chlorine in a certain quantity of chlorine solution (MAR).

Comparing Fig.1 with Fig.5, it is clear that the

α

stochastic regression model produces much better result. This slight adjustment to regression model yields unbiased parameter estimation in the case of MAR mechanises. However, stochastic regression imputation may not be able to guess the real error between the real and predicted values because it depends on random error values.

4 EM ALGORITHM

EM algorithm is an iterative technique, which is useful for incomplete data analyses, and it is an algorithm depending on a maximum likelihood technique to produce a group of data by using the relationships among all observed variables(Enders, 2010). The basic idea of this technique was developed in 1970s (Dempster et al., 1977). This algorithm consists of iterative procedures, which are divided into two steps, that is the expectation step and the maximization step (E and M steps, respectively). As an iterative algorithm it needs initial values to start, these initial values are represented by a mean vector and covariance matrix. To generate the initial values of the mean vector and the covariance matrix we can use much simple technique such as listwise deletion method (Enders, 2010). EM technique uses linear regression models to estimate the missing data and sometimes gives biased estimation especially when the system contains high nonlinearity behaviour (Smyth, 2002; Ng et al., 2012). This study proposes a modified iterative algorithm to deal with nonlinear system models, where there exist a number of latent variables. It follows that for small data set problems, the EM algorithm gives the same result as regression imputation technique (Baraldi and Enders, 2010).

5 NONLINEAR ESTIMATION BY GAUSS-NEWTON ALGORITHM

The linearization technique for nonlinear regression is an approach widely used in nonlinear regression model estimation (Montgomery et al., 2006). The basic idea of nonlinear estimation by linearization method consists of two steps, that is the linearization of the nonlinear system and the estimation of model parameters (Smyth, 2002). Linearization can be implemented by a Taylor series expansion of the nonlinear model regarding a specific operating point. For example for a nonlinear model $f(X,\beta)$ of n parameters (X is input and β is the estimated parameter vector) the linearization result with respect to the operation point β_0 is

$$f(X_k,\beta) = f(X_k,\beta_0) + \sum_{m=1}^n \left[\frac{\partial f(X_k,\beta)}{\partial \beta_m}\right]_{\beta=\beta_0} (\beta_k - \beta_{m0})$$
(1)

$$f_k^0 = f\left(X_k, \beta_0\right) \tag{2}$$

$${}^{0}_{m} = (\beta_m - \beta_{m0}) \tag{3}$$

 $J_{km}^{0} = \left[\frac{\partial f(X_{k},\beta)}{\partial \beta_{m}}\right]_{\beta=\beta_{0}} \text{ is } k \times n \text{ jacobian matrix. The residual between linear and nonlinear values for the nonlinear model is}$

$$e = Y_k - f_k^0 = \sum_{m=1}^n \alpha_m^0 J_{km}^0 + \varepsilon_k \tag{4}$$

The linear model (3) is assumed to be valid just around some specific operating point and ε is assumed to be white noise with zero mean and constant variance. Least squares method can be used to estimate parameter α

$$Y_0 = J_0 \alpha_0 + \varepsilon \quad \text{(5)}$$

$$\alpha_{0} = \left(J_{0}^{'}J_{0}\right)^{-1}J_{0}^{'}e \tag{6}$$

From equation (1),

$$\beta_1 = \alpha_0 + \beta_0 \tag{7}$$

The next step is to replace β_0 by β_1 in equation (1) which represents new initial value for the system and repeat same steps for $[\beta_2, \beta_3, \beta_4, \dots, \beta_l]$ where l is the number of required iterations to get the convergence. We can calculate the number of iterations m by determining the convergence ratio $\left(\left[\left(\alpha_{k,l+1}-\alpha_{kl}\right)/\alpha_{kl}\right]\right) < \delta$ at each iteration until it meets some pre-specified threshold (specific small value for δ) for example when the value less than 1×10^{-6} (Montgomery et al., 2006). The above procedures are called Gauss-Newton iteration method for nonlinear system analysis. Unfortunately, this technique cannot be used to estimate the parameters if there exist missing data because it depends on the error between the linear and nonlinear values and if there is a missing value on the output Y it is not possible to estimate the error. This study thus tries to use another optimization technique (that is the EM algorithm) to estimate the error and take it as an initial value in the Gauss-Newton iteration approach. It shows that the combination of EM and Gauss-Newton approach produces better results in comparison with linear analysis methods. To illustrate this, the same example taken from (Draper and Smith, 1981)was considered here.



Figure 6: Nonlinear scatterplot of the proportion of available chlorine in a certain quantity of chlorine solution (MAR).

Firstly, a nonlinear exponential growth model is used to fit the data

$$Y = \theta_1 \left(y_1 - \theta_1 \right) e^{\theta_2 (X - x_1)} \tag{8}$$

where x_1 and y_1 represent the first two values in the data set (initial values). The values generated by the estimated nonlinear model are shown in Fig.6. Comparing Fig.6 with Fig.4 and Fig.5, there is similarity between the linear estimation and the nonlinear estimation. This slight modification to nonlinear algorithm for missing data yields unbiased parameter estimation in the MAR case. Notice that the nonlinear regression model yields a correlation -0.94 between the output Y and input X, in contrast the correlation equals to -0.86 for the complete-data. Consequently, the nonlinear model produces less variability, for example, the standard deviation of the output Y estimated from the nonlinear model is 0.029, whereas it is equal to 0.025 for the complete data. Although nonlinear regression model gives unbiased estimation of standard deviation and correlation, it does produce biased estimate of the mean. In the above example, an exponential growth model was used to fit the data, which shows some disadvantage in comparison with linear models. Next, it presents the use of EM algorithm for linear model parameter estimation, and the use of the modified Gauss-Newton algorithm nonlinear model parameter estimation. (Enders, 2006; Graham, 2009; Schlomer et al., 2010; Seaman and White, 2013; Montez-Rath et al., 2014). To give more details let us consider another data set which is taken from (Montgomery et al., 2006), and shown in Table.2. In this example, the dependent variable (Y) is the tensile strength of Kraft paper and the independent variable (X) is the hardwood concentration for pulp, which produces the paper. The data set in this example contains complete data on the input and output of the system. The data set also includes the following missing data mechanism: data missing completely at random (MCAR) with 21%, 26% and 37% missing.

Note that unlike in the previous examples, the choice of this mechanism is to study the effect of different algorithms on different missing mechanisms. The ultimate purpose of this example is to compare the performance of linear algorithm (EM algorithm) and nonlinear algorithm (modified Gauss-Newton algorithm) in the presence of different percentages of missing data for a MCAR mechanism in term of correlations, residuals, standard deviations, and means. For illustration, the complete data are plotted in Fig.7. The EM algorithm is applied to estimate the parameters of the linear model:

$$Y = \theta_0 + \theta_1 X \tag{9}$$



Figure 7: NComplete data scatterplot of input/output data.

The modified Gauss-Newton algorithm was applied to estimate the parameters of the nonlinear model:

$$Y = \theta_0 + \theta_1 X + \theta_2 X^2 \tag{10}$$

Let us start by comparing the estimated values generated by the linear and nonlinear models (in case of MCAR with 21% missing data), with that of the complete data, where the mean value for full-observed output Y is 34.184, and mean value for the predicted values is 34.379, and 34.178, respectively. This result indicates that the nonlinear regression is just slightly better than the linear model for mean value estimation. By inspecting Fig.8 and Fig.9, it can be seen that the effect of linear regression on the system. In Fig.8, the predicted values from linear model fall directly on a straight line that has a slope 1.73, the same thing happens with the nonlinear model in Fig.9. The predicted values with linear and nonlinear regression have a correlation 0.54684 and 0.53117 respectively between the predicted output and input X, whereas the case of complete data has a correlation 0.55261. Table.3, summarises the effect of other two cases of percentage missing (MCAR 26% and MCAR 37%) on the linear and nonlinear model. For example, linear and nonlinear model give standard deviation estimates of 13.61 and 14.00, respectively, whereas the full-observed data standard deviation is 13.778. Not surprisingly, this is because the missing values are close to linear region area.

Y-MCAR							
X	Complete	(21%)	(26%)	(37%)			
1	6.3	6.3	6.3	6.3			
1.5	11.1	11.1	11.1	11.1			
2	20	-	20	-			
3	24	24	24	24			
4	26.1	26.1	26.1	26.1			
4.5	30	-	-	-			
5	33.8	33.8	33.8	33.8			
5.5	34	-	34	-			
6	38.1	38.1	-	38.1			
6.5	39.9	39.9	39.9	-			
7	42	42	-	42			
8	46.1	46.1	46.1	-			
9	53.1	53.1	53.1	-			
10	52	52	-	52			
11	52.5	52.5	52.5	52.5			
12	48	48		-			
13	42.8		42.8	42.8			
14	27.8	27.8	27.8	27.8			
15	21.9	21.9	21.9	21.9			

Table 2: The input and output of the system in MCAR with missing percentage (Montgomery et al., 2006) (Montgomery, Peck, and Vining, 2006).

Table 3: The effect of linear and nonlinear models on the system in different MCAR missing percentage.

Linear regression							
	21%	26%	37%				
Mean	34.379	31.744	31.106				
Correlation	0.5468	0.543	0.5541				
Standard deviation	13.61	13.778	13.778				
Nonlinear regression							
Mean	34.178	30.945	31.426				
Correlation	0.5312	0.5148	0.5372				
Standard deviation	14.01	12.438	12.356				



Figure 8: Linear regression model of input/output data in case of 21% missing data scatter plot.



Figure 9: Linear regression model residual e versus predicted values scatter plot in case of 21% missing.



Figure 10: Nonlinear regression model of input/output data in case of 21% missing data scatter plot.

6 CONCLUSIONS AND FUTURE WORK

The primary aim of this paper is to introduce a nonlinear modelling technique for missing-data analysis. Comparative studies on EM and Gauss-Newton approaches have been carried out. EM and Gauss-Newton algorithms are advantageous over traditional approaches. Although EM and Gauss-Newton algorithms have not produced same results specially in existing of high nonlinearity in the system and different missing data mechanism (i.e., MAR and different MCAR cases). Most studies in the literature focus on using of linear techniques because they hold the simplest assumptions that make these procedures easier for users especially in computerised environment. As mentioned previously, in existence of high nonlinearity parts in the system, EM does not always give good result. Although Gauss-Newton does need initial values to start iteration process and that gives it disadvantage because this needs more time to do in computerised environment. In summary, EM and Gauss-Newton algorithms require similar procedures and frequently produce similar parameter estimates (in case of small number of data for both MAR and MCAR mechanism), particularly if the distribution of data contains low nonlinear parts. As a future work,

for a nonlinear model, the form of the model must be specified, the parameters need to be estimated, and starting values for those parameters must be carefully provided.(Box and Tidwell, 1962) proposed the first technique for model selection. (Royston and Sauerbrei, 2008) suggested a class of regression models by fractional polynomials (FP), involving model choice from a specific number of models, but all of these methods work only in case of complete data. We will try to modify one of these approaches and apply it on missing data. To further improve and test the performance of the proposed method, we will try and incorporate good ideas of other methods for example those presented in (Luengo et al., 2012)also carry out comparative studies on real data sets, readers are referred to (Alcalá et al., 2010) for good sample data sets.

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