FORECASTING INNOVATION DIFFUSION WITH NEAR-OPTIMAL BERTALANFFY-PÜTTER MODELS

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ABSTRACT

Using a classical example for technology diffusion, the mechanization of agriculture in Spain since 1951, we considered the forecasting-intervals from the near-optimal Bertalanffy-Pütter (BP) models. We used BP-models, as they considerably reduced the hitherto best fit (sum of squared errors) reported in literature. And we considered near-optimal models (their sum of squared errors is almost best), as they allowed to quantify model-uncertainty. This approach supplemented traditional sensitivity analyses (variation of model parameters), as for the present models and data even slight changes in the best-fit parameters resulted in very poorly fitting model curves.

1. INTRODUCTION

1.1. BACKGROUND

Technology forecasting uses a wide range of methods (Firat et al., 2008). This paper focuses on a popular phenomenological approach, trend analysis for the diffusion of technologies by means of sigmoidal (S-shaped) model curves. Here, an often considered three-parameter model was the Verhulst model of logistic growth (e.g. Adamuthe & Thampi, 2019; Naseri & Elliott, 2013; Yamakawa et al., 2013). This paper proposes a five-parameter model to describe the success (growth, diffusion) of a technology, the Bertalanffy-Pütter (BP) model. It generalizes many

conventional three-parameter models (e.g. logistic growth) and therefore improves their fit. In addition, the two additional parameters allow to identify near-optimal three-parameter models that do not differ significantly from the best-fit BP-model. Comparing the forecasts from these near-optimal models with the forecast from the best-fit model results in new quantitative indicators for assessing model-uncertainty *ex ante*. We illustrate this approach for data from literature, where we explore, which levels of model-uncertainty occurred in the past for forecasting. We expect that such empirical studies will lead to sensible recommendations for practitioners about what model-uncertainty needs to be assumed for different timespans of prognosis.

1.2. PROBLEM

Model uncertainties arise, when gaps in knowledge about the true drivers and mechanisms of growth cannot be reduced by an analysis of the past observations. For instance, as was observed for the prognosis of cancer, many growth curves with different shapes in the future may fit well to given historic data (Kühleitner et al., 2019). The paper develops a new approach to assess model-uncertainty and it illustrates it for forecasting. In order to measure model-uncertainty quantitatively, Bai & Jin (2016) suggested to use the relative error of the prediction. However, *ex ante* we could not compute this future error of prediction.

We propose a different approach. We identify models that fit well to the current data and that therefore in a technical sense defined below have a certain "probability to be true". Thereby, we use the Akaike information criterion *AIC* (Akaike, 1974) and its associated probability (Akaike weights): For given data, the model with the lowest *AIC* is most likely to be true and comparing other models with this one, their probabilities to be true are computed from the differences in *AIC*.

Based on this notion, we define a forecasting interval by the lower and upper bounds of the predictions drawn from likely models. Thereby, we consider all BP-models with a certain probability to be true, when compared to the best-fitting one. The forecasts based on these models define the forecasting interval. This concept resembles the confidence interval, but the confidence interval assumes a fixed model that is fitted to random variations of the data, while for the forecasting interval the data remain fixed.

2. MATERIALS AND METHODS

2.1. MATERIALS

The computations used Mathematica 12.0 software of Wolfram Research. The results of optimization were exported to a spreadsheet (Microsoft Excel) and reimported into Mathematica for further analysis of the model-uncertainty.

2.2. DATA

We use data about the mechanization of agriculture in Spain by means of tractor ownership. The primary sources were census data and government reports over the period 1951-1976 (Mar-Molinero, 1980). While the data may appear to be outdated, they cover an interesting phase for agriculture in Spain: During the early 1950s, the ancient regime of Franco gave up its disastrous policy of economic autarky and in the 1960s and 70s this was followed by a policy of modernization of the agricultural sector (Táboas et al., 2019). Further, the data for 1951-1976 were used repeatedly to test approaches to forecasting (e.g. Nguimkeu, 2014; Franses, 1994; Meade, 1984; Mar-Molinero, 1980). Gurung et al. (2018) is a recent related study about the mechanization of agriculture in India.

The data were rescaled to start at $t = 0$, meaning the year 1951. (This rescaling was used in literature.) We used equation (1) to model the stock of tractors $y(t)$ over time t in years. Thereby, we first searched for the best fitting BP-model for the data till 1976. In order to assess prognosis, we also identified the best fitting BP-models to ten truncated data (number of tractors till the year 1966, 1967, … 1975) that we used to test the forecast for 1976 in hindsight. We supplemented this example by considering in addition the 1977-2009 data from the World Bank Open Data repository starting in 1961 (World Bank, 2019) and identifying the best-fit BP model for the extended data till 2009. The combined data are listed in Table 1.

Table 1: Stock of tractors in Spain during the period 1951-2009.[1]

Year[2]	Stock[3]	Year	Stock	Year	Stock	Year	Stock	Year	Stock	Year	Stock
0	1.3800	10	7.1080	20	28.2370	30	54.8080	40	75.5740	50	92.5690
1	1.5800	11	9.2750	21	30.6190	31	57.1170	41	76.6270	51	94.6050
2	1.9000	12	11.4410	22	33.0360	32	59.2010	42	77.5300	52	94.3650
3	2.1440	13	13.0130	23	35.5550	33	61.1430	43	78.9750	53	96.6600
4	2.6020	14	14.7880	24	37.9070	34	63.3210	44	80.5590	54	98.0810
5	2.9960	15	16.9190	25	40.0928	35	65.7830	45	82.3610	55	100.0220
6	3.4180	16	18.0720	26	42.1390	36	67.8680	46	84.1930	56	101.6040
7	4.0680	17	20.4360	27	45.5680	37	70.1930	47	86.2140	57	103.0440
8	4.7080	18	23.4540	28	49.1600	38	72.2660	48	88.1980	58	103.8730
9	5.6840	19	25.9820	29	52.3910	39	74.0830	49	89.9700		

1) Source: data combined from Figure 5 of Mar-Molinero (1980) and open data from World Bank (2019).
2) Start with 1951 (year 0); 1976 corresponds to year 25.
3) One unit is a stock of 10,000 tractors.

2.3. BERTALANFFY-PÜTTER (BP) MODEL

The growth function $y(t)$ of the BP-model is a solution of the following differential equation (Pütter, 1920), which can be solved analytically, though in general not by means of elementary functions (Ohnishi et al., 2014).

$$y'(t) = p \cdot y(t)^a - q \cdot y(t)^b$$

The five model parameters are determined from fitting the model to historical data: Four parameters are displayed in the equations, namely the non-negative exponent-pair $a < b$ and the constants p and q. An additional parameter is the initial value, i.e. $y(0) = c > 0$.

Each exponent-pair (a, b) defines a unique BP-model $BP (a, b)$ with three free parameters. Well-known examples are bounded exponential growth $BP (0, 1)$, logistic growth $BP (1, 2)$, the von Bertalanffy model $BP (1, 2/3)$, and the West model $BP (1, 3/4)$. The Solow (1957) model of economic growth is a class of BP-models; it coincides with the generalized Bertalanffy model ($b = 1$ and $a < 1$). Also, the Richards model is a class of BP-models ($a = 1$ and $b > 1$). The Gompertz-model is the limit case $BP (1, 1)$ with a different differential equation, where b converges to $a = 1$ from above (Marusic & Bajzer, 1993). These models have been used in forecasting, e.g. business trends (Dhakal, 2018), tumor growth (Murphy at al., 2016), or epidemic trajectories (Pell et al., 2018). In biology, these models have been proposed to model the growth of plants (Richards, 1959) or the mass growth of vertebrates (e.g. West et al., 2001; Bertalanffy, 1949).

In literature, there are several other five-parameter growth models, such as the model of Bass (1969) for market diffusion or the model of Monod (1949) for bacterial kinetics. We decided to use the BP-model, as it was very flexible. In comparison to other five-parameter models, this versatility had the disadvantage that for the BP-model the standard optimization tools (e.g. command Non-Linear Model Fit in Mathematica) did not always identify the best-fit parameters (numerical instability). However, as explained below, we could overcome this difficulty, whence this model is now feasible for practitioners. As to another limitation, the BP-model is not suitable in situations, where both growth and decay occur. Rather, it is intended to improve the fit to the data in situations, where initially e.g. logistic growth has been considered as a viable model.

2.4. DATA FITTING

The most common method for data-fitting, used also for this paper, is the method of least squares, which fits a (nonlinear) model to past data (Satoh & Matsumura, 2018). Thus, model selection aimed at finding parameters that minimized the sum of squared errors SSE. If $y(t)$ is a solution of equation (1), using certain exponents $a < b$ and parameters p, q, c, and if (t_i, y_i) are the N data, then SSE is defined by equation (2):

$$SSE = \sum_{i=1}^{N}(y_i - y(t))^2$$

As explained above, for model (1) the standard optimization tools did not find best-fit parameters to minimize (2). We did overcome this difficulty by considering exponent-pairs (a, b) on a grid with step size 0.01 in both directions; initially $0 \leq a \leq 2.5, a < b \leq a + 3.5$. (The grid was adaptively enlarged during optimization; for one dataset we searched about 200,000 grid points.) Figure 1 plots the search-grid (yellow area) and it displays the exponent-pairs of named models by dots (e.g. Verhulst model) or lines (e.g. Richards' model interpreted as a model class). Compared to the search-grid, these models were rather exceptional.
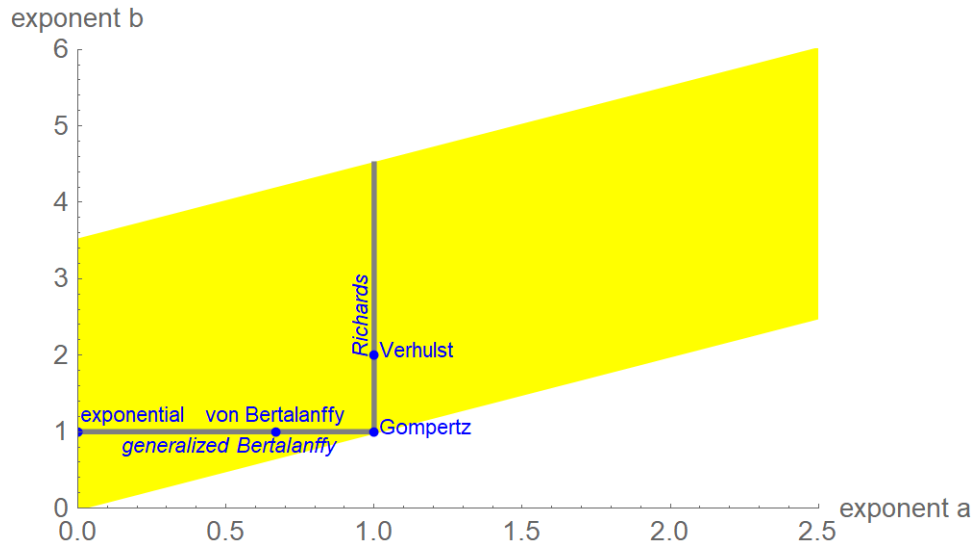

Figure 1: Named models (blue) and model classes (italics and lines) and part of the search region (yellow) of BP-models (plot using Mathematic 12.0).

For each exponent-pair of the grid we identified the best fitting model parameters (p, q, c) that minimized SSE. This defined the following function of equation (3), assuming for the minimization (right hand side) model (1) with exponents a, b:

$$SSE_{opt}(a, b) = \min_{c,p,q}(SSE)$$

The best fitting model had the overall least sum of squared errors (SSE_{min}). We identified its exponent-pair (a_{min}, b_{min}) with an accuracy of 0.01 (as we searched only grid-points) and its parameters $p_{min}, q_{min}, c_{min}$ that minimized $SSE_{opt}(a_{min}, b_{min}) = SSE_{min}$.

For each grid-point (a, b), the optimization of p, q, and c was done using a custom-made variant of the method of simulated annealing (Vidal, 1993). The details and the code were outlined in another paper (Renner-Martin et al., 2018, Kühleitner et al., 2019). The outcome was exported into a spreadsheet, whose rows listed the best fit parameters a, b, c, p, q, and SSE for each grid-point. The exponent-pair (a_{min}, b_{min}) was identified from the row, where the least value of SSE was attained.

2.5. COMPARISON OF MODELS

We use SSE of equation (2) as the primary measure to assess the fit of a model to data. Related measures used in forecasting literature (for a survey: Hyndman & Koehler, 2006) are the root-mean-square error, $RMSE = \sqrt{\frac{SSE}{N}}$, and R-squared, $R^2 = 1 - \frac{SSE}{SQT}$. Here, SQT is the total sum of squares (variance of the N data y_i times N–1 or N, depending on the estimator for the variance). The use of SSE was based on assuming normally distributed errors.

Different statistical assumptions have led to weighted sums of squared errors. In addition, we used the Akaike information criterion, $AIC = N \cdot \ln(SSE/N) + 2 \cdot K$; c.f. Burnham & Anderson (2002) or Motulsky & Christopoulos (2003). Here, N is the number of the data-points. For the 1951-1976 data, N = 26; for the truncated data, N ranges from 16 to 25; and for the 1951-2009 data, N = 59. Further, K = 4 is the number of optimized parameters (c, p, q and SSE as an implicit parameter). As we compared a finite set of three-parameter BP-models $BP(a, b)$ using exponent-pairs chosen from a grid, we did not penalize the best fitting model by a higher number of parameters (the optimal exponent-pair was roughly approximated, but not yet computed). Thus, for these models, the least AIC_{min} was achieved for the model defined from the exponent-pair (a_{min}, b_{min}).

If the model with AIC_{min} is compared to another model with larger AIC, then the probability that the other model is true (in an information theoretic meaning) is given by the relative Akaike weight $e^{-d/2}/(1 + e^{-d/2})$, using the difference $d = AIC–AIC_{min}$. This probability is at most 50% (comparing the model with the least AIC with an almost as good model).

2.6. FORECASTING INTERVALS

The starting point of our new approach are the data and SSE_{min} together with all u-near-optimal exponent-pairs (a, b). Thereby, an exponent-pair (a, b) is u-near-optimal with model-uncertainty u, if $SSE_{opt}(a, b) \leq (1+u) \cdot SSE_{min}$. For each exponent-pair we also consider the best fitting growth curve $y_{a,b}(t)$; it is specified by its parameters a, b, c, p, q. All models that are displayed in the yellow search region of Figure 1 by their exponent-pairs are meant to realize the best possible fit to the given data, i.e. depending on a and b (which defined the model) the model parameters p, q and c were optimized according formula (3). Therefore, for the data that represent the past, there was barely a difference between the model curves for models whose SSE did not differ much from SSE_{min}.

In analogy to confidence intervals we now define: For a point of time T the forecasting interval $I_u(T)$ for the level u of model-uncertainty has as its end-points the least upper and the largest lower bounds of the function values $y_{a,b}(T)$ associated to u-near-optimal exponent-pairs. For the computation of a forecasting interval $I_u(t)$, filtering in the table of optimal parameters identified the rows with $SSE \leq (1+u) \cdot SSE_{min}$. The parameters of each of these rows defined a growth function $y_{a,b}$ that was evaluated at T. The minimum and maximum of these values defined the boundaries of the interval.

In order to obtain a closer analogy to the confidence intervals, we related model-uncertainty in the following way to the probability that a model is true in the information theoretic sense, using AIC and more specifically, the relative Akaike weight. For, as follows from the above section, if the exponent-pair (a, b) is near-optimal with model-uncertainty u, then the probability that this exponent-pair is true is given by the following formula (4) for the relative Akaike-weight.

$$\text{prob}(a, b) = \frac{1}{1 + \sqrt{(1 + u)^N}}$$

3. RESULTS AND DISCUSSIONS

3.1. PREVIOUS OUTCOMES

The trend for tractors has been studied repeatedly. There is a consensus in literature that the growth of tractors would follow a logistic model. Mar-Molinero (1980) compared several models and for the 1951-1976 tractor data he reported SSE = 4.9768 as the best fit, obtained by the logistic model. Subsequent authors (e.g. Meade, 1984; Franses, 1994; Nguimkeu, 2014) confirmed this conclusion.

Mar-Molinero (1980) also reported an "unexplained residual sum of squares" of 2.57. However, he referred to autocorrelation, using a fit of a time series: $r_t = \rho \cdot r_{t-1} + \varepsilon_t$ for the residuals $r_t = y_t - y(t)$ and the unexplained error ε_t. This paper aims at improving the fit by using a better growth curve, but it does not follow up on the autocorrelation.

3.2. DATA FITTING

In order to identify the best-fit BP-model for the 1951-1976 tractor data, and for the truncated data, we searched between 0.9-1.3×10^5 grid-points. Figure 2 plots the best fitting growth curves. Their best-fit parameters are listed in Table 2 and their exponent-pairs are plotted in Figure 3.

Table 2: Parameters for the best fit of model (1) to the data from 1951 up to the indicated year.

Year[1]	Best fit parameters					Goodness of fit		
	a_{min}	b_{min}	c_{min}	p_{min}	q_{min}	SSE_{min}	$RMSE$	R^2
1966	1.91	2.12	1.47507	0.182778	0.0976106	0.581875	0.190702	0.998599
1967	1.89	2.13	1.47848	0.166224	0.0808923	0.58954	0.186223	0.998926
1968	1.72	1.9	1.37506	0.252761	0.14337	1.29791	0.268526	0.998208
1969	1.42	1.62	1.20355	0.312459	0.155705	2.92583	0.392417	0.996969
1970	1.34	1.42	1.13237	0.700413	0.519034	3.53807	0.420599	0.997196
1971	1.24	1.4	1.08056	0.423065	0.227006	3.64734	0.416753	0.997732
1972	1.22	1.38	1.08142	0.424588	0.22552	3.69308	0.409716	0.998164
1973	1.17	1.4	1.06337	0.341165	0.136074	3.74722	0.403637	0.998487
1974	1.17	1.37	1.07238	0.37085	0.165032	3.84279	0.400145	0.998725
1975	1.15	1.34	1.03507	0.396099	0.182001	3.89954	0.394945	0.998921
1976	1.12	1.32	0.997355	0.396746	0.173354	3.91475	0.38803	0.999085
2009	0.75	1.02	0.253028	0.590051	0.159631	64.9233	1.049	0.999085

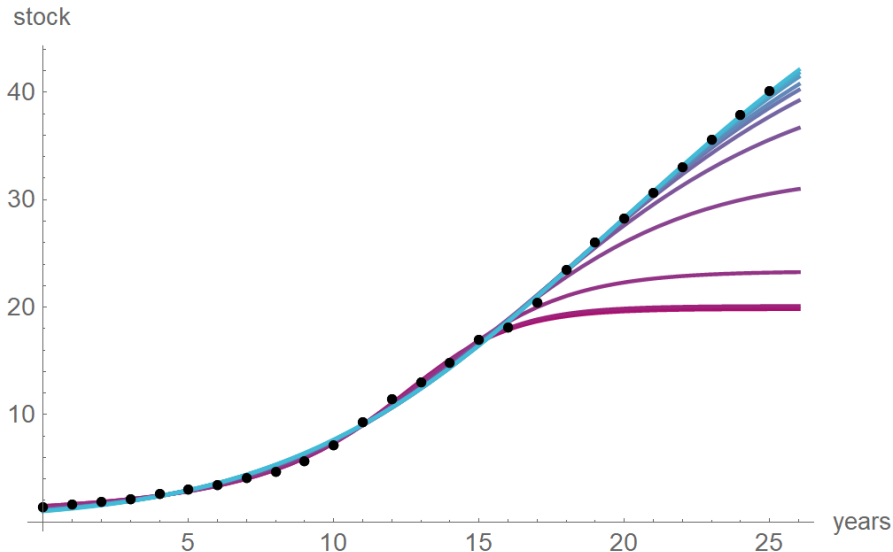1) This indicates the data from 1951 to the displayed year

Figure 2: Stock of tractors for 1951-1976 (black dots) with the best fitting growth curve of the BP-class (top line) and forecasts using the best fitting growth curves for the data till 1966, 1967, ... 1975 (increasing order of the curves); the best fit parameters are from Table 2 (plot using Mathematica 12.0).

Judging from R^2 (Table 2), for all (truncated) data the fit of all curves to these data was excellent (99.7-99.9% of the variance in the data was explained by the models). Further, the best fitting model curve for the 1951-1976 data with SSE = 3.91475 displayed a significant improvement of 21% over the previous SSE = 4.9768 reported in literature for logistic growth. However, the extrapolations of the growth curves for the truncated data to the remaining data underestimated the future growth (Figure 2). In particular, the best fitting growth curves to the data till 1966, 1967, ... and 1969 did rapidly approach their asymptotic limits and therefore their prognosis for T = 1976 remained considerably below the true value. However, the error became smaller, the more data were used. Further, the best fit exponent-pairs for different years were spread widely along a regression line (Figure 3). For comparison, we also plotted the optimal exponents for the extended data 1951-2009.
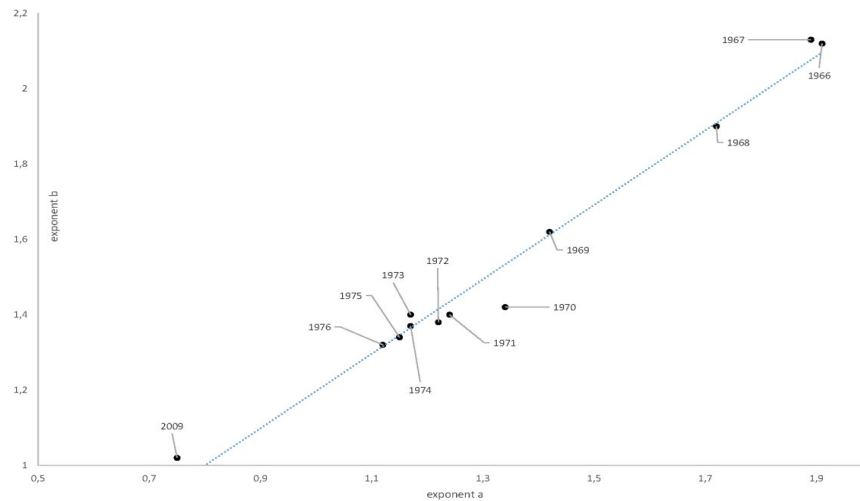
Figure 3: Optimal exponent-pairs (Table 2) and linear trend $b = 0.2094 + 0.988 \cdot a$ (dotted, plot using MS Excel).

3.3. FORECASTING

Figure 4 displays the near-optimal exponent-pairs for the truncated data for 1951-1971. This figure was obtained as a by-product of our approach to data-fitting, where for each of almost 127,000 exponent-pairs (a, b) the best-fit exponents to the truncated data were found by an optimization. The red area displays about 2700 near-optimal exponent-pairs, for which SSE_{opt} did not exceed the overall best SSE_{min} (attained at the black dot) by more than $u = 10\%$. The blue area corresponds to the near-optimal exponent-pairs with $u = 34\%$. The best fitting models using these exponent-pairs have a probability of 5% or more to be true, when compared to the best-fit model. We repeated these computations for the truncated tractor data till 1970, 1971, … and 1975. (In view of Figure 2, the data truncated at 1969 or earlier were unsuitable for prognosis and in view of Figure 3 their best-fit exponent-pairs were remote from the exponent-pair for the data till 1976.)
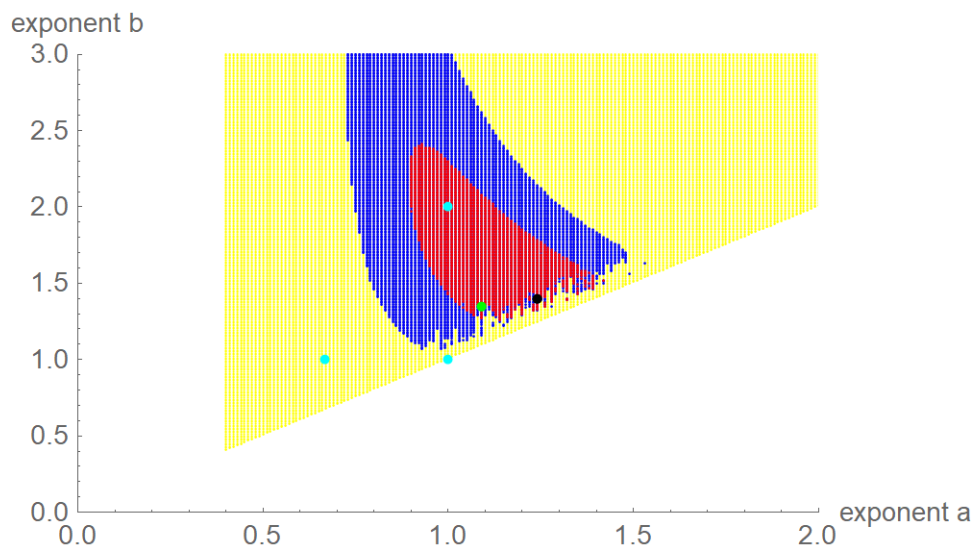

Figure 4: Part of the searched grid points (yellow) for the fit of model (1) to the tractor data for 1951-1971, near-optimal exponent-pairs assuming a model-uncertainty of $u = 34\%$ (blue: this corresponds to a probability of 5%) and of $u = 10\%$ (red: probability 28%), optimal exponent-pair for these data (black, see Table 2), exponent-

pair to obtain an upper bound for the prognosis for 1976 (green, see Table 3) and selected exponent-pairs of named models (light blue: logistic, Gompertz and von Bertalanffy); plot using Mathematica 12.0.

Next, for each of near-optimal exponent-pair (a, b) the best fitting growth curve $y_{a,b}(t)$ was identified and its "future" values were also evaluated ("future" referring to the perspective of the fitted data). Their upper and lower bounds defined forecasting intervals. Figure 5 plots the resulting forecasting band corresponding to Figure 4, prognosis for the stock of tractors based on the data for 1951-1971. For the present data and the chosen model-uncertainty all data points from 1972-1976 (plotted in green) were within this forecasting band.
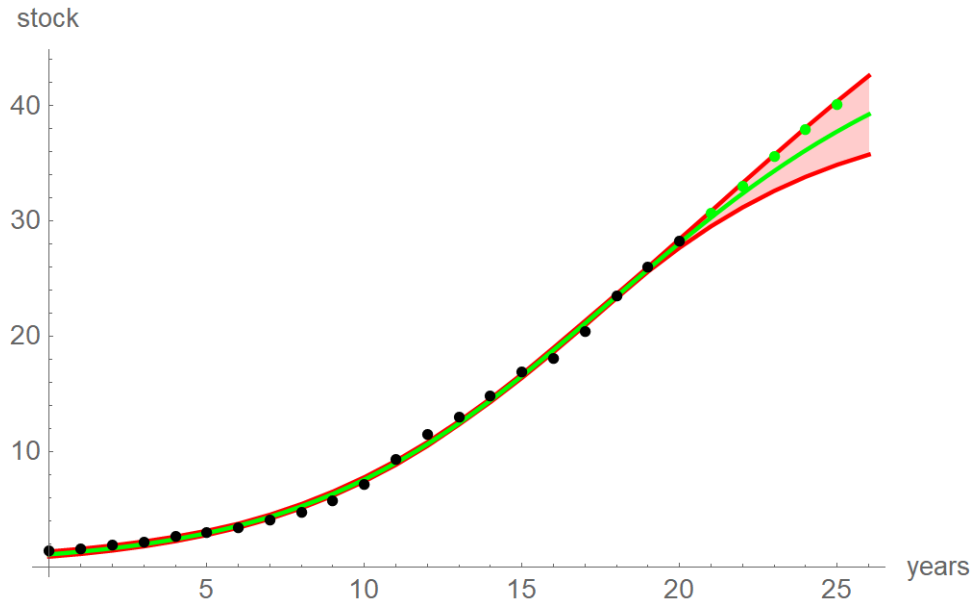

Figure 5: Forecasting band (red, defined from the red dots in Figure 4) around the best fitting growth curve (green) to the tractor data for 1951-1971 (black), and comparison with the data for 1972-1976 (green), assuming a model-uncertainty of u = 10%; plot using Mathematica 12.0.

These computations were repeated for all truncated data. Table 3 summarizes these results in the following way: It identifies the least model uncertainty that was needed to include the true value for 1976 in the forecasting interval. For instance, for each red exponent-pair (a, b) of Figure 5 (model-uncertainty u = 10%) the value of the growth curve $y_{a,b}$ was evaluated for the year 1976; the values ranged between 34.9 and 40.4. The observed value at 1976 was 40.1 and the best-fitting curve to the 1951-1971 data attained a lower value. For Table 3 (line for 1971) we identified all model curves $y_{a,b}$ that attained a higher value and selected the one with the least *SSE* (Table 3 displays it as "needed *SSE*").

Table 3: Minimal model-uncertainty so that the true value for 1976 was in the forecasting interval.

Year	Model that achieves the required bound[1]					Needed [2] *SSE*	Logistic[3]$SSE_{logistic}$	Model-uncertainty [4]	Probability [4]
	a	b	c	p	q				
1970	1.19	1.27	1.04613	0.76236	0.547886	3.84508	3.74498	8.677%	30.3197%
1971 [5]	1.09	1.35	0.984258	0.34281	0.116463	3.90232	3.83045	6.991%	32.9706%
1972	1.1	1.31	0.988966	0.388885	0.161407	3.959	3.92061	7.201%	31.7592%
1973	1.08	1.29	0.940007	0.406382	0.168379	3.99785	4.05518	6.689%	32.2009%
1974	1.12	1.26	0.955065	0.525042	0.29214	3.95846	4.35074	3.01%	41.1955%

1975	1.08	1.37	0.990765	0.322379	0.0968257	3.94831	4.68163	1.251%	46.1232%

1) For each year, we searched for the exponent pair (a, b), whose $SSE_{opt}(a, b)$ was minimal subject to the constraint that its best fitting growth curve $y_{a,b}$ was above the 1976 value. The parameters of this $y_{a,b}$ are listed.
2) SSE_{opt} of the displayed exponent-pairs; it was above SSE_{min} for the data (see Table 2) and "model uncertainty"
3) $SSE_{opt}(1, 2)$ of the logistic model.
4) The computations were based on SSE_{min} (7th column of Table 2).
5) This model is represented by the green dot in Figure 4.

Table 3 shows that forecasting of the true value based on the truncated data did not require unlikely models: The probabilities of the used models ranged between 30-46% and SSE_{opt} of these models exceeded SSE_{min} by 1-9%. Thus, the prognosis for up to six years remained within the range of variability that could be expected from the data. Note that for the forecast based on the years till 1973, 1974, or 1975, the logistic model was outside this minimal range (i.e. $SSE_{logistic}$ exceeded the needed SSE).

4. CONCLUSIONS AND RECOMMENDATIONS

Forecasting requires the use of models that are capable to represent the hitherto observed data accurately. Model class (1) has some obvious advantages: it is a very flexible class of growth models and it includes a wide range of common growth models. Therefore, in general the best-fitting model of the BP-class will fit better than any of the above-mentioned named model. Thus, for the tractor data the use of models from the BP-class resulted in a significant improvement over the fit by the logistic growth function that was previously used in forecasting.

This approach requires extensive computations, where about hundred thousand models from the BP-class need to be optimized (different models are defined from different exponent-pairs). Yet, these optimization results serve an additional important purpose, as they may be used to quantify the model-uncertainty of forecasting. As is displayed by the forecasting intervals (Figure 5), the near-optimal model curves remained close to the data (on which data-fitting was based). Nevertheless, subsequently there were considerable differences.

For the present data it was feasible to consider forecasting intervals based on all models with a probability of 5% or more to be true. Using this approach, we have shown that the considered data were suitable for a prognosis over a time span of five years.

APPENDICES

The method section lists the data and explains their sources. Further, the authors provided the supplementary material, namely the following spreadsheet (MS Excel) with the outcomes of the optimizations.

S-File. Computation of SSEopt(a, b), based on Table 1 for the stock of tractors for the period 1951-1971, for certain grid-points, namely exponents a and b, and for them the best fit-parameters (optimization results) initial number m0, p, q, and SSE.

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