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Enhancing simulation-based theory development in entrepreneurship through statistical validation

Roman Breig, Maximilian Coblenz*, Michael Pelz

Department of Economics and Management, Karlsruhe Institute of Technology (KIT), Kaiserstrasse 12, 76131 Karlsruhe, Germany

A R T I C L E I N F O

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A B S T R A C T

Recent research has called for new theory development because variables in entrepreneurship have been shown to follow power laws. Usually, simulation is used to validate these new theories. However, validation has been insufficient because it fails to provide a quantitative comparison of distribution parameters. This neglect can cause misleading conclusions. To address this insufficiency, we contribute a four-step method: the *possible simulation parameter range* (PSPR). The fundamental advantage of the method is to compare distribution parameters of both empirical data and simulation results. We demonstrate the method's usefulness with an illustrative example.

1. Introduction

Power law (PL) distributions have received considerable attention in recent entrepreneurship studies because they challenge the fundamental assumption of normally distributed (i.e. Gaussian) variables in this research field (Crawford et al., 2015, 2014). PL distributions are a specific form of heavy-tailed distributions, but other forms exist, such as lognormal. Recent findings make clear that researchers have to consider heavy-tailed distributions, as they characterize many variables that are central to entrepreneurship theories, such as revenue growth, company size, or venture debt. Recently, researchers have called for development of new theories that "explain and predict the mechanisms that generate these distributions and the outliers therein" (Crawford et al., 2015, p. 696).

New theories should contain generative mechanisms, which cause PL and other heavy-tailed distributions. Prior research provides a comprehensive overview of generative mechanisms (Andriani and McKelvey, 2009; Mitzenmacher, 2004; Newman, 2005). Theory development can benefit substantially from simulation (Davis et al., 2007). Recent work has developed theory and implemented simulations in the context of entrepreneurship, including a simple model for the distribution of several entrepreneurial variables over time, which was implemented and validated in a simulation based on a multiplicative process as a generative mechanism (Shim, 2016). Further work developed a bibliometric method to generate agent-based simulation models (Shim et al., 2017).

Empirical data can provide the basis for using numerical simulation, which generates its own set of data. Researchers have described the conventional approach for conducting agent-based simulation (e.g. Shim et al., 2017; Shim and Bliemel, 2017). The comparison of empirical data and simulation results can be used to assess whether heavy-tailed distributions in entrepreneurial research, such as PL distributions, can be explained by a newly developed theory that compares the type of distribution from both sets of data (Shim, 2016; Shim et al., 2017). Having the same type of distribution is used to show that a developed theory can sufficiently explain the heavy-tailed distributed data.

However, as this paper demonstrates, this approach lacks a final step, namely a quantitative comparison of the distribution parameters of both the empirical data and simulation results. Even when both sets have the same type of distribution, qualitatively

* Corresponding author.
E-mail address: maximilian.coblenz@kit.edu (M. Coblenz).

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Table 1
Descriptive statistics and data analysis results for PSED II Wave F data.[a].

Data description	
N	99
Mean	653.650
Standard deviation	3.688.200
Skewness	9
Excess kurtosis	85
p-value test for normality	< 0.0001
Distribution fit	
PL fit	$\hat{\alpha} = 1.75$; $\hat{xmin} = 104{,}500$ $n_{tail}/n = 38.4\%$
KS statistic PL	0.08
p-value PL fit	0.45
Lognormal fit	$\hat{\mu} = 10.85$; $\hat{\sigma} = 2.03$
KS statistic lognormal	0.05
p-value lognormal fit	0.50
Test statistic Vuong's test	+0.09 (n.s.)

[a] Data are right-skewed and exhibit heavy tails. A test for normality is highly significant (i.e. normality is rejected). Both lognormal distribution and PL distribution fit the data well; p-values of lognormal and PL from the bootstrapping procedure show a good fit of both models. The Vuong model comparison test is not significant. Thus, both the PL distribution and the lognormal distribution are reasonable distribution choices and are included in the candidate collection.

the specific distribution parameters might still be significantly different. Only a more detailed comparison allows drawing inferences about whether a developed theory sufficiently explains heavy-tailed distributions in the empirical data.

A quantitative comparison of empirical and simulation data is a form of validation, and the literature introduces several categories of validation. One distinction is between micro-level (i.e. behavior of simulated agents) and macro-level validation (i.e. simulation output) (Takadama et al., 2008). A second distinction is that between conceptual (i.e. assumptions of simulation model) and operational validation (i.e. output) (Heath et al., 2009). Statistical and non-statistical validation have also been distinguished (Heath et al., 2009).

The contribution of this paper is twofold. First, we introduce a four-step method that enables researchers to easily compare distribution parameters from simulation and empirical data, allowing a more sophisticated and comprehensive validation of developed theory. The method is embedded in the overarching framework of simulation-based theory development and refers to that framework's last step, "*Validate with empirical data*" (Davis et al., 2007, p. 482, Table 1). As the method is macro-level, operational, and statistical, we respond to the call for statistical validation techniques (Heath et al., 2009). Second, we apply the method in an illustrative example of the entrepreneurial variable venture debt (VD), thereby showing why taking the distribution parameters into account is important. Both contributions reduce the gap in the current literature significantly.

2. The four-step method

We present the method in detail and offer an illustrative application in the next section. The method consists of the following four steps:

1. *Analyze the data* according to the method outlined in Clauset et al. (2009) and form a collection of candidate distributions that fit the data.
2. *Build a theory-guided simulation* that implements a generative mechanism corresponding to one of the candidate distributions.
3. *Run and assess the simulation*. Assess the results by explicitly comparing the *specific distribution parameters* of both simulation and empirical data.
4. *Validate the results and refine if necessary*. Validation is achieved as soon as the specific distribution parameters of Step 3 match. If parameters do not match, refine Step 2 and repeat Step 3 until the simulation (and thus the model) is validated.

2.1. Step 1 – analyze the data

Empirical data are analyzed according to the method in Clauset et al. (2009), who describe how to fit a PL to data. To assess the distribution fit, they suggest calculating the Kolmogorov-Smirnov (KS) test statistic. A low value (i.e. a value close to 0) indicates a good distribution fit. However, the distribution fit must be further supported by a semi-parametric bootstrapping procedure based on the KS test statistic. The method yields a p-value where values above 0.1 are considered to be a strong indicator for a PL (Clauset et al., 2009).

Following Shim (2016), the analysis is extended to other possible heavy-tailed distributions, such as lognormal and exponential. Each distribution is fit using the method described above, and every distribution that fits the data well is added to a collection of

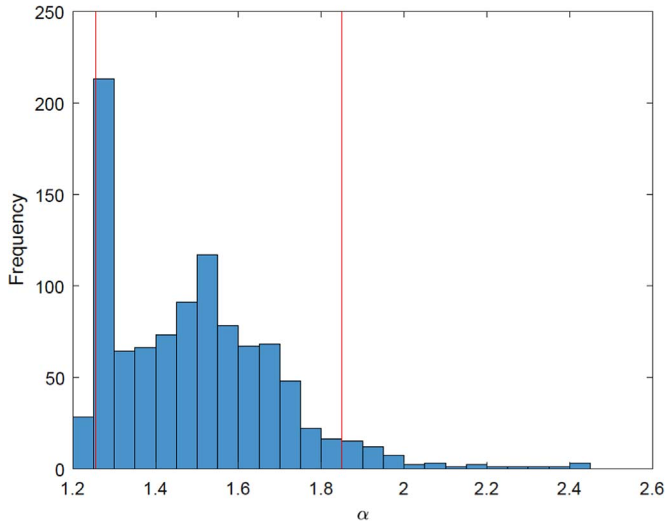

Fig. 1. Histogram of simulation results of distribution parameter (α) for Model 4. Red lines mark the 90% PSPR. Cutting off the top and bottom 5% of values is appropriate.

candidate distributions. Furthermore, a Vuong model comparison test (Vuong, 1989) is conducted on each distribution pair in the collection to check whether some distributions exhibit a superior fit compared to others. If so, the low fit distributions can be removed from the candidate set. A further way to augment the candidate set is to add distributions based on theoretical considerations, which may yield a specific distribution type, or based on expert knowledge. This approach can lead to a range of parameters for the various distributions in the candidate set.

2.2. Step 2 – build a theory-guided simulation

Select one distribution of the candidate collection (Step 1) and a plausible corresponding generative mechanism. Build a simulation model that closely reflects the underlying theory. Unless the simulation reflects the theory appropriately, conclusions about theory from simulation results are invalid.

2.3. Step 3 – run and assess the simulation

We suggest running the simulation at least 1000 times to generate simulation results sufficient to allow a sound analysis of the simulation output. For simulations with fewer than 1000 runs, we suggest an additional graphical check: The histogram of fitted distribution parameters should not exhibit a uniform distribution, but clearly show one or more peaks in frequency (see Fig. 1). If no peaks are present, the number of simulation runs should be increased. The results are then compared to empirical data. If they are in line with each other, the model is validated. However, note that as soon as the model is falsified (e.g. by new data), a new theory is needed.

Two assessments are necessary. First, check whether simulation yields the selected candidate distribution. For this, we suggest fitting the selected candidate distribution to each of the 1000 simulation outcomes. Then, report the average distribution parameter and its standard deviation. Calculate the KS test statistic for each simulation outcome and report the average (e.g. Shim, 2016; Shim et al., 2017). In addition, calculate *p*-values of the semi-parametric bootstrap for each simulation outcome and report the average. Second, compare the specific distribution parameters of the simulation and empirical data. We suggest sorting the 1000 estimated simulation parameters in ascending order. Then, form an interval leaving out the lowest 5% and highest 5% of parameter values, and retain 90% within the interval. We call this interval the *90% possible simulation parameter range* (90% PSPR).

2.4. Step 4 – validate the results and refine if necessary

Finally, check whether the empirical distribution parameter (obtained in Step 1) falls within the 90% PSPR. A result within this range offers strong support that the simulation explains the empirical data appropriately. Otherwise, the model has to be rejected because it does not reflect the empirical data sufficiently. In this case, refine Step 2 and repeat Step 3 until the simulation (and thus the model) is validated.

2.5. The PSPR

The PSPR resembles a confidence interval in a bootstrapping context (e.g. Efron and Tibshirani, 1998). However, strictly speaking, it is not a confidence interval for the empirically estimated parameter. Running the simulation once is not bootstrapping the original data. The PSPR shows in a limited number of simulation runs (here: 1000 runs) the parameter value range the simulation can actually generate. In principle, comparing the empirical parameter to the PSPR compares two different things. However, if the empirical parameter does not lie within the PSPR, the simulation model is unlikely to yield a value like this. Thus, the simulation model itself is flawed. It cannot represent the observed data appropriately, and theory validation has failed.

Excluding more than the top and bottom 5% simulation parameter values, for example to build an 80% PSPR, would reject a model more often since the range into which the empirical parameter can fall would be tighter. Another option would be to exclude fewer values, for example to build a 95% PSPR, or even to include all the values and form a 100% PSPR. However, we advise against doing this. Fig. 1 shows an example histogram of PL parameters from the simulation of Model 4 (see Section 3). Clearly, most values lie within the 90% PSPR, which should be the criterion for picking the value. The graph shows that choosing an asymmetric PSPR could be appropriate, leaving out for example the top 7.5% of values but only the bottom 2.5% of values.

As a marginal note, the PSPR could also be used to compare several validated simulation models based on the same empirical data. In this case, the model with the narrowest PSPR should be selected because it produces more stable results than the other models. Moreover, while the PSPR is influenced by both the input parameters of the simulation model and the number of simulation runs, it is reliable despite these two influences. Regarding the input parameters, we strongly advise researchers to verify and conceptually validate their model (e.g. Heath et al., 2009; Sargent, 2005), since validation directly guarantees a valid PSPR. However, conceptual validation and model verification go beyond the scope of this paper. A sufficiently large number of runs (1000) allows a profound evaluation of the model.

3. Illustrative example

We offer an illustrative example of the four-step method that highlights the importance of applying the method and also shows why neglecting the method can lead to misleading conclusions. The variable used is venture debt (VD) because it was shown to be PL-distributed (Crawford et al., 2015) and it is of general interest to entrepreneurship research.

The data for VD are taken from the second Panel Study of Entrepreneurial Dynamic (PSED II) (University of Michigan, 2017). VD refers to the variable *total amount of business loans*, which is the sum of 13 individually collected variables including different sources of loans, such as loans from venture capitalists, banks, and so on. Since we are not interested in the temporal behavior of the distribution parameters, we focus on Wave F of the PSED II. Wave F contains the latest data and resembles a broad picture of start-ups of different ages that is close to reality when considering the population of start-ups at any given point in time. After some data cleaning, 99 observations remained (Table 1 gives descriptive statistics). The data are highly right-skewed and exhibit heavy tails. Not surprisingly, a KS test for normality is rejected.

3.1. Illustration of Step 1 – analyze the data

Results of the data analysis are shown in Table 1. We first fit a PL to the data according to the method suggested in Clauset et al. (2009). The fitted distribution parameter is $\hat{\alpha} = 1.75$. The KS statistic is very low at 0.08, indicating a good distribution fit. The *p*-value of the semi-parametric bootstrapping method is 0.45 (we used 1000 repetitions for bootstrapping). The fraction of points in the tail of the distribution n_{tail}/n (i.e. the points x with xmin ≤ x) is 38.4%, which is quite high. Hence, the PL exhibits a good fit to the data and is added to the collection of plausible candidates.

Following Shim (2016), we take the analysis further and additionally fit a lognormal distribution to the data because more than one distribution could be plausible. The fitted parameters of the lognormal distribution are $\hat{\mu} = 10.77$ and $\hat{\sigma} = 2.12$. The lognormal distribution yields a low KS test statistic value of 0.05 and a high bootstrapping *p*-value of 0.50. Hence, the lognormal distribution is also plausible and joins the collection of candidates.

Furthermore, we employ a Vuong model comparison test (Vuong, 1989) to check whether one of the distributions yields a better fit. The test is not significant (test statistic: + 0.09) and thus we cannot decide which distribution fits better. Hence, both power law and lognormal distribution remain in the collection of candidate distributions.

At this point, it is possible – and also advisable – to consider even more distributions for the candidate collection, such as an exponential distribution (Shim, 2016). As mentioned above, it is also possible to include distributions based on theoretical considerations or expert knowledge. However, for simplicity, we focus on the PL and lognormal distributions. Importantly, the analysis in our example was limited to 99 data points owing to the magnitude of the underlying database. As the analysis was conducted for illustrative purposes, the distribution parameter should not be treated as a "stylized fact."

3.2. Illustration of Step 2 – build a theory-guided simulation

To build a simulation, it is important to know which generative mechanism causes which distribution (Mitzenmacher, 2004; Newman, 2005). For example, the lognormal is generated by a multiplicative process. On the other hand, a PL can be generated by, among others, preferential attachment. We focus on multiplicative process and preferential attachment.

We build our first model (Model 1) assuming the lognormal distribution as the true underlying distribution. Thus, we employ the multiplicative process as a generative mechanism. Suppose a growth process in which an individual unit grows or shrinks in each time step according to a random growth rate. Thereby, an important assumption is that the growth rate is independent of the size the individual unit has already reached. If the growth rate follows a normal distribution, over time the multiplicative process yields a lognormal distribution of VD (Mitzenmacher, 2004; Newman, 2005).

Table 2
Simulation results.[a].

Setting	Model 1	Model 2	Model 3	Model 4
Distribution	lognormal	PL	PL	PL
Mean (STD) parameter	$\overline{\mu}$ = 20.73 (0.08)	$\overline{\alpha}$ = 4.95 (1.16)	$\overline{\alpha}$ = 3.21 (1.88)	$\overline{\alpha}$ = 1.49 (0.20)
	$\overline{\sigma}$ = 2.48 (0.05)	$\overline{n_{tail}/n}$ = 14.6%	$\overline{n_{tail}/n}$ = 9.0%	$\overline{n_{tail}/n}$ = 33.0%
90% PSPR	$[20.60; 20.85]_{\mu}$	[3.46; 7.03]	[1.78; 6.82]	[1.26; 1.85]
	$[2.40; 2.57]_{\sigma}$			
Average KS statistic	0.02	0.06	0.11	0.06
Average *p*-value	.48	0.29	0.24	0.24

[a] Overall, the average KS statistic and average *p*-value from the bootstrapping method show a good fit for the respective distribution type. However, looking at the 90% PSPR of the simulation results, clearly the empirical parameter lies only within the range of Model 4. For Models 1, 2, and 3 the parameters of the data do not lie within the respective 90% PSPRs.

3.3. Illustration of Step 3 – run and assess the simulation

Model 1 is run in a Matlab simulation of 1000 start-ups over 120 periods corresponding to 10 years. Thus each period represents one month. Each start-up has a starting VD value that is the mean value of the VD in Wave A of the PSED II (which is the first wave recorded). In each period for each start-up, we draw at random a multiplicative factor that is multiplied to the current VD of a start-up yielding a decline or increase in VD. The range of multiplicative factors that can occur is determined from the VD increases and decreases in the PSED II data. Since the PSED II contains yearly data, we took the 12th root of the empirically determined VD range and ran the simulation 1000 times. A similar simulation has been used for employee and revenue variables in start-ups (Shim, 2016).

The crucial point of our method is to now adequately assess the simulation outcome – first by assessing the general distribution fit and second by comparing the specific distribution parameters of both simulation and empirical data. Table 2 reports our simulation results. The average KS test statistic of the 1000 simulation outcomes of Model 1 is 0.02. We employ the semi-parametric bootstrap to each simulation outcome and obtain an average *p*-value of 0.48. Thus, on average the simulation seems to reflect the predicted lognormal distribution well.

Previous research has stopped the assessment at this point and in this case would have concluded that the lognormal distribution would suit the data. However, comparison of the specific distribution parameters demonstrates that lognormal distribution of data and simulation do not coincide. Our proposed 90% PSPR resolves this issue. The 90% PSPR for μ is [20.60; 20.85] and the 90% PSPR for σ is [2.40; 2.57]. Since the empirical parameters lie outside these ranges, Model 1 cannot be validated. This example shows that the method we suggest helps to avoid misleading conclusions.

3.4. Illustration of Step 4 – validate the results and refine if necessary

As Model 1 cannot be validated in Step 3, we need to refine the simulation. Step 3 suggests that the multiplicative process might not be the underlying mechanism of the observed phenomenon. Thus, the developed theory should consider another generative mechanism. In our example, we replace multiplicative process by preferential attachment. Keep in mind that preferential attachment will cause a PL and not a lognormal distribution (Mitzenmacher, 2004; Newman, 2005).

Preferential attachment is a generative mechanism that can be observed in complex networks. Based on growth of the network, new edges between nodes are added every period. Compared to nodes with a low degree, nodes with a higher degree have a stronger ability to generate new edges. Thus, preferential attachment induces a rich-get-richer phenomenon within a growing complex network (Barabási et al., 1999). The new simulation model based on preferential attachment is called Model 2.

We implement Model 2 in a simple Matlab simulation. Again, there are 1000 start-ups and the number of simulation periods is 120, resembling a 10-year horizon. Model 2 contains one venture capitalist as a source of VD. The 1000 start-ups and the venture capitalist represent nodes in a network. At the beginning of the simulation, each start-up has one common edge with the venture capitalist. In each period, a random number of edges is added from a start-up to the venture capitalist, thus granting more VD. The amount of VD added is derived from the PSED II data. Start-ups that have accumulated more edges over time have a higher probability to establish new edges to the VD source. Again, the simulation is run 1000 times to generate a reliable 90% PSPR. The VD granted per edge is randomly drawn in the simulation.

Table 2 reports the simulation results. The average ratio of n_{tail}/n is at 14.6%, which means that on average, 146 of the 1000 simulated start-ups have a VD in the tail of the distribution (i.e. their VD is higher than xmin). The average KS statistic and bootstrapping *p*-value are 0.06 and 0.29, respectively, showing a seemingly good model fit. As with Model 1, comparison of the specific distribution parameters is crucial, because it reveals a different picture. The empirical parameter $\hat{\alpha}$ = 1.75 lies far outside the 90% PSPR of [3.46; 7.03]. Thus, we again reject Model 2.

We now repeat Step 4 and refine the assumptions of the underlying theory. For example, in Model 2 we did not account for the fact that in reality some start-ups are older than others. Older start-ups have had more time and, thus, a greater chance to accumulate VD.

In fact, another form of preferential attachment accounts for the factor *age* (Barabási, 2002). In this other version of preferential attachment, both the edges and the nodes of the network can grow. The new simulation model, based on another form of preferential attachment, is called Model 3. Instead of 1000 start-ups, the simulation now starts with 50 start-ups. During a simulation run, every 6 periods (corresponding to 6 months) 50 new start-ups enter the model. Thus, we try to enhance the rich-getting-richer effect by introducing a start-up age component into the simulation.

Table 2 shows the simulation results. The average n_{tail}/n ratio is low at only 9%. The ratio is low because some start-ups enter the model late. These start-ups are unlikely to attract VD. Thus, they remain around their initial VD value (which is below xmin in all cases). However, the average KS statistic of 0.11 and the average bootstrapping *p*-value of 0.24 still show a satisfying distribution fit. For Model 3, the 90% PSPR of [1.78; 6.82] comes close to the empirical parameter. However, the empirical parameter does not lie within the 90% PSPR and Model 3 has to be rejected.

We again repeat Step 4. This time, we take a different route and combine multiplicative process and preferential attachment into one simulation, similar to Shim et al. (2017). We call this Model 4. We take Model 3 and add a multiplicative process to it. Now, the simulation accounts for two generative processes: start-ups can establish new links to the VD source, and VD is multiplied by a random factor in each period. Table 2 summarizes the simulation results. The average n_{tail}/n ratio is at 33%, which means that on average, a substantial number of start-ups are in the tail of the distribution. The average KS statistic and average *p*-value of 0.06 and 0.24, respectively, again show a good overall distribution fit.

This time, the 90% PSPR of [1.26; 1.85] covers the empirically determined parameter. Fig. 1 shows a histogram of the fitted simulation parameters. Clearly, the bulk of simulation parameters lies within the 90% PSPR (red lines). Thus, our four-step method is completed because the simulation is validated by the empirical data.

We end our illustrative example with two further remarks. First, every time a researcher collects new empirical data, the validation of a model has to be repeated. For example, new data could yield different distribution parameters or show a different distribution than previously assumed. Second, we assume – in concordance with Shim et al. (2017) – that a combination of multiplicative process and preferential attachment causes a PL distribution. However, to our knowledge, a mathematical proof for this is missing.

4. Discussion and conclusion

This study enhances simulation-based theory development in entrepreneurship as described in prior work (e.g. Shim et al., 2017; Shim and Bliemel, 2017). We emphasize that the method presented should be combined with other validation methods. Specifically, to yield valid results, the conceptual validation of a simulation model must be established prior to using the PSPR. Moreover, we have applied the PSPR in an illustrative example only. Hence, we encourage future research on entrepreneurial theory development to apply and assess the PSPR in an actual research project.

This paper contributes to current knowledge on heavy-tailed distributions in entrepreneurship research by introducing a method (PSPR) to compare simulation results to empirical data. The purpose is to reduce the gap in existing literature with respect to the validation process of novel theory. We demonstrate the usefulness of our method with an illustrative example of the variable VD. We encourage researchers who develop new theory based on simulation to consider the proposed method to avoid misleading conclusions.

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Declaration of interest

None.

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