dissertation_writeup_draft

Alassane Ndour

23/08/2019

1 Introduction and Objectives

1.1 Background to the problem, Choice of project and beneficiaries

Growth model selection is a large literature in many domains which often takes into account the specificity of the subject matter. For instance, in biostatistics, bioassay data can be modeled using different logistic like functions (e.g. 4PL or 5PL) [CITATION] that are tested against each other. Generally, model selection is a basic scientific requirement that answers what functional form a set of data corresponds to. There are differrent requirements for a function to be chosen in a selection problem such as the simplicity of the model (Occramm's razor states that the simpler model should prevail), the estimation of parameters or even the "certainty" of the selection. For instance, in economics different models can be tested against each other to verify how well they explain GDP growth[CITATION]. In such a case, the main requirement of the models is interpretability as it is required for policy making. In contrast, for prediction interpretability of neural nets for example is not always necessary. Naturally, depending on the use case, it is crucial to select the best functional form as the real one is often unknown, and a wrong selection invalidates any following inference (Nguimkeu, 2014).

Most domains use statistical foundation to select models. It is often done comparing the relative likelihood that the data's underlying generating process was given by a model[CITATION]. This is a well known and documented problem. However, there is a specific context that is not tackled often by the current literature : if one were to classify a large pool of different datasets according to the functional form each one of them follows given a set of known functional forms, how would one go about it? This classification problem was posed here by our commercial partner and is the subject of matter. Therefore, by comparing several relevant model selection strategies, this project aims to obtain a growth model classification method that by construction classifies datasets accurately but also demonstrates the uncertainty level by which it is doing so and provides the estimated parameters.

The project was chosen for its application in a wide variety of domains as well as its relevance for the specific use case brought forth by our commercial partner. This analysis will therefore aim to contribute to the literature of model selection by offering an experimental evaluation of several model selection processes. Furthermore,it can also be used as a base for the commercial partner's model evaluation.

- [IF TIME PERMITS] Contribution to literature as unexplored method - combination of Bayes factor and Harris paper

1.2 Objectives, metrics and broad methods

The aim of the project is to construct a dataset classification method that can accurately identify the functional form the dataset is following. The challenge of this task arises when the dataset to be classified is noisy and the ratio of signal to noise weakens. Consequently, it is essential for the classification to be able to detect any underlying patterns in a noisy setting. Thus a large part of the study will focus on how well the classification performs as the noise increases. Ideally, the classifier will can quantify the noise level for a given dataset. Furethermore, our model should offer an estimation that identifies its classification "certainty" and an estimation of the parameters of the model. Finally, as the selection process must scale to a large amount of datasets, we record the computation cost of each method and will favour a less expensive but accurate classifier.

Section [methodology] provides more details on the methodology used. Here we offer a brief overview of the ways the classification task was handled. There are broadly speaking two ways of thinking of how one

might choose a model: a frequentist one which aims to compute a statistic on the data for which we know the distribution [citation] and a Bayesian approach which compares the posterior of different models using methods such as Bayes factor. Here we apply both views on a generated dataset and compare using the criteria described above.

- Furthermore, there have been interesting developments in combining Bayesian methods and cross validation as they are not mutually exclusive methods and can contribute to robust estimates. Such works include Bürkner et al. (2019) where the authors aim to improve upon leave-future-out cross-validation (LFO-CV) - an adaptation of leave-one-out cross-validation (LOO-CV) to timeseries - to reduce computation time.

2 Context and relevant literature

The analysis carried out in this project has two fundamental building blocks which are data simulation and model selection strategies. For this reason relevant literature on both these topics will be presented in this section.

2.1 Data simulation contextual elements

Data simulation simply refers to the process of generating random numbers from a distributional statements. It a common statistical technique to understand or forecast phenomenons that might occur in observational data, all so in a controlled context. Kery and Royle (2016) provide an insightful outline of the advantages of simulations. Here we highlight some of them as these were the principle reasons for simulations used in this study. According to them data simulations allow researchers to know the truth behind the data, in a parametric context for instance. This is partucularly important as the researcher has less insight on the internals of certain black box algorithms. The authors point out that having knowledge of parametric values before applying a Markov-Chain Monte Carlo (MCMC) simulation as is done in the present study, is necessary as it confirms that the simulation is not going astray. Additionally, it can be noted that MCMC by nature is a simulation and represents a corner stone of Bayesian statistical techniques (Gelman) therr gain emphasizing its importance. Kery and Royle (2016) also highlight that simulations help calibrate model parameters. More generally, it can added that simulations have also been used in order to study, compare and contrast particular models in many fields. For instance in Ploeg et al (2014), the authors study the effect of small sample size on different modelling techniques in patient survival rates; the data they use was simulated based on observed data. In Murari et al. (2019) the authors compare different information criteron in model selection problems using simulations. These examples not only show that simulation is present in many domains but also serves as a solid control to study intra and inter model specificities. Finally, Kery and Royle (2016) also point out that simulations allow researchers to include errors that can then be accounted for and studied as one should do with obersved phenomenon. This principle is important in our context and can be illustrated by Harris (2015) who use Bayesian techniques to account for sampling errors in a simulated dataset.

Although, simulation is undeniably an important and effective tool in the researchers aresenal, it must be noted that there exist different forms of data simulations. Since this research project originally stems from biological literature, examples in biology and biostatistics will be emphasized here. Broadly speaking simulation methods can be divided between Simulation Optimization methods and algebraic methods as described by Amaran et al (2015). The former refers to techniques used to optimize stochastic simulations that cannot be described algebraically. These are more black-box type simulations and can be found in projects such as Montagna et al (2015) which proposes a framework to optimise parameters in biological system development simulations. It can be stated that these models are very powerful in very specific settings anc can lack generalisation as pointed out by Fu et al (2000). In contrast algebraic solutions are more general but it cannot explicitly tackle more precise stochastic tasks. For instance, we know that population growth in ecological studies follows a logistic growth process (Brimlow et al. - 2013). This is a general result and observed data can be seen to fit this pattern as demonstrated when Buehler et al. (1991) adapt logistic growth functions to take into account the human activity impoact on the bald eagle population in the US. However, to model stochastic differential equations as is necessary in the seperation of DNA molecules (Cho

and Dorfman - 2010), stochastic simulations are necessary. In this study since generalisation was necessary the algebraic route described in section Data was taken.

CAN USE Sigman (2010) for inverse transform method to create data and can discuss tools in python - https://www.biorxiv.org/content/biorxiv/early/2017/12/21/088773.full.pdf - Morpheus and CompuCell3D - logistic regression for shape of population : QuantitativeConservationBiology - https://www.nature.com/scitable/knowledge/library/an-introduction-to-population-growth-84225544/ - https://www.sciencedirect.com/science/article/pii/S0888754383711808 * Ed Harris

2.2 Model selection contextual elements

The second building block of this research is statistical model selection which refers to the the step of selecting the most appropriote statistical model among a set of candidates for a given dataset (Ding et al - 2018). This can be diffentiating the number of regressors usind in a linear regression or selection the type of neural network to use. This step is performed in an array of domains: in ecological science where researchers use mark-recapture (marking an animal and recapturing in a latter period) in order to estimate the population and survavability probabilities of a species they make multiple statistical models compete and use the best for inference (Johnson et al - 2004); in cosmology, researchers make models whose parameters have been estimated compete to describe phenomenons such as the geometry of the expansion of the universe (Liddle et al. - 2006). Therefore the overarching importance of model selection is not contested; as pointed out by a Nguimkeu (2014) a wrong statistical selection invalidates any following inference. In addition to selection, as pointed out by Claeskens and Lid Hjort (2010), model averaging is a closely linked problem as researchers might wish to combine relevant competing models. Even though model selection's value is not contested it remains an open problem in statistics that often requires the combination of multiple methods. Furthermore, within the literature there are different ways of approaching the selection problem. Dormann (2018) outlines the schools of thought that are prevalent in model selection and averaging issues. This discussion is very relevant to understand and compare the different paths available.

On one hand, empirisits base model selection on the data. Their methods have proven effective and are extensively present in the machine learning literature [citation]. Popular methods in this line of thought include selection using algorithms such as cross validation (Allen, 1974; Stone, 1974; Geisser, 1975) or bootstrp aggregations. These methods are often computationally more expensive than others but have proven very effective (Dormann - 2018) leading them to have prominent supporters such as Lambert (2018) or Bishop (). In general the algorithms in this school of thought repeatidly and consitently sample data points and then compute an average metric based on the samples or use more brute force methods such as grid searches. [PLAN AND FINISH]

Intro : * what is model selection, why is it useful? * link to model averaging - Claeskens and Lid Hjort (2010) + Dormann (2018) * 3 types of model selection frameworks : - Empirical methods : Cross validation - Information Criterion - Bayesian model selection -combining these methods

- LOO-CV
- Bayesian books
- Bürkner et al. (2019)
- Claeskens and Lid Hjort (2010) (Model selection)

3 Data

The data used in this project was generated data. There are several practical and methodological reasons for doing so. First, methodogically, generating data makes sense: as advised by Kéry and Royle (2016) as this offers a ideal control environment under which parameters and hyper-parameters are known. Furthermore, in growth cell literature, from which this project stems (e.g. Harris et al. (2016)) synthetic data is standard practice. Second, data from the commercial partner that was meant was to be analysed here was unavailable due to legal restrictions and no open source equivalents were found. As the synthetic data is at the heart of the analysis this section will describe in greater detail the data meant to be mimicked and the process and tools used to do so.

The type of generated process in this project is similar to a cell counting process proposed by Morpheus or CompuCell3d with certain restrictions posed by the commercial partner's contextextual information which led to custom data generation. The restrictions posed by the commercial partner were as follows :

At any time x we must be able to estimate the number of a given cell count. We have knowledge of the growth function that the cells take (i.e. $f(x)$). We also know that introducing an agent in our cell sample alters the growth path that the sample follows to another process (say $g(x)$). Given this information, we should be able to obtain the number of cells for any given time on the condition that we have knowledge of the presence or absence of the agent. However, if we do not know if the agent has been introduced in the sample then we must choose whether we estimate the numbers of cells using $f(x)$ or $g(x)$ based on the count. At this point, a simple model selection is sufficient to capture the correct model or even combine the two models if necessary. However, the primary difficulty with this is that the counting process is subejct to a large amount of noise. Therefore, the problem at hand is to find the ideal model selection method under noisy conditions. In this case, the ideal model selection would favour a growth function that is able to identify the true growth process along with the corresponding parameters. Furthermore, it is interesting for the researcher to be able to jauge the uncertainty surrounding the selected model and its parameters. Note that the growth functions ($f(x)$ and $g(x)$) were not avaible and we therefore made simple assumptions to create them.

Within this context, the data generated was meant to mimic a growth process through time in which x represents the time through which the count y increases. To bound the problem the count was generated and then normalized (min-max normalization). Therefore we have :

$$x \sim U(0, 1000)$$

$$y \in [0, 1]$$

Although the normalization is clearly not realistic, it is ideal to bound the problem and does not undermine generalisation.

The two growth functions used to generate the data were a simple linear function (1) and a logistic function (2) of the following forms :

(1) $f(x) = \alpha + \beta \times x$

where α is the intercept and β the the coefficient of x and :

(2) $g(x) = \frac{L}{1+e^{(-k(x-x0))}}$

where L describes the maximum value the curve could take, k describes the growth rate of the logistic function and $x0$ represents the sigmoid's midpoint.

For all these parameters, the following values were uniformly drawn :

- $\alpha \sim U(0, 0.05)$
- $\beta \sim U(0, 0.2)$
- $L \sim U(0.9, 1.1)$
- $x0 \sim U(\frac{max(x)}{4}, \frac{3max(x)}{4})$
- $k \sim U(0.5, 2)$

In order to simulate the noise in the problem and analyze it in a coherent manner different levels of additive Gaussian errors were introduced. The Gaussian errors all had a mean of 0 and a a variance σ ranging from 0.1 to 1 by intervals of 0.1. In the following discussion we refer to each of these noise levels as noise buckets. Each noise bucket was comprised of 100 synthetic datasets. To generate the data, custom `numpy` based functions were created and caleld. The meta-data regarding the created dataset was stored along with the data in nested `pandas` dataframes.

To understand the robustness of any of the selection processes used, we add to the generated data a drift which distorts the growth functional. The drift was added to a rescaled dataset and and was unifomly distributed $drift \sim U[0.5, 1]$. From the synthtic data we record the x and y values (which are reffered to as the datasets) as well as the label (i.e. "linear" or "logistic"), the set of corresponding parameters and the

	dataset	parameters	noise_bucket	label	drift	x_array	y_array
23	[[0.564986417530553, 0.0], [0.1735136232889022...	{'x0': 535, 'L': 0.9165705331270448, 'k': 0.87...	0.4	logistic	True	[0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, ...	[0.564986417530553, 0.17351362328890227, 0.004...
90	[[0.4539524019419308, 0.0], [-0.29480440010406...	{'a': 0.028578324371486965, 'b': 0.16309959331...	0.2	linear	False	[0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, ...	[0.4539524019419308, -0.2948044001040612, 0.24...
79	[[0.05050089184510416, 0.0], [0.16100597714613...	{'x0': 73, 'L': 1.0116239241653049, 'k': 1.888...	0.1	logistic	True	[0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, ...	[0.05050089184510416, 0.16100597714613477, -0....
66	[[0.034405760571275416, 0.0], [-0.399020420328...	{'x0': 78, 'L': 1.0883084162085814, 'k': 0.860...	0.2	logistic	False	[0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, ...	[0.034405760571275416, -0.399020420328 4269, -0...
15	[[-0.47752743748456006, 0.0], [-0.589150730187...	{'a': 0.016564631720453717, 'b': 0.03606739348...	0.4	linear	False	[0.0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, ...	[-0.47752743748456006, -0.5891507301879397, -0...

Figure 1: Sample of data used in tabular format

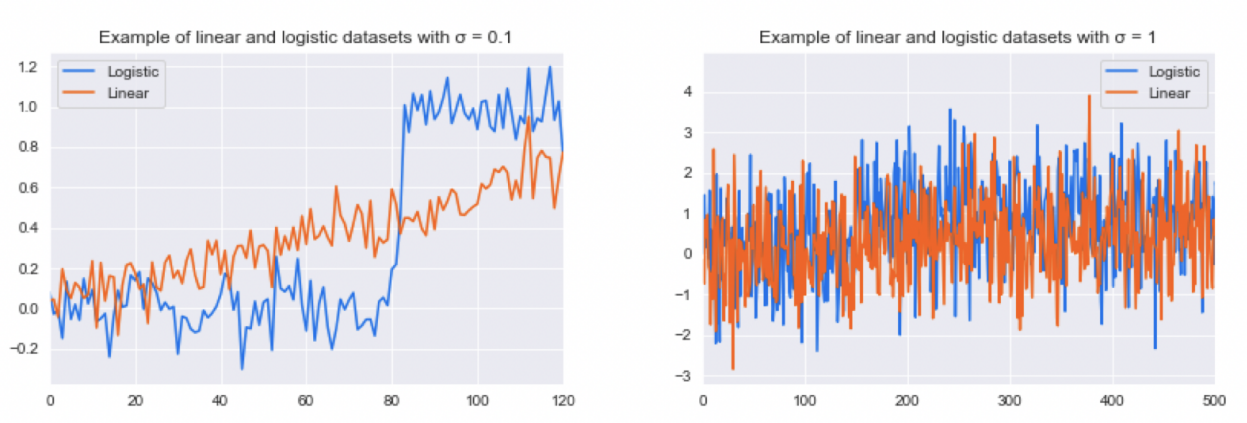


Figure 2: As noise increases the underlying process becomes harder to spot

associated noise bucket. A subset of the data used is presented in figure ... to provide clarity on the data used.

To clarify the problem we face in the selection process, figure ... illustrates the distortion that occurs as we increase the noise in the data. The grphic on the left shows very little noise (smallest noise bucket in the data). Here one could easily eyeball the functional form associated to each dataset. However, the figure on the right demonstrates that as we add noise in the data this task becomes less evident and requires a methodological selection process.

4 Methods

This section describes the different estimation strategies used for model selection. To compare how well the different methods performed, we look at how well the datasets are classified as well as how confident the method is in the classification. Furthermore, as the systematic error and the parameters are of interest, we also focus on the estimated parameter values for different noise levels as well as the estimation of the error itself when possible. Finally, the time/complexity required for the estimation is also an important aspect of the study. To structure this discussion we first focus on selection strategies that are more often regarded as Frequentist methods [describe more] and then we highlight Bayesian model selection processes.

4.1 Frequentist model selection

As discussed in section ... there are a battery of different methods to perform model selection, some of which shall be used in this study. However, before performing any selection it is important to estimate our models.

Fitting the models to the data or curve fitting refers to the process of obtaining a mathematical function that can approxite a data. There are many approches to solve such a problem but a common one is to solve the least square problem shown in formally shown equation.

$$\min_{\theta} \sum_{n=1}^{N} (y_n - \hat{y}(\theta, x))^2$$

where $y(\theta, x)$ is $f(x, \theta)$ or $g(x, \theta)$ depending on the functional form chosen and θ is the vector of parameters. Least square aims at minimizing the sum of the distances between the fitted curve and the data points. Here a noticable difference has to be noted between a linear functional form and a logistic one: The former represents an unbound problem whereas the logistic function is by contruction bounded. This implies that different algorithms must be used in order to solve apply curve fitting to the two functions.

- (i) Solving the linear least square problem : Solving the linear regression problem is straightforward and a commmon result. As such the details of solving it are not expanded on here. If needed, readers can refer to [add reference].
- (ii) Solving the bounded non-linear least square problem : To solve the logistic curve fitting problem, we employ the Trust Region reflective algorithm which given bounds subsets the region of the objective function (in this case the equation ...) and gradually expands it each time an adequate model fit is obtained. In our case, the normalization of the data was key as the bounds given to the algorithm were [0,1]. Taking a step back from the synthetic data framework, in general binding the problem with known bounds makes sense as researchers would normally have an idea of the growth they are evaluating and can often determine an upper and lower limit of the growth process.

Both (i) and (ii) were solved using `python`'s scientific library `scipy`.

Once each of the datasets were fit with a logistic and a linear regression, the model selection process can take place. We use a panel of different selection metrics and evaluate as a first priority how well each of these perform in terms of dataset classification and the computation time they require.

MSE, MAE - naive approach

We begin with a naive apporach to model selection by using the Mean Squared Error (MSE) and the Mean Absolute Error (MAE - defined as the average absolute value of the error). We do so as these are popular metrics in empirical data work. Both of these evaluate the average error that the model prediction would generate and are naturally meant to be minimized. Therefore a dataset is classified as linear if the MSE/MAE of the linear model is lower than the MSE/MAE of the logistic model (and vice-verca). However, we only use these metrics as a starting point : MSE and MAE are not the most suitable for selection outside of a cross valiadation [REF] process as they do not take into acount any model complexity. A model with more parameters will by construction tend to cause less error but can break the rules of an appropriate model which aim to make a selection which would not overfit and is as simple as necessary (i.e. Occram's razor) [REF]. With this in mind we use information criterion which are more appropriate tools here.

BIC, AIC, and entropy enhanced BIC and AIC

In order to penalize the complexity of a model the most popular metrics used are the Bayesian Information Criteria (BIC) and the Akaike Information Criteria (AIC). They both aim at estimating the likelihood of a model to predict future values [science_direct_ref] while balancing the benefit ofa good fit with the model's complexity. They are defined as :

$$AIC_a = -2ln(L) + 2k$$
$$BIC_a = -2ln(L) + 2ln(N)k$$

where L is the likelhihood of the model, k is the number of parameters and N is the sample size. These measures are meant for selection problems such as the one at hand. However in empirical work as the

likelihood is often difficult (if not impossible) to obtain, workarounds exist (often by making assumptions on the error term's distribution) such as the one applied here where using the `RegscorePy` package :

$$AIC_b = N \times ln(MSE) + 2k$$
$$BIC_b = N \times ln(MSE) + k \times ln(n)$$

This is done because the MSE is an estimate of the variance of the error and since the error has mean 0, given a constant that can be dropped (since we compare Information Criteria on the same samples) we can replace the likelihood by the MSE. Regardless of the minor definition changes, the rule for model selection using AIC/BIC is to make a decision based on the lower Information Criteria value. Therefore a similar classification rule as the MSE/MAE can be applied here. Since the problem at hand is to make appropriate model selection choices with respect to different noise levels in the data we make an addition to our Innformation Critirea suggested by Murari et al. (2019). In their research, Murari et al. (2019) demonstrate that including Shanon Entropy into the BIC and AIC can enhance the criteria, especially when the data is subject to a high amount of noise. The reasoning to this is holding everything else constant models which have a more uniform ditribution of error should be favoured because for a perfect model, noise would only be coming from the data. To quantify the degree of uniformity of the error, Entropy is added by the authors in the following manner :

$$BIC_c = N \times ln(\frac{\sigma_e^2}{H}) + k \times ln(N)$$
$$AIC_c = N \times ln(\frac{MSE}{H}) + 2k$$

where σ_e^2 is the variance of the error and H is the Shanon entropy. Using our definition of BIC and combining it with Murari et al. (2019) we have :

$$BIC_H = BIC_b - Nln(H)$$
$$AIC_H = AIC_b - Nln(H)$$

which we estimate in this work since model selection in low signal to noise ratio is the subject of study. Note that we can safely meet the assumption or error normality of Murari et al. (2019) by checking the distribution of the errors. One such check is presented in figure ...

This work also serves as an extension of Murari et al. (2019) since the authors concluded that comparing their entropy enhanced AIC/BIC should be compared to Bayesian selection approaches which we shall do in this study. The main pacakges used in this part of the analysis were `RegscorePy` along with custom `numpy` functions.

χ^2selection to estimate uncertainty

In order to have a test that better quantifies the degree through which we select one model over another, a hypothesis test is required. In a frequentist context, to do so the goal is to calculate a statistic that relates to a distribution of which we know the properties. In our case, we choose a χ^2 distribution. This part of the discussion follows VanderPlas (2014) who describes model selection using χ^2 model selection process. We assume that the errors are independent and normally distributed which would mean that the normalized sum of errors follows a χ^2 distribution. As outlined above, this assumption is not too strong for most of the fitted models and holds particularly true as the signal to noise ratio increases. Thereon we compute the χ^2 statistic which is the normalised sum of errors and follows a χ^2 distribution with the degrees of freedom related to the number of parameters in the model. From there we can obtain the χ^2 likelihood (by referring to the values in distribution table). This number can be interpreted as the likelihood of observing the error values given our model.

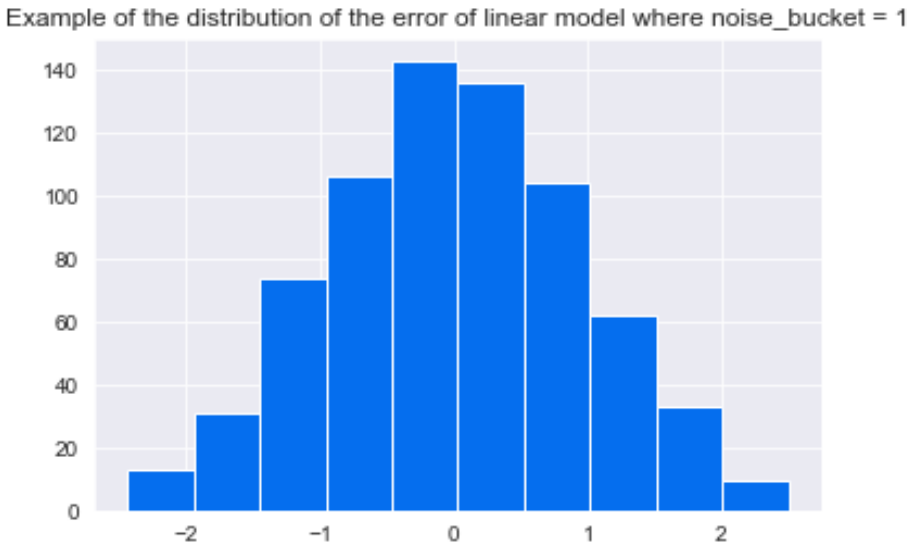


Figure 3: The assumption of normality of error has been checked - it is not a strong assumption in this case

This selection methodology is a useful addition to the methods outlined above because it can quantify the certainty of the classification made using hypothesis testing : by formulating a hypothesis and testing it on the difference of the χ^2 likelihoods as demonstrated by VanderPlas (2014). The only necessary condition is that the models must be nested which is the case here as we can write :

$$g(x) = S(f(x))$$

where :

$$S(u) = \frac{L}{1 + e^u}$$

and $\beta = -k$ and $\alpha = kx_0$.

Thesefore we could formulate our null hypothesis as the data following a linear generating process and find the p-values related to $\chi^2_f - \chi^2_g$.

It is noteworthy to mention that there are there may be in caveat in this process : Adrae et al (2014) point out that noise and non-linearity may adverserly affect a χ^2 test. These results should be kept in mind for interpretation. The computations were done using `scipy`'s `stats` module.

4.2 Bayesian model selection

Other cases in the literature use Bayesian approches to estimate models and the corresponding parameters. This methodology is more complex to implement which often hurdles practionners. Here we provide an overview of a Bayesian approach and the parameter settings used in this study.

As in the frequentist section we first contextualize and estimate the model before outlining the selection process. In general, a Bayesian model contains a set of parameters (and hyperparameters) θ. In the case of the logistic form $\theta = \{L, k, x_0, \sigma\}$ and for the linear model $\theta = \{\alpha, \beta, \sigma\}$. The modelling goal is to obtain the probability distribution of θ given the data (i.e. $P(\theta|D)$). Equation ... provides the standard Bayes rule approximation where D is the data, the right hand side is the posterior, the first term on the left hand side is

the likelihood and the second one is the prior.

$$P(\theta|D) \propto P(D|\theta) \times P(\theta)$$

One particularity with a Bayesian model is that the prior distribution assigned to the parameters plays a crucial role in the obtained model. In our case, this set of priors is considered : bounded flat priors (i.e. the values of the parameters are uniformly drawn within given bounds) for the parameters and a Gaussian prior for the nuisance hyperparameter (σ). Different bounds were tried but as our expectation in a growth model is positive growth with our count unable to be negative, the largest bounds chosen were all positive real numbers. These priors are similar than those used int the literature and are quite general similarly to Harris (2015) these priors can be seen as uninformative. Note that flat priors are not ncessarly uninformative and Jeffrey's prior can also be used (they were also tried in certain experiments here). As posterior distributions are difficult to express analytically, as generally done in Bayesian problems we turn to Monte Carlo Markov Chain (MCMC).

MCMC is a numerical simulation that samples data from a given distribution where each future chain is only dependent on the present and not on all past chains. In our context these simulations are important as convergence of MCMC to the target distribution is a known result and by sampling enough data points from the posterior we can estimate it. The parameters required to run the MCMC simulation consists of the number of "walkers" (the number of chains used), the "burn-in" amount (the number of steps to to discard from each chain) and the number of points sampled per chain. These parameters were set according to guidelines from documentation.

To implement MCMC, different `python` packages were tested: although `PyMC3` was the first option due to its popularity in the `python` community, it was too computationally expensive for the task at hand – it seems better suited when the number of datasets is small. Instead, the package `emcee` was used. `emcee` is an implementation of Goodman & Weare (2010)'s affine-invariant ensemble sampler for MCMC. It proved quick and reliable in the tests conducted likely due to the fact that it is written originally in `python` which speeds up sampling and compilation process. To use `emcee` well, it is important to express the posterior in log form. Hence equation ... we have :

$$log(P(\theta|D)) = log(P(D|\theta)) + log(P(\theta))$$

We then assume that the data is independently and identically distributed and following $y \sim N(\hat{y}(\theta, x); \sigma^2)$. Therefore the log-likelihood function is given by :

$$log(P(D|\theta)) = -\frac{1}{2} \times \sum_{i=1}^{N} log(2\pi\sigma^2) + \frac{(y_i - \hat{y}(\theta, x_i))^2}{\sigma^2}$$

The flat prior terms are set as $log(P(\theta)) = 0$ for all positive parameters in θ. Note that σ represents the noise parameter - sometimes called the nuisance parameter and is also estimated here. One of the advantages of a Bayesian model is that parameters are obtained as distributions which allows us to make decisions on the prefered model in different ways and model uncertainty more accuratly. Furethermore, plots such as ... to verify parameters spaces and distributions can be made when closer inspection is required.

Once a posterior is estimated for each model, classifications can be made using model selection techniques.

Bayes factor : Classic Bayesian model selection

One commun selection method in Bayesian approaches is to calculate Bayes factor (BF) and use the table described by Raffety(1995) to select the better model. BF is described as calculated as the ratio of the likelihoods for different models. For instance, if we define our hypothesis that the data D is generated by $f(x)$ as H_0 and the alternative H_1 that the data is generated by $g(x)$ then Bayes factor is defined as :

$$BF = \frac{P(\theta_{H_0}|D)}{P(\theta_{H_1}|d)} \times \frac{P(\theta_{H_0})}{P(\theta_{H_1})} = \frac{P(D|\theta_{H_0})}{P(D|\theta_{H_1})}$$

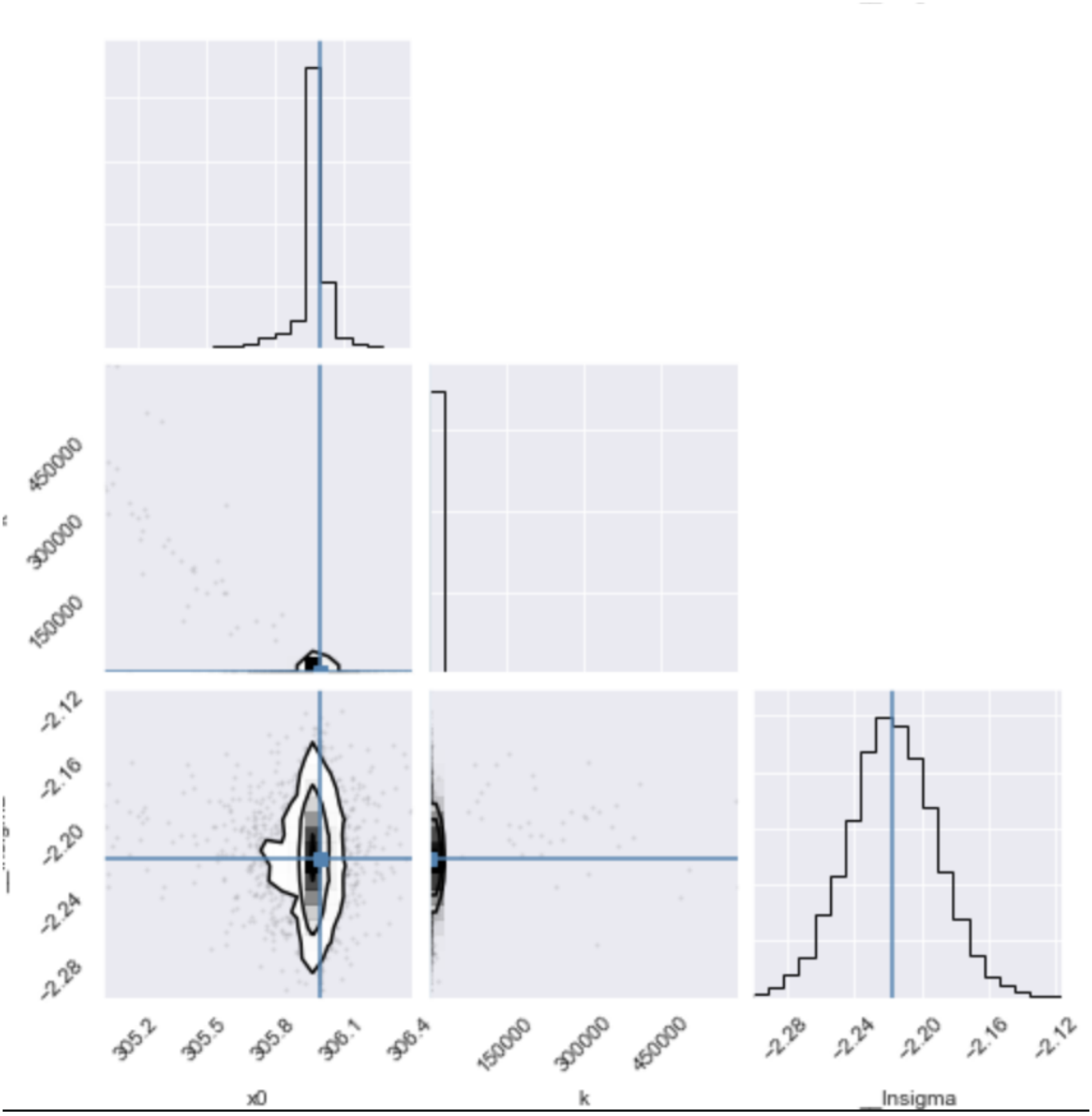


Figure 4: Caption for the picture.

Since there is no prior evidence favouring one model we set $\frac{P(\theta_{H_0})}{P(\theta_{H_1})}$ to 1. We can then compute BF by taking the ratio of the posterior distributions. From the MCMC computation it then necessary to obtain the posterior. Two main options are considered here:

(i) computing a harmonic mean of sampled values as advised by .... . This has been shown to be a consistent estimator but an approximation that should be interpreted with caution as the values obtained can stray away from the real value of distribution as shown by [citation].

(ii) compute the integral over the parameter space given of the marginal likelihoods given by $P(D|\theta_{H_i}) = \int_\theta P(D|\theta_{H_i}) \times P(\theta_{Hi}) d\theta_{H_i}$ where i correponds to the hypothesis. Note that for more complex models this computation is not possible as the number of integrations increases with the number of model parameters. Here for computation purposes we simplify the models in the by setting the value of L to 1 and during the calculation of the marginal likelihood we set σ to a constant in all datasets. The first of these assumptions is not strong because we know that the true value of $L \in [0.9, 1.1]$ - recall that L corresponds to the upper-limit of the logistic function. Also in practice, researchers could either estimate this parameter or set it equal to an known upperbound. The second assumption is stronger but multiple values were tested including the median value of the estimated posterior which seemed to be suitable in this case.

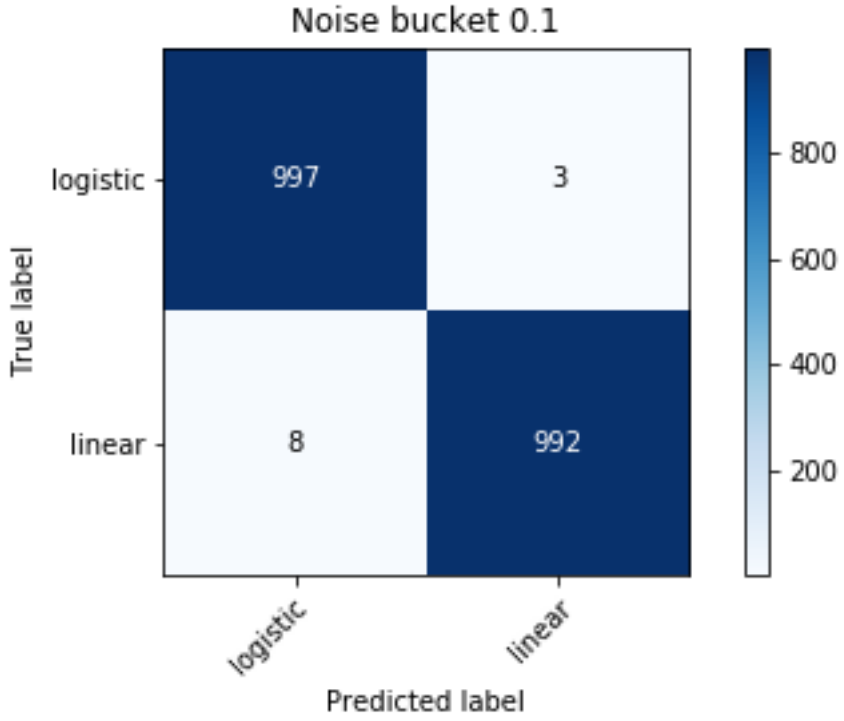
Once the computation of BF complete we can refer to the scale given by Raffety (1995) and for a clear classification fail to reject H_1 if $BF < 1$. In experiments, following ... we find that the median value of the posterior distributions can be helpful in analysis and seem to fit well to the data. These values are also recorded for the analysis as well as the distributional properties of the error term and all corresponding computation times.

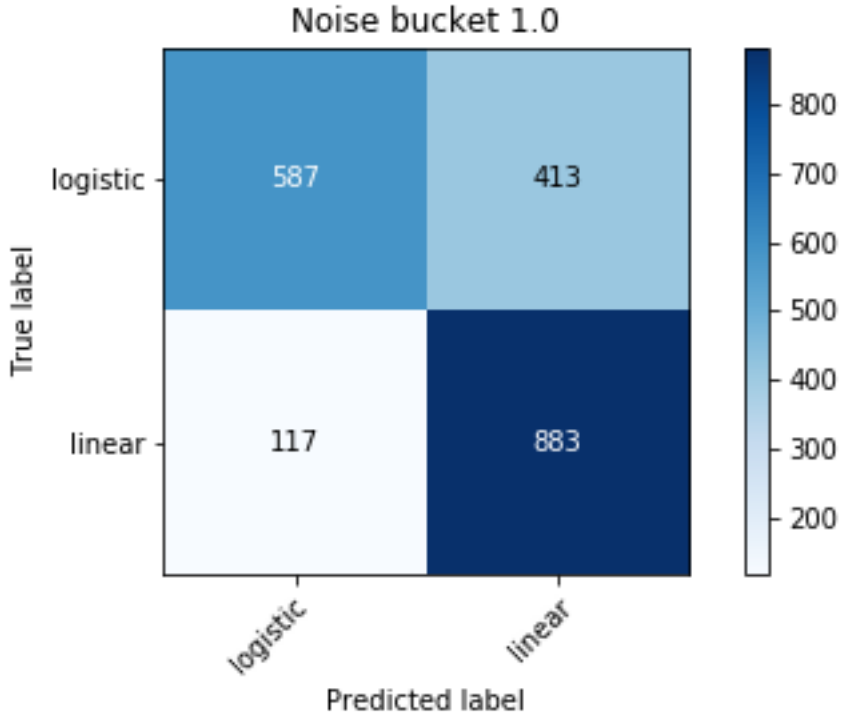
5 Results

To discuss the results we shall proceed by evaluating the datasets that do not contain a trend and then those that do :

5.0.1 Data without trend

We first focus on the frequentist approach. The average run time is ... which represents about ... per model evaluated. In terms of classification, with little noise ($\sigma = 0.1$) the datasets naturally seem to be classified correcly most of the time (0.99 accuracy).





This is expected as the signal to noise ratio is very high. However, the classification clearly becomes less accurate as the noise level increases. Figures X and Y represent the accuracy and F1 score for different levels of noise for the frequentist classification approaches: the accuracy drops quickly after $\sigma > 0.3$. When the noise reaches its peak at $\sigma = 1$ accuracy drops to 0.74 The frequentist approach although quick to estimate would lead to too many classification errors.

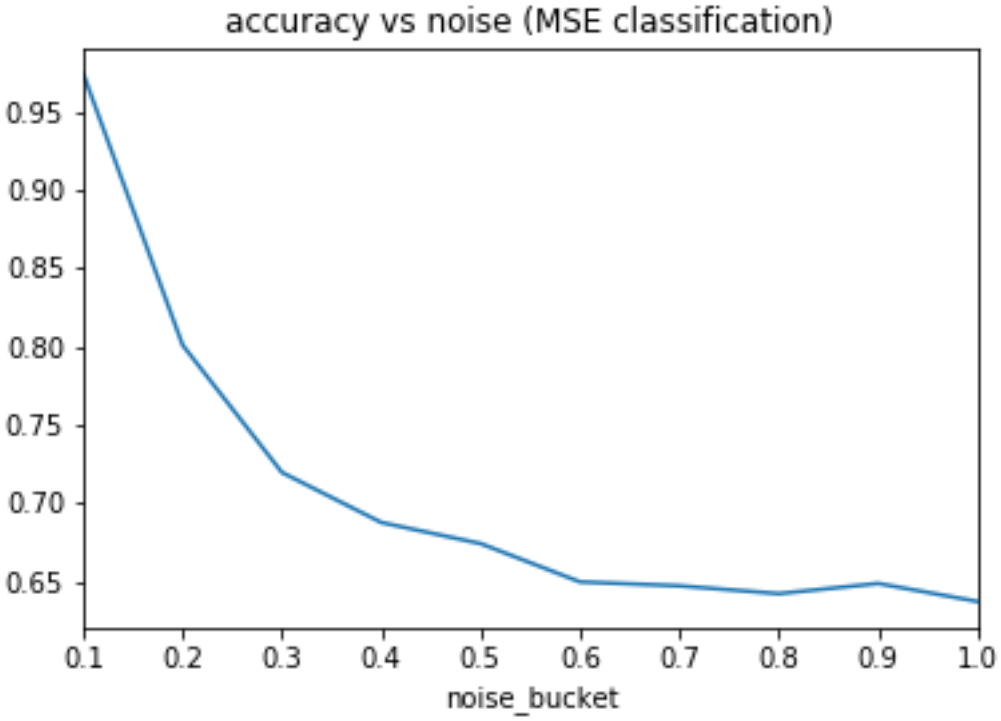


Figure 5: Caption for the picture.

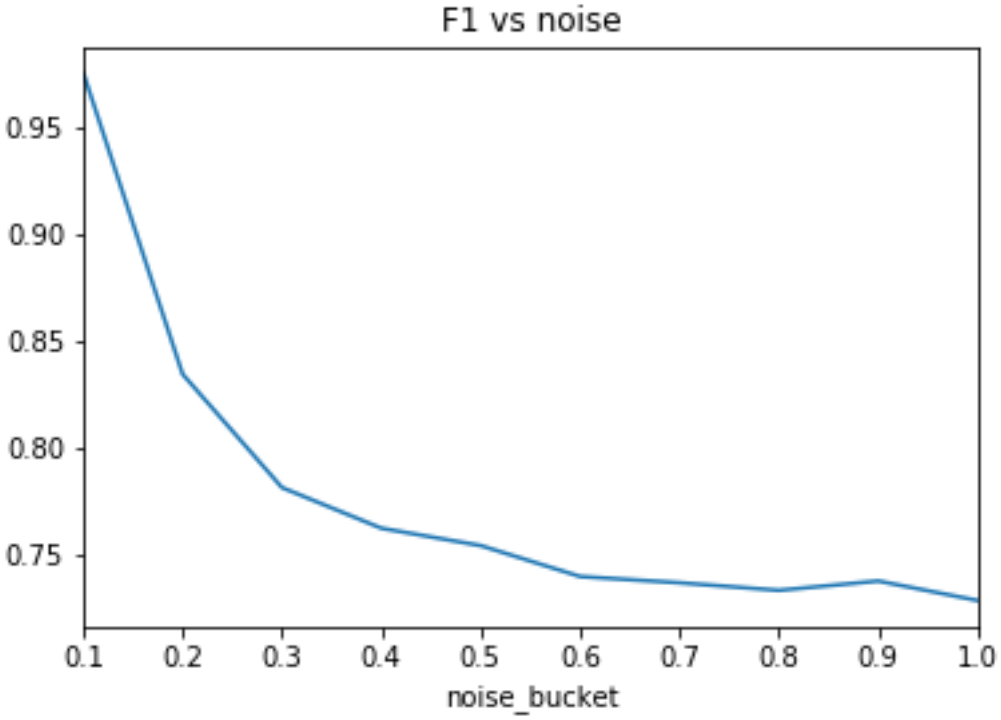


Figure 6: Caption for the picture.

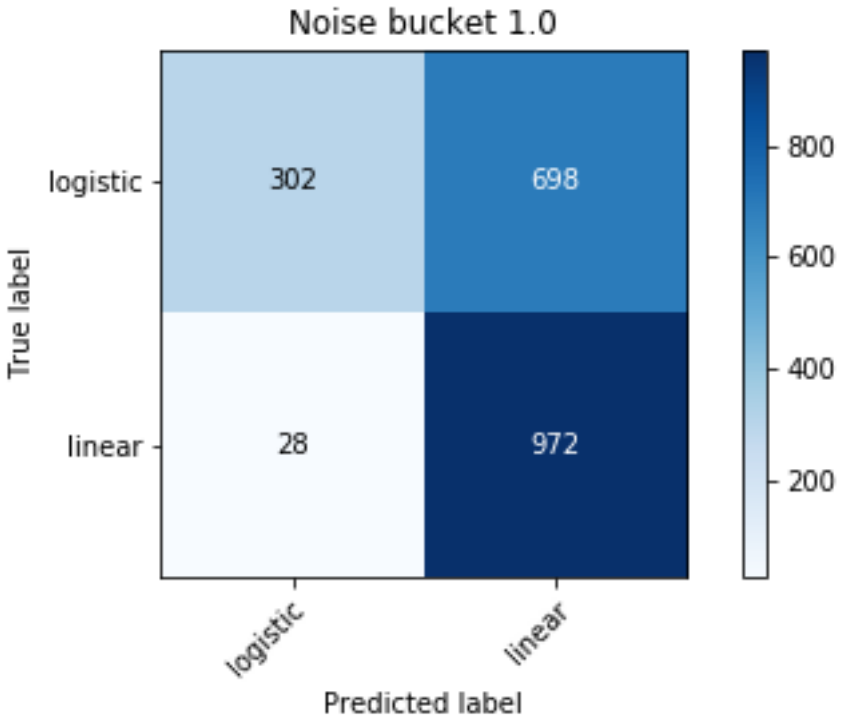


Figure 7: Caption for the picture.

In terms of parameters, we assume a Gaussian distribution in order to create parameter confidence intervals [TO DO]. To analyse this we observe how the parameter confidence changes as the noise level increases [TO DO]... Interestingly when observing the behaviour of the standard deviation of the parameters with regard to noise levels for the logistic form for instance, k seems to the slowest variance change compared to L and $x0$.

The MSE method can be contrasted with the BIC evaluation (or Chi square) which should in theory be more suitable [TO DO]. Here the results are ...

We compare the frequentist methods to the Bayesian classifications described in section [methodology]. The first noteworthy point is that the Bayesian methods were too computationally expensive to run on the whole dataset. The estimation of one model was about ... which would have been ... for tall the data. This is due to the computation cost of the MCMC. To still contrast the methodologies, we sample an even fraction for each noise bucket which we then use as our sample dataset. The first classification we use is to create a model based on the median values of each parameter distribution and then evalute the best model according to the BIC. This simple Bayesian method yielded surprisingly low classification results : for different levels of σ the accuracy was always situated between 0.5 and 0.6. This can be due to the prior settings or the too small number of chains used in the MCMC process (settings were number chians = ..., numbe of burns = ...).

Another possibility can be that the median value is not a good representative of the parameter distribution. To remedy this we consider the Bayes factor as our model selection process [TO DO]. One advantage of Bayesian modelling is the obtention of parameters as distribution. This is demonstrated by figure ... whcih provides an example of a contour plot for one of the dataset's parameter estimation.

6 Discussion

7 Evaluation, Reflections, and Conclusions