Apprentissage statistique et modélisation 0D/1D des systèmes : application au vieillissement des batteries

Statistical learning and 0D/1D modelling: application to battery ageing

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Résumé:
Un modèle de système 0D/1D est une représentation mathématique du comportement dynamique et des interactions entre les parties d'un système complexe. Modelica est un langage pour programmer de tels modèles à l'aide d'équations différentielles. Grâce au paradigme orienté objet, il permet de constituer des bibliothèques de parties de modèles réutilisables, ou *modules*. Enrichir ces modèles par apprentissage statistique et interpréter leurs prédictions en termes probabilistes constitue une excellente démarche pour la gestion des risques industriels. Nous illustrons comment elle peut-être mise en œuvre efficacement avec Python et la norme *functional mock-up interface*. L'exemple traité est la prédiction de la longévité des batteries de bus hybrides. D'abord du point de vue global, adopté lors des phases précoces de conception, puis pour des véhicules roulants suivis individuellement.

Summary:
A 0D/1D system model is a mathematical of the dynamic behaviour and interactions between the parts of a complex system. Modelica is a language for programming such models using differential equations. By leveraging the object oriented paradigm, it enables to reuse model components, collected in library of *modules*. Difficult industrial risk management problems can be tackled by supplementing these models with empirical information through statistical learning, and interpreting their predictions from a probabilistic standpoint. We illustrate how this can be efficiently achieved using the Python programming language and the *functional mock-up interface* standard. We studied the case of predicting the longevity of hybrid bus batteries. First in general, as called for in early design phases, and then for individually monitored vehicles.

Statistics meets 0D/1D system models

By *system model* we designate a global mathematical description of a complex physical system whose aim is more to reproduce the interactions between the parts of the system, than the detail of the individual physical phenomena. This voluntary loose definition does not draw a clear line between system models and what could be called *component* models. Indeed, such a delimitation depends on the context and especially on the *purpose* of the model, namely on what scientific or industrial problems it was designed to solve (Girard et al., 2017). The models we have in mind are usually sets of equations that are solved without resorting to computationally intensive methods such as finite elements, nor require the approximation of geometric domains by meshes, hence the denomination "0D/1D". As the dynamic behaviour of the system is often of great interest, these macroscopic descriptions are often formulated as *time differential* equations.

Modelica (*Modelica, A Unified Object-Oriented Language for Systems Modeling – Language Specification* 2014; Tiller, 2015) is a programming language particularly well suited for designing 0D/1D system models. A Modelica model is a system of differential equations written in almost natural (mathematical) language, efficiently organised and structured thanks to the object-oriented programming paradigm. The solution of these equations is obtained by dedicated multipurpose third-party tools such as the commercial software Dymola[1] or the open source OpenModelica[2].

Probabilistic modelling and statistical learning have the potential to vastly enrich the predictions of numerical model used to solve industrial problems. Uncertainty can be apprehended through *propagation*, *sensitivity analysis* provides insights to the design of model itself, *emulation* of models overcomes computational cost issues, statistics is an appropriate framework for *calibration* or parameter estimation, *data assimilation* allows to incorporate information from observations into the predictions *etc.* Many of the aforesaid methods are non-intrusive: they apply to inputs and outputs linked by a mathematical function representing the numerical model. This black box approach to computer experiments has been formalised into the *functional mock-up interface* (FMI) standard (*Functional mock-up interface for model exchange and co-simulation* 2014). It specifies input and output data interfaces to numerical models implemented by collecting into zip archives called *functional mock-up unit* (FMU) an XML file describing the variables of the model, and a set of possibly compiled C functions for carrying out the simulation. Most tools dealing with Modelica are compatible with the FMI standard, allowing to compile or pilot FMUs.

The PyFMI module[3] (Andersson et al., 2016) brought FMUs

[1] https://www.3ds.com/products-services/catia/products/dymola/
[2] https://www.openmodelica.org/
[3] http://www.jmodelica.org/page/4924

into the Python universe. Python is a very apt language for computer experiments and statistical analysis. It provides a plethora of specialised modules, for instance Dask for large scale problems or TensorFlow and Theano for designing neural networks, and generic packages, such as Numpy, Scipy, Scikit-learn, Statsmodels, Pandas... Among them, OpenTURNS was recently extended by a plugin module, Otfmi[4], relying on PyFMI to enable transparent calls to FMUs (Girard, 2017).

Python and Modelica both are user-friendly and encourage modularity. The case of battery longevity prediction studied here is an attempt to illustrate how the combination of these two languages offers opportunities for fast paced yet rigorous industrial problem solving. The physical and statistical models that were created to simulate the battery ageing process are first presented. Then two illustrative applications are presented in the second part of the article.

Physical and statistical models for battery longevity prediction

Batteries are responsible for about half of the price of an hybrid electric bus. Hence their longevity strongly impacts the cost of possession and is of prime interest to fleet operators. Battery ageing mechanisms are multiple and complex (Catton, 2017; Vetter et al., 2005) but can be regrouped into *calendar*, namely continuous physico-chemical reactions, and *cycling*, those driven by consecutive charge and discharge cycles. Both calendar and cycling ageing are strongly impacted by temperature. A commonplace rule of thumb is that batteries age twice as fast with every 10 °C increase. We devised a panoply of models to predict battery ageing while taking into account the uncertainty induced by temperature fluctuations. Section 1 presents the ageing model itself and the way it depends on temperature. The thermodynamical model described in section 2 outputs the temperature of the battery given an input ambient temperature time series. Finally, a stochastic model simulating battery temperature fluctuation based on past ambient input temperature observations is detailed in section 3.

1. Empirical ageing model

There is vast body of literature on models for predicting battery degradation ranging from essentially mechanistic models describing electrochemical reactions in details to more macroscopic models with much fewer parameters (Jin et al., 2018). We settled here for the latter and adopted an empirical formulation, assuming that battery damage, for instance measured as capacity loss, is the sum of calendar and cycling contributions (Shojaei et al., 2017b):

$$\delta = \delta_{cal} + \delta_{cyc}, \tag{1}$$

where the *cal* and *cyc* indices refer to calendar and cycling ageing.

A battery stored at constant temperature usually ages proportionally to the square-root of time. It was shown by Ploehn et al. (2004) that this could be explained as resulting from the diffusion-limited growth of a resistive film layer at the electrode surface. In order to perform dynamical simulations, we assumed film growth to be indeed the dominant mechanism and related the calendar ageing rate to the current state of health of the battery through the following differential formulation:

$$\delta \, \frac{\mathrm{d}\delta_{cal}}{\mathrm{d}t} = A_{cal}(T)^2/2, \tag{2}$$

where A_{cal} is a temperature dependent coefficient.

[4]https://github.com/openturns/otfmi

We assumed that cycling damage is proportional to the number of consecutive identical cycles of charge and discharge (Rugh et al., 2013), which we formulated as:

$$\frac{\mathrm{d}\delta_{cyc}}{\mathrm{d}t} = U(t)A_{cyc}(T), \tag{3}$$

where A_{cyc} is a temperature dependent coefficient, and $U(t)$ a factor varying in time according to battery usage. Given a reference cycle, with charge or discharge rate ρ_r, of duration τ_r and causing a damage of δ_r, the instantaneous usage factor is proportional to the current rate $\rho(t)$:

$$U(t) = \frac{\delta_r}{\rho_r \tau_r}\rho(t). \tag{4}$$

The temperature dependence of both mechanisms was assumed to follow Arrhenius' law:

$$A(T) = \alpha \exp(-\frac{E}{KT}), \tag{5}$$

where K denotes Boltzmann's constant. The two parameters α, the pre-exponential factor, and E, the activation energy, are to be estimated from experimental data.

The system of differential equations described above was programmed in Modelica and compiled to FMU using the OpenModelica compiler.

2. Thermodynamical model

Simply equating the battery temperature with the ambient temperature would be a very rough approximation: the battery is not in direct contact with the outside air, as any solid body it has a thermal inertia, its functioning generates heat, and it exchanges thermal energy with the vehicle cabin whose temperature is controlled during drive... We settled here for a lumped formulation that takes these factors into account while enabling fast simulation.

The main equation of the model stems from Newton's law of cooling:

$$C\frac{\mathrm{d}T}{\mathrm{d}t} = \dot{Q}_{ambiant} + \dot{Q}_{cabin} + \dot{Q}_{cool} + \dot{Q}_{generation}, \tag{6}$$

where $\dot{Q}$ denotes heat fluxes, T the battery temperature, and C its specific heat capacity whose value was set to 3000 J kg^{-1} K based on experiment conducted by EDF (Durcik, 2015). The heat exchanges with the cabin and ambient air were both modelled as

$$\dot{Q} = \frac{\Delta T}{R}, \tag{7}$$

where ΔT is the difference between the considered temperature and that of the battery, and R a thermal resistance. We used values given by Shojaei et al. (2017a). In particular, the heat exchange with ambient air is about twice as efficient when the bus is moving, meaning that the corresponding thermal resistance is halved. The dynamics of the temperature in the cabin was modelled in the same fashion as that of the battery: it exchanges heat with the exterior and, when on, with the air conditioning cold source. It was tuned such that the cabin temperature is around 22 °C during driving periods, and following ambient temperature in idle time. The battery cooling system is triggered when the battery temperature approaches 35 °C. It ensues a negative heat flux $\dot{Q}_{cool}$ which goes back to zero when the temperature rise is mitigated. The internal heat generation term $\dot{Q}_{generation}$ is null when the battery is not functioning, and constant during charge or drive. It was set to a value of 0,016 C based on the experiments of Pesaran (2002).

This thermodynamical model was programmed in Modelica and compiled to FMU using the OpenModelica compiler. The resulting dynamics is illustrated in figure 1 depicting the battery response to input ambient temperature measured at Perpignan in 1996. The battery is charging from 4:00 to 7:00,

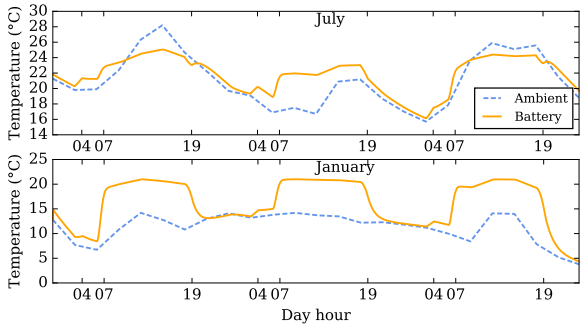


Figure 1. Simulation of the battery temperature dynamics in summer (top) and winter (bottom) in 1996 in Perpignan.

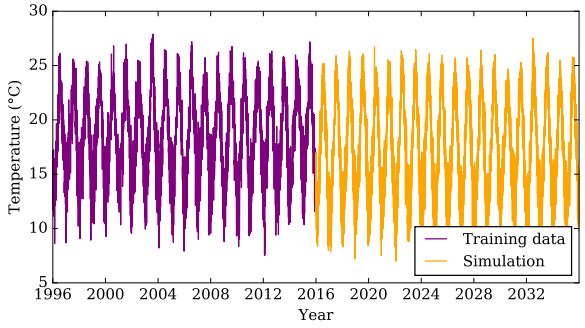


Figure 2. Example of battery temperature simulation (orange, right-hand side) prolonging the Perpignan training data (purple, left-hand side).

and the bus is driving from 7:00 to 19:00. Air conditioning is on when the bus is driving. In winter, the cabin is actually *heated* and pulls battery temperature to a plateau around 22 °C during the day, while it falls back to ambient temperature during the night. Battery temperature variation are smoother in summer when the ambient temperature span comprises the target cabin temperature.

3. Stochastic weather model

MétéoFrance freely provides meteorological data measured during the last twenty years by weather stations spread on the French territory (MétéoFrance, 2017). We collected ambient air temperature in two cities, Lille and Perpignan, sampled at a 3 h rate from 1996 to 2016. Lille (N50°38′14″ E3°3′48″), the "*Capital of French Flanders*", close to the Belgian border, has a temperate oceanic climate. Perpignan (N42°41′55″ E2°53′44″) was the capital of the former Kingdom of Majorca which straddled today's France and Spain. It has a Mediterranean climate.

These input data were fed to the thermodynamical model presented in the previous section to produce training signal of battery temperature. The Perpignan training signal is plotted in purple on the left-hand side of figure 2.

Temperature signals display repetitive structures at different periods, called *seasonal* pattern. The most obvious of these patterns are the cycle of actual seasons (winter is colder than summer), and the alternance of night and day. The erratic fluctuations on top of those structures are strongly auto-correlated, both because of the thermal inertia of the system and the dynamics of their causes, for instance the cloud cover.

Modelling these behaviours is but a means towards simulating battery ageing. Hence, we used the characteristic time period of the combined ageing mechanisms to decide which seasonal structures and correlations should be modelled, and which can be safely neglected. Consider for instance systematically exchanging Mondays, Tuesdays and Wednesdays with Thursdays, Fridays and Saturdays in the input temperature signal: the day-to-day correlation structure would be upset but the effect on the overall ageing would be negligible. Battery age by 1 % in about one month on average during the initial phase of the ageing process, from 0 % to 3 % of damage when ageing is the most rapid and non-linear in time, and has a determining effect on the subsequent evolution. Based on that consideration, the average temperatures during charge (from 4:00 to 7:00), drive (from 7:00 to 19:00) and idle time (from 19:00 to 3:00) were modelled independently.

Each signals was split into a sum of a seasonal and an erratic parts by separating the terms of its Fourier decomposition whose periods are above 30 days from the higher frequency ones. The low frequency part was sliced by year, producing a table with 20 rows (each year is an individual) and 365 columns (each day is a variable), whose principal components (Jolliffe et al., 2016) were computed. The yearly seasonal structure could be reasonably well captured by 2 principal components. We modelled the joint distribution of their scores by kernel density estimation (Hastie et al., 2001), which enables us to simulate years of low frequency temperature fluctuations. The unstructured remainder corresponding to the 363 unused principal components, was added to the high frequency part of the signal.

Then the high frequency part was modelled by kernel density estimation, conditionally on the day number using a window of 7 days. By doing so, we preserve the evolution of the daily variability during the year but abandon the correlation between the temperature of successive days.

An example of battery temperature simulation is plotted in orange on the right-hand side of figure 2. The annual patterns and year-to-year variability are adequately reproduced.

Uncertainty propagation and parameter estimation

The thermodynamical model described in section 2 was used only twice, once for each city, to simulate battery temperature time series from the 20 year ambient temperature records in Lille and Perpignan. The stochastic models fitted to these two time series, as accounted by section 3, allow us to sample the probability distribution of the battery temperature fluctuations during the, say, next 10 years. In section 1, 4 parameters governing the influence of temperature on ageing through Arrhenius' law, 2 for each mechanism, were introduced. The estimation of these parameters and the associated uncertainty is discussed in section 1. The uncertainty on both temperature and Arrhenius parameters was propagated through the ageing model to study the influence of the geographic location on ageing. The analysis of the resulting sample applies to all batteries of a given type. It would be typically carried out during the design phase, for instance to arbitrate technological decisions, or to build a business plan for a reprocessing and disposal process.

The case studied in section 2 lies downstream in the system's life cycle: hybrid buses are now driving and we would like to monitor the ageing process of their battery *individually*.

1. Influence of geographic location on ageing rate

The two pairs of Arrhenius parameters related to calendar and cycling ageing were estimated by classical regression techniques on experimental data representative of Li-Ion battery used by the automotive industry (Durcik, 2015; Grolleau, 2015; Rugh et al., 2013). This approach induces a strong dependence between parameters related to the same mechanism. Put another way, the likelihood of the observations is high in a narrow band of exponential shape

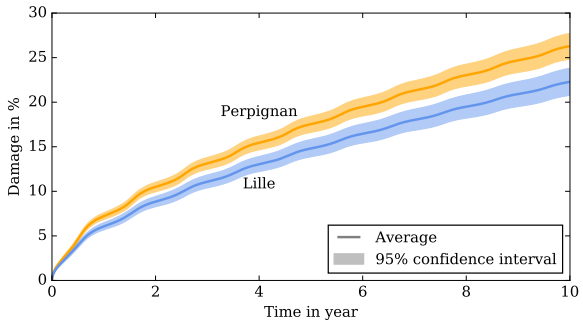


Figure 3. Ageing prediction and associated uncertainty for batteries in Perpignan and Lille.

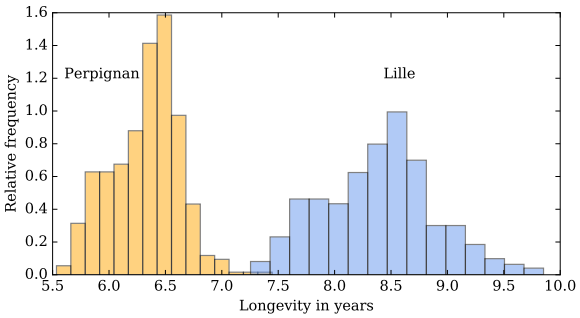


Figure 4. Relative frequencies of battery longevity in Perpignan and Lille for a threshold of 20 % of damage.

in the {pre-exponential factor ; activation energy} plan, and nearly zero everywhere else. Sampling the parameters independently would be obviously wrong. Instead, we modelled the uncertainty of the data points by confronting comparable experiments. Simulation of the joint probability of a pair of parameters was later carried out by repeated regression on data perturbed according to these experimental uncertainty models. Finally, our global black box ageing model can be thought to have 3 uncertain inputs: the temperature fluctuations and the two pairs of Arrhenius parameters.

We generated samples of 1000 ageing realisations in both Lille and Perpignan. The sample averages of the damage are plotted as lines in figure 3, surrounded by symmetric 95 % confidence intervals depicted as flat tints. The damage in Perpignan is significantly higher than in Lille after a little less than 5 months. The divergence occurs at an upwards inflexion of the damage slope, corresponding to the onset of the first summer of operation (simulations starts on the 1st of January).

The uncertainty of damage prediction, measured as the width of confidence interval, is roughly the same in the two cities. Its growth is very steep in the first few months, then decelerates to a constant rate of about 0,20 points per year after one semester. Recall that calendar ageing is proportional to the square root of time, while cycling ageing is linear in time because we applied constant cycles. At the end of the 10 years simulation interval, the battery damage reached 26,29 (95%CI: 24,85 to 27,72) points in Perpignan and 22,28 (95%CI: 20,77 to 23,81) points in Lille. The corresponding interval widths are therefore 2,88 points (10,94 % relative uncertainty) in Perpignan, and 3,04 points (13,63 % relative uncertainty) in Lille.

The longevity of a battery is defined as the time before it reaches a given damage threshold. Figure 4 displays the distribution of battery longevity in Perpignan and Lille for a threshold of 20 % of damage. The 20 % of damage longevity is significantly smaller in Perpignan, 6,32 (95%CI: 5,73 to 6,85) years, than in Lille, 8,39 (95%CI: 7,53 to 9,45) years. The same goes for the associated relative uncertainty: 17,81 % in Perpignan versus 22,88 % in Lille.

2. Predictive monitoring of a battery longevity

Let assume that the sate of health of a battery has been evaluated 3 times during its first year of usage. Damage observation are plotted as green dots in figure 5. We sampled 1000 sets of Arrhenius parameters from the prior distribution described in the previous section and simulated the corresponding damage trajectories using the same input ambient temperature, assumed to be known from measurement of a the Perpignan weather station.

Discrepancies between simulated damage trajectories and observations stem from the combination of modelling and

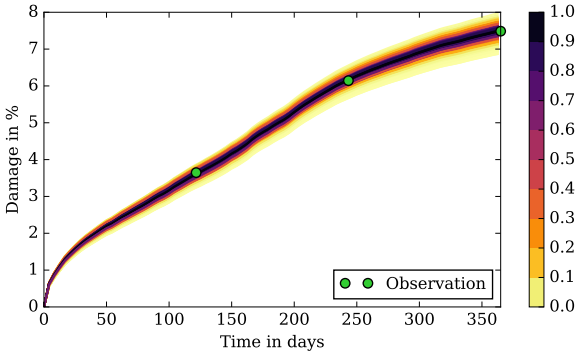


Figure 5. Damage observations (blue dots) and 1000 prior simulations for the year 1996 in Perpignan. The tint of the simulation line indicates their relative probability when sampling with replacement after weighting by the likelihood.

measurement errors. We postulated a Gaussian structure for the root mean squared of these difference, and derived likelihood values for each input set of Arrhenius parameters. The simulated damage trajectories are plotted in figure 5 under the observation dots with colours indicating the associated relative likelihood. The best match trajectory is drawn in black, and the worst in pale yellow.

Calling upon Bayes formula, we then sampled the posterior distribution of Arrhenius parameters. In practice we sampled with replacement from the 1000 previous parameter sets, weighted by their relative likelihood. Finally, for each set picked that way we simulated 9 years of battery temperature in Perpignan, and fed them to the ageing model. The resulting statistics obtained from 1000 such simulations are displayed in figure 6, with the same graphical conventions as in figure 3.

The average of damage trajectories is close to that of the generic a priori simulation (figure 3) because the observations happened to fall roughly in the middle of the support of the prior distribution of damages. At the end of the 10 years interval, the battery damage reached 26,56 (95%CI: 25,60 to 27,52) points. The prediction uncertainty has been substantially reduced by incorporating the information from the observations: the posterior relative uncertainty on damage after 10 years usage is 7,23 %, which is 3,71 points less than the prior relative uncertainty related in the previous section.

The same comment goes for longevity The 20 % damage longevity average posterior prediction, 6,19 (95%CI: 5,78 to 6,53) years, is close to the prior prediction, but we achieved a gain of 5,72 points in relative uncertainty, the posterior value being 12,09 %.

Interestingly, the relative uncertainty stays below 5 % dur-

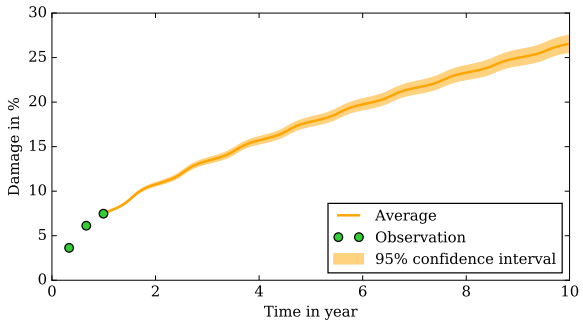


Figure 6. Posterior ageing prediction for a given battery after one year of observation in Perpignan.

ing 3 years following the last temperature and damage observations. Hence, the above procedure could be used as a means to monitor and anticipate battery degradation in order to assist maintenance planning and help making strategic decisions.

Conclusion

Bridging disciplines, such as different flavours of physical and probabilistic modelling, is a pivotal requirement for the safe design and operation of industrial systems. Python and Modelica are two versatile tools with relatively smooth learning curves. As a matter of fact, a single engineer or researcher may master both in a reasonable time, in addition to its core skills. Such concentrations of abilities are steps towards bridging disciplines. Hence, along with educational and organisational measures, a very pragmatic and efficient course of action to meet the said requirement is to develop technological interfaces between existing tools. This is driving idea of the FMI initiative, and the motivation behind the recent development of the open source Python module Otfmi.

Another important concept central to the FMI is obviously standardisation, which allows for automation. As they mature, mathematical methods usually get more streamlined, more robust, and their domain of application widen. This is both the result of the continuous research effort, and a selection process: the less practical methods are little used and gradually forgotten. Should technological tools adequately follow this process, we may hope for a lessening of the cost (manpower, computer, time) of mobilising advanced mathematical methods down to the point where they become common practice among non specialists. The recommendation that "sensitivity analysis should be used early in the modelling process, as a safeguard against irrelevant complexity" is a common trope of conferences on the topic. How often is it carried into effect? There is still some way to go, but a rapid survey of recent literature allows for optimism.

For the sake of pithiness, the physical models presented here were kept relatively simple. But, once again, we think that mathematical analysis of physical models should go alongside with the design of the model itself. Hence, such a collection of models should be always thought of as being in a transitory state, ready to evolve with the perpetual knowledge and data acquisition and the emergence of new problems. Keeping up with the hybrid vehicle battery example, are we interested into evaluating the energetic cost of temperature management? Then an extension of thermodynamical is called for, following for instance the example of Shojaei et al. (2017a). Some data about the driving cycles are now available? Maybe it's time to consider the more elaborate ageing models described by Jin et al. (2018). We are convinced that Python and Modelica, completed, while we are at it, by a version control system such as git[5], are great options for implementing such a workflow.

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