Handling uncertainties in industrial context? A statistical point of view

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CRAN-SAFT

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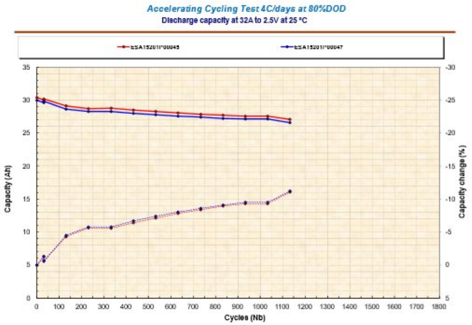
Industrial context

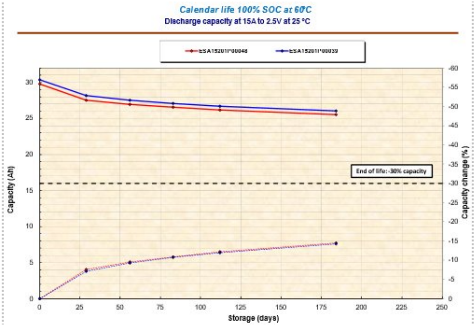
Global context on Lithium-ion batteries

- Growing demand of Lithium-ion batteries for electrical vehicles and energy storage
- Investments of TotalEnergies with SAFT on this field

Industrial context

- For a new battery design it is important to model its degradation
  - To set its price (lifetime models)
  - To understand the ageing mechanism
- Some long and expensive tests are performed (several months or even years)
- Several indicators of state-of-health can be considered
- Here we focus on the decreasing of the capacity of the battery with time





Industrial context

Lifetime prediction?

- Difficulties to predict batteries lifetime: complex ageing mechanisms, cost of testing ...
- Need to determine uncertainties to assess financial risks
- Explain battery lifetime, find solutions to improve it

Industrial context

Which data?

- Few industrial data available in our context!
- Increasing quantity of public data

Location with weblink	Paper ref	Cell (form size chemistry)	Test variables	Data given	No. of cells
NASA [53, URL]	[10]	18650 2 Ah (?)	Dhrg, T	Q, IR, V, I, T	34
	[9]	18650 2.2 Ah LCO	Chrg, Dhrg, T	Q, IR, V, I, T	28
CALCE [67, URL]	[68,70]	prismatic 1.1 Ah LCO	Chrg, Dhrg	Q, IR, E, V, I, T	15
	[68,70]	prismatic 1.35 Ah LCO	Chrg, Dhrg, T	Q, IR, E, V, I, T	12
	[13]	pouch 1.5 Ah LCO	Chrg, DOD	Q, V, I	16
TRI [71, URL]	[6]	18650 1.1 Ah LFP/gr	Chrg	Q, IR, V, I, T	124
	[72]		Chrg	Q, V, I, T	233

Industrial context

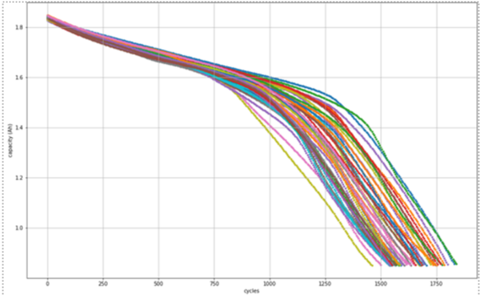
Goals

- Model with uncertainties the time evolution of state of health of a population of batteries given the experimental conditions
- Important focus on uncertainties modeling to assess the financial risk related to performance guarantees
- Choice to model the complete health degradation not only lifetime
- Not application dependant and provides a more complete understanding of the degradation process

Industrial context

Modelling uncertainties?

- Aachen university dataset
- 47 batteries, one experimental condition (25°C, CC at 2C until 3.9V and CV until 30 minutes)
- Ideal to model uncertainties and for forecasting



An important source of uncertainties is the inter-battery variability which increases with time

Industrial context

A Data-driven approach relying on Gaussian processes (GPs) [See Rasmussen 2006]

- Can automaticaly learn complex functions
- Naturally include uncertainties
- Allow use of prior knowledge
- Can be used with few data

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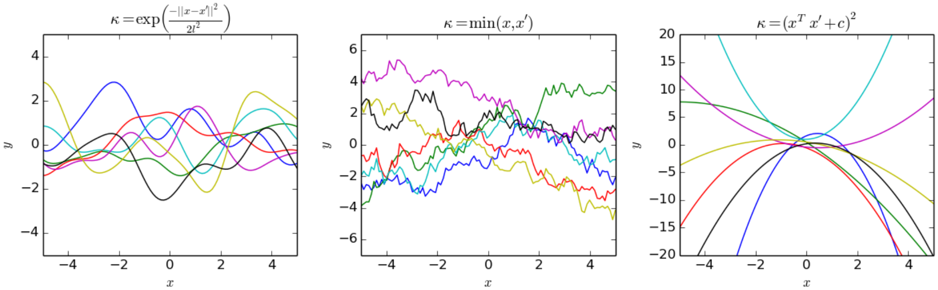
Background on GPs

- GPs are extensions of Gaussian vectors
- Random functions f defined thanks to
  - a mean function m : $m(t) = \mathbb{E}[f(t)]$
  - a kernel k encoding the covariance of $(f(t), f(t'))$:

$$k(t,t') = \mathbb{E}\left[(f(t) - m(t))(f(t') - m(t'))\right]$$

- The choice of the kernel has a major influence on the GP.



Gaussian processes regression (GPR)

Vanilla GPR considers the following regression model

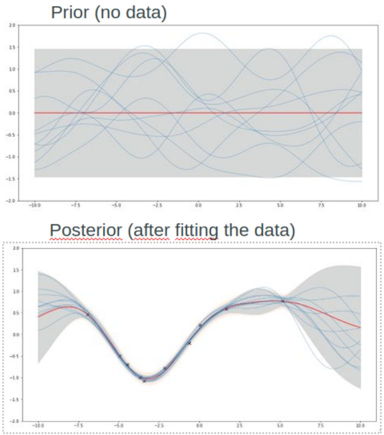
$$y = f(t) + \varepsilon$$

where

- y is the variable to explain (capacity of the battery here)
- t is the explanatory variable (time here)
- f is the mean function to estimate
- ε is a noise related to measurement error

Gaussian processes regression (GPR)

GPR is a Bayesian approach where we set a GP prior on f with mean m (usually set to zero) and a parametric kernel k



Gaussian processes regression (GPR)

- Estimation of hyperparameters of the GP by maximizing the marginal likelihood given the training data
$$p(y_1, \cdots, y_n | t_1, \cdots, t_n)$$
- After that, we can compute the posterior law of f at new inputs
- Vanilla GPs implemented in the Python library `GPflow` (see `https://www.gpflow.org/`)

Gaussian processes regression (GPR)

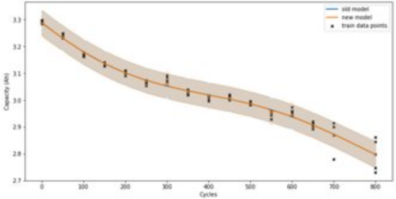
We applied vanilla GPs to obtain an interpretable model

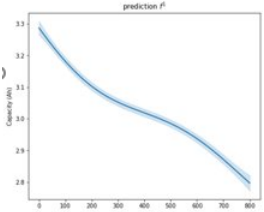
$$y = f_1(t) + f_2(t) + f_3(t, b) + \varepsilon$$

where

- f_1 : degradation trend
- f_2 : bias at each cycle
- f_3 : inter battery variability
- ε : noise measurement

Gaussian processes regression (GPR)





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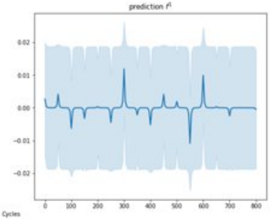

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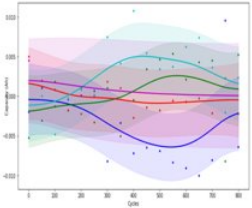

f_3

Prediction with Vanilla GPs

Gaussian processes regression (GPR)

Main drawbacks of Vanilla GPs

Two main physical features of the degradation process are not included

- The variance of the phenomena is increasing with time
- The capacity is decreasing with time

Our solution : chained GPs including monotonicity constraints

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Chained GPs [Saul et al. 2016]

- Chained GPs are models to handle models depending non linearly on several independent GPs
- Instead of considering

$$y = f_1(t) + f_2(t) + f_3(t, b) + \varepsilon$$

one consider

$$y = f_1(t) + f_2(t) + \sigma(t) f_3(t, b) + \varepsilon$$

where $\sigma(t) = g(\eta(t))$ with η GP, g positive function (sigmoid for e.g.)

Chained GPs [Saul et al. 2016]

Inference step

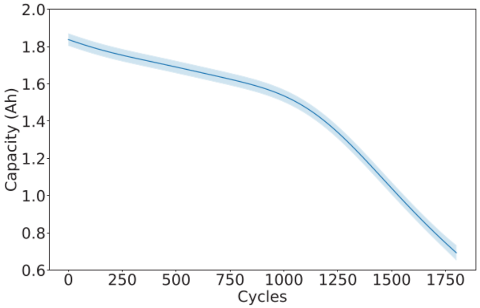
- Starting point : likelihood function

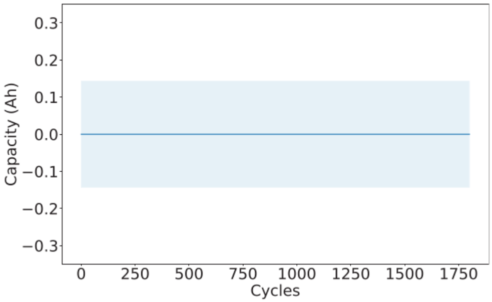
$$p(y|f_1, \cdots, f_3, \eta)$$

- One sets independent Gaussian process priors on f_1, f_2, f_3, η
- Model too complex to have an exact posterior law
  $\Rightarrow$ has to be approximated
- variational inference approach with optimization of the evidence lower bound (ELBO)

Chained GPs [Saul et al. 2016]

Qualitative results

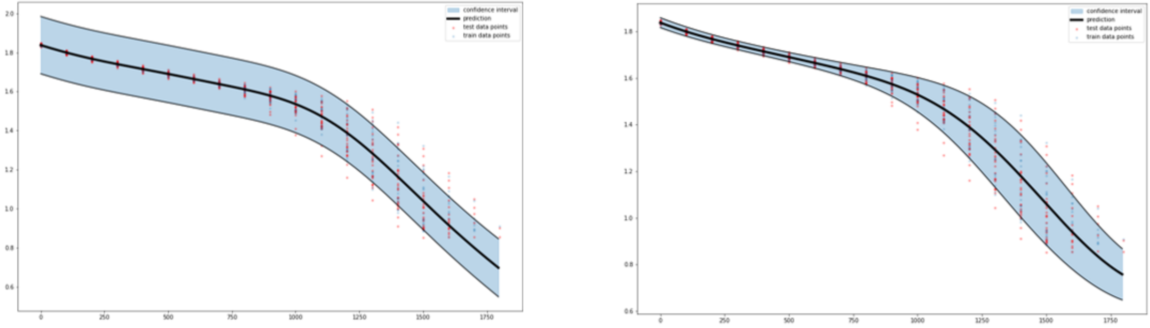




Prediction with CGPs

Chained GPs [Saul et al. 2016]

Qualitative results



Prediction with CGPs

Chained GPs [Saul et al. 2016]

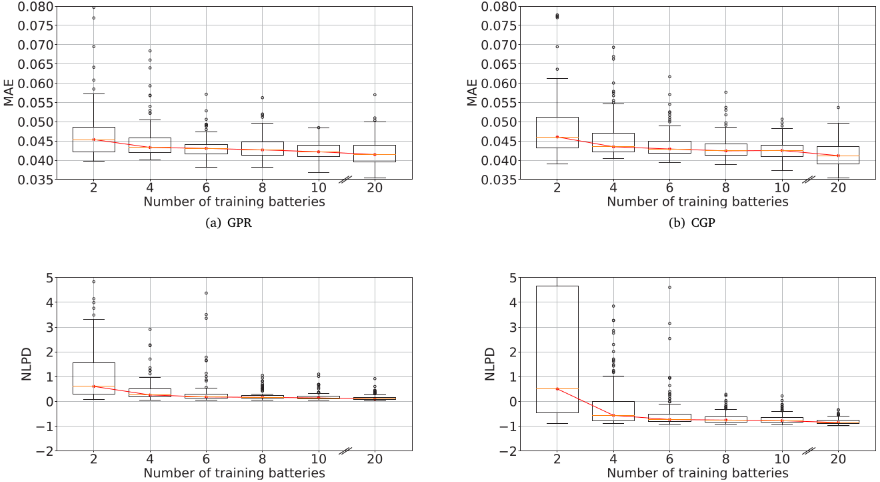
Quantitative comparison between GPR and CGP models

- Metric to validate prediction : mean absolute error (MAE)
- Metric to validate uncertainty quantification : negative log predictive density (NLPD) (Quinonro 2005)

$$\mathrm{NLPD} = -\frac{1}{n^*}\sum_{i=1}^{n^*} \log p(y_i^* | t_i^*)$$

Chained GPs [Saul et al. 2016]

Quantitative comparison between GPR and CGP models

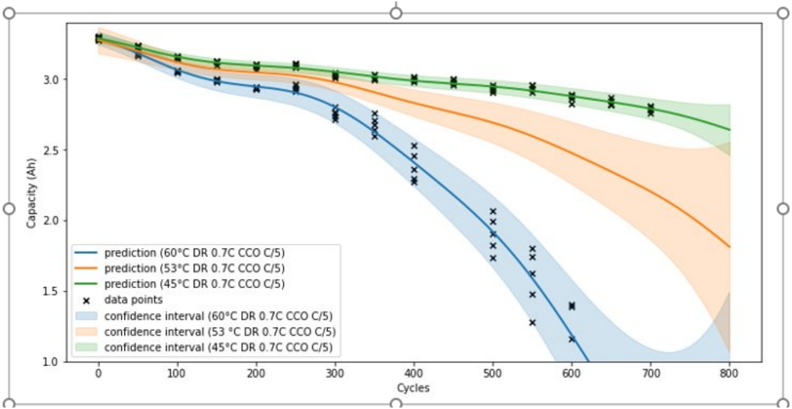


(a) GPR (b) CGP

(c) GPR (d) CGP

Chained GPs [Saul et al. 2016]

Previous model can be adapted to work on several experimental conditions



Prediction with CGPs at different temperature conditions

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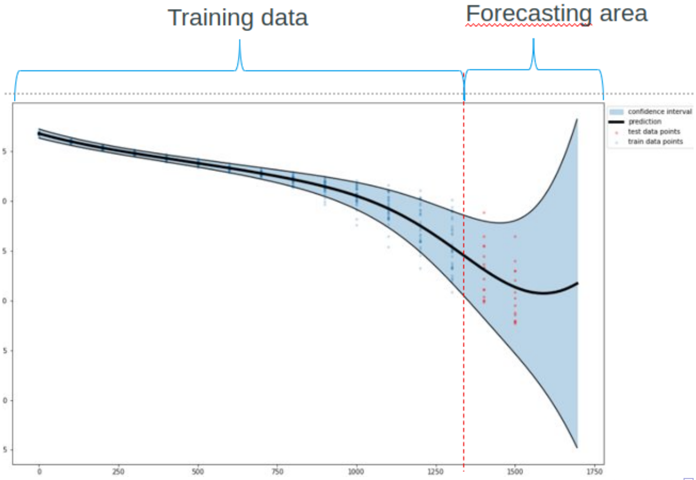
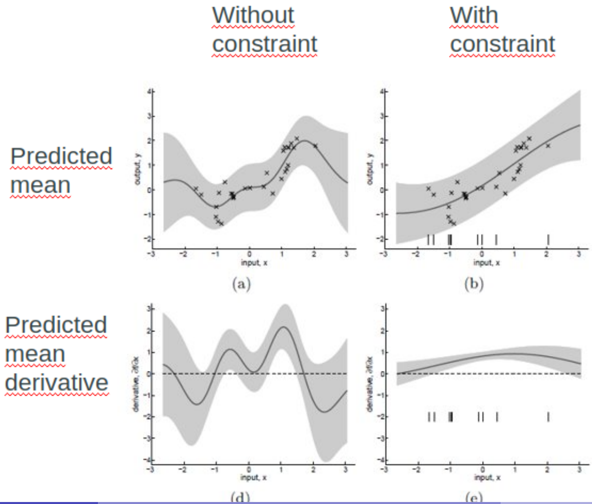
Limits of GPR and CGP for forecasting

- Methods using Gaussian processes face difficulties to forecast
- Predictions for future cycles should be decreasing



CGPs with monotonocity constraint (Lavaron et al. 2023)

- (Riihimaki, 2010) proposed a method to impose local monotonocity on GPR
- Extension of this method for CGPs?



CGPs with monotonocity constraint (Lavaron et al. 2023)

- We add virtual points translating our prior knowledge.
- At positions X^v we add virtual observations z^v taking values in $\{0, 1\}$, 0 if f_d should be decreasing, 1 if it should be increasing.
- To integrate them into our model, we suppose that

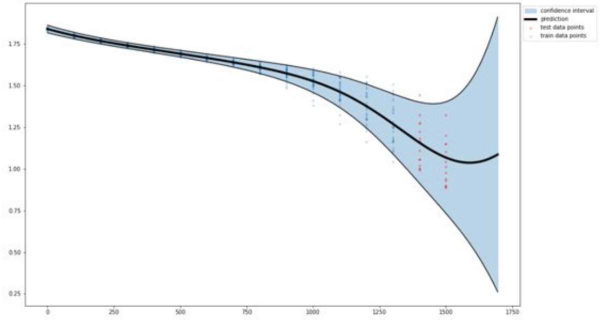
$$\mathrm{z}_i^v | \mathrm{f}'_{d,i} \sim \mathcal{B}(s(\mathrm{f}'_{d,i})),$$

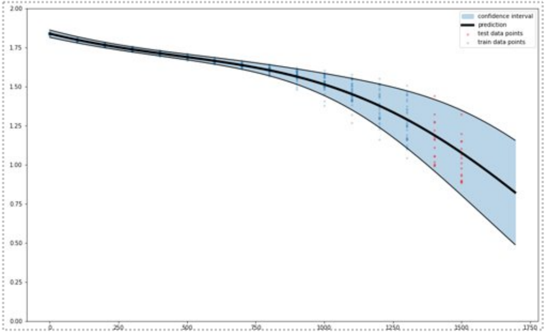
CGPs with monotonocity constraint (Lavaron et al. 2023)

- Including virtual observations, the model has an extended likelihood
- We use variational inference based on a ELBO for inference

CGPs with monotonocity constraint (Lavaron et al. 2023)

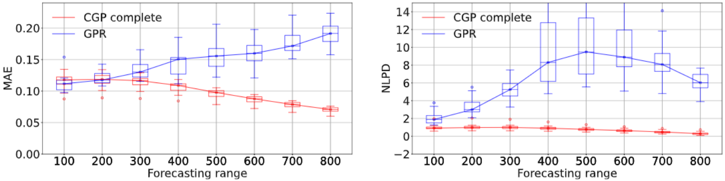
Qualitative comparison





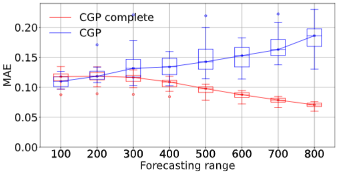
CGPs with monotonocity constraint Lavaron er al. 2023

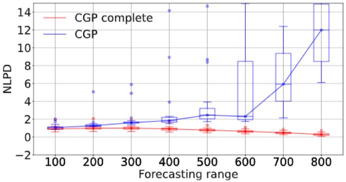
Quantitative comparison



CGPs with monotonocity constraint (Lavaron et al. 2023)

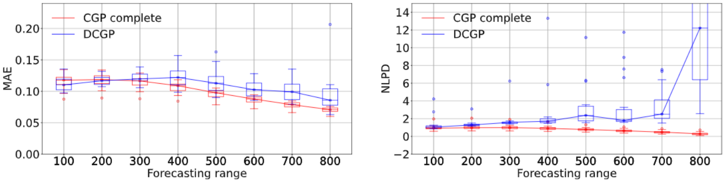
Quantitative comparison





CGPs with monotonocity constraint (Lavaron et al. 2023)

Quantitative comparison



CGPs with monotonocity constraint (Lavaron et al. 2023)

In practice several constraints can be included at the same time

- On each function of the Chained Gaussian process model : mean and inter-batteries variability
- On different directions when working with different experiental factors : mean of capacity decreases with time and temperature
- On different order of derivatives ; second order derivative to model acceleration of capacity degradation

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