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Information-Theoretic Measures and Sequential Monte Carlo Methods for Detection of Regeneration Phenomena in the Degradation of Energy Storage Devices

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This paper compares the performance of several approaches for anomaly detection that are based on a combination of information-theoretic measures and sequential Monte Carlo methods for state estimation in nonlinear, non-Gaussian dynamic systems. All approaches conveniently use properties of the differential entropy to quantify the impact of process measurements on the posterior probability density function (PDF) of the state, assuming that sub-optimal Bayesian estimation algorithms such as classic particle filters (PF) or risk-sensitive particle filters (RSPF) are to be used to obtain an empirical representation of the system uncertainty. The proposed anomaly detection strategies are tested and evaluated both in terms of (i) detection time (early detection) and (ii) false alarm rate, when utilized to identify the existence of capacity regeneration phenomena ([A-h]) in energy storage devices (particularly, Lithium-Ion batteries).

1. Introduction

The development of optimal energy storage devices (ESDs) has been an issue of study in the main scientific communities around the world. This is only a consequence of the exponential growth shown by the industry of electric/hybrid vehicles and electronic devices that require ESDs. Regardless of the main purpose for which an ESD is needed, it is critical that battery management systems are able to determine in a reliably manner the battery state-of-health (SOH); a measure that is associated to the degradation that the battery have suffered over the course of its life. This task can only be accomplished through precise estimation algorithms that allow the incorporation of real online measurements of the process and ambient variables to determine the amount of remaining charge cycles. Online estimation algorithms –more specifically Sequential Monte Carlo methods (a.k.a. Particle Filter, PF)– are especially suited to solve the aforementioned problem, given its capacity to combine the available system's measures information and analytic/empiric models. However, some ESDs suffer from sudden, momentary, and occasionally considerable regeneration of the ESD capacity. These changes, related to physicochemical aspects and temperature/loading conditions during charge and discharge cycles, are particularly important in the case of Li-Ion batteries because they often alter the trend of the SOH prediction curve, thus affecting the performance of estimation and prognosis modules based on Bayesian algorithms (Olivares et al., 2012). Here lies the importance of considering a detection module for these regeneration phenomena of the SOH, which allows to correctly isolating them in the SOH modelling.
This paper presents a solution to the aforementioned problem, which provides a framework capable of estimating the SOH while simultaneously detecting and isolating the effect of self-recharge phenomena through different detection techniques. The anomaly detection modules are based on a combination of a PF-based state estimators and information-theoretic measures that allows detecting rare events within the evolution of the battery degradation process under analysis. The selection criteria for the best suitable detection module, is based in the performance obtained when comparing type I vs type II errors, considering the impact they have over the SOH estimation in the MSE sense.

2. Problem Formulation

Capacity regeneration in ESD has been only briefly mentioned in literature (Olivares et al., 2012). Specifically in the case of lithium-ion batteries, this phenomenon has been represented as a self-charging in the logger, where certain operating conditions facilitate a sudden (and temporary) increment in the available capacity of the ESD at the next cycle (see Figure 1a), which can directly affect the accuracy and precision in SOH estimation algorithms if they are not correctly isolated, since these phenomena alter the initial condition and uncertainty on the prediction stage of the SOH (Olivares et al., 2012).
This paper analyses a solution for this problem considering an anomaly detection module that includes a PF-based SOH estimation framework; see Figure 1b, which illustrates the output of such a detection module when processing the degradation data that is shown in Figure 1a. The main focus of this research is to compare several detection methods, determining their performance in terms of type I and type II errors, and their effect in the SOH estimation bias. All detection methods used in the construction of the hypothesis test are based in PF algorithms, including its classic and the risk-sensitive version (Orchard et al., 2010). These methods are complemented by the utilization of information-theoretic measures (e.g., entropy) to generate a detection indicator that characterizes the PF-based estimate of state PDF.

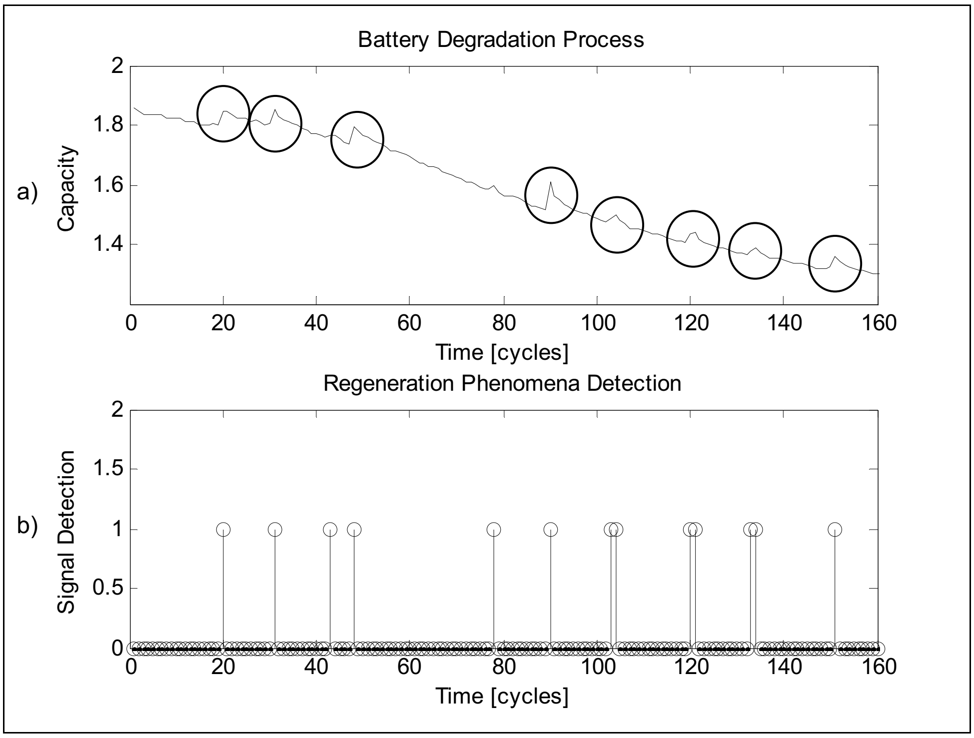

Figure 1: PF-based detection of capacity regeneration phenomena in Lithium-Ion batteries

The dynamic system that represents the battery degradation process considers the use of state-space stochastic models; mainly because of their ability to effectively combine empirical and phenomenological knowledge in the representation of nonlinear dynamic phenomena (such as an statistical characterization of self-recharge phenomena within the structure of the life cycle model).

State transition model

$$x(k+1) = f_k(x(k), U(k), \omega(k)) \tag{1}$$

Measurement equation

$$y(k) = h_k(x(k), U(k), v(k)) \tag{2}$$

where k is the cycle index; x is a vector state representing the battery SOH; $y(k)$ is the measured SOH; ω and v are non-Gaussian noises used to represent uncertainty sources within the parameter estimation procedure. The time-varying functions f_k and h_k are non-linear mappings.

Although state transition model (1)-(2) enables the implementation of Bayesian filtering techniques to monitor degradation processes in Li-Ion batteries, it may result inadequate when trying to detect and isolate the long-term effect of regeneration phenomena. This fact motivates the development of anomaly detection modules, either based on PF-algorithms as in (Orchard et al., 2011), or information-theoretic measures (Orchard et al., 2012) as the present research proposes. For this purpose an external input *U*, is included in the model to represent the output of the online detection module (Orchard et al., 2009). This module performs a test for a null hypothesis that affirms that self-recharge phenomena either does not exist or is fading in time. The framework considers a PF-based state estimator for model (1)-(2) that uses the output of the detection stage, where input variable *U*(*k*) is used to indicate if a regeneration phenomenon has occurred at time *k*. The selected detection measure must enable isolating events where the SOH estimation algorithm is unable to track the process measurements using a state transition model. The main aspects associated to the formulation of this type of detection modules follows next.

3. Anomaly Detection based on Particle Filtering Algorithms

Nonlinear filtering is defined as the process of using noisy observation data $Y = \{y_k, k \in \mathbb{N}\}$ to estimate at least the first two moments of a state vector $X = \{x_k, k \in \mathbb{N}\}$ governed by a dynamic nonlinear, non-Gaussian state-space model (Orchard et al., 2012). From a Bayesian standpoint, a nonlinear filtering procedure intends to generate an estimate of the posterior probability density function $p(x_k \mid y_{1:k})$ for the state, based on the set of received measurements. Particle Filtering (PF) is an algorithm that intends to solve this estimation problem by efficiently selecting a set of *N* >>1 particles $\{x_k^{(i)}\}_{i=1\cdots N}$ and weights $\{w_k^{(i)}\}_{i=1\cdots N}$, such that the state PDF may be approximated (Doucet *et al.*, 2001) by the empirical distribution:

$$\tilde{\pi}_k^N(x_k) = \sum_{i=1}^{N} w_k^{(i)} \delta(x_k - x_k^{(i)}) \tag{3}$$

and the values of the particles weights $w_t^{(i)} \propto w(x_t^{(i)})$ can be computed by:

$$w(x_k^{(i)}) = w_{k-1}^{(i)} \cdot \frac{p(y_k \mid x_k^{(i)}) p(x_k^{(i)} \mid x_{k-1}^{(i)})}{q_k(x_k^{(i)} \mid x_{k-1}^{(i)})} \forall i \in \{1,...,N\} \tag{4}$$

where $q_k(x_k)$ denotes the importance sampling density function (Arulampalam et al., 2002). The choice of this importance density function $q_k(x_k)$ is critical for the performance of the particle filter scheme. In the particular case of classical PF, the value of the particle weights $w_k^{(i)}$ is computed by setting the importance density function equal to the a priori PDF for the state, i.e., $q_k(x_k \mid x_{k-1}) = p(x_k \mid x_{k-1})$ (Arulampalam et al., 2002). Although this choice of importance density is appropriate for estimating the most likely probability distribution according to a particular set of measurement data, it does not offer a good estimate of the probability of events associated to high-risk conditions with low likelihood. Indeed, the Risk-Sensitive PF (RSPF) seeks to solve this issue.

This paper uses the PF- and RSPF-based state PDF estimates to implement detector modules. In addition, it explores the possibility of using information-theoretic measures to analyze those estimates, to perform early detection of SOH regeneration phenomena that may take place on ESDs.

3.1 Anomaly Detection based on Classic Particle Filtering Algorithms

PF-based anomaly detection modules (Orchard and Vachtsevanos, 2009) have been used in the past to identify abnormal conditions in nonlinear, non-Gaussian dynamic systems. The objective in this type of implementations is to fuse the information that is available at a feature vector (measurements) to generate estimates of the *a priori* state PDF that could be helpful when determining either the operating condition (mode) of a system or deviations from desired behavioral patterns. This compromise between model-based and data-driven techniques is accomplished by the use of a PF-based module built upon the nonlinear dynamic state model. PF-based detection modules provide a framework where customer specifications (such as false alarm rate and desired probability of detection) can be easily managed and incorporated within the algorithm design parameters.

This paper uses the PF-based detection module presented in (Olivares et al., 2012) as the baseline to compare other detection approaches. This module applies a hypothesis testing procedure, where the *a priori* PF-based PDF estimate at time *k* is used to compute a time-varying threshold $T(k)$, which is defined as the largest scalar such that the sum of the weights $w_k^{(i)}$, for all particles that satisfy $x_k^{(i)} \geq T(k)$, is greater than the desired false alarm rate α%. As a result, the detection module performs a hypothesis test (with a false alarms rate α% determined by the user) for the measurement y_k, considering the a priori one-step ahead prediction of the system output as the PDF that characterizes the null hypothesis (self-recharge phenomena either does not exist or is fading in time). On the other hand, if the null hypothesis is rejected at cycle *k*, then measurement y_k is larger than the detection threshold for α% statistical confidence of the one-step ahead prediction PDF.

3.2 Anomaly Detection based on Risk-Sensitive Particle Filtering

The problem of early detection using PF-based approaches has also been discussed in (Orchard et al, 2008), where a Risk-Sensitive PF framework complements the benefits of the classic approach, by representing the probability of rare events (in this particular case, the capacity regeneration phenomena on ESDs) within the formulation of an importance density function that aims at generating more particles in high-risk regions of the state-space. Mathematically, the importance distribution is set as:

$$q(d_k, x_k \mid d_{k-1}^{(i)}, x_{k-1}^{(i)}, y_{1:k}) = \gamma_k \cdot r(d_k) \cdot p(d_k, x_k \mid y_k) \tag{5}$$

where d_k is a set of discrete-valued states representing fault modes, x_k is a set of continuous-valued states that describe the evolution of the system given those operating conditions, $r(d_k)$ is a positive risk function that is dependent on the fault mode, and γ_k is a normalizing constant. Thus, a RSPF-based detection module should define a risk importance sampling distribution that ensures the existence of particles in the tails of the state PDF; to help representing the event of unlikely regeneration phenomena. In situations where effectively the data shows no signs of these events, the weights of the particles located at the tails of the PDF should decrease over time. The formulation of the hypothesis test and its corresponding threshold is similar to what has been already discussed in the case of PF-based detection modules.
The assumption that an anomaly should affect the qualitative behavior of the state PDF estimate motivates the use of information-theoretic measures (Cover and Thomas, 1991) to complements the paradigm of hypothesis testing procedures based on PF/RSPF-based anomaly detection modules. The following section focuses on the most important concepts that need to be taken into account when implementing these measures (in this case, entropy) to analyze and characterize sampled versions of the posterior PDF.

4. Information-Theoretic Measures Applied to PF Approach

Several examples that incorporate information-theoretic measures to analyze the outputs of particle filtering algorithms can be found in literature (Ajgl and Šimandl, 2011). This article aims at the formulation of anomaly detection modules based on PF, which are combined with the use of theoretical information measurements, particularly focused on the widely known information-theoretic measures like differential entropy (Cover and Thomas, 1991).

4.1 Differential Entropy

Entropy is a measure of uncertainty that is associated to a probability measure. In particular, the differential entropy *H* of a probability density function $p(x)$ is given by:

$$H(p) = -\int p(x)\log(p(x))dx \tag{6}$$

Few additional considerations are required when trying to compute it in the case of PF-based estimates of the conditional state PDF. Indeed, the differential entropy of PF-based estimates of the posterior state PDF, given a set of measurements $y_1,\ldots, y_k$, is computed as in (7):

$$H(p(x_k \mid y_k)) = \log\left(\sum_{i=1}^{N} w_{k/k-1}^{(i)} p(y_k \mid x_k^{(i)})\right) - \sum_{j=1}^{N} w_{k/k}^{(j)}\left[\log\left(p(y_k \mid x_k^{(j)})\right) + \log\left(\sum_{i=1}^{N} w_{k-1/k-1}^{(i)} p(x_k^{(j)} \mid x_{k-1}^{(i)})\right)\right] \tag{7}$$

where $w_{k/k-1}^{(i)}$ are the particle weights. The latter expression will be of use when evaluating the uncertainty associated to online estimates in dynamic processes. More details can be found in (Orguner, 2009).
Entropy-related applications for PF algorithms generally aim at evaluating how many i.i.d. samples does the filtering algorithm require to represent regions of the state space that accumulate the majority of the

probability mass, for a given state PDF estimate $p(x)$. This is useful because the entropy indicator should remain stable around a particular value while no regenerations of the SOH are detected. On the contrary, the entropy should suddenly increase when this phenomena is present, allowing to set a threshold to determine if an increment of the SOH is detected as a regeneration of its capacity. In this sense, the proposed anomaly detection scheme uses the fact that any sudden abnormal condition in the battery degradation process should affect the distribution of the PF-based posterior state estimate. This is caused by the fact that, under abnormal operating conditions, the system model no longer represents the best choice for the importance sampling distribution. As a consequence, the weights associated to particles with low-likelihood undergo strong corrections, increasing the differential entropy of the aforementioned conditional state PDF.

5. Case Study: Detection of Capacity Regeneration Phenomena in Lithium-ion Batteries

Self-recharge phenomena detection in Li-ion batteries has been selected as case of study to compare the different aforementioned detection modules. Verification of the proposed detection schemes is performed using simulated data for SOH accelerated degradation test (Olivares et al., 2012), to ensure absolute knowledge on the time instant where a regeneration phenomenon occurs. Performance is evaluated by computing several realizations of the stochastic process that defines each one of the proposed PF-based detection modules, and estimating the type I and II errors. Also, the impact that each detection scheme has on the Bayesian processor that estimates the battery SOH is measured in terms of the mean-squared error MSE for the posterior estimate. The analysis was made using 10 different data sets that capture the behavior of an accelerated degradation process for Li-ion batteries. The primary concept behind the proposed anomaly detection schemes is that any sudden abnormal behavior in the system should affect the posteriori distribution of the PF-based state estimate. The latter, based on the fact that under abnormal operating conditions the system model will no longer be represented by the importance sampling distribution. In this sense, the first proposed detection approach uses a PF algorithm based on model (1)-(2) as state estimator, in combination with PF-based hypothesis testing procedures ("Base Case/PF", Section 3.1). The second scheme considers the same type of state estimator, but a RSPF-based detection module instead ("Base Case/RSPF"). Two other anomaly detection approaches, implemented for completion purposes, use a threshold for the entropy of the posterior state PDF estimate: "Entropy/PF" and "Entropy/RSPF". The former uses a classic PF algorithm for estimation purposes, while the latter utilizes a risk-sensitive PF algorithm. Figure 2 shows the ROC curves for each proposed detection module, describing their performance in terms of the false alarm rate (α) and detection probability (β).

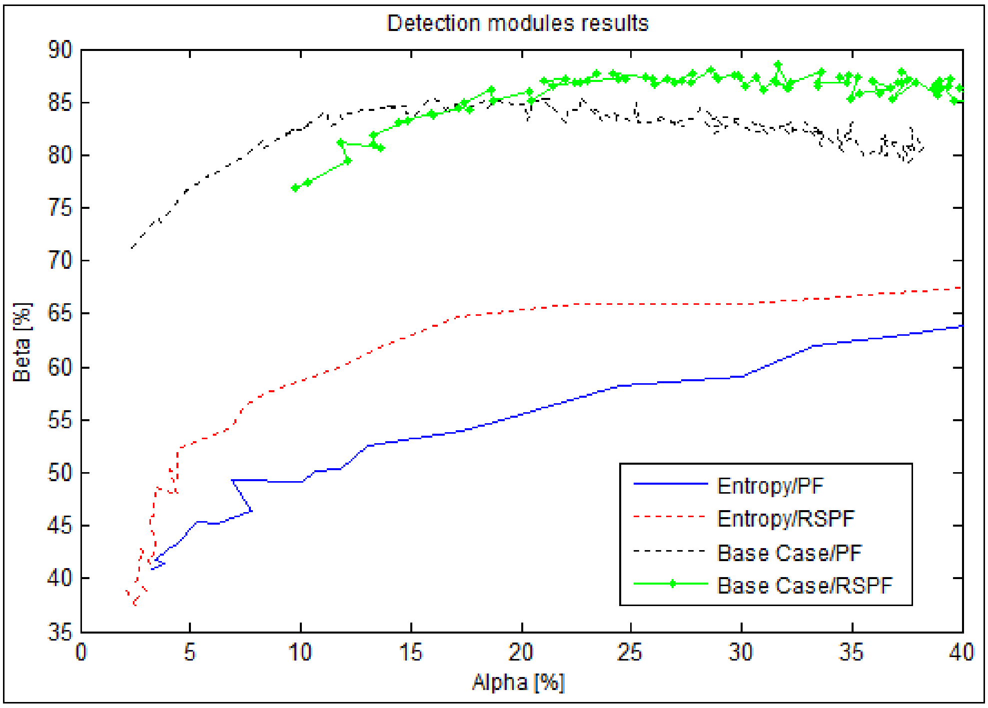

Figure 2: Performance comparison of detection approaches for capacity regeneration phenomena

Figure 2 shows that PF- and RSPF-based hypothesis testing procedures have better performance than other detection schemes. Evidences indicate that this is mainly caused by the fact that their construction emulates the implementation of a likelihood ratio test (best test of a simple hypothesis against an alternative), thus trying to maximize the probability of detection for a given probability of false alarm (α). Furthermore, it is important to note that both RSPF-based detection modules show improvements over the classic PF scheme, in terms of maximizing the probability of detection. Evidence, in this case, supports this statement mainly because these approaches incorporate the regeneration phenomena effect in the importance sampling distribution, allowing better detection rates and early detection. All proposed approaches obtained similar results in terms of the estimation MSE.

6. Conclusion

This paper presents a set of anomaly detection modules that are specifically used to identify capacity regeneration phenomena in ESDs, and more particularly in Li-ion batteries. All the proposed approaches use a PF-based SOH estimation procedure and incorporate information of detected regeneration phenomena as exogenous inputs in a state transition model for battery degradation. A throughout performance analysis that considered type I and type II detection errors and MSE of the state estimator was conducted to evaluate the contribution of entropy-based detectors with respect to hypothesis testing procedures based both on the classic PF and risk-sensitive algorithms. From obtained results, we surmise that the implementation of hypothesis testing procedures outperforms entropy-based approaches for detection of capacity regeneration; although the choice of classic PF algorithms versus risk-sensitive variants depends on the desired probability of detection. The latter, because a detector that computes a fault indicator from posterior state PDF estimate is more capable of isolating regeneration phenomena in the degradation curve, if the a priori PDF incorporates those in the importance sampling distribution.

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