MASTER

Mathematical strategies and experimental aspects for SOC estimation of the recharge battery

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MASTER'S THESIS

Mathematical Strategies and Experimental Aspects for State-of-Charge Estimation of the NiMH Rechargeable Battery

by

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Professor P.L. Davies

Eindhoven, November 2006
The work that resulted in this Master's thesis began back in September 2003, when I joined the Battery Modelling and Management project: A joint project of EURANDOM, Philips Research and the Eindhoven University of Technology. I am much indebted to all the participants of this project, as I am indebted to three of them in particular: William Rey, Evgeny Verbitskiy and Peter Notten. I would like to express all my gratitude to You. Thank you for being my Teachers, both in the research and in the formation of my life. I am grateful for all our talks/discussions/debates, for your always straightforward opinions, criticism when it was necessary and at the same time very strong encourage. I have hugely benefitted from their ability to come up with (and solve) new and challenging problems. Our joint work has led to the material covered in Chapter 2.

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Contents

1 Introduction .................................................. 7
   1.1 Battery technology and applications ....................... 7
       1.1.1 General operational mechanism of batteries .......... 8
       1.1.2 Battery types and characteristics .................... 10
   1.2 State-of-Charge indication .................................. 11
       1.2.1 Motivation of an accurate SoC indication ............... 11
       1.2.2 Possible State-of-Charge indication methods .......... 12
   1.3 Scope of this thesis .......................................... 12

2 Karhunen-Loève Expansion and its Application to SoC Estimation 15
   2.1 Orthogonal Transforms: Principal Component Analysis and Karhunen-Loève Expansion, are they different? ............... 15
       2.1.1 Introduction ............................................. 16
       2.1.2 Singular Value Decomposition ............................ 17
       2.1.3 Karhunen-Loève Expansion .............................. 18
       2.1.4 Principal Component Analysis ............................ 19
       2.1.5 Relationships and Conclusions .......................... 21
   2.2 Battery open-circuit voltage estimation by a method of statistical analysis 27
       2.2.1 Introduction ............................................. 27
       2.2.2 Experimental setup of the "constant current" experiment ...... 28
       2.2.3 Open-circuit voltage estimation: KLE and extrapolation .......... 29
       2.2.4 Open-circuit voltage estimation: experimental approach ........ 33
       2.2.5 Conclusions ............................................. 35

3 Single-Index Models and their Application to SoC Estimation 37
   3.1 A survey about Single-Index models theory ................ 37
       3.1.1 Definition .............................................. 37
<table>
<thead>
<tr>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1.2</td>
</tr>
<tr>
<td>3.1.3</td>
</tr>
<tr>
<td>3.2</td>
</tr>
<tr>
<td>3.2.1</td>
</tr>
<tr>
<td>3.2.2</td>
</tr>
<tr>
<td>3.2.3</td>
</tr>
<tr>
<td>3.3</td>
</tr>
<tr>
<td>3.3.1</td>
</tr>
<tr>
<td>3.3.2</td>
</tr>
<tr>
<td>3.3.3</td>
</tr>
<tr>
<td>3.4</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Section</th>
</tr>
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<tbody>
<tr>
<td>A</td>
</tr>
<tr>
<td>A.1</td>
</tr>
</tbody>
</table>
Chapter 1

Introduction

Due to the fact that people want to have a more mobile life, there is an increasing demand for mobile devices. When mains power supply is not available for power delivery of these devices they have to rely on a portable power supply such as a battery. From that point of view it becomes important that users can trust the indicated remaining run-time and the State-of-Charge (SoC), which is defined as the percentage of charge that is present inside the battery. Otherwise, users will charge the battery more often resulting in a faster wear out of the batteries Aylor et al. (1992).

First, this chapter will briefly describe the general operational mechanism of batteries and the characteristics of the best-known batteries with their applications. Secondly, the importance of an accurate State-of-Charge determination will be presented and possible SoC indication methods will be discussed. Finally, the area of actual research will be motivated and the scope of this thesis will be defined.

1.1 Battery technology and applications

Portable electronic devices have become ubiquitous in modern society. The recent rapid expansion in the use of portable computers, personal data assistants, cellular phones, camcorders and power tools creates a strong demand for fast deployment of battery technologies at an unprecedented rate. The design of such a portable device requires many battery-management features, including charge control, battery capacity monitoring, remaining
run-time information, compensation of battery capacity and remaining run-time due to environmental conditions, charge-cycle counting, etc, Pop et al. (2005).

Batteries have been around for a long time. In 1800, Volta discovered that a continuous flow of electrical force was generated when using certain fluids as conductors to promote an electrochemical reaction between two metals or electrodes Buchmann (2001). This led to the invention of the first voltaic cell, better known as the battery.

Later in 1859, the French physicist Gaston Plante invented the first rechargeable battery. This secondary battery was based on leadacid (LA) chemistry, a system that is still used today. In 1899, Waldmar Jungner from Sweden invented the nickelcadmium (NiCd) battery, which used nickel for the positive electrode and cadmium for the negative. Two years later, Edison produced an alternative design by replacing cadmium with iron. Due to high material costs compared to dry cells or LA storage batteries, the practical applications of the nickelcadmium and nickeliron batteries were limited. It was not until Schlecht and Ackermann invented the sintered pole plate in 1932 that large improvements were achieved. These advancements were reflected in higher load currents and improved longevity. The sealed nickelcadmium battery, as known today, only became available when Neumann succeeded in completely sealing the cell in 1947, Buchmann (2001). In the following years the hydride-forming electrode has proven to be a serious alternative to the cadmium electrode, which was widely employed in rechargeable nickelcadmium batteries. The nickelmetal hydride (NiMH) battery became commercially available in the 1990s, Notten and van Beek (2000).

1.1.1 General operational mechanism of batteries

In its simplest definition, a battery is a device capable of converting chemical energy into electrical energy and vice versa. The chemical energy is stored in the electro-active species of the two electrodes inside the battery. The conversions occur through electrochemical reductionoxidation (redox) or charge-transfer reactions, Bergveld et al. (2002). These reactions involve the exchange of electrons between electro-active species in the two electrodes through an electrical circuit external to the battery. The reactions take place at the electrode/electrolyte interfaces. When current flows through the battery, an oxidation reaction will take place at the anode and a reduction reaction at the cathode. The oxidation reaction yields electrons to the external circuit, while a reduction reaction takes up these electrons from the external circuit. The electrolyte serves as an intermediate between the electrodes. It offers a medium for the transfer of ions. Hence, current flow is supported by electrons inside the electrodes and by ions inside the electrolyte. Externally, the current
Figure 1.1: Electrochemical operation of a battery during charging a) and discharging b) 

flows through the charger or load, Bergveld et al. (2002). The charging and discharging of a battery are schematically illustrated in Figure 1.1 a) and b) respectively. In both cases, the negative electrode (-) is shown on the left and the positive electrode (+) on the right. Figure 1.1 shows that oxidation occurs at the positive electrode during charging, whereas reduction occurs at the negative electrode. The reverse takes place during discharging. The basic electrochemical unit of a battery is called a cell, but commonly the word battery is used for one cell or for two or more cells connected in series/parallel.

During the lifetime of a battery, its performance or health tends to deteriorate gradually due to irreversible physical and chemical changes that take place with usage and with age until eventually the battery is no longer usable. The State-of-Health is an indication of the point that has been reached in the life cycle of the battery and a measure of its condition relative to a fresh battery. Ageing of the battery is a complex process that involves many parameters of the battery (e.g., impedance, conductance, capacity) of which the most important is the capacity of the battery.

While the most significant progress in portable energy storage depends on the developments in chemical technology and material sciences, other areas such as charge regulation and battery monitoring can contribute significantly to the life-time performance of these batteries.

It is of most importance that the battery management system (BMS) which controls
charging and discharging of the battery, operates with an accurate estimate of the energy stored in the battery at any given time. The available fraction of the full capacity is called the State-of-Charge (SoC). An accurate estimation of the State-of-Charge is one of the main tasks of the BMS, Bergveld et al. (1999), Bergveld et al. (2002).

1.1.2 Battery types and characteristics

The general operational mechanism of a battery and characteristics of the most important rechargeable batteries available in the market today, e.g. NiCd, NiMH and Li-ion batteries will be given in the remainder of this section.

NiCd batteries. Advantages of the NiCd batteries are their fast charge and discharge times: it is possible to charge a battery in 10 min and large currents can be supplied. NiCd batteries have a cell voltage of 1.2 Volt and can be used in many devices. Especially in tools demanding much power the NiCd battery is often found. Other applications include cordless and mobile phones, shavers, camcorders, portable audio products and laptop computers. Disadvantages of the NiCd batteries are their low-energy density and their so-called memory effect. The memory effect causes the battery to deliver only the capacity, which was used during the repeated charge/discharge cycles before. Because of this the whole capacity of the NiCd batteries should be used for each discharge cycle to avoid a decrease of the maximum capacity, Bergveld et al. (2002). Another disadvantage is the presence of cadmium, which is an environmental hazard. This may lead to a complete ban on NiCd batteries in the future.

NiMH batteries. The major difference between NiCd and NiMH batteries is the fact that in a NiMH battery a metal hydride alloy is used for the electrode instead of the cadmium. In this way a higher energy density is obtained, the memory effect is reduced and the environmental impact is decreased. Besides, NiMH batteries can replace NiCd batteries because of the same cell voltage of 1.2V. Applications include cordless and mobile phones, shavers, camcorders, portable audio products and laptop computers. A disadvantage of the NiMH battery is the relatively high self-discharge rate and the relatively low robustness with respect to overcharging, which is made worse by the fact that it is more difficult to detect the battery-full condition during charging, Bergveld et al. (2002).

Li-ion batteries. The chemistry in Li-ion batteries is difficult to compare with Ni-based batteries. They have intercalation electrodes what means that they have a lattice structure in which the host material stays the same while guest species can be inserted or extracted. They are based on the rocking chair principle: lithium ions are transferred from the positive to the negative electrode during charging or vice versa during discharging.
Besides the chemistry of the Li-ion battery also some other properties differ a lot. The operating voltage has its average at 3.6 Volt which results in the fact that Li-ion and Ni-based batteries are not interchangeable and other charging and discharging methods are often required. Moreover Li-ion batteries have higher charge and discharge times making them unsuitable for appliance in high-power devices.

1.2 State-of-Charge indication

Almost as long as rechargeable batteries exist there are systems that are able to give some indication about the State-of-Charge (SoC) of the battery. These systems were mostly simple volt-gauges and they gave only a little clue about the charge that is present in the battery, Aylor et al. (1992). Especially at low SoC the indicated SoC was very inaccurate. Besides that the user has to know most times actual information about the battery in order to translate the indicated values to an estimate of the remaining run-time.

Nowadays there exist better SoC indication systems which measure more properties of the battery than only the voltage such as current, relaxation time which are dependent on the temperature. This results in more accurate systems. In real-world applications where the behavior of the battery as well as the user behavior is difficult to predict, the indication systems still perform not so accurate and more improvements must to be added.

1.2.1 Motivation of an accurate SoC indication

An accurate SoC determination method and an understandable and reliable SoC display to the user will improve the performance and reliability, and will ultimately lengthen the lifetime of the battery. Accurate SoC information allows the battery to be used within the design limits, so the pack does not need to be over-engineered. This allows a smaller, lighter battery, which costs less. However, many examples of poor accuracy and reliability can be found in practice. A poor reliability of the SoC indication system may induce the use of only part of the available battery capacity. For example, the user may be inclined to recharge the battery every day, even when enough battery capacity is indicated on the portable device. This will lead to more frequent recharging than strictly necessary, which in turn leads to an earlier wear-out of the battery. The effect of inaccuracy of SoC indication can be even worse when the SoC value is also used to control charging. The battery is either not fully charged or it is overcharged. In the former case, the battery will be recharged more often than needed, which will lead to an earlier wear-out. In the latter case, frequent overcharging will lead to a lower cycle life, Bergveld et al. (2002).
These examples motivate the request for an accurate and reliable SoC indicator system in portable applications.

1.2.2 Possible State-of-Charge indication methods

Several methods in the art of determining the SoC of a cell or battery of cells are known. Some older, very inexpensive fuel gauges simply measured voltage. This battery voltage is a highly inaccurate indication of a battery's capacity, because it changes with temperature, discharge rates and ageing. Another known method of measuring SoC involves impedance measurements utilizing bridge circuits that are manually adjusted. The measurements obtained are compared with previously generated standard reference curves. Still another prior-art method used to determine the battery SoC involves estimating the SoC by means of the battery response to current or voltage pulses. These pulse systems provide a rough means of determining the SoC and are used primarily to determine if a battery is still useful. This first group of methods will be called direct measurements.

Another known method is to measure the current flowing into and out of a battery and to integrate this current over time in order to determine its capacity, Bergveld et al. (1999). When utilizing these current integrators one must correct the estimation of the SoC obtained, since several battery-related factors affect the accuracy of this estimation. These factors include temperature, history, charge and discharge efficiencies and cycle life. The integration of current is referred to in literature as Coulomb counting, Bergveld et al. (2002). When this method is compensated for discharging efficiency, self-discharge and capacity loss then this method is presented as a book-keeping system, Bergveld et al. (2002).

The main problem in designing an accurate SoC indication system is the unpredictability of both battery and user behavior. In this case an adaptive system has to be used, which is based on direct measurement, book-keeping or a combination of the two, Bergveld et al. (2002).

1.3 Scope of this thesis

The goal of this Master's thesis is to propose several statistical methods applicable for the indication of the battery State-of-Charge. The statistical approach is selected in order to give a satisfactory prediction of battery performance, but be simple and accurate enough to enable on-line identification and adaptation of model parameters based on the
measurements of voltage during battery operation in the course of charge and discharge experiments under controlled conditions.

In the second chapter we propose a method for determining the open-circuit voltage (OCV). By definition, the open-circuit voltage is the battery voltage under the equilibrium conditions, i.e. the voltage when no current is flowing in or out of the battery, and, hence no reactions occur inside the battery. The OCV is directly proportional to the battery SoC and can be calculated using the following equation:

\[ \text{OCV} = V_{\text{term}} + IR, \]

where \( V_{\text{term}} \) is the battery terminal voltage, \( I \) the actual battery current considered as a positive value during discharge and as a negative value during charge and \( R \) is the internal resistance. Note that \( \text{OCV} = V_{\text{term}} \) when \( I = 0 \), but after current interruption this takes a while due to several relaxation processes occurring inside a battery. In addition to the OCV, the method presented by Eby (1978) also uses the voltage under load to determine the SoC of a LA storage battery during a discharge cycle.

Our approach is based on Karhunen-Loève (KL) dimension reduction and modelling the dependence of the KL coefficients on physical parameters of the experiment.

Karhunen-Loève expansion, as well as principal components analysis (PCA), form the basis for multivariate data analysis. Although similar in their goals and essence, one may be more appropriate than the other for a particular application. In this chapter, prior to the application, we review the concepts and basic derivations of the both methods, give appropriate geometric interpretations and compare the two methods. The goal for such an analysis is to emphasize the often ignored difference between the principal component analysis and the Karhunen-Loève expansion and to reveal advantages of appropriately choosing between the two.

In the third chapter we find ourselves under conditions that are closer to the real user's behavior (the charging and discharging of the battery is operated according to the specially designed scheme of "varying-currents") and estimate the amount of charge presented in the battery under these operational conditions.

To be able to extract information on SoC from the shape of voltage curves adapted to the different current regimes, we use Single-Index model's (SIM) theory, which is going to be present in the form of the literature survey with the main underlying results and basic techniques, as well as of a new approach we propose for estimation of unknown index-coefficients and a link-function in SIM by solving \( L_1 \)-problem under the monotonicity
constrains. We illustrate the performance of the proposed procedure for some simulated data sets, comparing the results with the existing methods, and apply it directly to our main problem of estimating State-of-Charge of the battery.

Technically speaking, our new approach offers a very simple and efficient way of estimating index-coefficients and appears to be computationally feasible. Results, obtained after applying this procedure to the problem of SoC estimation, confirm that information on SoC is present in voltage curves of the "varying-current" experiment and allow to conclude that the dynamic response of the system while the battery is under operation can be used for the reliable State-of-Charge indication.
2.1 Orthogonal Transforms: Principal Component Analysis and Karhunen-Loève Expansion, are they different?

The principal components analysis and the Karhunen-Loève expansion are two similar linear methods that have proven to be extremely useful in the study of physical, biological, electrochemical and other complex phenomena. By providing insight into the intrinsic structure of data, these techniques offer means to compress the data, to filter out and to estimate noise. Although similar in their goals and essence, one may be more appropriate than the other for a particular application.

In this section we review the concepts and basic derivations of both methods, give appropriate geometric interpretations and compare the two methods.
2.1.1 Introduction

Principal components analysis (PCA) and Karhunen-Loève expansion (KLE) form the basis for multivariate data analysis, see Hotelling (1933), Jackson (1991). These techniques have been used to examine a wide range of data sets in many disciplines as diverse as chemistry, sociology, economics, psychology, biology, etc. Being similar in their concepts and mathematical implementations, they remain different and each of them has characteristics that may be appropriate for particular applications.

In the literature on data analysis much attention is devoted to the orthogonal transforms of a data matrix. Many authors refer to KLE while treating the PCA. So, Ahmed and Rao (1975), treat the Karhunen-Loève expansion in the context of data compression and refer to the similar technique of principal components analysis in statistics. Their definition of KLE is identical with the definition of PCA given by Anderson (1958). We found these remarks confusing and will try to unravel the situation around these techniques.

The goal of this section is to emphasize the often ignored difference between the principal component analysis and the Karhunen-Loève expansion and to reveal advantages of appropriately choosing between the two.

KLE is an approximation technique: the data are projected onto a lower dimensional linear subspace which minimizes the sum of the squared deviations of the data vectors from their projections onto that subspace. This results in the representation of the data in terms of an orthogonal basis for that subspace. This representation is the most efficient in the mean-square sense, and in particular, no other representation with fewer basis functions can achieve the resulting accuracy. PCA is a statistical method designed to extract and display the systematic variation in the data.

Although the viewpoints are quite different, the implementations are very closely related: Singular Value Decomposition (SVD) is applied in both cases to determine unique orthogonal basis functions (eigenvectors) and the corresponding singular values. This difference of viewpoints delineates the fields of applicability of each of these methods.

In technical terms, principal components analysis centers the observations by subtracting their means, and the SVD is then carried out on the covariance matrix. By capturing the variance over their respective domains as efficiently as possible, the basis functions catch the structure of the data. The Karhunen-Loève expansion does not transform the data prior to the SVD. Hence, unlike PCA, KLE is not translation-invariant. At the same time, KLE allows one to interpret the retained eigenvectors as the most dominant and significant components of the data. The corresponding singular values represent the amplitude explained in the original data, but not the variance. These mathematical con-
Orthogonal Transforms: Principal Component Analysis and Karhunen-Loève Expansion, are they different? 17

straints help to recognize interesting structures in the data and to describe relationships within the data.

In this section we give comparative assessment of both methods and illustrate geometric perspective in order to poster an intuitive understanding of the techniques. In subsection 2.1.2 we define the singular value decomposition and mention some of its properties and applications. In subsection 2.1.3 the Karhunen-Loève expansion will be given the same treatment, followed in subsection 2.1.4 by principal component analysis. In subsection 2.1.5 the relationships between these transforms are investigated and their similarities and dissimilarities are exposed.

2.1.2 Singular Value Decomposition

According to a well-known result of linear algebra, a fundamental matrix decomposition theorem, Lanczos (1961), any real $n \times m$ matrix $X$ of rank $k \leq \min \{n, m\}$ can be decomposed as

$$X = U\Sigma V',$$  \hspace{1cm} (2.1)

where $U$ is an $n \times k$ orthogonal matrix, $\Sigma = \text{diag}(\sigma_1, ... \sigma_k)$ is $k \times k$ diagonal matrix with elements $\sigma_1 \geq ... \geq \sigma_k \geq 0$, and the transpose of $m \times k$ column-orthogonal matrix $V$. The various shapes of these matrices will be made clearer by Figure 2.1. The orthogonal $n \times k$ matrix $U$ and the orthogonal $m \times k$ matrix $V$ are defined by

$$XX' = U\Sigma^2 U', \quad X'X = V\Sigma^2 V'. \hspace{1cm} (2.2)$$

Hence, the columns of $U$ are eigenvectors of $XX'$ and the columns of $V$ are eigenvectors of $X'X$. Consequently,

$$U'U = V'V = I_p. \hspace{1cm} (2.3)$$

The diagonal entries of $\Sigma$, called the singular values of $X$, are the positive square roots of the eigenvalues of $XX'$ as well as $X'X$. They are ordered in decreasing values. The decomposition (2.1) is usually referred to as the Singular Value Decomposition (SVD). With $U = (u_1, ..., u_k)$ and $V = (v_1, ..., v_k)$, equation (2.1) can be written as

$$X = \sum_{j=1}^{k} \sigma_j u_j v_j', \hspace{1cm} (2.4)$$

where the product $u_j v_j'$ is an $n \times m$ matrix. Equation (2.4) shows that the SVD constitutes an expansion of $n \times m$ matrix $X$ into a sum of rank-1 matrices.
Karhunen-Loève Expansion and its Application to SoC Estimation

![Figure 2.1: Singular value decomposition of a matrix of rank k those number of columns m is greater than or equal to its number of rows n.](image)

If we consider the approximation of $X$ given by

$$X_p = \sum_{j=1}^{p} \sigma_j u_j v_j'$$

with $p < k$, $k$ being the rank of $X$, then it is a best approximation of $X$ in the sense that

$$\|X - X_p\|^2 = \text{min}.$$  \hspace{1cm} (2.6)

In other words, the approximation of $X$ obtained by (2.5) is the best approximation of rank not greater than $k$ in the least-square sense.

### 2.1.3 Karhunen-Loève Expansion

Given a data set, Karhunen-Loève expansion (KLE) can be used as a tool to project these data onto a lower dimensional linear subspace which minimizes the sum of the squared deviations of the data vectors from their projections onto that subspace. Thereby it helps to select interesting structures in the data and to describe relationships within the data.

Let $Y$ be an $n \times m$ matrix with $n$ objects sampled in $m$ points in time, $n < m$. For $p \in [1, n]$, the Karhunen-Loève rank $p$ approximation $Y_p$ of $Y$ is:

$$Y \approx Y_p = AF' \text{ or } y_i \approx \sum_{j=1}^{p} \alpha_{i,j} f_j';$$

where $i = 1, \ldots, n$ and the $p$ columns of $F$ are the first $p$ eigenvectors of the $m \times m$ matrix $Y'Y$. The matrix $Y'Y$ is non-negative definite, its eigenvectors are orthogonal to one another. Therefore they constitute an orthogonal basis for the space of the data called Karhunen-Loève basis functions. Such an orthogonal decomposition gives the best representation that is achieving minimization of the mean-square error while making use
Orthogonal Transforms: Principal Component Analysis and Karhunen-Loève Expansion, are they different?

of a limited number, $p$, of terms:

$$\hat{A}, \hat{F}' = \arg \min_{A,F'} \{\|Y - AF'\|^2\}$$

(2.8)

under restriction $F'F = I_p$.

The global minimum to this minimization problem is obtained by performing the singular value decomposition (2.1). Then the Karhunen-Loève rank $p$ approximation $Y_p$ of $Y$ (2.7) can be written in the following form:

$$Y_p = U_p \Sigma_p V_p'$$

(2.9)

where $\Sigma_p = \text{diag}(\sigma_1, \ldots, \sigma_p)$, $U_p$ is an $n \times p$ matrix (first $p$ columns of $U$), and $V_p$ is an $m \times p$ matrix (first $p$ columns of $V$).

The Karhunen-Loève approximation $Y_p$ of $Y$ can be interpreted as follows. Denote by $y_1, \ldots, y_n \in \mathbb{R}^m$ the rows of $Y$. Suppose that we are looking for a linear subspace $W \subset \mathbb{R}^m$, $\dim(W) = p$, such that

$$\sum_{i=1}^{n} \|y_i - P_W(y_i)\|^2$$

(2.10)

is minimal, where $P_W(y)$ denotes the projection of vector $y$ to $W$. Then the rows of $V_p'$ form the basis $F'$ of the optimal subspace $W$, and the optimal projections are given by

$$P_W(y_i) = [\alpha_{i,1}, \ldots, \alpha_{i,p}] V_p', \quad i = 1, \ldots, n.$$ 

(2.11)

The matrix of Karhunen-Loève coefficients $A = (\alpha_{i,j})_{i=1,j=1}^{n,p}$ satisfies $A = U_p \Sigma_p$.

In practical applications, where KLE is used as a dimensionality reduction method, the choice of the parameter $p$ depends on the associated singular values, see Karlis et al. (2003).

2.1.4 Principal Component Analysis

Principal component analysis (PCA), a statistical method designed to extract and display the systematic variation in the data, has been well established in the literature and it has become one of the most useful tools for data modelling, compression and visualization. In this subsection, we show that the SVD solves the PCA.

The goal of the principal component analysis is to find a projection of the data onto subspace with a maximum spread of the data points, as measured by the covariance.

We first examine the more intuitive geometric approach to PCA. That is, one tries to find a subspace $S$ where the data points are as separated as possible. Starting with the
Karhunen-Loève Expansion and its Application to SoC Estimation

$n \times m$ data matrix $Y$, let us assume that the dimension of the subspace $p$ is known. Then every point $y_i$ on a $p$-dimensional subspace in $\mathbb{R}^m$ can be represented as

\[ y_i = y_0 + \beta_i G_p', \quad i = 1, \ldots, n, \quad (2.12) \]

where $y_0 \in \mathbb{R}^m$ is any fixed point in the subspace, $G_p$ is $m \times p$ with $p$ orthonormal column vectors, and $\beta_i \in \mathbb{R}^p$ is simply the vector of new coordinates of $y_i$ in the subspace. Therefore, we need some additional constraints in order to end up with a unique solution to the problem of finding a subspace where the data points become to be as separated as possible. A common constraint is to impose that the mean of $\beta_i$ is zero:

\[ \tilde{\beta} = \frac{1}{n} \sum_{i=1}^{n} \beta_i = 0, \quad (2.13) \]

and this yields to $\tilde{y}_0 = \tilde{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$.

We define the "optimal" subspace to be the one that minimizes the sum of squared error between $y_i$ and its projection on the subspace:

\[ \min_{G_p\{\beta_i\}} \sum_{i=1}^{n} \|y_i - \tilde{y} - \beta_i G_p'\|^2, \quad \text{s.t. } G_p' G_p = I_p. \quad (2.14) \]

By differentiation, we obtain the normal equations and

\[ \hat{\beta}_i = (y_i - \tilde{y}) G_p'. \quad (2.15) \]

The vector $\hat{\beta}_i \in \mathbb{R}^p$ is simply the coordinates of the projection of $y_i \in \mathbb{R}^m$ in the subspace $S$.

Then the original objective becomes one of finding an orthogonal $m \times p$ matrix $G_p$ that minimizes

\[ \min_{G_p} \sum_{i=1}^{n} \|(y_i - \tilde{y}) - (y_i - \tilde{y}) G_p G_p'\|^2. \quad (2.16) \]

Let us consider the centered $n \times m$ matrix $Y_{\text{centre}} = Y - \tilde{Y}$, where all rows of $\tilde{Y}$ are identical and equal to $\tilde{y}$.

Let $Y_{\text{centre}} = U \Sigma V'$ be the singular value decomposition of the matrix $Y_{\text{centre}}$. Then for any given $p \leq \min \{n, m\}$, a solution to PCA problem, $\hat{G}_p$ is exactly the first $p$ columns of $V'$; and $\hat{\beta}_i$ is the $i$th row of the $n \times p$ submatrix $U_p \Sigma_p$ of the matrix $U \Sigma$.

Thus, the SVD gives the solution to the PCA problem. The resulting matrix $V_p$ (together with the mean $\tilde{y}$ if the data is not zero-mean) provides a geometric description of the dominant subspace structure for all the points. The rows of the matrix $U_p \Sigma_p = (\hat{\beta}_1, \ldots, \hat{\beta}_n) \in \mathbb{R}^{n \times p}$ are the so-called principal components.
Orthogonal Transforms: Principal Component Analysis and Karhunen-Loève Expansion, are they different?

From the statistical standpoint, the column vectors of $V_p$ give the directions in which the data $Y$ has the largest variance. Then the $p$ principal components are defined to be $p$ uncorrelated linear components and the criterion can be formulated as follows:

Chose $G_p$ in a way such that points $(\beta_1, \ldots, \beta_n) \in \mathbb{R}^{n \times p}$ be as separated as possible, i.e.

$$
\hat{G}_p = \arg \max_{G_p} \{ \text{Var}(y_1G_p, \ldots, y_nG_p) \} \text{ and } G_p'G_p = I_p, \quad (2.17)
$$

where

$$
\text{Var}(y_1G_p, \ldots, y_nG_p) = \frac{1}{n-1} \sum_{i=1}^{n} [(y_i - \bar{y})G_p]^2, \quad \bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i. \quad (2.18)
$$

Combining (2.17) and (2.18), the criterion (2.17) becomes

$$
\hat{G}_p = \arg \max_{G_p} \{ \text{tr}(G_p' \text{Cov} G_p) \} \text{ and } G_p'G_p = I_p, \quad (2.19)
$$

where

$$
\text{Cov} = \frac{1}{n-1} Y'_{\text{centre}} Y_{\text{centre}}. \quad (2.20)
$$

Hence, $m \times p$ matrix $G_p$ is made of the first $p$ eigenvectors of $\text{Cov}$.

Indeed, if $Y_{\text{centre}}$ has the singular value decomposition $Y_{\text{centre}} = U \Sigma V'$, then $Y_{\text{centre}}' Y_{\text{centre}} = V \Sigma^2 V'$ is the eigenvalue decomposition of $Y_{\text{centre}}$. And if $\Sigma$ is ordered, then the first $p$ columns of $V$ are exactly the leading $p$ eigenvectors of $Y_{\text{centre}}' Y_{\text{centre}}$, which give the $p$ principal components $(\beta_1, \ldots, \beta_n)$.

Thus, in technical terms, PCA centers the observations by subtracting their means, and the SVD is then carried out on the covariance matrix, what allows extracting and displaying the systematic variation in the data.

### 2.1.5 Relationships and Conclusions

In this subsection we explore the relationships between the Karhunen-Loève expansion and principal component analysis, give appropriate geometric interpretations and compare the two methods.

Consider a matrix $Y$ with $n$ observations and $m$ variables. For this matrix we construct a variable space with as many dimensions as there are variables. Each variable represents one coordinate axis. Then each observation (each row) of the matrix $Y$ is placed in the $m$-dimensional variable space. Consequently, the rows in the data table form a swarm of points in this space, see the Figure 2.2a (for simplicity only two variable axes are displayed).

As it was shown in the subsection 2.1.2 the Karhunen-Loève expansion does not transform the data prior to the SVD, as opposed to the PCA, which centers the observations by
Figure 2.2: a). KLE: the observations in the data matrix \( Y \) can be understood as a swarm of points in the variable space; b). PCA: the mean-centering procedure corresponds to moving the origin of the coordinate system to coincide with the average point.

subtracting their averages from the data, and the SVD is then carried out on the covariance matrix. The subtraction of the averages from the data corresponds to a repositioning of the coordinate system, such that the average point now is the origin, see Figure 2.2b.

A geometric interpretation of the Karhunen-Loève expansion is in terms of a rotation of the coordinate system, see Figure 2.3a,c. The KL coefficients are the lines that best approximate the data in the mean-square sense. The principal components method can be described as a shift of the origin of the coordinate system to the average point, followed by the rotation as well, see Figure 2.3b,d. The principal components then are the lines which best account for the shape of the point swarm and represent the maximum variance directions in the data.

When two KL coefficients and principal components have been derived by applying SVD on the data matrix/covariance matrix correspondingly, and data has been rotated such that the KL coefficients/PC line along the axes, a plane into the \( m \)-dimensional variable space is defined. By projecting all the observations onto the low-dimensional subspace and plotting the results, it is possible to visualize the structure of the investigated data set. The coordinate values of the observations on this subspace form basis functions.

Frequently, one or two KL coefficients/PC are not enough to adequately summarize the information in a data set. In such cases, the descriptive ability of the orthogonal expansion is improved by using more KL coefficients/principal components. There are
Orthogonal Transforms: Principal Component Analysis and Karhunen-Loève Expansion, are they different?

Figure 2.3: a). The points in the data space and the first two KL coefficients; b). The points in the data space and the first two principal components; c). The points in the projected space by the KL coefficients; d). The points in the projected space by the principal components. Observe the rotation and, as well, the change of scale.
several approaches that can be used to evaluate how many of them are appropriate, see Jackson (1991).

Thus, giving a geometric interpretation of the KLE in terms of a rotation of the coordinate system and of the PCA in terms of a shift of the origin of the coordinate system to the average point, followed by the rotation as well, "you cannot say that any rotation is better than any other rotation from a statistical point of view: all rotations are equally good statistically. Therefore, the choice among different rotations must be based on non-statistical grounds...", (SAS/STAT User's guide, Vol.1, p.776).

In the case of using KLE, this technique allows one to interpret the retained KL basis functions as the most dominant and significant components of the data. KLE decomposes the data set into components that are of decreasing importance; these components are the basis functions and their importance is measured by the KL coefficients. By opposition, PCA is derived from the covariance matrix and therefore, it ignores the mean. In case the data set presents an important offset, its clearly appears in the first KLE component and could be missed in PCA. This difference of viewpoints delineates the fields of applicability of each of these methods.

Often, when the data observations are performed across many variables, it is not possible to make a visual inspection of the relationship between them. One way to make sense of this data is to reduce its dimension. Principal component analysis is an appropriate
Orthogonal Transforms: Principal Component Analysis and Karhunen-Loève Expansion, are they different?

Figure 2.5: a). Pressure during charging period of NiMH battery. b). First two KL basis functions.

technique for that. The goal of the PCA is to find a projection of the data onto a subspace with a maximum spread of the data points, as measured by the variance; the corresponding shift of the origin of the coordinate system to the average point is just a trick to relocate the observations, that helps to model the systematic variation of a data set. Thus, for example, to classify Iris data of Fisher (1939), PCA is applied to the covariance matrix, see Figure 2.4.

By opposition, the KLE is an approximation technique and it results in the representation of the data in terms of an orthogonal basis for the subspace which minimizes the sum of the squared deviations of the data from their projections onto that subspace. KLE can be recommended when data reduction is the main goal, see Figure 2.5a, where the curves have been obtained from the experiment during the charging period of a NiMH battery. The first two KL basis functions are the most significant components of the data, see Figure 2.5b. Typically, for the data sets with some intrinsic smoothness, most of the original amplitude is captured by the first few basis functions. KLE can be used to visualize data, as well; the plots obtained can appear similar to those of PCA, although they are usually of less quality. Similarly, PCA can be used to approximate a data set; but, as you must add one component for the average, the approximation is non-optimal.

Both methods, PCA and KLE, combine the original variables to define the projections. Hence, they are little interesting to identify variables in the original space. When variable selection is a feature of concern, a factor analysis rotation can be run after PCA or KLE.
to foster some of the variables.

Thus, in this section we illustrated the often ignored difference between the two orthogonal transforms, principal component analysis and the Karhunen-Loève expansion. We stressed advantages of choosing between them based on the specific characteristics of these methods.
2.2 Battery open-circuit voltage estimation by a method of statistical analysis

The basic task of a battery management system (BMS) is the optimal utilization of the stored energy and minimization of degradation effects. It is critical for a BMS that the State-of-Charge (SoC) is accurately determined. Open-circuit voltage (OCV) is directly related to the State-of-Charge of the battery, accurate estimation of the OCV leads to an accurate estimate of the SoC.

In this section we describe a statistical method to predict the open-circuit voltage on the basis of voltage curves obtained by charging batteries with different currents. We employ a dimension reduction method (Karhunen-Loève expansion) and linear regression. Results of our modelling approach are independently validated in a specially designed experiment.

2.2.1 Introduction

Several conventional approaches exist for determining the State-of-Charge. For Nickel-Metal Hydride (NiMH) batteries, one of these approaches is based on the measurements or estimation of electrical properties of the battery, such as its open-circuit voltage (OCV). By definition, the open-circuit voltage is the battery voltage under the equilibrium conditions, i.e. the voltage when no current is flowing in or out of the battery, and, hence no reactions occur inside the battery.

The open-circuit voltage is a function of State-of-Charge, \( OCV = f(\text{SoC}) \), and the function \( f \) is expected to remain the same during the life-time of the battery, i.e. it does not depend on the age of the battery. Note, however, that other battery characteristics do change with time, e.g. capacity is gradually decreasing as a function of the number of charge-discharge cycles. In this section we only consider the problem of estimating the OCV. The question of how exactly the OCV depends on the SoC will be addressed elsewhere, for example in Bergveld et al. (2005).

In this section, we study the voltage of the battery, which is being charged with a constant current. Roughly speaking, with twice the current the battery is charged in half the time. Therefore, to compare the results of charging experiments with different currents, we study the battery voltage not as a function of time, but of the so-called Depth-of-Charge (DoC),

\[
\text{DoC}(t) = \frac{It}{Q_{\text{nom}}},
\]

where \( I \) is the charging current, \( t \) is the charging time and \( Q_{\text{nom}} \) is the nominal capacity.
If one charges an empty battery, then, typically, in the first half of the charging period the State-of-Charge and the Depth-of-Charge coincide. Later, due to the presence of so-called side-reactions, the SoC increases slower than the DoC. Therefore, in the figures below the DoC can reach values larger than 100%, while SoC, by definition, does not exceed 100%.

The open-circuit voltage corresponds to equilibrium conditions. Therefore we estimate OCV as a limit of voltage curves corresponding to the decreasing sequence of currents. More specifically, using voltage curves obtained when various currents flow into the battery while it is being charged, we extrapolate to the current value equal to 0, hence obtaining the open-circuit voltage of the battery.

The second approach is based on a different limiting behavior. If a battery is left to "rest", then neglecting some physical processes such as self-discharge, we can assume that the battery voltage will stabilize to a certain value, which is the value of the open-circuit voltage at a given Depth-of-Charge. The relaxation period can take some time and the OCV is determined at the end of the resting period.

The first approach uses statistical methods to predict the OCV. The method maps a voltage curve to a small number of its Karhunen-Loève (KL) coefficients; each curve becomes a point in a low-dimensional space and each point describes a voltage curve obtained for a specific current. A polynomial regression is then applied to model the dependence of the KL coefficient on the current. Extrapolating the regression model to zero current yields an estimate of the KL coefficient of the OCV curve.

The second approach is purely experimental. It requires a large number of partial charging experiments followed with substantial resting periods. This approach, however, is not very suitable for the application in battery management systems.

A good agreement between the results in OCV estimation by both methods is demonstrated.

### 2.2.2 Experimental setup of the "constant current" experiment

All the experiments were performed with commercial AA size NiMH batteries of the type HHR110AAOK (Matsushita Battery Industries, Japan). The nominal battery capacity was about 1100 mAh at room temperature. The battery was placed on a special holder to ensure electrical connections. A pre-calibrated thermocouple is pasted on the battery to monitor the battery temperature. The set up was then placed in an ambient temperature controlled chamber. The battery voltage and temperature were measured during the experiment. Electrochemical measurements were performed using Maccor Systems (Maccor Inc, Tulsa, OK, USA Series 2300). Prior to all experiments, the battery was activated ac-
Battery open-circuit voltage estimation by a method of statistical analysis

According to a standard activation procedure to ensure battery stability and hence increase reproducibility of the experiments and similarity between different used batteries. The activation procedure consisted of 5 cycles each containing the following steps: charging with 0.55A followed by a discharge phase containing a rest period of 1 h then discharging with -0.55A, a rest period of 15 min, further discharging with -0.11A and a final rest period of 15 min. The discharge steps have a battery voltage cut-off value of about 0.9V, see Figure 2.6.

2.2.3 Open-circuit voltage estimation: KLE and extrapolation

Let us consider a group of voltage curves $V(t)$ obtained in an experiment when a NiMH battery was charged till 200% DoC with a given current value then completely discharged according to the discharge phase described in the activation regime and then charged again with a different current. The charging-discharging cycle was repeated for increasingly charging currents ranging from 0.011A to 2.2A.

Since the measurements were performed across many parameters, such as varying currents, voltages and time points, it is not possible to make a visual inspection of the relationship between these parameters in such a multi-dimensional matrix. One way to make sense of this data is to reduce its dimension. Several data decomposition techniques are available for this purpose: Karhunen-Loève expansion is one of such techniques.

Indeed, the representation given by the KL expansion with a limited number of KL coefficients is optimal in the mean-square sense. Such a dimensionality reduction has important benefits. First, noise is reduced, as the data not contained in the first coefficients is most probably due to noise. Secondly, in some cases, visualization becomes possible.

Let $Y$ be an $n \times m$ matrix representing the battery voltage during charging with $n$
Karhunen-Loève Expansion and its Application to SoC Estimation

Figure 2.7: Voltage during charging with various currents: 0.011A, 0.022A, 0.055A, 0.077A, 0.11A, 0.55A, 1.1A, 1.65A, 2.2A (bottom-up).

different currents and sampled in $m$ points in time. We assume that $n < m$. Figure 2.7 shows a typical experimental result.

The singular value decomposition (SVD) of matrix $Y$ is given by

$$ Y = V \Sigma U', $$

where $V$ is an $n \times n$ unitary matrix, $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n)$ is an $n \times n$ diagonal matrix, with $\sigma_1 \geq \ldots \geq \sigma_n \geq 0$, and $U$ is an $m \times n$ matrix, whose columns are the first $n$ columns of a unitary matrix. For $p \in [1, n]$, the Karhunen-Loève rank $p$ approximation $Y_p$ of $Y$ is:

$$ Y_p = V_p \Sigma_p U_p', $$

where $\Sigma_p = \text{diag}(\sigma_1, \ldots, \sigma_p)$, $V_p$ is an $n \times p$ matrix (first $p$ columns of $V$), and $U_p$ is an $m \times p$ matrix (first $p$ columns of $U$).

Karhunen-Loève approximation $Y_p$ of $Y$ can also be interpreted as follows. Denote by $y_1, \ldots, y_n \in \mathbb{R}^m$ the rows of $Y$. Suppose that we are looking for a linear subspace $W \subset \mathbb{R}^m$, $\dim(W) = p$, such that

$$ \sum_{k=1}^{n} \| y_k - P_W(y_k) \|^2 $$
Battery open-circuit voltage estimation by a method of statistical analysis

is minimal, where $P_W(y)$ denotes the projection of vector $y$ to $W$. Then the rows of $U_p'$ form the basis of the optimal subspace $W'$, and the optimal projections are given by

$$P_W(y_k) = [\alpha_{k,1}, \ldots, \alpha_{k,p}] U_p', \quad k = 1, \ldots, n.$$  

The matrix of Karhunen-Loève coefficients $A = (\alpha_{k,j})_{k=1,j=1}^{p,n}$ satisfies $A = V_p \Sigma_p$.

In a practical application of the KL dimension reduction method, the choice of the parameter $p$ depends on the importance of KL basis vectors for the description of the data, which is measured by the associated singular values, see Karlis et al. (2003). Typically, for the data sets with some intrinsic smoothness, most of the original variability is captured by the first few basis functions. For our experimental data the first three Karhunen-Loève coefficients seem to be sufficient: the heuristic indicators $a_1 + a_2 + a_3 = 0.99$ and $a_2 + a_3 = a_1 + \ldots + a_n a_2 + \ldots + a_n = 0.83$ are appropriately large. Therefore, we put $p = 3$, see also Figure 2.8, showing the first 3 components.

If one wants to construct "experimental" voltage curves that have never been measured, under conditions that have never been used, one is forced to interpolate or extrapolate in the space of voltage curves, or, equivalently, in the space of KL coefficients. Therefore, one has to model the dependence of the KL coefficients on the parameters, influencing the
Karhunen-Loève Expansion and its Application to SoC Estimation

Figure 2.9: Dependence of Karhunen-Loève coefficients on current value in low and high current regimes: dotted lines represent linear regression.

experiment, e.g. current, temperature, age of the battery, etc. In our experiments, the value of the applied current is the only parameter that has been varied. Let $(a_{k,1}, a_{k,2}, a_{k,3})$ be the KL coefficients describing the voltage curve obtained in the $k$-th experiment when the current $I_k$ was applied. Figure 2.9 shows the dependence of the first KL coefficient $a_{k,1}$ on $I_k$. Figure 2.9 is quite interesting from the electrochemical point of view as well. There are clearly two different slopes in the dependence of $a_{k,1}$ on $I_k$ for low and high values of $I_k$, respectively. The presence of two different slopes is related to the fact that the reaction mechanism of oxygen evolution has two rate-determining steps, see Notten et al. (2005).

In this section we are primarily interested in the open-circuit voltage, i.e. zero current. Therefore we apply a linear regression model for the KL coefficients using only low currents 0.011-0.11A, i.e., the first 5 points in Figure 2.9. If one is interested in voltage curves corresponding to moderate currents (0.1-0.5A), kinetic equations derived in Notten et al. (2005) provide a model for interpolation.

Since we adopted a linear model for the dependence of $(a_{k,1}, a_{k,2}, a_{k,3})$ on $I_k$ in low-current regime, we have to find only 6 regression parameters $(a_1, b_1), (a_2, b_2)$ and $(a_3, b_3)$,
Battery open-circuit voltage estimation by a method of statistical analysis

Figure 2.10: Partial charging experiment. Battery relaxation period is 6 hours, after which the OCV is sampled (dots). To ensure that the battery reaches equilibrium state in 6 hours, a very low current has been used for charging.

which are determined by

$$
\sum_{k=1}^{K} \left| \alpha_{k,j} - (a_j + b_j I_k) \right|^2 \rightarrow \min, \quad j = 1, 2, 3,
$$

where $K = 5$ is the number of low currents. Finally, setting current to 0 in the linear model, we obtain extrapolated values of the KL coefficients $\hat{a}_1 = a_1, \hat{a}_2 = a_2, \hat{a}_3 = a_3$, and the prediction for the OCV curve

$$
\hat{V} = [\hat{a}_1 \hat{a}_2 \hat{a}_3] U_3'.
$$

2.2.4 Open-circuit voltage estimation: experimental approach

The values of the OCV for various values of the Depth-of-Charge can be measured in a separate experiment. Comparing these results with the results of our statistical approach we can independently validate our modelling assumptions.
In this experiment, the battery is charged with a constant current to a specific Depth-of-Charge, the current is then interrupted and the battery is allowed to rest for a certain period of time. The basic idea of that after current interruption, the battery reaches the equilibrium state (6 hours in our experiment) and hence the battery voltage is the value of the OCV at the given DoC. Figure 2.10 shows the voltage curves obtained in such experiments for 5 values of DoC. Figure 2.11 shows a good agreement between the results of our data analysis (solid line) and several experimentally observed values of OCV (dots).

The experimental approach to the evaluation of the OCV is extremely time-consuming. Every point on the OCV curve is obtained by performing a separate charging experiment. On the other hand, the modelling approach allows a simultaneous estimation of the OCV for all values of the DoC based only on a few charging experiments with various currents. This aspect of our approach makes its application in adaptive battery management systems feasible.
2.2.5 Conclusions

In this section we proposed a method for determining the open-circuit voltage. Our approach is based on Karhunen-Loève dimension reduction and modelling the dependence of the KL coefficients on physical parameters of the experiment. The method is also suitable for interpolation in the space of experimental voltage curves. Strikingly, results of our statistical analysis also detect an interesting electrochemical phenomenon recently observed for Ni-based rechargeable batteries. We also performed a series of independent experiments in which the OCV was evaluated directly for several values of the DoC. Results of both approaches are in a good agreement.

The method presented in this section suggests a significant potential of the dimension reduction techniques in the development of battery management systems.
Karhunen-Loève Expansion and its Application to SoC Estimation
Chapter 3

Single-Index Models and their Application to SoC Estimation

This chapter aims at giving an idea on how Single-Index models can be used for State-of-Charge estimation of the battery. Basic techniques, existing estimators and a new approach for the estimation of the index-coefficients by solving $L_1$-problem will be demonstrated and discussed through the "varying-current" experiment, that was specially designed in a way to allow extracting information on SoC from the shape of voltage curves adapted to the different current regimes.

3.1 A survey about Single-Index models theory

One of the most referred semiparametric regression models in the literature is the Single-Index model (SIM). In this section we propose a summary of the theory of the SIM: definition, estimation of the index-coefficients and estimation of the link-function, comparison of the existing methods.

3.1.1 Definition

Ichimura (1993) gives the following definition of a Single-Index model:

Definition 3.1 Let $n$ and $m$ be positive integers. The model

$$\ Y = f[h(X, \beta)] + \varepsilon,$$

where

$\bullet \ Y \in \mathbb{R}, \ X \in \mathbb{R}^n; $
Single-Index Models and their Application to SoC Estimation

- \( \varepsilon \in \mathbb{R} \) is unobserved random error;
- \( \beta \in \mathbb{R}^m \) parameter vector (index-coefficient) to be estimated;
- the function \( h: \mathcal{S} \times \Theta \rightarrow \mathbb{R} \), for some \( \mathcal{S} \times \Theta \subset \mathbb{R}^n \times \mathbb{R}^m \) is known up to a parameter \( \beta \);
- the function \( f: \mathbb{R} \rightarrow \mathbb{R} \) (link-function) is not known;

is a Single-Index model.

Great simplifications in most of the results can be obtained by choosing

\[
h(X, \beta) = \beta' X = \sum_{k=1}^{n} \beta^{(k)} X^{(k)},
\]

where \( \beta^{(k)} \) and \( X^{(k)} \) represent the \( k \)th components of vectors \( \beta \) and \( X \). Ichimura (1993) calls such a model "linear Single-Index model". By sake of simplicity, and as this form for the function \( h \) is almost ever supposed, "Single-Index model" will always refer to linear Single-Index model in this chapter. Hence, all the methods examined hereafter rest on the main following hypothesis:

\[
E(Y|X = x) = f(\beta' x). \tag{3.1}
\]

### 3.1.2 Estimation of the link-function \( f \)

Suppose that \( \beta \) is known. Then \( f \) can be estimated by classical means of univariate nonparametric regression of \( Y \) on \( U = \beta' X \). Various methods are proposed in Härdle (1990). Although it is known that it is not the most efficient one, the Nadaraya-Watson kernel estimator is used in many situations because of its easiness of implementation and interpretation and its mathematical tractability. It is defined in the following way.

Let \( \{X_i, Y_i\} \) be the sample and define \( U_i = \beta' X_i \). Let \( K \) be the kernel function, usually taken to be a bounded symmetric probability density, and \( h \) a bandwidth, i.e. a smoothing parameter. Then the Nadaraya-Watson estimator of the regression function is

\[
f_{\hat{\beta},h} (u) = \frac{1}{nh\hat{p}_{\beta,h}(u)} \sum_{i=1}^{n} K \left( \frac{u - U_i}{h} \right) Y_i, \tag{3.2}
\]

where \( \hat{p}_{\beta,h} \) is the kernel estimator of the density \( p \) of \( U \):

\[
\hat{p}_{\beta,h}(u) = \frac{1}{nh} \sum_{i=1}^{n} K \left( \frac{u - U_i}{h} \right). \tag{3.3}
\]

Obviously, these estimations cannot be implemented since \( \beta \) is not known. If an estimator \( \hat{\beta} \) of \( \beta \) is known, an estimator of \( f \) can be obtained by:

\[
f_{\hat{\beta},h} (u) = \frac{1}{nh\hat{p}_{\beta,h}(u)} \sum_{i=1}^{n} K \left( \frac{u - \hat{U}_i}{h} \right) Y_i. \tag{3.4}
\]
with \( \hat{U}_i = \hat{\beta}'X_i \) and
\[
\hat{p}^{\beta,h}(u) = \frac{1}{nh} \sum_{i=1}^{n} K \left( \frac{u - \hat{U}_i}{h} \right).
\] (3.5)

### 3.1.3 Estimation of the index-coefficient \( \beta \)

Many methods of estimating \( \beta \) have been proposed in the literature. We review some of them in this section. The estimators of \( \beta \) can be classified into two main groups, according to whether they require solving nonlinear optimization problem (M-estimators) or not (direct estimators).

**M-estimators**

If \( f \) were known, a M-estimator of \( \beta \) should have the following form:
\[
\hat{\beta} = \arg\max_{\beta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \Psi(Y_i, f(\beta'X_i)),
\] (3.6)

where \( \Psi : \mathbb{R}^2 \rightarrow \mathbb{R} \) is a function verifying some mild regulatory conditions. In the SIM context, we substitute for the unknown fits leave-one-out Nadaraya-Watson estimator, so that the criterion to maximize becomes
\[
\frac{1}{n} \sum_{i=1}^{n} \Psi(Y_i, f^{\beta,h}_{(-i)}(\beta'X_i)).
\] (3.7)

The leave-one-out estimator of \( f \) at the point \( \beta'X_i \), denoted by \( f^{\beta,h}_{(-i)}(\beta'X_i) \), is equal to the Nadaraya-Watson estimator (3.4) based on all observations except the \( i \)th, and is used because of bias reasons.

We describe hereafter two important particular M-estimators: generalization of the parametric least squares and maximum likelihood estimators.

**Semiparametric Least Squares (SLS)**

As in a parametric least squares problem, the idea is to minimize the mean square distance between the observed values \( Y_i \) and the values given by the model \( f(\beta'X_i) \). If \( f \) were known, we should have the classical weighted least squares estimator given by
\[
\hat{\beta} = \arg\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} w(X_i)[Y_i - f(\beta'X_i)]^2,
\] (3.8)

where \( w \) is a positive bounded weight function.
In the Single-Index context, the least squares criterion to minimize becomes

\[
\frac{1}{n} \sum_{i=1}^{n} w(X_i)[Y_i - \hat{f}_{(-i)}^{\beta,h}(\beta'X_i)]^2,
\]

where \( \hat{f}_{(-i)}^{\beta,h}(\beta'X_i) \) is the leave-one-out estimator of \( f \) at the point \( \beta'X_i \).

The choice of the weight function \( w \) affects the efficiency of the estimator. It was found that in the SIM context the semiparametric least squares estimator achieves the efficiency bound, see Newey and Stoker (1993), if

\[
w(x) = 1/\sigma^2(x),
\]

where \( \sigma^2(x) \) is a variance function, which can be unknown. Then its estimator is obtained by using the two-steps procedure proposed in Newey and Stoker (1993).

**Semiparametric Maximum Likelihood (SLS)**

This optimization based method is inspired by the parametric maximum likelihood methods. In the Single-Index context, the joint distribution of \( X \) and \( Y \) and the conditional density of \( Y \) given \( X \) clearly depend on \( \beta \) and \( f \). Suppose this conditional density depends upon \( X \) only through \( \beta'X \) and denote them by \( l_{f,\beta}(\ldots) \) and \( l_{f,\beta}(\ldots|.) \) respectively. Then the likelihood is

\[
L_f(\beta) = \prod_{i=1}^{n} l_{f,\beta}(X_i, Y_i) = \prod_{i=1}^{n} l_{f,\beta}(Y_i|\beta'X = \beta'X_i) g(X_i),
\]

where \( g \) is the marginal density of \( X \). Hence the log-likelihood is

\[
LL_f(\beta) = \sum_{i=1}^{n} \log l_{f,\beta}(Y_i|\beta'X = \beta'X_i) + \sum_{i=1}^{n} \log g(X_i).
\]

Since the term \( \sum_{i=1}^{n} \log g(X_i) \) does not depend on \( f \) and \( \beta \), the maximizing \( LL_f \) amounts to maximizing \( \sum_{i=1}^{n} \log l_{f,\beta}(Y_i|X = X_i) \). If \( f \) known, the maximum likelihood estimator of \( \beta \) should be given by the following maximization problem

\[
\hat{\beta} = \arg \max_{\beta \in \Theta} \sum_{i=1}^{n} \log l_{f,\beta}(Y_i|\beta'X = \beta'X_i).
\]

In the SIM context, if \( f \) is unknown, \( \beta^* \) is not feasible, but if the conditional distribution of \( Y \) given \( X \) is known up to \( f \) and \( \beta \), we overcome the problem by replacing \( f \) in (3.11) with its Nadaraya-Watson leave-one-out estimator, thus forming a pseudo-likelihood. The estimator is finally given by

\[
\hat{\beta} = \arg \max_{\beta \in \Theta} \sum_{i=1}^{n} \log l_{f_{(-i)}^{\beta,h},\beta}(Y_i|\beta'X = \beta'X_i).
\]
If the conditional distribution of $Y$ given $X$ is not known, it can be estimated in a fully nonparametric way like it was proposed in Delecroix et al. (2003).

**Bandwidth selection**

In order to construct an estimator (3.7), a bandwidth $h$ is needed. ? propose an empirical rule for selecting it. Actually, extend of the methodology first introduced by Härdle et al. (1993) for the SLS estimator. Define

$$
\hat{S}(\beta, h) = \frac{1}{n} \sum_{i=1}^{n} \Psi(Y_i, \hat{f}_{ih}^{\beta}(\beta'X_i))
$$

(3.13)

the criterion to be maximized. One way to select the bandwidth is to consider it as an extra parameter of the model, and to maximize the cost function with respect to it as well. That is:

$$
(\hat{\beta}, \hat{h}) = \arg \max_{\beta \in \Theta, h \in \mathbb{R}^+} \hat{S}(\beta, h).
$$

(3.14)

This semiparametric criterion (3.13) can be split into a parametric part $\hat{S}(\beta)$ and a nonparametric part $T(h)$, where $\hat{S}(\beta)$ is an approximation of $S(\beta) = E(\Psi(Y, f(\beta'X)))$ and $T(h)$ is the cross-validation criterion for choosing $h$ when $\beta$ is known. This result leads to a simple way of simultaneously maximizing with respect to both $\beta$ and $h$ as it is very much like separately maximizing $\hat{S}(\beta)$ with respect to $\beta$ and $T(h)$ with respect to $h$.

**Direct estimators**

Whereas M-estimators require solving an intricate optimization problem in a high-dimensional space, see Hristache et al. (2001), direct estimators provide the estimator in an analytic form.

**Average Derivatives Estimator (ADE)**

We set $u = \beta'x$ and $m(x) = f(\beta'x)$. Average derivatives method based on the fact that

$$
\nabla m(x) = \frac{\partial f}{\partial u}(\beta'x)\beta,
$$

which induces that

$$
\delta_w \doteq E[w(X)\nabla m(X)] = E[w(X)\frac{\partial f}{\partial u}(\beta'X)]\beta
$$

(3.15)

for any bounded continuous weight function $w$. The quantity $\delta_w$ is called a weighted average derivative of $f$ with weight function $w$. It appears from (3.15) that any weighted average derivative is proportional to $\beta$, provided $E[w(X)\frac{\partial f}{\partial u}(\beta'X)]$ is not zero. Note that
this condition is in particular violated when \( w \equiv 1 \), \( f \) is an even function and \( X \) is symmetrically distributed.

**Unweighted Average Derivatives (UADE)**

Härdle and Stoker (1989) take \( w \equiv 1 \) and use nonparametric estimation of the marginal density of \( X \). Let \( g(x) \) be this marginal density, \( \nabla g = \frac{\partial g}{\partial x} \) its gradient vector and let \( l = -\nabla g / g \) the negative log-density derivative. By definition we have

\[
\delta = \int \nabla f(\beta'x)g(x)dx.
\]

Assuming that \( g(x) = 0 \) on the boundary of \( x \) values, integration by parts gives \( \delta = E[Y I(X)] \).

The proposed estimator is an analog of this last expression, using a nonparametric estimator of \( l(x) \), that is

\[
\hat{\delta} = \frac{1}{n} \sum_{i=1}^{n} \hat{l}^h_{(i)}(X_i)Y_i,
\]

where

\[
\hat{l}^h_{(i)}(x) = \frac{1}{\hat{g}^h_{(i)}(x)} \nabla \hat{g}^h_{(i)}(x),
\]

\( \hat{g}^h \) can be the classical leave-one-out multivariate kernel density estimator.

By dividing this vector \( \hat{\delta} \) by its first component, one gets an estimate of \( \beta \).

**Density-weighted Average Derivatives (DWADE)**

The previous method requires the estimation of both the density \( g \) and its gradient. To avoid this estimation, Powell et al. (1989) have proposed to set \( w(x) = f(x) \). With this weight function we have from (3.15),

\[
\delta_g = \int \nabla f(\beta'x)g^2(x)dx.
\]

Assuming again that \( g(x) = 0 \) on the boundary of the support of \( X \),

\[
\delta_g = -2 \int \nabla f(\beta' x) \nabla g(x) g(x) dx = -2E[Y \nabla g(X)],
\]

so that we can estimate \( \delta_g \) with

\[
\hat{\delta}_g = \frac{-2}{n} \sum_{i=1}^{n} Y_i \nabla \hat{g}^h_{(i)}(X_i),
\]
where only the gradient of $g$ has to be estimated, which can be done by the formula for the gradient of a leave-one-out version of the kernel density estimator, see Klein and Spady (1989).

**Iterative Average Derivative Estimator (IADE)**

The major drawback of the previous two procedures is the need to estimate the density of $X$ and/or its gradient in a fully nonparametric way, what can lead to poor performance due to the curse of dimensionality. Hristache et al. (2001) propose another type of direct estimator of $\beta$, which can be regarded as an iterative improvement of the average derivative estimator. The idea is the following. Suppose for the moment that $p = 2$ and that the observations $X_i$ are scattered uniformly over the square $[0, 1]^2$. The expected gradient of $m$, appearing in (3.15) with $w \equiv 1$, will be estimated by a sample average of estimates of this $\nabla m$ at each point $X_i$. At $X_i$, a kind of local least squares problem is used:

\[
\left( \frac{\hat{m}(X_i)}{\nabla m(X_i)} \right) = \arg \min_{c \in \mathbb{R}, \theta \in \mathbb{R}^p} \sum_{j=1}^{n} [(Y_j - c) - \theta'(X_j - X_i)]^2 K \left( \frac{X_j - X_i}{h} \right).
\]

As kernel, it is here recommended, see Hristache et al. (2001), to choose a function depending only on the squared euclidean norm of its argument, that is

\[
K \left( \frac{X_j - X_i}{h} \right) = K_0 \left( \frac{||X_j - X_i||^2}{h^2} \right),
\]

so that the weights of all points $X_j$ outside a spherical neighborhood $V_h(X_i)$ of diameter $h$ around $X_i$ vanish. Hence, the expected gradient

\[
\theta^* = E[\nabla m(X)]
\]

can be estimated by

\[
\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} \nabla \hat{m}(X_i)
\]

leading to an estimate of $\beta$ being

\[
\hat{\beta} = \frac{\hat{\theta}}{\hat{\theta}(1)}.
\]

Recall that we are working for the moment in a two-dimensional space for $X$. We can stretch $V_h(X_i)$ along the direction orthogonal to $\beta$. This is so because of a well-known property of the gradient: it points towards the direction in which the function increases most, and this function is locally constant in the orthogonal direction. Although $\beta$ is not known, we can use the first estimate (3.19): at any $X_i$ define an elliptic window $V_{h,\rho}(X_i)$,
centered at $X_i$, with small axis of size $O(\rho h)$ (with $\rho < 1$) oriented along $\hat{\beta}$, and large axis of size $O(h)$ orthogonal to $\hat{\beta}$. If $\rho$ is small and $\hat{\beta}$ a good approximation of $\beta$, we can expect that the approximation error of $m$ by a linear function in the neighborhood $V_{h,\rho}$ would be small. We can deal with such an elliptic window by replacing the weights $K_0(h^{-2}\|X_j - X_i\|^2)$ in (3.18) with $K_0(h^{-2}\|\Lambda_{\rho,\hat{\beta}}(X_j - X_i)\|^2)$, where the positive definite symmetric matrix

$$\Lambda_{\rho,\hat{\beta}} = I + \rho^{-1}\hat{\beta}\hat{\beta}'$$

(3.20)
defines the elliptic geometry of the window. The estimate of the gradient at $X_i$ is now given by

$$\left( \frac{\hat{m}(X_i)}{\sqrt{m}(X_i)} \right) = \arg \min_{c \in \mathbb{R}, \theta \in \mathbb{R}^p} \sum_{j=1}^n [(Y_j - c) - \theta'(X_j - X_i)]^2 K_0 \left( \frac{\Lambda_{\rho,\hat{\beta}}(X_j - X_i)\|\|^2}{h^2} \right),$$

(3.21)

that is, from classical least-squares theory,

$$\hat{\theta}_i = W_{k,\Lambda_{\rho,\hat{\beta}}}(X_i) \sum_{j=1}^n Y_j \begin{pmatrix} 1 \\ X_j - X_i \end{pmatrix} K_0 \left( \frac{\Lambda_{\rho,\hat{\beta}}(X_j - X_i)\|\|^2}{h^2} \right)$$

with

$$W_{k,\Lambda_{\rho,\hat{\beta}}}(x) = \sum_{j=1}^n \begin{pmatrix} 1 \\ X_j - X_i \end{pmatrix} \begin{pmatrix} 1 \\ X_j - X_i \end{pmatrix}' K_0 \left( \frac{\Lambda_{\rho,\hat{\beta}}(X_j - X_i)\|\|^2}{h^2} \right).$$

After averaging, we can compute the estimator $\hat{\beta}$ of $\beta$ the same way as in (3.19). The procedure is iterated, each time flattening the elliptic window in the direction of the current estimate and stretching it in the orthogonal direction.

**Sliced Inverse Regression (SIR)**

In a dimension reduction purpose, Li (1991) proposed a simple and easy to implement algorithm. Duan and Li (1991) adapted this method in the Single-Index context. It is based on the relationship between $\beta$ and the inverse regression $E(X|Y = y)$. Unfortunately, their results require an important design condition:

*For any $\beta \in \mathbb{R}^p$, the conditional expectation $E(\beta' X | \beta_0' X = u)$ is linear in $u$. If it is not the case, a bias has to be taken into account.*

The advantage of considering the inverse regression $\xi(y) = E(X|Y = y)$ is to avoid the curse of dimensionality. Indeed, $\xi(y)$ can be nonparametrically estimated in a reliable way since $Y$ is a scalar. It is noteworthy that we have

$$\xi(y) = \mu + \Sigma\beta_0 \kappa(y),$$

(3.22)
where $\mu = E(X)$, $\Sigma = \text{cov}(X)$ and

$$\kappa(y) = E[\beta_\theta^\prime(X - \mu|Y = y)] / \beta_\theta^\prime \Sigma \beta_\theta.$$ 

This follows from the fact that

$$E(X|\beta_\theta^\prime X = \beta_\theta^\prime x) = \mu + \frac{\beta_\theta^\prime (x - \mu) \Sigma \beta_\theta}{\beta_\theta^\prime \Sigma \beta_\theta}$$

due to the design condition and $\xi(y) = E[E(X|\beta_\theta^\prime X)|Y = y]$.

Hence, from (3.22) appears that $\beta_0$ is proportional to $\Sigma^{-1}(\xi(y) - \mu)$, with the proportionality constant $1/\kappa(y)$. For any $y$ such that $k(y) \neq 0$, we can estimate $\beta_0$ by suitably scaling an estimate of $\Sigma^{-1}(\xi(y) - \mu)$. In order to combine the information from all $y$'s, consider $\Gamma = \text{cov}(\xi(Y))$. We have, according to (3.22), that

$$\Gamma = \text{var}(\kappa(Y)) \Sigma \beta_0 \beta_0^\prime \Sigma.$$ 

From Cauchy's inequality, it is found that $\beta_0$ solves the maximization problem

$$\beta_0 = \arg \max_{\beta \in \Theta} \frac{\beta^\prime \Gamma \beta}{\beta^\prime \Sigma \beta}.$$ 

(3.23)

$\beta_0$ is thus the suitably scaled principal eigenvector for $\Gamma$, with respect to the inner product $\langle a, b \rangle = a^\prime \Sigma b$. The maximum value of the quotient is the principal eigenvalue. The spectral decomposition for $\Gamma$ is trivial: all eigenvalues except the first are zero, since the rank of $\Gamma$ is one (the only degree of freedom of $\xi$ is $y$).

Other estimators

The previous ideas are historically the most popular ones in order to estimate $\beta$. Nevertheless, much more estimators have been proposed in the literature. Han (1987) proposes an estimator based on the rank correlation between the observed values and the values fitted by the model. This method requires the link-function $f$ to be strictly monotonic. In a dimension reduction purpose, Li (1992) suggests a method called Principal Hessian Directions, which can be adapted to the Single-Index context. The main results are based on Stein's lemma, which assumes that $X$ has a normal distribution. Naik and Tsai (2000) extend the method of Partial Least Squares to the case of Single-Index models. Xia et al. (2002) propose an adaptive approach for dimension reduction, called the Minimum Average Variance Estimation (MAVE). This is a kind of M-estimation method, inspired by the SIR method, the ADE method and the idea of local linear smoothers. Huh and Park (2002) derive an extension of ADE, where the gradient of the regression function is evaluated in any $X_i$ via local polynomial fits based on kernel weighted conditional likelihoods.
3.2 Estimation of index-coefficients under the assumption of monotonicity

In many applications, it is natural to expect a monotonic relationship between a response variable and an associated index.

In this section, we introduce a new approach for estimation index-coefficients in the monotonic linear Single-Index models. This estimator exploits monotonicity between a response variable and an associated index in a natural way and may allow more flexibility in balancing robustness and efficiency objectives, cover a wider range of models, and in general, is far more computationally efficient than the other estimators under the assumption of monotonicity, see Ichimura (1993) and Han (1987).

3.2.1 Problem formulation

Suppose that the observations \((y_i, x_i), i = 1, \ldots, n\) are generated by the following Single-Index model:

\[
y = f(\beta' x) + \varepsilon,
\]

where \(y_i\) are response variables; \(x_i \in \mathbb{R}^d\); \(\varepsilon_i\) are random errors. We assume that \(f: \mathbb{R}^d \rightarrow \mathbb{R}\) is an unknown link function and a \(d\)-vector \(\beta\) is an unknown index vector.

Two estimation problems are involved here. The first consists of estimation of the unknown function \(f(\cdot)\), the objective of the second is to recover the index-vector \(\beta\). We will focus on the second one, to be precise, we will suggest an efficient method for the estimation of the orientation vector \(\beta\) based on the minimization of an \(L_1\)-problem.

3.2.2 Estimation procedure

We start with the informal description of the proposed estimator. The estimator \(\hat{\beta}\) of \(\beta\) is constructed by minimization of the following \(L_1\)-functional with respect to \(\beta\):

\[
\hat{\beta} = \arg \min_\beta \sum_{i=2}^n |(\beta' x)_i - (\beta' x)_{i-1}|,
\]

subject to \(|\beta_1|^2 + \ldots + |\beta_d|^2 = 1\).

The global minimum to this minimization problem is obtained by sorting the observations according to the values of \(y\) which will give us \(y(1), y(2), \ldots, y(n)\) with \(y(1) \leq y(2) \leq \ldots \leq y(n)\) and the corresponding values of \(\beta' x\): \((\beta' x)(1), \ldots, (\beta' x)(n)\) with \((\beta' x)(1) \leq \ldots \leq (\beta' x)(n)\).
It follows from the following theorem:

**Lemma 3.1** \( U^n \sum_{i=2}^n [z_{i-1}, z_i] = [\inf(A), \sup(A)] \).

**Proof.** For \( n = 2 \) this is obvious. For \( n = k + 1 \), observe that \( z_1 \) and \( z_{k+1} \) appear only once in the sum, while all other terms appear twice.

By induction \( U^n \sum_{i=2}^n [z_{i-1}, z_i] = [\inf(A_k), \sup(A_k)] \). If \( z_{k+1} > \sup(A_k) \), then \( [z_k, z_{k+1}] \) covers \( [\sup(A_k), z_{k+1}] \) and so \( U^{n+1} \sum_{i=2}^n [z_{i-1}, z_i] = [\inf(A_{k+1}), \sup(A_{k+1})] \) (similarly if \( z_{k+1} < \sup(A_k) \)). Otherwise \( z_{k+1} \in [\inf(A_k), \sup(A_k)] \) and therefore \( [\inf(A_k), \sup(A_k)] = [\inf(A_{k+1}), \sup(A_{k+1})] \), so the result still holds.

**Theorem 3.1** For a set of real numbers \( A_n = \{z_1, z_2, \ldots, z_n\} \), the sum of the absolute deviations \( \sum_{i=2}^n |z_i - z_{i-1}| \) is minimized when the set \( A_n \) is ordered: \( z(1), z(2), \ldots, z(n) \), where \( z(1) \leq z(2) \leq \ldots \leq z(n) \).

**Proof.** For any permutation of the elements in \( A_n \) the deviation \( |z_i - z_{i-1}| \) is the length of the interval \([z_{i-1}, z_i]\) (without loss of generality, \( z_i > z_{i-1} \)).

It follows immediately from the above Lemma 3.1 that any permutation of \( A_n \) gives a sum of lengths of intervals that cover \([\inf(A_n), \sup(A_n)]\), and therefore that sum is greater than or equal to \( \ell[\inf(A_n), \sup(A_n)] \). When \( A_n \) is ordered, the sum \( \sum_{i=2}^n |z_i - z_{i-1}| \) is exactly \( \ell[\inf(A_n), \sup(A_n)] \) so this ordering is a minimum.

If \( A_n \) is not ordered, then the intervals defined by this permutation \([z_{i-1}, z_i]\) must overlap and the sum of the absolute deviations \( \sum_{i=2}^n |z_i - z_{i-1}| \) will be strictly larger (by at least the length of the overlap) than \( \ell[\inf(A_n), \sup(A_n)] \).

### 3.2.3 Simulation study

In this section we illustrate the performance of the proposed procedure for some simulated data sets.

The performance of the method is illustrated by the means of the following examples. We consider the model described by (3.24)

\[
y = f(\beta' x) + \epsilon,
\]

where \( y_i \) are response variables; \( x_i \in \mathbb{R}^d \); \( \epsilon_i \) are random errors, \( i = 1, \ldots, n \), when \( f \) is a function of normal distribution:

\[
f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{t} e^{-\frac{s^2}{2}} ds,
\]
Figure 3.1: Simulated data sets by the model (3.24), where link-function is a function of normal distribution.

where \( x \sim \mathcal{N}(0, I) \), \( \varepsilon \sim \mathcal{N}(0, \sigma) \). The simulations are made with \( \sigma = 0.02, 0.05, 0.1 \), \( n = 200, 400 \) and \( d = 2, 3, 4 \), see Figure 3.1. We set

\[
\beta^* = (1, 0, \underbrace{0, \ldots, 0}_{d-2}).
\]

Plotting of \( y \) against any pair of coordinate variables, say \( x_1 \) and \( x_2 \), can only give a picture which is too shadowy to reveal the nonlinear structure in the data. So a critical question is how to find the better projection angles without knowing where the data were generated from.

The direction of \( \beta \) is called the effective dimension reduction (e.d.r.) direction because the relationship between \( y \) and \( x \) hinges entirely on the associated projection \( \beta' x \). For visualization purpose, it is the most informative statistical profile to find the nonlinear structure of the data. If that direction is given, then we can visualize perfectly the functional relationship between \( y \) and \( x \) by plotting \( y \) against \( \beta' x \).

Our proposed procedure, based on the minimization of \( L_1 \)-problem, offers a very simple
and efficient way of estimating index-coefficients $\beta$. It requires no iteration, it is very computationally advisable.

The estimation error is measured in the $L_1$-norm in $\mathbb{R}^d$:

$$||\hat{\beta} - \beta^*||_1 = \sum_{i=1}^{d} |\hat{\beta}_i - \beta^*_i|,$$

which allows to easily evaluate the "error per parameter".

The empirical results for the mean absolute value (MAE) $E||\hat{\beta} - \beta^*||_1$ based on 100 replicates of two estimation procedures (proposed $L_1$-method and SIR-method presented in the Section 3.1.3) are collected in Table 3.1 for the comparison.

Table 3.1: MAE $E||\hat{\beta} - \beta^*||_1$ based on $L_1$-procedure and SIR method for the link function

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{t} e^{-\frac{s^2}{2}} ds.$$
### Single-Index Models and their Application to SoC Estimation

<table>
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<th>n</th>
<th>d</th>
<th>σ</th>
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Compared to the Sliced Inverse Regression estimator, the proposed procedure provides superior results. The table clearly illustrates that the losses of the $L_1$-estimator are essentially proportionally to the noise level $\sigma$ and to $n^{-\frac{1}{2}}$. The general conclusion of the simulation study is that proposed procedure works well, it outperforms the SIR-estimator almost in all situations and since the method is based on the minimization of the $L_1$-problem, it is far more computationally efficient.
3.3 Single-Index model as an approach to SoC indication

In recent years a clear change has become evident in the requirements of accurate indication of battery State-of-Charge (SoC) that would warn of imminent power loss of the system. The increasing demands have been partly met by improvements in measurement precision and developments of methods for achieving higher levels of accuracy in SoC estimation. However, the need to provide some applications with much better State-of-Charge information calls for radical new solutions based on deep understanding of the battery response to currents that are "varying" during the load or discharge phases and its dependence on parameters such as charge/discharge profile, temperature, battery age. It turns out that the peculiarities of voltage response require sophisticated analysis of collected data.

The main questions that we will naturally arise and consider are the following:
- How should we describe a shape of voltage curves?
- How should we use Single-Index models in order to estimate State-of-Charge of the battery?

3.3.1 Experimental setup of the "varying-current" experiment

The objective of this experiment is to learn about the reactions to "varying-currents". The analysis of that experiment permits to get information under conditions that are closer to the real user's behavior and to estimate the amount of charge presented in the battery under these operational conditions.

The organization of each cycle is in several phases including charge, discharge and rest periods satisfying the battery operation.

The charging and discharging of the battery is operated according to the following scheme: currents varying from 0.275A to 2.2A as further described in Figure 3.2;

The current changes according to a repeated sequence of 24 steps:

\[ ABDBADCACBCDABDBADCBCACD \]

Hence, we get the 24 steps followed by, again, the same 24 steps and so on. This sequence has the following properties: the length of the sequence of 4 symbols is 24. Each symbol is present exactly 6 times. Each pair of different symbols is present exactly 2 times.

Each step corresponds to 1 of the 4 symbols \( A, B, C \) and \( D \). Each step is applied during the basic period \( T = 20 \) sec. During the charge and discharge phases, the symbols
correspond to the next currents:

\[ A = 0.275\text{A}, B = 0.55\text{A}, C = 1.1\text{A} \text{ and } D = 2.2\text{A}; \]

the average current value is 1.03125A.

The charge takes place during varying durations attaining up to DoC = 125\%.

The discharge takes place during varying durations attaining up to first reach of voltage 0.9V.

The battery reaction to “varying-currents” will be analyzed based on the discharge phase of the battery operation. Figure 3.3 illustrates voltage behavior adapted to the different current regimes.

It turns out that the peculiarities of voltage response require sophisticated analysis of collected data, such as data screening (interpolation and data cleaning) and statistical shape analysis.

### 3.3.2 Data screening

Measuring equipment delivers sampling points that are irregularly spaced in time. Hence, two similar events are sampled at time that do not correspond to one another. A solution to
Figure 3.3: Voltage behavior during discharging as a response to currents varying in time according to the introduced current-scheme.
this problem is obtained by the interpolation: segments on a common basis. By “segment”
we refer to the $V$-variations during each of the 24 steps of sequence, see Figure 3.3. Each
segment is known by its samples.

Let $V(t)$ be the observed voltage segment, $t \geq 0$.

The sampling scheme is designed to properly follow the rise/fall of voltage curves:
$V(t) = V(u(t))$ with $V(u)$ approximately linear in $u$, where $u(t)$ is approximated by

$$
\begin{align*}
    u &= u(v) = -a(1 - e^{\frac{v}{b}}), \\
    v &= v(t) = b(1 - e^{-\frac{t}{c}}),
\end{align*}
$$

where parameters $a$, $b$, $c$ are obtained by fitting that model to the experimental data and
they are found to be the following: $a = 0.2$, $b = 0.7$, $c = 0.25$.

The proposed sampling scheme guaranties a high density of points at the beginning of
the segments and it is efficient involving as few sample points as possible.

Due to hazards in the data acquisition, some of the segments are of little value. The
goal is to identify the possible outliers and discard such segments. A solution to this prob­
lem is obtained by data cleaning. The cleaning must keep on the data properties, data
integrity and discard the irrelevant features. Singular Value Decomposition (SVD) permits
to do this.

**Algorithm**

1. Characterize each of the $n$ segments by $m$ sampling points and organize them into
   a $[n \times m]$-data matrix

   $$
   X = (x_1, \ldots, x_n), \quad x_i \in \mathbb{R}^m, \quad i = 1, \ldots, n.
   $$

2. Project $X$ onto a subspace of dimension $p$ by SVD:

   $$
   X_{[n \times m]} \approx U_{[n \times p]} \Sigma_{[p \times p]} V'_{[p \times m]}.
   $$

   Each row of a $[n \times p]$-matrix $Y = U\Sigma$ is a set of $p$ coefficients that characterize a segment.

3. Discard contributions of the current before the transition and current after transition
   from $Y$:
   - construct the $[n \times 2]$-matrix $Z = (I_{\text{before}}, I_{\text{after}})$;
   - derive a corresponding orthogonal basis. It is $U_Z$ in $Z = U_Z \Sigma_Z V'_Z$;
   - estimate the contributions: $Y U'_Z U_Z$. 

Single-Index model as an approach to SoC indication

- discard the contributions: \( Y = Y - Y U_Z U_Z^\prime \).

4. As a good outlier detector use a combination of the standard deviation as an outlier sensitive measure with a measure which is insensitive. Such a robust measure for the dispersion is the median of the absolute deviation (MAD), proposed by Hampel (1985), which is maximally robust (it has a breakdown point of 1/2), see Davies and Gather (1993)

For \( Y = (y_1, ..., y_n) \), \( y_i \in \mathbb{R}^p \), \( i = 1, ..., n \) estimate

\[
    r_i = |y_i - \text{Median}_j \{y_j\}|, \quad i = 1, ..., n, \quad j = 1, ..., p.
\]

Estimate

\[
    \text{MAD} = \text{Median}\{r_1, ..., r_n\},
\]

then

\[
    \sigma_{\text{MAD}} = 1.483 \text{MAD}
\]

is robust estimate of the standard deviation, where the factor 1.483 is the ratio of the standard deviation of a normal random variable to its median absolute deviation.

5. A value \( r_i, \ i = 1, ..., n \) is considered as being indicating an outlier,

\[
    i \text{ is an outlier if } r_i > 3.5\text{MAD}.
\]

Let \( k \) be the number of outliers, then

- if \( k = 0 \), the segment cleaning is over and we obtained a matrix \( X \)
- if \( k > 0 \), discard from \( X \) the corresponding rows. Make \( n = n - k \). Restart algorithm and continue.

As a result of applying the introduced sampling scheme and the data cleaning procedure, we describe a V-shape based on the information that remains when location of the voltage curves due to the current transitions, rotational effects and measurements error are filtered out from the segments. In order to illustrate the outcome, Figure 3.4, the discharge phase of the “varying-current” experiment of a cell with 20 seconds segments is considered. There are 60 segments and each of them is known by 12 samples.
Figure 3.4: Voltage-shapes during discharging after applying the sampling and cleaning procedures. The different colors of $V$-segments correspond to different currents varying in time.
3.3.3 SoC estimation by Single-Index model

Characterizing each of the $n$ voltage-segments by $m$ sampling points and organizing them into a $[n \times m]$-data matrix $X = (x_1, ..., x_n)$, $x_i \in \mathbb{R}^m$, $i = 1, ..., n$, we are interested in the estimation of SoC, denoted by $Y = (y_i), i = 1, ..., n$, via described above Single-Index model

$$Y = f(\beta'X) + \varepsilon$$

with an unknown link-function $f$ and an unknown index-vector $\beta$.

The objective of the first estimation problem is to recover the index-vector $\beta$, assuming that the relationship between SoC and voltage-segments hinges entirely on the associated projection $\beta'X$. For visualization purpose, it is the most informative statistical profile to find the nonlinear structure of the data.

Our proposed procedure, based on the minimization of $L_1$-problem

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=2}^{n} |(\beta'X)_i - (\beta'X)_{i-1}|,$$

subject to $|\beta_1|^2 + \ldots + |\beta_m|^2 = 1$,

offers an efficient way of estimating index-coefficients $\hat{\beta} = (\hat{\beta}_1, ..., \hat{\beta}_m)$, $m = 12$, and as a result, finds the best projection angle without knowing where the data were generated from in such a way that we can visualize perfectly the functional relationship between SoC and voltage-segments by plotting $Y$ against $\beta'X$. State-of-Charge $Y$ as a function of the estimated projection $\beta'X$, $\hat{\beta} = \{\hat{\beta}_i\}, i = 1, ..., 12$ is illustrated in the Figure 3.5 for the discharge phase of the “varying-current” experiment of a cell with 20 seconds segments, presented in the Figure 3.4.

The estimated index-vector here $\hat{\beta} = (\hat{\beta}_1, ..., \hat{\beta}_m)$, $m = 12$ is found to be the following:

$$\hat{\beta} = (-0.000057, -0.048088, 0.154636, -0.095250, -0.000619, -0.040518, -0.208600, 0.249334, 0.000001, -0.000001, 0.094913, -0.107981).$$

Taking as an aim reduction of the dimensionality, we set $\hat{\beta}_1 = \hat{\beta}_5 = \hat{\beta}_9 = \hat{\beta}_{10} = 0$ and run the proposed $L_1$-optimization algorithm to estimate the index-coefficients, but now achieving to reduce $m$ from 12 to 8:

$$\hat{\beta} = (0.005233_2, -0.000586_3, -0.001014, 0.087556, -0.208600, 0.249334, 0.000001, -0.000001, 0.094913, -0.107981).$$

State-of-Charge as a function of the estimated projection $\beta'X$, where the dimension $m$ was reduced from 12 to 8, is illustrated in the Figure 3.6 for the discharge phase of the
"varying-current" experiment of a cell with 20 seconds segments, presented in Figure 3.4.

The second estimation problem consists of estimation of an unknown function \( f(\cdot) \). We assume here that the functional relationship between SoC and voltage-segments’ associated projection is smooth and monotone.

The problem of monotonic smoothing on a set \( \{Z_i, Y_i\}_{i=1}^n \), \( Z_i = \beta^T X_i \) can be formalized as follows. Sort the data \( \{Z_i, Y_i\}_{i=1}^n \) by \( Z \) into \( \{Z(i), Y(i)\}_{i=1}^n \).

Find \( \{\hat{f}(Z(i))\}_{i=1}^n \) to minimize

\[
\sum_{i=1}^{n-1} (Y(i) - \hat{f}(Z(i)))^2
\]

subject to the monotonicity restriction

\[
\hat{f}(Z(1)) \leq \hat{f}(Z(2)) \leq \cdots \leq \hat{f}(Z(n)).
\] (3.28)

Such a solution exists and can be obtained from the pool adjacent violators (PAV) algorithm, Barlow et al. (1972). The pool adjacent violators algorithm can be formalized as follows.

**STEP 1.**

Start with \( Y(1) \), move to the right and stop if the pair \((Y(i)), Y(i+1))\) violates the monotonicity constraint, that is, \( Y(i) > Y(i+1) \). Pool \( Y(i) \) and the adjacent \( Y(i+1) \), by replacing them both by their average,

\[
Y^*_i = Y^*_i = (Y(i) + Y(i+1))/2.
\]

**STEP 2.**

Next check that \( Y(i-1) \leq Y^*_i \). If not, pool \( \{Y(i-1), Y(i), Y(i+1)\} \) into one average. Continue to the left until the monotonicity requirement is satisfied. Then proceed to the right. The final solutions are \( \hat{f}(Z(i)) \).

There are three remarkable facts about this solution. First, if the data are already monotone, then the PAV algorithm will reproduce the data. Second, since each \( \hat{f}(Z(i)) \) is an average of the observations near \( Z(i) \) the solution is a step function. Third, if there are outliers the PAV algorithm will produce long, flat levels.

Thus, in view of monotonicity, an estimator may be obtained via isotonizing the response values via the PAV algorithm. The resulting estimator may be called an \( I \)-estimator.

In view of smoothness, one may employ some kind of smoother, for example, smoothing spline, see Green et al. (1994). The resulting estimator may be called a \( S \)-estimator.

Note that an \( I \)-estimator may not admit smoothness while an \( S \)-estimator may not possess monotonicity. In fact, an \( I \)-estimator is often just a step function rather than a smooth function while an \( S \)-estimator is often just a smooth function rather than a monotone function.
Figure 3.5: State-of-Charge as a function of voltage-segments, presented as \( \hat{\beta}'X \), \( \hat{\beta} = \{\hat{\beta}_i\}, \ i = 1, \ldots, 12 \), for the discharge phase of the "varying-current" experiment. The different colors of SoC-points correspond to the different currents. Black line is the resulting estimation of SoC as a smooth and monotone link-function.
Figure 3.6: State-of-Charge as a function of voltage-segments, presented as $\hat{\beta}'X$, $\hat{\beta} = \{\hat{\beta}_i\}$, $i = 1, \ldots, 8$, for the discharge phase of the "varying-current" experiment. The different colors of SoC-points correspond to the different currents. Black line is the resulting estimation of SoC as a smooth and monotone link-function.
Therefore, there is space to improve an $I$-estimator or an $S$-estimator via applying a smoother to a resulting $I$-estimator (PAV algorithm) to an $S$-estimator, resulting in $SI$-estimator or an $IS$-estimator, respectively. An $SI$- or $IS$-estimator may be simply called a monotone smoother. Although $IS$- and $SI$- estimators are satisfactory in many practical applications, they are still not very desirable. This is because an $SI$-estimator may still be not smooth while an $IS$-estimator may still be not monotone.

We make a further improvement with a price of more computational effort via employing B-splines with the $L_1$-norm. Hence, Figure 3.6 shows the $IS$-estimator $\hat{f}$ (black line) obtained by applying the smoother (B-spline) to the resulting $I$-estimator (PAV algorithm) to find a relationship between SoC and voltage-segments described by the Single-Index model (3.26).

The obtained result confirms that information on SoC is present in voltage-segments.
3.4 Conclusions

In this chapter we illustrated how Singel-Index models can be used for State-of-Charge estimation of the battery. We made a summary of the SIM-theory, by presenting main definitions and the basic techniques for estimation of index-coefficients and a link-function, comparing the existing methods.

We proposed a new approach for the estimation of the index-coefficients by solving $L_1$-problem, which offers very simple and efficient way of estimating $\beta$, requires no iteration and is very computationally advisable. We demonstrated and discussed this idea through the "varying-current" experiment, that was specially designed in a way to allow extracting information on SoC from the shape of voltage curves adapted to the different current regimes.

The obtained results in State-of-Charge indication allow to conclude that the dynamic response of the system while the battery is under operation can be used to "see" how much energy remains.
Bibliography


Appendix A

Program Codes

A.1 Procedure for IS-estimation of a link-function $f$ in Section 3.3.3

function [sortx,mony] = ISestimation(xx,yy);
regim='IS';
[sortx, ind]=sort(xx);
y=yy(ind);

% monotone spline
if regim=='S'
    h=0.0001;
mflag=1;
method=1;
indfig=1;
    params=[h,mflag,method,indfig];
data(:, 1)=xx;
data(:, 2)=yy';
[mony]=monospline(data,params);
end;

% PAV regression
if regim=='I'
    n = length(y);
    mony = y;
    bb = 0;
eb = 0;
while (eb < n)
    bb = eb + 1;
end;
eb = bb;
while eb < n & mony(bb) == mony(eb+1)
    eb = eb + 1;
end
poolflg = -1;
while poolflg ^= 0
    if eb >= n | mony(eb) <= mony(eb+1)
        poolflg = 1;
    end
    if poolflg == -1
        br = eb+1;
        er = br;
        while er < n & mony(er+1) == mony(br)
            er = er + 1;
        end
        pmn = (mony(bb)*(eb-bb+1) + mony(br)*(er-br+1))/(er-bb+1);
        eb = er;
        mony(bb:eb) = pmn;
        poolflg = 1;
    end
    if poolflg == 1
        if bb <= 1 | mony(bb-1) <= mony(bb)
            poolflg = 0;
        else
            bl = bb-1;
            el = bl;
            while bl > 1 & mony(bl-1) == mony(el)
                bl = bl - 1;
            end
            pmn = (mony(bb)*(eb-bb+1) + mony(bl)*(el-bl+1))/(eb-bl+1);
            bb = bl;
            mony(bb:eb) = pmn;
            poolflg = -1;
        end
    end
end
end;

% PAV regression + smoothing spline
if regim=='IS'
n = length(y);
mony = y;
bb = 0;
Procedure for IS-estimation of a link-function $f$ in Section 3.3.3

\[
\begin{align*}
\text{eb} &= 0; \\
\text{while (eb < n)} & \\
\text{bb} &= \text{eb} + 1; \\
\text{eb} &= \text{bb}; \\
\text{while eb < n & mony(bb) == mony(eb+1)} & \\
\text{eb} &= \text{eb} + 1; \\
\text{end}
\end{align*}
\]

\[
\begin{align*}
\text{poolflg} &= -1; \\
\text{while poolflg ~= 0} & \\
\text{if eb} &\geq n \text{ | mony(eb) <= mony(eb+1)} \\
\text{poolflg} &= 1; \\
\text{end}
\end{align*}
\]

\[
\begin{align*}
\text{if poolflg} &= -1 \\
\text{br} &= \text{eb+1}; \\
\text{er} &= \text{br}; \\
\text{while er < n & mony(er+1) == mony(br)} & \\
\text{er} &= \text{er} + 1; \\
\text{end}
\end{align*}
\]

\[
\begin{align*}
\text{pmn} &= (\text{mony(bb)}*\text{eb-bb+1} + \text{mony(br)}*\text{er-br+1})/(\text{er-bb+1}); \\
\text{eb} &= \text{er}; \\
\text{mony(bb:eb)} &= \text{pmn}; \\
\text{poolflg} &= 1;
\end{align*}
\]

\[
\begin{align*}
\text{if poolflg} &= 1 \\
\text{if bb} &\leq 1 \text{ | mony(bb-1) <= mony(bb)} \\
\text{poolflg} &= 0; \\
\text{else} & \\
\text{bl} &= \text{bb-1}; \\
\text{el} &= \text{bl}; \\
\text{while bl > 1 & mony(bl-1) == mony(el)} & \\
\text{bl} &= \text{bl - 1}; \\
\text{end}
\end{align*}
\]

\[
\begin{align*}
\text{pmn} &= (\text{mony(bb)}*\text{eb-bb+1} + \text{mony(bl)}*\text{el-bl+1})/(\text{eb-bl+1}); \\
\text{bb} &= \text{bl}; \\
\text{mony(bb:eb)} &= \text{pmn}; \\
\text{poolflg} &= -1;
\end{align*}
\]

\[
\begin{align*}
\end{align*}
\]

[sp,values,param] =spaps(sortx,mony,1.e-8); 
[mony]=fnval(sp,sortx); 
end;