Physics-based Li-ion Battery Modelling

Towards Online Vehicular Applications

Thesis submitted by
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towards the degree requirements of

Doctor of Philosophy
Ph.D.

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Internal Examiner: TBD
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London 2018

Abstract

Put your abstract here...

Dedicated to ...

Acknowledgements

I would like to acknowledge the thousands of individuals who have coded for open-source projects for free. It is due to their efforts that scientific work with powerful tools is possible.

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Glossary

BMS Battery Management System(s) 9

DFN Doyle-Fuller-Newman 9

EIS Electrochemical Impedance Spectroscopy 11

SOC State of Charge 11

Abbreviations

ATP adenosintriphosphat 1

1
Introduction

[1] provide a comprehensive survey of the wide range of battery models out there.

1.1 put section name here

Write your text without any further commands, like this:.... Any organised system requires energy, be it a machine of some kind or a live organism. Energy is needed to win the uphill battle against entropy and pull together lifeless molecules to be able to do something in this world, like complete a PhD.

1.1.1 Name your subsection

Different organised systems have different energy currencies. The machines that enable us to do science like sizzling electricity but at a controlled voltage[1]. Earth's living beings are no different, except that they have developed another preference. They thrive on various chemicals.

Most organisms use polymers of glucose units for energy storage and differ only slightly in the way they link together monomers to sometimes gigantic macromolecules. Dextran of bacteria is made from long chains of α-1,6-linked glucose units.

Starch of plants and glycogen of animals consists of α-1,4-glycosidic glucose polymers [2]. See figure 1.1 for a comparison of glucose polymer structure and chemistry.

Two references can be placed separated by a comma [2, 3].

Insulin stimulates the following processes:

- muscle and fat cells remove glucose from the blood,
- cells breakdown glucose via glycolysis and the citrate cycle, storing its energy in the form of ATP,

[1]Footnote example

- liver and muscle store glucose as glycogen as a short-term energy reserve,
- adipose tissue stores glucose as fat for long-term energy reserve, and
- cells use glucose for protein synthesis.

Gene	GeneID	Length
human latexin	1234	14.9 kbps
mouse latexin	2345	10.1 kbps
rat latexin	3456	9.6 kbps

Table 1.1: title of table - Overview of latexin genes.

1.2 SI-Units

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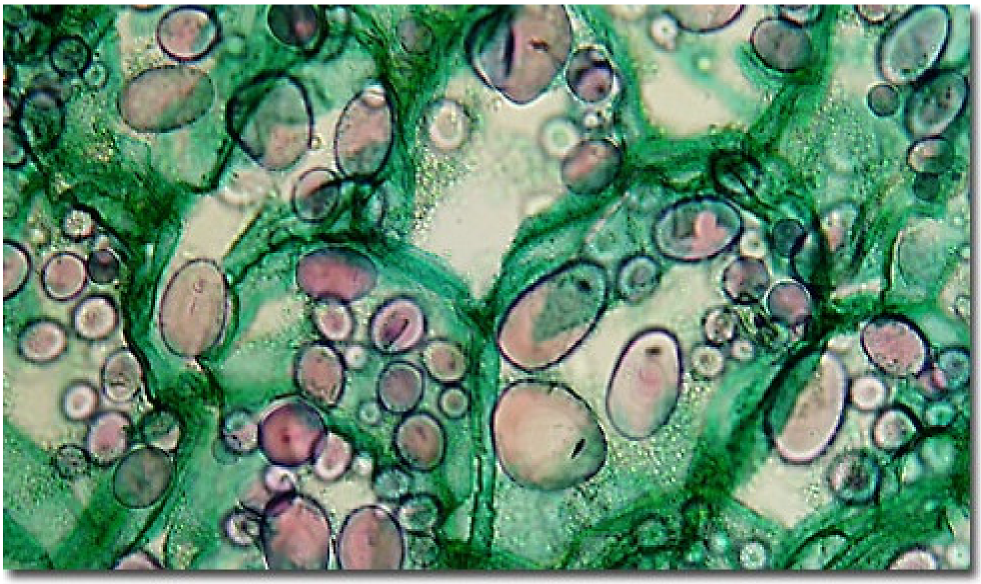

Figure 1.1: A common glucose polymers - The figure shows starch granules in potato cells, taken from Molecular Expressions.

2

State of the Art

2.1 Lorem ipsum

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3. three

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2.2 Some math

Theorem 1 (Residue Theorem) *Let f be analytic in the region G except for the isolated singularities $a_1, a_2, \dots, a_m$. If γ is a closed rectifiable curve in G which does not pass through any of the points a_k and if $\gamma \approx 0$ in G, then*

$$\frac{1}{2\pi i}\int_\gamma f = \sum_{k=1}^{m} n(\gamma; a_k)\mathrm{Res}(f; a_k)\,.$$

2.2.1 More math

$y = \sin(x)$:

$$y = \int_0^x \cos(x)\,\mathrm{d}x = \frac{e^{\mathrm{i}x} - e^{-\mathrm{i}x}}{2\mathrm{i}} \tag{2.1}$$

Normal text output. This is written with textsf! **And this text with textbf!** `This is Courier font.`

2.3 Preliminary aims

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3

Including tikz

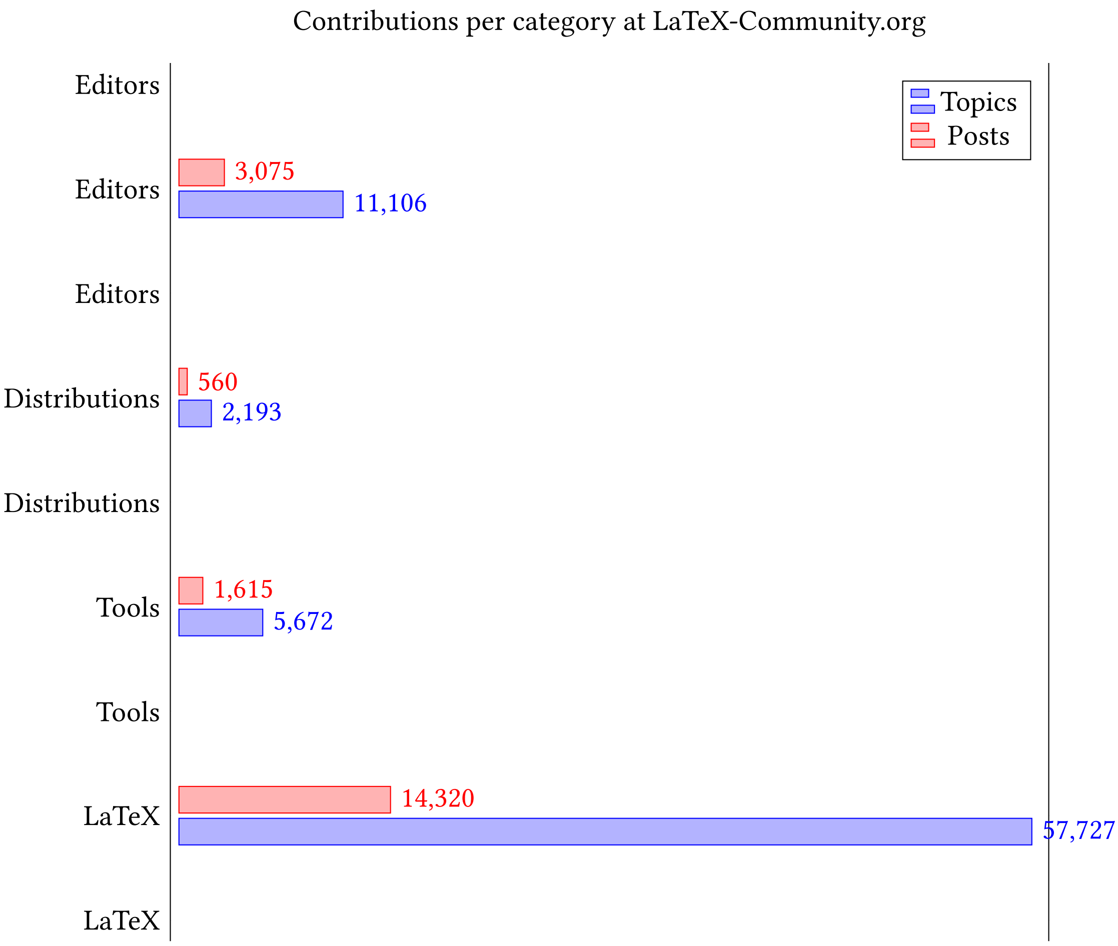

Figure 3.1: Tikz Example.

4

Physics-Based Controls-Oriented Time-Domain Modelling

Battery modellers face the classic conundrum of conjuring physics-based battery models that remain amenable for control applications. Firstly, the contrasting nature of this modelling objective is presented. Secondly, prior attempts by the research community to tackle this issue is briefly examined. A suitable family of models from the broad category of reduced-order models is identified as a promising candidate for implementation in controls applications. Next, the drawbacks of this family of models is discussed in detail. The state of the art implementation for tackling these drawbacks is presented and their inadequacies are discussed.

The following efforts/trials were done (failures)

write the chapter first. Come back to summarize this.

- first attempt

- second attempt

The following successes were achieved.

- first attempt

- second attempt

At the end of this chapter, we have a control oriented reduced order battery model amenable for use in real-time applications for SOC, SOH etc. estimations.

Control-Oriented models can be considered synonymous with the term ‘Reduced Order Models’. This is because the complexity of physics-based models inherently necessitates the use of a low order model. In this thesis, the two terms are used interchangeably.

4.1 Introduction to Control-Oriented Models

Jokar *et al.* [4] provide a comprehensive review of the various categories of reduced order physics based battery modelling. However, a notable omission in [4] is that it does not distinguish between models based on time-vs-frequency domains. Fan *et al.* [5] performed a similar review of reduced order battery models, but only provide a brief comparative overview of models derived and implemented in these dual domains. Unlike [4], this review did not aim to provide a classification of various reduced order models, but instead emphasises on a broad survey of relevant methodologies and tools towards obtaining such models. Hence, neither [4] nor [5] provide specific emphasis on the rubrics and implication of the choice of modelling in either of these dual domains. Although in principle, the transformation between them follows standard mathematical practices, availability of models for final implementation in the time domain aids immediate uptake by industry for adoption in online BMSes. Treatment of reduced order models from this aspect is so germane to the central hypothesis of this chapter, that the author of this thesis feels compelled to undertake a simpler classification exercise within the context of implementation. In this discussion, the various modelling methodologies and the resulting models are viewed as a continuum and hence this thesis discusses them with a unified perspective. Furthermore, there is also a need to highlight the salient works among the more recent advances and extensions to then-prevailing models published since [4] and [5]. Hence, the specialised review of reduced order modelling literature covered in this section intends to supplement — not supplant — the breadth of modelling art covered between them. In particular, care has been taken to minimize repetition of background art analysed in these aforementioned review articles, ensuring that only a subset of prior research that is pertinent to illustrate the new classification scheme introduced here shall be discussed.

citation(s) needed?

can a simple time-domain model do the job?

Physics-based Control-Oriented Models can be classified as belonging to one of the following categories. It is important to distinguish between models that are derived directly in the time domain versus those that are derived first in the frequency domain and later converted to time domain.

just enumerate in-line here

write this better

In principle, a modelling method that yields a time-domain mathematical description of physical phenomena that is lower in computational complexity by an arbitrary magnitude than the original DFN model can be considered for further investigation. In the absence of a quantitative definition of what can be considered as a true reduced order model, the number of candidate family of models to consider is large and overwhelming. In practice, the constraints of realtime implementation limits the choice of candidate modelling families. For instance, models relying primarily on classical finite difference [6] and Galerkin Finite Element [7] methods for transformation and order reduction of one or more field variables of the DFN model are immediately excluded, owing to the impracticability of implementing them in a resource-constrained environment.

Owing to the low entry-barrier for adoption in a real-time controller that logs samples of measurement data at specific time intervals, this thesis focusses on models that are cast for implementation in the time domain. Such a decision implies the exclusion of those models that are derived and implemented entirely in the frequency-domain. For the interested reader wishing to peruse the sizeable literature in this field, the discussion here briefly alludes to a few popular frequency domain modelling techniques.

The transfer-function oriented Padé approximation method for low order physics-based battery modelling pioneered by Forman *et al.* [8] has gained widespread adoption in the areas of cell design [9], charge trajectory optimisation [10], controller design [11] and state estimation [9, 12, 13]. Although online identification of a subset of aging parameters using a Padé model and a recursive least squares algorithm was presented in Prasad and Rahn [14], a detailed treatment was not given on the specific implementation details such as the transformation of the Padé reduced impedance to discrete-time difference equations. Padé models are typically limited to offline applications owing to the aggressive trade-offs required in the approximation order to maintain accuracy. Traditionally, models truncated to very low Padé order exhibit poor fidelity and perform no better than classical equivalent circuit models, although recent research attempts have focussed to mitigate this drawback [15, 16].

Smith *et al.* [17] pioneered the possibility of a semi-hybrid modelling approach by obtaining independent closed form expressions for all electrochemical field variables in the frequency domain except electrolyte concentration and potential, which were separately solved with the classical finite difference discretization method. This is the earliest published instance to the author's knowledge wherein the dynamics of the full order model were retained in the frequency domain, enabled through the innovative use of transcendental transfer functions without being forced to resort to truncation techniques such as Padé approximation. A composite impedance model was obtained which was then converted by residue grouping and truncation techniques to a 12th order state space model thereby introducing this hybrid modelling workflow. This model was capable of predicting the battery terminal voltage within 1% of a full-order DFN model. The frequency domain impedance-based model was derived for the frequency range of interest from 0–10 Hz through Model order reduction of the DFN model. The singular drawback of this model is its complexity for an online implementation. Furthermore, extensive parametrisation efforts are required to render the model useful for practical applications. The difficulties associated with such extensive parametric requirements coupled with inherent uncertainties in such obtained values act as a deterrent to stakeholders outside academia to adopt this model for online BMS implementations. Nevertheless, this model was the first of its kind to provide a physics-based battery model in the classical state-space formulation

at the end, count and substitute the canonical number of parameters here

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx + Du \end{aligned} \tag{4.1}$$

Although the matrices A, B, C and D do not directly involve physical parameters of the DFN model, computation of their numeric values through the model reduction procedure has a direct relationship with them. The presence of 12 states dilutes the effectiveness of state estimation algorithms. In the classical isothermal implementation of this model, with only output voltage being available to measure, the observablity of the model degrades. Although observablity analysis was proven in a noise-free

might have to re-write as being common with Plett and offer my comments to both as an informed researcher context, the presence of process noise (via unmodelled phenomena and parameter uncertainty) and sensor noise makes this model unattractive for implementation in a vehicular BMS application.

The identification of individual parameters of the DFN model remains a key area in battery modelling that remains only partially explored, and is key to implementation of the advanced models and control algorithms.. The state of the art in this area, the challenges involved and current efforts in this direction are explored in chapter 6. Although sensitivity analysis of the DFN parameters has been performed in literature, the extent to which parameter uncertainties influence the numerical values in the A, B, C and D matrices has not yet been attempted. In continuation of this research aspect, the order of magnitude shift in eigen/singular values of the relevant system matrix also need to be quantified to enable an informed choice about stability of such models for realtime implementations.

does this fit better in the introduction chapter?

citation here

A key drawback of Smith *et al.* [17] is the requirement for linearisation at a specific SOC. In [17], the operating point was chosen to be 50% for the derivation of the state-space model. This counteracts to a high degree, the usability of the model for state estimation tasks, wherein the SOC is itself the unknown quantity to be estimated. Furthermore, the need to interpolate between matrices from a look-up table pre-computed at different states of charge/temperature combinations is an ad-hoc approach to quantifying the model across the entire operating range of the battery. This renders the robustness of cross-over between models during state-estimation questionable, and demands the need for smoothing filters and other ad-hoc apparatus to obtain acceptable SOC estimations during online operation. The requirement of linearisation also renders the model usable only for a small range of SOCs.

Several attempts have been undertaken, with varying degrees of success, to improve and extend this controls-oriented model from Smith *et al.* [17].

write plett's group work in the next couple of paragraphs explaining the DRA. DRA was a way forward in bringing all the internal quantities closer to time-domain implementation rather than resorting to a lumped impedance parameter

Physics-inspired equivalent circuit models [18–20] are a class of hybrid models that have rapidly gained prominence since the publication of[4] and [5]. Such models are first derived in the frequency domain and later converted to an equivalent circuit representation. Prasad and Rahn [19] extended their Padé order reduced model first presented in [14] to convert the impedance model into standard equivalent circuits. approximation or EIS measurements, and later on converted to equivalent circuit models. In these family of models, the classical Randles equivalent circuit model structure is retained. However, the values of the electrical circuit components such as series resistance and equivalent capacitance are obtained through various mechanisms . The biggest advantage of such models is that they serve as drop-in replacements to traditional equivalent circuit models whilst still retaining their origins in physical principles rather than empirical curve-fitting. Merla *et al.* [18] introduced an equivalent circuit model that can be parameterised through a systematic decoupling of the kinetics and diffusion at both electrodes and in the electrolyte. Although these interacting phenomena can be complex to resolve over all length and time-scales, acceptable trade-offs in accuracy was demonstrated to be achievable from a system-level simulation perspective. A drawback of such models is that there exists an ad-hoc attribution of key model parameters such as the diffusion coefficients among the two electrodes through non-verifiable assumptions. Furthermore, in [18], notable discrepancies exist in

such as ...

the values of parameters such as electrolyte conductivity (obtained through calculations from EIS measurements) to that typically reported in literature. Chapter 6 discusses the author's efforts towards obtaining a similar physics-informed equivalent circuit model based on the results from the improved DRA reported in Gopalakrishnan*et al.* [21] and detailed in chapter 3. This physics-inspired equivalent circuit model seeks to explore the present gap in impedance modelling by forming an equivalent composite impedance value as laid out in [17]. The preliminary work towards this hitherto unexplored direction is briefly presented in chapter 6. This physics-informed impedance model can be extended to fit parameter values of components in an equivalent circuit model. The scope of this attempt differs from [18] in that, the author's efforts are focussed on suitability for online implementation for control applications as opposed to the objective of degradation diagnosis in Merla *et al.* [18]. It should be emphasised that in these category of models, there exists no direct link between the final value of the circuit components and the physical parameters. Nevertheless, the author believes that these models have the potential to elicit interest from stakeholders owing to the need for minimal code changes, thereby facilitating instant adaptability to existing BMS control architectures.

tikz picture here, showing a nice layout classifying various models

5

PGF-plots from python

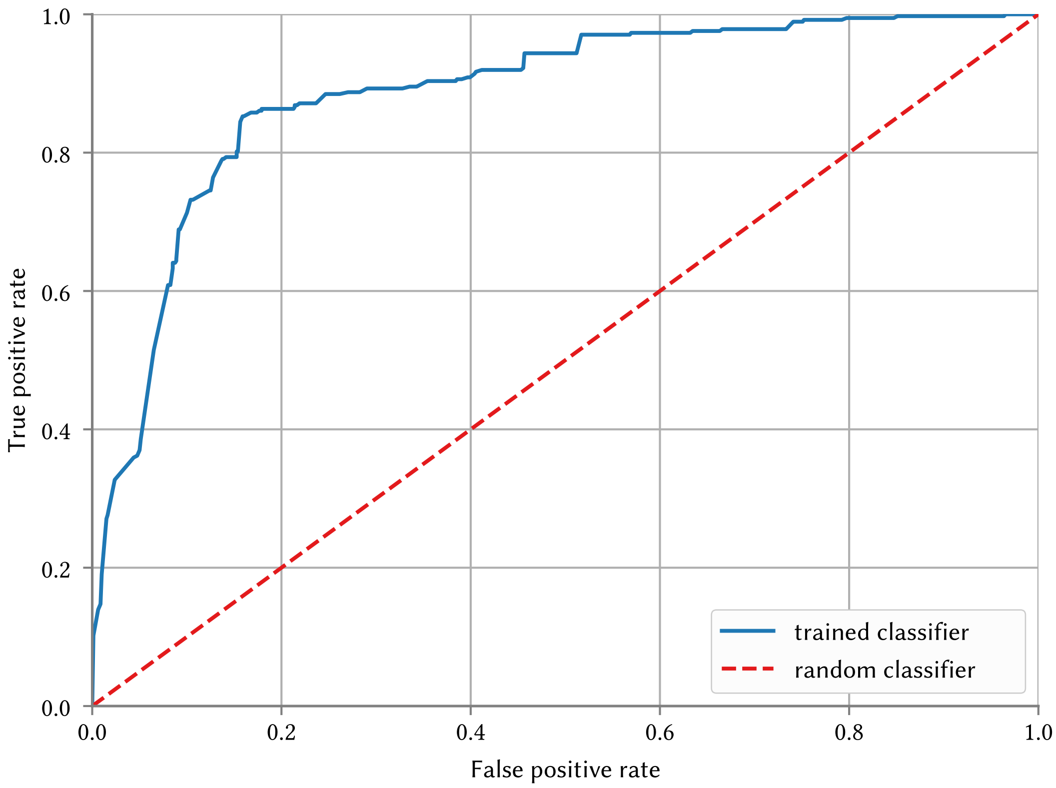

Figure 5.1: Example of using python to generate a pgf-figure which has the same fonts as the main latex document. Run python plot_exemplary_roc.py from the Python directory to generate the pgf-file.

6
Discussion and Future Work

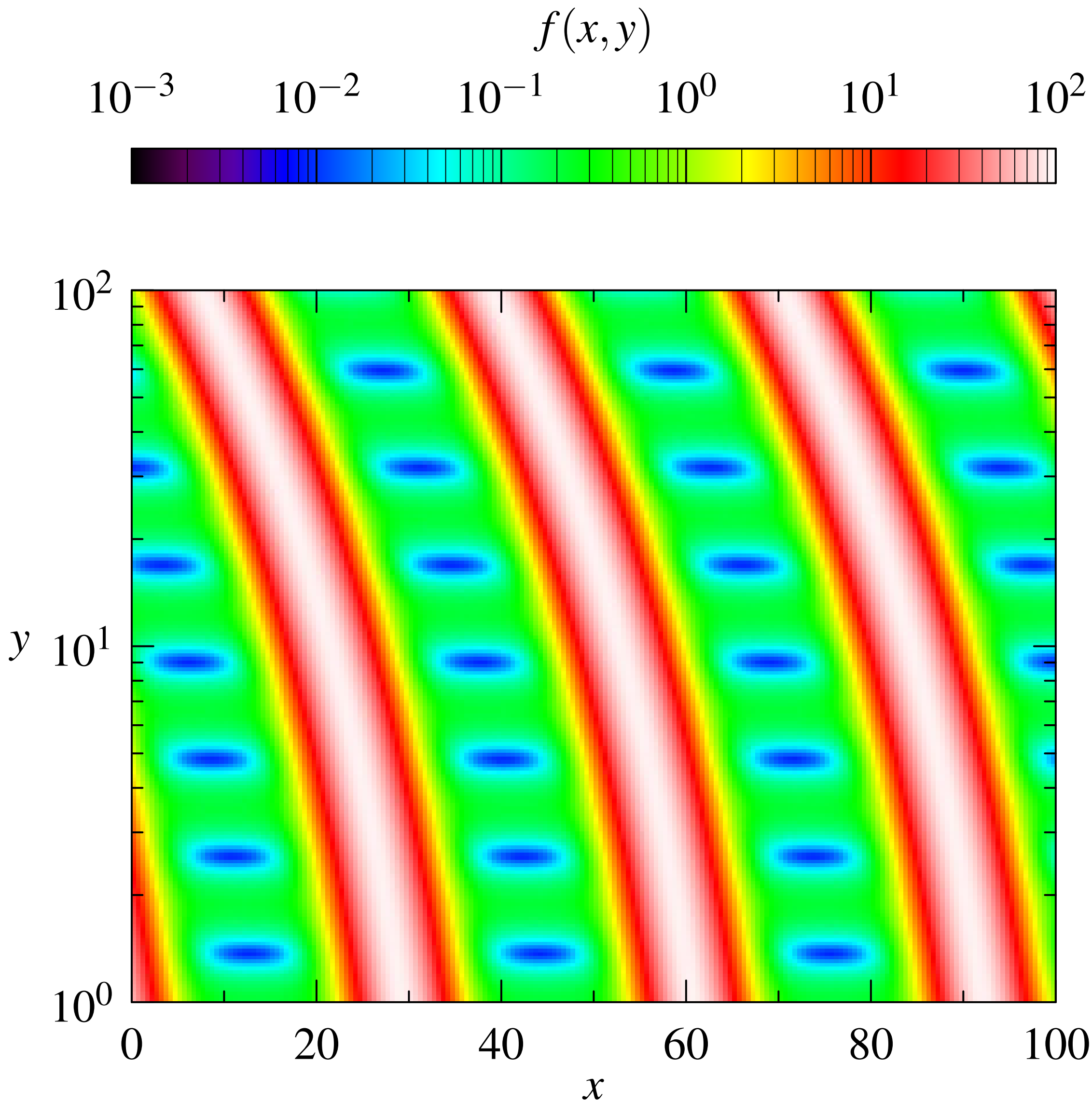

Figure 6.1: Example for plotting with asymptote

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Appendix A