2021

Projects on Process Optimization and Control

Johannes Jäschke and team

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1. Model Predictive Controller approaches while considering long term degradation in Batteries

Supervisor: Associate Professor Johannes Jäschke (johannes.jaschke@ntnu.no)
Co-Supervisor: PhD Candidate Sandeep Prakash (sandeep.prakash@ntnu.no)

Are you curious about how electricity markets work, and the role that energy storage devices play in the renewable energy future? Me too !!!, then this project could be of interest to you.

The big problem

One of the challenging aspects of powering the world with more and more solar panels and wind turbines is that we cannot really control when the sun shines or the wind blows. So, what do we do when the demand for electricity does not match up with its production? This is where energy storage technologies play a crucial role – storing energy during periods of low demand and discharging it to satisfy the excess demand.

The act of balancing the grid in short time scales (seconds to a few hours) is where grid scale battery energy storage applications are becoming more and more prevalent these days (The most well-known known one being the **Tesla Big Battery** in Australia – Thank Elon for the publicity).

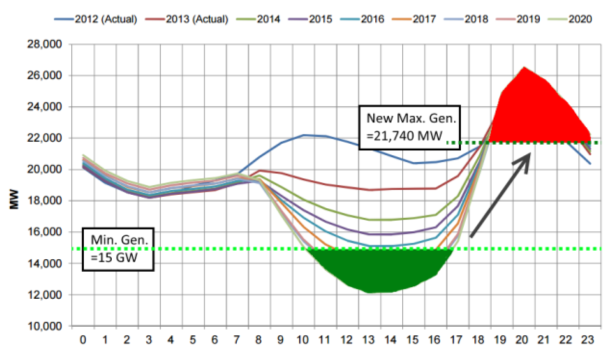

Figure 1: The Duck curve to explain the philosophy of load shifting using energy storage (Burnett, M)

Figure 2: Stock photo of Tesla Big Battery in Australia

But here lies the issue that I want to try and look more closely in this project. You could charge and discharge your "Big Battery" to capitalize even on the smallest frequent fluctuations in the grid – which can make you money now (Think charging for 1 sec, discharging for the next 3 secs and charging again because the electricity prices changed enough and was tempting enough for you to do this). Operating the battery so "fast and furiously" would be able to maximize your immediate profits, but this would be a very short sighted approach to take, because this can cause the battery to degrade faster and hence it would need to be replaced sooner than initially expected (for a good analogy of battery degradation – think of how the battery life in your phone gets poorer over time and it's not even able to last a full day's use).

There is this trade-off that exists between **maximizing short term profits** and **long term equipment degradation** (which in turn translates to maintenance/ replacement costs which happens in the distant future). In the case of batteries, the replacement costs are significant enough that you would be wise to care about in the short terms too.

In this project

Since we are not electrochemists, we would take for granted a mathematical model which is given to us which captures 1) Some detailed relations happening inside a battery and 2) relationship between how charging/ discharging affects the battery's state of health. We are currently using the Single Particle model for batteries for this purpose as seen in the paper (Cao et al., 2020). We would focus more on exploring methods in Numerical Optimization that can help us manage this trade-off.

During the Specialization project, we expect that you would be able to implement the mathematical model in Julia and simulate some operating profiles. This should give you a good understanding of the process and the build familiarity with the concepts we would later use.

During the Master Thesis, you should then be able to compare and implement some methods for the control of such a system that considers both economic performance and degradation.

The tasks outlined above are for both a specialization project and a further master's thesis project and can be divided accordingly.

What are we looking for in the student for this project?

- Be interested in, and have a basic understanding of process modelling, control, and optimization
    - Having done courses on these previously on these subjects are an advantage, but not necessary. Ideally you could consider just doing the MPC module as part of the specialization course – as this would introduce and get you some hands-on experience with most of the concepts you will need in the project.
- Be familiar with programming in general
    - We will help you get started and get comfortable on Julia
- (Lastly and most importantly) Motivation to learn and be self-driven
    - In the end - this is YOUR PROJECT

For more information about the project, contact Associate Professor Johannes Jäschke (johannes.jaschke@ntnu.no) or PhD candidate Sandeep Prakash (sandeep.prakash@ntnu.no)

References

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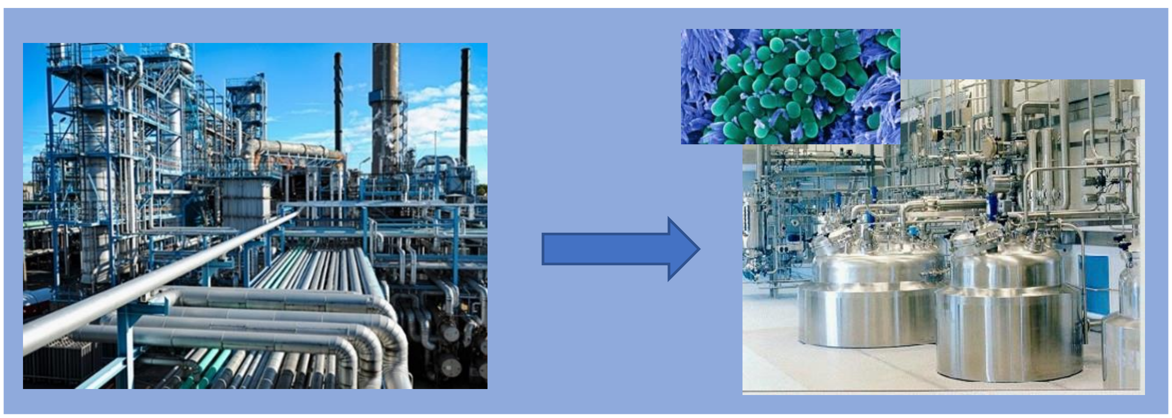
2. Optimal control of bioprocesses using metabolic modeling

Supervisor: Johannes Jäschke (johannes.jaschke@ntnu.no)
Co-supervisor: Caroline Satye Nakama (caroline.s.nakama@ntnu.no)

Why is it important?

One of the outcomes of the growing environmental awareness has been the increasing interest in the usage of renewable resources as an alternative to the traditional chemical industry. As a result, alternative production routes have been widely studied. Biochemical production of fuel and chemicals is one of such alternative routes and is often carried out as fed-batch processes. Ethanol and insulin are examples of biochemicals that are produced in large-scale in a fed-batch process. Many organic molecules have the potential of being produced or having equivalent substances developed via microbial platforms. However, switching the industry focus to biochemical production still requires extensive research in every level, from genetic comprehension and manipulation to process design and operation. This project focuses on the latter, aiming to study and evaluate optimal control strategies based on the metabolic modeling.



What are we going to do?

Control of fed-batch biological processes is often based on models that describe the dynamics of cellular growth, substrate consumption and external product secretion. However, they usually are not able to precisely describe all transient conditions that may occur in a fed-batch process [1]. An alternative is to use a metabolic model, that is, a model that can also describe the internal metabolism of the microorganism, such as dynamic flux balance analysis (dFBA) [2]. This approach is challenging to implement, but possible strategies have been reported in literature [1,3,4]. The idea of this project is to implement and evaluate control strategies for fed-batch fermentation using dFBA.

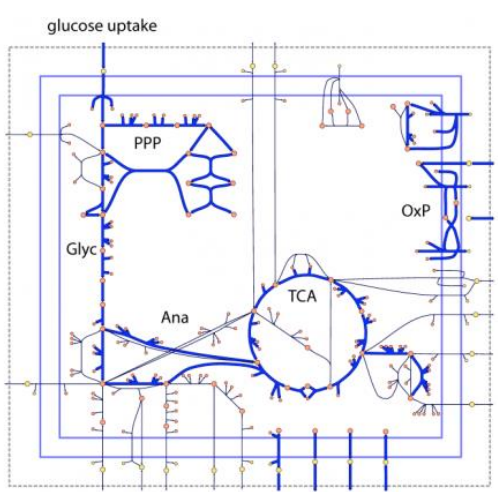


Figure 3. Example of a pathway in a metabolic network calculated with flux balance analysis.

What are we looking for in a candidate?

This is a mathematical and computationally focused project that can be extended to a master's project in the following semester. The plan is to use the Julia programming language for implementation. We do not expect the candidate to know Julia (learning it will be part of the process), but they should preferably be familiar with programming and, more important, eager to learn.

For more information about the project, you can contact one of the supervisors.

References:

[1] Hjersted, J.L. and Henson, M.A., 2006. Optimization of fed-batch Saccharomyces cerevisiae fermentation using dynamic flux balance models. *Biotechnology progress*, *22*(5), pp.1239-1248.

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3. Evaluation of strategies for solving mathematical programs with complementarity constraints

Supervisor: Johannes Jäschke (johannes.jaschke@ntnu.no)
Co-supervisors: Peter Maxwell (peter.maxwell@ntnu.no),
Caroline Satye Nakama (caroline.s.nakama@ntnu.no)

Why is it important?

Mathematical programming with complementarity constraints (MPCC) is a class of optimization problems that have one or more constraints of the type $0 \leq x \perp y \geq 0$, that is, if x is greater than zero, then y is zero and vice-versa. While both variables can be zero, if one is greater than zero, the other one must be zero. This type of formulation originated from equilibrium relations in economics, but there are many applications in engineering. Specifically, in process engineering, these problems can arise when dealing with phase change, flow reversal, safety valve operation, and discrete events in general [1]. MPCC is an active area of research and is of interest in both academia and industry. Solving an MPCC problem can be challenging due to some inherit mathematical properties, and different approaches and contributions have been proposed in literature [2,3].

What are we going to do?

We can start by looking at some toy models and relevant case studies in process engineering to understand how MPCC models work, while contributing to our group's MPCC problem library (https://carolinesnakama.github.io/). A possible avenue to develop these ideas further would be implementing some of the common algorithms for solving MPCCs such as Leyffer and Munson's SLPEC-EQP method [1] and a popular interior point method penalty formulation [2]. Properties such as convergence and robustness of solution can be investigated for selected problems. Similarly, challenging aspects that are particular to MPCCs can be investigated.

What are we looking for in a candidate?

This is a mathematical and computational project focused on formulating and solving MPCC models with basic approaches during the specialization project, and on algorithm implementation during the master's project. The plan is to use the Julia programming language for both parts. We do not expect the candidate to know Julia (learning it will be part of the process), but they should preferably be familiar with programming and, more important, eager to learn.

For more information about the project, you can contact one of the supervisors.

References:
[1] Biegler, L.T., 2010. Nonlinear programming: concepts, algorithms, and applications to chemical processes. Society for Industrial and Applied Mathematics.
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4. Designing subsea oil field layouts using artificial intelligence

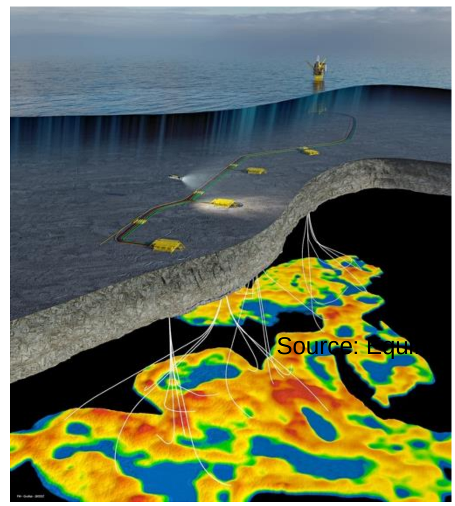
Supervisors: Johannes Jäschke and Milan Stanko Cosupervisor: Leonardo Sales

Project goals

Develop a field layout optimization model using artificial intelligence (genetic algorithms) and implement it in a case study.

Why this project?

Designing a subsea oil field is a task that takes several months to complete by a experienced team of engineers. Many factors play a role in the decisions, such as number of wells, production profile, oil economics, current technology, reservoir characteristics, and many more. Using optimization techniques such as genetic algorithms to tackle this problem can point us to designs that provide the largest profit in a much shorter time span, and also give insights about the problem and the efficient use of natural resources.



In overall, by proposing an optimization tool for field layout, we want to automate large-scale decisions in an oil field development.

How this will be useful?

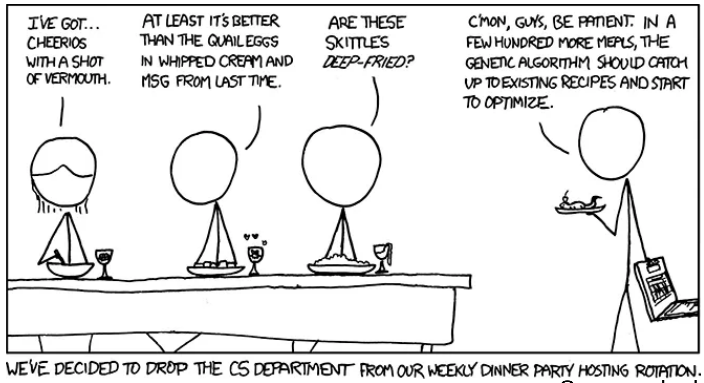
As the oil industry has interest in developing such tools, this master project will be part of an ongoing project at NTNU SUBPRO center, a research-based innovation center in partnership with the most important industrial players in subsea oil production.

What I am supposed to do in this project?

You will be developing a genetic algorithm to tackle the oil field layout problem. Note that this is a heuristic method, i.e., it is a practical method to generate solutions that may not be the perfect one, but are good ones given a limited timeframe or deadline. You can read more about them in Mohaghegh (2000) and Goldberg (1988). Not only the solutions by this method are interesting, but it is planned to compare the designs obtained by your algorithm with the one obtained by exact algorithms. These algorithms guarantee the best solution possible, however they take much more time to solve the problem, sometimes infeasible to practical purposes.

Sounds good! What the candidate should know?

The project is challenging, but will give you more understanding of oil & gas field development process, and a chance to learn (in practice) how to model, develop and implement an artificial intelligence optimization technique. To successfully complete the project, you should:



Source: xkcd

- Be interested in modeling and optimization;
- Be familiar and interested in programming (any language suited to engineering is good);
- Be creative and eager to learn.

For more information about the project, contact PhD student Leonardo Sales (leonardo.sales@ntnu.no), Assoc. Prof. Milan Stanko (milan.stanko@ntnu.no), or Assoc. Prof. Johannes Jäschke (johannes.jaschke@ntnu.no).

References

Goldberg, D. E. (1988). *Genetic Algorithms in Search, Optimization and Machine Learning* (13th ed.). Addison-Wesley Professional.

Mohaghegh, S. (2000). Virtual-Intelligence Applications in Petroleum Engineering: Part 2—Evolutionary Computing. *Journal of Petroleum Technology*, *52*(10), 40–46. https://doi.org/10.2118/61925-JPT

5. Modeling reliability and maintenance in field layout optimization

Supervisors: Johannes Jäschke and Milan Stanko Cosupervisor: Leonardo Sales

Project goals

Consider reliability and maintenance aspects in a field layout optimization model and implement it in a case study.

Why this project?

Maintenance and reliability are important aspects while developing a subsea oil field. Without proper maintenance, even the best engineering solutions are doomed to fail. However, considering maintenance and reliabilty in the design decisions is a challenge, and many other factors in the field layout play a role, such as number of wells, production profile, oil economics, current technology, reservoir characteristics, and many more. To economically compare two or more alternatives, a maintenance and reliability estimation procedure is yet to be developed.

By proposing a cost estimation procedure for reliability and maintenance, we want to automate large-scale decisions in an oil field development.

How this will be useful?

As the oil industry has interest in developing such tools, this master project will be part of an ongoing project at NTNU SUBPRO center, a research-based innovation center in partnership with the most important industrial players in subsea oil production.

What I am supposed to do in this project?

You will be developing a reliability and maintenance cost estimation procedure for the subsea field layout. Your method will be applied into an optimization model, so it must be developed in a way that is computationally fast, while capturing important costs and aspects of reliability and maintenance. For more information about reliability and maintenance in petroleum production systems, please check Verheyleweghen (2020).

Sounds good! What the candidate should know?

The project is challenging, but will give you more understanding of oil & gas field development process, and a chance to learn (in practice) how to develop and implement an maintenance and reliability cost model. To successfully complete the project, you should:

- Be interested in modeling, optimization and a bit of programming;
- Be familiar with maintenance and reliability;
- Be creative and eager to learn.

For more information about the project, contact PhD student Leonardo Sales (leonardo.sales@ntnu.no), Assoc. Prof. Milan Stanko (milan.stanko@ntnu.no), or Assoc. Prof. Johannes Jäschke (johannes.jaschke@ntnu.no).

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Verheyleweghen, A. (2020). *Control Degrees of Freedom for Optimal Operation and Extending Remaining Useful Life* [NTNU]. https://ntnuopen.ntnu.no/ntnu-xmlui/handle/11250/2656034

6. High Precision Numerical Optimization: Results you can count on

Floating point arithmetic is the mainstay of modern scientific computing but this apparently reliable workhorse can occasionally lead us astray: these computations may produce erroneous results, which can be difficult to detect.

A practical example of this is the failure of a Patriot missile system to intercept an incoming Scud in 1991, resulting in the death of 28 US soldiers [Par]. The system's internal clock value was an integer representation of the number of elapsed tenths of seconds since start-up. However, calculations were done with 24-bit registers. To convert the clock value to seconds, it was multiplied by the binary representation of `0.1 = 0.00011001100110011001100b = 209715/2097152`. Unfortunately, the system had been active for circa 100 hours so the error was [Wol], `(1/10 − 208715/2097152) × 3600000 ≈ 0.34` seconds. Given the Scud was travelling at circa 1,676 meters per second, the location estimate would have been off by over a kilometer. See also, presentation slides from Kahan [Kah12] (primary architect of IEEE 754-1985 and inventor of Kahan summation algorithm). These type of issue –and more importantly, how to avoid them– comprise much of numerical analysis

Despite numerical optimisation algorithms generally having favourable numerical properties, problems can still occur. For example, models that are inherently multi-scale often require reformulation and use of special techniques to process; even so, one can still encounter issues with computed solutions being infeasible or having an appreciable error.

These issues can often be ameliorated by use of high precision arithmetic. Instead of calculating using 64-bit double precision as usual, longer word lengths are used. A common choice is quad: twice the length of double, it is often sufficient to remedy these issues, and it can be an efficient choice with fast software implementations. Other choices are the use of rational arithmetic or using arbitrary precision.

Most solvers cannot calculate in precision better than double (or the intermediate extended). Reliance on dependencies such as highly efficient linear algebra libraries means the development cost of refactoring software to use higher precision arithmetic is substantial, and the demand has traditionally not been strong enough to justify this. However, there was some recent efforts in this direction: a quad precision version of MINOS was successfully used to solve a large ill-conditioned problem concerning a growth maximization for macromolecular expression model, see [Yan; Ma+17]. Also see the discussion in the presentation slides, [Sau15; Sau17].

It is anticipated that the specialisation project would largely comprise use of supplied tools to test various difficult or pathological problems. The student will acquire or further their knowledge in aspects of numerical analysis, how to approach numerical experiments in a consistent manner, and manage a larger body of work in a coherent manner. Depending on the student's interests, there are several directions in which these ideas can be further developed including a larger programming project, theoretical work, or application to specific optimisation problems of industrial importance.

To be able to successfully undertake this project, the student should:

• be a reasonably competent programmer, ideally in (or willingness to learn) MATLAB and/or Julia;

• have an interest in tackling 'difficult' and unusual problems; and,
• have some mathematics grounding in linear algebra, numerical optimisation, etc.

The project aims to develop competencies in several areas that are valuable both in industrial and academic work contexts:

• building the confidence and tolerance to 'sit' with difficult problems until a solution is found;

• skills in programming and algorithm design;
• understanding of concepts such as roundoff error, truncation error, ill-conditioning, etc; and,

• gaining experience of managing and directing one's own project.

Please send any queries to Johannes Jäschke (Associate Professor) johannes.jaschke@ntnu.no or Peter Maxwell (Postdoc) peter.maxwell@ntnu.no.

References

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7. Vertical Multiphase Flow: Gas Lift (collaboration with EPT and Tanzania)

Cosupervisors: Jose Matias, Ole Jørgen Nydal (EPT)

This student project concerns gas-liquid flow in vertical pipes. A particular concept for wells and risers is gas-lift, were gas is injected into the riser to reduce the gravitational pressure drop such that the production rate from a reservoir into the vertical pipe can increase.

Gas lift systems can become unstable, if the choke operates at subcritical conditions.

Dynamic flow phenomena in gas-lift systems can be studied in both small scale and large scale systems at NTNU. A small scale system (3m) is available at Dept. of Chemical Engineering and a larger scale system at Dept. of Energy and Process Engineering, EPT (15m). Two students can collaborate on the case of gas-lift, one from each laboratory.

Tasks at the EPT laboratory can included:

- Experiments in vertical flow: effect of inlet conditions on flow regimes in the vertical riser

- Demonstration of unstable flow conditions

- Implementation of a frequency controller on the pump, to obtain constant pressure boundary conditions for the inflow to the riser.

The flow observations can be compared with dynamic simulations, using OLGA and/or LedaFlow.

The work is linked with a NORPART mobility project “UDSM-NTNU mobility program in energy technology” which includes exchange of master students between NTNU and University of Dar es Salaam, Tanzania. NTNU students can typically have a period of stay (one month) at UDSM, during the master thesis period. A student from UDSM will join the gas-lift student group at NTNU for 4 months during the autumn 2021.

8. Control of a continuous-flow microreactor

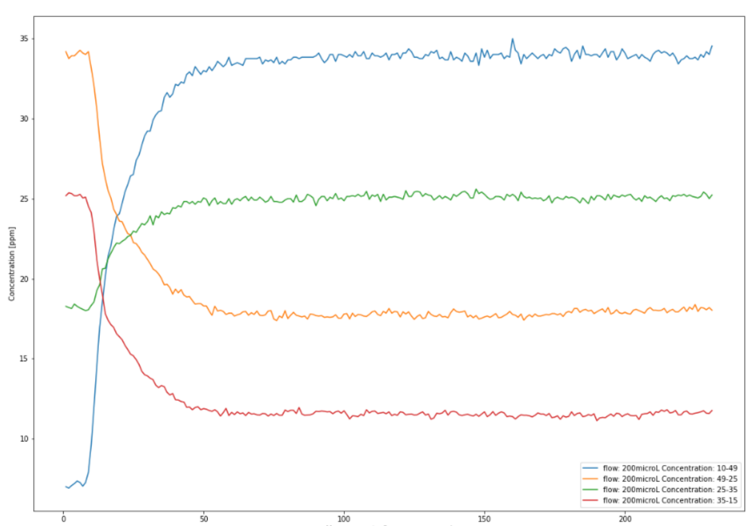
Cosupervisor: (Marcin Dudek – Ugelstad laboratory)

Background:

Controlling processes in flow is a crucial factor affecting the outcome of a number of industrial operations. In order to avoid deviations in the product quality and keeping up with the production yield, advanced control models are often implemented. These take into account readings from various sensors and instruments, and decide on various parameters of the process. In a lab, this process can be simulated and studied with a continuous-flow microreactor. Microreactor technology has recently gained a lot of attention within chemistry, biomedicine and biology applications. Due to its small dimensions and easy control of the process parameters, it is also an excellent tool for testing both simple and more complex control models.

Objective:

In this project, a flow setup, integrated in Python environment, is going to be used as a simplified production process. A fluidic system, composed of syringe pumps, valves and an inline spectrophotometer will be used to test different variables affecting the outcome of the experiment. Two or more fluids will be mixed together at different ratios, producing a solution of a specific concentration, measured online by the spectrophotometer (see Figure for an example of a dynamic change of concentration upon changing the flow rates of the pumps). A previously developed control model will be further modified to account for various disturbances that can affect the outcome of the process. In addition, some constraints, such as minimum concentration of the product or total flow rate will be introduced to bring the simulated process closer to real-life conditions. A combination of creating a model and observing its outcome in simulated and experimental environments will provide an opportunity to learn about both the theoretical approach, as well as experimental factors affecting the process.



9. Scientific Machine Learning – tuning out the noise

Supervisor: Johannes Jäschke Cosupervisor: Evren Turan

Scientific machine learning is defined as the combination of domain knowledge with machine learning. You've surely heard of machine learning – it seems to be everywhere these days. This project offers the opportunity to learn more about machine learning, while also improving your programming skills! If you are unfamiliar with machine learning methods you will learn what is behind the hype, while those with familiarity will have the chance to explore further.

In this project, we will use machine learning methods to perform optimisation in the presence of noise. Also, see the related project "Scientific Machine Learning – Uncertainty and first principle models"

The project

It would be ideal if we could operate a process at its optimum. Typically this requires having a model, but we often do not have perfect models of processes. If we have measurements of the system, we can overcome this model mismatch [1]. However, reality is noisy – sensors fluctuate and often we cannot get accurate measurements, and classical methods will fail. Modern machine learning methods, such as Gaussian Processes, allows us to rigorously model a noisy system [3], and furthermore, use integrate this modelling process with some optimisation algorithm.

This project will focus on developing machine learning models for optimisation of a noisy system, using different amounts of data/information. This could include providing the machine learning model a simplified model of the system or noisy estimates of process gradients. We will examine how this influences the optimisation of toy models and could potentially be applied to a relevant case study.

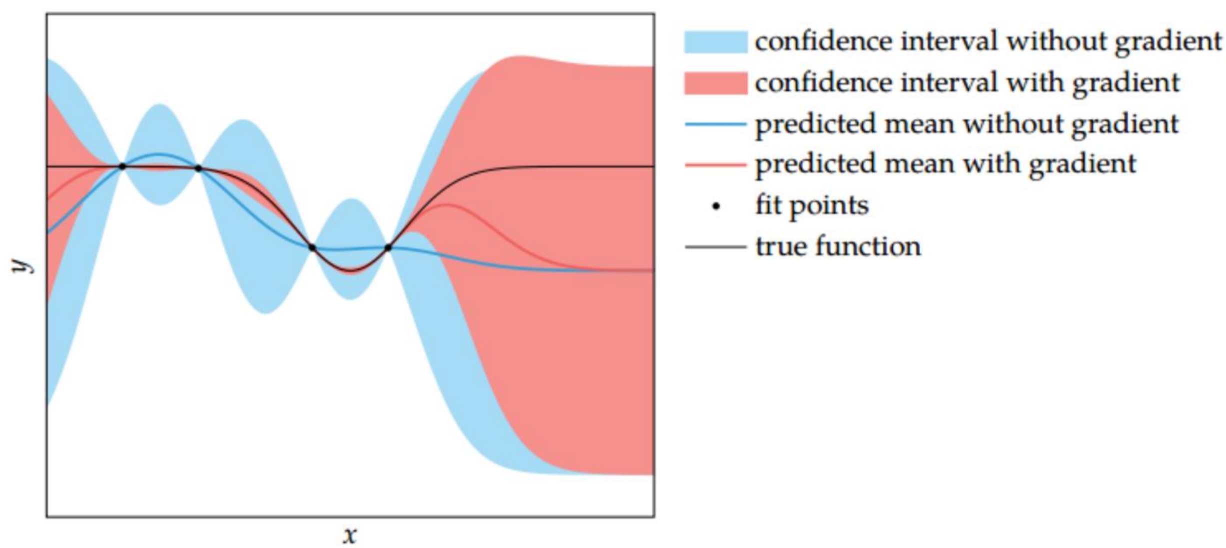


Figure showing the influence of using gradient information with a Gaussian Process, taken from [2]

What are you looking for in candidates?

This is a computationally focused project that can be extended as a master's project in the following semester. Basic familiarity with programming (in any language) is preferable. The candidate is not expected to have prior experience in machine learning or data science, only to be interested and willing to learn!

For more information about the project, contact Associate Professor Johannes Jäschke (johannes.jaschke@ntnu.no) or Evren Turan (evren.m.turan@ntnu.no).

References

[1] Marchetti, A. G., François, G., Faulwasser, T., & Bonvin, D. (2016). Modifier adaptation for real-time optimization—methods and applications. Processes, 4(4), 55.

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[3] del Rio Chanona, E. A., Graciano, J. A., Bradford, E., & Chachuat, B. (2019). Modifier-adaptation schemes employing Gaussian processes and trust regions for real-time optimization. IFAC-PapersOnLine, 52(1), 52-57.

10. Scientific Machine Learning – Uncertainty and first principle models

Supervisor: Johannes Jäschke Cosupervisor: Evren Turan

Scientific machine learning is defined as the combination of domain knowledge with machine learning. You've surely heard of machine learning – it seems to be everywhere these days. This project offers the opportunity to learn more about machine learning, while also improving your programming skills! If you are unfamiliar with machine learning methods you will learn what is behind the hype, while those with familiarity will have the chance to explore further.

In this project, we will combine neural networks with first principal models and quantify uncertainty in these predictions. Also see the related project "Scientific Machine Learning – tuning out the noise."

The project

Source: XKCD.com

Machine learning has received a lot of hype, due to the development of popular and flexible methods that have been successfully applied to incredibly complex problems in a variety of fields. Although machine learning methods are flexible, they are also incredibly data intensive and can have issues relating to generalizing to new data. Numerous ways have been proposed to alleviate these problems, including to combine these machine learning methods with first principal scientific models [1, 2]. This combination allows the combined model to better approximate the true system, while taking advantage of the structure of the scientific model [2]. Using Bayesian based methods, we can not only obtain predictions, but can also estimate the uncertainty of our predictions. This gives our models the ability to say "I don't know" instead of just giving out wrong answers.

In this project we will look at augmenting scientific models with neural networks while quantifying our uncertainty in the combined model. We will showcase this approach on toy models, and potentially a case study.

What are you looking for in candidates?

This is a computationally focused project that can be extended as a master's project in the following semester. Basic familiarity with programming (in any language) is preferable. The candidate is not expected to have prior experience in machine learning or data science, only to be interested and willing to learn!

For more information about the project, contact Associate Professor Johannes Jäschke (johannes.jaschke@ntnu.no) or Evren Turan (evren.m.turan@ntnu.no).

References

[1] Chen, R. T., Rubanova, Y., Bettencourt, J., & Duvenaud, D. (2018). Neural ordinary differential equations. *arXiv preprint arXiv:1806.07366*.

[2] Rackauckas, C., Ma, Y., Martensen, J., Warner, C., Zubov, K., Supekar, R., ... & Edelman, A. (2020). Universal differential equations for scientific machine learning. *arXiv preprint arXiv:2001.04385*.

11. Multiphase flow modelling for virtual flow metering applications

Supervisors – Johannes Jäschke, IKP & Christian Holden, MTP; Co-supervisor- Md Rizwan, MTP

Keywords: Virtual flow metering, First principles model, Digital twins, Uncertainty quantification

Motivation:

Oil and gas production systems usually consist of multiple oil wells connected to a production facility with the flowlines. These oil wells can be onshore or offshore. The well heads of these production wells can be located on a platform or even sitting on the ocean floor under water. Therefore, the produced fluids from these wells is transported across large distances through the flowlines.

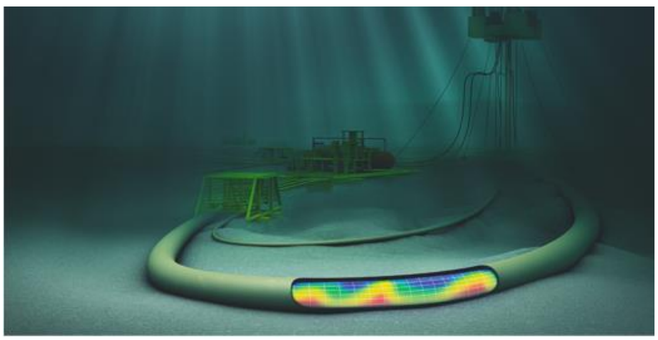

Figure 1: Typical offshore production system with subsea wells [2].

Typically the produced fluid is a multiphase mixture of oil, gas, water and solids such as sand or asphaltenes. For economic operation of the production systems it is important to know the oil, gas and water flowrates from each well. The information about the flowrates of the associated phases is crucial to make decisions regarding the production optimization, rate allocation, reservoir management and to predict the future performance of the field [1]. Direct measurement of these flowrates using multiphase flowmeters (MPFMs) is expensive and has high maintenance costs. Hence we plan to use virtual flow metering (VFM) to estimate these multiphase flowrates without actually measuring them directly. The idea behind VFM is to collect the available field data and use it in a numerical model to estimate these multiphase flowrates. Hence, in this project the focus is to develop first principle models for the virtual flow metering systems as it allows to make inexpensive and accurate estimate the multiphase flowrates.

Tasks

The tasks involved in this project are as follows:

- Development of simulation framework based on first principles model for virtual flow metering. For this prior experience with the multiphase modeling softwares like Ledaflow [2] or OLGA will prove to be of advantage.
- Sensitivity analysis to quantify the effect of measurement uncertainties on flowrate estimates. These uncertainties can be attributed to the measurement noise or drifts usually present in the data from a real field applications. Hence this study will help to identify how the first principle

based VFM systems react to these uncertainties. This can be done in any standard programming language like Python or MATLAB.

This master project will be part of an ongoing project in SUBPRO. The student can take advantage of the cross disciplinary supervision and shall get an opportunity to interact with the associated SUBPRO industry partners.

References

[1] Bikmukhametov, T. (2020). Machine learning and first principles modeling applied to multiphase flow estimation. PhD thesis, NTNU Norway

[2] Product Sheet, K- Spice® Meter, Kongsberg, https://www.kongsberg.com/globalassets/digital/oil-and-gas/k-spice-process-simulation/k-spice-meter.pdf

12. Robust Model Predictive Control of a State-of-the-art Electrolyzer Plant

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Do you like programing and want to learn more about control and optimization, then this is the project for you. In this project you will get to implement a nonlinear Model Predictive Controller nMPC on a state-of-the-art electrolyzer plant. This project is a continuation of a previous master project in cooperation with Yara where a mathematical model of an electrolyzer plant was developed.

Motivation:

So why is an electrolylzer plant an interesting process you should spending the next year of your life on, designing a control-structure for. Well, here are some reasons: With the invention of the Haber-Bosch process the highly reactive component ammonia could be formed from nitrogen gas and hydrogen gas. Using ammonia as a raw material agricultural fertilizer can be produced. Due to the Haber-Bosch process large scale industrial production of fertilizers which has had a huge impact on the food production of the world [1], is possible. This production, however, requires hydrogen gas. In the conventional process hydrogen gas is obtained from steam-methane reforming of natural gas. By switching to hydrogen production using green alternatives like water electrolysis, the carbon-footprint from fertilizer production can be reduced.

What will you do?

You will use the mathematical model developed in [2] to implement a nonlinear model predictive controller of the electrolyzer plant, in Julia and do run some simulations. Assuming nonlinear optimization is a new concept, the specialization project will focus on familiarizing yourself with the electrolyzer model, learning Julia, and implementing a nonlinear MPC on the electrolyzer plant. Having familiarized yourself with the process in the specialization project, you can explore more advanced robust MPC formulations in the spring thesis project, however many different possibilities are available.

What are the prerequisites for this project?

We expect you to be interested in optimization and control theory. It is not necessary to be an expert in any of these fields but some knowledge from e.g., previous courses are preferable. We also expect you to be interested in programming and possessing some elementary skills in at least one language. We do not expect you to know any Julia beforehand however, as learning it will be part of the specialization project. Most important, however, is that you are motivated and willing to learn.

If you have any questions about the project, please contact either Associate Professor Johannes Jäschke (johannes.jaschke@ntnu.no) or PhD candidate Simen Bjorvand (simen.bjorvand@ntnu.no)

References

[1] Erisman J. W., Sutton M. A., Galloway J., Klimont Z. and Winiwarter W, How a century of ammonia synthesis changed the world. Nature Geoscrience, 636-639, 2008

[2] Rizwan M., Plantwide control of alkaline water electrolyzer plant for hydrogen production, Master thesis, Norwegian University of Science and Technology, 2020