

MOD300-1 Anvendt Python programmering og modellering

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Let me first introduce US



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Before to be here...

- Chemical engineer graduated from the Politecnico di Torino
- PhD at M&ST university of Rolla, Missouri, USA
- Post Doc at TUD Darmstadt, Germany
- Researcher at NTNU, Trondheim, Norway
- Post Doc UiO, Oslo, Norway
- Assoc. Prof. at Uis, Stavanger, Norway
- Prof. at Uis, Stavanger, Norway from 28.8.2025!!

Course objectives (second half)

Understanding of

- Data sources and data properties
- Monte Carlo simulations
- Basis of machine learning
- modeling

Metalearning

- Pedagogic empiricism teaches us that good learning happens in social contexts where the students are actively participating in the classroom dialogue
- In general, the number of questions, and the dialogue in general, drops significantly when lectures are recorded
- Remote attendance can lead to empty classrooms and higher failure rate.

Teaching method

!Active Learning!

- There will be a combination of lectures and tutorials.
- Tutorial and hands-on will be presented during the course.
- Study groups are strongly encouraged.
- In class discussions are encouraged at any stage.
- Flip classroom approach: problem first (when possible).
- Feedback expected from you!
- Note: each teacher, even if coordinated, will have a different approach/expectations.

A personal considerations on generative AI

With great power comes great responsibility (Spider-Man)

LLMs can and shall be used in a **production** phase . Their usage is encouraged, but they **DO** hinder learning.

If you want to be a student (i.e. whom is learning), you shall take the responsibility in delivering original output.

Hard and soft modeling

Models allow us to predict 'the future', or describe the past and present (what is the present...?). They can be wrong on porpose!

Remember

Models are always wrong, but some are useful. (George Box)

Three main families:

- ① Hard models (physics)
- ② Soft models (statistic)
- ③ Machine learning

Soft modeling

- Soft-modeling describes systems without the need of an *a priori* physical or (bio)chemical model postulation. They are **data driven** models.
- Soft models are much easier to make than hard models.
- Soft modeling can be used to understand complex relationships.
- Soft modeling needs (much) more data than hard-modeling.
- Soft models have a poor extrapolating capabilities (compared with hard-modeling)

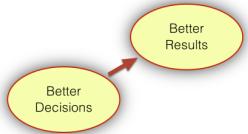
Why are we here? Why this course?

- Decisions are the hinge. What influences your decisions has value.

Life lesson?!

Life is a sum of all your choices (Albert Camus)

The only way you can purposefully influence your life, your family, your organization, your country or your world is through **the decisions you make**.



Models can be useful only when they can influence decisions

Hard modeling

- Based on an accurate physical description of the system and mathematical modeling (e.g. differential equations). Hard models are often deterministic.
- Hard modeling methods usually use optimization methods to find out the best values for the parameters of the model.
- Hard modeling is preferable in laboratory experiments, where all the variables are controlled and the physicochemical nature of the dynamic model is known and can be fully described using a known mathematical model.
- Hard modeling, if successful, usually gives better understanding of a system and better extrapolations. Wrong assumptions often lead to non-sense results.

How to create hard models?

After understanding the problem to be solved we need to:

- ① Link mathematics to physics.
- ② Define boundary conditions and constitutive equations.
- ③ Make tons of assumptions.
- ④ Solve the constitutive equation in space and time.
- ⑤ Check solution stability and sensitivity analysis.
- ⑥ A long set of judicious approximations have to be taken.
- ⑦ It is hard (but we are engineers!).
- ⑧ Get quite some money for the awesome job.

How to create soft models?

After understanding the general problem to be solved we need to:

- Determine a suitable **numerical description**.
- Choose a suitable **model** to which parameters are fitted.
- Train, test, validate the model.
- Perform **data analysis** with chosen method(s).
- Link predictions with expectations.

Hard models vs Soft models

Requirements

Deterministic:

- physics and expert knowledge
- integration of various information sources
- very complicated

Statistical:

- quick
- uncertainty assessment
- data driven approach
- physics can be included
- stochastic modeling

Hard models vs Soft models

Behaviour

Deterministic:

- predictable
- defined error

Statistical:

- outcome uncertainty
- undefined error
- sampling resolution issues

Uncertainty or Probability?

Our aim here is to provide good guidance on how to link data, models and output to value creation.

- First we need to understand uncertainty and probability, and the difference between the two.
- Spoiler: Probability is the language of uncertainty!
- We will analyse, quantify and structure models as a function of uncertainty.
- Clarity of language in probability is one of the hallmarks of decision analysis and of modeling.

Data properties (i.e. statistics!)

- All starts from data: what are data-properties?
- Are there such things as good data and bad data?

Life lesson (or exam question, same thing ;))

- Data **DO NOT always** have value.

- TRASH in TRASH out

Quantifying uncertainty

On the **data sources** side

- Confidence intervals
- Relevance
- Significance
- Correlation
- Causation
- Data Filters
- Biases identification

Quantifying uncertainty

Fields of application

On the **modelling** side

- Clustering
- Regression
- Principal components
- Decision tree (random forests)
- Neural network
- Performance metrics

- Spatial estimation of energy and mineral resources
- Weather modeling: from aviation to agriculture
- Maintenance forecasting
- Commodity, currency, stock and financial markets
- Market analysis
- Risk analysis
- ... and much much more!