# TTK4260 - introduction to multivariate data analysis

## Lesson L1

## January 6, 2020

Big Data Cybernetics gang

Welcome to TTK4260 !

# Bigdatacybernetics

- Instructors
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  - Damiano VARAGNOLO
  - Frank Ove WESTAD
  - Adil RASHEED

Homework: Who is who ?

# Some suggestions, just to start

- Sit together and at the ‘center’ of the first rows
  *(this to interact better)*

- Write your names on some ‘nametags’
  *(this to learn your names – please write them sufficiently big!)*

# Today's lesson

- Practical information about the course
- Why multivariate data analysis
- Overview of the data analysis methods types and traditions

# Practical information about the course

# What is multivariate data analysis?

= data analysis of more than one statistical outcome variable at a time

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Aim: take advantage of the multitude of information sources available now

# Intended learning outcomes *(in brief)*

- Get an in-depth understanding of commonly used Multivariate Data Analysis tools
- Make an informed choice of tools to solve a particular problem
- Understand their relationship to more advanced but black box machine learning methods
- Apply the knowledge gained from the course to solve real life problems *(on realistic data sets)*

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- Do the flipped classrooms, and thus
  - Register on www.scalable-learning.com
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- Reserve some time for interacting with your peers
- Make sure to understand everything

# What do we expect you to do?

- Provide feedback in real time (preferably directly but in a nice way without hampering the progress in the class)
- Send the feedback directly to the lecturer (preferably as soon as possible so that the following lectures can be adapted on the fly)

# What do you expect from us?

(think and discuss this 1 minute also with your peers)

# Schedule of the lectures

https://www.ntnu.no/studier/emner/TTK4260#tab=timeplan

# Overarching division of the course

- Part 1: Refreshing the background knowledge
- Part 2: Detailed analysis of some core algorithms / problems
- Part 3: Overview and demonstration of the capabilities / working strategies of other relevant algorithms

# Part 1: refreshing the background knowledge

- L1: Motivations, underlying points of view, overview of the course, and notation
- L2: Use cases through analysing datasets and problems relative to the marine and medical domains
- L3: Use cases through analysing datasets and problems relative to the process industry and robotics domains
- L4: Least squares, in all its interpretations and flavors
- L5: Maximum Likelihood and Maximum A Posteriori
- L6: Statistical performance indexes
- L7: Bias vs variance tradeoff, and model validation algorithms
- L8: Assessment

# Part 2: Detailed analysis of some core algorithms / problems

L9: Design of experiments

L10-11: Principal components analysis

L12: Model order selection

L13: Independent component analysis

L14-16: Principal component regression and partial least squares

L17: Metamodelling

L18: Summary of the various types of plots and their meanings

L19: Multiblock algorithms

L20: PARAFAC algorithms

L21-22: Time series modelling, identification, and prediction

L23: Assessment

# Part 3: overview and demonstration of the capabilities / working strategies of other relevant algorithms

L24: Change detection and subspace identification

L25: IDLE and informative converse methods

L26: Neural networks and random forests

L27: Support vector machines and t-SNE

L28: Other clustering and classification methods

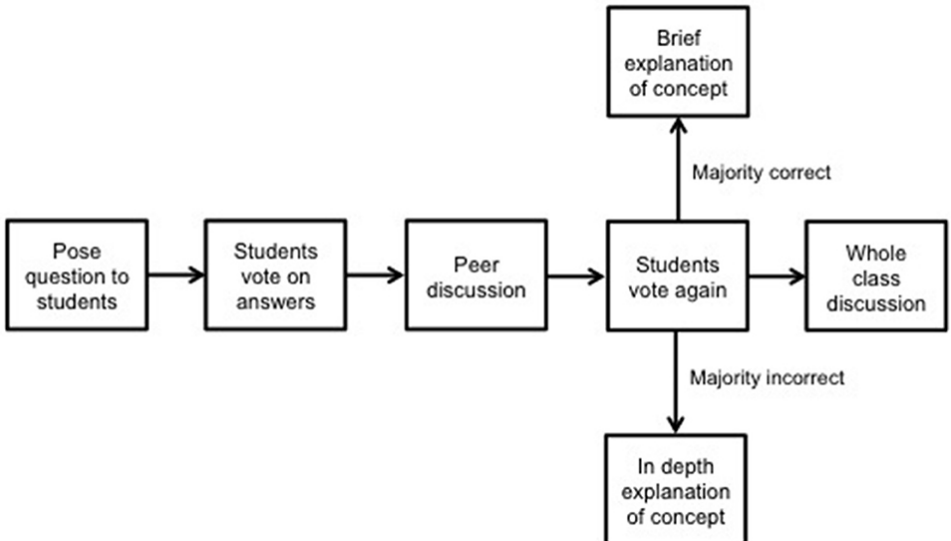
# Peer instructions - example

# Peer instructions

**Why?**

- discussions among and with students
- sharpen focus and understanding

# Peer instructions: working



example: which of these are reasons for the seasons?

go to www.kahoot.it

# Scalable Learning

# Introduction to Scalable-Learning

- Register on `www.scalable-learning.com`
- Watch the videos before the lessons
- Check scalable learning before the lessons

Any data put in is fully annonymized

# Scalable learning - how to enroll in the portal

1. Register an account in `https://www.scalable-learning.com/#/users/login` using your institutional email (i.e., `xxx@ntnu.no`)
2. Go to `https://www.scalable-learning.com/#/courses/enroll?id=GUKXE-22315` and follow the instructions
3. In case the portal asks, use `GUKXE-22315` as the course enrollment key

direct link to the course:
`https://www.scalable-learning.com/#/courses/4363/course_information`

# Exams and evaluation

Written exams: tentative date, assignments

# Data to work with

- A selected set of data will be shared in the Lecture 2
- Students are expected to search for more relevant dataset on websites like Kaggle
- Bring a laptop with Matlab, Python and Unscrambler installed to preprocess the data for the subsequent lectures

# To do list (before Lecture 2)

- Install Matlab (Damiano)
  `https://innsida.ntnu.no/wiki/-/wiki/English/Matlab+for+students`
- Install Python (Adil)
  `https://www.anaconda.com/distribution/`
- Install Unscrambler (Frank)

# Evaluation of the prerequisites

*Today @ 14.15 in R9, realfag*

What are you supposed to do?
→ do module *"assessment of the prerequisites"* in Scalable-Learning

direct link: `https://www.scalable-learning.com/#/courses/4363/modules/17002/courseware/lectures/53828`

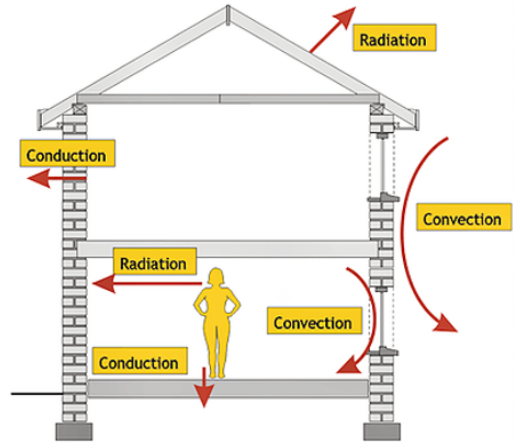
# Expectation from today's lecture

- Why data driven models when first principle mechanistic models are available in abundance?
- Why to take a course in Multivariate Data Analysis when so many courses on ML are available?
- What makes this course different from other courses on similar topics?
- Some taste of Big Data Cybernetics
- Get to know each other and encourage to prepare our own data
- Install the required softwares
- Get familiar with the content and schedule of the course

# Overview

- Mechanistic Modeling
- Data-driven modeling (Deep Learning)
- Big Data Cybernetics
- Preparing the grounds for Multivariate Data Analysis

# Mechanistic modeling approach

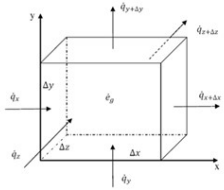


# Modeling

$$\dot{q}_{x+dx} = \dot{q}_x + \frac{\partial \dot{q}_x}{\partial x}\,dx$$

or,

$$\dot{q}_x - \dot{q}_{x+dx} = -\frac{\partial \dot{q}_x}{\partial x}\,dx$$




## Fourier's law of heat conduction

$$\dot{q}_x = -k\,dy\,dz\,\frac{\partial T}{\partial x}$$

$$\dot{q}_x - \dot{q}_{x+dx} = \frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right)dx\,dy\,dz$$

$$\dot{q}_y - \dot{q}_{y+dy} = \frac{\partial}{\partial y}\left(k\,\frac{\partial T}{\partial y}\right)dx\,dy\,dz$$

and,

$$\dot{q}_z - \dot{q}_{z+dz} = \frac{\partial}{\partial z}\left(k\,\frac{\partial T}{\partial z}\right)dx\,dy\,dz$$

*Rate of heat input + Rate of heat generation*

*= Rate of heat output*

*+ Rate of change of heat energy within the body*

$$\dot{u} = (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

$$(\dot{q}_x + \dot{q}_y + \dot{q}_z) + (\dot{e}_g\,dx\,dy\,dz) = (\dot{q}_{x+dx} + \dot{q}_{y+dy} + \dot{q}_{z+dz}) + (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

$$(\dot{q}_x - \dot{q}_{x+dx}) + (\dot{q}_y - \dot{q}_{y+dy}) + (\dot{q}_z - \dot{q}_{z+dz}) + (\dot{e}_g dx\,dy\,dz) = (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

or,

$$\left\{\frac{\partial}{\partial x}\left(k\,\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\,\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\,\frac{\partial T}{\partial z}\right)\right\}(dx\,dy\,dz) + (\dot{e}_g\,dx\,dy\,dz) = (\rho dx\,dy\,dz)c_p\left(\frac{\partial T}{\partial t}\right)$$

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# Model simplification

- Reducing dimension (eg.using symmetry)

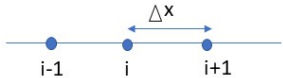
$$\frac{\partial T}{\partial t} = \nu \frac{\partial^2 T}{\partial x^2}$$

- Approximating thermophysical properties
- Approximating shapes
- ....
- ....

# Numerical Discretization

1D diffusion equation

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2}$$




$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x}\bigg|_i + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\bigg|_i + \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}\bigg|_i + O(\Delta x^4)$$

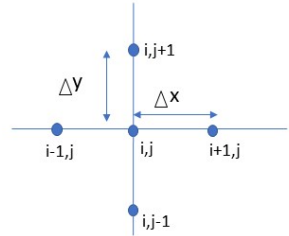
$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x}\bigg|_i + \frac{\Delta x^2}{2}\frac{\partial^2 u}{\partial x^2}\bigg|_i - \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3}\bigg|_i + O(\Delta x^4)$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(\Delta x^2)$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

$$u_i^{n+1} = u_i^n + \frac{\nu \Delta t}{\Delta x^2}(u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

2D diffusion equation

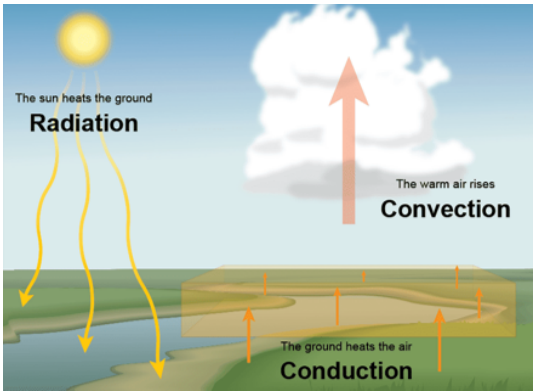


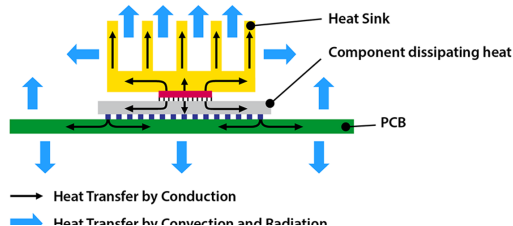

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} + \nu \frac{\partial^2 u}{\partial y^2}$$

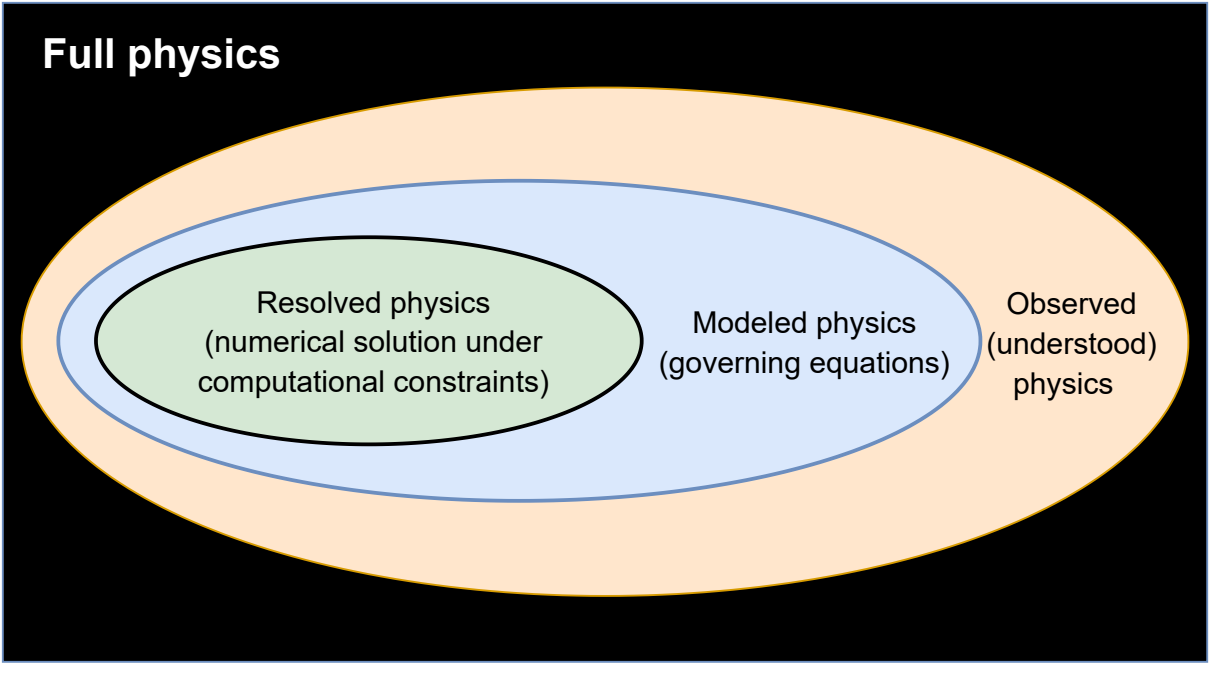
$$\frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} = \nu \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + \nu \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2}$$

$$u_{i,j}^{n+1} = u_{i,j}^n + \frac{\nu \Delta t}{\Delta x^2}(u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n) + \frac{\nu \Delta t}{\Delta y^2}(u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n)$$

# Generalization to other problems



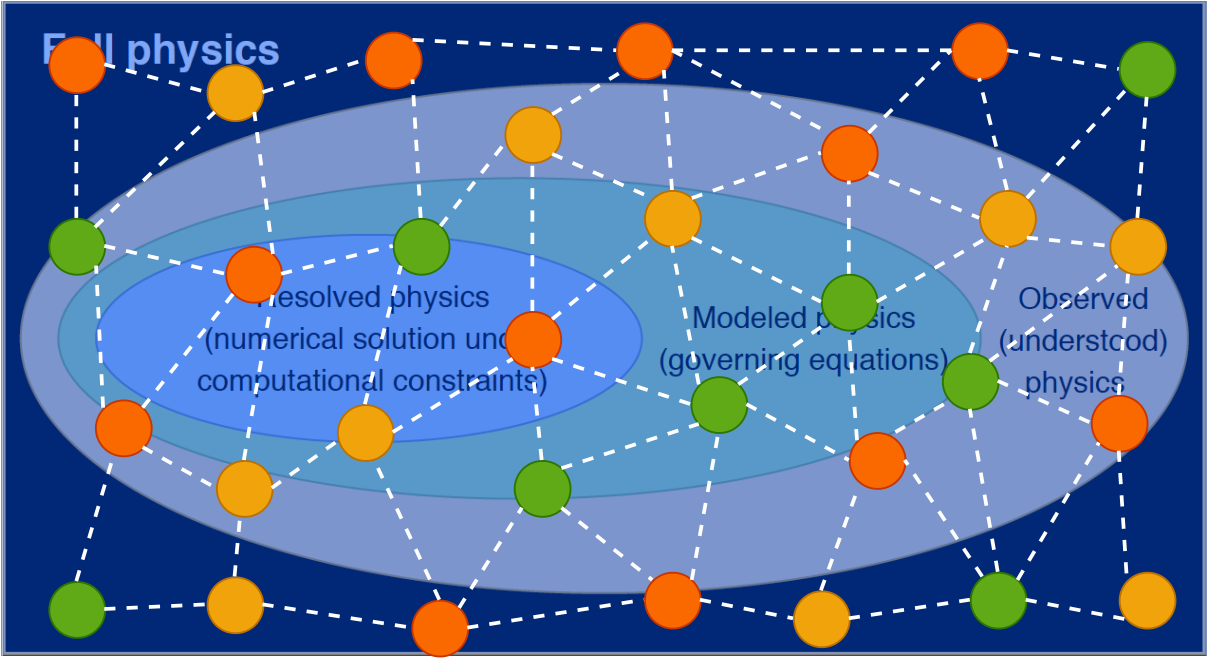




Full physics
Resolved physics
(numerical solution under
computational constraints)
Modeled physics
(governing equations)
Observed
(understood)
physics

# Assignment 1

- Figure out a phenomena governed by the 1D, 2D
- Decide on the initial condition and boundary condition
- Solve it using the numerical methods
- Convince yourself about the generalizability of the mechanistic models

https://github.com/adil-rasheed/TK8117/blob/master/Lecture1/Physicsbased.ipynb


Full physics
Observed
(understood)
physics

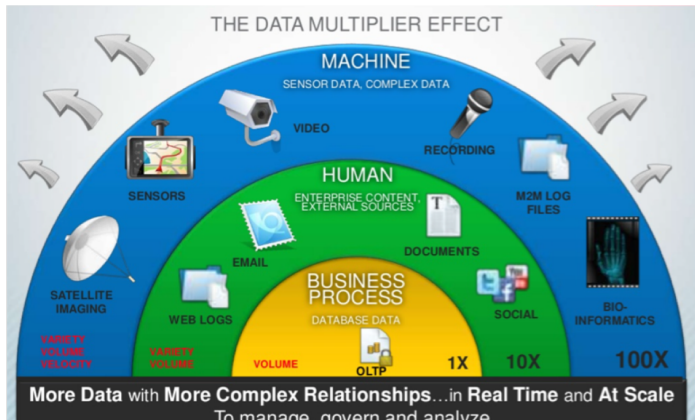
# Technology push and Market pull

- New and existing algorithms
- Digitalization wave
- Cheap sensors and observation data (mobile data, cams)
- Easy-to-use software libraries
- Cheap GPU's and TPUs

- Digital Twin
- Internet of Things
- Smart Cities
- Autonomy
- Precision in predictions
- Real time control systems

# Sources of big data

- Multichannel sensor data
- Web log data/log files
- Computer simulation data
- 4Vs



# Supervised Learning

Classification

- Binary
- Multiclass
- Multilabel

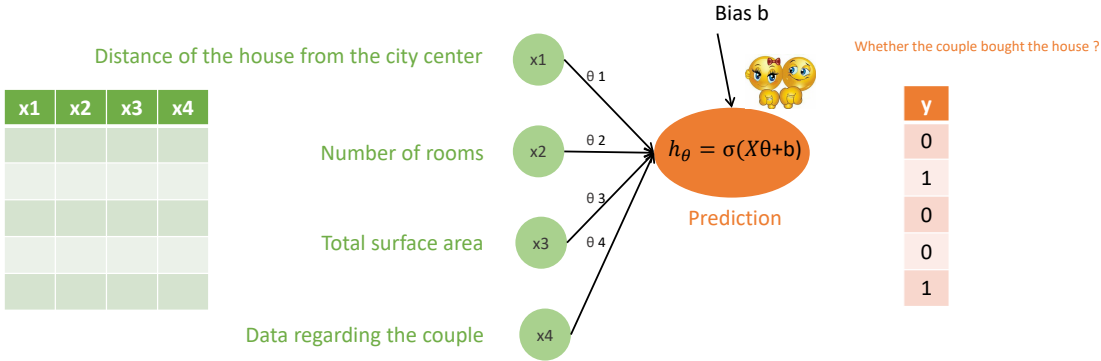
Regression

- Continuous output
- Curve fitting

# Unsupervised Learning

1. Given an input $X$, find interesting structure in the data
2. More general than a supervised approach
3. Compares to human and animal learning

# Logistic Regression

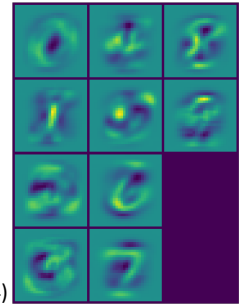



Categorically cross entropy loss

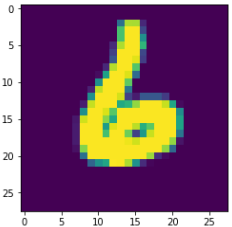
$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}log(h_\theta(x^{(i)})) + (1-y^{(i)})log(1-h_\theta(x^{(i)}))]$$

https://github.com/adil-rasheed/TK8117/blob/master/Lecture1/BinaryClassLogisticRegression.ipynb

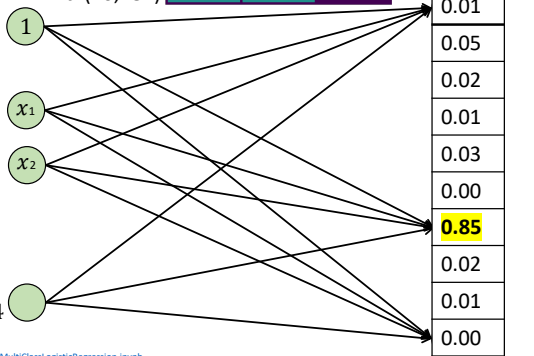
# Logistic Regression



$\theta$ (10,784)




X(1,784)



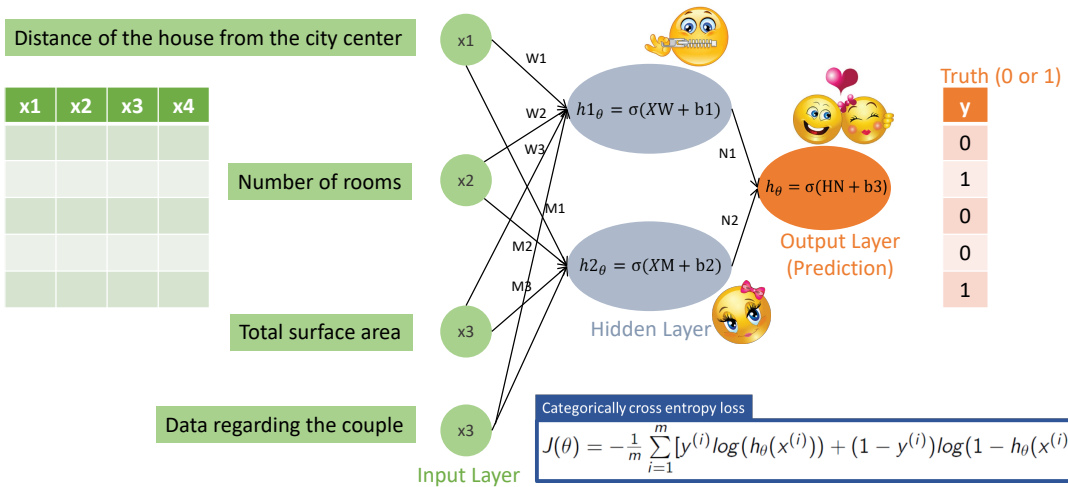

$\sigma(\theta X + b)$

| |
|---|
| 0.01 |
| 0.05 |
| 0.02 |
| 0.01 |
| 0.03 |
| 0.00 |
| **0.85** |
| 0.02 |
| 0.01 |
| 0.00 |

92% accuracy

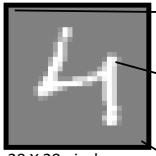
https://github.com/adil-rasheed/TK8117/blob/master/Lecture1/MultiClassLogisticRegression.ipynb

# Artificial Neural Networks

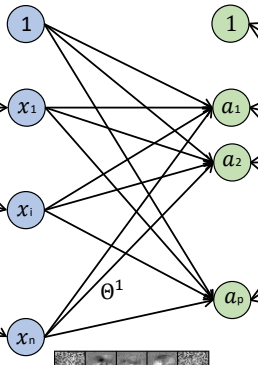



https://github.com/adil-rasheed/TK8117/blob/master/Lecture1/Aritifial_Neural_Network.ipynb

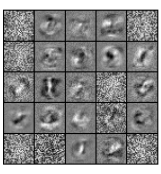
# Shallow neural network

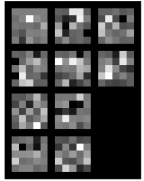


28 X 28 pixels




| Prediction | 1-Hot-Encode | Label |
|---|---|---|
| 0.05 | 0 | 0 |
| 0.01 | 0 | 1 |
| 0.02 | 0 | 2 |
| 0.05 | 0 | 3 |
| **0.8** | **1** | **4** |
| 0.1 | 0 | 5 |
| 0.04 | 0 | 6 |
| 0.01 | 0 | 7 |
| 0.04 | 0 | 8 |
| 0 | 0 | 9 |





96% accuracy

https://github.com/adil-rasheed/TK8117/blob/master/Lecture1/Aritifial_Neural_Network.ipynb

# Deep Neural Networks

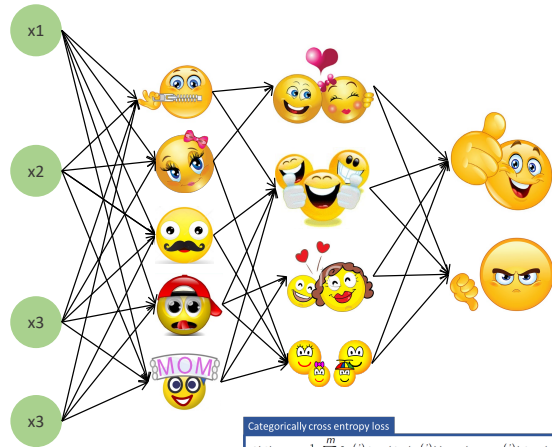
Distance of the house from the city center

| x1 | x2 | x3 | x4 |
|---|---|---|---|
| | | | |
| | | | |
| | | | |
| | | | |
| | | | |

Number of rooms

Total surface area

Data regarding the couple

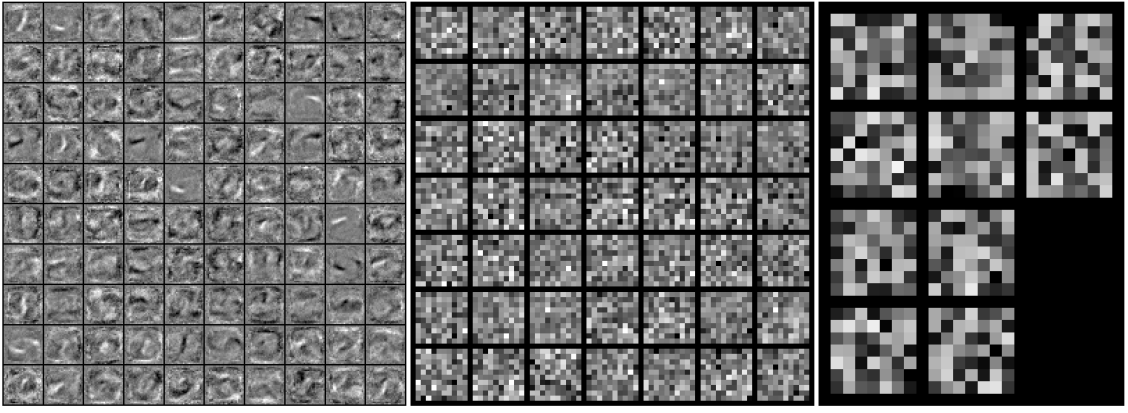



| Truth |
|---|
| y |
| 0 |
| 1 |
| 0 |
| 0 |
| 1 |

Categorically cross entropy loss

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y^{(i)}log(h_\theta(x^{(i)})) + (1-y^{(i)})log(1-h_\theta(x^{(i)}))]$$

# How the weights look



98% accuracy on the validation data

https://github.com/adil-rasheed/TK8117/blob/master/Lecture1/Aritifial_Neural_Network.ipynb

Trained a Conditional adversarial nets on NVIDIA GEFORCE 1080 Ti for 10 hours on 2000 images to come up with a model that can convert any grayscale image to its colored version.

Some other applications

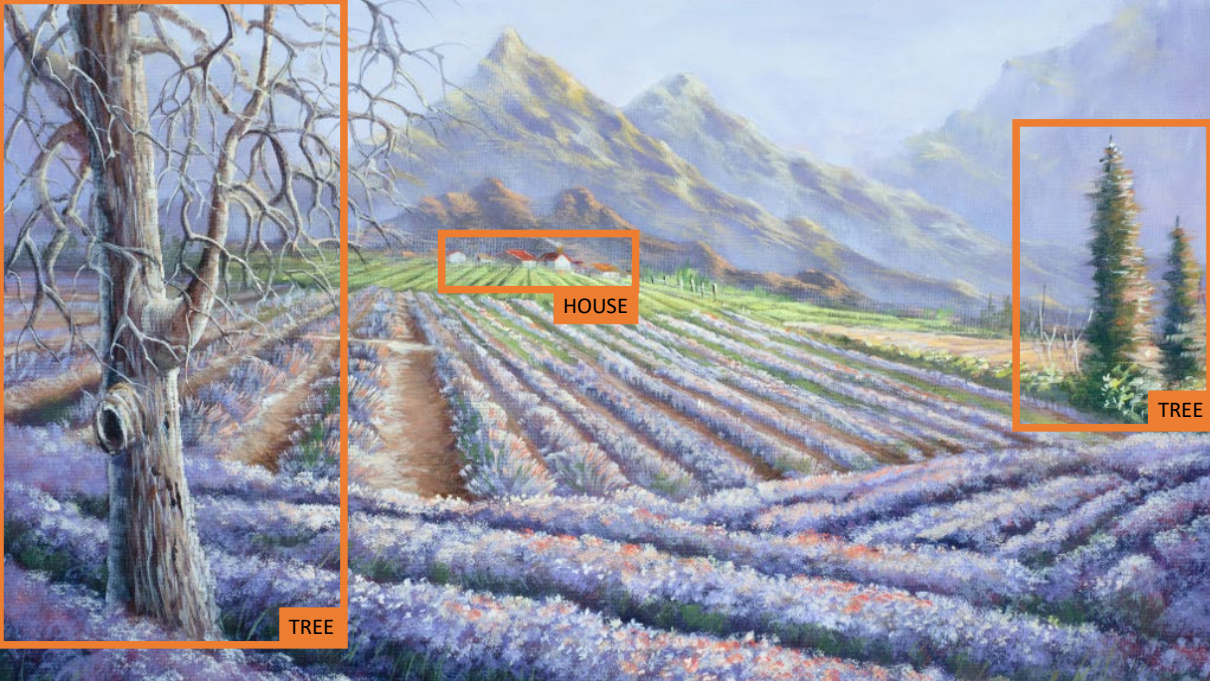
- Converting summer scenes to winter
- Landscape images to sea scapes
- Convert boats into ships

Missing Pixels

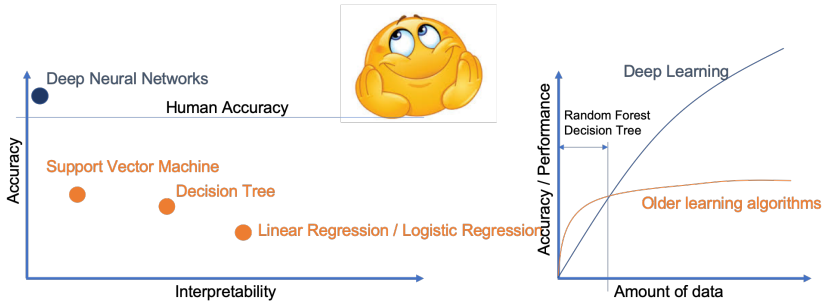
Computer Generated

Original


Outline
Computer generated
Original

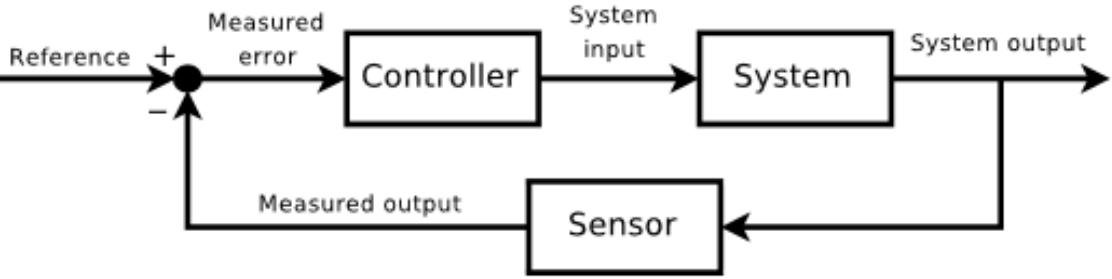

HOUSE
TREE
TREE

# Accuracy, interpretability and scalability

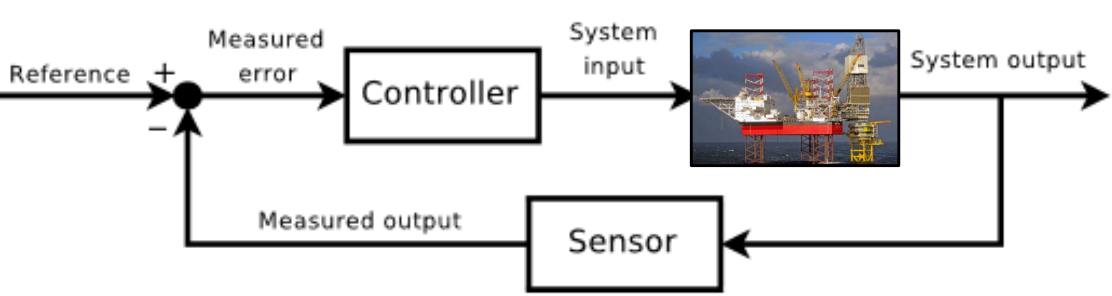


# Mechanistic vs data driven modeling

| Mechanistic modeling | Data-driven modeling |
|---|---|
| +Solid foundation based on physics | – Mostly black-boxes |
| – Difficult to assimilate very long term historical data into the computational models | + Takes into account long term historical data and experiences |
| – Computationally expensive, sensitive and susceptible to numerical instability | + Once the model is trained, it is very stable and efficient for making predictions / inferences |
| + Errors / uncertainties can be bounded and estimated | – Not possible to bound errors / uncertainties |
| + Less susceptible to bias | – Bias in data is reflected in the model prediction |
| + Generalizes well to new problems with similar physics | – Poor generalization on unseen problems |




Modelling ***known*** **and** ***unknown*** **structures**
within the Framework of *Big Data Cybernetics*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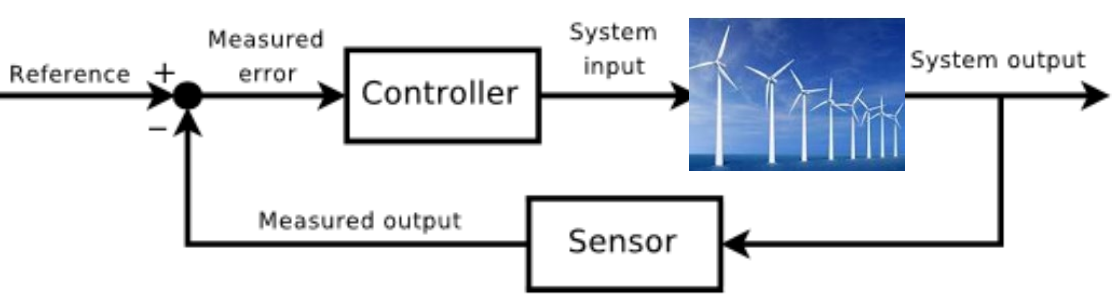
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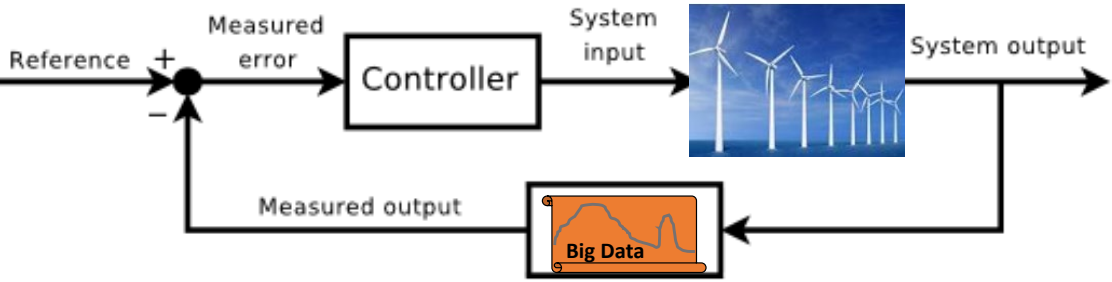
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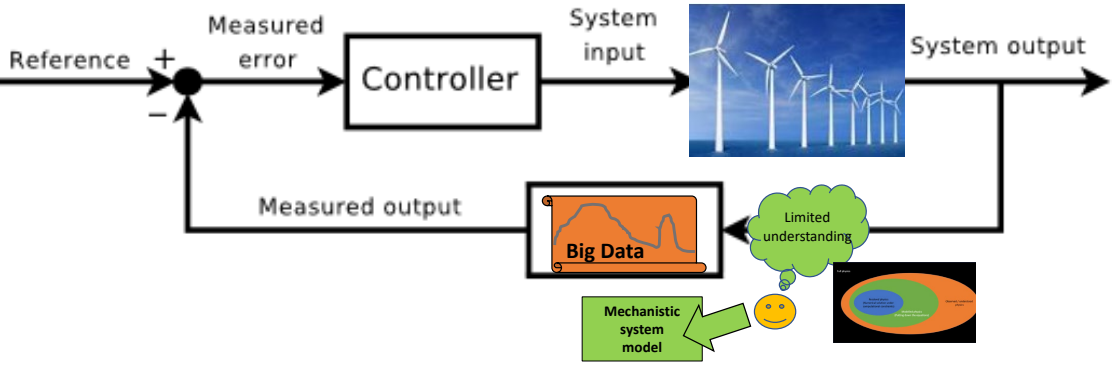
Big Data
$y_j$
time
Channels j=1,2,...,J
symbolized as
4Vs: Volume (amount), Velocity (rate), Veracity (quality), Variety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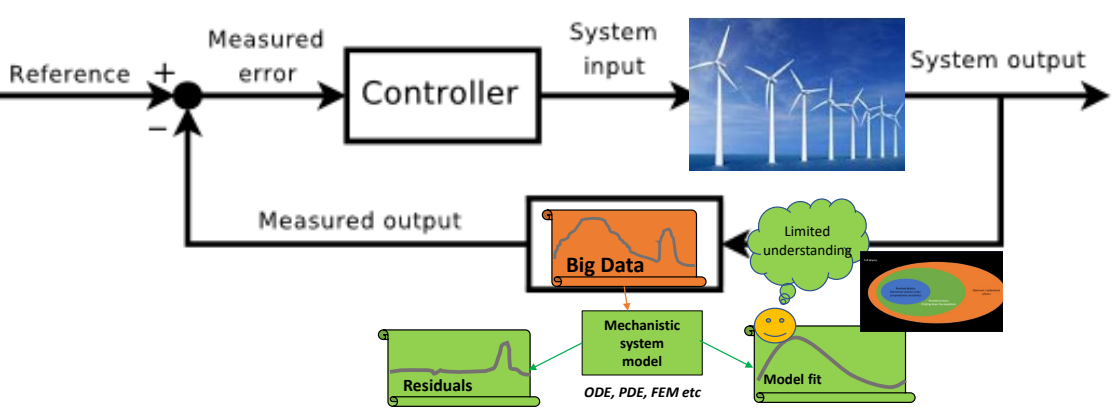
Big Data
Limited understanding
Mechanistic system model
ODE, PDE, FEM etc,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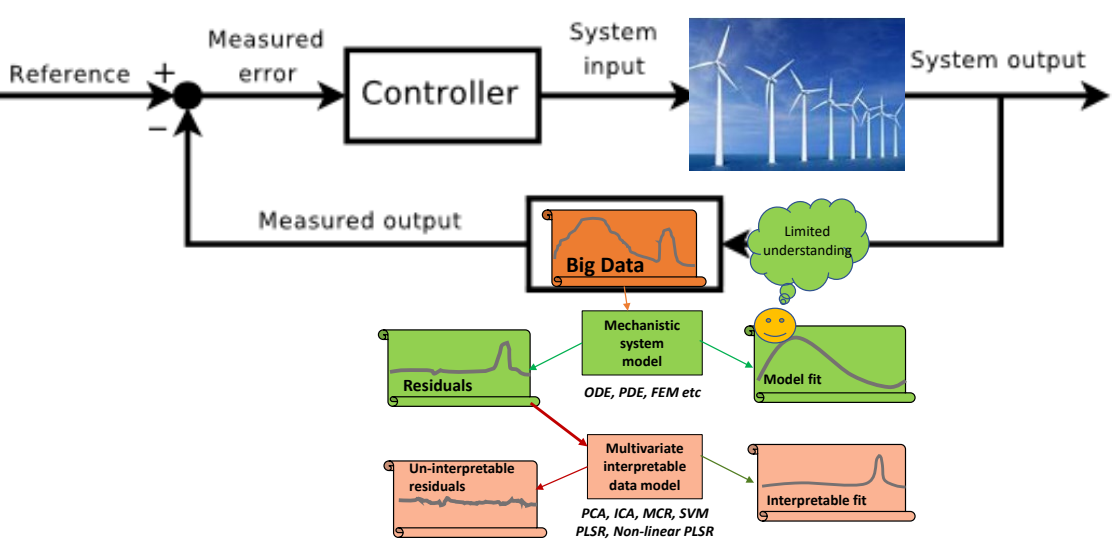
Mechanistic
system
model
ODE, PDE, FEM etc
Residuals
Model fit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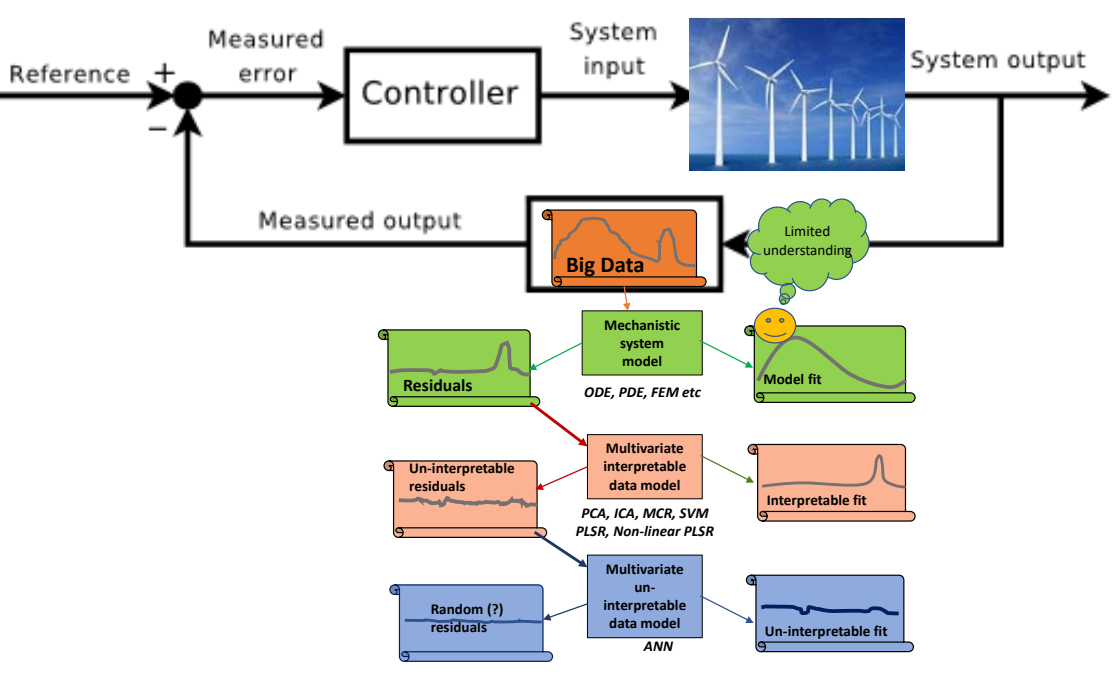
Model fit
Multivariate interpretable data model
PCA, ICA, MCR, SVM
PLSR, Non-linear PLSR
Un-interpretable residuals
Interpretable fit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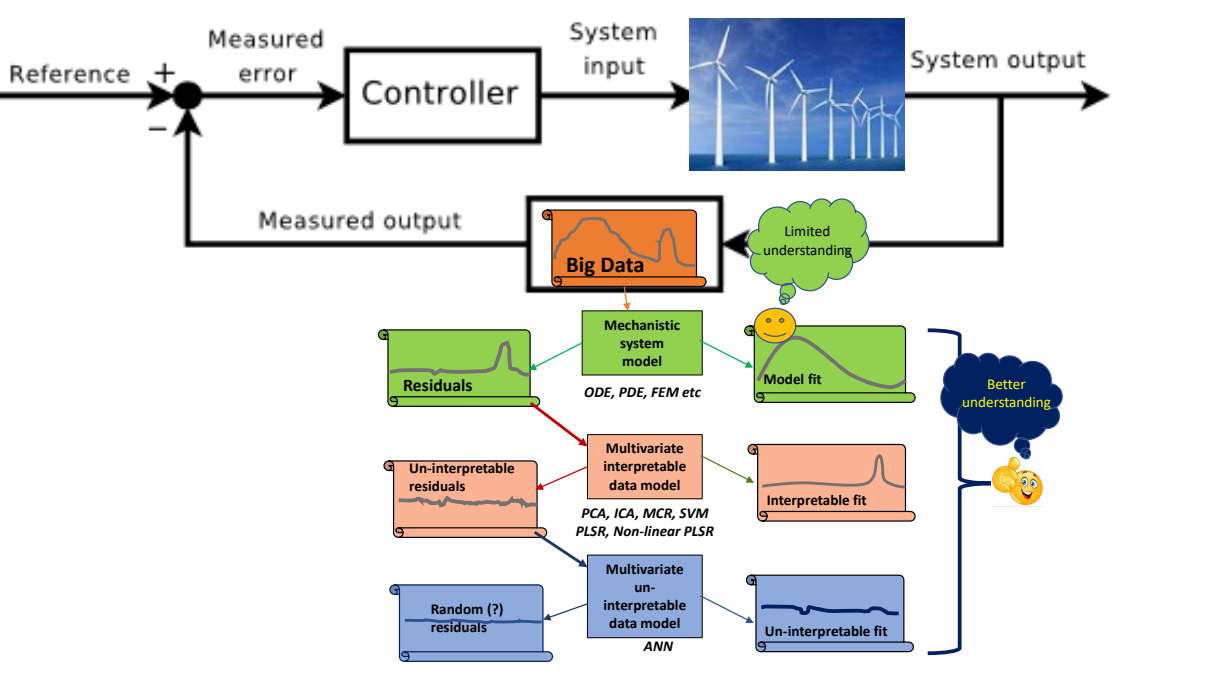
PLSR, Non-linear PLSR
Un-interpretable residuals
Interpretable fit
Multivariate un-interpretable data model
ANN
Random (?) residuals
Un-interpretable fit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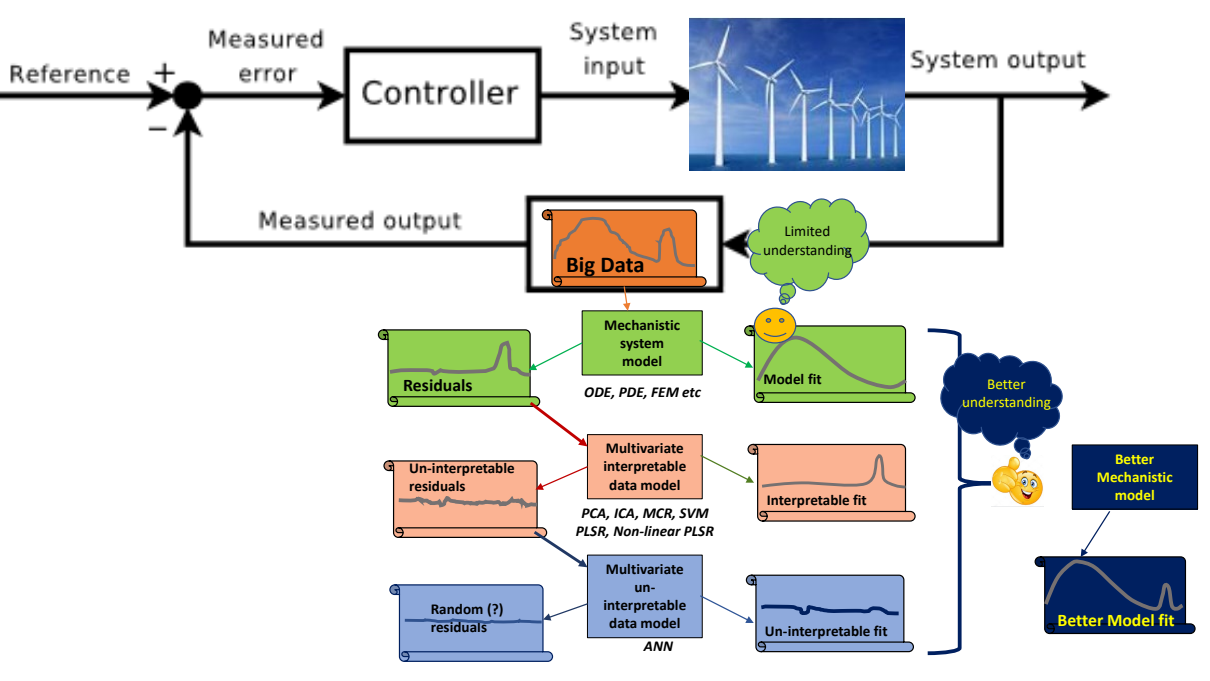
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Interpretable fit
Better Mechanistic model
Multivariate un-interpretable data model
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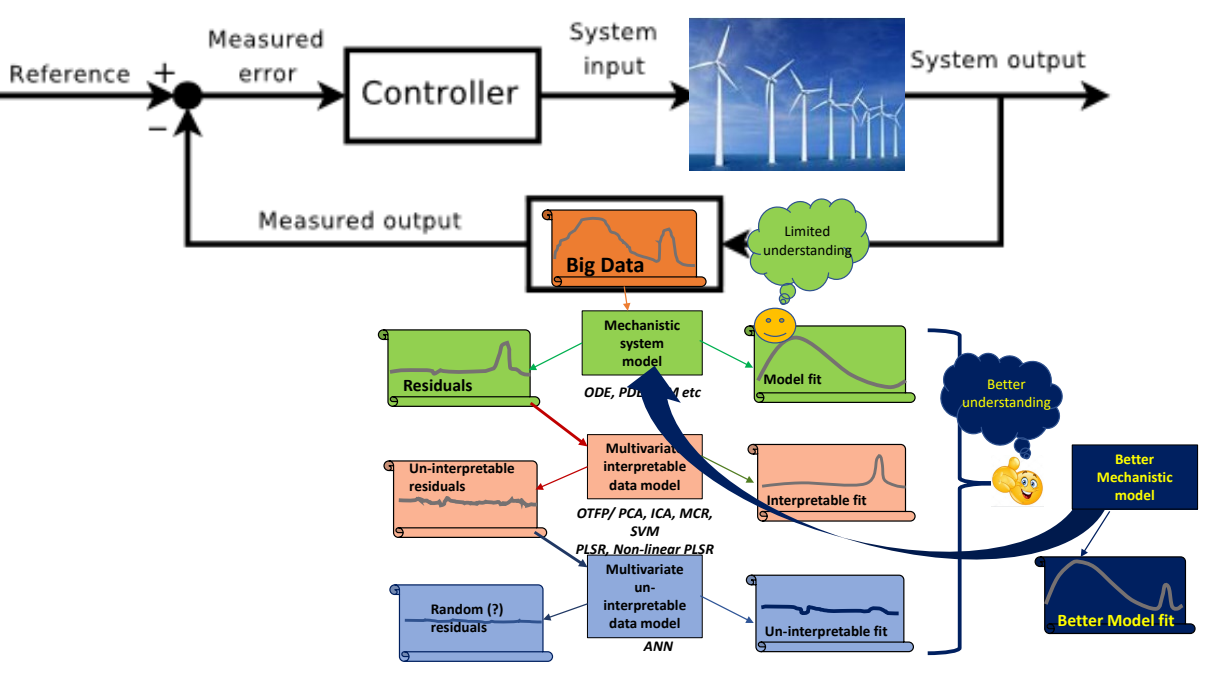
Random (?) residuals
Un-interpretable fit
Better Model fit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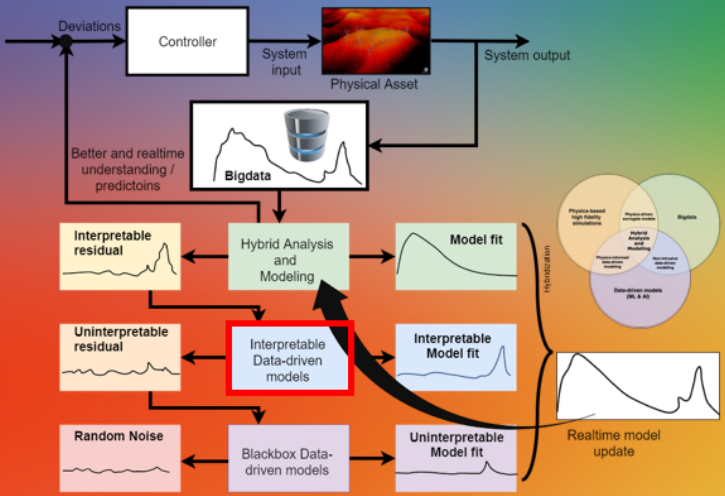
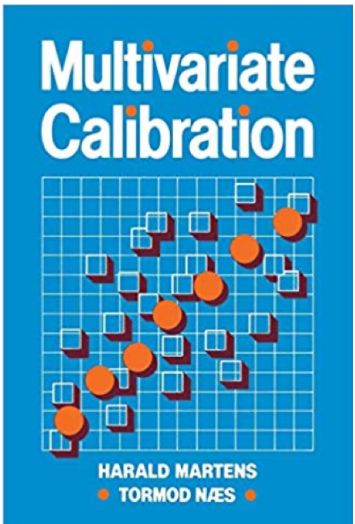
Un-interpretable fit
Better Model fit

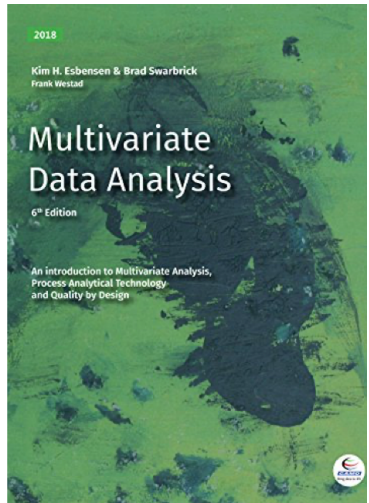
# Big Data Cybernetics

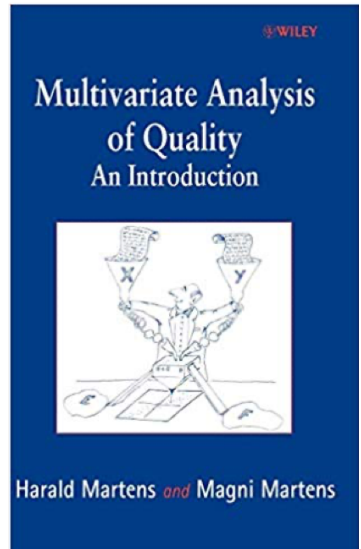



*A new paradigm in steering the world with big data characterized by high volume, high velocity, high vareity and high veracity*

# Additional Reading Materials




Additional articles, reports and papers will be shared

motivations and underlying points of view

overview of the data analysis methods types and traditions

# What is modelling?

Important topics to consider:

- The difference between significance and relevance
- Causality vs. indirect correlation
- "No prediction without interpretation"
- "No interpretation without a valid model"
- Is the model good enough to be applied on individual objects?
  - Classification: Accuracy in terms of sensitivity/selectivity
  - Quantification: Prediction error and uncertainty in prediction
- Estimation of model robustness by proper validation
- Do we find the true signal in our system?

# Modelling strategies

- First principle models: Physics, flow theory, reaction kinetics etc.
- Numerical simulations e.g. ‘Ab initio’, Molecular Dynamics, CFD, finite element
- Metamodelling
- Hybrid modelling
- Models based on empirical data (collected by means of proper designed experiments)

# Which variables are present in our process/system?

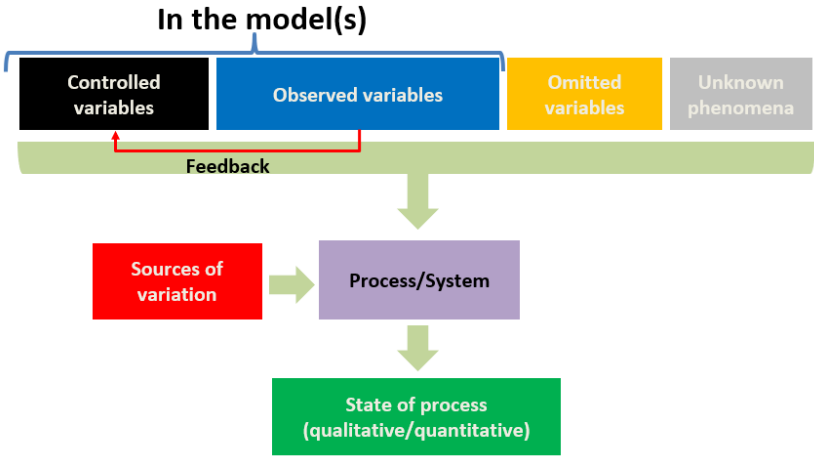



Figure: Variables in a system

# What's in our toolbox?

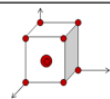
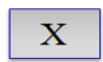
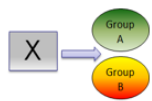
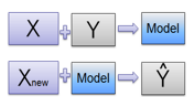
| Tool | Symbol | Purpose |
|---|---|---|
| Design of Experiments (DoE)<br><br>Full and Fractional Factorial Designs, Optimisation Designs |  | Gain maximum information from a minimum of experimental effort |
| Exploratory Data Analysis (EDA) |  | Find important sample groups or variable relationships in large data sets. Define classes. |
| Classification/Discrimination |  | Classify samples. Identify raw materials. Is the process under control (MSPC)? |
| Regression and Prediction |  | Predict quality for new samples and/or find out which variables that most influence a process |

Figure: Multivariate tools

# Considerations when choosing a specific method

Source, type and structure of data

- How to include theory and first principle models
- How to handle missing values
- How to deal with outliers
- Setting up validation schemes
- Interpretation using domain expertise and background information
- Dynamic model updates
- Applicability for prediction in real-time

# The dimensionality of a model

- Most systems are observed with more sensors/variables than the actual underlying dimensionality (rank)
- Methods based on latent variables will summarize the information in terms of "super variables" and reveal the individual variable's contribution to these
- What do we mean by *rank* ?
  - The numerical rank (this will for all real data be the smallest dimension of the data table)
  - The statistical rank (found by some statistical criterion, e.g. the chosen validation scheme or maximum likelihood)
  - The application specific rank based on experience and interpretation

# Redundancy and selectivity

- Most sensors are not measuring directly the inherent state or property of a system; 'das Ding an Sich'
- Although individual sensors are not selective, we can still use them for observing the system:
  - Qualitative: Is the system under control?
  - Quantitative: What is the water content in this rock on Mars?
- Sensor redundancy helps in making the models robust and to detect anomalies
- Using ten instead of two temperature sensors in e.g. a distillation process does not add eight new underlying dimensions to the system, but will describe the process better

Thanks for your attention and see you in the afternoon !!