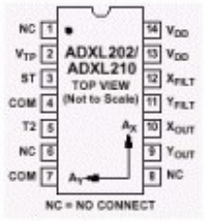
ENM 531: Data-driven Modeling and Probabilistic Scientific Computing

Lecture #1: Introduction, motivation and course logistics

Paris Perdikaris
January 16, 2020

Roadmap to Trillion Sensors



Accelerometer


Gyro


Pendulum Resistive
Tilt Sensors


Piezo Bend Sensor

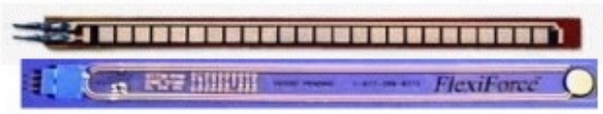

Metal Detector

Gas Sensor


Gieger-Muller
Radiation Sensor


Digital Infrared Ranging


CDS Cell
Resistive Light Sensor



Resistive Bend Sensors

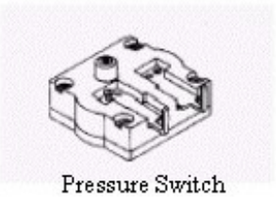

UV Detector

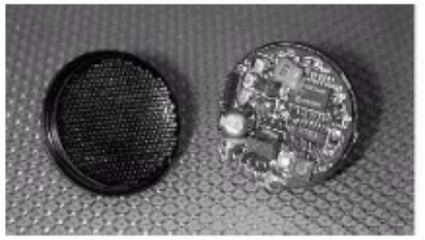

Pyroelectric Detector

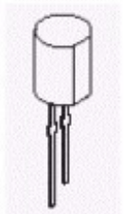

Limit Switch

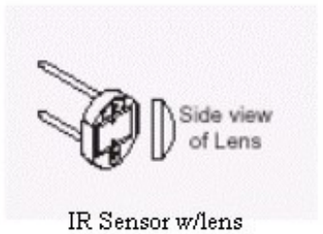

Mechanical Tilt Sensors


Touch Switch


Pressure Switch

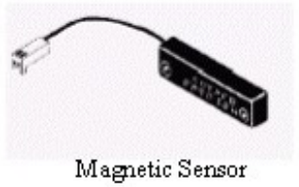

Miniature Polaroid Sensor

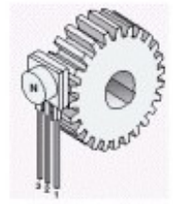

IR Pin
Diode

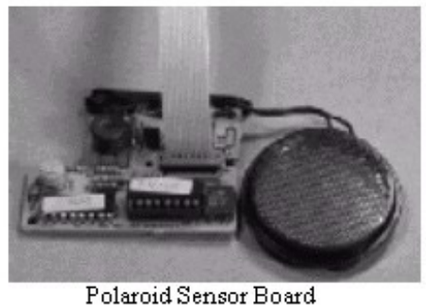


IR Sensor w/lens

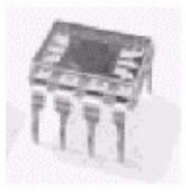

Thyristor


Magnetic Sensor


Hall Effect
Magnetic Field
Sensors

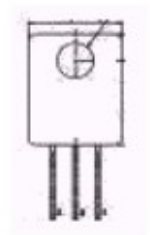

Polaroid Sensor Board

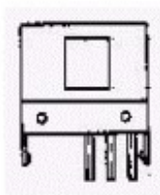

IR Reflection
Sensor


IR Amplifier Sensor


IRDA Transceiver


Magnetic Reed Switch

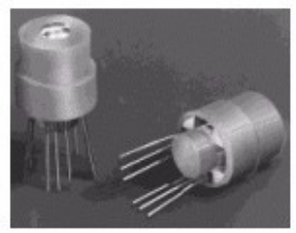

Lite-On IR
Remote Receiver

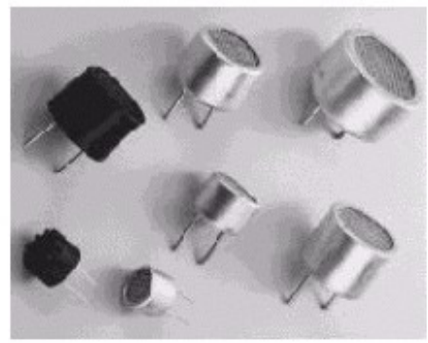

Radio Shack
Remote Receiver


IR Modulator
Receiver


Solar Cell

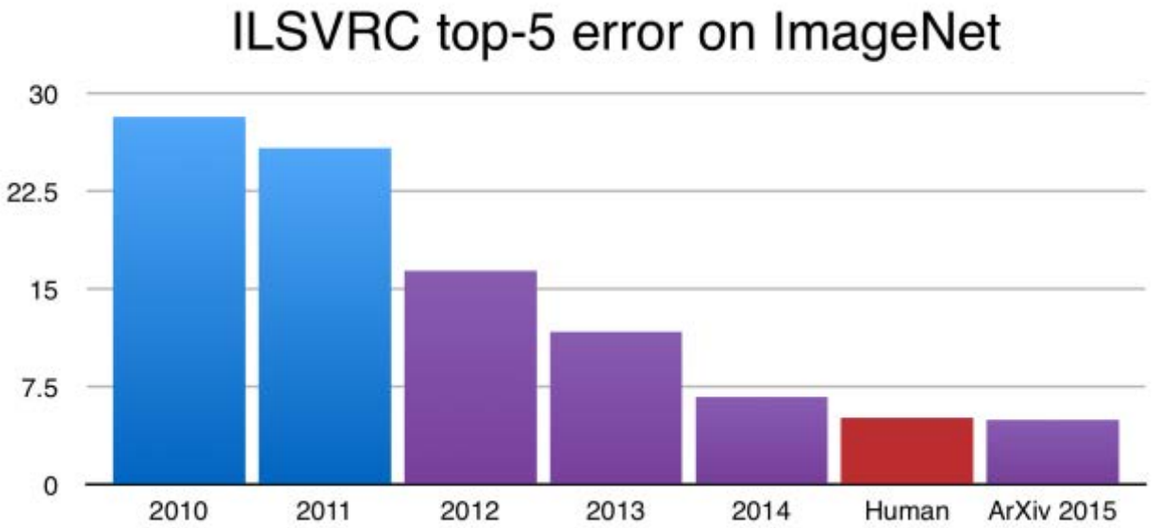

Compass

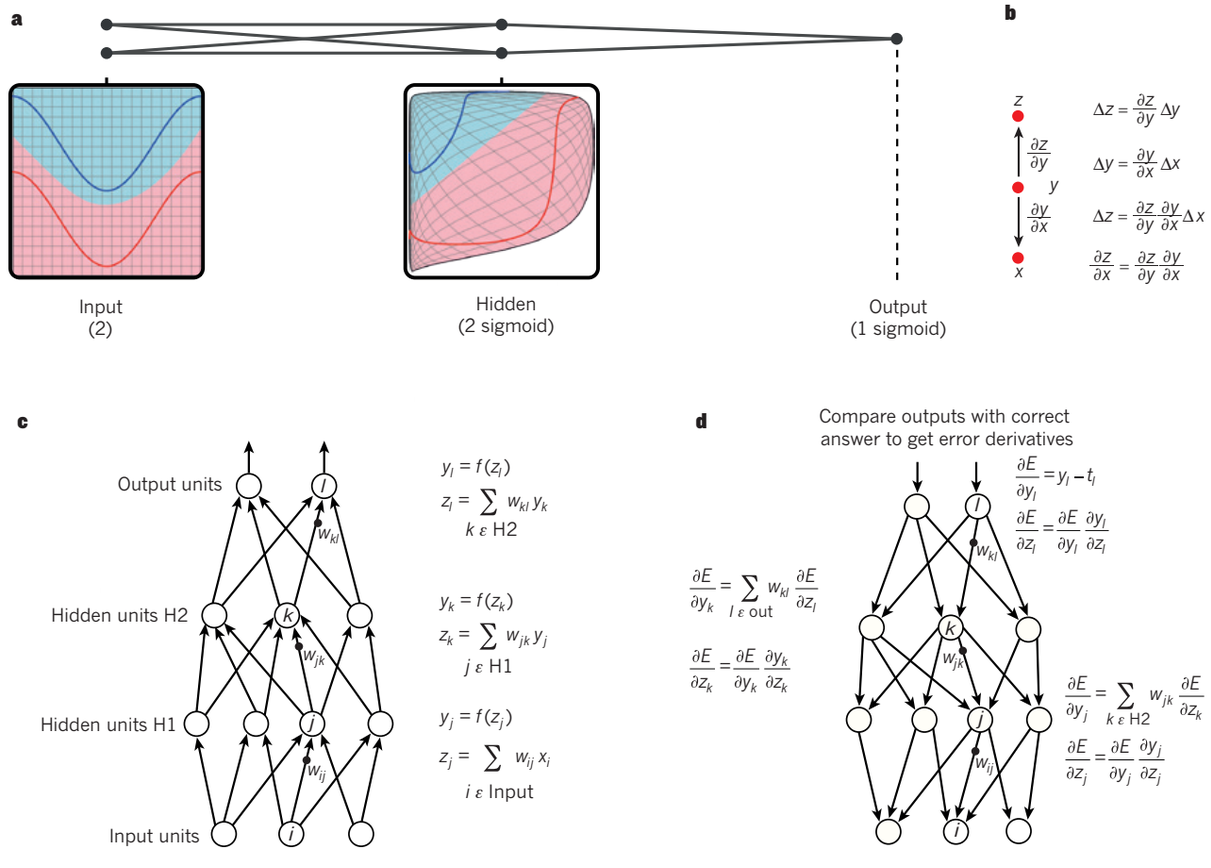

Compass


Piezo Ultrasonic Transducers

Sensors are expected to generate a bronto-bytes (1000 trillion trillion) of data by 2025!

Recent success of machine learning

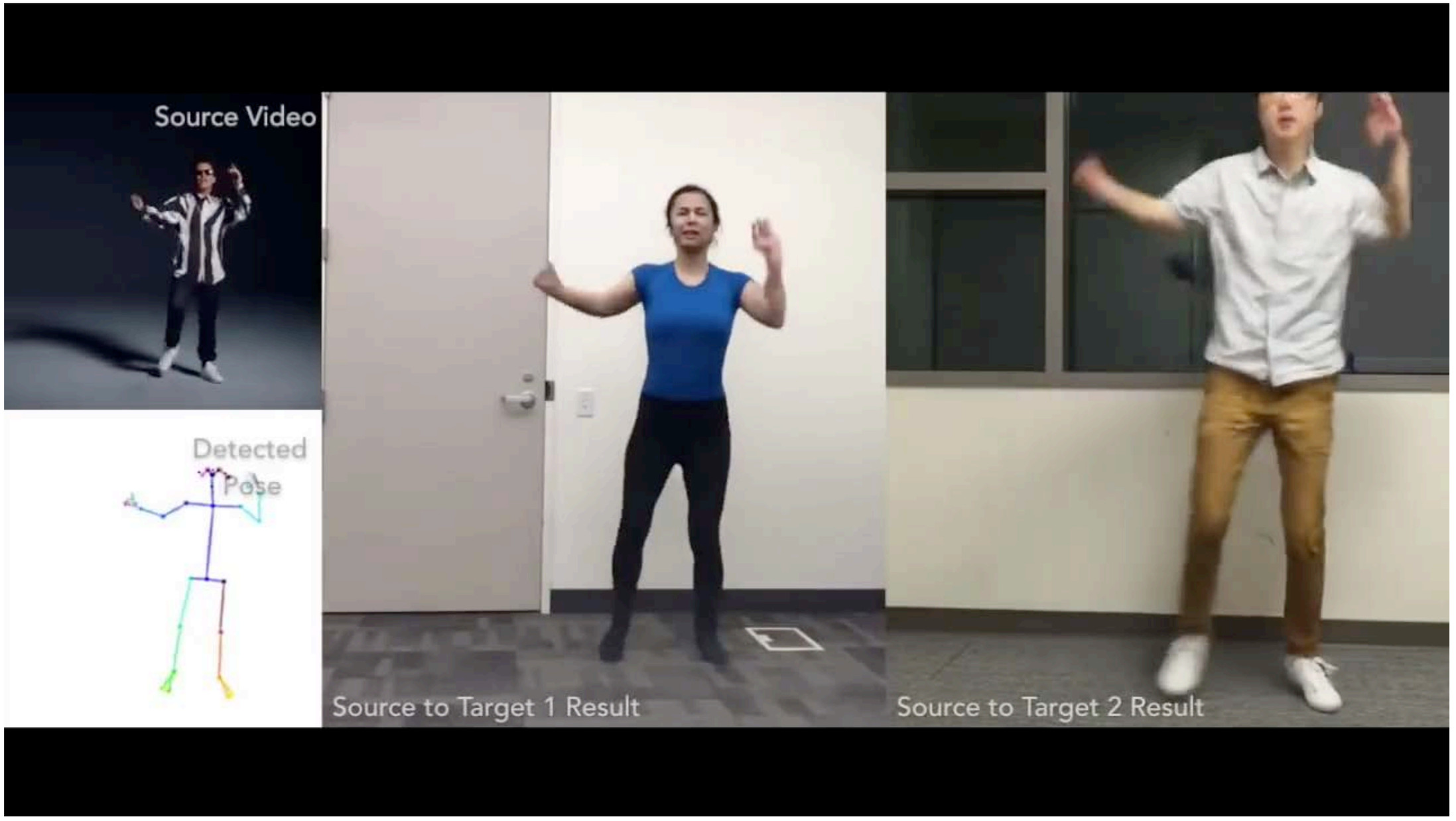




Working with high-dimensional data

Karras, T., Aila, T., Laine, S., & Lehtinen, J. (2017). Progressive growing of GANs for improved quality, stability, and variation. arXiv preprint.

Working with high-dimensional data



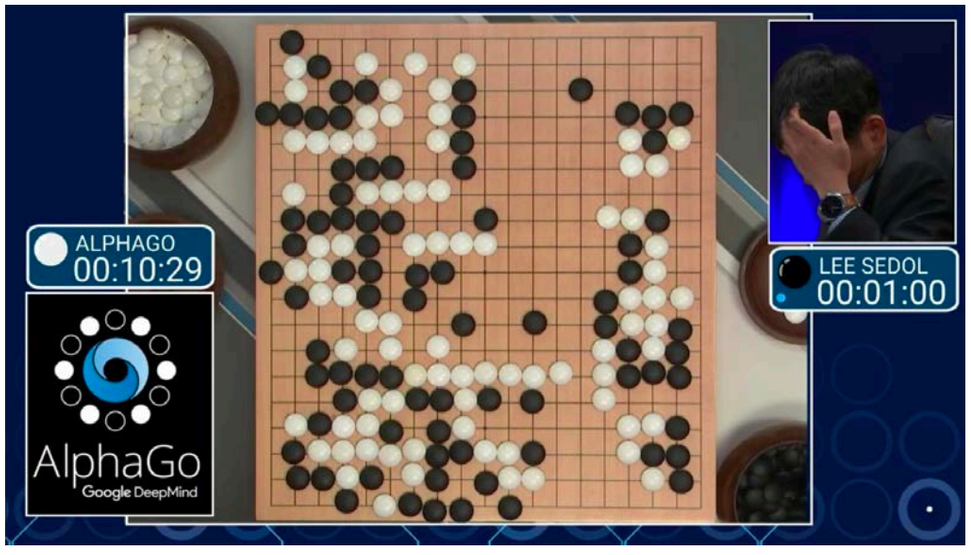
Chan, C., Ginosar, S., Zhou, T., & Efros, A. A. (2018). Everybody Dance Now. arXiv preprint arXiv:1808.07371.

Working with high-dimensional data

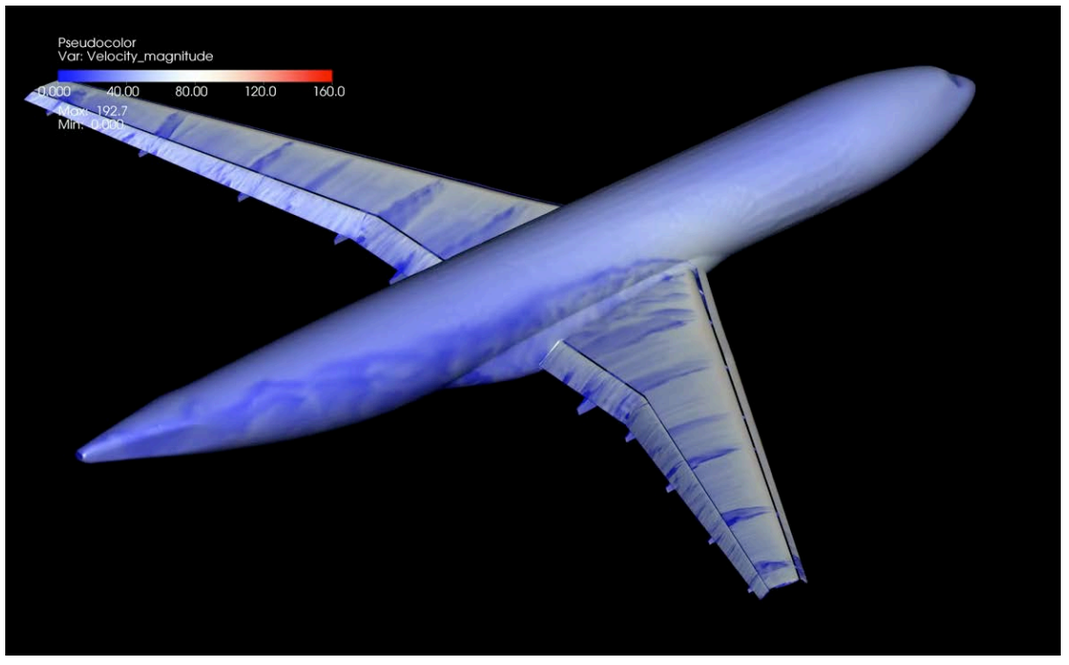
Google DeepMind's
Deep Q-learning

The algorithm will play Atari breakout.

The most important thing to know is that all the agent is given is sensory input (what you see on the screen) and it was ordered to maximize the score on the screen.



Motivation and open challenges



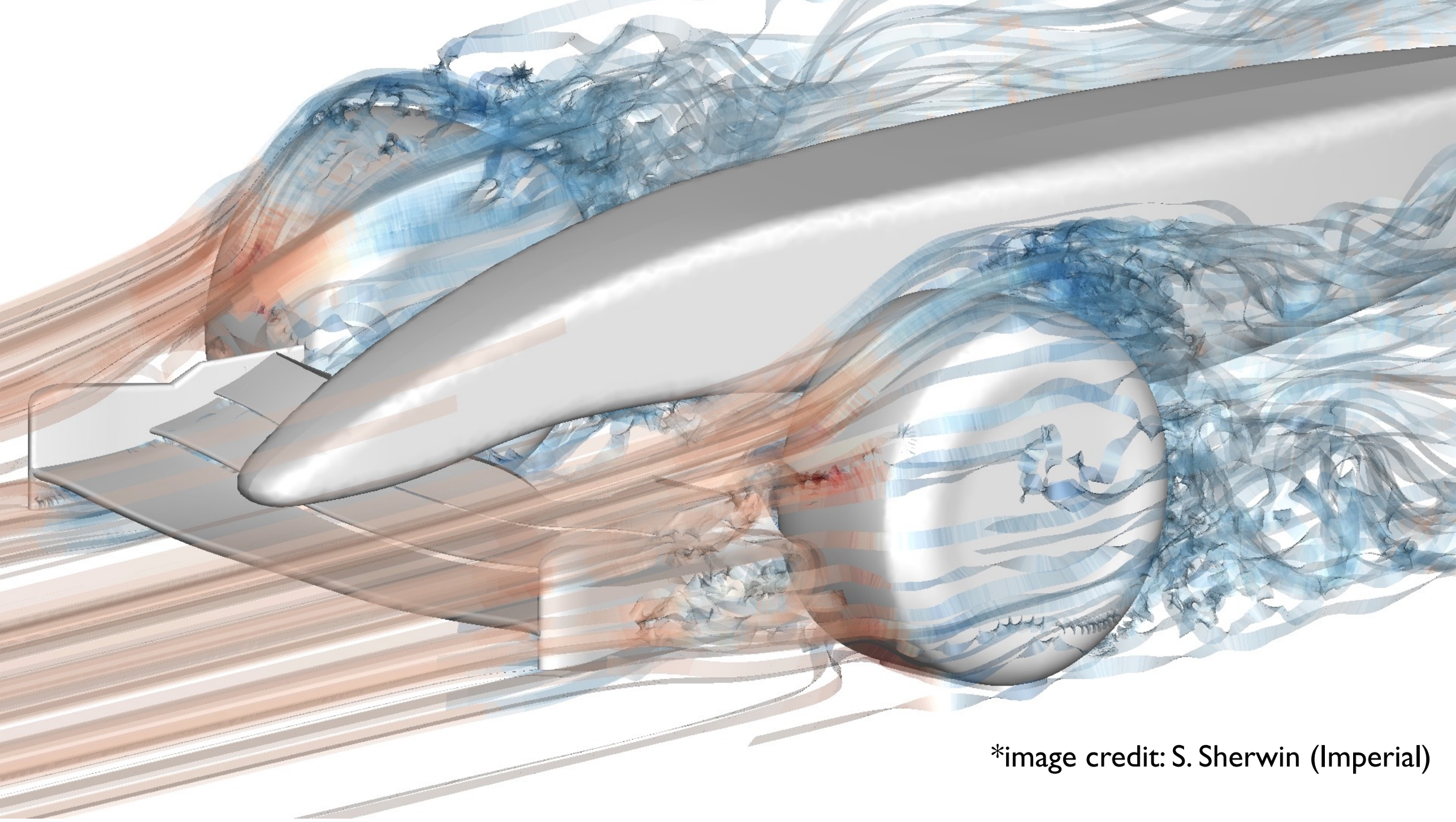
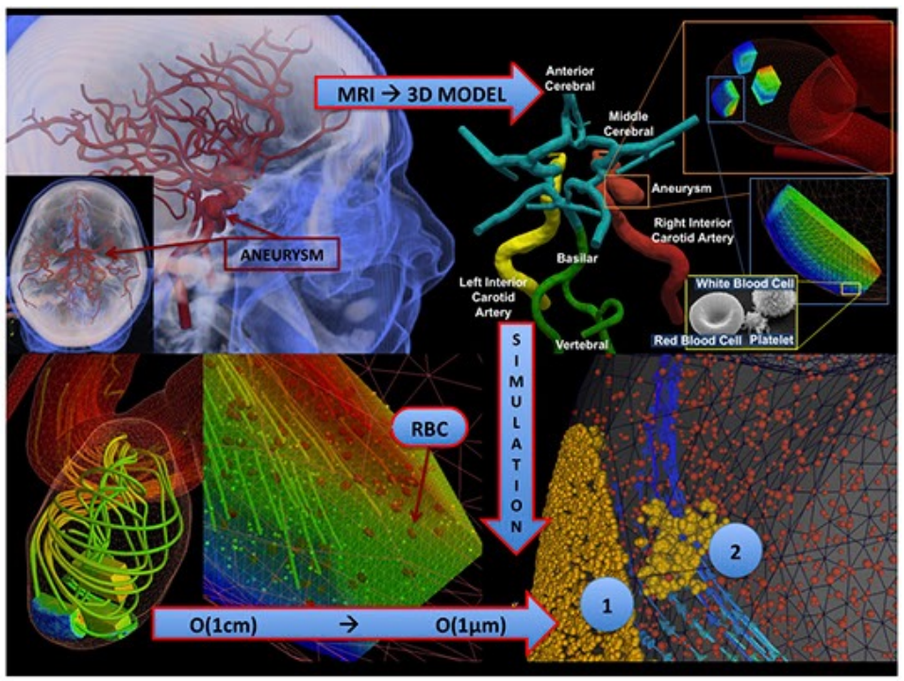


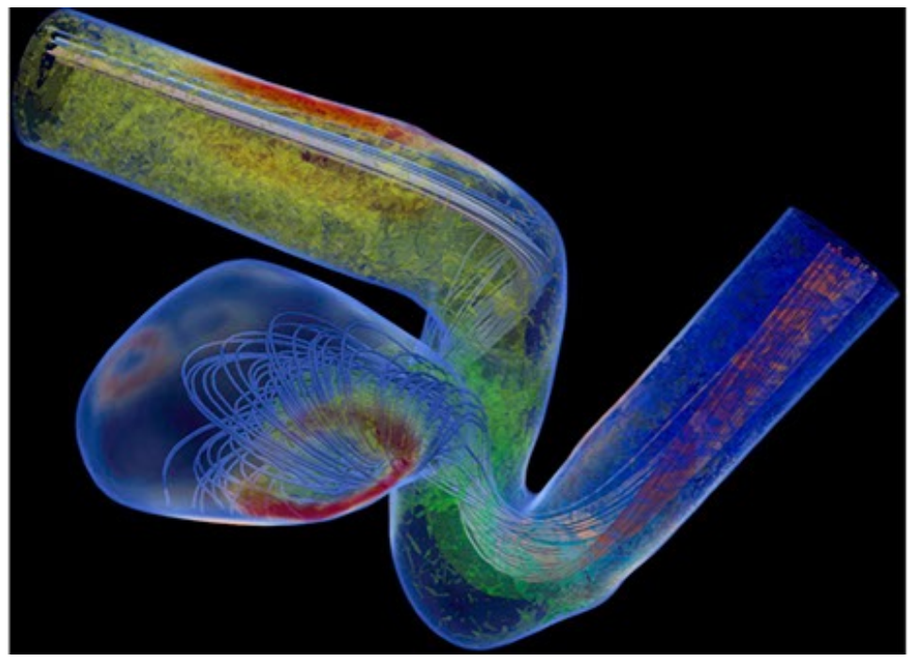
*image credit: S. Sherwin (Imperial)

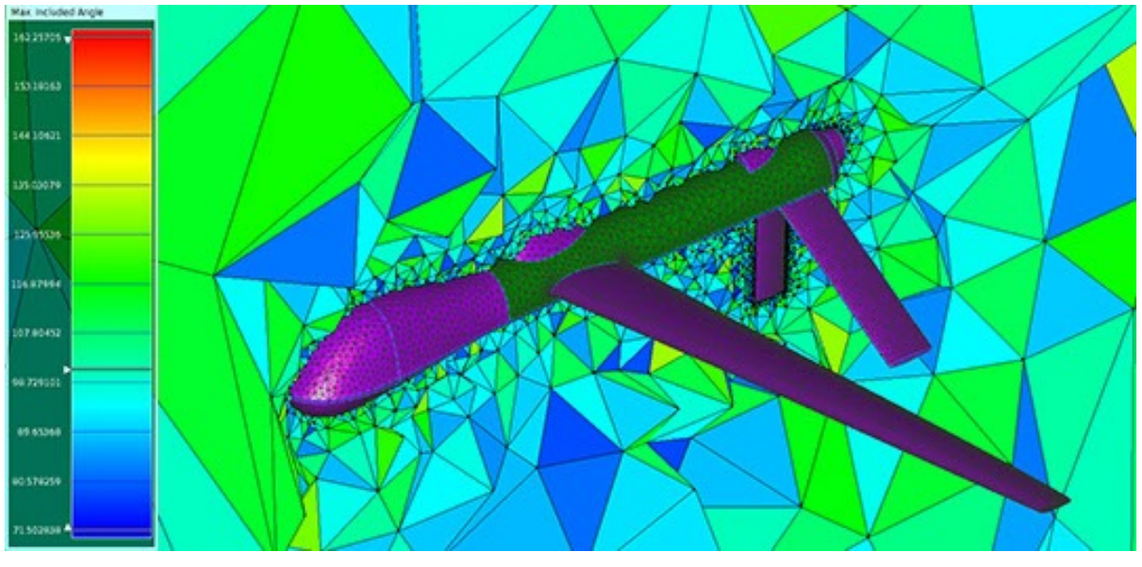
$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \boldsymbol{u}$$

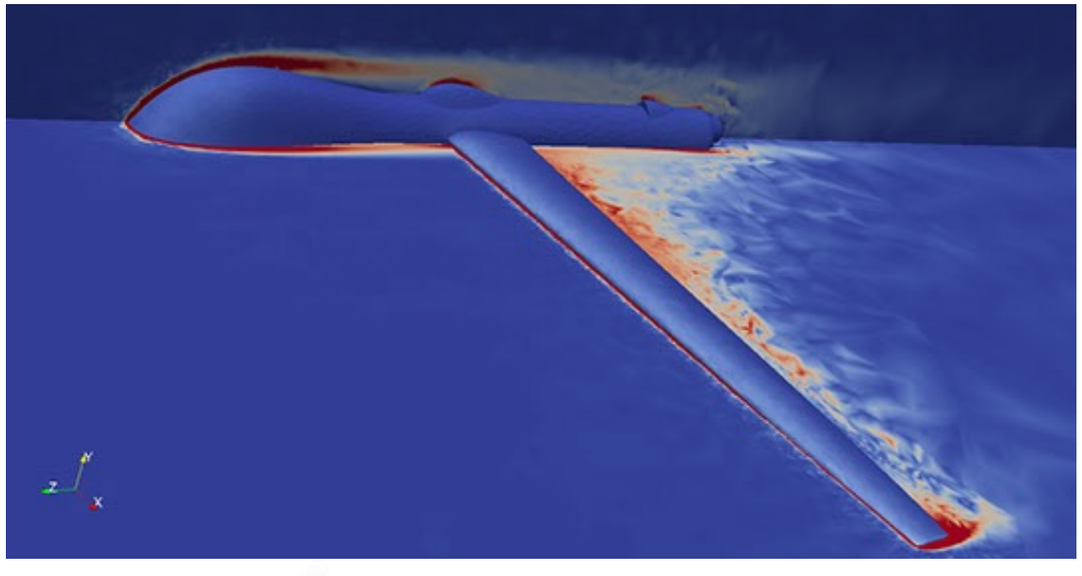
$$\nabla \cdot \boldsymbol{u} = 0$$

Computational science & engineering









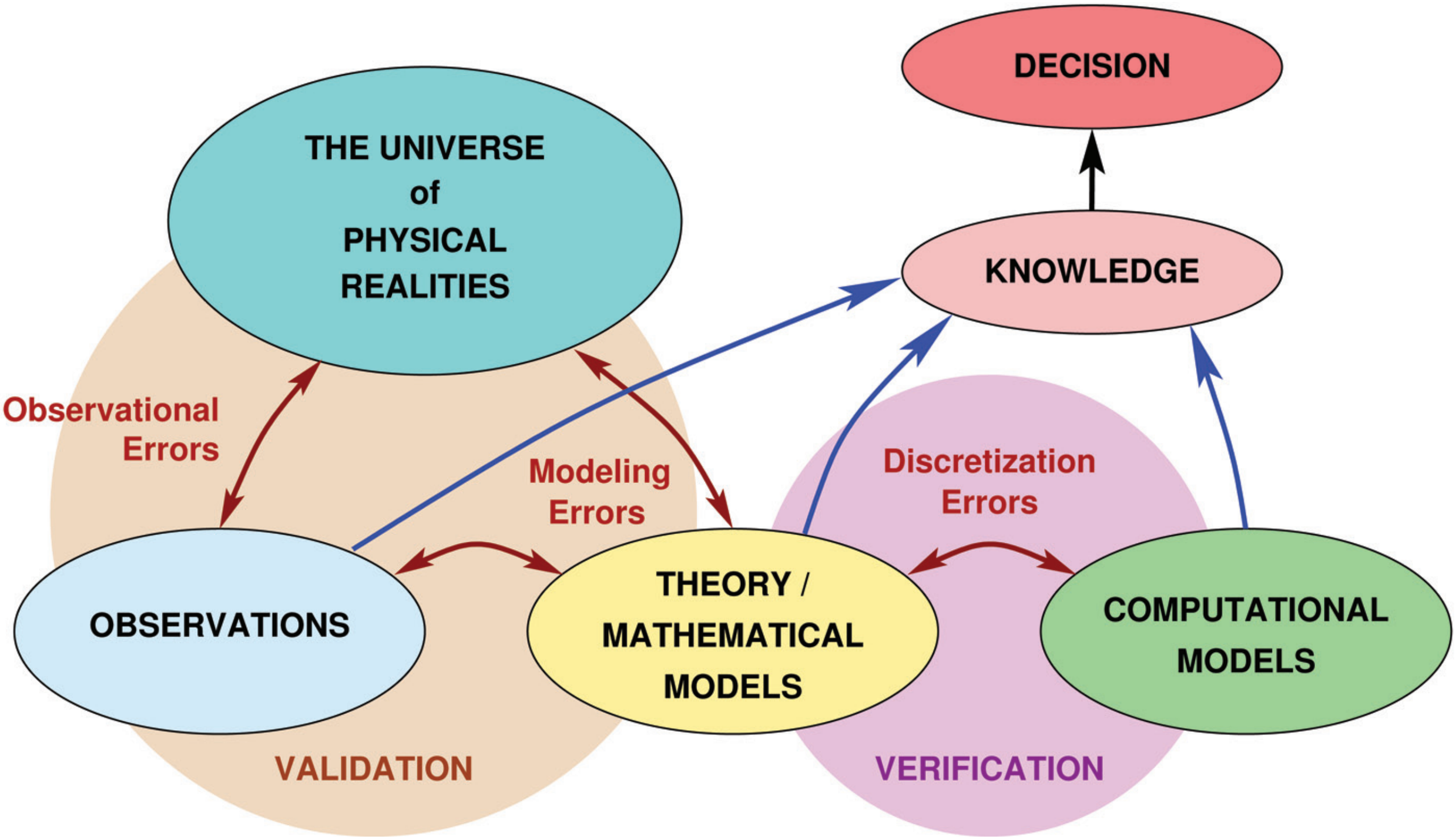
One exaflop is a thousand petaflops or a quintillion (10^18) floating point operations per second!

All models are wrong

but some are useful

George E.P. Box

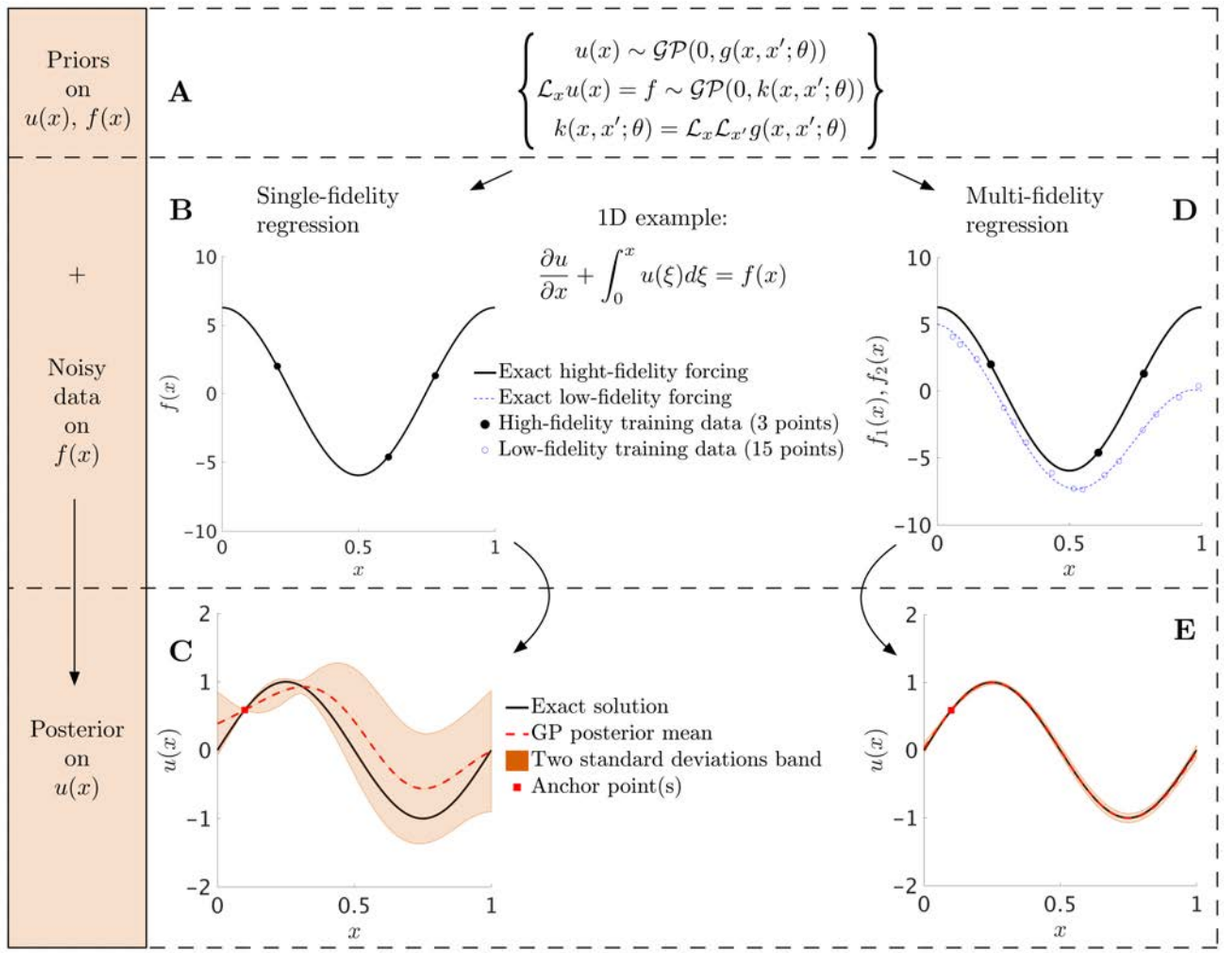
Predictive science



Oden, T., Moser, R., & Ghattas, O. (2010). Computer predictions with quantified uncertainty, part I. SIAM News, 43(9), 1-3.

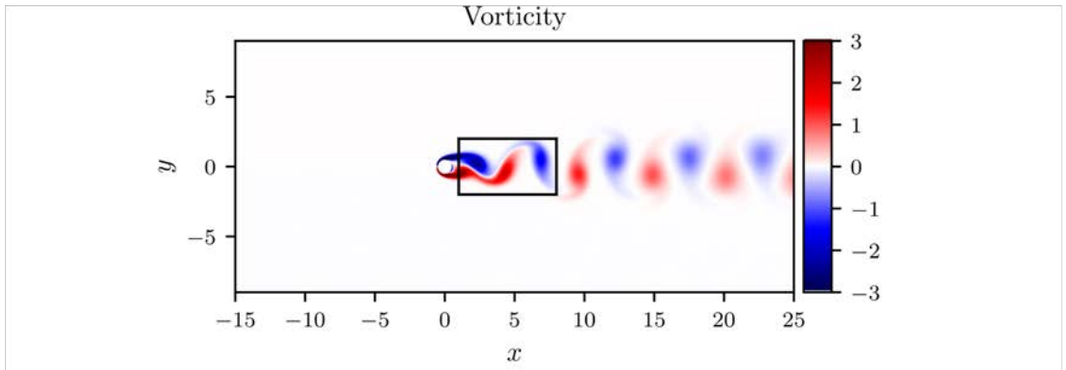
CSE for ML

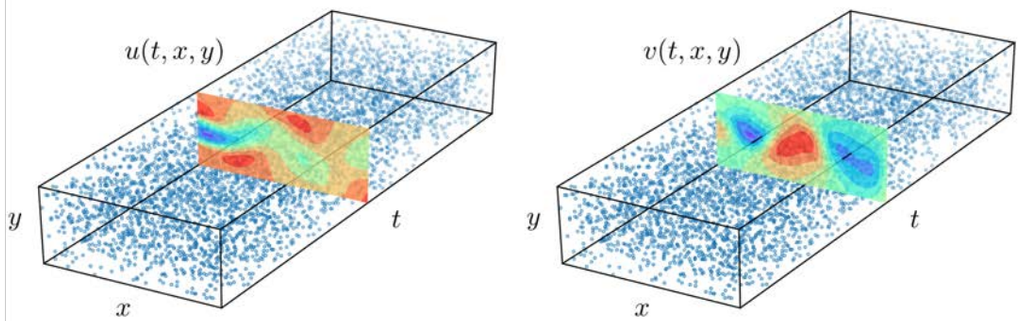
Leverage domain-specific prior information to construct more structured, interpretable, and accurate and data-efficient learning algorithms.

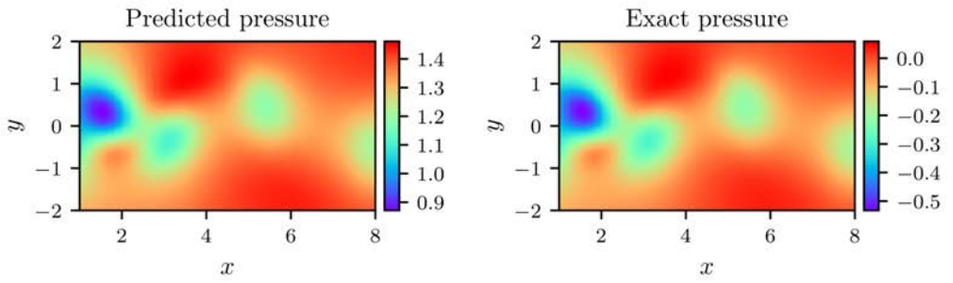


ML for CSE

Leverage recent developments in machine learning to construct robust data-driven solvers, discover new models, and address longstanding challenges in scientific computing (e.g. high-dimensional problems, UQ, etc.)







Correct PDE	$u_t + (uu_x + vu_y) = -p_x + 0.01(u_{xx} + u_{yy})$ $v_t + (uv_x + vv_y) = -p_y + 0.01(v_{xx} + v_{yy})$
Identified PDE (clean data)	$u_t + 0.999(uu_x + vu_y) = -p_x + 0.01047(u_{xx} + u_{yy})$ $v_t + 0.999(uv_x + vv_y) = -p_y + 0.01047(v_{xx} + v_{yy})$
Identified PDE (1% noise)	$u_t + 0.998(uu_x + vu_y) = -p_x + 0.01057(u_{xx} + u_{yy})$ $v_t + 0.998(uv_x + vv_y) = -p_y + 0.01057(v_{xx} + v_{yy})$

$$f : \mathcal{X} \to \mathcal{Y}$$

Supervised learning

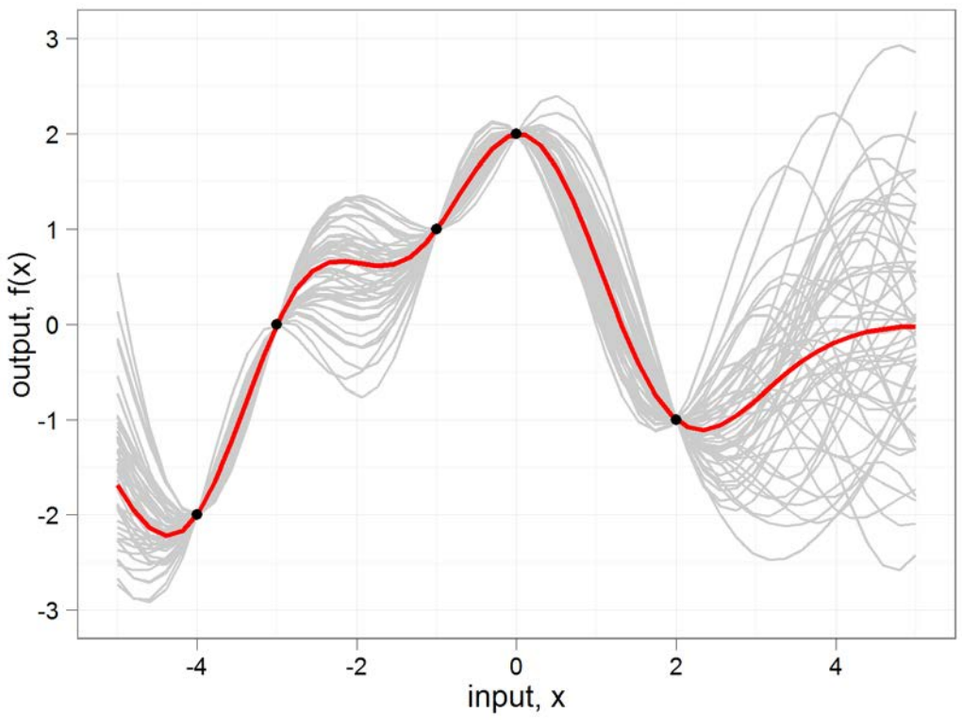
$$f : \mathcal{X} \to \mathcal{Y}$$

$$\mathcal{D} = \{\boldsymbol{x}, \boldsymbol{y}\},\ \boldsymbol{x} \in \mathcal{X},\ \boldsymbol{y} \in \mathcal{Y}$$

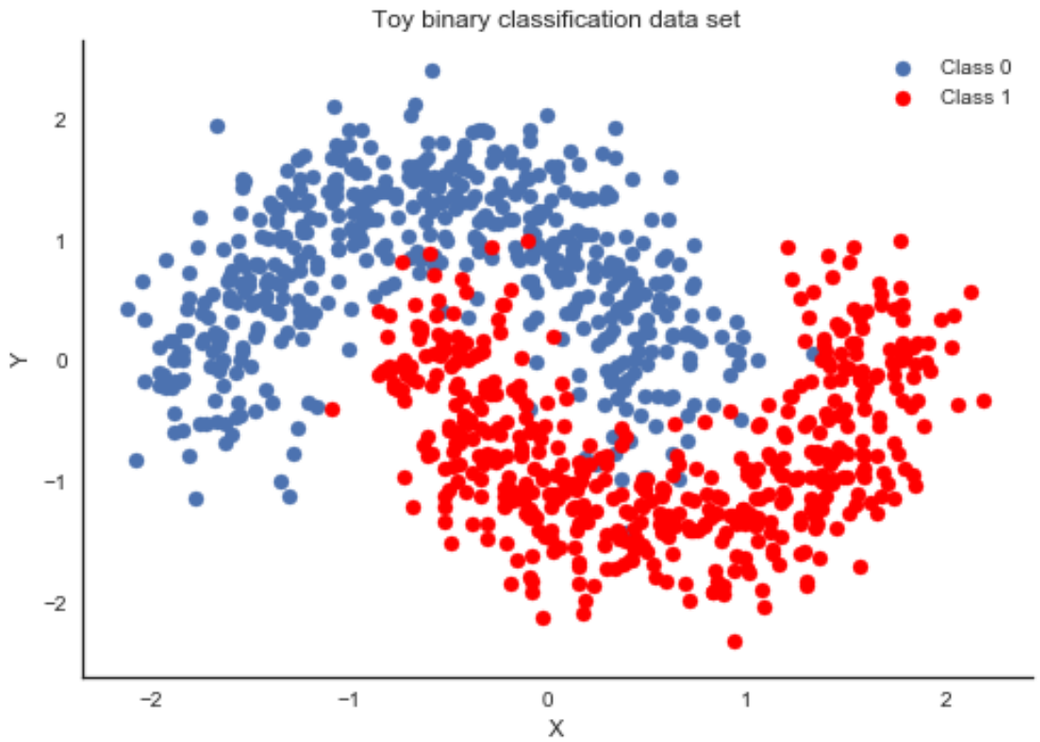
$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon$$

$$p(f(\boldsymbol{x}^*)|\boldsymbol{x}^*, \mathcal{D})$$

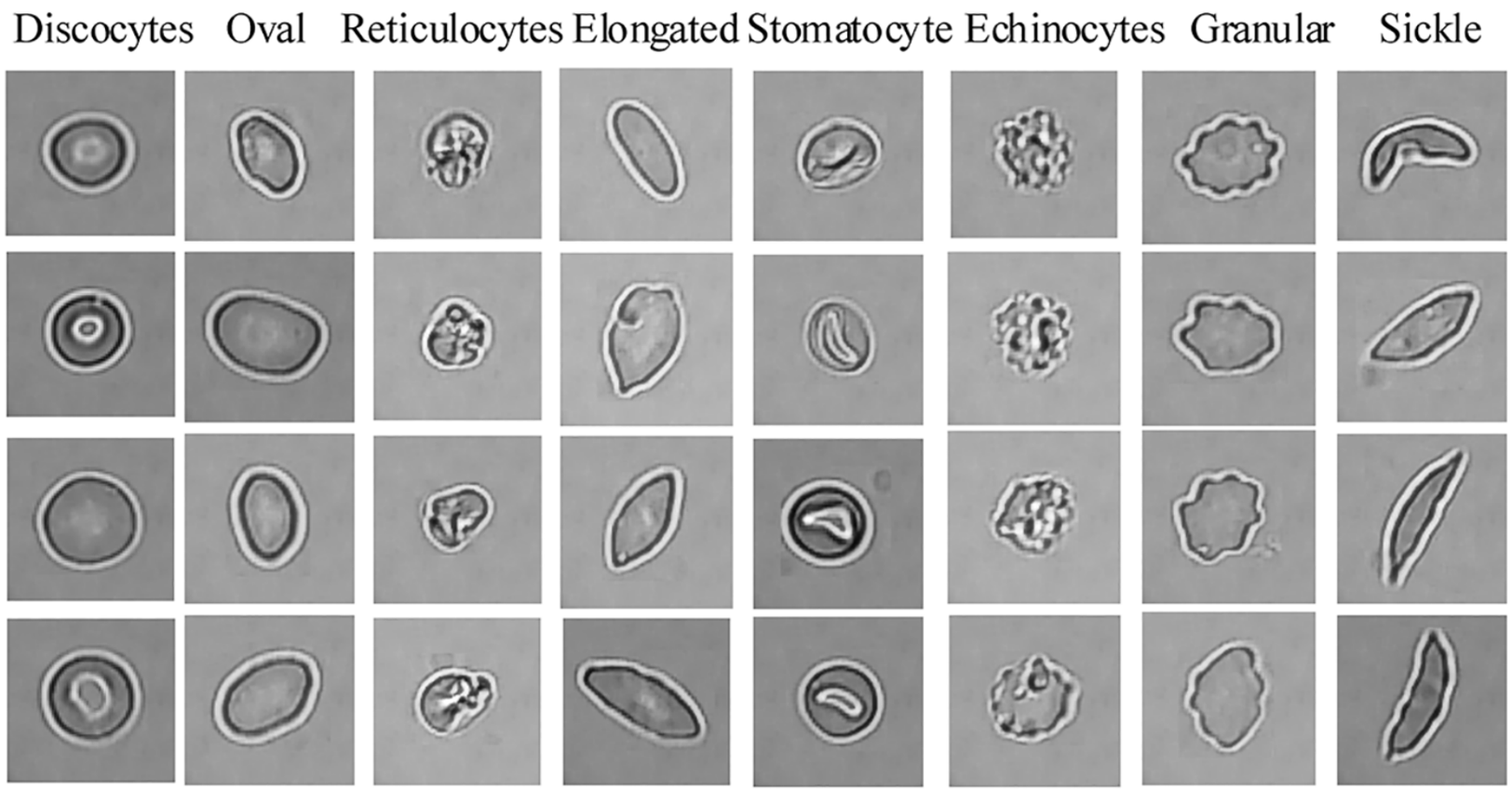
Regression



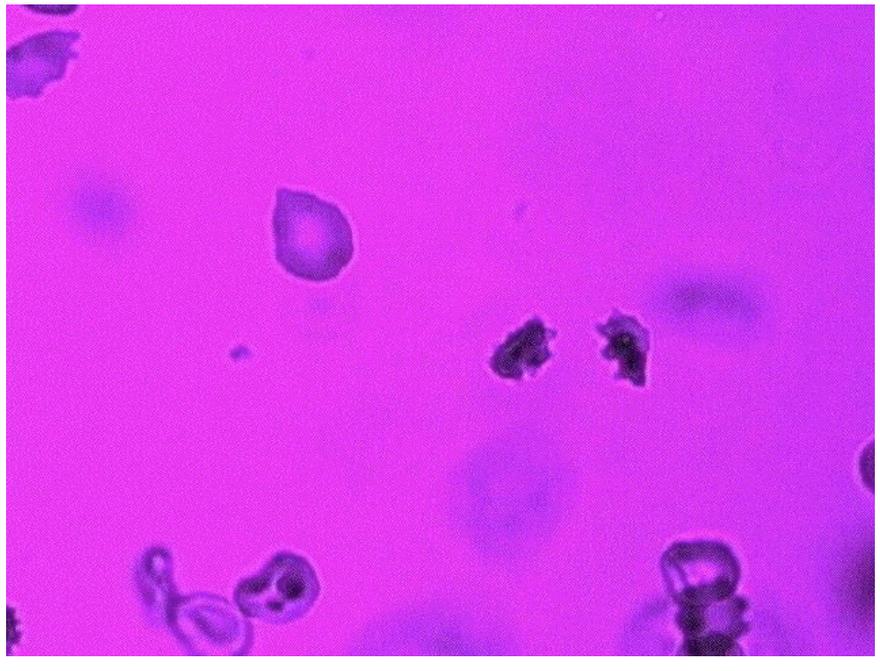
Classification



Classification



$$\mathcal{D} = \{\boldsymbol{x}, \boldsymbol{y}\},\ \boldsymbol{x} \in \mathcal{X},\ \boldsymbol{y} \in \mathcal{Y}$$



$$\boldsymbol{y} = f(\boldsymbol{x}) + \epsilon$$

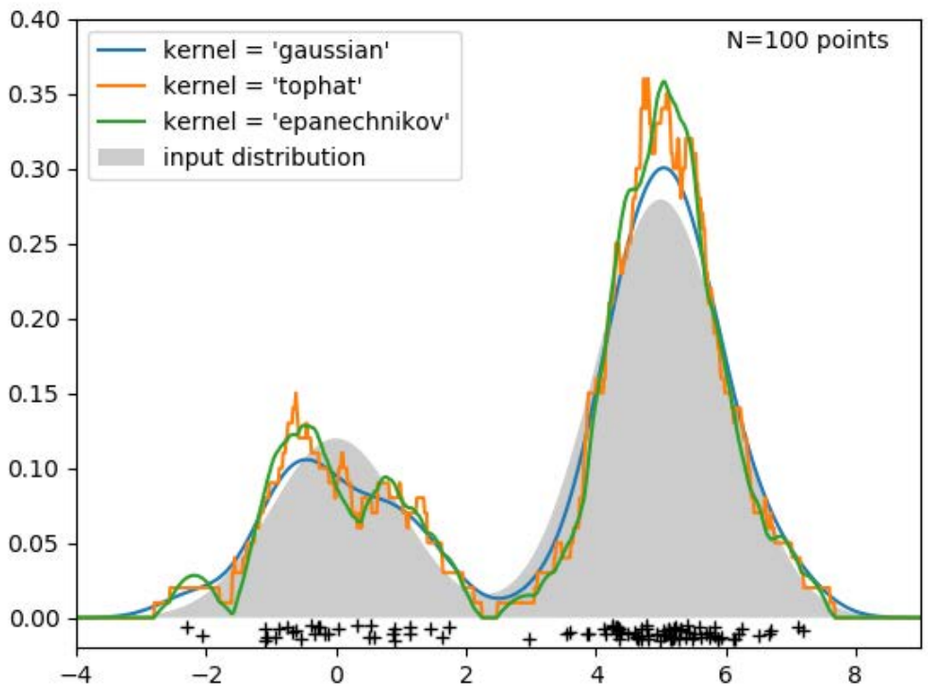
Unsupervised learning

$$\{\boldsymbol{y}\},\ \boldsymbol{y} \in \mathcal{Y}$$

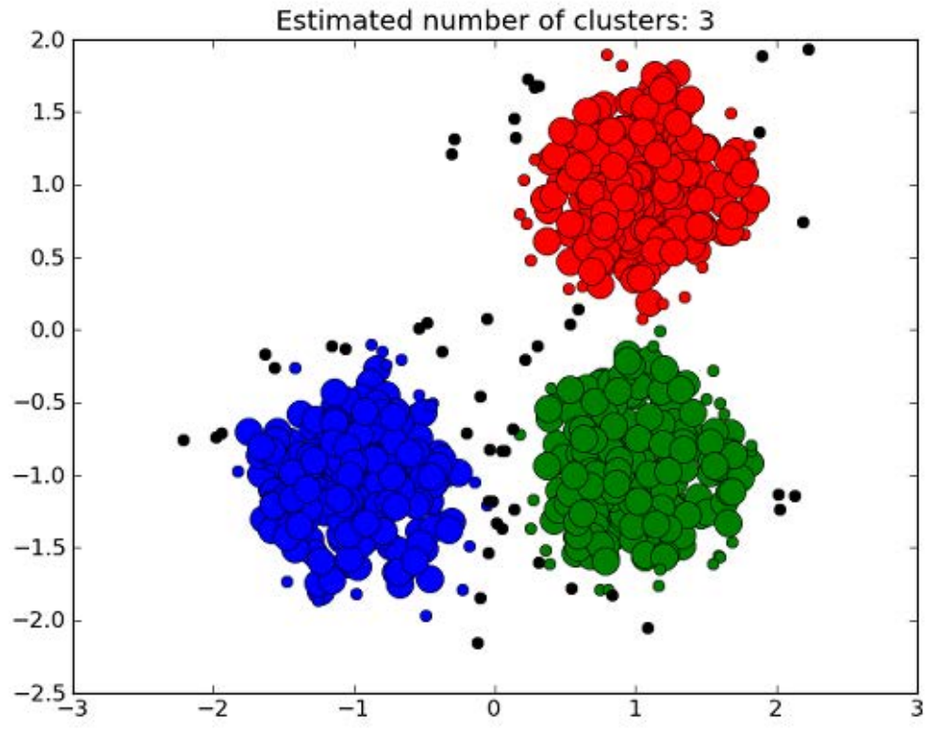
$$\boldsymbol{y} = f(\boldsymbol{z}) + \epsilon$$

$$p(\boldsymbol{y}),\ \boldsymbol{z} \sim p(\boldsymbol{z})$$

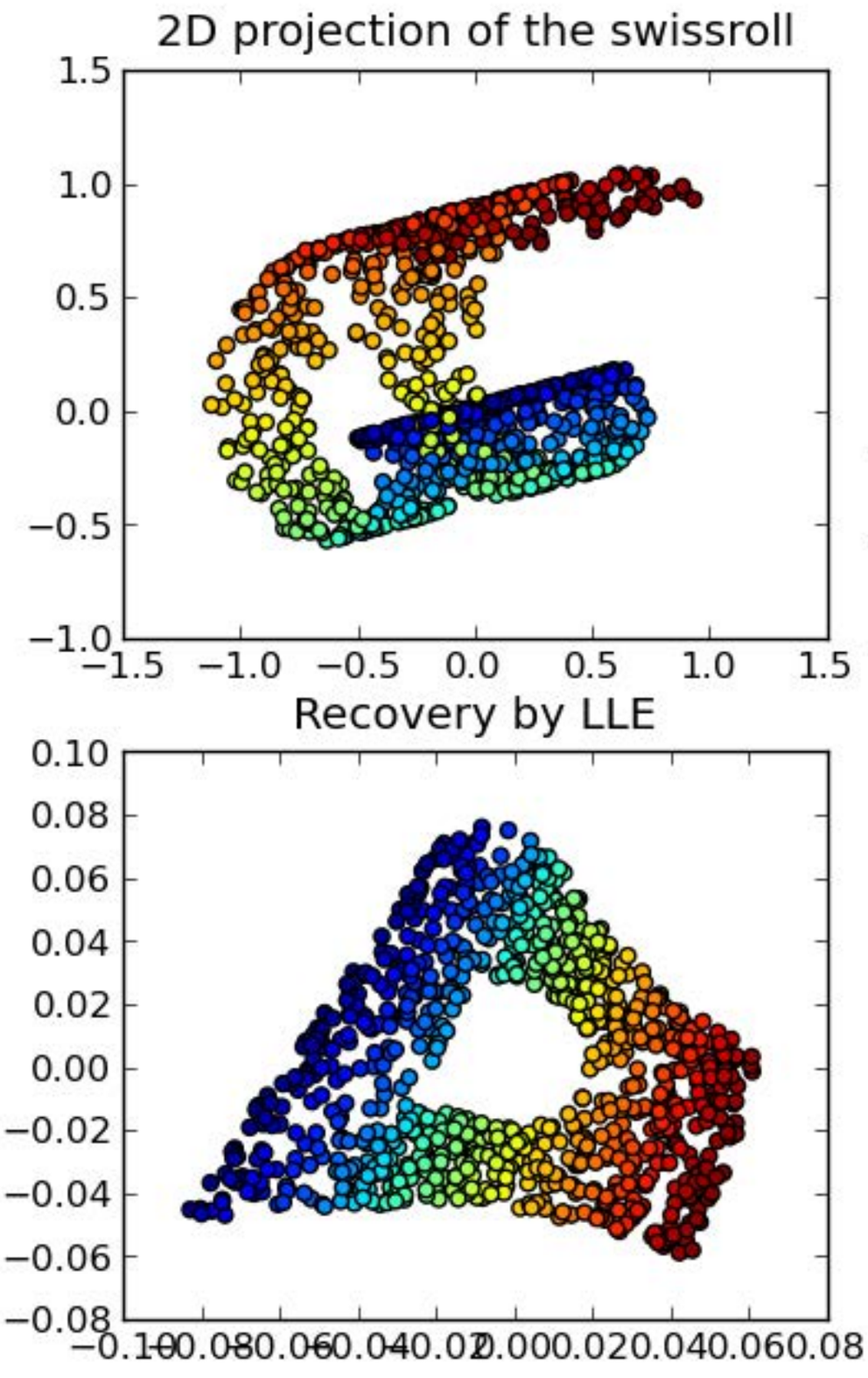
Density estimation

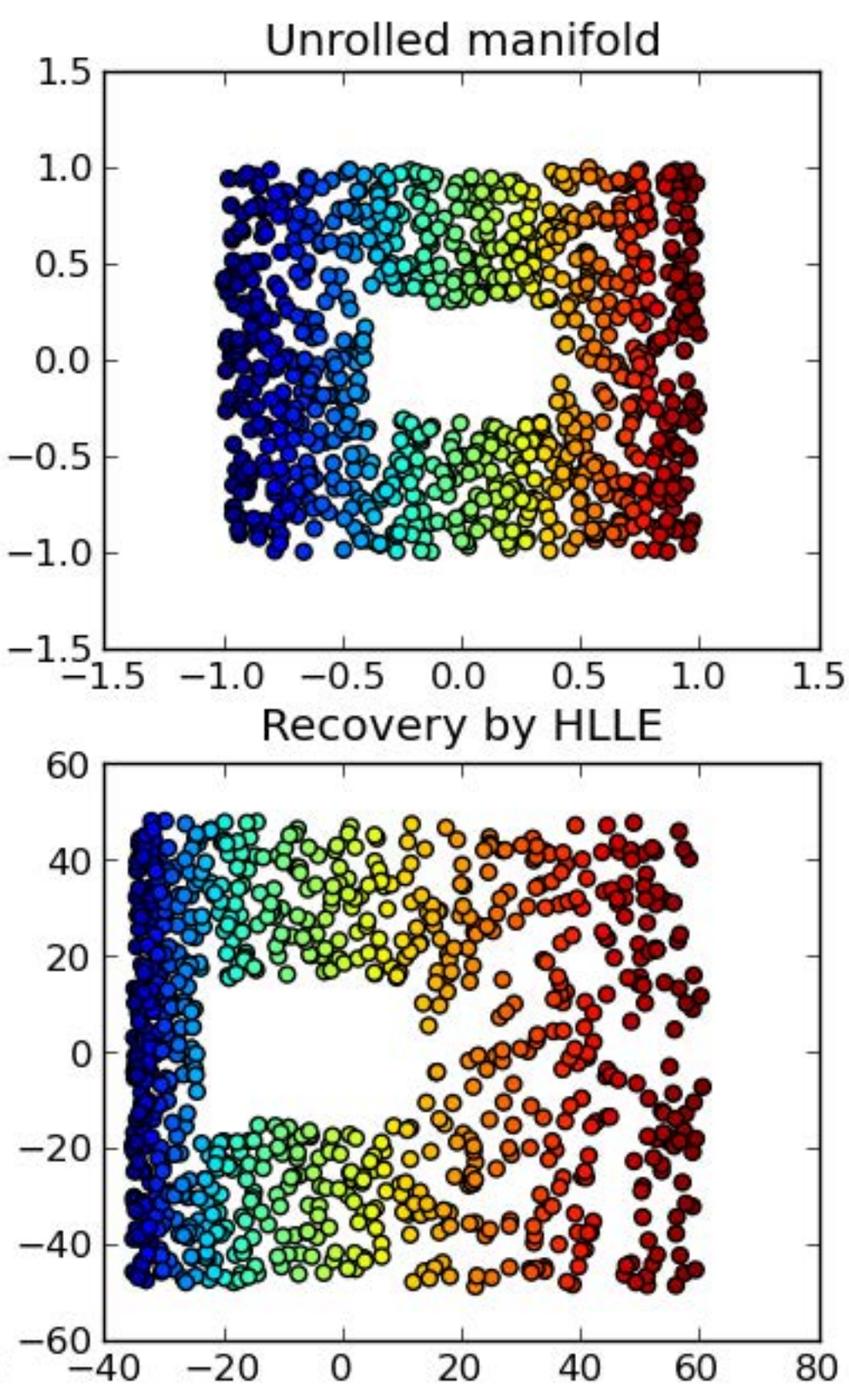


Clustering



Dimensionality reduction

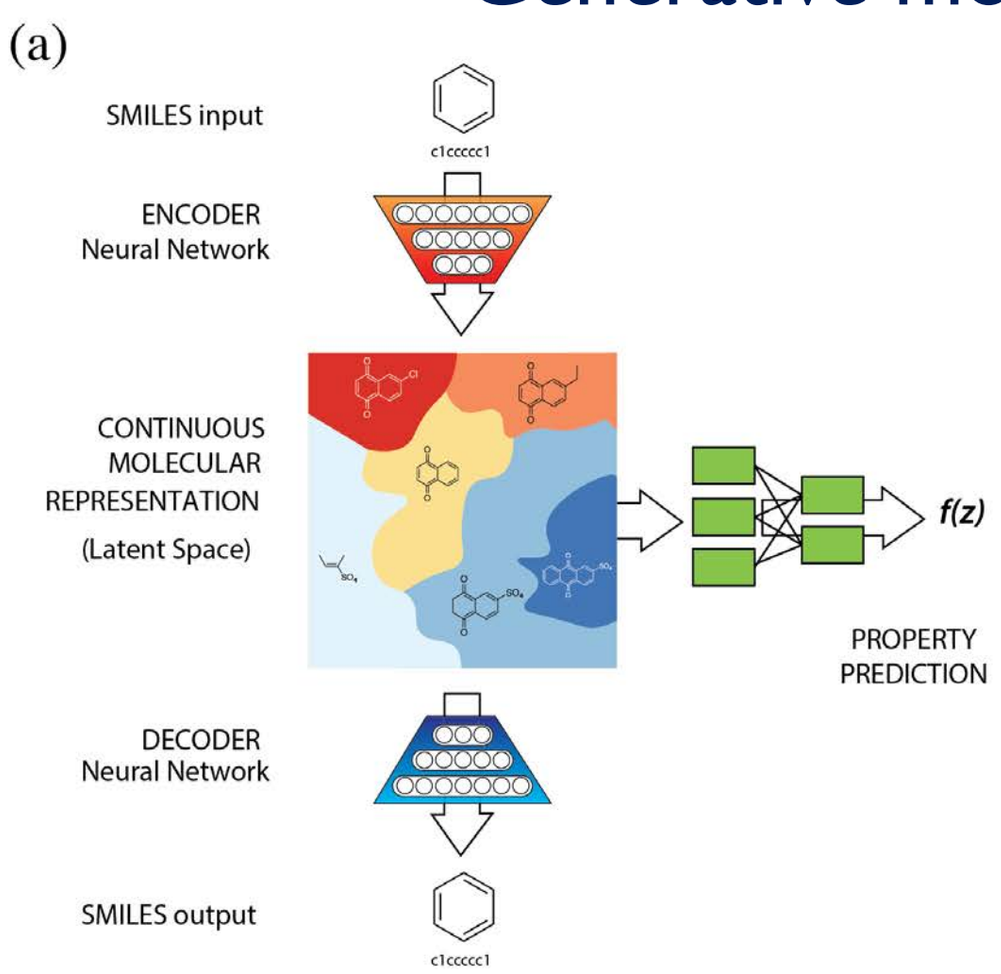


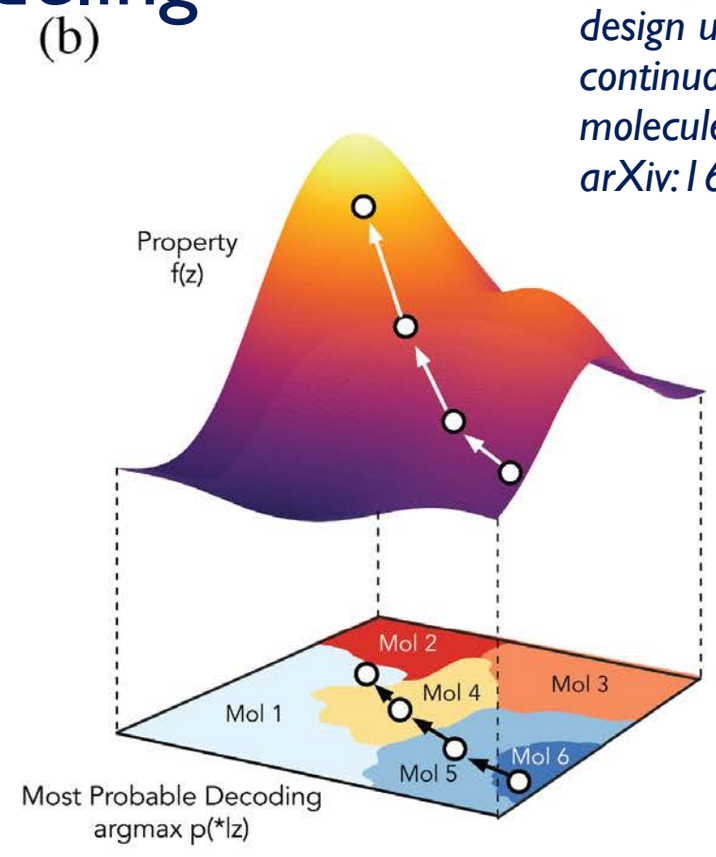


Generative modeling

Generative modeling

Gómez-Bombarelli, R., el. al. (2016). Automatic chemical design using a data-driven continuous representation of molecules. arXiv preprint arXiv:1610.02415.





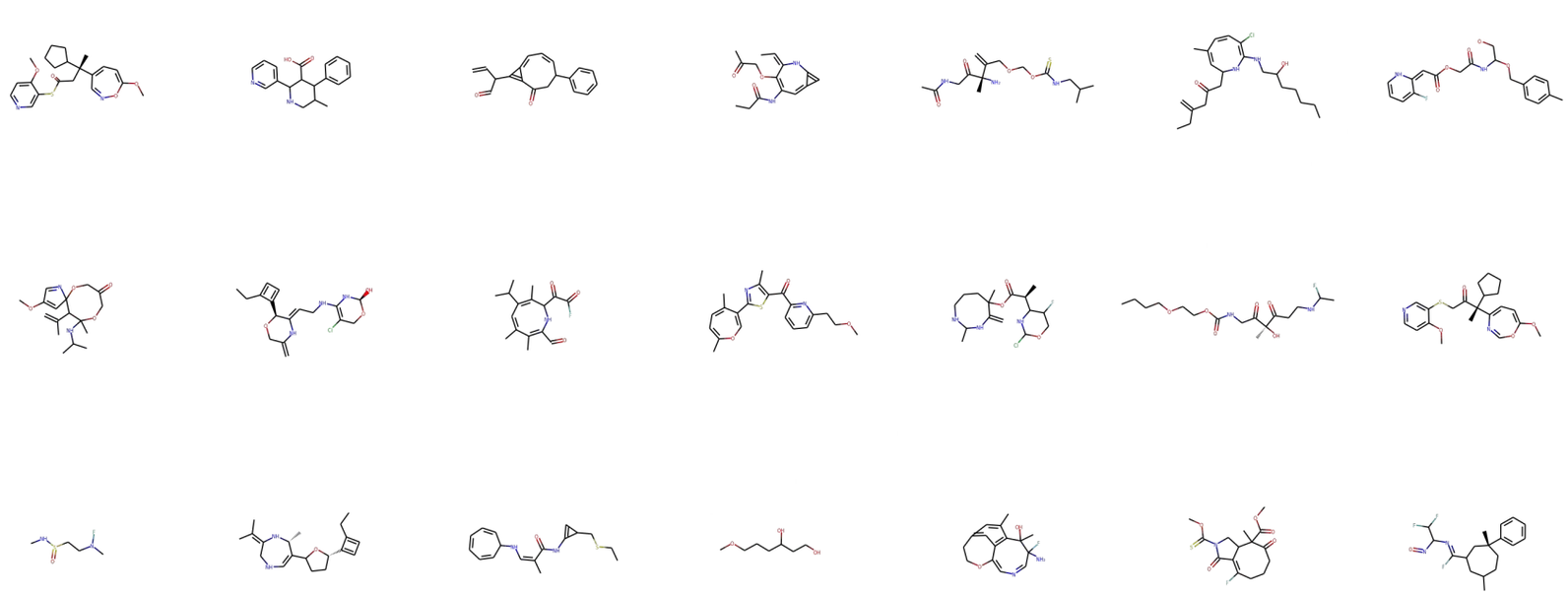
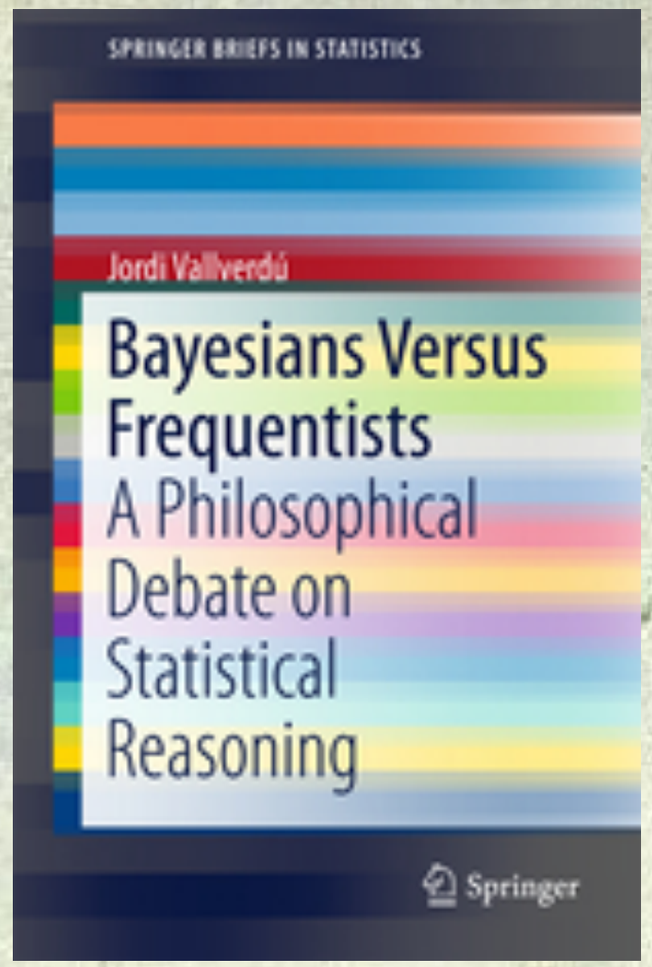
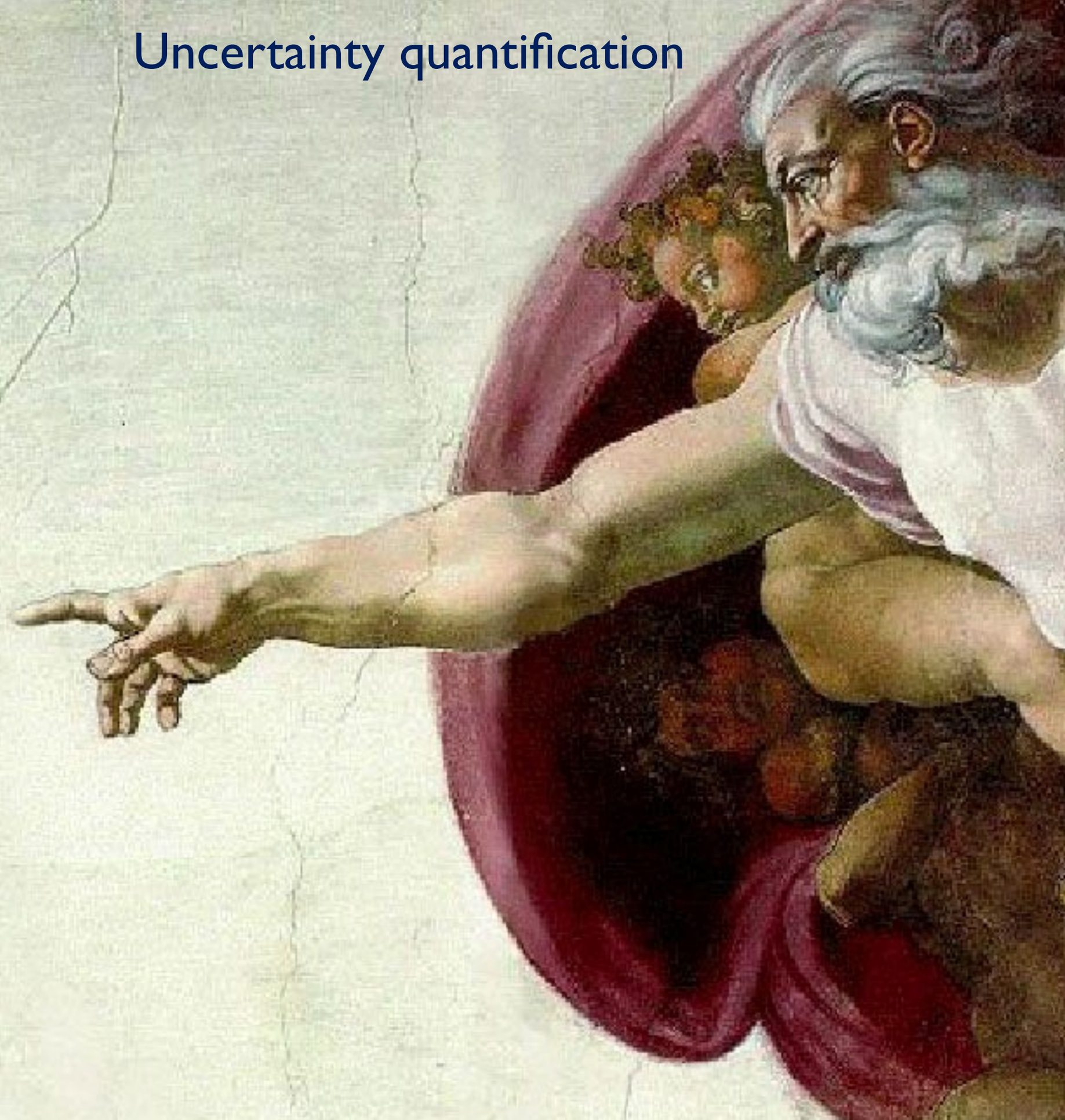


Figure 8: Molecules decoded from randomly-sampled points in the latent space of the ZINC VAE.

Uncertainty quantification





Course goals

- Learning how to analyze and synthesize data towards enhancing their understanding and ability to model physical, biological, and engineering systems.
- Hands-on skills on contemporary machine learning tools enabling them to construct prediction models, extract patterns and characterize the statistical properties of data.
- Applications of these tools spanning a diverse set of engineering disciplines, including fluid dynamics, heat transfer, mechanical design, and biomedical engineering.

<u>Key motifs:</u>

- Representation
- Approximation
- Optimization
- Control

Course logistics

- Duration: 14 Weeks
- Time: Tuesdays and Thursdays, 4:30 pm to 6:00 pm
- Dates: January 16 to April 28, 2020. No classes on Tuesday, March 10 and Thursday, March 12.
- Location: Towne Building, Room 309
- Office Hours: Thursdays 11:00 am to 1:00 pm at Office 527A (3401 Walnut Street).
- Weekly/bi-weekly homework assignments, mid-term exam, final project.

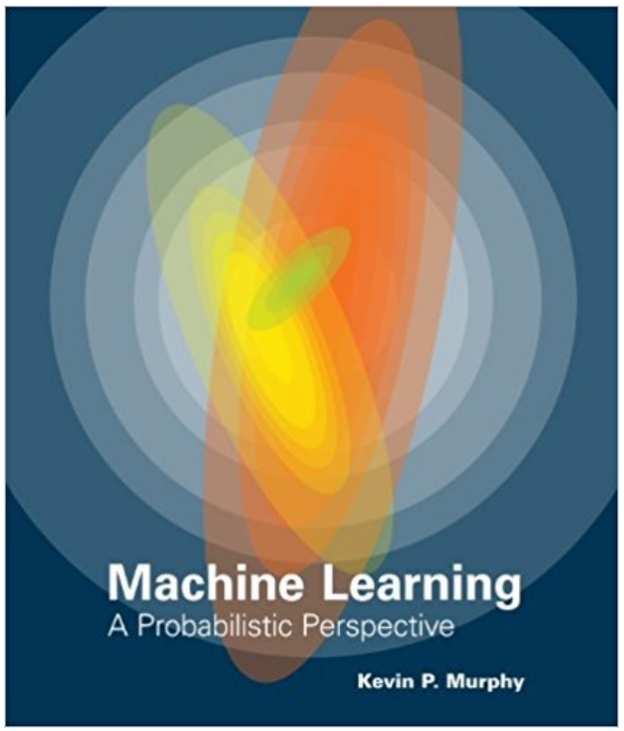
For more details visit the course website:
https://www.seas.upenn.edu/~enm531/

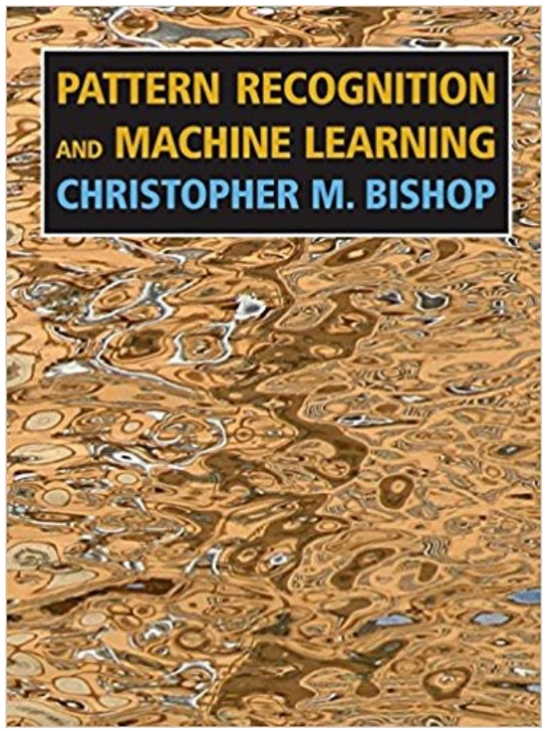
Slides and code can be found on Github:
https://github.com/PredictiveIntelligenceLab/ENM531

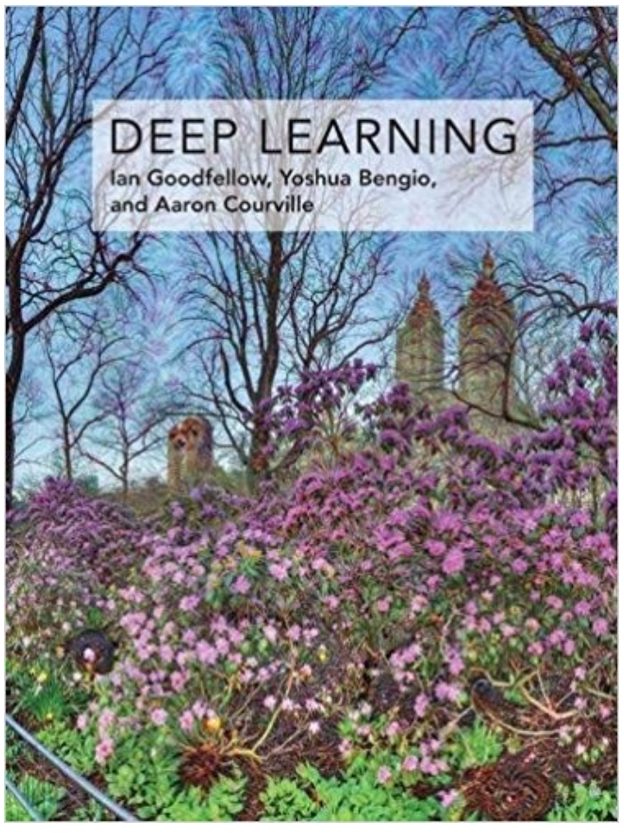
Course outline

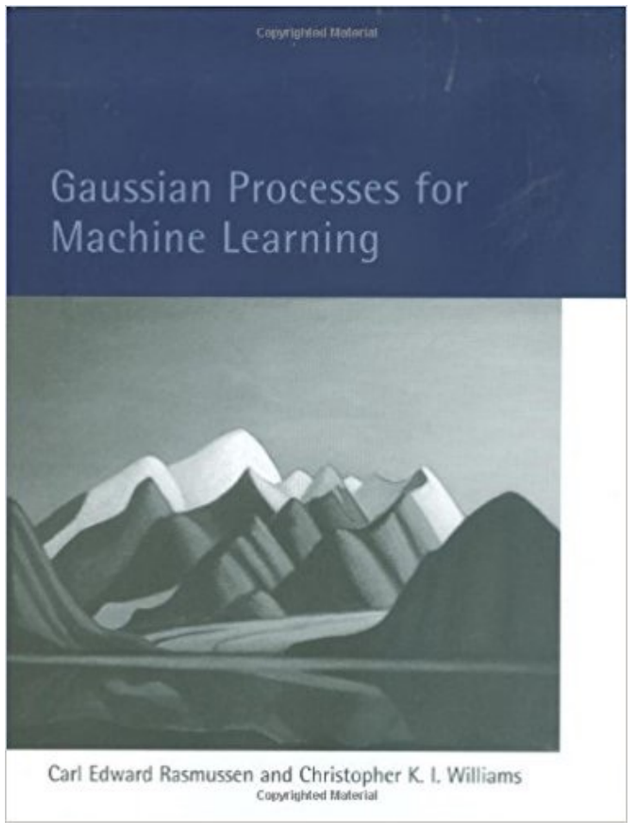
- Week 1: Introduction to data-driven modeling, motivating examples and course outline.
- Week 2: Probability theory primer through the lens of Bayesian linear regression.
- Week 3: Optimization: gradients and Hessians, gradient descent, Newton's algorithm, stochastic gradient descent.
- Week 4: Deep neural networks: back-propagation, over-fitting and regularization, automatic differentiation.
- Week 5: Image classification with convolutional neural networks.
- Week 6: Recurrent neural networks and LSTMs.
- Week 7: Sampling and quantification of uncertainty.
- Week 8: Gaussian processes, multi-output Gaussian processes and multi-fidelity modeling.
- Week 9: Bayesian optimization and active learning.
- Week 10: Probabilistic scientific computing: Gaussian process regression meets differential equations.
- Week 11: Unsupervised learning: principal component analysis, Gaussian process latent variable models.
- Week 12: Variational auto-encoders and conditional variational auto-encoders.
- Week 13: Generative adversarial networks.
- Week 14: Class presentations of final papers.

Textbook


Machine Learning
A Probabilistic Perspective
Kevin P. Murphy


PATTERN RECOGNITION
AND MACHINE LEARNING
CHRISTOPHER M. BISHOP


DEEP LEARNING
Ian Goodfellow, Yoshua Bengio,
and Aaron Courville


Copyrighted Material
Gaussian Processes for
Machine Learning
Carl Edward Rasmussen and Christopher K. I. Williams
Copyrighted Material

Reading

- Introduction
- Syllabus review
- Presentation of diverse applications that showcase the use of data, modeling, and scientific computation.
- Overview of the main themes and goals of this course
- Primer on Probability and Statistics

Reading

- The Emergence of Predictive Computational Science:
  - Computer predictions with quantified uncertainty (Oden, Moser, & Ghattas, 2010)
  - Lecture by J.T Oden.
- Review papers on recent advances in machine learning:
  - Probabilistic machine learning and artificial intelligence (Ghahramani, 2015)
  - Deep learning (LeCun, Bengio, & Hinton, 2015)
  - Machine learning: Trends, perspectives, and prospects (Jordan & Mitchell, 2015)
- Scientific computing in Python:
  - Lectures and code by Robert Johansson.

1. Oden, T., Moser, R., & Ghattas, O. (2010). Computer predictions with quantified uncertainty, part I. *SIAM News*, *43*(9), 1–3.
2. Ghahramani, Z. (2015). Probabilistic machine learning and artificial intelligence. *Nature*, *521*(7553), 452–459.
3. LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. *Nature*, *521*(7553), 436–444.
4. Jordan, M. I., & Mitchell, T. M. (2015). Machine learning: Trends, perspectives, and prospects. *Science*, *349*(6245), 255–260.

Software

Consult the Web for instructions and make sure you have the following software properly installed and working on your laptop:

- A Python 3.7 distrubution configured for scientific computing. The simplest way to set this up is by installing the Anaconda distribution.
- PyTorch. If you have access to GPU hardware, make sure you install a version with GPU support.
- Autograd. Efficiently computes derivatives of numpy code.
- Jupyter notebook. You will need this in order to follow some of the in-class tutorials.
- Git. You will need this in order to download and stay in sync with the latest code we will develop in class.

jupyter rht-stock-price (autosaved)

Logout

File Edit View Insert Cell Kernel Help

Python 3

Code CellToolbar

In [1]:
```
%matplotlib inline
```

In [2]:
```
import datetime
```

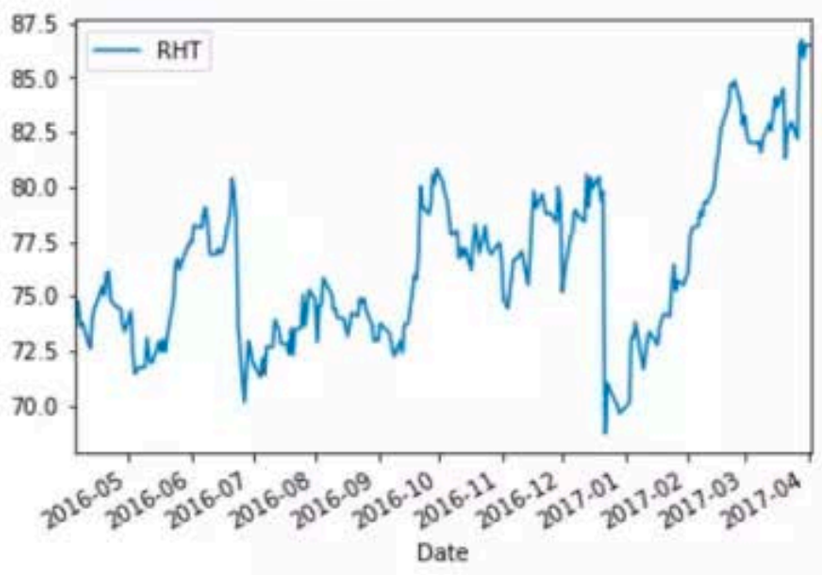
In [3]:
```
import pandas_datareader.data as web
```

In [4]:
```
end = datetime.date.today()
start = end - datetime.timedelta(days=365)
```

In [5]:
```
values = web.get_data_yahoo(["RHT"], start, end)['Adj Close']
```

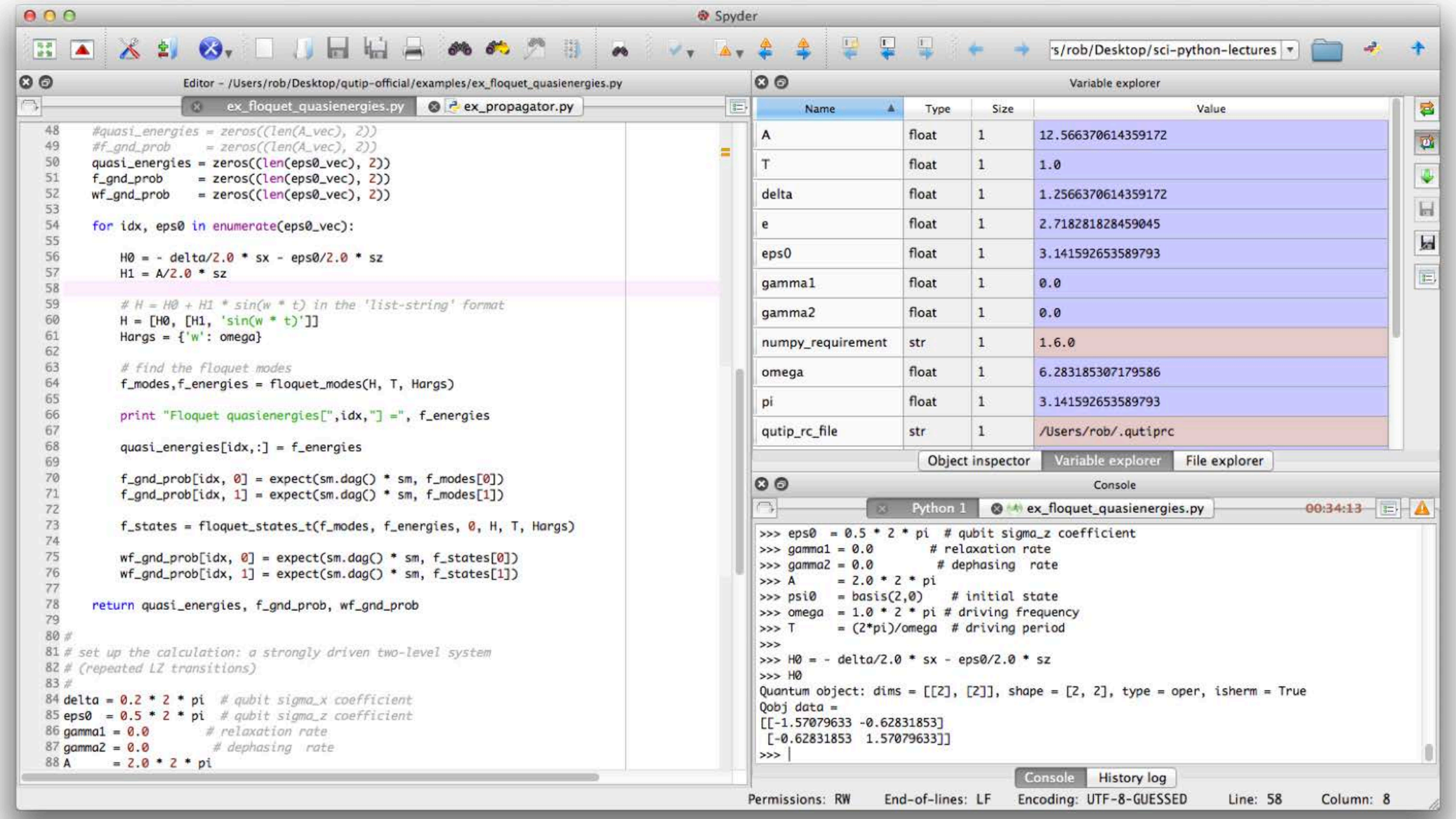
In [6]:
```
values.plot()
```

Out[6]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7f5845889780>
```



Spyder

Spyder is a MATLAB-like IDE for scientific computing with python. It has the many advantages of a traditional IDE environment, for example that everything from code editing, execution and debugging is carried out in a single environment, and work on different calculations can be organized as projects in the IDE environment.



Some advantages of Spyder:

- Powerful code editor, with syntax high-lighting, dynamic code introspection and integration with the python debugger.
- Variable explorer, IPython command prompt.
- Integrated documentation and help.