Machine Learning for Modelling Physical Systems

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4TU.AMI Models and Data in Digital Twins
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Finnish Center for Artificial Intelligence
FCAI – from science to impact

RESEARCH PROGRAMMES
- Agile Probabilistic AI
- Simulator-based inference
- Data-efficient deep learning
- Privacy-preserving and secure AI
- Interactive AI

AI ACROSS FIELDS
- Humanities, social sciences & education
- Engineering
- Health
- Economics
- Environmental sciences
- Natural sciences
- Information technologies

DATA EFFICIENCY
UNDERSTANDABILITY
TRUST & ETHICS

INDUSTRY AND SOCIETY
- Bring research result to practice
- Create FCAI ecosystem
- Promote effective and ethical application of AI
- Support governmental decision-making

EDUCATION
- Provide new AI professionals
- Educate professionals in industry and public sector
- Increase general public's understanding

IMPACT
- Systematic evaluation

IMPACT PROGRAMS AND ACTIONS
Outline

Machine learning and AI overview

Learning for differential equations with probabilistic models

Other interesting probabilistic models

Probabilistic programming
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What is AI?

- Two types of AI
  - Symbolic/logical
  - Machine learning (ML): imitation-based AI
- Current revolution in machine-learning-based AI
  - Combination of big data, models that benefit from big data, more computing power (GPUs) and accessible programming environments
- We are nowhere close to human-level intelligence
  - Imitation of examples in the data, not thinking
Flavours of ML

- **Supervised learning**
  - E.g. classification, regression, time series prediction, emulators for expensive simulators
  - Outcome: map: $x \mapsto y$

- **Reinforcement learning**
  - Planning
  - Outcome: policy: (state, observations) $\mapsto$ actions

- **Unsupervised learning**
  - E.g. dimensionality reduction, generative modelling
Big data revolution in ML

- Deep neural networks
- Classical machine learning

Accuracy vs. amount of training data
Deep neural networks and data

- Most typical applications in *supervised learning*
  - Require annotated (input, target output) pairs
- Current methods need a lot of data
- 100,000 cases is a good start, the more the better!
  - Upper limit still has not been found!
- Research viewpoint: less data may be OK, but more work and expertise needed for good results
Limitations of deep neural networks (DNNs)

- DNNs are susceptible to *adversarial examples*
  - In classification: selected examples with imperceptible differences are seriously misclassified
Limitations of deep neural networks (DNNs)

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"pig" (91%) + 0.005 x noise (NOT random) = "airliner" (99%)

Limitations of deep neural networks (DNNs)

- DNNs are susceptible to adversarial examples
  - In classification: selected examples with imperceptible differences are seriously misclassified

- This is a feature, not a bug
  - Robustness–accuracy trade-off
  - More prior knowledge (e.g. structured models) can help

- Major challenge for reinforcement learning and optimisation
  - Algorithms will learn to exploit any weaknesses of the model
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Probabilistic modelling and differential equations

- Inference of unknown parameters $\theta$ and initial conditions $x_0$ in an ODE from noisy observations $Y = [y(t_1), \ldots, y(t_n)]$, where

$$\begin{align*}
x'(t) &= g(x(t), \theta), \quad x(0) = x_0 \\
y(t_i) &= x(t_i) + \eta_i
\end{align*}$$

- Inference of latent driving functions $f(t)$ (latent force models)

$$\begin{align*}
x'(t) &= g(x(t), f(t), \theta), \quad x(0) = x_0 \\
y(t_i) &= x(t_i) + \eta_i
\end{align*}$$
Modelling latent driving functions: Gaussian processes

- Gaussian process priors on driving functions $f(t)$
  - Functional prior, specified by mean and covariance functions
  - No need for time discretisation
  - Can capture diverse activation profiles

$$f(t) \sim \mathcal{GP} (\mu(t), k(t, t'))$$

where

$$\mu(t) = \mathbb{E}[f(t)] = \langle f(t) \rangle$$

$$k(t, t') = \mathbb{E}[(f(t) - \mu(t))(f(t') - \mu(t'))]$$
Gaussian process examples: squared exponential covariance
Gaussian process examples: Matern covariance
Gaussian processes and ODEs (Lawrence et al., NIPS 2006)

- Assume $x \sim \mathcal{N}(\mu, \Sigma)$
- Affine transformation $Ax + b$ follows

$$(Ax + b) \sim \mathcal{N}(A\mu + b, A\Sigma A^T)$$
Gaussian processes and ODEs (Lawrence et al., NIPS 2006)

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- Insight: an analogous property applies to Gaussian processes:
  For suitable $g()$, the solution for $x(t)$ in

$$\frac{dx(t)}{dt} = g(x(t), f(t), \theta)$$

is an affine operator $x(t) = L_g(f(t))$ of $f(t)$

$\Rightarrow$ Joint Gaussian process over $f(t), x(t)$
ODE Gaussian process

- Assuming $x(t) \sim \mathcal{GP}(\mu_x(t), k_{xx}(t, t'))$, how to evaluate the mean function $\mu_x(t)$ and covariance $k_{xx}(t, t')$?

$$
\mu_x(t) = \mathbb{E}_{p(f(t))}[\mathcal{L}_g(f(t))] \\
k_{xx}(t, t') = \mathbb{E}_{p(f(t), f(t'))}[(\mathcal{L}_g(f(t)) - \mu_x(t))(\mathcal{L}_g(f(t)) - \mu_x(t))^T]
$$

- For suitable $k_{ff}(t, t')$ and linear $g$, these can be evaluated in closed form, leading to very efficient computation

- E.g. squared exponential covariance:

$$
k_{ff}(t, t') = \alpha \exp\left(\frac{(t - t')^2}{2\ell^2}\right)
$$
Single input motif gene regulation (Lawrence et al., NIPS 2006; Gao et al., Bioinformatics 2008):

\[
\frac{dx_i(t)}{dt} = B_i + S_if(t) - D_ix_i(t)
\]

- \( x_i(t) \) target gene expression
- \( f(t) \) regulator activity
ODE Gaussian process applications II

Translation + transcription model of gene regulation (Honkela et al., PNAS 2010; Gao et al., Bioinformatics 2008):

\[
\frac{dp(t)}{dt} = f(t) - \delta p(t)
\]

\[
\frac{dx_i(t)}{dt} = B_i + S_i p(t) - D_i x_i(t)
\]

- \(x_i(t)\) target gene expression
- \(p(t)\) regulator activity
- \(f(t)\) regulator mRNA expression
Modelling transcription+expression (Honkela et al., PNAS 2015):

\[
\frac{dx(t)}{dt} = B + Sf(t - \Delta) - Dx(t)
\]

- \(x(t)\) gene expression
- \(f(t)\) transcriptional activity
Non-linear ODEs

- If $L_g$ is not affine, $x(t)$ will not follow Gaussian process
- Approximations still possible
- E.g. non-linear gene regulation model by Titsias et al. (BMC Systems Biology, 2012):

\[
\frac{d p_i(t)}{d t} = f_i(t) - \delta_i p_i(t)
\]
\[
\frac{d x_j(t)}{d t} = b_j + s_j G(p_1(t), \ldots, p_I(t); \theta_j) - d_j x_j(t)
\]

with

\[
G(p_1(t), \ldots, p_I(t); w_j, w_{j0}) = \frac{1}{1 + e^{-w_{j0} - \sum_{i=1}^{I} w_{ji} \log p_i(t)}}
\]
Gene transcription and expression model (Honkela et al., PNAS 2015)

\[
\frac{dm(t)}{dt} = \beta p(t - \Delta) - \alpha m(t), \quad \alpha = \ln \frac{2}{t_{1/2}}
\]

ODE model
Gene transcription and expression fits (Honkela et al., PNAS 2015)
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![Diagram](image)
Gene transcription and expression fits (Honkela et al., PNAS 2015)
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Inferring simulators from data

How to fit a model to data when no standard tools apply

- only indirect observations
- likelihoods intractable

**FCAI**

BOLFI: Gutmann & Corander 2016
Example: Probabilistic modelling in cosmology (Regier et al., ICML 2015)

Figure 1. An image from the Sloan Digital Sky Survey (SDSS, 2015) of a galaxy from the constellation Serpens, 100 million light years from Earth, along with several other galaxies and many stars from our own galaxy.
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Implementation: Probabilistic programming

- Probabilistic inference is hard
  - Typically expert derivations, coding & tuning are required for good results
  - Some easy-to-use frameworks exists, but often limited in scope
  - Almost all real applications require computational approximations
  - Non-trivial to judge if these are accurate enough
- Idea of probabilistic programming: user writes a description of the model, the machine takes care of the rest
- Cf. writing machine code in assembly language vs. high level code
- Key challenge: how to perform inference efficiently
- Emerging solutions: Stan, Edward, PyMC3, Pyro, ELFI, ...
parameters {
  simplex[K] theta[M];  // topic dist for doc m
  simplex[V] psi[K];    // word dist for topic k
}
model {
  for (m in 1:M)
    theta[m] ~ dirichlet(alpha);  // prior
  for (k in 1:K)
    psi[k] ~ dirichlet(beta);     // prior
  for (n in 1:N) {
    real gamma[K];
    for (k in 1:K)
      gamma[k] <- log(theta[doc[n],k]) + log(psi[k,w[n]]);   
      increment_log_prob(log_sum_exp(gamma));  // likelihood
  }
}
Conclusion

- Deep neural networks (most) useful for unstructured problems with massive data
- Probabilistic models allow incorporating structure such as known physics
- Likelihood-free inference can incorporate existing simulators
- Gaussian processes are a powerful tool for modelling latent functions
- Probabilistic programming big help for implementation

http://mc-stan.org  http://edwardlib.org