Machine Learning for Modelling Physical Systems

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4TU.AMI Models and Data in Digital Twins
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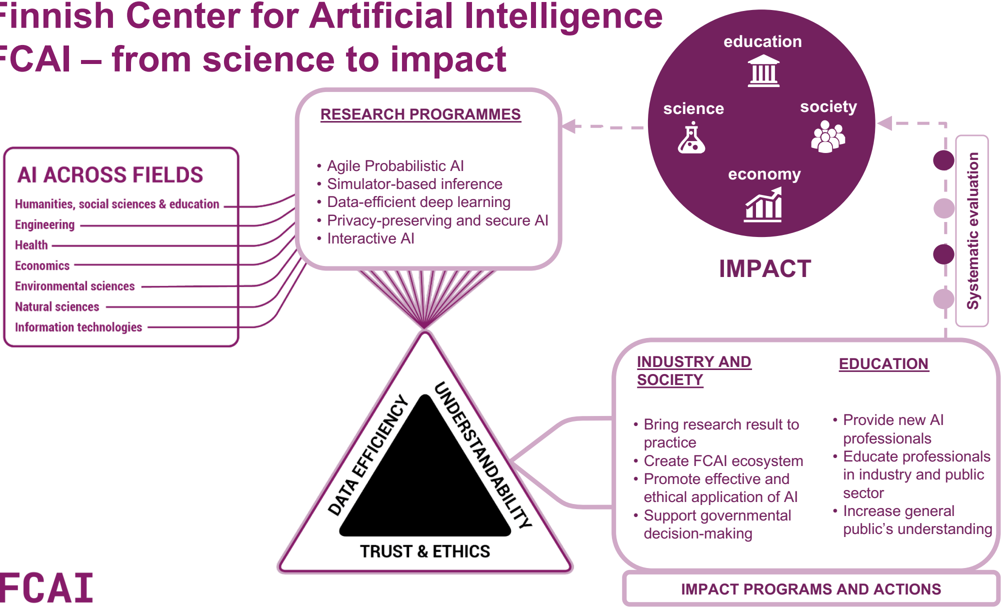
FCAI Finnish Center for Artificial Intelligence

Finnish Center for Artificial Intelligence FCAI – from science to impact



FCAI

Outline

Machine learning and AI overview

Learning for differential equations with probabilistic models

Other interesting probabilistic models

Probabilistic programming

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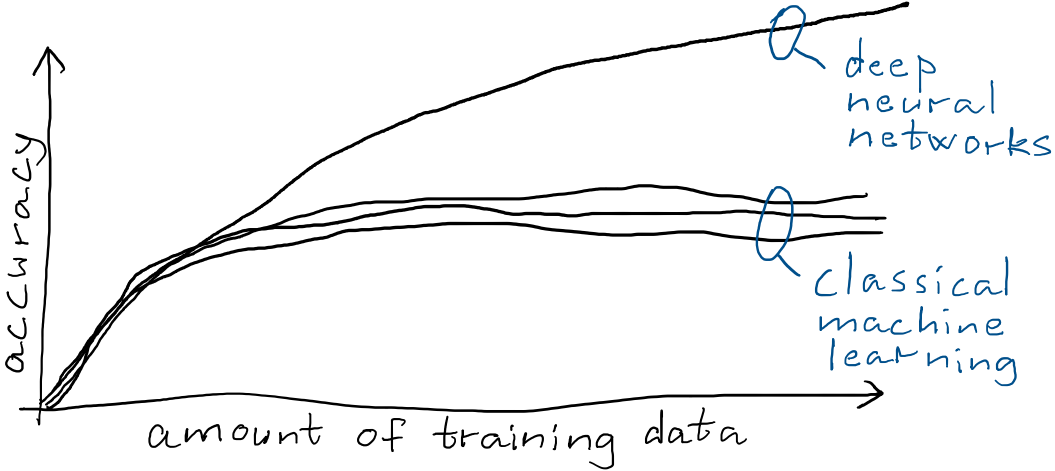
What is AI?

- 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: $(\text{state}, \text{observations}) \mapsto \text{actions}$
- Unsupervised learning
  - E.g. dimensionality reduction, generative modelling

Big data revolution in ML



Deep neural networks and data

- Most typical applications in *supervised learning*
  - Require annotated (input, target output) pairs
- Current methods need a lot of data
- 100000 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

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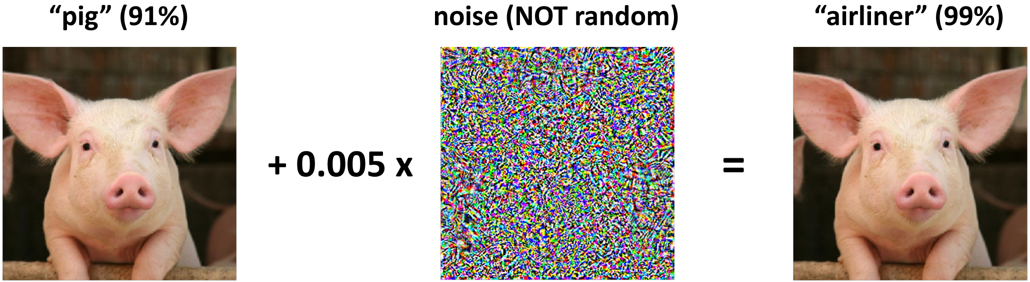

Szegedy et al. (arXiv:1312.6199) via https://adversarial-ml-tutorial.org/

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 θ and initial conditions x_0 in an ODE from noisy observations $Y = [y(t_1), \dots, y(t_n)]$, where

$$x'(t) = g(x(t), \theta), \quad x(0) = x_0$$
$$y(t_i) = x(t_i) + \eta_i$$

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

$$x'(t) = g(x(t), f(t), \theta), \quad x(0) = x_0$$
$$y(t_i) = x(t_i) + \eta_i$$

Modelling latent driving functions: Gaussian processes

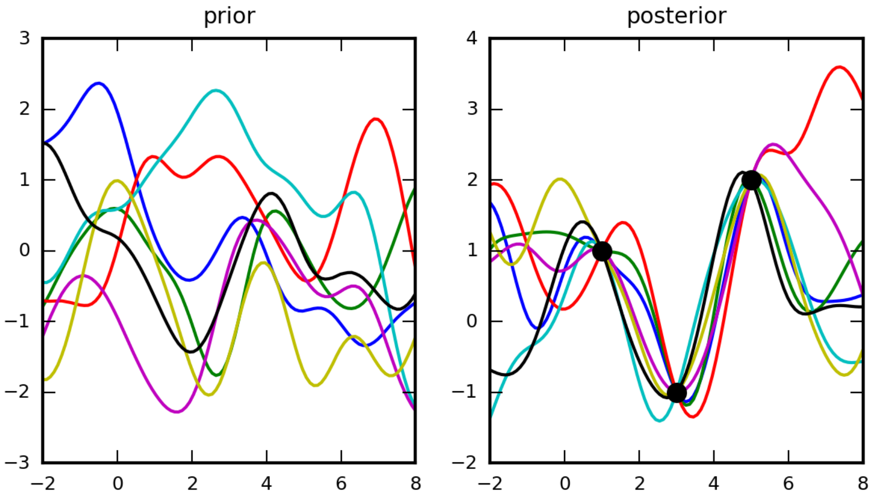
- Gaussian process priors on driving functions $f(t)$
  - Functional prior, specified by mean and covariance functions
  - No need for time discretisation
  - Can capture diverse activation profiles

$$f(t) \backsim \mathcal{GP}\left(\mu(t), k\left(t, t'\right)\right)$$

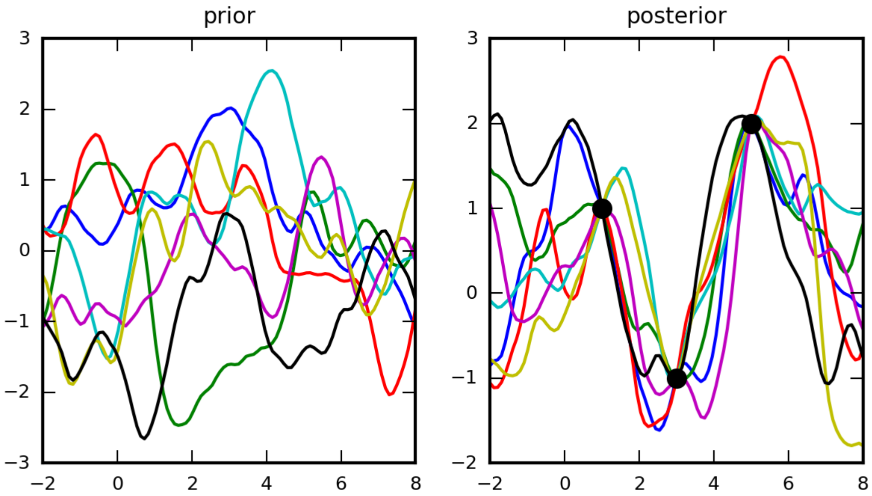
where

$$\begin{aligned}\mu(t) &= \mathbb{E}\left[f(t)\right] = \langle f(t) \rangle \\ k\left(t, t'\right) &= \mathbb{E}\left[\left(f(t) - \mu(t)\right)\left(f\left(t'\right) - \mu\left(t'\right)\right)\right]\end{aligned}$$

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

$$(Ax + b) \sim \mathcal{N}(A\mu + b, A\Sigma A^T)$$

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

$$\frac{\mathrm{d}\, x(t)}{\mathrm{d}\, t} = g(x(t), f(t), \theta)$$

  is an affine operator $x(t) = \mathcal{L}_g(f(t))$ 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 $k_{xx}(t, t')$?

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

- 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:

$$k_{ff}(t, t') = \alpha \exp\left(\frac{(t - t')^2}{2\ell^2}\right)$$

ODE Gaussian process applications I

- Single input motif gene regulation (Lawrence et al., NIPS 2006; Gao et al., Bioinformatics 2008):

$$\frac{\mathrm{d}\, x_i(t)}{\mathrm{d}\, t} = B_i + S_i f(t) - D_i x_i(t)$$

  - $x_i(t)$ 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):

$$\frac{\mathrm{d}\,p(t)}{\mathrm{d}\,t} = f(t) - \delta p(t)$$
$$\frac{\mathrm{d}\,x_i(t)}{\mathrm{d}\,t} = B_i + S_i p(t) - D_i x_i(t)$$

  - $x_i(t)$ target gene expression
  - $p(t)$ regulator activity
  - $f(t)$ regulator mRNA expression

ODE Gaussian process applications III

- Modelling transcription+expression (Honkela et al., PNAS 2015):

$$\frac{\mathrm{d}\, x(t)}{\mathrm{d}\, t} = B + Sf(t - \Delta) - Dx(t)$$

  - $x(t)$ gene expression
  - $f(t)$ transcriptional activity

Non-linear ODEs

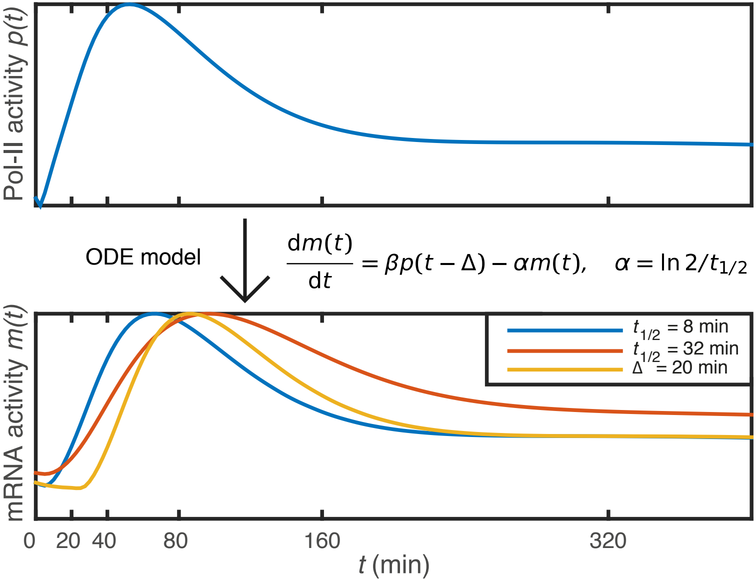
- If $\mathcal{L}_g$ is not affine, $x(t)$ will not follow Gaussian process
- Approximations still possible
- E.g. non-linear gene regulation model by Titsias et al. (BMC Systems Biology, 2012):

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

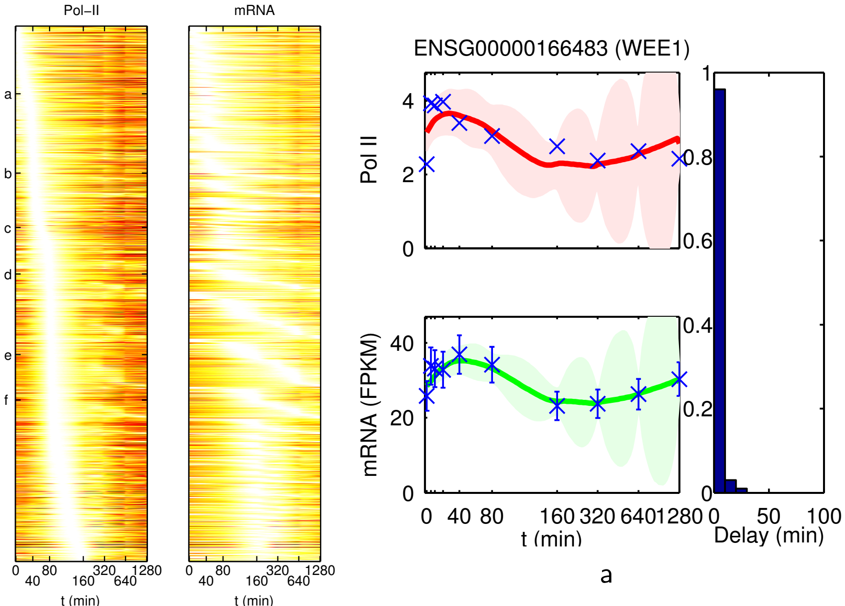
with

$$G(p_1(t), \ldots, p_I(t); \mathbf{w}_j, w_{j0}) = \frac{1}{1 + e^{-w_{j0} - \sum_{i=1}^{I} w_{ji} \log p_i(t)}}$$

Gene transcription and expression model (Honkela et al., PNAS 2015)



Gene transcription and expression fits (Honkela et al., PNAS 2015)



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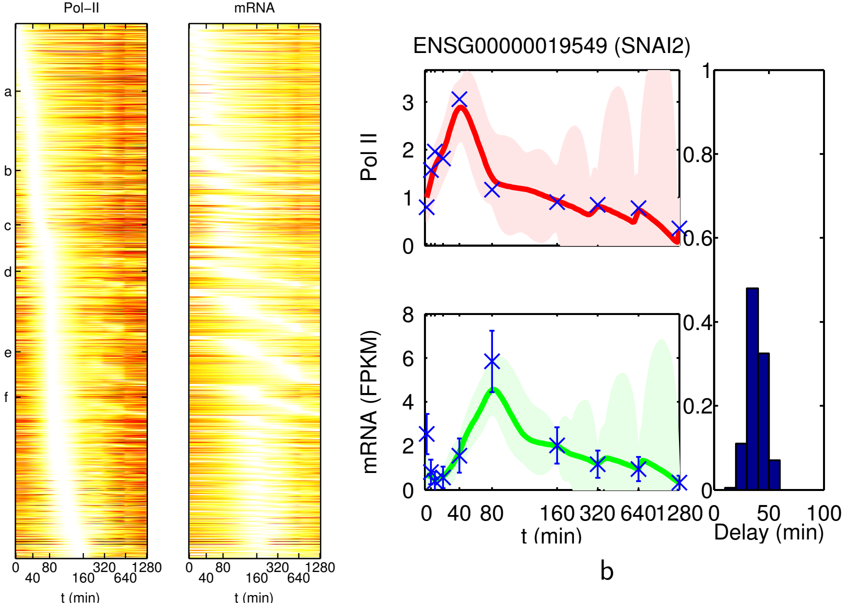

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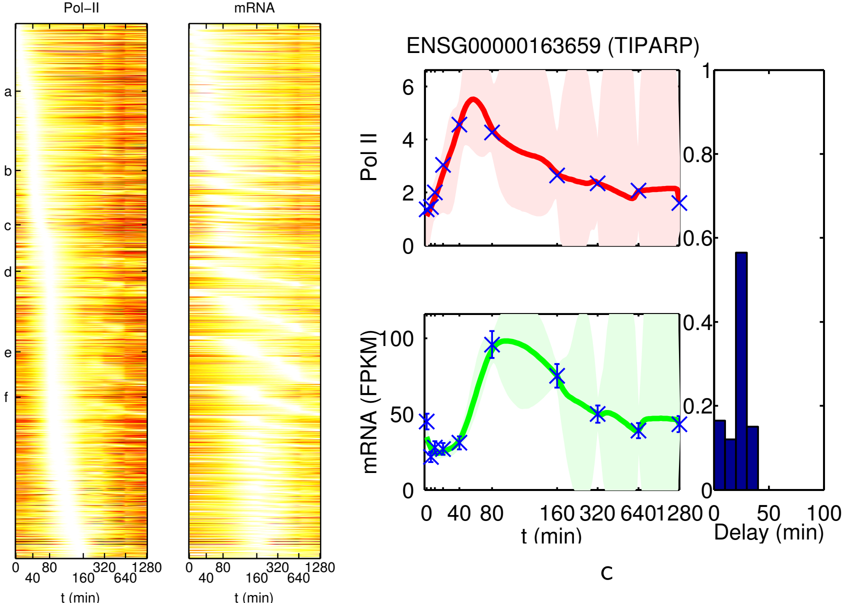

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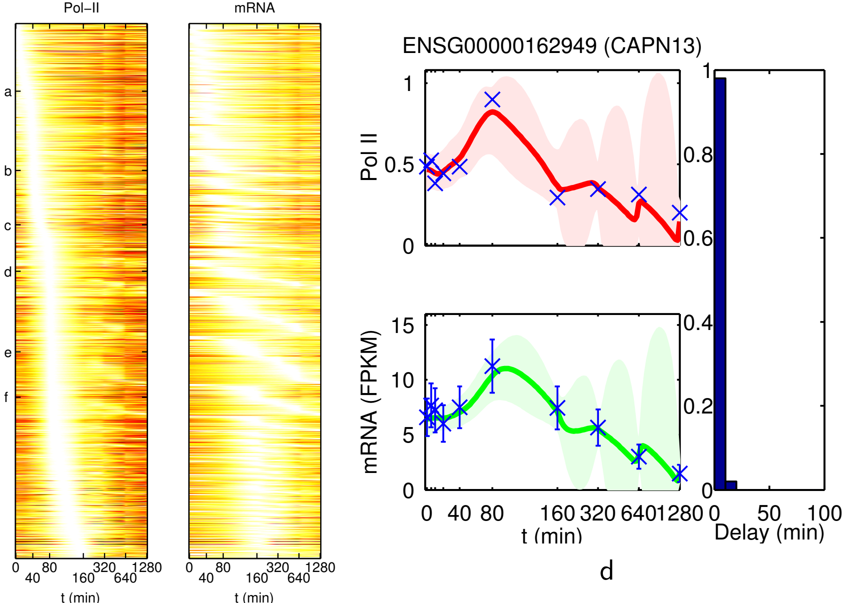

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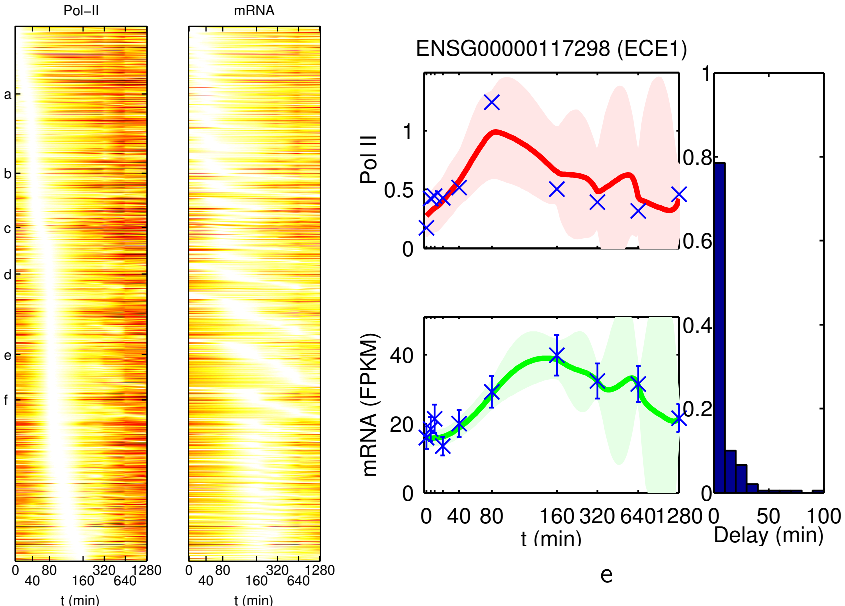

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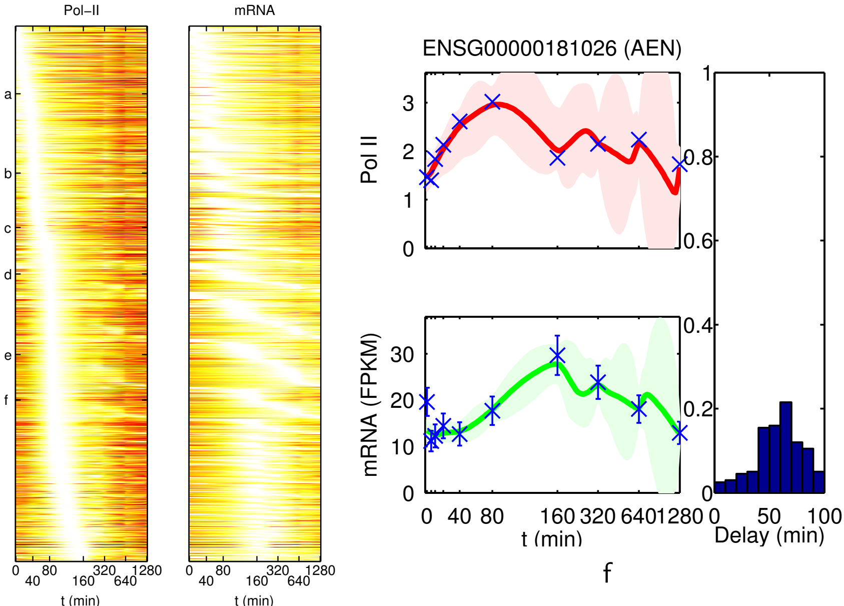

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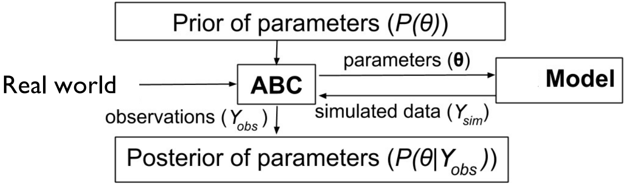
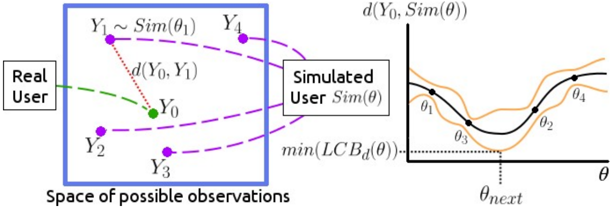
Inferring simulators from data

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

- only indirect observations
- likelihoods intractable

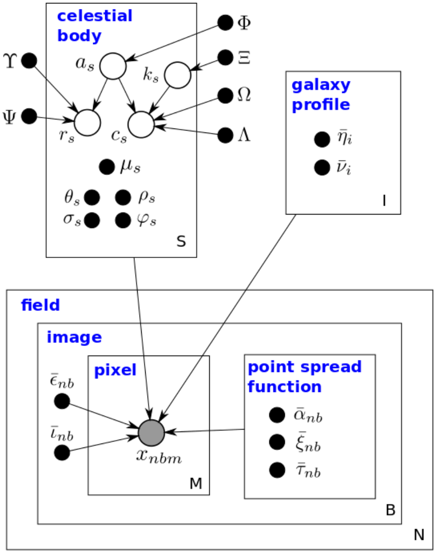




BOLFI: Gutmann & Corander 2016

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, ...

Probabilistic programming example (Carpenter et al., JASS 2016)

```
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

http://pyro.ai

http://gpflow.org

http://elfi.ai