Introduction

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Welcome!

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Outline

- Motivation
- A practical example
- Probabilistic programming
- Structure
  - Syllabus
  - Method
  - Requirements
  - Evaluation

Motivation - focus on the problem!

- Traditional machine learning
  - A very wide range of algorithms (k-Means, NN, SVM, PCA,...)
  - When faced with a new problem, map it onto one of the existing machine learning methods
  - **Focus is on algorithms**
- Model-based machine learning (MBML)
  - No need to learn about the huge range of traditional methods
  - When faced with a new problem, think about
    - the number and types of variables in the problem domain
    - which variables affect each other
    - what the effect of changing one variable is on another variable
    - encode that knowledge in the form of a model
  - **Focus is on the problem**
    - includes all the assumptions about the problem domain
    - highly tailored models for specific scenarios

MBML in a nutshell

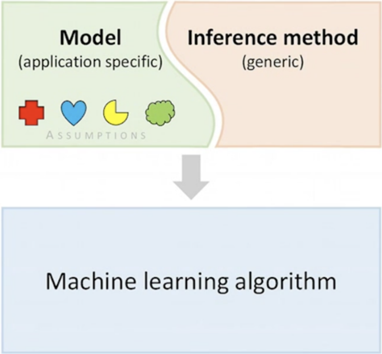

Figure: MBML big picture[1]

[1] In Christopher Bishop's Keynote, "Model-Based Machine Learning"
https://www.microsoft.com/en-us/research/video/keynote-model-based-machine-learning

Motivation - Why probabilistic models?

- **Uncertainty** in the real world
  - partial knowledge of state of the world
  - noisy observations
  - inherent stochasticity
- It is essential to account for uncertainty when building models of reality!
- **Probability theory** provides us with a consistent framework for quantifying and manipulating uncertainty

Motivation - A recent example...

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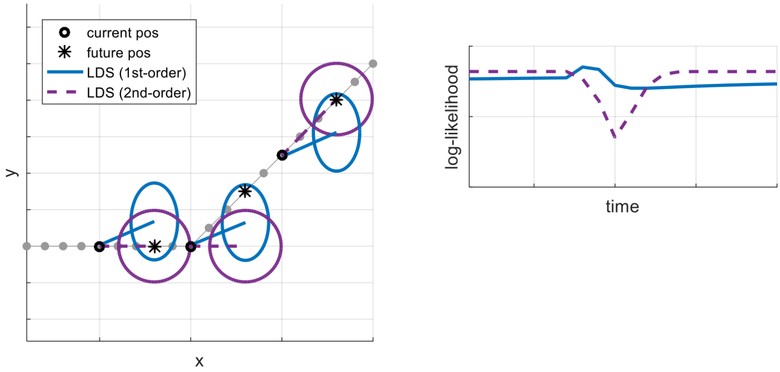
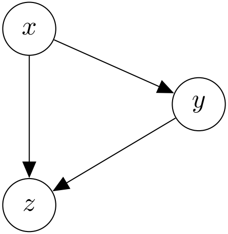


Figure: From Julian Kooij, TUDelft

Motivation - A recent example...

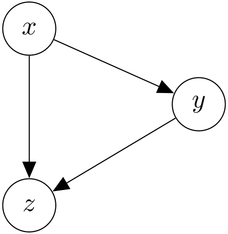
- Video

Motivation - Why probabilistic graphical models (PGMs)?



- **Nodes** - Represent random variables
- **Arrows** - Represent causal relationships

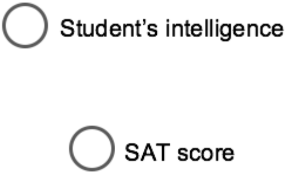
Motivation - Why probabilistic graphical models (PGMs)?



- Provide an **intuitive** and **compact** way of representing the structure of a probabilistic model
  - gives us insights about the properties of the model (e.g. relationships between variables, conditional independencies)
  - helps us communicate and design new models

A practical example

- A recruiter looking for the most intelligent students



A practical example

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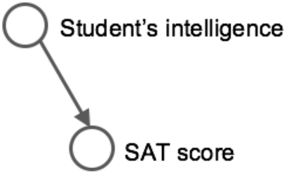

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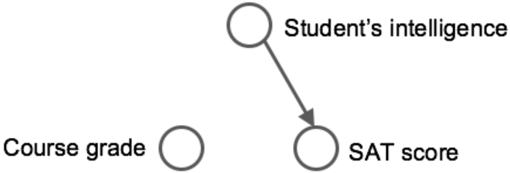

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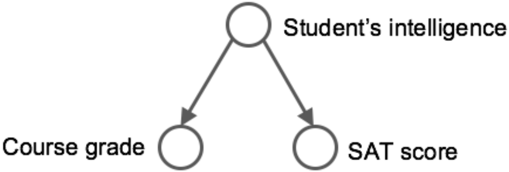

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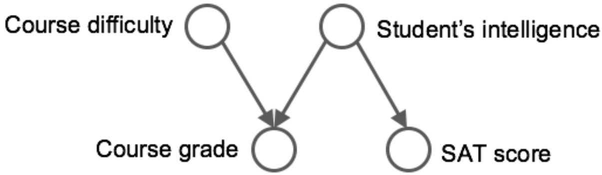

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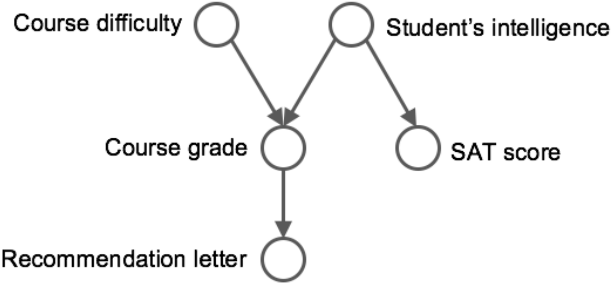

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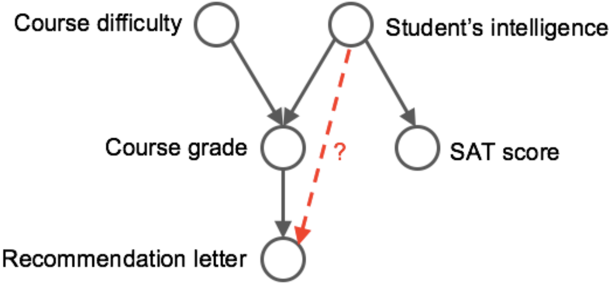

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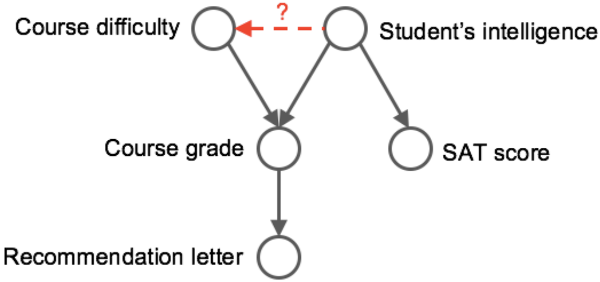

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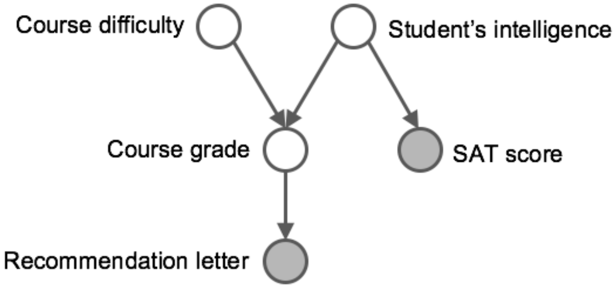


Playtime!

- Your first exercise!
- In pairs, build a graphical model that you think best represents this problem involving the following variables:
  - Climate change
  - GHG emissions
  - Energy demand
  - Earth's natural variability
  - Food supply
  - Population growth
  - Water quality
- Duration: 5 min.
- Exchange your graphical models between groups (and check if they are similar...)

A (familiar) example - Linear regression

- y - target (a.k.a. response or dependent variable)
- $\mathbf{x}$ - vector of explanatory variables
  (a.k.a. predictor or independent variables)
- Target y is assumed to be a function of $\mathbf{x}$

$$y = f(\mathbf{x})$$

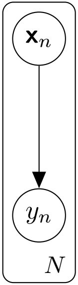
- Linear regression assumes f to be a **linear function** of $\mathbf{x}$

$$y = \boldsymbol{\beta}^T \mathbf{x} + \epsilon$$

- $\boldsymbol{\beta}$ is a vector of coefficients
- $\epsilon \sim \mathcal{N}(0, \sigma^2)$ is an error term (accounts for observation noise)

Linear regression

- Linear regression as a graphical model
  - We have a set of N observations of the targets y_n which depend on their corresponding explanatory variables $\mathbf{x}_n$



Linear regression

- Linear regression as a graphical model
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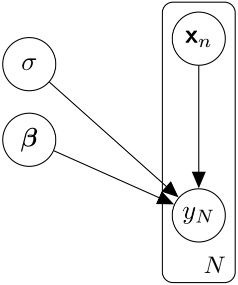
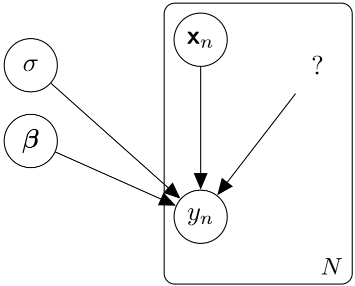


- We need to include parameters

Linear regression

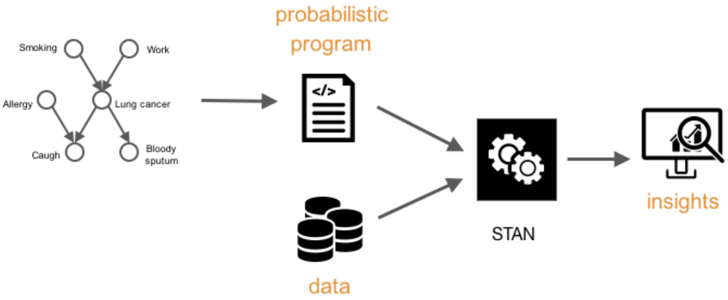
- Linear regression as a graphical model
  - We have a set of N observations of the targets y_n which depend on their corresponding explanatory variables $\mathbf{x}_n$



- In fact, we can even include other models (within our model)!

$$y = \boldsymbol{\beta_{lr}}^T \mathbf{x} + \boldsymbol{\beta_k} \textit{kernel\_model} + \boldsymbol{\beta_{dl}} \textit{deep\_learning\_model} \ldots$$

Probabilistic programming



- Popular probabilistic programming languages
  - **STAN** - we will use this throughout the course
  - **Pyro** - NEW! we will have Pyro versions of the notebooks (experimental)
  - PyMC3
  - Edward2

About STAN and Pyro

- **STAN** is a state-of-the-art platform for statistical modeling and high-performance statistical computation
- It allows for specification of a graphical model
- We will use STAN quite a bit in our course - you'll see it's pretty easy! :-)
- Check http://mc-stan.org

- **Pyro** is a universal probabilistic programming language written in Python and supported by PyTorch on the backend
- Pyro enables flexible and expressive deep probabilistic modeling
- Unifies the best of modern deep learning and Bayesian modeling
- Check https://pyro.ai

Example with Linear Regression

- Linear Regression with STAN:

```
model="""
data {
    int<lower=0> N; // data points
    vector[N] x;    // independent variable
    vector[N] y;    // depedent variables
}

parameters {
    real beta0;             // intercept
    real beta1;             // coefficient of x
    real<lower=0> sigma;    // observation noise parameter
}

model {
    y ~ normal(beta0 + beta1*x, sigma);
}
"""
```

- Linear Regression with Pyro:

```
def model(x, y):
    beta0 = pyro.sample("beta0", dist.Normal(0., 1.))   // intercept
    beta1 = pyro.sample("beta1", dist.Normal(0., 1.))   // coefficient of x
    sigma = pyro.sample("sigma", dist.Uniform(0., 10.)) // observation noise
    with pyro.plate("data", N):
        pyro.sample("obs", dist.Normal(beta0 + beta1*x, sigma), obs=y)
```

Example with Linear Regression

- Running inference in Python+STAN:

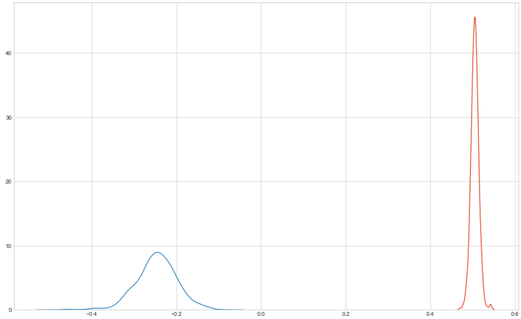
```
data_dict = {'N': N,
             'x': x,
             'y': y}

sm = pystan.StanModel(model_code=model)
fit = sm.sampling(data=data_dict, iter=1000, chains=4)
print(fit)
```

- Running inference in Pyro:

```
from pyro.infer import MCMC, NUTS
nuts_kernel = NUTS(model)
mcmc = MCMC(nuts_kernel, num_samples=1000, warmup_steps=200)
mcmc.run(x, y)
```

Example with Linear Regression

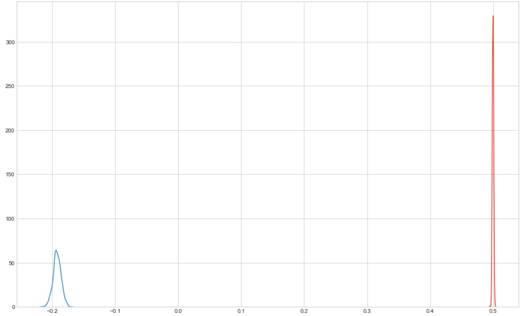
- Running inference... (N=10)



	mean
beta1	0.51
beta0	-0.25
sigma	0.1

Example with Linear Regression

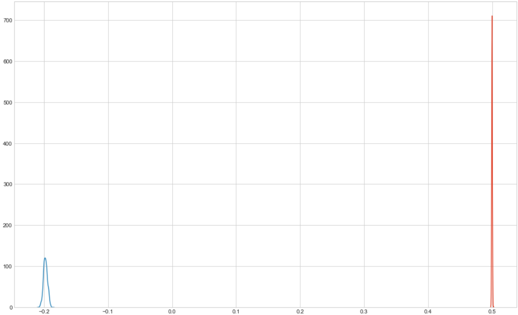
- Running inference... (N=200)



	mean
beta1	0.5
beta0	-0.19
sigma	0.1

Example with Linear Regression

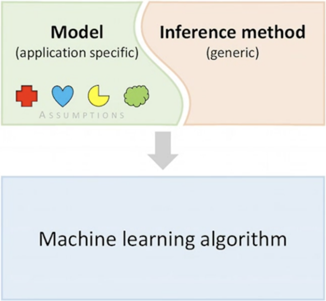
- Running inference... (N=1000)



	mean
beta1	0.5
beta0	-0.2
sigma	0.1

Course structure

- 3 main blocks:
  - Foundations of probabilistic graphical models (PGMs) and probabilistic programming - 4 lectures
  - Probabilistic modelling in various contexts (with practical examples of popular models) - 5 lectures
  - Bayesian inference (exact and approximate) - 3 lectures
- These are the key ingredients of MBML!



Syllabus: Lectures

1. Intro to MBML + probability and statistics review (F. Pereira)
2. PGM foundations 1 (F. Pereira)
3. PGM foundations 2 + Mixture models (F. Pereira)
4. Frequentist vs Bayesian + Prob. Programming (F. Rodrigues)
5. Regression models (F. Rodrigues)
6. Classification models (F. Rodrigues)
7. Temporal models (F. Rodrigues)
8. Topic models (F. Rodrigues)
9. Exact inference (F. Rodrigues)
10. Markov-chain Monte Carlo (F. Rodrigues)
11. Variational inference (F. Rodrigues)
12. Gaussian processes (F. Rodrigues)

What we expect you to get out of this course

- In-depth understanding of Probabilistic Graphical Models and the Bayesian framework
    - Easily understand new models (e.g. by relating them with others)
    - New unifying perspective to models that you already know
    - Exploit your domain knowledge to build new models
    - Break out of the suite of the standard ML algorithms
- Good knowledge of a broad class of probabilistic modelling approaches
    - Modelling ideas that you can "re-use"
    - Great starting point when tackling a new problem
- Experience with a state-of-the-art probabilistic programming language
    - Easily specify a model and run inference on it
    - Flexibility to try new ideas/variants
- Excitement about MBML and its application to solve real-world problems :-)

What we DON'T expect from you

- To know in detail every single topic mentioned
  - Curriculum is large, but we try to be reasonable!
  - Many lectures could be the topic of an entire course
  - Some topics we require that you know in depth
  - Other topics we will just cover at the conceptual level and provide pointers to where to learn more

Method

- Interleaved blocks of theory and practice
  - Theory: slides
  - Practice: Jupyter notebooks; Python and STAN/Pyro

Requirements

- Programming is important (preferably Python)
- Confident knowledge about basic statistics and probability
- Creativity and domain knowledge

Evaluation

- 2 Tests (approx. 1h duration; with aid), 25% each (March 20, May 12)
- Project, 50% (deadline: TBD)