TUTORIAL I

Liesel Devs

WELCOME

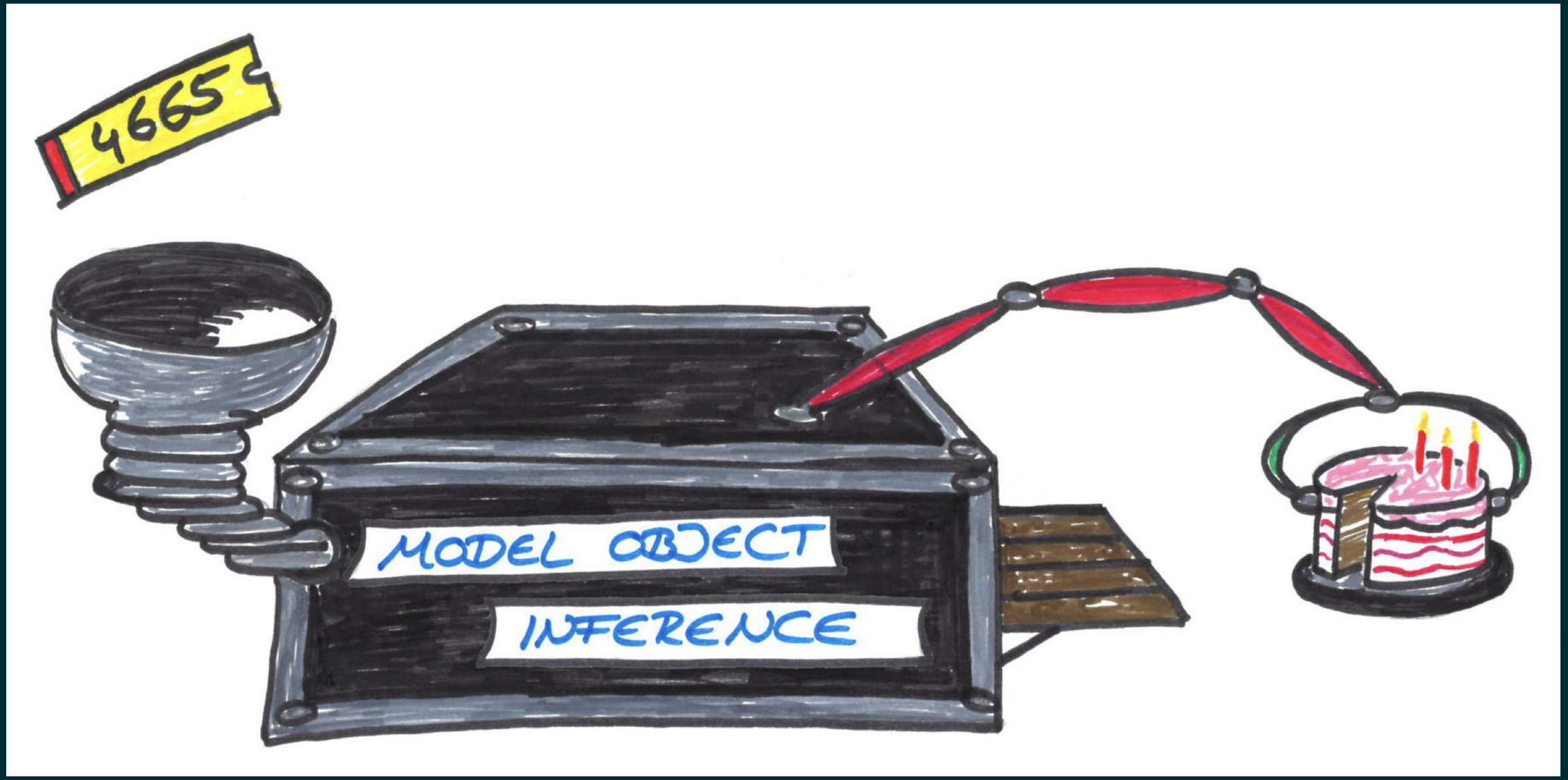
AGENDA

- In the tutorial, you will gain some hand-on experience working on Bayesian models with Liesel
- We start simple and will make our way to Bayesian distributional regression
- Some tutorials have small lecture-like parts where we introduce some software / concepts
- In all tutorials, we will give you exercise sheets with tasks you can work on in the class
- We will actively support you

WHAT IS LIESEL?

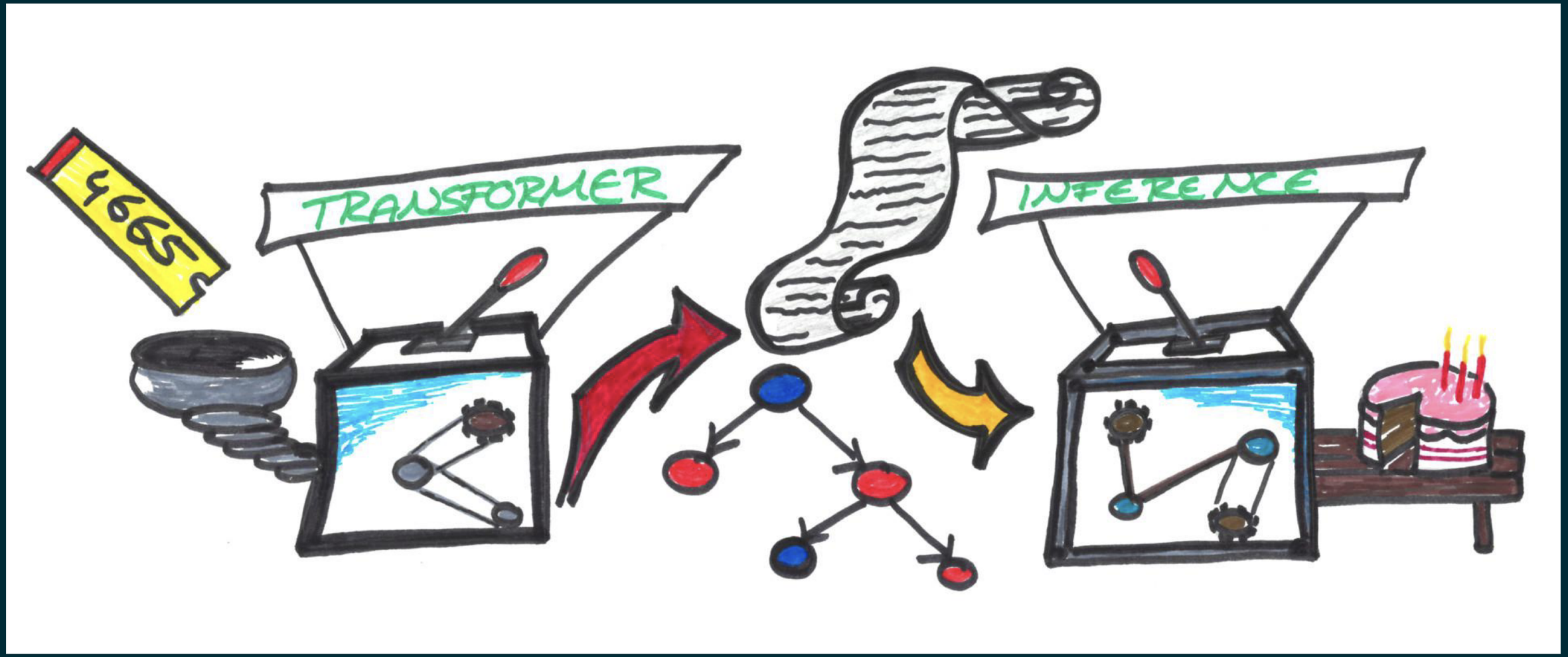
Wait for it.

A LOT OF STATISTICAL SOFTWARE WORKS LIKE THIS...



blackbox

...BUT LIESEL TRIES TO BE LIKE THIS

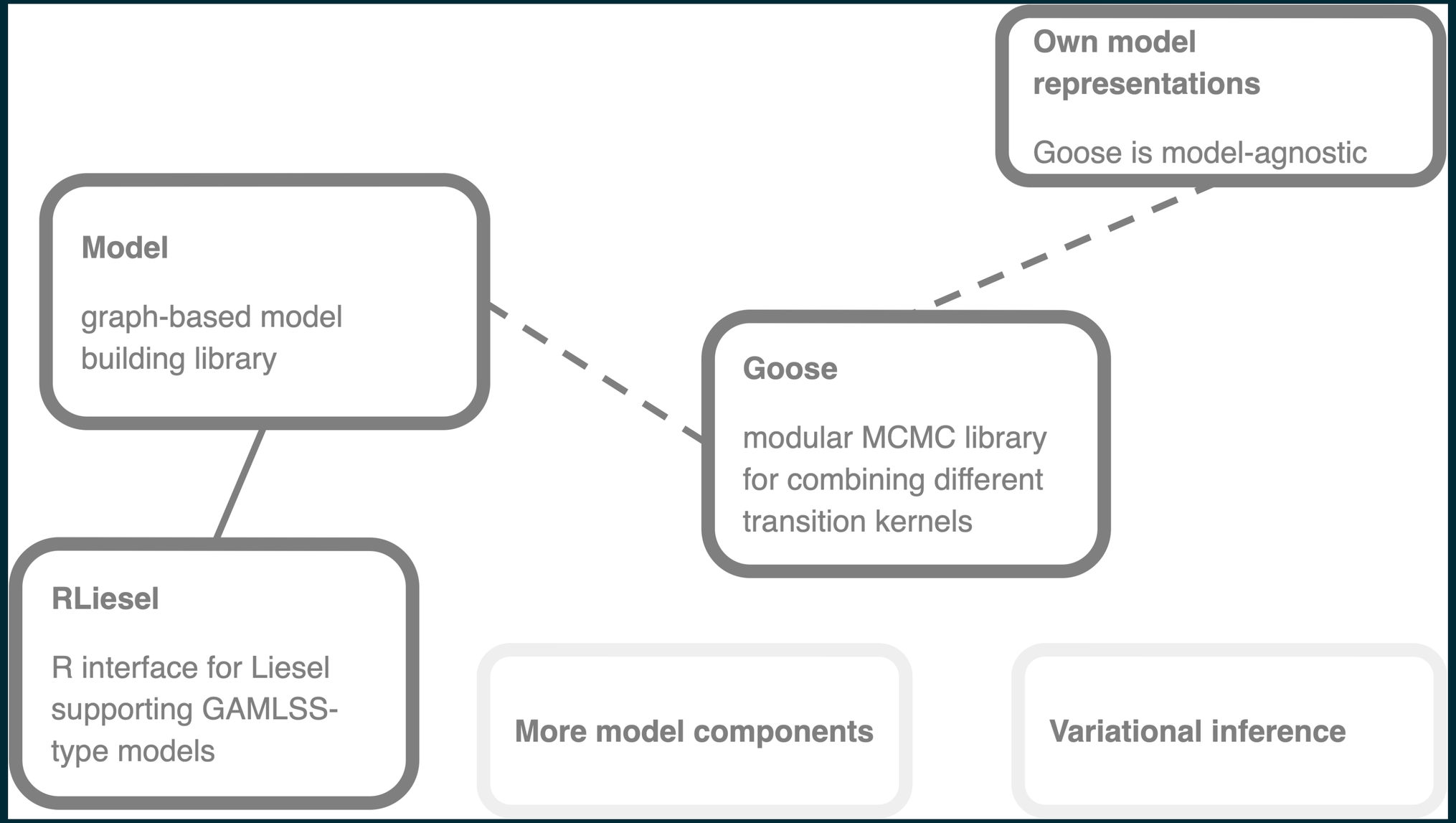


lieselbox

WHAT IS LIESEL?

- Liesel is a software framework for research on semi-parametric regression models and Bayesian inference.
- Liesel aims to provide
  - easy modeling
    with full programmatic access to manipulate the model
  - an easy way to set up an MCMC sampler
    and the building blocks to tailor the inference algorithm for your problem
  - extensible
  - well-tested
- Liesel builds on good software.
- Liesel uses modern tools.
- Liesel is partially funded by the German Research Foundation (DFG) since April 2022 ❤️

WHAT IS LIESEL?



components

WHAT IS LIESEL?

- a Python package with an R interface
- based on the *JAX* machine learning library…
  - automatic differentiation
  - vectorization & parallelization
  - just-in-time compilation
  - CUDA support
- …and BlackJAX
  - Goose wraps their HMC & NUTS algorithms (kernels)

WHY NOT X?

X does not mean Twitter!

STAN

- great probabilistic programming language which allows the user to specify their models
- models are compiled, cannot be examined with a REPL
- inference not as flexible, strong focus on MCMC with NUTS
  - models sometimes need to be re-parameterized to be sampled efficiently
  - no discrete parameters / no Gibbs sampling
- use them if they fit your problem

GAMLSS / BAMLSS / MGCV

DEVELOPERS

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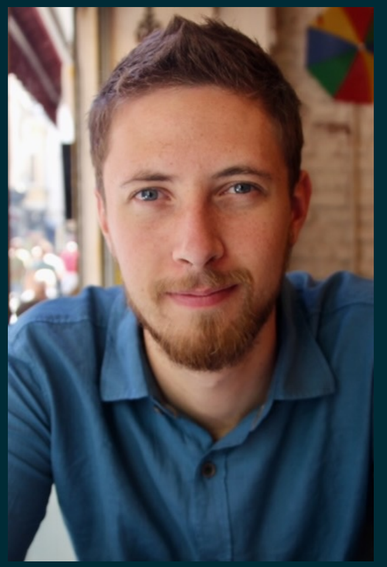


Johannes Brachem
University of Göttingen

JAX

INTRODUCTION TO JAX

- a library for numerical computing in Python
- the design follows numpy very closely
  - JAX uses the same concept of multi-dimensional arrays
  - JAX provides high-level mathematical functions Operating on those arrays
  - many functions have the same names and arguments as in numpy
  - sometimes there are subtle differences
- focused on performance and automatic differentiation
- developed by Google for machine learning

```
1 import jax
2 import jax.numpy as jnp
```

KEY CONCEPTS

- functional programming paradigm
- transformable functions
- auto-vectorization and jit compilation
- automatic differentiation

FUNCTIONAL PROGRAMMING PARADIGM

- functions need to be pure
- the output depends only on the input
- does not change the state of the world

EXAMPLE

```
1  def pure(a, b):
2      return a + b
3
4
5  b = 2
6  def non_pure(a):
7      launch_rockets()  # changes state of the world
8      return a + b      # depends on state of the world
```

...

ADVANTAGE

- pure functions are easier to reason about; for humans and compilers.
- enables jit, automatic differentiation, and more

AUTOMATIC DIFFERENTIATION

A technique to algorithmicly determine the partial derivatives of a function $\mathrm{f} : \mathbb{R}^{\mathrm{M}} \to \mathbb{R}^{\mathrm{N}}$.

- two types:
  - forward mode. More effective when $\mathrm{M} < \mathrm{N}$
  - reverse mode. More effective when $\mathrm{M} > \mathrm{N}$
  - in stats and ML, we usually have $\mathrm{N} = 1$, e.g., loss function, log-likelihood, log unnormalized posterior and a potentially large M
  - for $\mathrm{N} = 1$, reverse mode can evaluate $\nabla \mathrm{f}(\mathrm{x})$ in the same time as $\mathrm{f}(\mathrm{x})$ (up to a constant) but needs more memory
- `jax.grad` takes a scalar-valued function f as argument and calculates $\nabla \mathrm{f}$ using the reverse mode.

```
1 def ll_poisson(lambda_, x):
2     t0 = x * jnp.log(lambda_) - lambda_
3     t1 = -jax.scipy.special.gammaln(x + 1) # \Gamma(x) = (x - 1)!
4     return t0 + t1
5
6 dll_poisson = jax.grad(ll_poisson, argnums = 0)
7 dll_poisson(1.0, 2)
```

```
Array(1., dtype=float32, weak_type=True)
```

SECOND ORDER DERIVATIVES

We can chain the transformations, for example, to get the second order derivative.

```
1 ddll_poisson = jax.grad(dll_poisson, argnums = 0)
2 ddll_poisson(1.0, 2)
```

```
Array(-2., dtype=float32, weak_type=True)
```

or we use the function `jax.hessian` (recommended) to calculate the Hessian matrix of f.

```
1 hll_poisson = jax.hessian(ll_poisson, argnums = 0)
2 hll_poisson(1.0, 2)
```

```
Array(-2., dtype=float32, weak_type=True)
```

For details and pretty advanced details you might want to refer to the documentation:

- Taking derivatives with `grad`
- Advanced Automatic Differentiation in JAX
- The Autodiff Cookbook
- API Reference `jax.grad`

JIT - JUST IN TIME COMPILATION

- JAX can compile function such that recurrent calls are faster.
- this is done with the function transformation `jax.jit`

```
jll_poisson = jax.jit(ll_poisson)
jdll_poisson = jax.jit(dll_poisson)

@jax.jit
def my_func(a):
    return a + 1.0

jll_poisson(1.0, 2)
```

```
Array(-1.6931474, dtype=float32, weak_type=True)
```

MORE TRANSFORMATIONS

VMAP

- use vmap to vectorize a function
- $\mathrm{f} : \mathbb{R} \to \mathbb{R}$
- $\mathrm{g} : \mathbb{R}^N \to \mathbb{R}^N$ with $\mathrm{g}(\boldsymbol{x}) = (\mathrm{f}(\mathrm{x}_1), \ldots, \mathrm{f}(\mathrm{x}_N))^T$
- instead of looping over f, `vmap` pushes the vectorization to the primitive operations for performance reasons
- no need to carry a batch dimension on all operations

PMAP

SPMD - Single Programm Multiple Data

Lifts a jax programm to accelerators like GPUs which can enable faster computation

JAX HAS SHARP BITS

- there are some sharp bits - most of them are (easily) avoidable
- however, this requires adaptation

MOST NOTABLY

- constraints on python's control flow statements in jitted functions
  - for example, `if` does not work
  - however, there are alternatives `jax.lax.cond(cond, f_true, f_false)`
  - this is also true for loops, `for`, `while` have counterparts in `jax.lax`
- by default, single precision instead of double precision
- random numbers work differently
  - JAX uses pure functions, thus there is no global state
  - ⟶ The state of the Pseudo random number generator (PRNG) needs to be passed
- refer to the JAX' documentation The Sharp Bits

EXTENDED EXAMPLE

One parameter Poisson model

EXTENDED EXAMPLE

Consider 5 iid observations of $Y \sim \text{Poi}(\lambda)$, $y_1 = 3, y_2 = 4, y_3 = 4, y_4 = 6, y_5 = 3$. We place a prior on λ, namely $\lambda \sim \text{Gamma}(1, 1)$. The goal is to estimate the posterior mode of λ. The posterior mode is defined as the parameter value that maximises the posterior density.

STEPS:

IMPLEMENTATION STEPS

1. implement the log-likelihood for one observation
2. use vmap to transform the log likelihood into a vectorized function
3. implement the log prior
4. implement the log unnormalized posterior
5. implement the optimization loop

IMPLEMENT THE LOG LIKELIHOOD

The probability mass function of a Poisson distribution random variable Y with rate parameter $\lambda > 0$ is

$$\Pr(Y = y|\lambda) = \frac{\lambda^y e^{-\lambda}}{x!}$$

```
1 def ll_poisson(x, lambda_):
2     t0 = x * jnp.log(lambda_) - lambda_
3     t1 = -jax.scipy.special.gammaln(x + 1) # \Gamma(x) = (x - 1)!
4     return t0 + t1
5
6 ll_vec = jax.vmap(ll_poisson, (0, None)) # map along the first axis of the first argument, do not map over the second argument
```

Comment: Many jax functions are already vectorized. We would not need to use `vmap` here.

ALTERNATIVE

There are different libraries that implement jax compatible distributions. Tensorflow probability is one of them.

```
1 import tensorflow_probability.substrates.jax as tfp
2
3 def ll_vec2(x, lambda_):
4     dist = tfp.distributions.Poisson(lambda_)
5     lps = dist.log_prob(x)
6     return lps
7
8 print(ll_vec(jnp.array([1, 2]), 1.5))
```

```
[-1.0945349 -1.3822172]
```

```
1 print(ll_vec2(jnp.array([1, 2]), 1.5))
```

```
[-1.0945349 -1.3822172]
```

IMPLEMENT THE LOG PRIOR

$$\lambda \sim \text{Gamma}(1, 1)$$

```python
import tensorflow_probability.substrates.jax.distributions as tfd

def log_prior(lambda_):
    dist = tfd.Gamma(1, 1)
    return dist.log_prob(lambda_)
```

and now in terms of ψ

```python
def log_prior_psi(psi):
    lambda_ = jnp.exp(psi)
    lp = log_prior(lambda_)
    cov_cor = psi
    return lp + cov_cor
```

IMPLEMENT THE LOG POSTERIOR (UNNORMALIZED)

```
@jax.jit
def log_upost(ys, psi):
    lambda_ = jnp.exp(psi)
    ll = ll_vec(ys, lambda_).sum()
    lprior = log_prior_psi(psi)

    return ll + lprior
```

NEWTON'S METHOD

Algorithm:

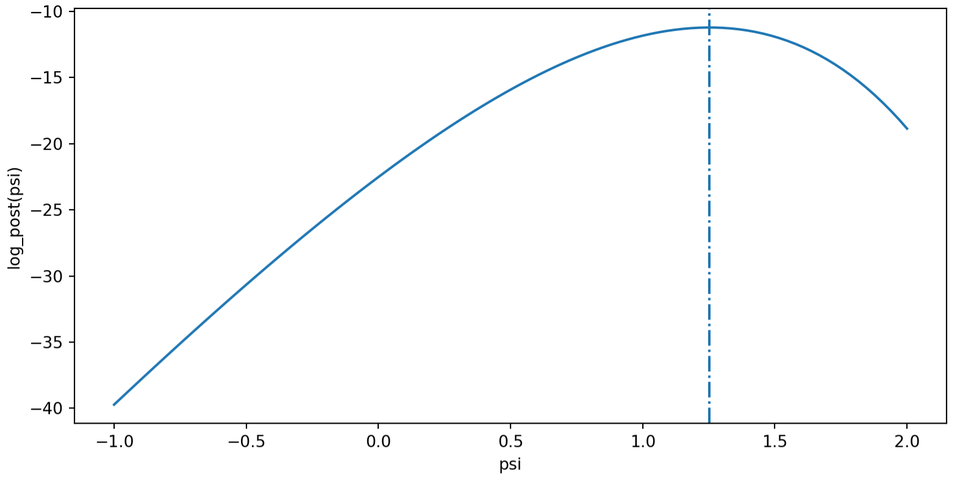
- Choose ψ^0.
- For $t = 1, \ldots, 10$ do (or until convergence)

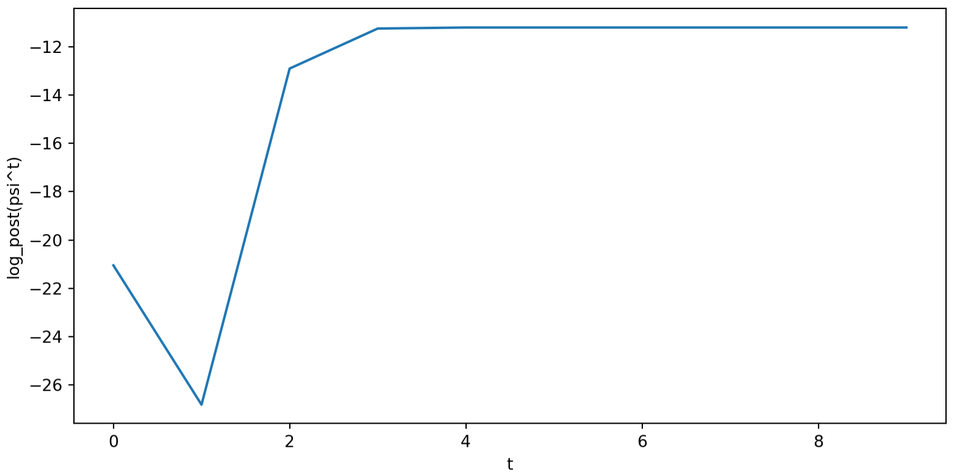
$$\psi^{t+1} = \psi^t - \frac{p'(\psi|y)}{p''(\psi|y)}$$

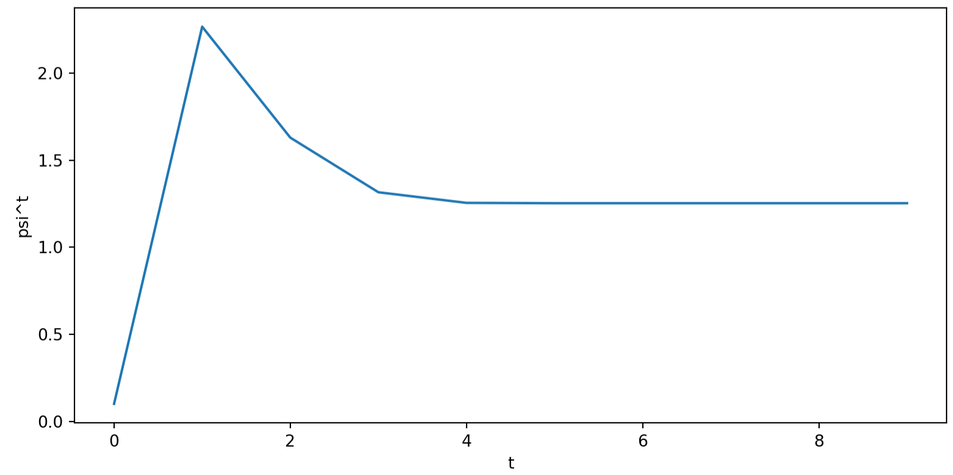
IMPLEMENTATION

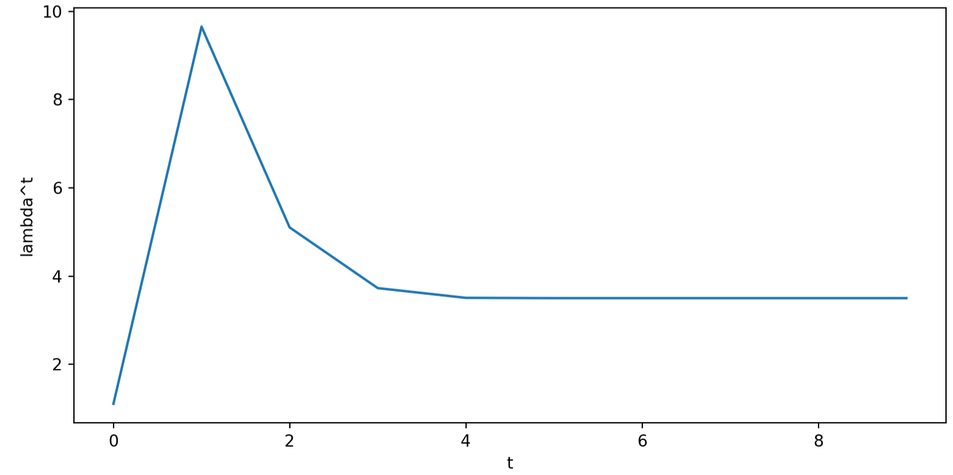
```
 1 ys = jnp.array([3, 4, 4, 6, 3])
 2 dlp = jax.grad(log_upost, argnums=1)
 3 ddlp = jax.hessian(log_upost, argnums=1)
 4
 5 jdlp = jax.jit(dlp)
 6 jddlp = jax.jit(ddlp)
 7
 8 psis = []
 9 lambdas = []
10 log_uposts = []
11
12 psi = 0.1
13 for i in range(10):
14     psis.append(psi)
15     lambdas.append(jnp.exp(psi))
16     log_uposts.append(log_upost(ys, psi))
17     psi = psi - jdlp(ys, psi) / jddlp(ys, psi)
```

PLOT


log_post(psi)
psi
−10
−15
−20
−25
−30
−35
−40
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


log_post(psi^t)
t
−12
−14
−16
−18
−20
−22
−24
−26
0
2
4
6
8


psi^t
t
2.0
1.5
1.0
0.5
0.0
0
2
4
6
8


lambda^t
t
10
8
6
4
2
0
2
4
6
8

CODE TO CREATE THE PLOTS

```python
import matplotlib.pyplot as plt

psi_grid = jnp.linspace(-1, 2, 100)
l_upost_grid = []
for psi in psi_grid:
    l_upost_grid.append(log_upost(ys, psi))

fig, axs = plt.subplots(2, 2)
axs[0][0].plot(psi_grid, l_upost_grid)
axs[0][0].set_xlabel("psi")
axs[0][0].set_ylabel("log_post(psi)")
axs[0][0].axvline(psis[-1], linestyle='-.')

axs[0][1].plot(log_uposts)
axs[0][1].set_xlabel("t")
axs[0][1].set_ylabel("log_post(psi^t)")

axs[1][0].plot(psis)
```

EXERCISE SHEET

Please start working on the exercise sheet