Programming in Python[1]

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Lecture XXII: Probabilistic programming

How science works

Describing one single "scientific method" is problematic, but a schema many will accept is:

1. Imagine a hypothesis
2. Design (mathematical/convenient) models consistent with the hypothesis
3. Collect experimental data
4. Discuss the fitness of data given the models

It is worth noting that the falsification of models is not *automatically* a rejection of hypotheses (and, more obviously, neither a validation).

The role of Bayes Theorem

In this discussion, a useful relationship between data and models is Bayes Theorem.

$$P(M, D) = P(M|D) \cdot P(D) = P(D|M) \cdot P(M)$$

Therefore:

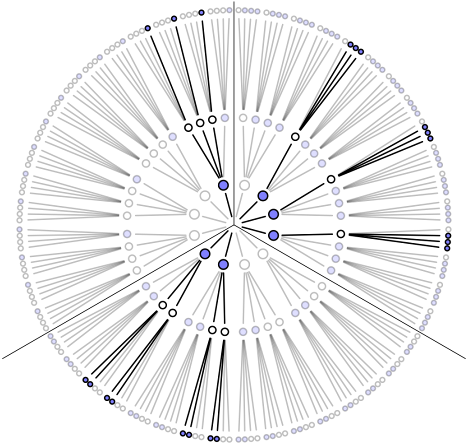
$$P(M|D) = \frac{P(D|M) \cdot P(M)}{P(D)}$$

The plausibility of the model given some observed data, is proportional to the number of ways data can be *produced* by the model and the prior plausibility of the model itself.

Simple example

- Model: a bag with 4 balls in 2 colors `B/W` (but we don't know which of `BBBB`, `BBBW`, `BBWW`, `BWWW`, `WWWW`)
- Observed: `BWB`
- Which is the plausibility of `BBBB`, `BBBW`, `BBWW`, `BWWW`, `WWWW`?

Bayes Theorem is counting



Picture from: R. McElreath, Statistical Rethinking

A computational approach

This Bayesian strategy is (conceptually) easy to transform in a computational process.

1. Code the models
2. Run the models
3. Compute the plausibility of the models based on observed data

Classical binomial example

- Which is the proportion p of water covering Earth? The models are indexed by the float $0 < p < 1$
- Given p, the probability of observing some W,L in a series of independent random observations is: $P(W, L|p) = \frac{(W+L)!}{W!\cdot L!}p^W \cdot (1-p)^L$ (binomial distribution).
- Do we have an initial (prior) idea?
- Make observations, apply Bayes, update prior!

A conventional way of expressing the model

$$\begin{aligned} W &\sim \mathit{Binomial}(W + L, p) \\ p &\sim \mathit{Uniform}(0, 1) \end{aligned}$$

Probabilistic programming is systematic way of coding this kind of models, combining predefined statistical distributions and Monte Carlo methods for computing the posterior plausibility of parameters.

In principle you can do it by hand


```
def dbinom(success: int, size: int, prob: float) -> float:
    fail = size - success
    return np.math.factorial(size)/(np.math.factorial(success)*np.math.factorial(fail))*p
    ↪ rob**success*(1-prob)**(fail)
```

```
W, L = 7, 3
p_grid = np.linspace(start=0, stop=1, num=20)
prior = np.ones(20)/20

likelihood = dbinom(W, n=W+L, p=p_grid)

unstd_posterior = likelihood * prior

posterior = unstd_posterior / unstd_posterior.sum()
```

Unfeasible with many variables!

PyMC

```
import pymc as pm

W, L = 7, 3
earth = pm.Model()
with earth:
    p = pm.Uniform("p", 0, 1)  # uniform prior
    w = pm.Binomial("w", n=W+L, p=p, observed=W)
    posterior =  pm.sample(2000)

posterior['p']
```

Behind pymc3

The probabilistic programming approach of `pymc3` is built on two “technologies”:

1. A library that mixes numerical and symbolic computations (Theano, soon becoming Aesara)
2. Markov Chain Monte-Carlo (MCMC) algorithms to estimate posterior densities

Theano

It bounds numerical computations to its symbolic structure ("graph")

```
import theano
from theano import tensor

a = tensor.dscalar('alpha')
b = tensor.dscalar('beta')

c = a + b**2

f = theano.function([a,b], c)

assert f(1.5, 2) == 5.5
```

Symbolic manipulations

Variables can be used to compute values, but also symbolic manipulations.

```
d = tensor.grad(c, b)

f_prime = theano.function([a, b], d)

assert f_prime(1.5, 2) == 4.
```

Note you still need to give an a because the symbolic structure needs it.

Markov Chain Monte-Carlo

It's way of estimating (relative) populations of "contiguous" states.

- It needs the capacity of evaluate the population/magnitude of any two close states (but a global knowledge of all the states *at the same time*)
- It's useful to estimate *posterior* distribution *without explicitly computing* $P(D)$: $P(M|D) = \frac{P(D|M) \cdot P(M)}{P(D)}$

Metropolis

The easiest MCMC approach is the so-called Metropolis algorithm (in fact appeared as Metropolis, N., **Rosenbluth, A., Rosenbluth, M.**, Teller, A., and Teller, E., 1953)

```
steps = 100000
positions = np.zeros(steps)
populations = [1,2,3,4,5,6,7,8,9,10]
current = 3

for i in range(steps):
    positions[i] = current
    proposal = (current + np.random.choice([-1,1])) %
    ↪  len(populations)
    prob_move = populations[proposal] /
    ↪  populations[current]
    if np.random.uniform(0, 1) < prob_move:
        current = proposal
```

Convergence

Eventual convergence is guaranteed, but it can be painful slow (and you dont't know if you are there...). Many algorithms try to improve: Gibbs, Hamiltonian-MC, NUTS...

Putting them together

```
import pymc3 as pm

linear_regression = pm.Model()

with linear_regression:
    # Theano variables
    sigma = pm.Uniform('sigma_h', 0, 50)
    alpha = pm.Normal('alpha', 178, 20)
    beta = pm.Normal('beta', 0, 10)
    mu = alpha + beta*(adult_males['weight'] -
    ↪  adult_males['weight'].mean())
    # Observed!
    h = pm.Normal('height', mu, sigma,
    ↪  observed=adult_males['height'])

    trace = pm.sample() # MCMC sampling
```