Programming in Python[1]

Mattia Monga

Dip. di Informatica
Università degli Studi di Milano, Italia
mattia.monga@unimi.it

Academic year 2020/21, II semester

Lecture XIX: Behind pymc3

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

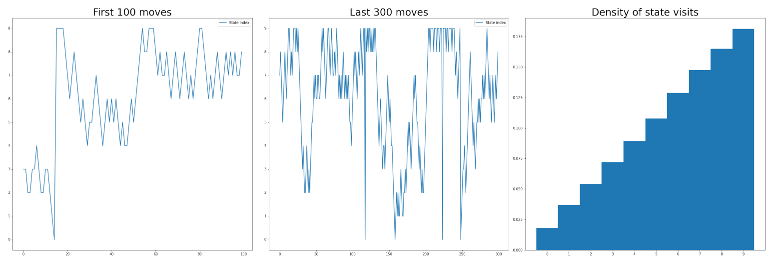
Metropolis

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
```