

Lecture 2. Computational methods

Markov Chain Monte Carlo, Laplace approximation

18.03.2024-22.03.2024 Instructors: Alina Bazarova, Oleg Filatov. Technical issues: Alexandre Strube

Why computational methods?

Recall that in our target formula for posterior $p(\theta | x) = \frac{p(\theta)p(x | \theta)}{\int_{\mathbb{R}} p(\theta)p(X | \theta)d\theta}$

where θ are our parameters the **integral** below can get **really nasty**!

BUT: this integral is just a constant! Rewrite $p(\theta | x) = \frac{1}{Z}p(x, \theta)$, where Z is just a normalising constant, although possibly varying over a large range.

What to do?

Markov Chain Monte Carlo (MCMC) algorithm

Monte Carlo integration.

Assume we want to compute $E f(\theta | X) = \frac{\int f(\theta) p(\theta) p(X | \theta) d\theta}{\int p(\theta) p(X | \theta) d\theta}$

where f is some function of parameters θ given the data X .

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(law of large numbers)

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2. Good news: $\{\theta_t\}$ does not necessarily need to be independent. One of the ways of tackling the above problem is to do it through a Markov chain having $p(\theta | X)$ as its stationary distribution.

This is called Markov chain Monte Carlo.

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Each time $t \geq 0$ the next state θ_{t+1} is sampled from a distribution $P(\theta_{t+1} \mid \theta_t)$, which depends **only on the current state of the chain** θ_t and does not depend on its history $\{\theta_0, \dots, \theta_{t-1}\}$.

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Important: We can construct an MCMC algorithm which will have $p(\theta | X)$ as the stationary distribution!

Metropolis-Hastings sampler

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where $\alpha(\theta, Y) = \min \left(1, \frac{p(Y)p(X|Y)q(\theta|Y)}{p(\theta)p(X|\theta)q(Y|\theta)} \right)$.

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rejection of all possible candidates Y

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Hence, once sample from stationary has been obtained, all subsequent samples are going to be from it. This means MCMC has converged. The period before convergence is called burn-in

Metropolis-Hastings: how it works in practice

1. Start at **current position** X .
2. Propose moving to a **new position** Y using proposal $q(Y|X)$
3. Accept/Reject the new position based on the position's adherence to the data and prior distributions using $\alpha(X, Y)$
 - If you accept: Move to the new position Y . Return to Step 1.
 - Else: Do not move to new position, stay at X . Return to Step 1.
4. After a large number of iterations, return **all accepted positions**.

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2. Even if the chain converged it may **mix** slowly (move around the states). And hence one needs to **run it for longer** to obtain **reliable estimates**.
3. Proposal has to **explore the space efficiently**, sometimes it requires to perform experimentation and craftsmanship to construct a good one.

Jupyter notebook 2

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3. This can be used during burn-in **to reach the desired acceptance** rate.

Single component MH and Gibbs sampler

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Acceptance probability will then be $\alpha(\theta_{-i}, \theta_i, Y_i) = \min \left(1, \frac{\pi(Y_i | \theta_{-i}) q(\theta_i | Y_i, \theta_{-i})}{\pi(\theta_i | \theta_{-i}) q(Y_i | \theta_i, \theta_{-i})} \right)$

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Acceptance probability will then be $\alpha(\theta_{-i}, \theta_i, Y_i) = \min \left(1, \frac{\pi(Y_i | \theta_{-i})q(\theta_i | Y_i, \theta_{-i})}{\pi(\theta_i | \theta_{-i})q(Y_i | \theta_i, \theta_{-i})} \right)$

Gibbs sampler: $q(Y_i | \theta_i, \theta_{-i}) = \pi(Y_i | \theta_{-i})$. **Acceptance probability in this case is always equals to 1!**

Single component MH and Gibbs sampler

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Gibbs sampling uses the property of tractability of all **conditional** posterior distributions to get samples from the unknown **full** posterior distribution of all model variables.

Gibbs sampling scheme

Assume we have data $X \sim p(X | \theta_1, \theta_2)$

1. Randomly initialize $\theta_1^{(0)}$ and sample $\theta_2^{(0)} \sim p(\theta_2 | X, \theta_1^{(0)})$

2. For step $t = 1, \dots, T$

(a) Sample $\theta_1^{(t)} \sim p(\theta_1 | X, \theta_2^{t-1})$

(b) Sample $\theta_2^{(t)} \sim p(\theta_2 | X, \theta_1^{t-1})$

Laplace approximation

The idea: find parameters μ and Σ such that $p(\theta | X) \approx N(\mu, \Sigma)$

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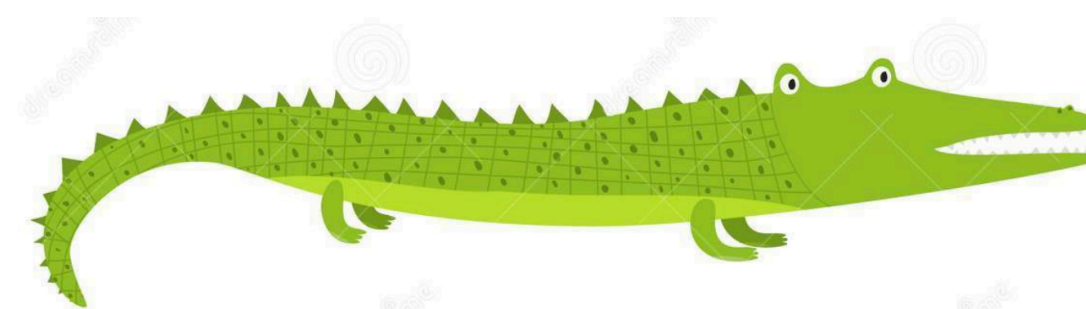
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Even a crocodile is shorter than this expression!



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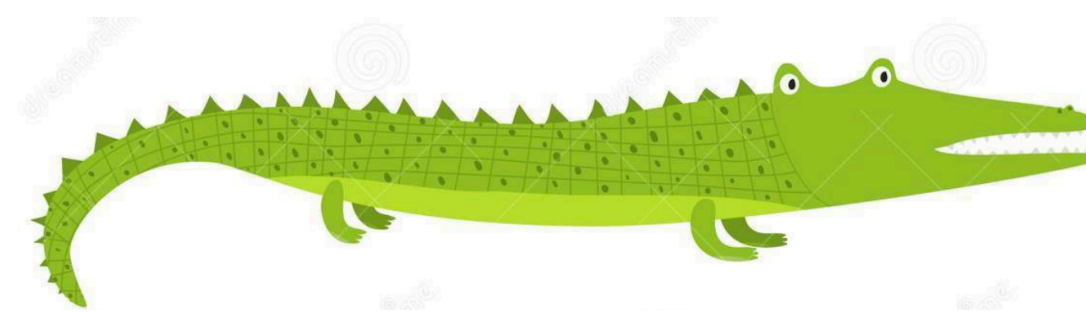
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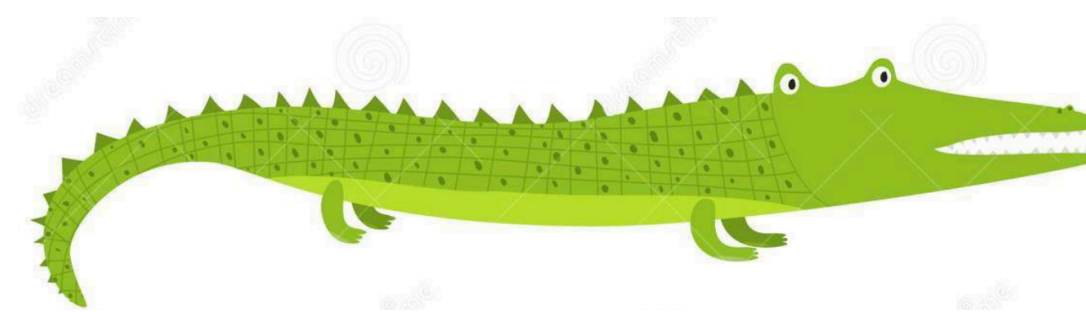
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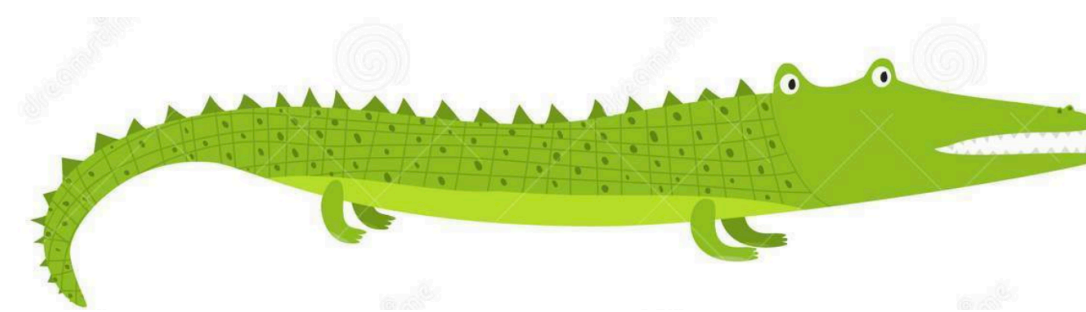
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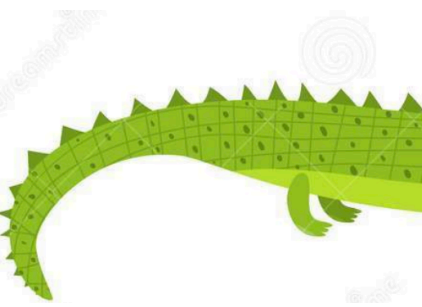
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Hence $\nabla f(\theta_{MAP}) = 0$ and the second term of the “crocodile” conveniently gets zeroed down:

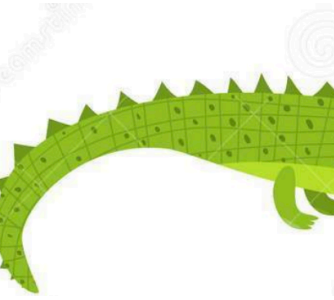


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Hence $\theta | X \sim N(\theta_{MAP}, -(\nabla^2 \ln p(X, \theta_{MAP}))^{-1})$

Laplace approximation 2. What is good about MAP?

1. **How to find MAP?** Iterative procedure, gradient ascent.

In **pymc** function **find_map** which we already used in the first Jupyter notebook.

2. **How to find Hessian $\nabla^2 \ln p(X, \theta)$?:**

In **pymc** function **find_hessian**

However with the large number of parameters this also becomes too computationally challenging, hence one needs another method

Jupyter notebook 2 Laplace approximation