Lecture 2. Computational methods

Markov Chain Monte Carlo, Laplace approximation

20.03.2023-24.03.2023 Instructors: Alina Bazarova, Sebastian Starke, Steve Schmerler. Technical issues: Alexandre Strube

Why computational methods?

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

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 $E\, f(\theta \mid X) = \dfrac{\int f(\theta)p(\theta)p(X \mid \theta)d\theta}{\int p(\theta)p(X \mid \theta)d\theta}$

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

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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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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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Most typical one: **random walk**, $q(Y \,|\, \theta) = q(\,|\,Y - \theta\,|\,)$.

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

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

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This means that instead of $q(Y \mid \theta)$ we will have $q(Y_i \mid \theta_{-i}, \theta_i)$, where $\theta_{-i} = \{\theta_1 \dots \theta_{i-1}, \theta_{i+1} \dots \theta_h\}$.

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

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

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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 $X \sim p(X \mid \theta_1, \theta_2)$

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

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

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

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

Laplace approximation

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

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$p(\theta \mid X) = \dfrac{p(\theta, X)}{p(X)} = \dfrac{e^{\ln p(\theta,X)}}{\int e^{\ln p(\theta,x)} d\theta}$, concentrate on $\ln p(\theta, X)$ as a function of θ

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Taylor series up to the 2nd term: $f(\theta) \approx f(\theta_0) + (\theta - \theta_0)^T \nabla f(\theta_0) + \dfrac{1}{2}(\theta - \theta_0) \nabla^2 f(\theta_0)(\theta - \theta_0)^T$

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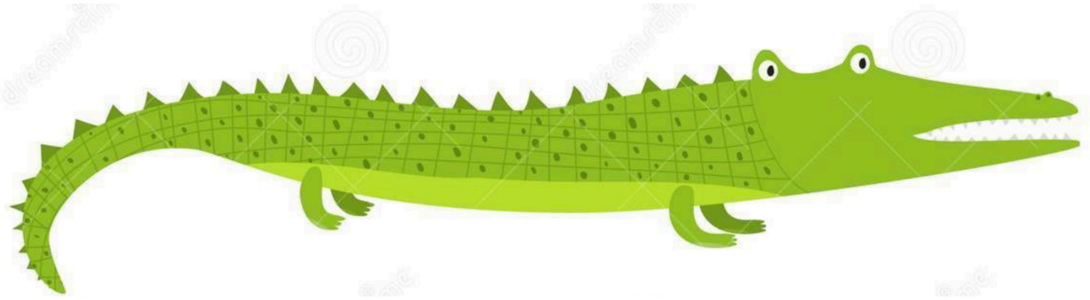
Even a crocodile is shorter than this expression!



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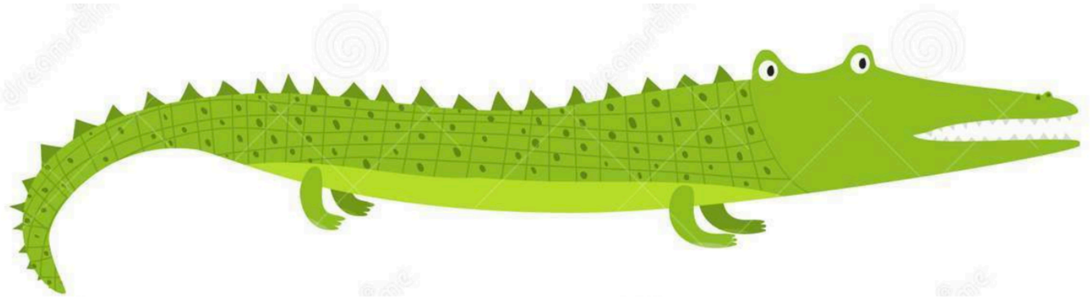

Hence finding a good point (MAP):

$$\theta_0 = \theta_{MAP} = \arg\max_{\theta} p(\theta | X)$$

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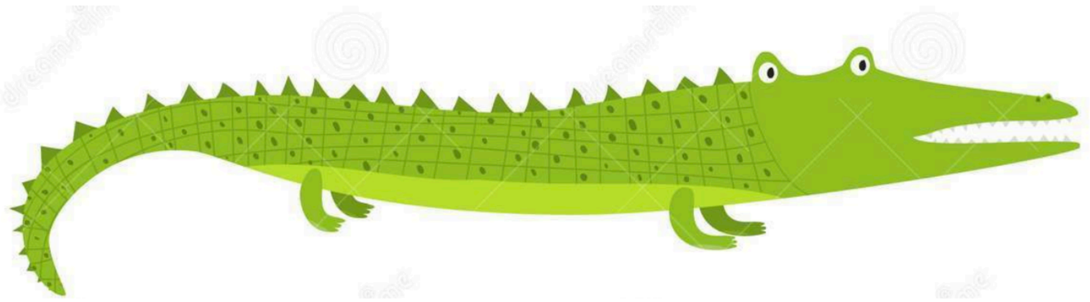

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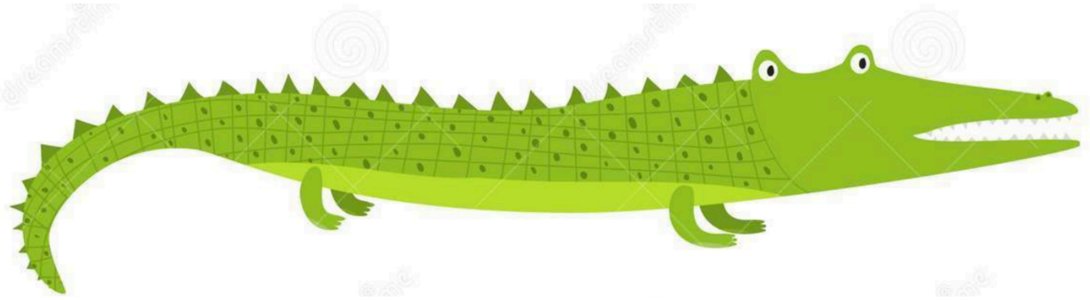

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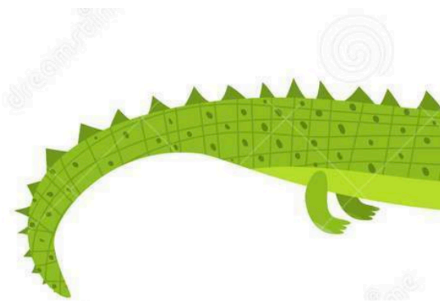
Laplace approximation 2. What is good about MAP?

Note, that θ_{MAP} corresponds to **local maximum of the posterior**



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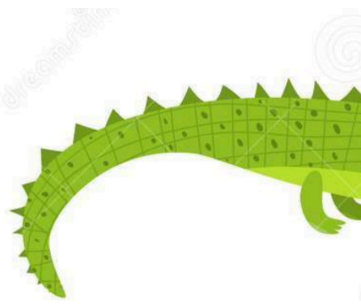

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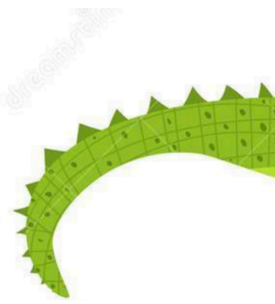

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Hence $\theta | X \sim N(\theta_{MAP}, -(\nabla^2 \ln p(X, \theta_{MAP}))^{-1})$

Laplace approximation 2. What is good about MAP?

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

In **pymc3** function **find_map** which we already used in the first Jupyter notebook.

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

In **pymc3** 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