Homework 2
Due Date: 20th of November EOD
Course: Stochastic Methods in Mathematical Modelling
Instructor: Prof. Vladimir Palyulin
Teaching Assistant: Maria Larchenko

Problem 1 Fluctuations and KL Divergence (5 points)
Let's consider a general physical system, described by a probability density $P^a(\omega)$, where ω denotes the degrees of freedom of the system. For example, we may take $\omega = x$ to be the coordinates of a diffusing particle and $P^a(\omega)$ to be the probability density of the particle's position at time t. We further specify an observable $r(\omega)$. Depending on ω, such an observable may, e.g., be a function of the particle's position. We denote the average of $r(\omega)$ by $\langle r \rangle^a = \int d\omega r(\omega) P^a(\omega)$. Since ω is a random variable, the observable $r(\omega)$ will likewise fluctuate. We can characterize the fluctuations of $r(\omega)$ by its deviations from the average $\Delta r(\omega) = r(\omega) - \langle r \rangle^a$. We now perturb the system, e.g., by applying an external force. The perturbation changes the probability density $P^b(\omega)$ and the average of the observable to $\langle r \rangle^b$. We refer to a and b as the reference and perturbed systems, respectively. Provided that $P^a(\omega)$ and $P^b(\omega)$ have the same support (i.e., $\frac{P^a(\omega)}{P^b(\omega)}$ is finite for all ω):

1. First write down the cumulant generating function of fluctuations $(r(\omega) - \langle r \rangle^a)$ in the unperturbed system.
2. Use the fact that $P^a(\omega)$ and $P^b(\omega)$ have the same support and re-write cumulant generating function.
3. Apply the Jensen's inequality to cumulant generating function (Since the logarithm is a concave function, you are eligible) .
4. Find the relation between response of the system to the perturbation $(\langle r \rangle^b - \langle r \rangle^a)$ and KL divergence.
5. Apply your results to the special case when r follows a Gaussian distribution.

Problem 2 Maximum Likelihood Estimation (2 points)

In this task one needs to find which source distribution was most likely used to generate given random sample

- Gamma distribution, where k is shape, $\theta = 1$ is scale, Γ is Gamma function

$$P_{gamma}(x) = x^{k-1} \frac{e^{-x/\theta}}{\theta^k \, \Gamma(k)}$$

- or Gumbel distribution, where μ is the mode, and $\beta = 1$ is the scale

$$P_{gumbel}(x) = \frac{e^{-(x-\mu)/\beta}}{\beta} e^{-e^{-(x-\mu)/\beta}}$$

You will need "unknown_sample.txt" file and additionally we provide jupyter notebook template for your convenience. Using them answer the following questions

1. What is the most probable value of shape $\hat{k}$ if the source distribution was P_{gamma}?

2. What is the most probable value of mode $\hat{\mu}$ if the source distribution was P_{gumbel}?
3. Which distribution has the highest probability to be the true one?

Ensure that your solution is correct by plotting PDFs with found $\hat{k}$ and $\hat{\mu}$ over the histogram of the sample. Then look through the autograd example and change the optimization method. Answer the remaining questions

4. Is there any difference between running the BFGS optimiser with and without a jacobian?
5. Do you spot any changes in an iterations number between BFGS and Nelder-Mead optimizers?

Problem 3 Markov chains (3 points)

I have 4 sun glasses, some at home, some in the office. I keep moving between home and office. I take glasses with me only if it is sunny. If it is not sunny I leave the glasses behind (at home or in the office). It may happen that all glasses are in one place, I am at the other, sun starts shining and I must leave, so I will suffer.

1. If the probability of sunny weather is p, what is the probability that I will suffer from the sun?
2. Current estimates show that $p = 0.6$ in Sochi. How many sun glasses should I have so that, if I follow the strategy above, the probability of my suffering is less than 0.1?