Exercises 3 for Computational Physics (physik760)
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Generalized inverse transform method

1: Use the *generalized inverse transform method* to sample $X \sim f_X$ with

$$f_X(x) = \frac{1}{\pi} \frac{1}{\sqrt{x\,(1-x)}}\,,$$

for $0 < x < 1$.

a) derive the c.d.f., F_X, and its inverse

b) confirm numerically that your derivation is correct by computing $F_X^{-1}\left(F_X(x)\right)$

c) use the inverse function method to sample $X \sim f_X$, plot a histogram to confirm visually that the distribution lines up with the target p.d.f.

Central Limit Theorem

2: In this exercise we will study the convergence properties of the central limit theorem (CLT). Consider $X_1^\alpha, X_2^\alpha, \ldots$ i.i.d. random variables with p.d.f.

$$f_\alpha(x) = \frac{1}{2\alpha}\,|x|^{-1-\frac{1}{\alpha}}\,\mathbb{1}_{\{|x|\geq 1\}}\,,$$

where $\alpha \in (0,1)$.

a) Determine the cumulative distribution function, F_α, and its inverse analytically.

b) Set up the *generalized inverse transform method* for sampling $X \sim f_\alpha$. Verify your sampling visually by comparing your observed distribution via the known pdf and cdf.

c) Consider the partial sums

$$S_K^\alpha = \frac{1}{\sqrt{K\,\mathrm{Var}(X_1^\alpha)}} \sum_{n=1}^{K} X_n^\alpha\,, \quad X_n \sim f_\alpha\,\forall\, n\,.$$

Implement the sampling of S_K^α.

d) Sample S_K^α for $\alpha = 0.1$, 0.25, 0.45 and $K = 100$ and compare your observed distribution to $\mathcal{N}_{0,1}$ in a Q-Q-plot. Use $N = 10^6$ samples. You can employ *Sturges' formula* $N_{\mathrm{bin}} = \log_2(N) + 1$ for the binning.

e) How does the distribution of S_{100}^α behave as a function of α and why? *Bonus:* Derive the variance as a function of α analytically. Which constraint on α does this suggest for the validity of the CLT?

Simulation of the Ising model in two dimensions

3: Continue to work on your simulation package for the Ising model, making sure that around November 20^{th} you ...

a) are able to use the Metropolis algorithm to generate several million spin configurations on lattices of size $L^2 \sim 32^2$ or larger on your work machine in a few minutes.

   - Normally, a "new" spin configuration is taken to be the one that results from attempting L^2 spin flips, you thus need to be able to go through $\mathcal{O}(L^2 \cdot 10^6)$ spin flips in a relatively short amount of time.
   - Further, you will be asked to scan (portions of) the parameter space, you will thus need many billions of spin configurations in total.
   - If your code is too slow, compare with your peers and ask your tutors for hints.

b) have confirmed that you obtain the same equilibrium estimates for the magnetisation when you start your simulation "*hot*" (randomly arranged spins) or "*cold*" (all spins aligned).

c) Are able to write a data file with the magnetisation and the average energy per spin for all sampled configurations.

d) Have employed a good PRNG such as Mersenne-twister or RANLUX at high luxury level.

   - It is instructive to test PRNGs using the Metropolis algorithm for the $2d$ Ising model.

In the weeks following November 20^{th}, many of the exercises will rely on the analysis of data generated with your simulation package.