# Exercises 4 for Computational Physics (physik760)
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## The accept-reject method

As we have seen in the previous exercises, transform methods can be used to sample from arbitrary distributions if we are able to compute the Jacobian or the inverse of the c.d.f. of the target distribution. However, when neither of these is possible or if the evaluation of the inverse of the c.d.f. is costly, the *accept-reject* method offers a powerful alternative.

**1:** Consider the one-parameter family of probability density functions

$$f_\alpha(x) = b_\alpha \sqrt{1-x^2}\cos(\alpha x)^2$$

defined on the set $x \in [-1, 1]$ and with normalization $b_\alpha$

$$b_\alpha = \left[\int_{-1}^{1} \sqrt{1-x^2}\,\cos(\alpha x)^2\right]^{-1} .$$

Tasks:

a) Take first $\alpha = 0$. Sample from $X \sim f_0$ using the accept-reject method with uniform instrumental density $g \sim \mathcal{U}(-1, 1)$

$$g(x) = \frac{1}{2}\,\mathbb{1}_{[-1,1]}(x)\,.$$

Determine $b_0$ analytically and compare your observed distribution with the true p.d.f.

b) Now generalize to $\alpha \neq 0$. Sample $X \sim f_\alpha$ with the accept-reject method and use $f_0$ as your instrumental density. Implement the accept-reject method and explore it for $\alpha \in (0, 16]$ in a rough stepping.

c) Why does the accept-reject algorithm not require explicit knowledge of $b_\alpha$?

d) An important measure of efficiency is the *acceptance ratio* (AR), which is the ratio of accepted $x$ divided by the number of tests. How does it vary with $\alpha$ and why?

e) Based on the previous two tasks, can you determine a numerical estimate for $b_\alpha$ from your sampling?

f) *Fun question:* For those who are interested, what is the limiting AR for $\alpha \to \infty$?

g) The generalization of the accept-reject method to multiple dimensions is easy. We can sample from the distribution with p.d.f.

$$f_\alpha^D = \sqrt{1-|x|^2}\,\prod_{i=1}^{D}\cos(\alpha^i\,x_i^i)^2\,\mathbb{1}_{|x|^2<1}$$
$$|x|^2 = x_1^2 + \cdots + x_D^2\,,$$

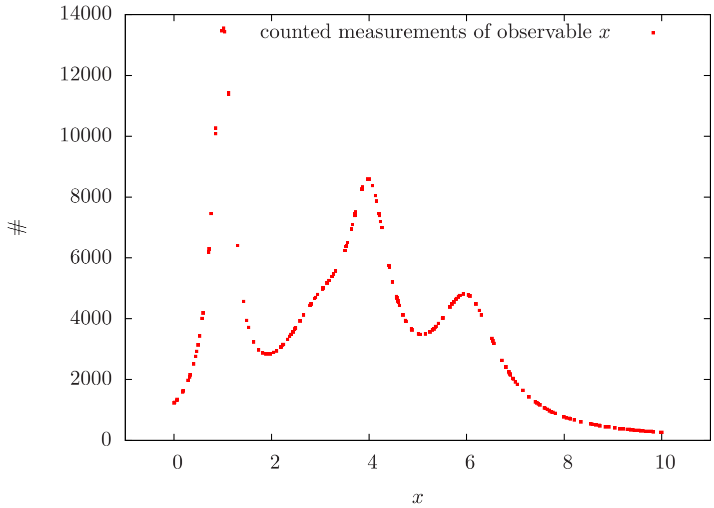
by generating $D$-tuples $[x_1, x_2, \ldots, x_D]$ and performing the same test as above, accepting or rejecting the entire tuple.

i) Implement the accept-reject method for $D \in \{2, 3, \ldots, 5\}$.

ii) For $\alpha = 2$, what can you say about the acceptance ratio as a function of $D$?

## Sampling from an empirical distribution

Here is another example for the usefulness of accept-reject, namely when we don't even know the target density in closed form. As an example, consider the following experimentally obtained distribution (counts) of measurements of observable $x$.




**2:** Based on the observed discrete distribution of measurements, sample from the underlying continuous distribution $f_X$ using the *accept-reject method*. Use e.g. piece-wise linear interpolation to approximately evaluate at intermediate points.

The data set can be downloaded from `https://ecampus.uni-bonn.de/goto_ecampus_file_1135752_download.html`

## Simulation of the Ising model in two dimensions

**3:** Keep working on your simulation code using the Metropolis algorithm.

a) As a test, try to reproduce these values for the (absolute value of the) magnetization

| $L$ | $J/T$ | $\|\bar{m}\|$ |
|---|---|---|
| 12 | 1/5 | 0.1127 (6) |
| 24 | 1/5 | 0.0570 (4) |
| 32 | 1/5 | 0.0419 (3) |

b) Time your code on your machine. Estimate the cost in *core hours* to produce $N_{\text{sample}}$ spin configurations depending on the lattice size $L$.