Homework 2. Due Thursday, Feb. 18

1. **(20 pts)** The invariant probability measure for the system evolving in the double-well potential $V(x) = x^4 - 2x^2 + 1$ according to the overdamped Langevin dynamics at temperature one is given by the Gibbs pdf

$$f(x) = \frac{1}{Z}e^{-(x^4-2x^2+1)}, \quad \text{where} \quad Z = \int_{-\infty}^{\infty} e^{-(x^4-2x^2+1)}dx. \tag{1}$$

   (a) Use the standard Gaussian pdf

$$g_1(x) = \frac{1}{\sqrt{2\pi}}e^{-x^2/2}$$

   to find the normalization constant Z in Eq. (1). Use at least 10^6 samples, better even 10^8. Check your answer using numerical quadrature by the composite trapezoidal rule on the interval $[-a, a]$ where a is large enough so that $e^{-(a^4-2a^2+1)} < 10^{-16}$.

   (b) Find the optimal value of σ in order to use the pdf of the form

$$g_\sigma(x) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-x^2/(2\sigma^2)}$$

   for sampling RV with pdf $f(x)$ (Eq. (1)) by means of the acceptance-rejection method [1]. The optimal σ minimizes the constant c.
   Hint: First find analytically

$$x^* = \arg\max_{x\in\mathbb{R}} \frac{f(x)}{g_\sigma(x)}$$

   as a function of σ. Then you can find the optimal σ using e.g. the function `fminbnd` *in MATLAB. If you use a programming language that does not have standard function to find a minimum of a function in 1D, plot a graph $c(\sigma)$ and pick σ close to the optimal one.*

   (c) Sample RV η with pdf $f(x)$ (Eq. (1)) using the acceptance-rejection method. Check that the ratio of the total number of samples and the number of accepted samples is close to C. Plot a properly scaled histogram for the obtained samples and compare it with the exact distribution (with Z found numerically). An example of generating such a histogram is given in the code in Section 3.3 in `sampling.pdf`.
   Hint: to generate samples of $\mathcal{N}(0, \sigma^2)$, generate samples from $\mathcal{N}(0, 1)$ and multiply them by σ.

   (d) Find $E[|x|]$ for the pdf $f(x)$ using the Monte Carlo integration.

   Submit a single pdf document. *Link your codes to it, or print them to pdfs and append them to the main pdf.*

References

[1] http://www.columbia.edu/ ks20/4703-Sigman/4703-07-Notes-ARM.pdf.
K. Sigman's lecture notes on the acceptance-rejection method for sampling random variables.