Reweighting and Taylor Expansion

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A Gaussian integral

$$
\begin{aligned}
Z(s) &\equiv \exp[-F(s)] = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} \mathrm{e}^{-(x-s)^2/2} = 1 \\
\overline{x}(s) &= s, \qquad \text{and} \qquad V(s) = 1,
\end{aligned}
$$

where V denotes the variance of x. The Taylor coefficients of $F(s)$, $\overline{x}(s)$ and $V(s)$, in expansions around $s = 0$, can be read off from here.

The Monte Carlo procedure for $s = 0$ is well-known. Draw two random deviates from an uniform distribution $0 \leq r_1, r_2 \leq 1$. These give two Gaussian random numbers

$$
x_1 = \sqrt{-2 \ln r_1} \cos(2\pi r_2) \quad \text{and} \quad x_2 = \sqrt{-2 \ln r_1} \sin(2\pi r_2).
$$

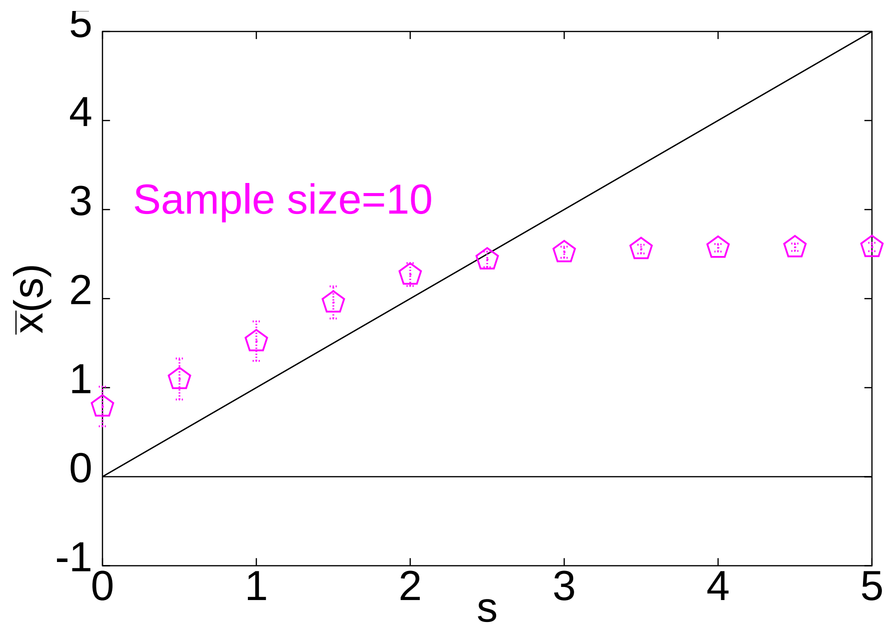
Perform this Monte Carlo. Values of x in the range X and $X + dX$ are then obtained with frequency proportional to the unit Gaussian.

Reweighting and Taylor expansion

In reweighting each point sampled by Monte Carlo is given an extra weight

$$w(x, s) = \mathrm{e}^{-(s^2 - 2xs)/2}$$

The statistical estimates of any quantity one wishes to evaluate are made using this weight for each sampled value of x. Taylor expand w and average.



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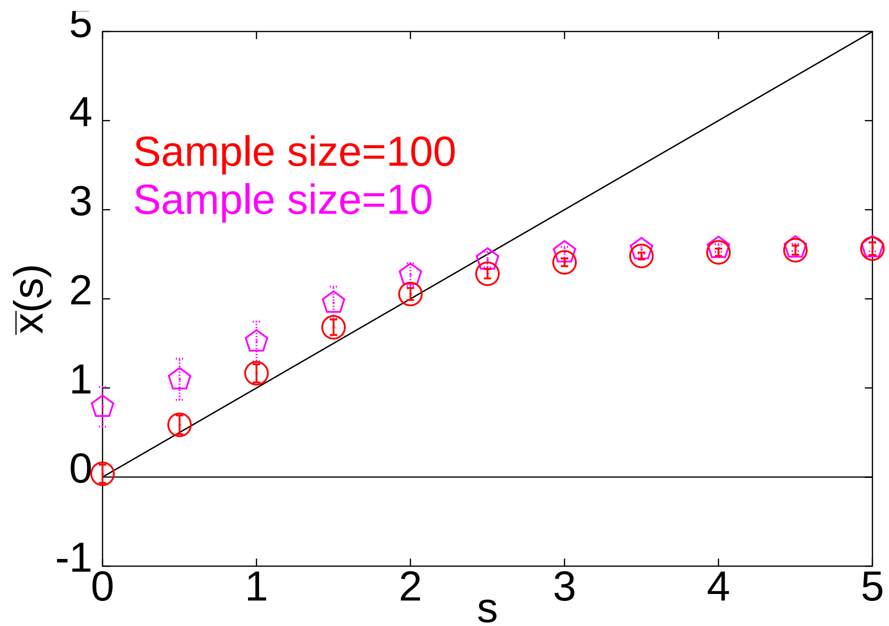

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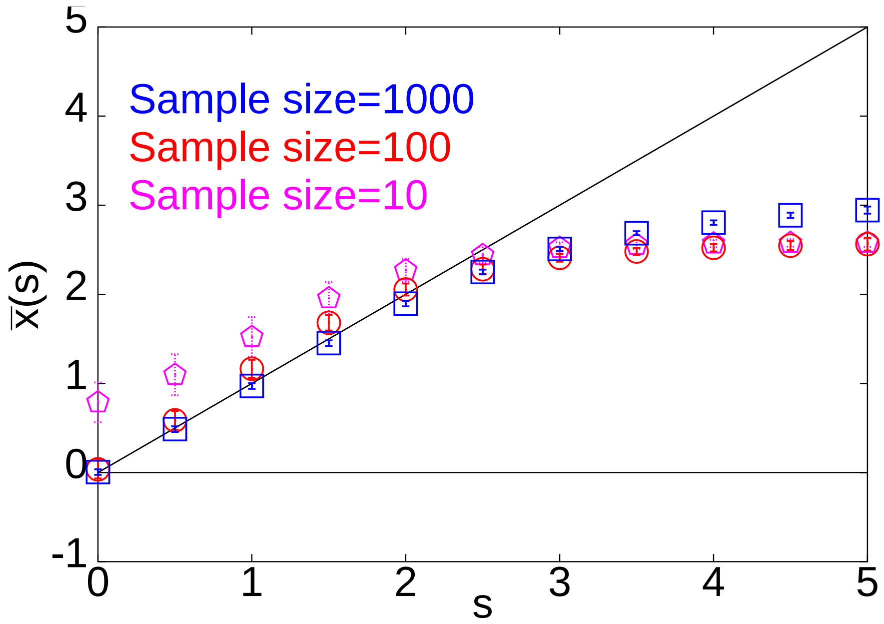

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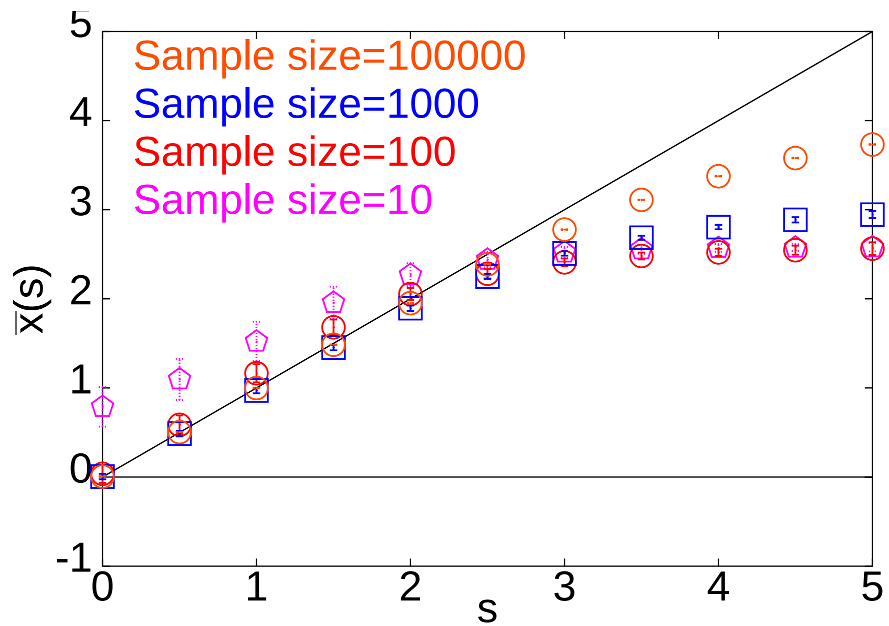

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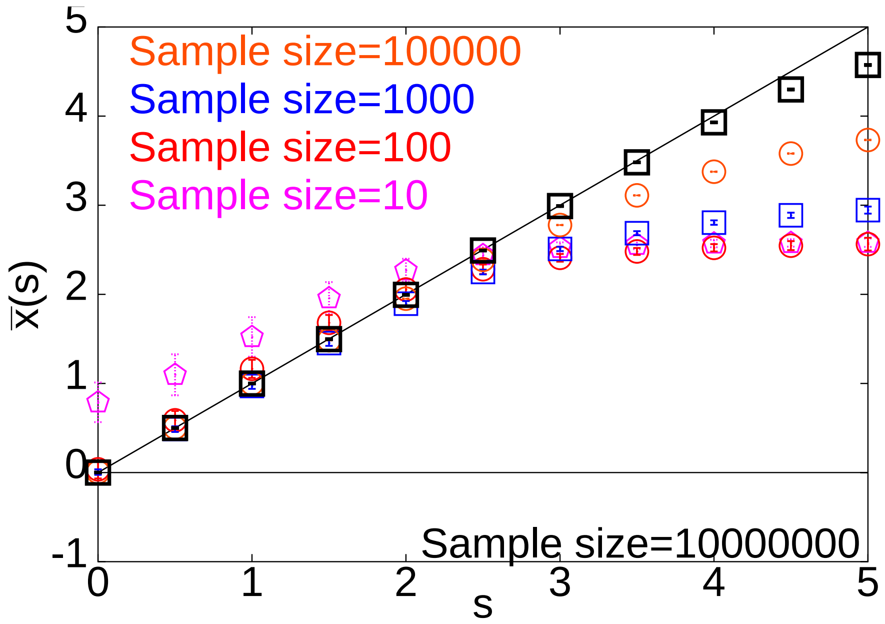

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$$w(x, s) = e^{-(s^2 - 2xs)/2}$$

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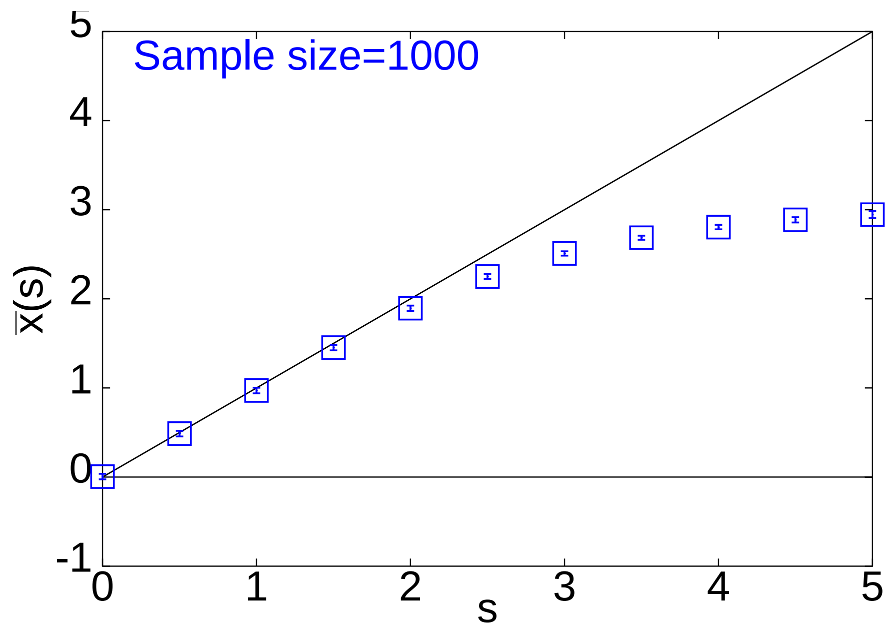

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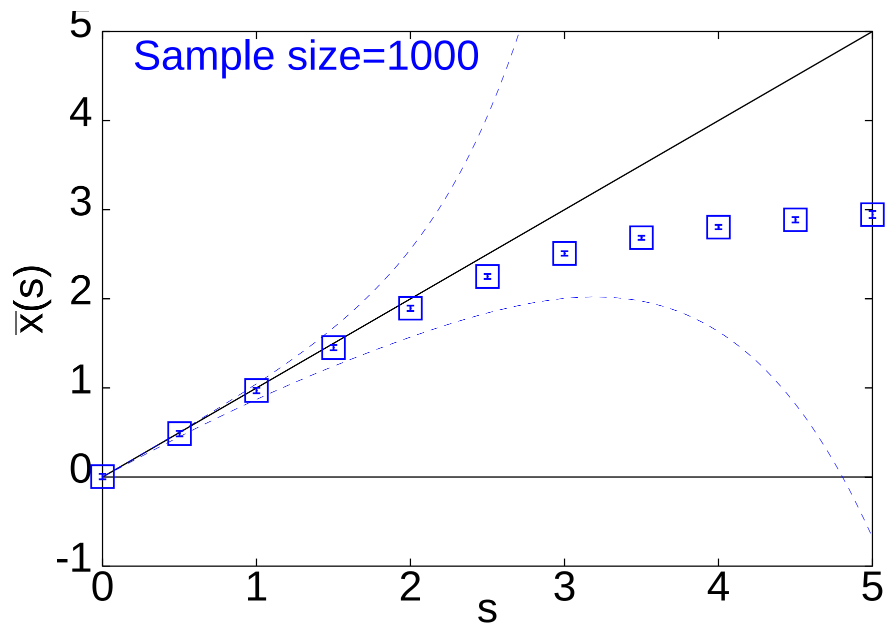

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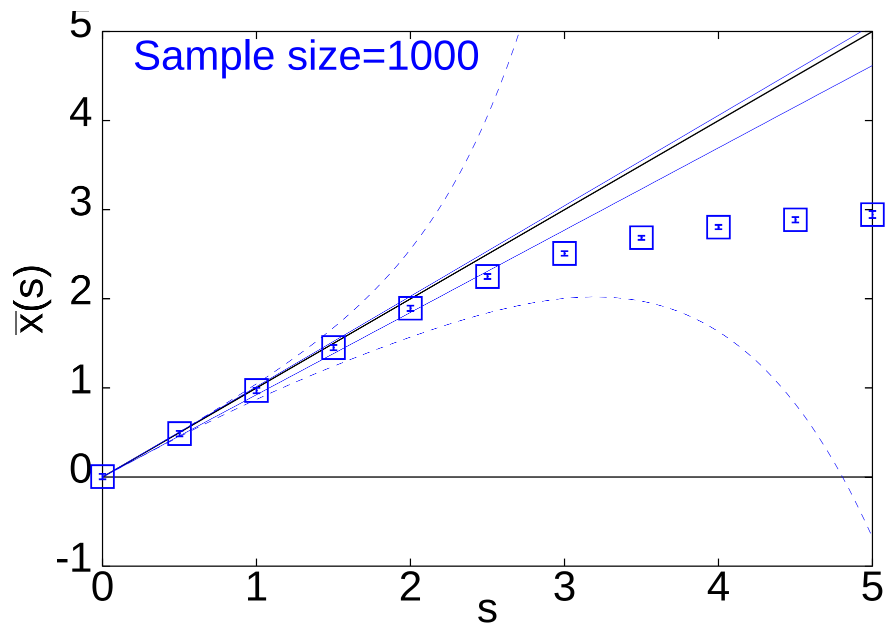

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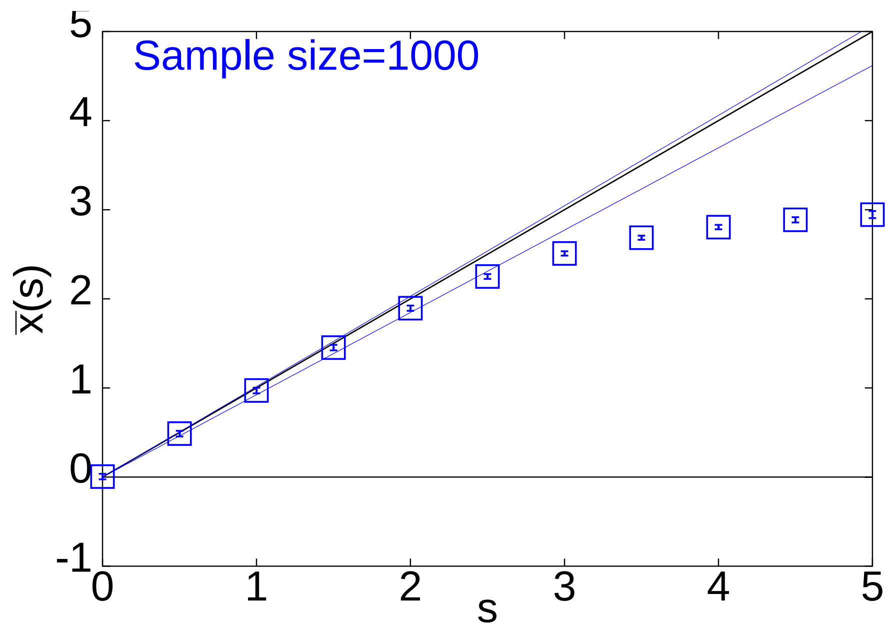
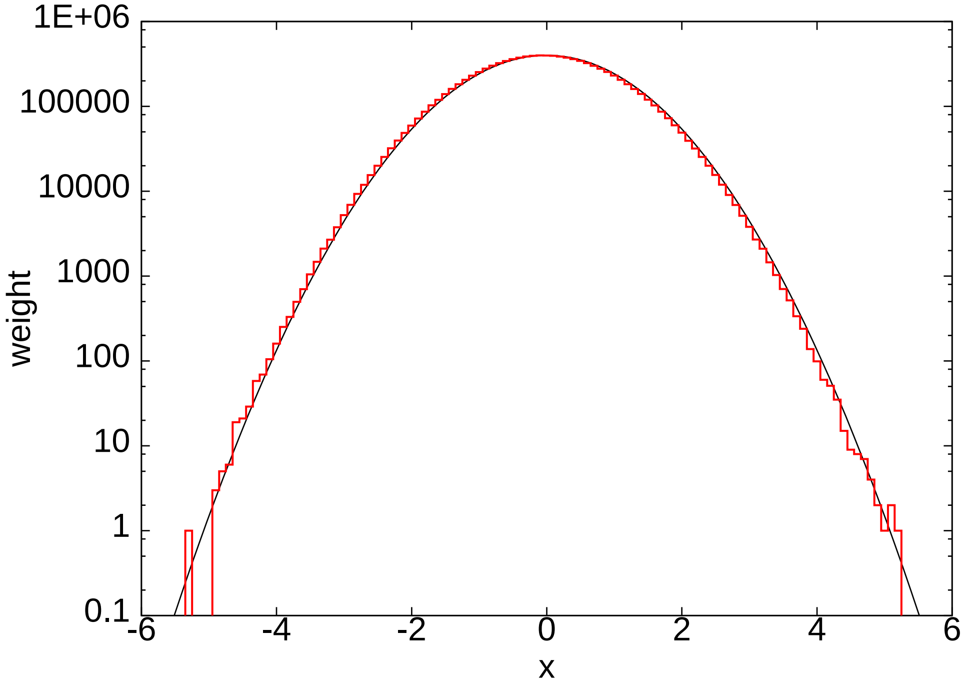


Why reweighting goes crazy

Simple: finite statistics means tail of the distribution is always badly sampled. On reweighting, what was once the tail eventually becomes the peak. Reweighting is exponentially hard.



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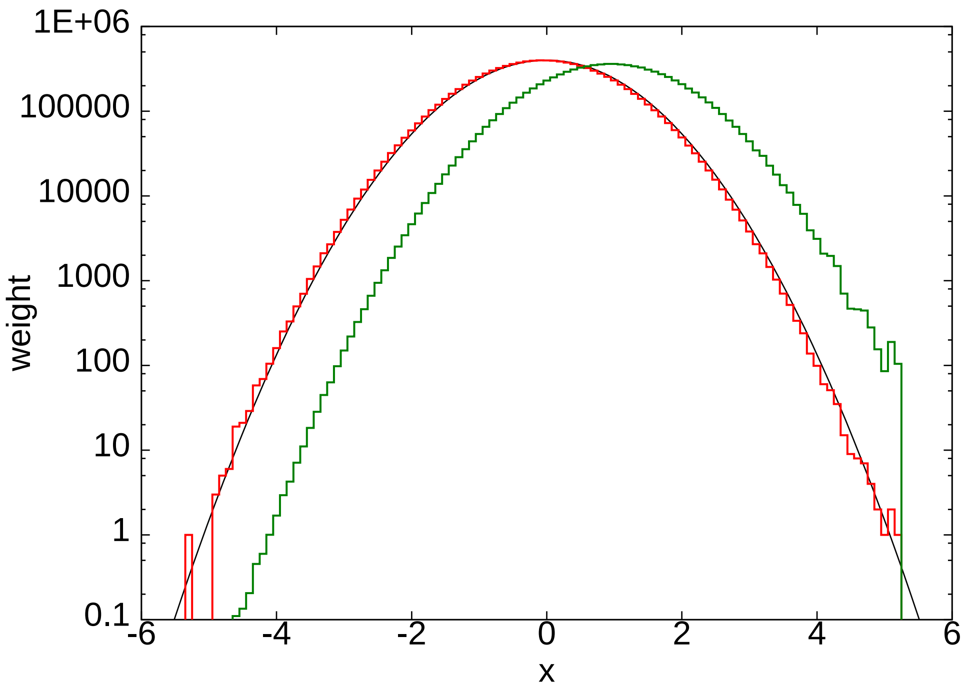

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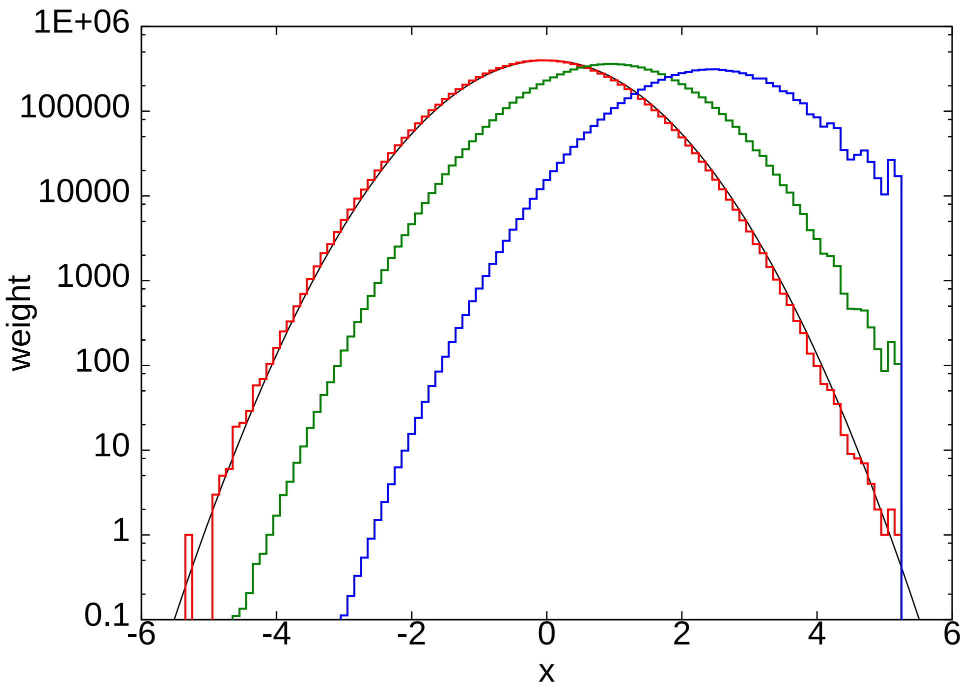

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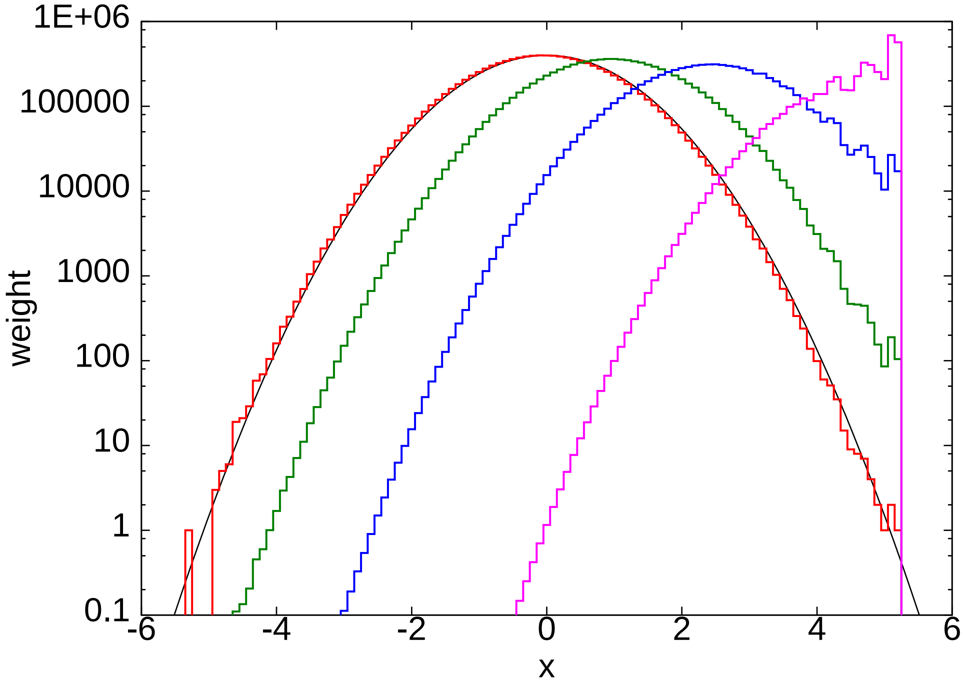

Why the Taylor expansion remains sane

The Taylor expansion can be rearranged in terms of cumulants—

$$
\begin{aligned}
1!t_1 &= \langle x^2 \rangle \equiv \left[x^2\right], \\
2!t_2 &= \langle x(x^2-1) \rangle \equiv 0, \\
3!t_3 &= \langle x^2(x^2-3) \rangle \equiv \left[x^4\right] + 3\left[x^2\right]\left(\left[x^2\right]-1\right), \\
4!t_4 &= \langle x(3-6x^2+x^4) \rangle \equiv 0, \\
5!t_5 &= \langle x^2(15-10x^2+x^4) \rangle \equiv \left[x^6\right] + \left[x^4\right]\left(15\left[x^2\right]-10\right) + 15\left[x^2\right]\left(\left[x^2\right]-1\right)^2.
\end{aligned}
$$

The symmetries of the Gaussian for $s = 0$ imply that alternate coefficients vanish. The central limit theorem says that only the second cumulant is non-vanishing. As a result, for a Gaussian of unit variance, only the first Taylor coefficient is non-vanishing.