Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information
Log-Gaussian Gamma Processes for Training Bayesian Neural Networks in Raman and CARS Spectroscopies

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A Additional results for validation of the log-Gaussian gamma process

Figure 1 illustrates the distribution of cost function values for synthetic coherent anti-Stokes scattering spectra generated using the Gaussian process and log-Gaussian gamma process formulations. Additionally, the figure shows cost function values for spectra generated with the point estimates for the experimental spectra shown in the paper. We generated 40 partially synthetic CARS measurements by replacing the log-Gaussian gamma distributed synthetic spectra in the CARS forward model with the point estimates for the experimental spectra. Difference in these cost function distributions would imply that the synthetic spectra would not adequately model the true underlying Raman spectra.

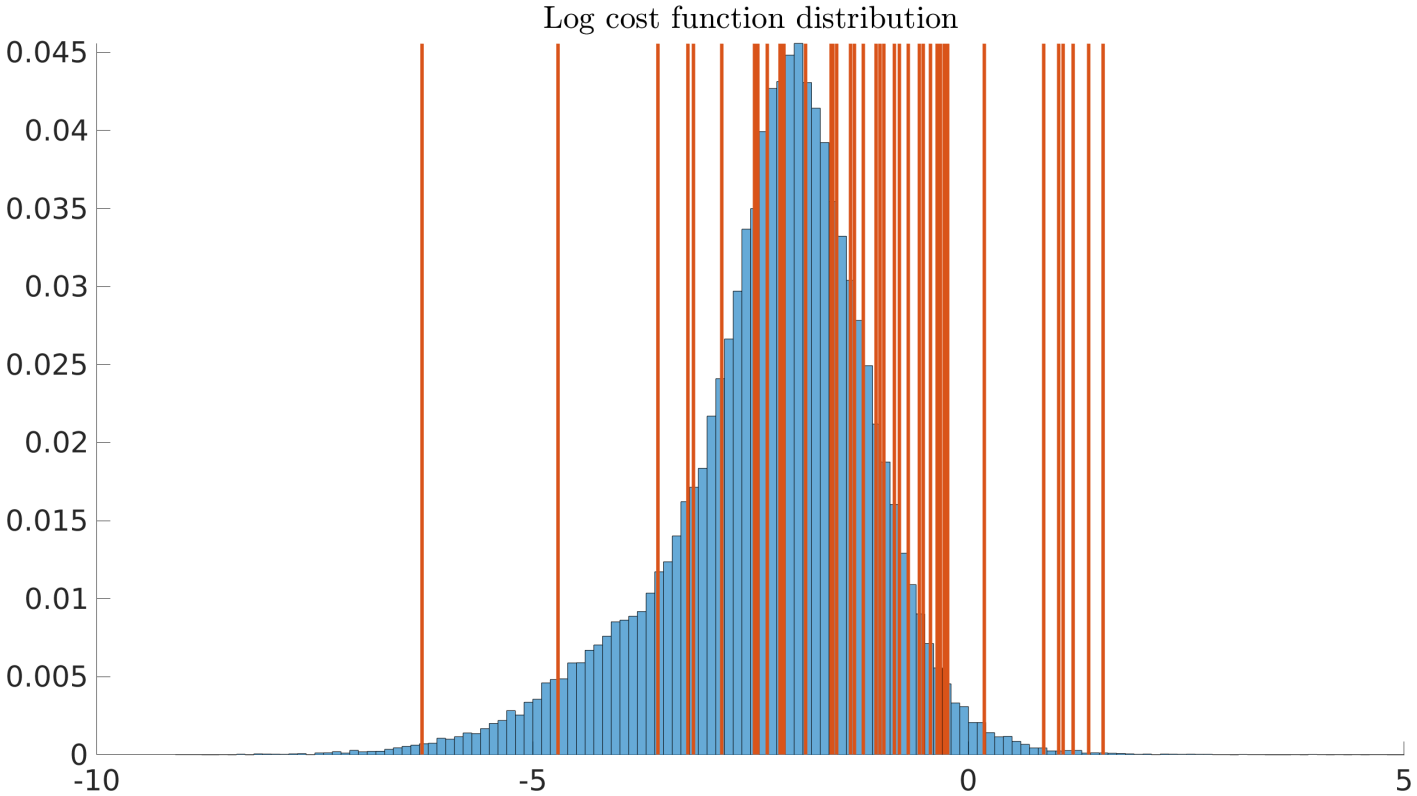

Figure 1: In blue, distribution of logarithmic cost function values for synthetic spectra generated using the log-Gaussian gamma and Gaussian process formulations. In red, logarithmic cost function values obtained for CARS spectra generated using the point estimates for the experimental spectra shown in Figure 9 of the paper. The results are in agreement, indicating that the log-Gaussian gamma process is capable of generating appropriate Raman spectra for the purpose of training a neural network.