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Supplementary Information for *Harnessing Deep Neural Networks to Solve Inverse Problems in Quantum Dynamics: Machine-Learned Predictions of Time-Dependent Optimal Control Fields*

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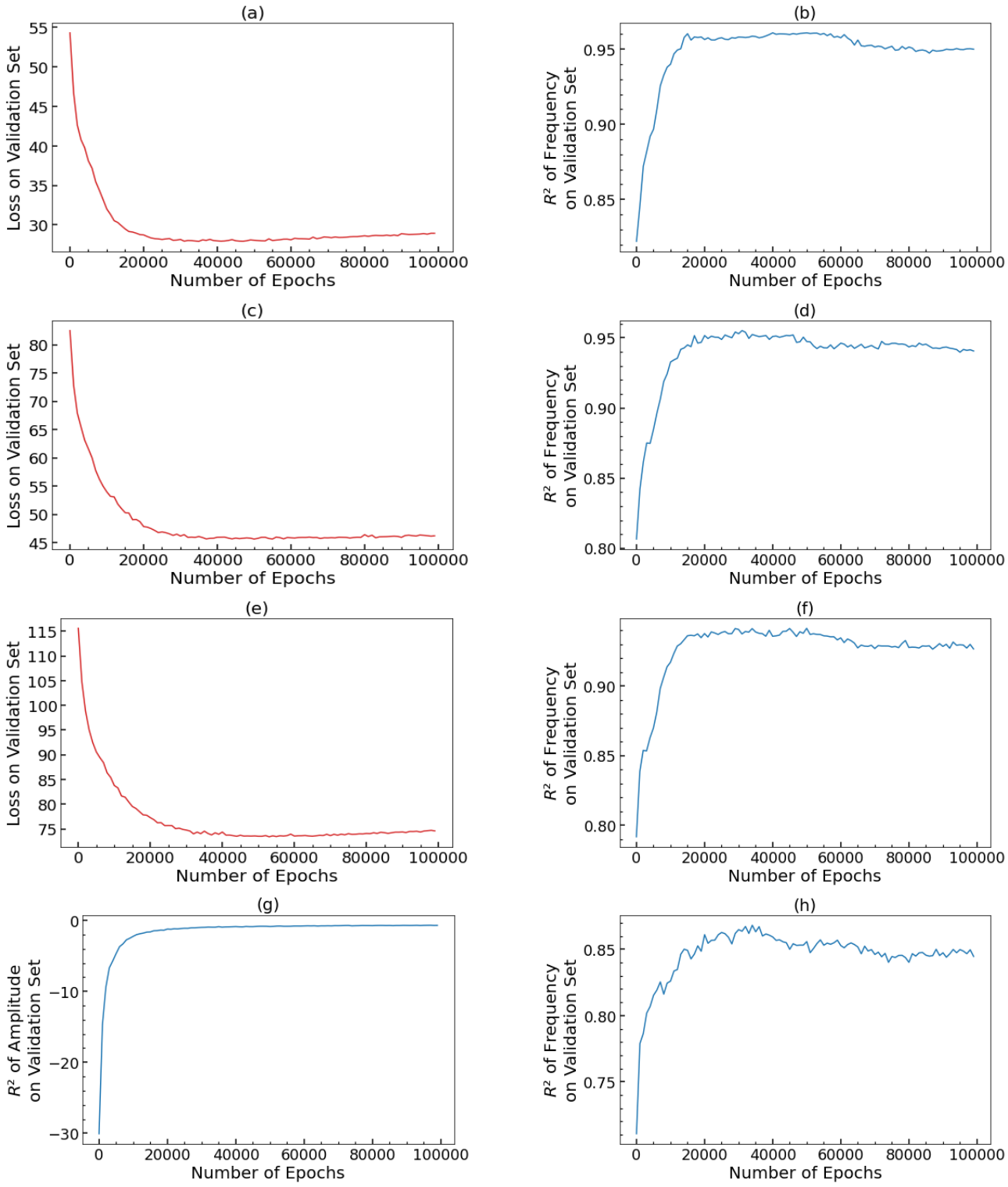

FIG. 1: Plots of the loss vs. the number of epochs for the (a) 600-, (c) 800-, and (e) 1000-output-layer-unit model for the validation dataset. Plots of R^2 values for the predicted frequency vs. the number of epochs for the (b) 600-, (d) 800-, and (f) 1000-output-layer-unit model for the validation dataset. (g) Plot of R^2 values for the predicted amplitude vs. the number of epochs for the 1000-output-layer-unit model for the validation dataset. Using the R^2 definition in the main text, the amplitude R^2 becomes negative-valued, which also manifests itself in the the 600- and 800-output-layer-unit models (not plotted here). (h) Plot of R^2 values for the predicted frequency vs. the number of epochs for the 1000-output-layer-unit model when only 2 hidden layers are used.

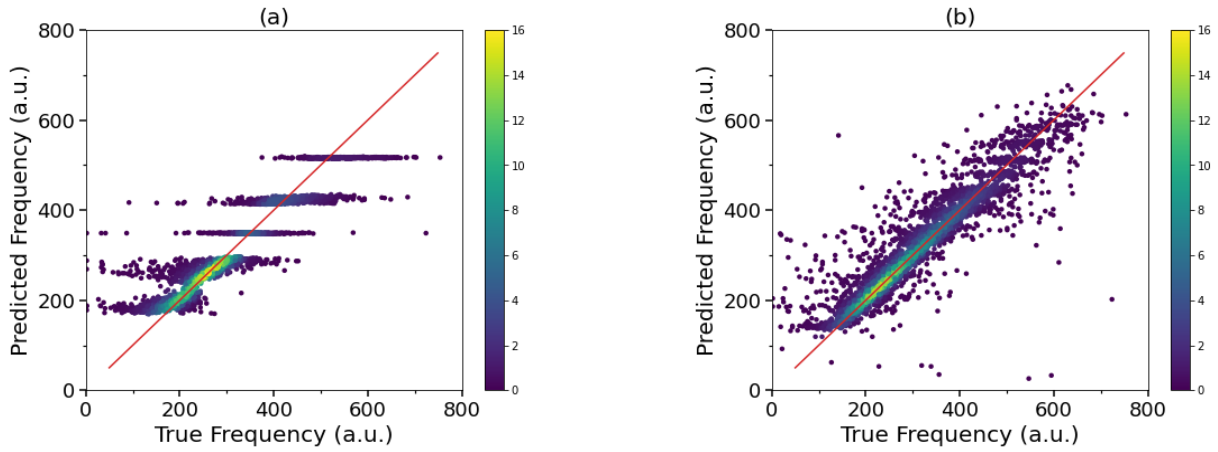

FIG. 2: Density plot of the predicted and true resonance frequencies for the (a) 600-output-layer-unit model for the unscaled amplitude (i.e., when the amplitude is not multiplied by 80), and (b) 1,000-output-layer-unit model with only 2 hidden layers. The diagonal line in each plot represents a perfect match between the machine-learned predictions and the true values. The vertical color bar in each sub-plot indicates the density of the data points.