Code and Data
for "Using a Single Circuit to Compute the Gradients with Respect to All Parameters of a Quantum Neural Network"

Overview:

All the output data of the experiments in the paper are in the "data" directory.
All the software code of the Python programs for generating these data are located in the "code" directory.
Operating environment: Python 3.8.10 with Qiskit 0.21.2.

About the programs:

- File list:
  1_grad_conventional_real_8d.py
  2_grad_conventional_sim_8d.py
  3_grad_conventional_sim_784d.py
  4_grad_improved_real_8d.py
  5_grad_improved_sim_8d.py
  6_grad_improved_sim_784d.py
  7_individual_shot_loader.py
  8_input_data_generator.py
  9_grad_conventional_sim+noise_8d.py
  10_grad_conventional_sim+noise_784d.py
  11_grad_improved_sim+noise_8d.py
  12_grad_improved_sim+noise_784d.py

- File name explanation:
  "*8d*": taking the 8-dimensional input dataset *input_data_8d.pickle* generated by program 8.
  "*784d*": taking the 784-dimensional input data, i.e., the MNIST dataset*.
  "*real*": using a real quantum hardware.
  "*sim*": using a quantum simulator.
  "*conventional*", "*conv*": using the conventional approach.
  "*improved*", "*impr*": using the improved approach.
  "*+noise*": with noise.

  * The MNIST dataset *mnist.pkl.gz* is available at:
  https://github.com/mnielsen/neural-networks-and-deep-learning/archive/master.zip

- Programs 1-3 read *input_data_8d.pickle* (8-dimensional input) or *mnist.pkl.gz* (784-dimensional input) and *parameters.csv*, and output the following files:
  gradient_conv.csv: the gradients with respect to the adjustable parameters of the VQC.
  job_result_conv.pickle: raw data generated by the quantum simulator or real quantum hardware.
  mapped_data_conv.pickle: the processed result of the data generated by the quantum simulator or real quantum hardware.
  other_results_conv.csv: runtimes and other related informations.
  cost_conv.csv (for program 3 only): the values of all the unshifted and shifted cost functions.

- Programs 4-6 read *input_data_8d.pickle* (8-dimensional input) or *mnist.pkl.gz* (784-dimensional input) and *parameters.csv*, and output the following files:
  gradient_impr.csv: the gradients with respect to the adjustable parameters of the VQC.
  job_result_impr.pickle: raw data generated by the quantum simulator or real quantum hardware.
  mapped_data_impr.pickle: the processed result of the data generated by the quantum simulator or real quantum hardware.
  other_results_impr.csv: runtimes and other related informations.
  individual_shot_impr.pickle: the individual shot numbers for all the unshifted and shifted cost functions.
  cost_impr.csv (for program 6 only): the values of all the unshifted and shifted cost functions.

- Program *7_individual_shot_loader.py*:
  Load the file *individual_shot_impr.pickle* and convert it into *individual_shot_impr.csv*.

- Program *8_input_data_generator.py*:
  Generate the dataset *input_data_8d.pickle*.

- Programs 9-10 read *input_data_8d.pickle* (8-dimensional input) or *mnist.pkl.gz* (784-dimensional input) and *parameters.csv*, and output the following files:
  result_conv.csv: the cost functions and gradients with respect to the adjustable parameters of the VQC.

- Programs 11-12 read *input_data_8d.pickle* (8-dimensional input) or *mnist.pkl.gz* (784-dimensional input) and *parameters.csv*, and output the following files:
  result_impr.csv: the cost functions and gradients with respect to the adjustable parameters of the VQC.

About the data files:

- *parameters.csv*:
  The initial values of all adjustable parameters of all the variational quantum circuits (VQCs) used in the paper.
  The VQC with 8-dimensional classical input uses the first 6 data in the file only.
  The VQC with 784-dimensional classical input uses all the 30 data in the file.
  The values are generated randomly, uniformly distributed over the interval $[0,\pi)$.

- *input_data_8d.pickle*:
  The input dataset for the VQC with 8-dimensional classical input.
  Generated randomly by the program *8-input_data_generator.py*, uniformly distributed over the interval [0,1).

- *fig4_data.csv*:
  Data for Fig.4.
  Each row contains the individual shot numbers corresponding to each input data point. The individual shot numbers in the 1st column are for the unshifted cost functions, while the individual shot numbers in the 2nd to 13rd columns are for the shifted cost functions.
  Computed by *5_grad_improved_sim_8d.py,* then converted from the output file *individual_shot_impr.pickle* using *7_individual_shot_loader.py*.

- *fig5_data.csv*:
  Data for Fig.5.
  The content is self-explained.
  The data for Fig.5a is computed using programs 2 and 5.
  The data for Fig.5b is computed using programs 1 and 4.
  The data for Fig.5c is computed using programs 3 and 6.
  (The value of "num_data" in these programs needs to be adjusted manually for different data point in the figures.)

- *fig6_data.csv*:
  The data in green are for Fig.6.
  The content is self-explained.
  The data for Fig.6a is computed using programs 9 and 11.
  The data for Fig.6b is computed using programs 10 and 12. (The value of "prob_1" in these programs needs to be adjusted manually for different data point in the figures.)

- The data for Table 1 of the paper (not shown here) is computed using programs 2 and 5.