# Project 1

Neural-Network Models of a Spray Measurement
and a Hybrid Solar Gas Turbine

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*Submitted individually. One set of Part 1 tables is given below and is identified with Adnan Ahali.*

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# 1 How the work was divided

I completed this project alone. Task P1.6 was omitted, as allowed for a student working alone. The work was as follows:

1. program changes for Part 1 (completion of the backpropagation code and the Keras comparison);
2. interpretation of the Part 1 weights, predictions, and initial-condition test;
3. preparation of the turbine data and the median normalization;
4. the Part 2 network, training schedule, and design variations;
5. the surface plot and the test-set comparison;
6. this write-up.

# 2 Part 1: a three-neuron network

Part 1 compares a first-principles implementation of backpropagation with a Keras model of the same network. The network has three inputs and one neuron in each of three layers. The activation at every neuron is the exponential linear unit,

$$\sigma(z) = \begin{cases} z & z \geq 0, \\ e^z - 1 & z < 0, \end{cases} \qquad \sigma'(z) = \begin{cases} 1 & z \geq 0, \\ e^z & z < 0. \end{cases} \tag{1}$$

The forward map is

$$z_1 = w_{01}x_{01} + w_{02}x_{02} + w_{03}x_{03} + b_1, \qquad a_1 = \sigma(z_1), \tag{2}$$
$$z_2 = w_{12}a_1 + b_2, \qquad a_2 = \sigma(z_2), \tag{3}$$
$$z_3 = w_{23}a_2 + b_3, \qquad a_3 = \sigma(z_3). \tag{4}$$

The squared error on one record is $E_3 = (a_3 - y_3)^2$.

## 2.1 Equations that were added

The supplied program already accumulated $\partial E_3/\partial w_{01}$ and $\partial E_3/\partial w_{02}$ and already applied a batch update to every parameter. The missing derivatives, equations (2c)–(2h), were added with the same chain rule:

$$\frac{\partial E_3}{\partial w_{03}} = 2(a_3 - y_3)\,\sigma'(z_3)\,w_{23}\,\sigma'(z_2)\,w_{12}\,\sigma'(z_1)\,x_{03}, \tag{5}$$
$$\frac{\partial E_3}{\partial b_1} = 2(a_3 - y_3)\,\sigma'(z_3)\,w_{23}\,\sigma'(z_2)\,w_{12}\,\sigma'(z_1), \tag{6}$$
$$\frac{\partial E_3}{\partial w_{12}} = 2(a_3 - y_3)\,\sigma'(z_3)\,w_{23}\,\sigma'(z_2)\,a_1, \tag{7}$$
$$\frac{\partial E_3}{\partial b_2} = 2(a_3 - y_3)\,\sigma'(z_3)\,w_{23}\,\sigma'(z_2), \tag{8}$$
$$\frac{\partial E_3}{\partial w_{23}} = 2(a_3 - y_3)\,\sigma'(z_3)\,a_2, \tag{9}$$
$$\frac{\partial E_3}{\partial b_3} = 2(a_3 - y_3)\,\sigma'(z_3). \tag{10}$$

After a pass over the batch, the program replaces each sum by its average. The red-box updates (1c)–(1h), written with those averages as in equations (3a)–(3h), are

$$w^{\text{new}} = w + \gamma \frac{(0 - \overline{E}_3)}{\partial \overline{E}_3 / \partial w}, \tag{11}$$

and the same form is used for every bias. The factor $\gamma$ is the learning rate. It is of order 1/8 because eight parameters share the correction.

### 2.2 Data

Both Part 1 programs were trained on the eight records stored in the supplied notebooks, normalized by the reference scales already written in those files: $x_{01}/20.2$, $x_{02}/14.5$, $x_{03}/308$, and $y_3/32.4$. The Keras inputs were corrected so that they are exactly those records. In the supplied Keras file, row 6 used $x_{01} = 20.2$ where the first-principles file uses 20, and row 8 used $x_{03} = 308.2$ where the first-principles file uses 308.1. The output scale in the Keras file was 32.401 rather than 32.4. Task P1.2 asks for the same data and the same normalization, so both programs now use Table 1.

Table 1: Part 1 records used for both models.

| $x_{01}$ | $x_{02}$ | $x_{03}$ | $y_3$ |
|---|---|---|---|
| 20.0 | 13.0 | 310.8 | 30.99 |
| 20.0 | 14.5 | 308.0 | 32.20 |
| 20.0 | 15.3 | 306.0 | 31.70 |
| 20.2 | 13.0 | 310.8 | 30.92 |
| 20.0 | 14.5 | 308.0 | 32.40 |
| 20.0 | 15.3 | 306.0 | 31.40 |
| 24.0 | 13.0 | 310.8 | 35.53 |
| 36.0 | 14.4 | 308.1 | 46.41 |

Two input rows are repeated with different measured outputs: $(20, 14.5, 308)$ is paired with both 32.2 and 32.4, and $(20, 15.3, 306)$ is paired with both 31.7 and 31.4. A deterministic network produces one output for each input, so those pairs set a floor on the error. The printed array in the handout differs in the fourth row ($x_{01} = 20$ instead of 20.2) and in the eighth row (22, 14.5, 308, 46.4). That eighth row places $y_3 = 46.4$ next to inputs that are almost the same as a row whose output is near 32. With the specified initial weights, the batch-average squared error on that handout array stalled near 0.015, above the required cutoff of 0.00035. The coded eighth row, with $x_{01} = 36$, is consistent with the large output and is the set on which the cutoff is reachable. It is also the set shared by the two supplied programs.

### 2.3 First-principles training

The initial weights were left at the specified values

$$w_{01} = 1.23,\ w_{02} = 0.40,\ w_{03} = 0.70,\ b_1 = -0.15,$$
$$w_{12} = 0.72,\ b_2 = -0.12,\ w_{23} = 0.70,\ b_3 = 0.01.$$

The cutoff on the batch-average squared error $\overline{E}_3$ was changed from 0.001 to 0.00035. The learning rate was

$$\gamma = \begin{cases} 0.015 & \text{when } \overline{E}_3 \geq 0.001, \\ 0.001 & \text{when } \overline{E}_3 < 0.001. \end{cases}$$

The smaller rate is used once the iteration is close to the minimum, where the Newton step $\overline{E}_3/(\partial \overline{E}_3/\partial w)$ becomes sensitive to a small derivative. The error first fell below 0.00035 at epoch 134. The iteration was then continued until $\overline{E}_3$ stopped decreasing, and the parameter set with the lowest error was kept. That minimum is

$$\overline{E}_3 = 2.139 \times 10^{-4} \quad \text{at epoch 484,} \qquad \text{rms} = \sqrt{\overline{E}_3} = 0.01462, \qquad \text{MAE} = 0.01382. \tag{12}$$

The rms and MAE above are in the normalized output. In the original units of $y_3$ the rms error is $0.01462 \times 32.4 = 0.474$.

### 2.4 Keras training

The Keras model has the same three ELU layers, one neuron each, and the same initial weights. The loss is the mean absolute error of the normalized output, and the optimizer is RMSprop. Cell 4 was run in successive stages, with the learning rate reduced as the loss dropped:

0.0035 for 400 epochs, 0.001 for 400, 0.0004 for 400, 0.0001 for 400.

The weights from the epoch of lowest loss were restored. The lowest loss is 0.01181, at epoch 1586, which is below the requested level of 0.014.

### 2.5 Weights and predictions

Tables 2 and 3 are the Part 1 tables for Adnan Ahali.

Table 2: Trained parameters. The rms value is $\sqrt{\overline{E}_3}$ on the normalized output. The Keras loss is the mean absolute error on the same normalized output.

| | First principles | Keras |
|---|---|---|
| $w_{01}$ | 1.2018 | 1.2122 |
| $w_{02}$ | 0.3685 | 0.3580 |
| $w_{03}$ | 0.6805 | 0.7119 |
| $b_1$ | −0.1295 | −0.1437 |
| $w_{12}$ | 0.7054 | 0.7058 |
| $b_2$ | −0.1054 | −0.1104 |
| $w_{23}$ | 0.6931 | 0.6824 |
| $b_3$ | 0.0203 | 0.0229 |
| | rms = 0.01462<br>MAE = 0.01382 | MAE = loss = 0.01181 |

Table 3: Measured $y_3$ and the two predictions, in the original units.

| $x_{01}$ | $x_{02}$ | $x_{03}$ | $y_3$ data | First principles | Keras |
|---|---|---|---|---|---|
| 20.0 | 13.0 | 310.8 | 30.99 | 31.200 | 31.007 |
| 20.0 | 14.5 | 308.0 | 32.20 | 31.706 | 31.484 |
| 20.0 | 15.3 | 306.0 | 31.70 | 31.958 | 31.720 |
| 20.2 | 13.0 | 310.8 | 30.92 | 31.389 | 31.194 |
| 20.0 | 14.5 | 308.0 | 32.40 | 31.706 | 31.484 |
| 20.0 | 15.3 | 306.0 | 31.40 | 31.958 | 31.720 |
| 24.0 | 13.0 | 310.8 | 35.53 | 34.970 | 34.752 |
| 36.0 | 14.4 | 308.1 | 46.41 | 46.749 | 46.432 |

## 2.6 Do the two models agree?

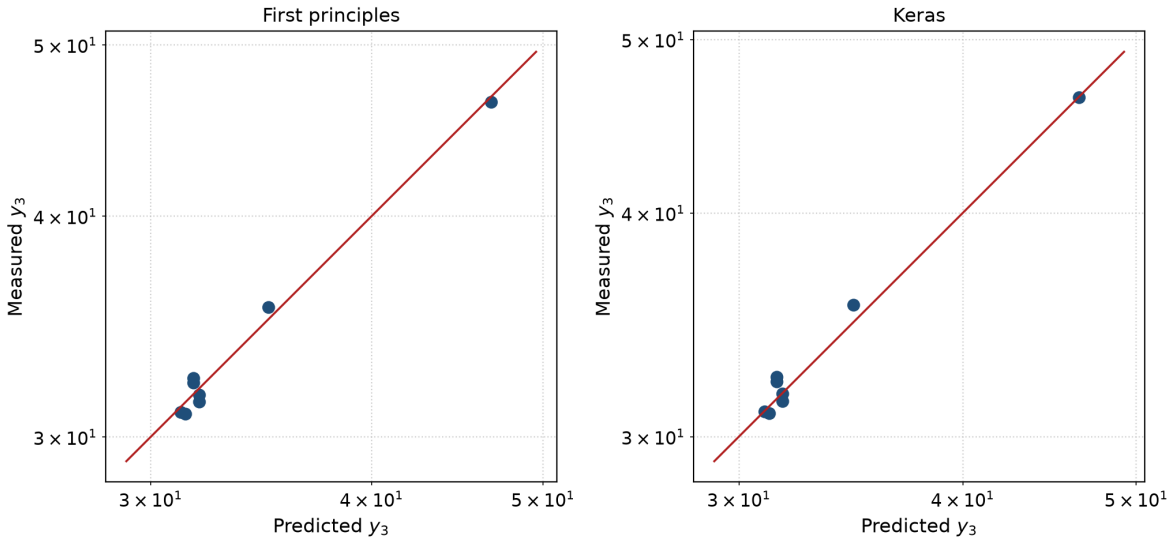



Figure 1: Log–log comparison of predicted $y_3$ (horizontal) with measured $y_3$ (vertical). The line is perfect agreement. Repeated input rows fall on top of each other because each model returns one value per input.

The predictions agree well. On the eight records the two models differ from each other by at most 0.24 in $y_3$, and both follow the measured values, including the point at $x_{01} = 36$. Repeated inputs receive one prediction. For $(20, 14.5, 308)$ both models sit below the two measurements (31.71 and 31.48 against 32.2 and 32.4). For $(20, 15.3, 306)$ the Keras value 31.72 falls between 31.4 and 31.7, while the first-principles value 31.96 sits just above that pair. The three-neuron map is smoothing the local scatter rather than averaging each repeated pair by itself. The normalized MAE values, 0.0138 and 0.0118, are close to each other.

The weights are close in magnitude and in sign, and they are not the same numbers. That is the expected outcome. The two programs minimize different losses: the first-principles code drives the batch-average squared error toward zero with the Newton update (11), while Keras minimizes mean absolute error with RMSprop. The step sizes and the path through parameter space therefore

differ. In addition, while every hidden activation stays in the linear part of the ELU, the three layers collapse to one affine function of the inputs. Several combinations of $(w_{12}, w_{23}, b_2, b_3)$ then produce nearly the same input–output map, so equal predictions do not require equal weights. The meaningful comparison is the map, and on that comparison the two models agree.

### 2.7 Initial weights raised by 20 percent

Task P1.2(d) repeats both trainings from initial weights and biases 1.2 times the specified values, so the start is

$$w_{01} = 1.476,\ w_{02} = 0.480,\ w_{03} = 0.840,\ b_1 = -0.180,$$
$$w_{12} = 0.864,\ b_2 = -0.144,\ w_{23} = 0.840,\ b_3 = 0.012.$$

For the first-principles model the batch error at this start is $\overline{E}_3 = 0.752$, against 0.00225 from the original start. The learning-rate pair used there, 0.015 then 0.001, lets the error fall and then jump back up, because a Newton step divided by a small derivative becomes large. The retained run therefore uses $\gamma = 0.01$ while $\overline{E}_3 \geq 0.05$ and $\gamma = 0.002$ below that. The cutoff 0.00035 is crossed at epoch 2011. The best point, kept rather than the last oscillating step, is

$$\overline{E}_3 = 2.080 \times 10^{-4} \quad \text{at epoch } 2633, \qquad \text{rms} = 0.01442, \qquad \text{MAE} = 0.01296.$$

The mean absolute error is below 0.025. For Keras the stages are 0.0035 (400 epochs), 0.001 (600), 0.0003 (600), and 0.0001 (400). The lowest loss is 0.01190, also below 0.025.

Table 4: Trained weights and biases from the original start and from the start raised by 20 percent.

| | First principles | | Keras | |
|---|---|---|---|---|
| | Original start | +20% start | Original start | +20% start |
| $w_{01}$ | 1.2018 | 1.0316 | 1.2122 | 1.2378 |
| $w_{02}$ | 0.3685 | 0.2579 | 0.3580 | 0.3968 |
| $w_{03}$ | 0.6805 | 0.7817 | 0.7119 | 0.8381 |
| $b_1$ | −0.1295 | −0.1524 | −0.1437 | −0.1907 |
| $w_{12}$ | 0.7054 | 0.7343 | 0.7058 | 0.7090 |
| $b_2$ | −0.1054 | −0.1331 | −0.1104 | −0.1533 |
| $w_{23}$ | 0.6931 | 0.7555 | 0.6824 | 0.6649 |
| $b_3$ | 0.0203 | 0.0204 | 0.0229 | 0.0043 |
| error | $\overline{E}_3 = 0.000214$ | $\overline{E}_3 = 0.000208$ | loss = 0.01181 | loss = 0.01190 |

The fit quality is essentially unchanged. The first-principles rms stays at 0.014, and the Keras loss stays at 0.012. The weights do change. From the raised start the first-principles solution moves $w_{01}$ from 1.202 to 1.032 and $w_{02}$ from 0.368 to 0.258, while $w_{23}$ rises from 0.693 to 0.756. On Keras the largest shift is $w_{03}$, from 0.712 to 0.838. The predictions do not follow those shifts: the two first-principles predictions differ by at most 0.38 in $y_3$, and the two Keras predictions by at most 0.04. Several different parameter vectors implement nearly the same input–output map, so the trained weights are sensitive to the initial condition and the predictions of a trained model are not. The Newton update needs a smaller $\gamma$ when the start is farther away, because its step is divided by the derivative. RMSprop reaches the same conclusion from the raised start with no change of schedule.

# 3 Part 2: hybrid solar gas turbine

The second network maps the operating condition $(T_1, \gamma, \dot{Q}_s)$ to the molar air-to-fuel ratio $\alpha$ and the system efficiency $\eta$. The turbine inlet temperature is held at 1473 K by adjusting the fuel flow, which is why $\alpha$ is an output rather than an input. The training set is the 60 records in `CodeP1.3F26`. Four inlet temperatures (318, 303, 288, and 268 K), propane mole fractions from 0 to 0.5, and solar inputs from 500 to 2500 kW are represented. Two solar values are entered as 2501 kW and one propane fraction as 0.51; those values were kept as recorded.

## 3.1 Median normalization

Each column was divided by its own median. With 60 rows the median is the average of the 30th and 31st sorted entries.

Table 5: Medians used to normalize the turbine data. The placeholder scales in the skeleton (293, 0.25, 1250, 60, 0.4) were replaced by these values. The gamma median happens to equal the placeholder.

| Variable | Median | Central pair |
|---|---|---|
| $T_1$ | 295.5 K | 288 and 303 |
| $\gamma$ | 0.25 | 0.25 and 0.25 |
| $\dot{Q}_s$ | 1500 kW | 1500 and 1500 |
| $\alpha$ | 61.18935 | 60.8067 and 61.572 |
| $\eta$ | 0.432 | 0.4315 and 0.4325 |

After this scaling, inputs and outputs are of order one, so a mean absolute error near 0.05 is small relative to the data. The dimensional arrays are printed before normalization, and the normalized arrays are printed after it, by the first cell of `CodeP1.4F26`.

## 3.2 Network and training

The network required by Task P1.4 is a sequential model with hidden widths 4, 8, and 4, ReLU activations, and a linear output of width 2. The kernel initializer is uniform on $[-0.9, 0.9]$. The loss is the mean absolute error of the two normalized outputs. Updates are full-batch RMSprop, so there is one weight update at the end of each epoch, as the handout describes.

A first pass at the specified learning rate 0.001 does get under the target of 0.04, but the loss remains in the range 0.025–0.05 after a few thousand epochs and depends strongly on the random seed. The model used for every prediction below was trained from seed 2 with the schedule

$$0.005 \text{ (1200 epochs)}, \; 0.001 \text{ (1000)}, \; 0.0003 \text{ (800)}, \; 0.0001 \text{ (600)}.$$

The lowest normalized MAE is

$$\text{loss} = 0.01710 \quad \text{at epoch } 3577 \text{ of } 3600. \tag{13}$$

On the training set this corresponds to an rms error of 3.13 in $\alpha$ and 0.00243 in $\eta$. Figure 2 shows the loss. The drops near epochs 1200 and 2200 occur when the learning rate is reduced.

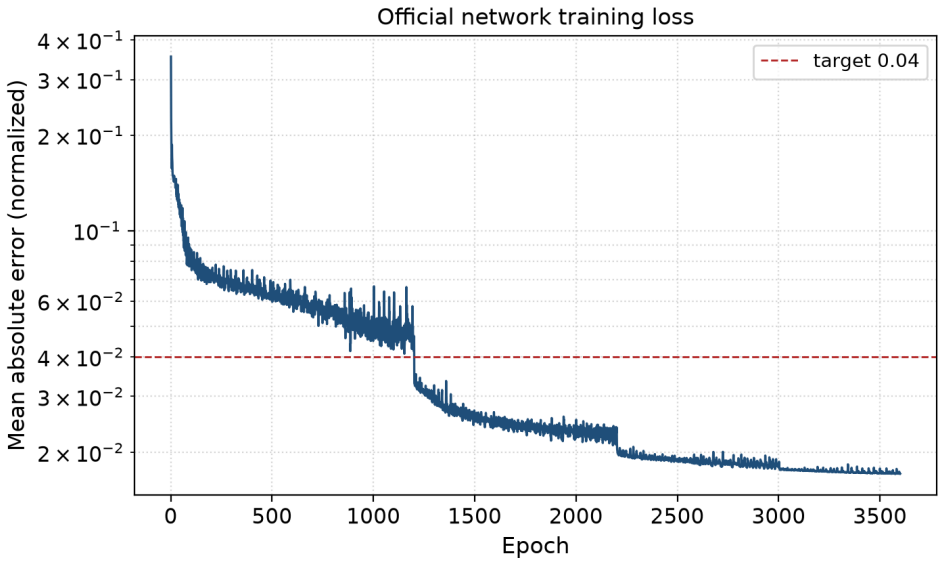



Figure 2: Normalized mean absolute error of the retained turbine network. The horizontal line is the target of 0.04.

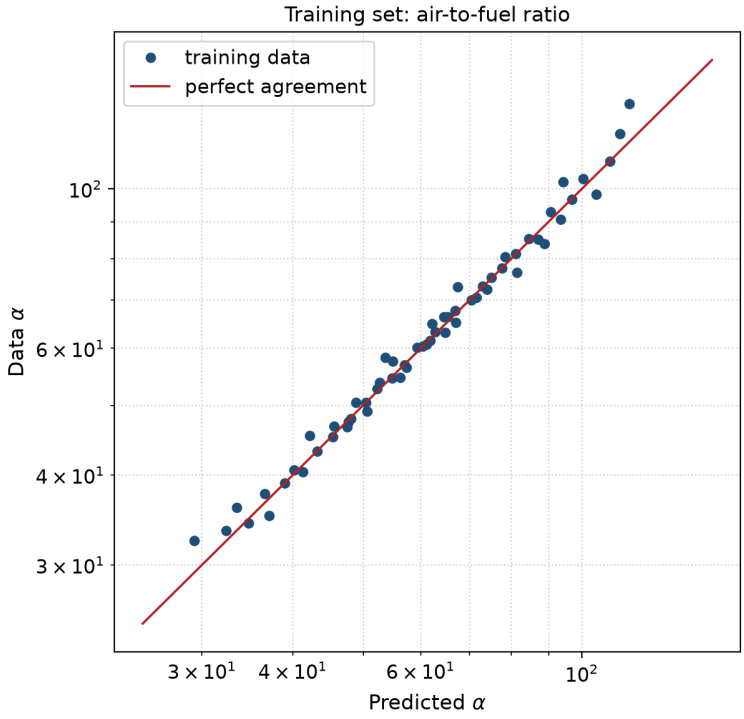



Figure 3: Training-set parity for $\alpha$. Predicted values are on the horizontal axis.

### 3.3 Surface at a propane fraction of 0.25

Figure 4 is the predicted air-to-fuel ratio on $268 < T_1 < 318\,\mathrm{K}$ and $500 < \dot{Q}_s < 2500\,\mathrm{kW}$, with $\gamma$ fixed at 0.25. The surface rises from about $\alpha = 42$ at the cold, low-solar corner to about $\alpha = 94$ at

the hot, high-solar corner. Both inlet temperature and solar input increase $\alpha$. The solar trend is the stronger of the two: at fixed $T_1 = 268\,\mathrm{K}$, raising $\dot{Q}_s$ from 500 to 2500 kW raises the predicted $\alpha$ from 42 to 81. That is the expected direction. Added solar heat leaves less temperature rise to be supplied by the burner, so less fuel is injected and the air-to-fuel ratio increases. The surface is smooth. It does not reproduce the sharp rise in the training data at the single point $T_1 = 318\,\mathrm{K}$, $\gamma = 0.5$, $\dot{Q}_s = 2501\,\mathrm{kW}$, where $\alpha = 131$; that point is outside the $\gamma = 0.25$ slice plotted here and is discussed with the test set.

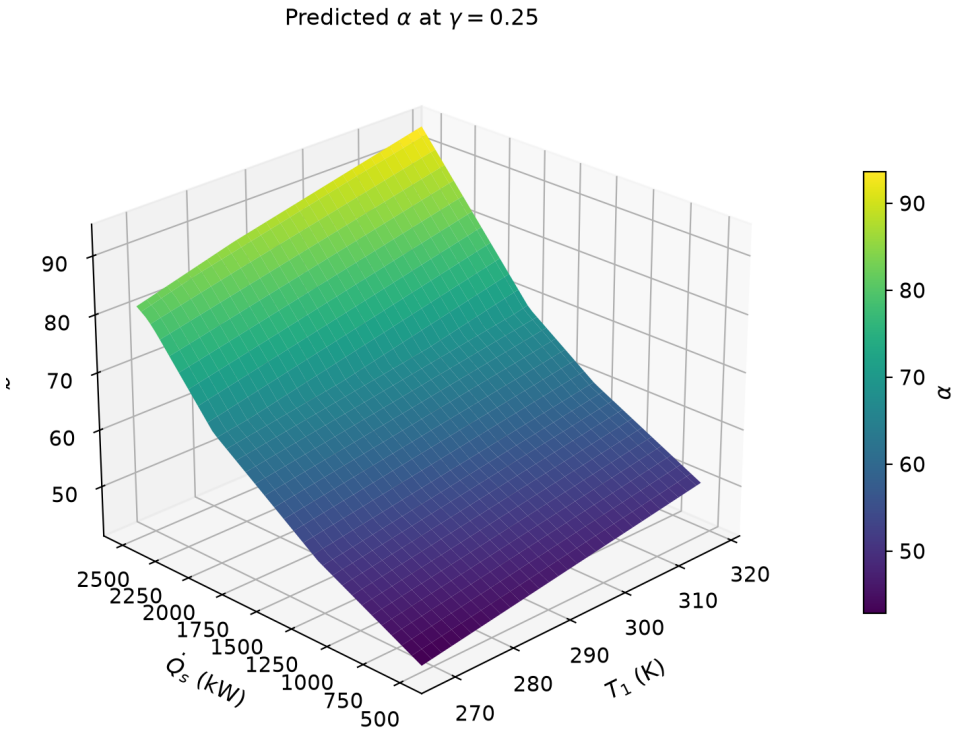



Figure 4: Predicted molar air-to-fuel ratio at propane mole fraction $\gamma = 0.25$.

### 3.4 Design variations

Four additional trainings were run to see which modeling choices actually change the fit. All of them use RMSprop, the same median-normalized data, and an initializer on $[-0.9, 0.9]$.

Table 6: Normalized MAE for the retained network and four variations. The epoch counts are the lengths of those runs, which are shorter than the retained schedule except for the seed-6 case.

| Model | Training | Lowest loss |
|---|---|---|
| ReLU 4–8–4–2, seed 2 (retained) | $0.005 \to 0.0001$, 3600 epochs | 0.01710 |
| ReLU 4–8–4–2, seed 6 | 0.001 then 0.0003, 2400 epochs | 0.02457 |
| ELU 4–8–4–2, seed 2 | $0.005 \to 0.0003$, 1800 epochs | 0.01998 |
| ReLU 8–16–8–2, seed 2 | $0.005 \to 0.0003$, 1600 epochs | 0.01901 |
| ReLU 4–8–4–2, seed 42 | $0.005 \to 0.0003$, 1800 epochs | 0.16307 |

The assigned width is enough. Widening every hidden layer, or replacing ReLU by ELU, changes the loss by only a few thousandths under the budgets in Table 6. The learning rate and the initializer seed matter more. Holding the learning rate at the specified value 0.001 still beats the target of 0.04 (loss 0.0246 from seed 6), and the decreasing schedule from seed 2 reaches 0.017. Seed 42, drawn from the same allowed interval $[-0.9, 0.9]$, stalls at a loss of 0.16. ReLU units that start off for every training input stay off, and that draw never recovered. For this architecture the practical design choices are therefore the learning-rate schedule and a check of more than one initialization, rather than a wider network.

The residual that none of these models removes cleanly is the steep corner of $\alpha$ at high inlet temperature, high propane fraction, and high solar input. There $\alpha$ jumps from 103 at 2000 kW to 131 at 2501 kW. A smooth ReLU surface under-predicts that single jump. Efficiency, which varies only from about 0.38 to 0.48, is fit much more tightly than $\alpha$.

### 3.5 Test set

The 20 test conditions were normalized with the training medians, passed through `model.predict`, and multiplied back by the output medians. Figure 5 is the requested log–log plot of test $\alpha$ against predicted $\alpha$.

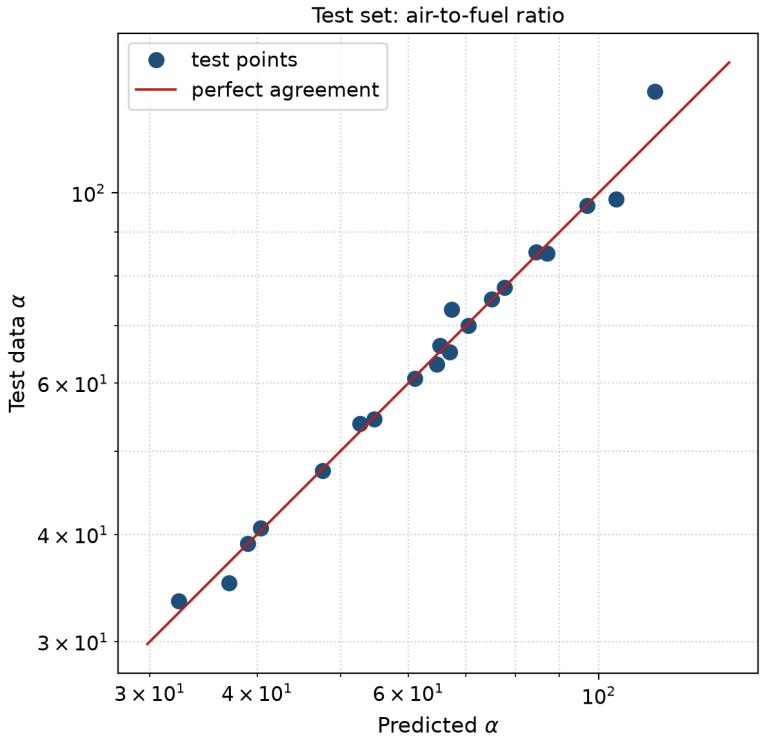



Figure 5: Test-set log–log plot. Predicted $\alpha$ is on the horizontal axis and the test value is on the vertical axis.

Table 7: Test Data 1. Predicted values use the retained network.

| $T_1$ | $\gamma$ | $\dot{Q}_s$ | $\alpha$ data | $\alpha$ pred. | $\eta$ data | $\eta$ pred. |
|---|---|---|---|---|---|---|
| 318 | 0.00 | 500 | 35.13 | 37.11 | 0.3808 | 0.3793 |
| 318 | 0.00 | 1500 | 47.46 | 47.68 | 0.3930 | 0.3897 |
| 318 | 0.00 | 2500 | 73.12 | 67.43 | 0.4061 | 0.4060 |
| 318 | 0.25 | 1500 | 66.34 | 65.35 | 0.4098 | 0.4114 |
| 318 | 0.50 | 500 | 63.09 | 64.80 | 0.4154 | 0.4223 |
| 318 | 0.50 | 1500 | 85.23 | 84.52 | 0.4197 | 0.4215 |
| 318 | 0.50 | 2500 | 131.32 | 116.13 | 0.4242 | 0.4259 |
| 303 | 0.00 | 1000 | 38.99 | 38.98 | 0.4012 | 0.3995 |
| 303 | 0.00 | 2000 | 53.80 | 52.72 | 0.4136 | 0.4131 |
| 303 | 0.25 | 1000 | 54.51 | 54.79 | 0.4215 | 0.4213 |
| 303 | 0.25 | 2000 | 75.22 | 75.01 | 0.4290 | 0.4301 |
| 303 | 0.50 | 1000 | 70.04 | 70.49 | 0.4337 | 0.4341 |
| 303 | 0.50 | 2000 | 96.65 | 96.89 | 0.4382 | 0.4387 |
| 288 | 0.00 | 500 | 33.45 | 32.40 | 0.4091 | 0.4112 |
| 288 | 0.00 | 2500 | 60.80 | 61.07 | 0.4334 | 0.4341 |
| 288 | 0.25 | 2500 | 85.044 | 87.06 | 0.4477 | 0.4465 |
| 288 | 0.50 | 1500 | 77.56 | 77.66 | 0.4516 | 0.4515 |
| 269 | 0.00 | 1500 | 40.68 | 40.35 | 0.4393 | 0.4423 |
| 268 | 0.25 | 2000 | 65.24 | 67.01 | 0.4628 | 0.4651 |
| 268 | 0.50 | 2500 | 98.23 | 104.65 | 0.4760 | 0.4754 |

The rms deviations on this test collection are

$$\mathrm{rms}(\alpha) = 4.02, \qquad \mathrm{rms}(\eta) = 0.00218. \tag{14}$$

The corresponding mean absolute errors are 2.03 in $\alpha$ and 0.00157 in $\eta$. Most points lie on the agreement line. One point dominates the $\alpha$ residual: at $T_1 = 318\,\mathrm{K}$, $\gamma = 0.5$, $\dot{Q}_s = 2500\,\mathrm{kW}$ the test value is 131.32 and the prediction is 116.13. That is the same steep corner already visible in the training data. Efficiency at that point is still predicted to 0.0017. Elsewhere the $\alpha$ errors are a few units, which is a few percent of a typical air-to-fuel ratio near 60. The efficiency model is accurate to a few thousandths on data it did not train on, inside the range of the training inputs.

## 4 Conclusions

The three-neuron ELU network can be trained from the written Newton updates to a batch-average squared error of $2.14 \times 10^{-4}$, below the cutoff 0.00035, without changing the specified initial weights. The Keras model of the same network reaches a normalized mean absolute error of 0.0118. The two predictions agree to a few tenths in $y_3$. Their weights differ because the losses, the optimizers, and the redundant parameterization of a linear ELU chain are different. Raising every initial weight by 20% changes the trained weights of both models and leaves the predictions almost unchanged. The error minimum is therefore not unique.

For the turbine, median normalization and the assigned 4–8–4–2 ReLU network reach a normalized MAE of 0.017, below the target of 0.04. The fit of efficiency is tight on both the training records and the test records (test rms 0.0022). The air-to-fuel ratio is also well predicted except for the steep high-$T_1$, high-$\gamma$, high-$\dot{Q}_s$ corner, which accounts for most of the test rms of 4.02. At $\gamma = 0.25$ the predicted $\alpha$ increases with both inlet temperature and solar input. Among the design changes that were tried, the learning-rate schedule and the initializer seed change the loss more

than replacing ReLU by ELU or widening the layers. One seed inside the allowed initializer range fails to train. Task P1.6 was omitted because the project was done by one student.

# A CodeP1.1F26

```
"""ME249 Project 1, Task P1.1
First-principles backpropagation for the three-neuron network in Figure 1.

The red-box relations (1c)-(1h) and (2c)-(2h) are implemented below.
Initial weights are the values specified in the supplied notebook.
The batch-average squared-error cutoff is 0.00035.
"""

from __future__ import print_function

import math
import os

import matplotlib.pyplot as plt
import numpy as np

# Eight-point set coded in the supplied CodeP1.1 / CodeP1.2 notebooks.
# Columns: x01, x02, x03, y3. Both Part 1 programs use this same set.
RAW = [
    [20.0, 13.0, 310.8, 30.99],
    [20.0, 14.5, 308.0, 32.2],
    [20.0, 15.3, 306.0, 31.7],
    [20.2, 13.0, 310.8, 30.92],
    [20.0, 14.5, 308.0, 32.4],
    [20.0, 15.3, 306.0, 31.4],
    [24.0, 13.0, 310.8, 35.53],
    [36.0, 14.4, 308.1, 46.41],
]

# Reference scales already used to normalize the supplied programs.
SX01, SX02, SX03, SY3 = 20.2, 14.5, 308.0, 32.4

xydata = [
    [row[0] / SX01, row[1] / SX02, row[2] / SX03, row[3] / SY3] for row in RAW
]
print("normalized xydata:")
for row in xydata:
    print(row)

# Specified initial weights and biases. These stay fixed.
w01n = 1.23
w02n = 0.40
w03n = 0.70
b1n = -0.15
w12n = 0.72
b2n = -0.12
w23n = 0.70
b3n = 0.01

# Retain the parameter set with the lowest batch-average squared error.
best_E3 = 1.0e99
best_params = None
```

```
best_epoch = None
stall = 0
first_below = None

for k in range(0, 2500):
    icount = 0
    E3ti = 0.0
    dE3dw01ti = 0.0
    dE3dw02ti = 0.0
    dE3dw03ti = 0.0
    dE3db1ti = 0.0
    dE3dw12ti = 0.0
    dE3db2ti = 0.0
    dE3dw23ti = 0.0
    dE3db3ti = 0.0

    w01 = w01n
    w02 = w02n
    w03 = w03n
    b1 = b1n
    w12 = w12n
    b2 = b2n
    w23 = w23n
    b3 = b3n

    for i in range(0, 8):
        # ELU activation and its derivative at each neuron.
        z1 = w01 * xydata[i][0] + w02 * xydata[i][1] + w03 * xydata[i][2] + b1
        sig1 = z1
        sigp1 = 1.0
        if z1 < 0.0:
            sig1 = math.exp(z1) - 1.0
            sigp1 = math.exp(z1)
        a1 = sig1

        z2 = w12 * a1 + b2
        sig2 = z2
        sigp2 = 1.0
        if z2 < 0.0:
            sig2 = math.exp(z2) - 1.0
            sigp2 = math.exp(z2)
        a2 = sig2

        z3 = w23 * a2 + b3
        sig3 = z3
        sigp3 = 1.0
        if z3 < 0.0:
            sig3 = math.exp(z3) - 1.0
            sigp3 = math.exp(z3)
        a3 = sig3

        # Squared error and Eqs. (2a)-(2h).
        # dE3/da3 = 2 (a3 - y3) multiplies every chain-rule factor.
        E3ti = E3ti + (a3 - xydata[i][3]) * (a3 - xydata[i][3])
        dE3da3 = 2.0 * (a3 - xydata[i][3])

        dE3dw01ti = dE3dw01ti + dE3da3 * sigp3 * w23 * sigp2 * w12 * sigp1 * xydata[i][0]
        dE3dw02ti = dE3dw02ti + dE3da3 * sigp3 * w23 * sigp2 * w12 * sigp1 * xydata[i][1]
        # (2c)
```

```
        dE3dw03ti = dE3dw03ti + dE3da3 * sigp3 * w23 * sigp2 * w12 * sigp1 * xydata[i][2]
        # (2d)
        dE3db1ti = dE3db1ti + dE3da3 * sigp3 * w23 * sigp2 * w12 * sigp1
        # (2e)
        dE3dw12ti = dE3dw12ti + dE3da3 * sigp3 * w23 * sigp2 * a1
        # (2f)
        dE3db2ti = dE3db2ti + dE3da3 * sigp3 * w23 * sigp2
        # (2g)
        dE3dw23ti = dE3dw23ti + dE3da3 * sigp3 * a2
        # (2h)
        dE3db3ti = dE3db3ti + dE3da3 * sigp3

        icount = i + 1

    E3 = E3ti / icount
    dE3dw01 = dE3dw01ti / icount
    dE3dw02 = dE3dw02ti / icount
    dE3dw03 = dE3dw03ti / icount
    dE3db1 = dE3db1ti / icount
    dE3dw12 = dE3dw12ti / icount
    dE3db2 = dE3db2ti / icount
    dE3dw23 = dE3dw23ti / icount
    dE3db3 = dE3db3ti / icount

    if E3 < best_E3:
        best_E3 = E3
        best_epoch = k + 1
        best_params = (w01, w02, w03, b1, w12, b2, w23, b3, E3, icount)
        stall = 0
    else:
        stall = stall + 1

    if first_below is None and E3 < 0.00035:
        first_below = k + 1

    # Learning rate on the order of 1/8, reduced near the minimum.
    gam = 0.015
    if E3 < 0.001:
        gam = 0.001

    # Batch updates (3a)-(3h), which are the red-box relations (1c)-(1h)
    # written with batch-averaged error and derivatives.
    w01n = w01 + gam * (-E3) / dE3dw01
    w02n = w02 + gam * (-E3) / dE3dw02
    w03n = w03 + gam * (-E3) / dE3dw03
    b1n = b1 + gam * (-E3) / dE3db1
    w12n = w12 + gam * (-E3) / dE3dw12
    b2n = b2 + gam * (-E3) / dE3db2
    w23n = w23 + gam * (-E3) / dE3dw23
    b3n = b3 + gam * (-E3) / dE3db3

    if k % 50 == 0 or E3 < 0.00035 and stall == 0:
        print("last w01, w02, w03, w12, w23:")
        print("last b1, b2, b3:")
        print(w01, w02, w03, w12, w23)
        print(b1, b2, b3)
        print("E3 = ", E3, "icount =", icount)
        print("next ws:", w01n, w02n, w03n, w12n, w23n)
        print("next bs:", b1n, b2n, b3n)
```

```
171
172     # Cutoff lowered from 0.001 to 0.00035. Training continues until the
173     # error has stopped improving, and the best parameter set is restored.
174     if E3 < 0.00035 and stall >= 250:
175         break
176
177 w01, w02, w03, b1, w12, b2, w23, b3, E3, icount = best_params
178 rms = math.sqrt(E3)
179
180 print("==============================")
181 print("last w01, w02, w03, w12, w23:")
182 print("last b1, b2, b3:")
183 print(w01, w02, w03, w12, w23)
184 print(b1, b2, b3)
185 print("E3 = ", E3, "icount =", icount)
186 print("rms = sqrt(E3) =", rms)
187 print("first epoch with E3 < 0.00035:", first_below)
188 print("epoch of best E3:", best_epoch)
189
190 abs_err = []
191 pred_phys = []
192 print("x01, x02, x03, y3(data), ypredicted:")
193 for i in range(0, 8):
194     z1 = w01 * xydata[i][0] + w02 * xydata[i][1] + w03 * xydata[i][2] + b1
195     sig1 = z1 if z1 >= 0.0 else math.exp(z1) - 1.0
196     a1 = sig1
197     z2 = w12 * a1 + b2
198     sig2 = z2 if z2 >= 0.0 else math.exp(z2) - 1.0
199     a2 = sig2
200     z3 = w23 * a2 + b3
201     sig3 = z3 if z3 >= 0.0 else math.exp(z3) - 1.0
202     a3 = sig3
203     yhat = a3 * SY3
204     pred_phys.append(yhat)
205     abs_err.append(abs(a3 - xydata[i][3]))
206     print(RAW[i][0], RAW[i][1], RAW[i][2], RAW[i][3], yhat)
207
208 print("mae =", sum(abs_err) / len(abs_err))
209
210 measured = np.array([row[3] for row in RAW])
211 predicted = np.array(pred_phys)
212 fig, ax = plt.subplots(figsize=(6.2, 6.0))
213 ax.loglog(predicted, measured, "o", ms=8, color="#1f4e79", label="data points")
214 lo = min(predicted.min(), measured.min()) * 0.94
215 hi = max(predicted.max(), measured.max()) * 1.06
216 ax.loglog([lo, hi], [lo, hi], color="#b22222", lw=1.3, label="perfect agreement")
217 ax.set_xlabel("Predicted y3")
218 ax.set_ylabel("Measured y3")
219 ax.set_title("First-principles network")
220 ax.grid(True, which="both", ls=":", alpha=0.6)
221 ax.legend(loc="upper left")
222 fig.tight_layout()
223 out_dir = os.path.join(os.path.dirname(__file__), "..", "figures")
224 os.makedirs(out_dir, exist_ok=True)
225 fig.savefig(os.path.join(out_dir, "p1_loglog_first_principles.png"))
226
227 # Task P1.2(d). Same update, initial weights and biases 20 percent higher.
228 # The schedule used for the original start makes the error jump back up from
229 # this farther start, so the learning rate is kept smaller.
```

```
print("---- Task P1.2(d): initial weights +20% ----")
w01n, w02n, w03n = 1.23 * 1.2, 0.40 * 1.2, 0.70 * 1.2
b1n = -0.15 * 1.2
w12n, b2n = 0.72 * 1.2, -0.12 * 1.2
w23n, b3n = 0.70 * 1.2, 0.01 * 1.2
best_E3 = 1.0e99
best_params = None
best_epoch = None
stall = 0
first_below = None
for k in range(0, 4000):
    E3ti = 0.0
    dsum = [0.0] * 8
    w01, w02, w03, b1 = w01n, w02n, w03n, b1n
    w12, b2, w23, b3 = w12n, b2n, w23n, b3n
    for i in range(0, 8):
        z1 = w01 * xydata[i][0] + w02 * xydata[i][1] + w03 * xydata[i][2] + b1
        a1, sigp1 = (z1, 1.0) if z1 >= 0.0 else (math.exp(z1) - 1.0, math.exp(z1))
        z2 = w12 * a1 + b2
        a2, sigp2 = (z2, 1.0) if z2 >= 0.0 else (math.exp(z2) - 1.0, math.exp(z2))
        z3 = w23 * a2 + b3
        a3, sigp3 = (z3, 1.0) if z3 >= 0.0 else (math.exp(z3) - 1.0, math.exp(z3))
        E3ti += (a3 - xydata[i][3]) ** 2
        dE3da3 = 2.0 * (a3 - xydata[i][3])
        g3 = dE3da3 * sigp3
        g2 = g3 * w23 * sigp2
        g1 = g2 * w12 * sigp1
        dsum[0] += g1 * xydata[i][0]
        dsum[1] += g1 * xydata[i][1]
        dsum[2] += g1 * xydata[i][2]
        dsum[3] += g1
        dsum[4] += g2 * a1
        dsum[5] += g2
        dsum[6] += g3 * a2
        dsum[7] += g3
    E3 = E3ti / 8.0
    deriv = [v / 8.0 for v in dsum]
    if E3 < best_E3:
        best_E3 = E3
        best_epoch = k + 1
        best_params = (w01, w02, w03, b1, w12, b2, w23, b3, E3)
        stall = 0
    else:
        stall += 1
    if first_below is None and E3 < 0.00035:
        first_below = k + 1
    gam = 0.002 if E3 < 0.05 else 0.01
    step = [gam * (-E3) / p for p in deriv]
    if max(abs(s) for s in step) > 2.0:
        print("stopped: step too large at epoch", k + 1)
        break
    w01n, w02n, w03n, b1n, w12n, b2n, w23n, b3n = [
        p + s for p, s in zip((w01, w02, w03, b1, w12, b2, w23, b3), step)
    ]
    if first_below is not None and stall >= 300:
        break

w01, w02, w03, b1, w12, b2, w23, b3, E3 = best_params
print("w01, w02, w03, b1, w12, b2, w23, b3:")
```

```
print(w01, w02, w03, b1, w12, b2, w23, b3)
print("E3 =", E3, "rms =", math.sqrt(E3), "epoch =", best_epoch)
print("first epoch with E3 < 0.00035:", first_below)
abs_err = []
print("x01, x02, x03, y3(data), ypredicted:")
for i in range(0, 8):
    z1 = w01 * xydata[i][0] + w02 * xydata[i][1] + w03 * xydata[i][2] + b1
    a1 = z1 if z1 >= 0.0 else math.exp(z1) - 1.0
    z2 = w12 * a1 + b2
    a2 = z2 if z2 >= 0.0 else math.exp(z2) - 1.0
    z3 = w23 * a2 + b3
    a3 = z3 if z3 >= 0.0 else math.exp(z3) - 1.0
    abs_err.append(abs(a3 - xydata[i][3]))
    print(RAW[i][0], RAW[i][1], RAW[i][2], RAW[i][3], a3 * SY3)
print("mae =", sum(abs_err) / len(abs_err))
plt.show()
```

# B CodeP1.2F26

```
"""ME249 Project 1, Task P1.2
Keras model of the same three-neuron ELU network used in Task P1.1.

Cell layout follows the supplied notebook:
  cell 1 data, normalized the same way as the first-principles model
  cell 2 network and the specified initial weights
  cell 3 RMSprop learning rate
  cell 4 successive training runs; the lowest-loss weights are kept
  cell 5 weights, biases, and predictions
  cell 6 Task P1.2(d), initial weights raised by 20 percent
"""

from __future__ import print_function

import os

os.environ["KMP_DUPLICATE_LIB_OK"] = "True"
os.environ["TF_CPP_MIN_LOG_LEVEL"] = "2"

import keras
import numpy as np
import tensorflow as tf

# Same raw records as CodeP1.1F26.
RAW = np.array(
    [
        [20.0, 13.0, 310.8, 30.99],
        [20.0, 14.5, 308.0, 32.2],
        [20.0, 15.3, 306.0, 31.7],
        [20.2, 13.0, 310.8, 30.92],
        [20.0, 14.5, 308.0, 32.4],
        [20.0, 15.3, 306.0, 31.4],
        [24.0, 13.0, 310.8, 35.53],
        [36.0, 14.4, 308.1, 46.41],
    ],
    dtype=np.float64,
)
```

```
SX = np.array([20.2, 14.5, 308.0])
SY = 32.4
xarray = (RAW[:, :3] / SX).astype(np.float32)
yarray = (RAW[:, 3] / SY).astype(np.float32)
print("x01/20.2, x02/14.5, x03/308.0, y3/32.4")
for i in range(len(RAW)):
    print(float(xarray[i, 0]), float(xarray[i, 1]), float(xarray[i, 2]), float(yarray[i]))

W0 = np.array([1.23, 0.40, 0.70, -0.15, 0.72, -0.12, 0.70, 0.01], dtype=np.float64)


def build_model(scale):
    tf.keras.utils.set_random_seed(1)
    initializer = keras.initializers.RandomUniform(minval=-0.2, maxval=1.2, seed=1)
    model = keras.Sequential(
        [
            keras.layers.Input(shape=(3,)),
            keras.layers.Dense(1, activation="elu", kernel_initializer=initializer, name="
                dense_one"),
            keras.layers.Dense(1, activation="elu", kernel_initializer=initializer, name="
                dense_two"),
            keras.layers.Dense(1, activation="elu", kernel_initializer=initializer, name="
                dense_three"),
        ]
    )
    vals = W0 * scale
    model.layers[0].set_weights(
        [vals[:3].astype(np.float32).reshape(3, 1), np.array([vals[3]], dtype=np.float32)]
    )
    model.layers[1].set_weights(
        [np.array([[vals[4]]], dtype=np.float32), np.array([vals[5]], dtype=np.float32)]
    )
    model.layers[2].set_weights(
        [np.array([[vals[6]]], dtype=np.float32), np.array([vals[7]], dtype=np.float32)]
    )
    return model


class BestWeights(keras.callbacks.Callback):
    """Keep the weights from the epoch with the lowest loss."""

    def __init__(self):
        super().__init__()
        self.best = 1.0e99
        self.weights = None
        self.best_epoch = 0
        self.seen = 0

    def on_epoch_end(self, epoch, logs=None):
        self.seen += 1
        loss = float(logs.get("loss"))
        if loss < self.best:
            self.best = loss
            self.best_epoch = self.seen
            self.weights = self.model.get_weights()


def train(scale, stages):
    model = build_model(scale)
```

```
    tracker = BestWeights()
    for lr, epochs in stages:
        es = keras.callbacks.EarlyStopping(
            monitor="loss", mode="min", patience=80, restore_best_weights=False, verbose=0
        )
        model.compile(
            loss="mean_absolute_error",
            optimizer=keras.optimizers.RMSprop(learning_rate=lr),
        )
        print("learning rate", lr, "epochs", epochs)
        model.fit(
            xarray,
            yarray,
            epochs=epochs,
            batch_size=len(xarray),
            verbose=0,
            callbacks=[tracker, es],
        )
    model.set_weights(tracker.weights)
    return model, tracker.best, tracker.best_epoch


def report(model, tag):
    pred = model.predict(xarray, verbose=0).ravel()
    mae = float(np.mean(np.abs(pred - yarray)))
    w01 = float(model.layers[0].get_weights()[0][0, 0])
    w02 = float(model.layers[0].get_weights()[0][1, 0])
    w03 = float(model.layers[0].get_weights()[0][2, 0])
    b1 = float(model.layers[0].get_weights()[1][0])
    w12 = float(model.layers[1].get_weights()[0][0, 0])
    b2 = float(model.layers[1].get_weights()[1][0])
    w23 = float(model.layers[2].get_weights()[0][0, 0])
    b3 = float(model.layers[2].get_weights()[1][0])
    print("----", tag, "----")
    print("w01 =", w01, "w02 =", w02, "w03 =", w03)
    print("b1 =", b1)
    print("w12 =", w12, "b2 =", b2)
    print("w23 =", w23, "b3 =", b3)
    print("mae = loss =", mae)
    print("x01, x02, x03, y3, a3*32.4")
    for i in range(8):
        print(RAW[i, 0], RAW[i, 1], RAW[i, 2], RAW[i, 3], float(pred[i] * SY))
    return pred * SY


# Task P1.2(a,b). Learning rate is reduced as the loss gets smaller.
# Each stage continues from the weights left by the previous stage.
nominal_stages = [(0.0035, 400), (0.001, 400), (0.0004, 400), (0.0001, 400)]
model, best_loss, best_epoch = train(1.0, nominal_stages)
print("best epoch =", best_epoch)
print("smallest loss =", best_loss)
pred_nominal = report(model, "nominal initial weights")

# Task P1.2(d). A fresh network, initial weights 20 percent higher.
model20, best_loss20, best_epoch20 = train(
    1.2, [(0.0035, 400), (0.001, 600), (0.0003, 600), (0.0001, 400)]
)
print("best epoch (+20%) =", best_epoch20)
print("smallest loss (+20%) =", best_loss20)
```

```
pred20 = report(model20, "initial weights +20%")

import matplotlib.pyplot as plt

measured = RAW[:, 3]
fig, axes = plt.subplots(1, 2, figsize=(10.4, 5.1))
for ax, pred, title in (
    (axes[0], pred_nominal, "Keras, nominal start"),
    (axes[1], pred20, "Keras, start +20%"),
):
    ax.loglog(pred, measured, "o", ms=7, color="#1f4e79")
    lo = min(np.min(pred), measured.min()) * 0.94
    hi = max(np.max(pred), measured.max()) * 1.06
    ax.loglog([lo, hi], [lo, hi], color="#b22222", lw=1.3)
    ax.set_title(title)
    ax.set_xlabel("Predicted y3")
    ax.set_ylabel("Measured y3")
    ax.grid(True, which="both", ls=":", alpha=0.6)
fig.tight_layout()
out_dir = os.path.join(os.path.dirname(__file__), "..", "figures")
os.makedirs(out_dir, exist_ok=True)
fig.savefig(os.path.join(out_dir, "p1_loglog_keras.png"))
plt.show()
```

# C CodeP1.3F26

```
"""ME249 Project 1, CodeP1.3F26
Data arrays for the hybrid solar / fossil-fuel gas turbine.

xdata columns: T1 (K), propane mole fraction gamma, solar input Qs (kW)
ydata columns: air-to-fuel ratio alpha, system efficiency eta
"""

xdata = [
    [318, 0, 500],
    [318, 0, 1000],
    [318, 0, 1500],
    [318, 0, 2000],
    [318, 0, 2500],
    [318, 0.25, 500],
    [318, 0.25, 1000],
    [318, 0.25, 1500],
    [318, 0.25, 2000],
    [318, 0.25, 2500],
    [318, 0.5, 500],
    [318, 0.5, 1000],
    [318, 0.5, 1500],
    [318, 0.5, 2000],
    [318, 0.5, 2501],
    [303, 0, 500],
    [303, 0, 1000],
    [303, 0, 1500],
    [303, 0, 2000],
    [303, 0, 2500],
    [303, 0.25, 500],
    [303, 0.25, 1000],
```

```
    [303, 0.25, 1500],
    [303, 0.25, 2000],
    [303, 0.25, 2500],
    [303, 0.5, 500],
    [303, 0.5, 1000],
    [303, 0.5, 1500],
    [303, 0.5, 2000],
    [303, 0.5, 2501],
    [288, 0, 500],
    [288, 0, 1000],
    [288, 0, 1500],
    [288, 0, 2000],
    [288, 0, 2500],
    [288, 0.25, 500],
    [288, 0.25, 1000],
    [288, 0.25, 1500],
    [288, 0.25, 2000],
    [288, 0.25, 2500],
    [288, 0.51, 500],
    [288, 0.5, 1000],
    [288, 0.5, 1500],
    [288, 0.5, 2000],
    [288, 0.5, 2500],
    [268, 0, 500],
    [268, 0, 1000],
    [268, 0, 1500],
    [268, 0, 2000],
    [268, 0, 2500],
    [268, 0.25, 500],
    [268, 0.25, 1000],
    [268, 0.25, 1500],
    [268, 0.25, 2000],
    [268, 0.25, 2500],
    [268, 0.5, 500],
    [268, 0.5, 1000],
    [268, 0.5, 1500],
    [268, 0.5, 2000],
    [268, 0.5, 2500],
]

ydata = [
    [35.1316, 0.3808],
    [40.3764, 0.38686],
    [47.462, 0.393],
    [57.5639, 0.39949],
    [73.1286, 0.40612],
    [49.111, 0.4023],
    [56.4428, 0.40605],
    [66.3479, 0.4098],
    [80.4695, 0.4133],
    [102.2276, 0.4175],
    [63.0904, 0.4154],
    [72.5092, 0.4175],
    [85.2338, 0.4197],
    [103.375, 0.42192],
    [131.3266, 0.4242],
    [34.273, 0.3952],
    [38.99026, 0.4012],
    [45.2133, 0.4073],
```

```
    [53.8, 0.4136],
    [66.413, 0.4201],
    [47.922, 0.4178],
    [54.518, 0.4215],
    [63.22, 0.4252],
    [75.226, 0.429],
    [92.862, 0.4329],
    [61.572, 0.4315],
    [70.0468, 0.43373],
    [81.226, 0.43597],
    [96.653, 0.4382],
    [119.3124, 0.44045],
    [33.4521, 0.40913],
    [37.6911, 0.415],
    [43.1602, 0.4209],
    [50.4858, 0.4271],
    [60.8067, 0.4334],
    [46.7865, 0.4328],
    [52.7151, 0.43646],
    [60.36425, 0.44016],
    [70.6099, 0.443926],
    [85.0447, 0.4477],
    [60.1208, 0.44721],
    [67.7391, 0.4494],
    [77.5683, 0.4516],
    [90.7341, 0.4538],
    [109.2828, 0.456],
    [32.4123, 0.42694],
    [36.0807, 0.4325],
    [40.6854, 0.4383],
    [46.6374, 0.4442],
    [54.6293, 0.4503],
    [45.3472, 0.4519],
    [50.4796, 0.4555],
    [56.9219, 0.4591],
    [65.2492, 0.4628],
    [76.4304, 0.4665],
    [58.2822, 0.4672],
    [64.8785, 0.4693],
    [73.1584, 0.4715],
    [83.861, 0.4738],
    [98.2316, 0.476],
]

print("dimensional xdata, n =", len(xdata))
for row in xdata:
    print(row)
print("dimensional ydata, n =", len(ydata))
for row in ydata:
    print(row)
```

# D CodeP1.4F26

```
"""ME249 Project 1, Tasks P1.3 through P1.5
Keras model of the hybrid solar / fossil-fuel gas turbine.
Task P1.6 is omitted because this project was done by one student.
```

```
4
5  Cell 1 full data set, medians, normalization
6  Cell 2 network 4-8-4-2, ReLU hidden layers, linear output
7  Cell 3 RMSprop, learning rate starts at the value used for the retained model
8  Cell 4 training; lowest normalized MAE is kept
9  Cell 5 training parity plot and the alpha surface at gamma = 0.25
10 Cell 6 Task P1.5 test set
11 """
12
13 import os
14 os.environ["KMP_DUPLICATE_LIB_OK"] = "True"
15 os.environ["TF_CPP_MIN_LOG_LEVEL"] = "2"
16
17 import keras
18 import matplotlib.pyplot as plt
19 import numpy as np
20 import tensorflow as tf
21 from mpl_toolkits.mplot3d import Axes3D # noqa: F401
22
23 # --- cell 1: data from CodeP1.3F26, then median normalization ---
24 xdata = [
25     [318, 0, 500],
26     [318, 0, 1000],
27     [318, 0, 1500],
28     [318, 0, 2000],
29     [318, 0, 2500],
30     [318, 0.25, 500],
31     [318, 0.25, 1000],
32     [318, 0.25, 1500],
33     [318, 0.25, 2000],
34     [318, 0.25, 2500],
35     [318, 0.5, 500],
36     [318, 0.5, 1000],
37     [318, 0.5, 1500],
38     [318, 0.5, 2000],
39     [318, 0.5, 2501],
40     [303, 0, 500],
41     [303, 0, 1000],
42     [303, 0, 1500],
43     [303, 0, 2000],
44     [303, 0, 2500],
45     [303, 0.25, 500],
46     [303, 0.25, 1000],
47     [303, 0.25, 1500],
48     [303, 0.25, 2000],
49     [303, 0.25, 2500],
50     [303, 0.5, 500],
51     [303, 0.5, 1000],
52     [303, 0.5, 1500],
53     [303, 0.5, 2000],
54     [303, 0.5, 2501],
55     [288, 0, 500],
56     [288, 0, 1000],
57     [288, 0, 1500],
58     [288, 0, 2000],
59     [288, 0, 2500],
60     [288, 0.25, 500],
61     [288, 0.25, 1000],
62     [288, 0.25, 1500],
```

```
    [288, 0.25, 2000],
    [288, 0.25, 2500],
    [288, 0.51, 500],
    [288, 0.5, 1000],
    [288, 0.5, 1500],
    [288, 0.5, 2000],
    [288, 0.5, 2500],
    [268, 0, 500],
    [268, 0, 1000],
    [268, 0, 1500],
    [268, 0, 2000],
    [268, 0, 2500],
    [268, 0.25, 500],
    [268, 0.25, 1000],
    [268, 0.25, 1500],
    [268, 0.25, 2000],
    [268, 0.25, 2500],
    [268, 0.5, 500],
    [268, 0.5, 1000],
    [268, 0.5, 1500],
    [268, 0.5, 2000],
    [268, 0.5, 2500],
]

ydata = [
    [35.1316, 0.3808],
    [40.3764, 0.38686],
    [47.462, 0.393],
    [57.5639, 0.39949],
    [73.1286, 0.40612],
    [49.111, 0.4023],
    [56.4428, 0.40605],
    [66.3479, 0.4098],
    [80.4695, 0.4133],
    [102.2276, 0.4175],
    [63.0904, 0.4154],
    [72.5092, 0.4175],
    [85.2338, 0.4197],
    [103.375, 0.42192],
    [131.3266, 0.4242],
    [34.273, 0.3952],
    [38.99026, 0.4012],
    [45.2133, 0.4073],
    [53.8, 0.4136],
    [66.413, 0.4201],
    [47.922, 0.4178],
    [54.518, 0.4215],
    [63.22, 0.4252],
    [75.226, 0.429],
    [92.862, 0.4329],
    [61.572, 0.4315],
    [70.0468, 0.43373],
    [81.226, 0.43597],
    [96.653, 0.4382],
    [119.3124, 0.44045],
    [33.4521, 0.40913],
    [37.6911, 0.415],
    [43.1602, 0.4209],
    [50.4858, 0.4271],
```

```
    [60.8067, 0.4334],
    [46.7865, 0.4328],
    [52.7151, 0.43646],
    [60.36425, 0.44016],
    [70.6099, 0.443926],
    [85.0447, 0.4477],
    [60.1208, 0.44721],
    [67.7391, 0.4494],
    [77.5683, 0.4516],
    [90.7341, 0.4538],
    [109.2828, 0.456],
    [32.4123, 0.42694],
    [36.0807, 0.4325],
    [40.6854, 0.4383],
    [46.6374, 0.4442],
    [54.6293, 0.4503],
    [45.3472, 0.4519],
    [50.4796, 0.4555],
    [56.9219, 0.4591],
    [65.2492, 0.4628],
    [76.4304, 0.4665],
    [58.2822, 0.4672],
    [64.8785, 0.4693],
    [73.1584, 0.4715],
    [83.861, 0.4738],
    [98.2316, 0.476],
]

x_raw = np.array(xdata, dtype=float)
y_raw = np.array(ydata, dtype=float)
print("dimensional xdata")
print(x_raw)
print("dimensional ydata")
print(y_raw)

# Even number of rows: the median is the average of the two central values.
med_x = np.median(x_raw, axis=0)
med_y = np.median(y_raw, axis=0)
Tmed, gamed, qsmed = med_x
almed, efmed = med_y
print("medians T1, gamma, Qs, alpha, eta")
print(Tmed, gamed, qsmed, almed, efmed)

x_norm = x_raw / med_x
y_norm = y_raw / med_y
print("normalized xdata")
print(x_norm)
print("normalized ydata")
print(y_norm)

xarray = x_norm.astype(np.float32)
yarray = y_norm.astype(np.float32)

# --- cell 2: 4, 8, 4, 2 network ---
SEED = 2
tf.keras.utils.set_random_seed(SEED)
initializer = keras.initializers.RandomUniform(minval=-0.9, maxval=0.9, seed=SEED)
model = keras.Sequential([
    keras.layers.Input(shape=(3,)),
```

```
    keras.layers.Dense(4, activation="relu", kernel_initializer=initializer),
    keras.layers.Dense(8, activation="relu", kernel_initializer=initializer),
    keras.layers.Dense(4, activation="relu", kernel_initializer=initializer),
    keras.layers.Dense(2, kernel_initializer=initializer),
])
model.summary()

# --- cell 3: learning rate. The retained schedule begins at 0.005 ---
# Task P1.4 first asks for 0.001. A pass at 0.001 is reported as a
# design variation in the written report. The schedule below is the one
# that produced the model used for Tasks P1.5 and P1.6.
learning_rate = 0.005
rms = keras.optimizers.RMSprop(learning_rate=learning_rate)
model.compile(loss="mean_absolute_error", optimizer=rms)

# --- cell 4: successive runs, full batch, keep the lowest loss ---
class BestWeights(keras.callbacks.Callback):
    def __init__(self):
        super().__init__()
        self.best = 1.0e99
        self.weights = None
        self.best_epoch = 0
        self.seen = 0

    def on_epoch_end(self, epoch, logs=None):
        self.seen += 1
        loss = float(logs["loss"])
        if loss < self.best:
            self.best = loss
            self.best_epoch = self.seen
            self.weights = self.model.get_weights()

stages = [(0.005, 1200), (0.001, 1000), (0.0003, 800), (0.0001, 600)]
tracker = BestWeights()
history = []
for lr, epochs in stages:
    model.compile(
        loss="mean_absolute_error",
        optimizer=keras.optimizers.RMSprop(learning_rate=lr),
    )
    print("learning rate", lr, "epochs", epochs)
    hist = model.fit(
        xarray, yarray, epochs=epochs, batch_size=len(xarray), verbose=0, callbacks=[tracker]
    )
    history.extend(hist.history["loss"])
model.set_weights(tracker.weights)
print("best epoch =", tracker.best_epoch)
print("smallest loss =", tracker.best)
model.save(os.path.join(os.path.dirname(__file__), "..", "results", "turbine_model_rerun.keras")
    )

fig, ax = plt.subplots(figsize=(7.2, 4.4))
ax.plot(np.arange(1, len(history) + 1), history, color="#1f4e79", lw=1.1)
ax.axhline(0.04, color="#b22222", ls="--", lw=1, label="target 0.04")
ax.set_xlabel("Epoch")
ax.set_ylabel("Mean absolute error (normalized)")
ax.set_title("Training loss")
ax.set_yscale("log")
ax.grid(True, which="both", ls=":", alpha=0.5)
```

```
ax.legend()
fig_dir = os.path.join(os.path.dirname(__file__), "..", "figures")
os.makedirs(fig_dir, exist_ok=True)
fig.tight_layout()
fig.savefig(os.path.join(fig_dir, "p2_loss_history.png"))

def predict_physical(x_phys):
    xn = (np.array(x_phys, dtype=float) / med_x).astype(np.float32)
    return model.predict(xn, verbose=0) * med_y

# --- cell 5: training comparison and surface at gamma = 0.25 ---
pred_train = predict_physical(x_raw)
print("row [0] data: T1 =", x_raw[0, 0], ", gam =", x_raw[0, 1],
      ", qsol =", x_raw[0, 2], ", alpha =", y_raw[0, 0],
      ", predicted alpha =", pred_train[0, 0])

fig, ax = plt.subplots(figsize=(6.2, 6.0))
ax.loglog(pred_train[:, 0], y_raw[:, 0], "o", ms=5, color="#1f4e79", label="training data")
lo = min(pred_train[:, 0].min(), y_raw[:, 0].min()) * 0.85
hi = max(pred_train[:, 0].max(), y_raw[:, 0].max()) * 1.15
ax.loglog([lo, hi], [lo, hi], color="#b22222", lw=1.3, label="perfect agreement")
ax.set_xlabel("Predicted alpha")
ax.set_ylabel("Data alpha")
ax.set_title("Training set: air-to-fuel ratio")
ax.grid(True, which="both", ls=":", alpha=0.6)
ax.legend()
fig.tight_layout()
fig.savefig(os.path.join(fig_dir, "p2_train_parity_alpha.png"))

t_vals = np.linspace(268.0, 318.0, 60)
q_vals = np.linspace(500.0, 2500.0, 60)
tt, qq = np.meshgrid(t_vals, q_vals)
grid = np.column_stack([tt.ravel(), np.full(tt.size, 0.25), qq.ravel()])
alpha_s = predict_physical(grid)[:, 0].reshape(tt.shape)
fig = plt.figure(figsize=(7.6, 5.8))
ax = fig.add_subplot(111, projection="3d")
surf = ax.plot_surface(tt, qq, alpha_s, cmap="viridis", linewidth=0, antialiased=True)
ax.view_init(elev=25, azim=-135)
ax.set_xlabel("T1 (K)", labelpad=8)
ax.set_ylabel("Qs (kW)", labelpad=8)
ax.set_zlabel("alpha", labelpad=8)
ax.set_title("Predicted alpha at gamma = 0.25")
fig.colorbar(surf, shrink=0.62, pad=0.1, label="alpha")
fig.tight_layout()
fig.savefig(os.path.join(fig_dir, "p2_surface_alpha.png"))

# --- cell 6: Task P1.5 ---
test_x = np.array([
    [318.0, 0.0, 500.0],
    [318.0, 0.0, 1500.0],
    [318.0, 0.0, 2500.0],
    [318.0, 0.25, 1500.0],
    [318.0, 0.5, 500.0],
    [318.0, 0.5, 1500.0],
    [318.0, 0.5, 2500.0],
    [303.0, 0.0, 1000.0],
    [303.0, 0.0, 2000.0],
    [303.0, 0.25, 1000.0],
    [303.0, 0.25, 2000.0],
```

```
    [303.0, 0.5, 1000.0],
    [303.0, 0.5, 2000.0],
    [288.0, 0.0, 500.0],
    [288.0, 0.0, 2500.0],
    [288.0, 0.25, 2500.0],
    [288.0, 0.5, 1500.0],
    [269.0, 0.0, 1500.0],
    [268.0, 0.25, 2000.0],
    [268.0, 0.5, 2500.0],
], dtype=float)
test_y = np.array([
    [35.13, 0.3808],
    [47.46, 0.3930],
    [73.12, 0.4061],
    [66.34, 0.4098],
    [63.09, 0.4154],
    [85.23, 0.4197],
    [131.32, 0.4242],
    [38.99, 0.4012],
    [53.80, 0.4136],
    [54.51, 0.4215],
    [75.22, 0.4290],
    [70.04, 0.4337],
    [96.65, 0.4382],
    [33.45, 0.4091],
    [60.80, 0.4334],
    [85.044, 0.4477],
    [77.56, 0.4516],
    [40.68, 0.4393],
    [65.24, 0.4628],
    [98.23, 0.4760],
], dtype=float)
pred_test = predict_physical(test_x)
rms_alpha = float(np.sqrt(np.mean((pred_test[:, 0] - test_y[:, 0]) ** 2)))
rms_eta = float(np.sqrt(np.mean((pred_test[:, 1] - test_y[:, 1]) ** 2)))
print("T1, gamma, Qs, alpha data, alpha pred, eta data, eta pred")
for i in range(len(test_x)):
    print(test_x[i, 0], test_x[i, 1], test_x[i, 2],
          test_y[i, 0], pred_test[i, 0], test_y[i, 1], pred_test[i, 1])
print("rms alpha =", rms_alpha)
print("rms eta =", rms_eta)

fig, ax = plt.subplots(figsize=(6.2, 6.0))
ax.loglog(pred_test[:, 0], test_y[:, 0], "o", ms=8, color="#1f4e79", label="test points")
lo = min(pred_test[:, 0].min(), test_y[:, 0].min()) * 0.92
hi = max(pred_test[:, 0].max(), test_y[:, 0].max()) * 1.08
ax.loglog([lo, hi], [lo, hi], color="#b22222", lw=1.4, label="perfect agreement")
ax.set_xlabel("Predicted alpha")
ax.set_ylabel("Test data alpha")
ax.set_title("Test set: air-to-fuel ratio")
ax.grid(True, which="both", ls=":", alpha=0.6)
ax.legend(loc="upper left")
fig.tight_layout()
fig.savefig(os.path.join(fig_dir, "p2_test_loglog_alpha.png"))
plt.show()
```