

## 1 Author Response

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3 We thank three reviewers for their valuable feedback. We address the comments and the concerns as follows.

### 4 5 To Reviewer #2

6 **a) Feature independence.** Our model **does not** work on the feature independence assumption but in a performance-driven manner. If a subset of combined features yields the optimal performance, the feature subset will be selected. Our experiments suggest that the importance of a feature correlated with others in the selected subset is ranked higher than that of an independent feature less relevant to the target. It is hence **not** biased towards linear solutions.

10 **b) Related work.** (1) REINFORCE and LTPA were proposed for **instancewise** FIR while ours tackles **populationwise** FIR problems. In fact, instancewise FIR for **local** explanations is quite distinct from populationwise FIR for **global** explanations and converting instancewise to populationwise FIR requires non-trivial mechanisms (see <https://arxiv.org/pdf/1907.03039.pdf>). Thus, we cannot directly compare ours to such instancewise methods.

14 (2) Technically, **LTPA does not work on input features and hence cannot conduct feature selection.** REINFORCE works only for visual input while ours works for different input types including visual input. REINFORCE was implemented with reinforcement learning due to its non-differentiable nature while our model is carried out with supervised learning.

17 **c) Connection to evolutionary computation (EC).** We really appreciate your insight by understanding our work from an EC perspective. This insight may allow us to highlight our contributions from another angle: for feature selection, (1) ours uses a **single learning model** (enabling different feature masks to be used simultaneously during learning) to carry out the functionality of a **population of learning models** in EC; (2) instead of **purely stochastic operations** on population in EC, ours uses a more efficient **gradient-guided local stochastic search strategy**. We will add this insight in revision.

22 **d) Computational cost.** Indeed, computational cost of our dual-net model is high due to the use of two DNNs and the alternate learning routine. We will re-run all experiments on the same environment and report detailed results.

24 **e) Performance and motivation.** (1) Our model works well for a large feature set when there are enough training examples required by deep learning. For demonstration, we have just conducted an experiment on the UCI gene expression cancer RNA-Seq data set (<https://archive.ics.uci.edu/ml/datasets/gene+expression+cancer+RNA-Seq>), where there are 801 instances and 20,531 features. With 4-fold cross-validation (450, 150 and 201 instances used for training, validation and test, respectively), our model yields **99.38 ± 0.00% testing accuracy on 49 selected features ( $s = 49$ )**. In literature, to the best of our knowledge, the best performance in the same settings on this data set is **98.81%** (see Highlight and Table 7, <https://doi.org/10.1016/j.ygeno.2019.11.004>). For your information, the code provided by the authors of CCM [14] (the strongest method in our comparative study) does not work on our server as it requires 158GB+ memory for this data set. (2) The motivation of our training procedure is generally described in paragraph 1 of Sect. 3.3 and the input-gradient guided local search idea was motivated by the work presented in [12], as stated in Phase II-A.

### 35 36 To Reviewer #3

37 **1. Convergence analysis.** We agree to this point. We will summarize empirical observations in the revised main text and make a formal convergence analysis of our alternate learning algorithm in our ongoing research.

39 **2. Connection to latest work.** Thanks for pointing out two papers related to our work. Our work distinguishes those from the following aspects: a) those methods yield populationwise FIR by aggregating or integrating instancewise FIR in a **sub-optimal** manner, while our models directly learns populationwise FIR in an **optimal** way; b) for feature selection, those methods work as **filtering** so another learner has to be re-trained on the selected subset for a target task, while ours works as **embedding** by accomplishing feature selection and a target task together in an **end-to-end** manner. We will make a connection to two papers and report comparative results between ours and those methods in revision.

45 **3. Instancewise vs. populationwise.** We entirely agree to this point. We will be extending our model to instancewise FIR and study a connection between population and instancewise FIR in our ongoing work.

47 **4. Computational cost and scalability.** a) Regarding the computational overhead issue, **see our response d) to reviewer #2**; b) We will investigate scalability issues although any deep learning models effectively working for a large dataset can be used as an operator in our dual-net model.

### 50 51 To Reviewer #4

52 **Number of important features.** Our problem formulation for a fixed  $s$  is a **common setting in feature selection**, e.g., CCM [14]. When the ground-truth is unknown in real applications, results yielded by different  $s$  values (sub-solutions to feature selection) are still useful to reveal some meaningful relationship between selected features and the target. To find out the optimal value of  $s$ , the common setting allows a model like ours to work on different  $s$  values in parallel.

56 **Other questions.** a) in all the experiments,  $2d$  is the input dimension of the operator in ours while  $d$  is the input dimension of all other methods; b) In Eq.(2b), dividing 2 in the MSE loss is default to facilitate the gradient computation.