

1 **Reviewer 1, 3, 4** Thank you for all the reviewers time and effort. Regarding  
2 the comments on experiments, we would like to emphasise that we have made  
3 significant effort into design of experiments in this work. In particular, we have  
4 designed one unsupervised example to explain our methodology, as well as 3 additional  
5 simulated regression/classification examples to demonstrate the behaviour  
6 of our methodology vs that of the baselines. In addition, we have demonstrated  
7 our methodology on two real life datasets, Parkinson (Appendix C.5) and a real  
8 life protein-ligand binding problem. In the latter, we especially vary the target  
9 task to be a different protein, enabling 7 different problems of transfer. To ensure  
10 the proposed method applies to different models, we also consider two separate  
11  $f$ s, namely C-SVM and Random forest (with 5 hyperparameters). In many of  
12 these cases, distGP/distBLR was able to outperform its baselines.

13 **Reviewer 1** Thank you for your detailed review. Regarding the limitation to a  
14 single class model and instance space, while we do constrain broad applicability,  
15 we believe that there are still many applications in this setting, including ride-  
16 sharing, customer analytics model and online inventory system (discussed in [1]).  
17 Here, the idea is to re-train our model when new data is available. Furthermore, we demonstrate that our methodology  
18 is applicable to a real life protein-ligand binding problem in the area of drug design, which typically require significant  
19 efforts to tune hyperparameters of the models for different targets [2].

20 Here we explain our design space (see additional details in Appendix A.3, B and C); (i) *Choice of embedding (joint vs*  
21 *marginal+conditional)*: We investigate this in Appendix C.1. The results are fairly invariant, as the same information  
22 is encoded. (ii) *Acquisition function*: We only investigate the modelling of  $f^{\text{target}}$  in this work, and hence we use the  
23 standard expected improvement (Appendix A.3). (iii) *Optimisation*: We follow the same regime as in [3] (Section 4.3),  
24 but ADAM is used instead, please see reviewer 4 comments below for more information. (iv) *BLR NN structure*: We use  
25 the same structure as in [3] for a fair comparison. 5) *Embedding structure*: We choose a small two layer neural network  
26 to avoid over-parameterisation, as the number of evaluations,  $N$  is small. We also provide new experiments in Figure 1  
27 to show that our methodology is indeed robust to this choice (note that for classification, we use a one hot encoding for  
28  $\phi_y$ , and that here the difference of accuracy between various NN structures is on order of 0.2% – 0.3% only).

29 *initGP and manualGP vs distGP*: While initGP is indeed simple to use, we disagree that its performance is similar to  
30 that of distGP, as in many experiments, initGP performance is very poor. Even in the real life protein experiment, its  
31 convergence was much slower compared to other methodologies, especially for the case where  $f$  is a random forest with  
32 5 hyperparameters in Figure 3 of Section 5. This is to be expected, considering the target task is often different to the  
33 source tasks (note hyperparameters are fairly high dimensional here), and that there is no joint model making use of all  
34 evaluations. In the case of manualGP, utilisation is not easier than that of distGP, partially as the framework is the same,  
35 except that the data embedding is replaced by the manual meta-features (the list is provided in Appendix B.1). Here,  
36 there is a design choice of what meta-features to use, and the computation of *landmarker* meta-features can involve  
37 substantial effort, as we run simple algorithms to obtain characteristics of the problem (e.g. we use 1-NN classifier,  
38 LDA, naive Bayes and decision tree classifier landmarkers in this work for classification). Regarding performance,  
39 although distGP does not significantly outperforms manualGP in the real life experiment, we do demonstrate that such  
40 use of meta-features can perform poorly in a regression experiment in Section 5. It is also noted that manualGP that can  
41 jointly model tasks, while performing feature selection of meta-features is novel in our work.

42 **Reviewer 3** Thank you for your review, and for comments regarding experiments, please see above.

43 **Reviewer 4** Thank you for your positive comments regarding the quality of the paper. Regarding your comments  
44 on clarity, indeed the criterion to learn the NN embeddings, kernel parameters and other parameters  $\mu$ ,  $\nu$  and  $\sigma$  is  
45 the marginal likelihood of the GP or BLR. All these parameters are learnt simultaneously, in an end-to-end fashion.  
46 Regarding extensive benchmarks, we have not used the datasets found in [3], as these datasets' covariate space lies in  
47 various  $\mathcal{X}$  (i.e. of different dimensions), whilst our work focuses on scenarios where  $\mathcal{X}$  is the same across all tasks.  
48 For additional comments regarding experiments and application, please see above. We use ADAM as an optimiser,  
49 because for each iteration of the training, we use a sub-sample (batch) of the training data to estimate the embedding of  
50 distribution, in order to reduce computational cost. Hence, we decided to use ADAM which in general works well with  
51 stochastic gradients. In experiments, the loss converges and the model performs well given a reasonable learning rate.  
52 However, we agree with the author that L-BFGS can be used as an alternative to remove the choice of the learning rate.  
53 Finally, thank you for the comment on frequent Appendix referencing - we will make sure to improve the flow.

54 [1] Matthias Poloczek, et al. "Warm starting Bayesian optimization". pages 770–781. IEEE Press, 2016.

55 [2] Ross, G.A., et al. "One size does not fit all: the limits of structure-based models in drug discovery." JCTC 9.9 (2013)

56 [3] Perrone, Valerio, et al. "Scalable hyperparameter transfer learning." NeurIPS. 2018.

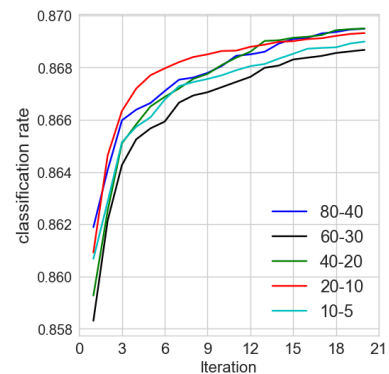


Figure 1: Protein with random forest across 140 evaluations with different NN structure for distGP's  $\phi_x$ .