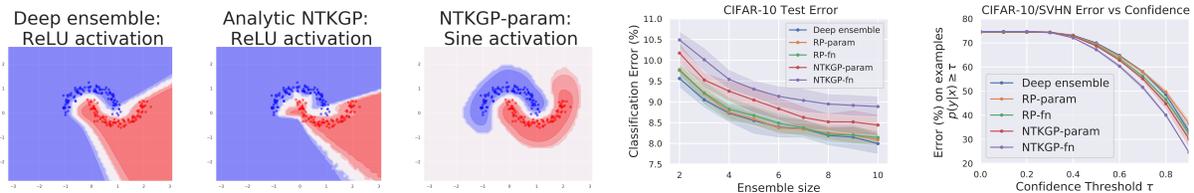


1 We thank reviewers **R1**, **R2**, **R3**, **R4** for their time and constructive reviews on our submission, which we will incorporate
 2 to improve our paper. Due to limited space, we will only be able to address the major points from the reviews:

3 **Benefits of a GP posterior ensemble interpretation** (addressed to **R1** & **R4**) We agree with **R2** that a key strength of
 4 our work is that it “provides a formal treatment of the relationship between deep ensembles and Bayesian posterior
 5 predictive distributions”. Posterior inference offers a principled way to convert prior beliefs into predictive uncertainties,
 6 and provides o.o.d. robustness via Bayesian marginalisation [14]. Moreover, Bayesian ML has a rich history [3] and is
 7 an active research frontier. One practical benefit to the GP posterior interpretation is selecting hyperparameters, like
 8 activation, of the NTK/NN architecture (akin to choosing GP kernel) that best model prior beliefs about data. For
 9 example, the NNGP/NTK correspondence allows one to deduce that Sine activation can alleviate overconfidence (see
 10 [43]) of ReLU deep ensembles on Two Moons classification. This is because the ReLU kernels do not decay away
 11 from the training data, as can be seen in Eqns S14,15 of [21], unlike the Sine kernels, as can be seen in `stax.py` of
 12 the Neural Tangents library [31]. In the left 3 plots below, we demonstrate this empirically (with two layer NNs of
 13 width 500, MSE trained with scaled one-hot regression targets and no observation noise, which are then fed into cross
 14 entropy to get probabilities): we see that both deep ensembles [11] and NTKGP analytic (with small noise $\sigma^2 > 0$ added
 15 for numerical stability, for **R4**) are overconfident with ReLU activation (denoted by blue and red shaded regions), but
 16 NTKGP-param with Sine activation has low confidence (white regions) away from the training data (points), as desired.



17 **Additional experiment on CIFAR-10** (**R2**, **R3**) We repeated the MNIST/NotMNIST experimental setup using the
 18 Myrtle-10 CNN with 100 channel width (Shankar et al., arXiv:2003.02237) trained on CIFAR-10 with SVHN o.o.d.
 19 test set. We changed our classification methodology to use MSE loss (using scaled one-hot regression targets with scale
 20 selected via moment-matching with NTK, small $\sigma^2 > 0$) before temperature scaling on a validation set. In the right 2
 21 plots above, we see that our NTKGP methods perform slightly worse on in-distribution test accuracy (<1% higher error),
 22 but outperform all baselines on o.o.d. detection in the Error vs Confidence plot (far right). For instance, NTKGP-fn
 23 exceeds baselines by between 8-10% accuracy on (combined in-dist+o.o.d.) test points with confident predictions (e.g.
 24 confidence $\tau=0.8$). This o.o.d. performance gain is crucial for safety-critical applications (e.g. self-driving cars).

25 **Computational overhead** (**R1**, **R2**, **R4**) We would like to clarify that for a training set of fixed-size (e.g. CIFAR-10)
 26 the train-time overhead of our methods is negligible compared to standard deep ensembles [11]: one can obtain and
 27 store our fixed additive JVPs δ in a single pass over the training data. This was mentioned on lines 528-531. For
 28 test-time constrained applications, we could apply distillation techniques, as is common with standard deep ensembles.
 29 **Novelty** (**R1**, **R4**) Though presentation has been simplified, we respectfully disagree that the novelty of our paper is
 30 straightforward. We are (to our knowledge) the first to consider $GP(0,NTK)$ prior instead of $GP(0,NNGP)$, in order
 31 to align posterior inference with optimisation of *all* NN layers. Our contributions are distinct to, not extensions of,
 32 [22, 23], and give different limiting predictive distributions to [22], see Table 1. Also, if there is no modelling of
 33 observation noise, $\sigma^2=0$, then RP-param [22, Eq. 4] and anchored ensembles with MSE [23, Eq. 8] become standard
 34 deep ensembles [11]. On the other hand, NTKGP-param still retains its posterior interpretation (Corollary 1), using
 35 fixed additive JVP corrections with no regularisation nor noisy targets. This is the case in the two moons ensembles
 36 above. It is only when modelling observation noise that we synergise our methods with [22].

37 **Individual responses** (**R1**) We contest the “marginal” empirical improvement of our work: Figure 3 (right) depicts
 38 significant gains of our methods for o.o.d. NotMNIST detection over baselines. The NTK & standard parameterisations
 39 are introduced in Appendix A. (**R2**) We believe the slightly worse in-distribution test performance of our methods
 40 can be alleviated with thorough NTK hyperparameter tuning. (**R3**) When modelling observation noise, $\sigma^2 > 0$, our
 41 regularisation scheme (Appendix D) enables closer alignment to the kernel regime in standard parameterisation (lines
 42 492-499) and nullifies problems caused by the fast decay of NTK eigenvalues (lines 84-86). (**R4**) $\Theta_{\succeq \mathcal{K}}$ follows from the
 43 NTK being a sum of p.d. contributions from different layers and \mathcal{K} is the contribution from last layer, see Eq. S29 of [21].
 44 JVPs are more memory-efficient in forward-mode than reverse-mode AD; we will add this. Please see lines 511-513
 45 for discussion of parameter and function space methods; our code is open-source and we are working with the Neural
 46 Tangents authors [31] to integrate our work. It is unclear if analytic NTKGPs are preferable to analytic NNGPs when
 47 both are tuned, due to cost and predictive-mean performance (see §3.2 of Lee et al., arXiv:2007.15801); we focus on
 48 giving a posterior interpretation to deep ensembles for wide but finite NNs, and lack the compute needed for comparisons
 49 of large-scale analytic NTKGP/NNGPs. For the prediction decomposition, setting $\Theta_{\mathcal{X}\mathcal{X}}^{\sigma} = \Theta(\mathcal{X}, \mathcal{X}) + \sigma^2 I$, we obtain:

$$50 \tilde{f}_{\infty}(x^*) = \underbrace{\Theta(x^*, \mathcal{X})[\Theta_{\mathcal{X}\mathcal{X}}^{\sigma}]^{-1}\mathcal{Y}}_{f_0} + \underbrace{f_0(x^*) - \Theta(x^*, \mathcal{X})[\Theta_{\mathcal{X}\mathcal{X}}^{\sigma}]^{-1}f_0(\mathcal{X})}_{\delta} + \underbrace{\delta(x^*) - \Theta(x^*, \mathcal{X})[\Theta_{\mathcal{X}\mathcal{X}}^{\sigma}]^{-1}\delta(\mathcal{X})}_{\delta}$$