

1 We thank the reviewers for their helpful comments. First, we briefly recap our contributions. We provide the first
2 computationally efficient and accurate method for approximate cross-validation (ACV) in the following setting:
3 structured models fit with MLE or MAP, where the task is a structured prediction. In so doing, we show (theoretically
4 and empirically) that IJ-style ACV ideas can be applied at an inexact (MLE or MAP) optimum; the latter is a new
5 result even for traditional ACV. By contrast, previous IJ approximations (e.g. Giordano et al. [2019]) do not apply to
6 structured prediction and also assume an exact optimum; Newton-step (NS) methods (e.g. Rad and Maleki [2020]) *could*
7 be applied to structured prediction, but we show (lines 118–121, Appendix G) they are not computationally efficient;
8 and Bürkner et al. [2020] focus on leave-future-out for time series (but not other forms of structured prediction) within
9 a fully Bayesian (rather than MLE or MAP) framework.

10 **Novelty:** (A) R2 is concerned that we are applying a “general framework for ACV from a previous paper.” But note that
11 Giordano et al. [2019], Beirami et al. [2017], Koh & Liang [2017], Koh et al. [2019], Stephenson & Broderick [2020],
12 and Wilson et al. [2020] all work in the framework of Eq. (1) of Giordano et al. [2019], whose additive form does not
13 allow for the structured tasks we consider here. Observe that Bürkner et al. [2020] extend Bayesian ACV methods to
14 leave-future-out CV for time series models; that work demonstrates the non-trivial nature of extensions to structured
15 tasks. (B) R2 also describes our new theoretical error bounds as applying to HMMs and CRFs. But note that our error
16 bound (Prop. 2) applies much more broadly — both to all of the structured tasks we consider here, including more
17 general MRFs — as well the Giordano et al. [2019] framework with inexact optima (a result which was not previously
18 established but is more practically relevant than results requiring exact optima). (C) R2 is concerned that our methods
19 apply only to models with latent processes. While we believe models with latent structure represent a widely used and
20 interesting class of models, we note that we do present methodology (Sections E, F, and Algorithm 4) and experiments
21 (Section 5, lines 265–291) for CRFs, which contain no latent variables. And our inexact optimum theory applies beyond
22 structured models.

23 **Additional experiments:** R2 asks for comparisons against pre-existing IJ or NS ACV methods. Unfortunately, there
24 are no existing IJ methods that apply to the tasks we consider. To the best of our knowledge, NS has not previously
25 been applied to these problems, but we do consider it. In lines 118–121 and Appendix G, we discuss the computational
26 challenges of NS methods, which arise from computing and inverting a new Hessian for each CV fold. E.g., for the
27 time-varying Poisson process problem ($T = 50,400$), IJ computation across all 1,000 folds took about 12 minutes. By
28 contrast, the NS approximation here would take roughly *113 hours*. On sufficiently small datasets, though, the NS and
29 our IJ can be much closer in performance. We will include NS timing across datasets, and discussion, in a revision of
30 our main text.

31 **Assumptions:** We fully agree with R1 that our assumptions could be stated more clearly. We will collect them in the
32 text, and we note them here for clarity. We require (1) a model fit via optimization, (2) twice differentiability of the
33 model objective and invertibility of the Hessian matrix at the initial model fit $\hat{\Theta}$, and (3) the ability to write the model
34 fits across CV folds, $\hat{\Theta}^{\circ}$, as optima of the same weighted objective for all folds \circ . These conditions are satisfied
35 by a broad class of empirical/regularized risk minimization problems, including widely used probabilistic models of
36 structured data fit via MLE or MAP. We further clarify that *any* optimization method (stochastic or exact; with or
37 without early stopping; etc.) may be used to obtain the initial fit $\hat{\Theta}$ for input to Algorithm 1. When computing the
38 actual derivatives in Algorithm 1, we assume that the gradients are computed exactly at $\hat{\Theta}$. Computing these gradients
39 involves a single pass through the dataset before approximating CV for all folds.

40 **Structured tasks:** R1 notes that we need to clarify that our novelty here is for the combination of structured models
41 *paired with* structured tasks. We completely agree and will be sure to make this point very early in a revised manuscript.

42 **Number of folds:** R4 is concerned that 500 folds in our neural CRF experiment is “too large to use in practice.” Fig. 1
43 of Rad and Maleki [2020] show leave-one-out CV (with hundreds of folds) substantially outperforming $\{3, 5, 10\}$ -fold
44 CV at estimating out-of-sample error. A goal of modern ACV methods is to allow a larger number of folds, and
45 therefore more accurate final estimate overall, in practice.

46 **Quantitative results:** R4 is concerned that our paper “lacks quantitative results.” We interpret this concern to mean
47 that the reviewer would like to see approximation error and timing reported in numbers, in addition to being plotted in
48 the figures we have included in our submission. We will be sure to include both numbers and figures in a revision.

49 **Inexact initial fit:** R4 is would like us to clarify how our method provides a solution to the inexact initial fit problem.
50 We prove (Section 4) that the IJ approximation error increases smoothly with the error in the initial fit. Proposition 2
51 explicitly bounds the approximation error and suggests that we can use “good enough” initial fits without substantively
52 sacrificing ACV accuracy. Our neural CRF experiments in Section 5 provide empirical confirmation.

53 *References* (beyond original paper) ◦ P. W. Koh, K. S. Ang, H. Teo, P. Liang. NeurIPS’19.

54 ◦ A. Wilson, M. Kasy, L. Mackey. AISTATS’20.