



FACCE-MACSUR

## C4.1-D Overview paper on comprehensive framework for assessment of error and uncertainty in crop model predictions

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**Abstract/Executive summary**

Crop models are important tools for impact assessment of climate change, as well as for exploring management options under current climate. It is essential to evaluate the uncertainty associated with predictions of these models. Several ways of quantifying prediction uncertainty have been explored in the literature, but there have been no studies of how the different approaches are related to one another, and how they are related to some overall measure of prediction uncertainty. Here we show that all the different approaches can be related to two different viewpoints about the model; either the model is treated as a fixed predictor with some average error, or the model can be treated as a random variable with uncertainty in one or more of model structure, model inputs and model parameters. We discuss the differences, and show how mean squared error of prediction can be estimated in both cases. The results can be used to put uncertainty estimates into a more general framework and to relate different uncertainty estimates to one another and to overall prediction uncertainty. This should lead to a better understanding of crop model prediction uncertainty and the underlying causes of that uncertainty. This study was published as (Wallach et al. 2016)

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## Introduction

Past crop model uncertainty studies can be grouped into three different approaches. The first is based on comparing model hindcasts to observed data. In a second approach, the uncertainties in the model inputs or parameters are of primary concern. The third, more recent approach is based on multi-model ensembles (MMEs). All three approaches give information about crop model prediction uncertainty, but to date there have been no studies that attempt to relate them. It is important to do so, in order to obtain a better overall understanding of prediction uncertainty and how best to estimate it. We will focus on two sets of questions: (1) What are pertinent criteria of uncertainty, how can they be estimated, and how are the different approaches described above related to estimation of those criteria? (2) Given an overall criterion of uncertainty, how can one estimate the separate contributions from different sources of uncertainty?

## Methods

We define prediction uncertainty as the distribution of simulated minus true values. This can be summarized using the mean squared error of prediction. Two different versions are possible. If one treats the model predictions as fixed quantities, then we have

$$MSEP_{fixed} = E \left[ \left( y - \hat{f}(\hat{X}; \hat{\theta}) \right)^2 \mid \hat{f}, \hat{X}, \hat{\theta} \right] \quad (1)$$

The notation is that the expectation is over all random variables, except those specified as fixed and that appear after the vertical bar. In eq. (1) the model structure  $\hat{f}$ , the approximation  $\hat{X}$  of  $X$  and the parameter vector  $\hat{\theta}$  are fixed, while  $X$  and  $y$  are treated as random variables. The second criterion based on MSEP is

$$MSEP_{uncertain}(X) = E \left[ \left( y - \hat{f}(\hat{X}; \hat{\theta}) \right)^2 \mid X \right]$$

Here the expectation is over the distribution of model structures  $P_{\hat{f}}$ , over the parameter vectors for each structure  $P_{\hat{\theta}|\hat{f}}$  and over the approximations to the input vector for each prediction  $P_{\hat{X}|X}$ , as well as over  $y$  for the given  $X$ .

$MSEP_{uncertain}$  can be decomposed into two terms:

$$\begin{aligned} MSEP_{uncertain}(X) &= E \left\{ \left[ \left( y - E \left[ \hat{f}(\hat{X}; \hat{\theta}) \mid X \right] \right)^2 \mid X \right] \right\} + \text{var} \left[ \hat{f}(\hat{X}; \hat{\theta}) \mid X \right] \quad (2) \\ &= \text{squared bias} + \text{model variance} \end{aligned}$$

The first term is the squared bias when predicting using an average over model structures, approximations to  $X$  and parameter vectors, and the second term is the variance of the predictor. The model variance term in eq (2) can be further decomposed into contributions from the different sources of uncertainty as

$$\text{var} \left[ \hat{f}(\hat{X}; \hat{\theta}) \mid X \right] = \sigma_f^2 + \sigma_{\hat{X}}^2 + \sigma_{\hat{f}\hat{X}}^2 + \sigma_{\hat{\theta}}^2 \quad (3)$$

where the terms on the right are respectively the first order effect of model structure, the first order effect of approximating  $X$  by  $\hat{X}$ , the interaction of model structure and approximating  $X$  by  $\hat{X}$  and finally the effect of uncertainty in parameter values  $\hat{\theta}$ , averaged over model structures and over  $\hat{X}$ .

$MSEP_{fixed}$  can be estimated from hindcasts.  $MSEP_{uncertain}$  can be estimated using hindcasts for the squared bias term, and a simulation experiment for the variance term. The variance term can be decomposed into separate contributions using a random effects ANOVA.

## Results

Using previously published data from a multi-model ensemble of crop models (Asseng et al. 2013), we can illustrate how the proposed framework can be applied. See (Wallach et al. 2016).

## Discussion

The framework proposed here can provide the basis for obtaining information on the relative contributions of model uncertainty, parameter uncertainty, input uncertainty and bias to overall prediction mean squared error. Furthermore, since the  $MSEP_{uncertain}(X)$  criterion that we propose is specific to each prediction situation, it can help to determine, for each specific problem, how well crop models are likely to perform.

$MSEP_{fixed}$  and  $MSEP_{uncertain}(X)$  are complementary criteria for estimating prediction accuracy of models. Both are useful because they give different types of information about prediction error. If possible, both should be evaluated.

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## References

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