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Efficient stabilization of crop yield prediction in the Canadian Prairies

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ABSTRACT

This paper describes how spatial dependence can be incorporated into statistical models for crop yield along with the dangers of ignoring it. In particular, approaches that ignore this dependence suffer in their ability to capture (and predict) the underlying phenomena. By judiciously selecting biophysically based explanatory variables and using spatially-determined prior probability distributions, a Bayesian model for crop yield is created that not only allows for increased modelling flexibility but also for improved prediction over existing least-squares methods. The model is focused on providing efficient predictions which stabilize the effects of noisy data. Prior distributions are developed to accommodate the spatial non-stationarity arising from distinct between-region differences in agricultural policy and practice. In addition, a range of possible dimension–reduction schemes and basis expansions are examined in the pursuit of improved prediction. As a result, the model developed has improved prediction performance relative to existing models, and allows for straightforward interpretation of climatic effects on the model's output.

1. Introduction

This paper presents a method for forecasting wheat crop yields in the Canadian Prairie Provinces—a challenging task due to dramatic variability in yield over space and time. Its importance, however, should not be understated: wheat is one of Canada's primary exports, accounting for 12% of wheat and barley traded in the world market. Thus variation in yield has considerable impact both within and beyond Canadian borders (Schmitz and Furtan, 2000). Enabling effective crop management, handling, and marketing thus requires accurate predictions of crop yield that account for and explain these variations. For example, these forecasts are helpful in setting insurance premiums and futures prices as well as in managing grain transport. Since spatial and temporal climate variability affect crop yields (Stone and Meinke, 2005; Potgieter et al., 2006), a crop yield forecasting method must include climate as an essential component if it is to be successful.

Several process-based models have been successfully used for crop yield prediction including the Agricultural Production Systems Simulator (APSIM) in Australia (Keating et al., 2003) as well as a web-based tool developed by the United States' Southeast Climate Consortium (Jagtap et al., 2002). These process-based models typically employ tunable and user adjustable deterministic and stochastic models to simulate biological and physical processes related to crop yield. While these models use knowledge pertaining to the individual processes, they often require significant input from the user, including a wide range of meteorological and environmental variables which may be difficult or expensive to obtain.

In contrast to the above, traditional statistical techniques are purely empirical. While these methods may result in accurate predictions, they typically lack the interpretability of process-based models (Barnett, 2004). As a result of this criticism, recent years have seen the development of statistical models that also provide interpretation of the underlying biophysical process (see, for example, Stephens (1995), Hansen et al. (2002)). One such process knowledge-based approach involves water stress indices (Potgieter et al., 2005, 2006; Qian et al., 2009a,b), the result of which has been of tremendous use and benefit to stakeholders, allowing for prediction and understanding of crop yield anomalies. While these models have improved the prediction of crop yield, there exists scope for improvement through (a) providing an efficient dimension reduction of explanatory variables; (b) accounting for uncertainty in the estimated technology trend; (c) modelling spatial correlation between regions.

This paper describes the results of a project coordinated by Agriculture and Agri-foods Canada to develop a model that explains and predicts wheat yield and its relation to climatic variables. With plans for an online implementation in the future, efficiency was required as a feature of the model, as was the ability to stabilize the effects of noisy measurements. Building on earlier work, we employ a crop water stress index (SI) to provide explanatory power for a new crop yield predictor (De Jong and Bootsma, 1996). To improve prediction over existing approaches, we extract

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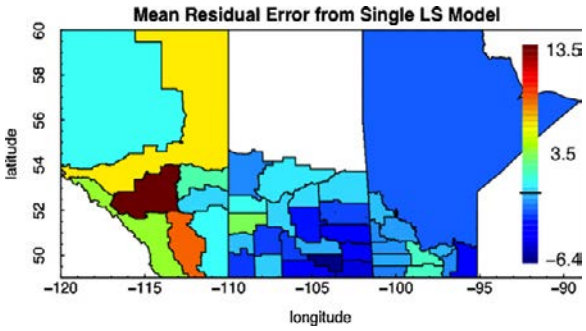

Fig. 1. Mean residuals from model (1). We observe that the model residuals are spatially correlated.

a sensitive yet low-dimensional summary of this stress index, comparing various alternatives and bases before ultimately selecting principal components. We then demonstrate its improved prediction performance compared to currently used windowed average approaches. In contrast to previous work which models each agricultural region separately, we create a unified model that allows strength to be borrowed from adjacent and nearby regions, thus stabilizing both inference and prediction. By employing a spatially-motivated context-specific prior distribution on the parameters of interest, we account for and use spatial correlation between sites while smoothing and consequently improving predictions.

Following this introduction, Section 2 describes the crop yield forecasting problem and available data. This section works through a series of successively improved models, eventually leading to a Bayesian model in Section 2.3 which jointly models all regions simultaneously. Model testing and diagnostics are explored in Section 3. Lastly, Section 4 concludes the work.

2. Materials and methods

This paper models crop yield in the Canadian Prairies as a function of climate-related explanatory variables. The data include annual wheat yields (in bushels per acre) along with associated measurements of a crop water stress index and growing degree day (both described later) for 40 agricultural regions (plotted in Fig. 1) across the Canadian Prairies from 1976 to 2006. The agricultural regions are those used in the 2006 Canadian Census of Agriculture, through which the data are also obtained, and are determined from climate and soil information. For each of the 31 years and 40 regions, yield is an aggregated average across the region. Likewise, stress index and growing degree day are calculated regionally, but on a daily basis throughout the growing season (April 1 to September 30).

2.1. Incorporating soil water

The well recognized influence of soil water on crop yields dictates its inclusion in any yield prediction model (De Jong and Bootsma, 1996). However, due to the time-consuming and costly process of measuring soil water content, in practice its effects must be inferred from more widely available environmental variables such as precipitation, temperature, and easily measured crop and soil-related factors. A suite of models have been developed which attempt to understand soil water availability in the context of these environmental variables. Beginning with simple water balance approaches that balance precipitation and soil water storage with evapotranspiration and water runoff, these models have increased in their complexity over the years (Thornthwaite, 1948; De Jong and Bootsma, 1996). For the reasons given below we focus on budget models, which build on the premise that above a certain threshold (called the 'field capacity'), soil cannot absorb any more water and therefore any additional water is drained off through runoff or drainage. Also, if the soil water fails to be replenished through precipitation, irrigation, or other sources, the soil reaches a point where plant roots are no longer capable of uptaking water. This stage is known as the 'wilting point'.

Evapotranspiration, which describes the sum of evaporation and plant transpiration, measures the water lost from plants, soil, and other land surfaces into the atmosphere. There are two key components in the budget model, potential evapotranspiration (PET) and actual evapotranspiration (AET). PET represents the atmospheric demand for evapotranspiration; specifically, it accounts for the energy available to evaporate water and transport it into the lower atmosphere. AET is the actual water content available for evaporation and transpiration, and relies on plant physiology and soil characteristics for its calculation. When the soil has ample water, the actual evapotranspiration (AET) can equal the PET. However when the soil is not at its field capacity, AET will be less than PET. More details on these concepts and soil science in general may be found in Brady et al. (1999).

Budget models are straightforward to implement since they require a minimum of meteorological data as well as soil field capacities and wilting points. While more advanced models have been built which include soil hydraulic characteristics and more complex relationships between soil, plant, and meteorological systems, these models require considerably more information from the user, including detailed soil and plant characteristics. Because of the additional variables required by these models, we employ a budget model in the remainder of this work. Our model uses crop water stress index (SI) over agricultural land, defined as 1-AET/PET (Qian et al., 2009a,b). This quantity will be near 0 when water is plentiful in the soil and near 1 when the plant is stressed by a lack of available moisture. Intuition might suggest directly including precipitation, temperature, soil and plant information into the model. However, doing so would add a large number of variables, especially considering that many of these variables are observed for every day of the growing season. Using the SI instead provides an economical reduction in the dimensionality of the description space in a way that respects the biophysical processes involved in soil water movement and availability.

2.1.1. Predicting yield with SI

We begin by detailing the process of fitting a regression model to crop yield using least squares (LS). First let $y_{j,t}$, $j = 1, \ldots, 40$ be the yield from region j for years $t = 1976, \ldots, 2006$. Since SI is a daily value, we create an annual average for each year and region; let $\overline{si}_{j,t}$ denote the vector of these means in year t for each region j. We begin by fitting a common regression model to all regions, specifically

$$y_{j,t} = \beta_0 + \beta_1 t + \beta_2 \overline{si}_{j,t} + \epsilon_{j,t}. \quad (1)$$

Here $\epsilon_{j,t}$ for year t and region j represents a combination of model and measurement error. While previously developed statistical models for crop yield account for a technology trend by first fitting a regression on time and then modelling the residuals, such approaches yield little understanding about the uncertainty associated with forecasting. In particular, while forecasts that use detrended data may be similar, their associated variances will be biased as uncertainty in the trend model is ignored. In fact, to properly account for all sources of variability the technology trend should be an integral part of any forecasting model.

To begin, note that the simple model in Eq. (1) relies on only 3 parameters—all regions are described by the same equation. The validity of inference for such a model relies on assumptions including for instance that the errors $\epsilon_{j,t}$ are stochastically independent

for all j, t. To test this assumption, we plot the mean residual (averaged over the 31 years) for each of the 40 stations in Fig. 1. This figure makes it clear that the residuals are spatially correlated. For instance, the residuals in Alberta (the western-most Prairie Province) are much larger than the other two provinces, highlighting the fact that the model is biased, particularly in central Alberta. Considering the mean and standard deviation of crop yield across the Prairies are 30.9 and 8.2, respectively, the average residual value of 13.5 in this region indicates that the model is consistently underestimating the crop yield there.

To gain descriptive power, researchers have expanded the above model by fitting a different regression model to each region, specifically

$$y_{j,t} = \beta_{0,j} + \beta_{1,j}t + \beta_{2,j}\overline{si}_{j,t} + \epsilon_{j,t}. \quad (2)$$

The expanded model now accounts for 61% of crop yield variation, compared to 33% for (1), albeit at the expense of additional parameters in its mean structure. In fact, by assigning a unique parameter to each region, this expanded model has $3 \times 40 = 120$ parameters. By using such models, albeit with potentially modified/additional explanatory variables, several authors have been able to create fairly accurate predictions of crop yield (Potgieter et al., 2005; Qian et al., 2009b). It is important to note that the large number of predictor variables (120) makes this model prone to overfitting; while some authors have used cross-validation to prevent this (i.e. Qian et al., 2009b), others have sought to further improve model fit by conducting extensive calibration to tune the explanatory variables (i.e. Potgieter et al., 2005). It is well understood that smoothed, or penalized, models have better prediction properties than larger, more variable models (Hastie et al., 2009). This leads us to prefer the most parsimonious model yielding accurate forecasts and to select explanatory variables which provide optimal prediction power for crop yield. While earlier models have been examined with regards to their model fit (as measured through R^2), a much preferred metric is model prediction performance (as measured through cross-validation).

While the availability of SIs for every day of the growing season (in our case April 1 to September 30) means its vector of measured values is of very large dimension, good modelling practice requires that this dimension be reduced before introducing the vector into the regression model. At one extreme, we could do what we did previously, and use just the mean of these daily SI values over the growing season, a one-dimensional feature, as our explanatory variable. However, that would oversimplify the SI's role, since plant growth is influenced more at certain times than others during the growing season. As an extreme example, if the crop is harvested in early September, the SI values in late September would aid little in predicting crop yield. To find a low-dimensional feature that provides good predictive power for crop yield, we could average over a reduced window, that is, exclude SI values early and late in the season (Qian et al., 2009b). This reflects the point just made that SIs early and late in the season may not be correlated with crop yield. Fig. 2 shows this correlation between SI and crop yield for each day in the summer, organized by province. This figure suggests we average over days 80 through 160, rather than the entire growing season. However, this produces only a modest improvement, 60.72% of crop yield's variability now being explained instead of 60.56% using the average over the entire season as before. This plot also reveals large spatial variability, particularly between provinces. We explore this issue in more detail later.

There exists considerable scope for tuning this window; for instance Potgieter et al. (2005) select unique window start and end points for each region to achieve an excellent fit—over 75% of variation explained. However such tuning entails much attention to detail. On top of the upper and lower limits for the averaging to take place, Potgieter et al. (2005) calibrate potential available soil water capacities, the maximum number of sowings and the rainfall amount triggering planting in each region. In other words, in addition to the corresponding regression coefficients, this tuning in effect adds 5 additional parameters per region, which in our case would increase the number of parameters being fitted in (2) from 120 to 320, leading most likely to serious over-fitting when considering that such an approach still uses an average SI over the growing season, not accounting for temporally-varying impact of SI. To quote John von Neumann:

> With four parameters I can fit an elephant and with five I can make him wiggle his trunk.

As such, a preferred alternative would be a lower dimensional feature which captures the key components of the stress index. In addition, we would like to include information which allows for the impact of SI on yield to vary over the growing season.

To capture more information from the SI values than would be available from simple averaging, we extract the principal components and hence main sources of variation from the stress index. To be more precise, after subtracting the average SI from each day, the first principal component is the linearly transformed vector of growing season SI values that accounts for the most variability in the SI values. The second, which is orthogonal to the first, explains the next largest amount of variation, and so on. Each observation, in this case each region—year combination, also has a set of loadings that, when multiplied by the corresponding principal components, return the original observation. Fig. 3 shows the subtracted mean process as well as the first four principal components that together show the SIs history over the growing season of our study. Fig. 3(a) reveals firstly the primary shape of the stress index, showing that initially – from April 1 – the stress is moderate, increasing until May, followed by a gradual decline until it bottoms out in July. It then returns to its highest values by the end of September. The first component (Fig. 3(b)), which describes 46.9% of the variation in SI, captures a valley in the SI cycle around late August. The second component, which accounts for 14.6% of the variation, shows SI's decline into its July valley followed by its rise to its early September peak. The orthogonality of the first two components is apparent from (b). The third and last major component of SI's variation captures its low April start. Altogether, the first 4 principal components account for 78.5% of the variation in SI over the growing season. Beyond 4 principal components we observed little in terms of improved modelling fit and a reduction in prediction performance, as shown in Figs. 4 and 5. Thus by including the

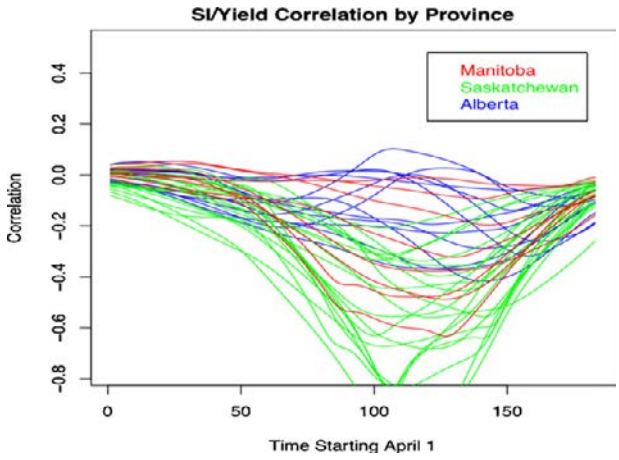

Fig. 2. Correlation of SI and yield over time. Correlations smoothed with Lowess smoothing. From this we see that SI is most correlated with yield in an intermediate part of the season, namely days 80 through 160.

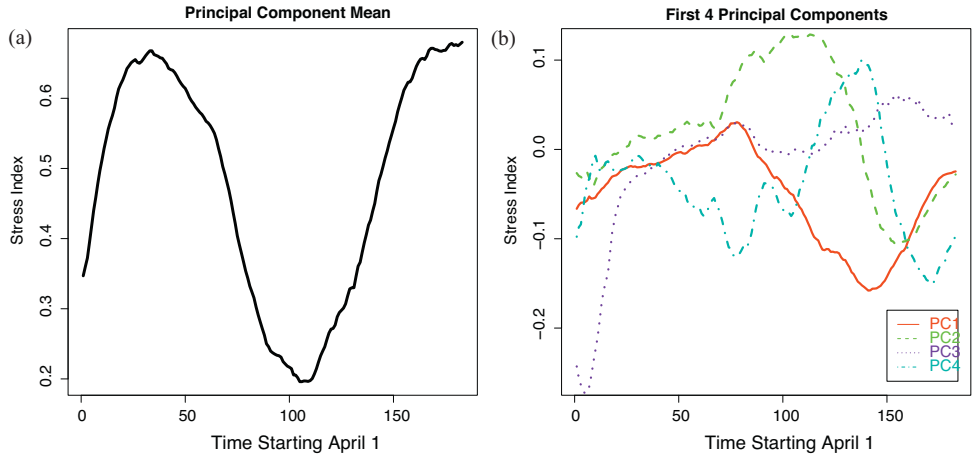

Fig. 3. Principal components and mean for SI. This figure depicts the major patterns in the variation of the stress index (unitless) over the growing season. Observe how the first four principal components pick up deviations from the overall pattern in (a), and reveal the peaks and valleys of the stress cycle over the course of the summer induced by things like patterns in precipitation and temperature. Together these four components capture most of the variation in stress in a very economical way and eliminate the need for the high dimensional vector of daily SI values.

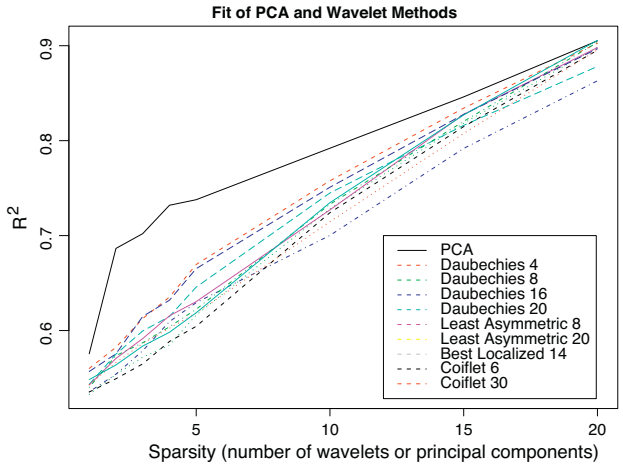

Fig. 4. R^2 of the crop yield model for a range of bases and sparsity levels. From this we notice that principal components (PCA) provide better model fit for all sparsity levels.

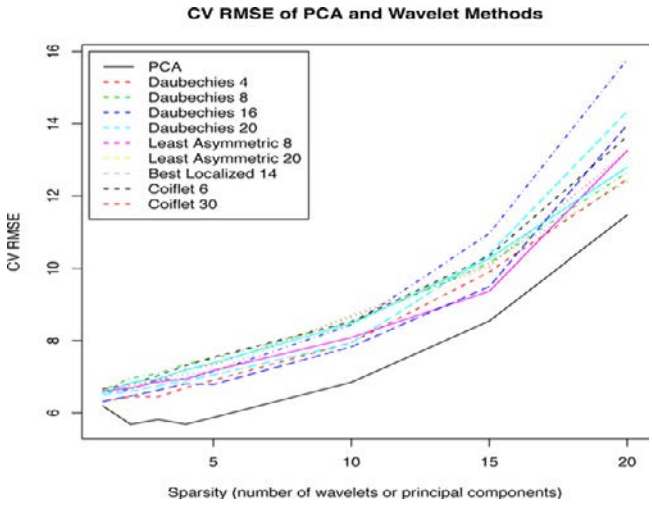

Fig. 5. Cross-validation RMSE (bushels per acre) of the crop yield model for a range of bases and sparsity levels. From this we notice that principal components (PCA) provide better prediction than the wavelet bases for all sparsity levels.

loadings for these 4 principal components as explanatory variables, we have created a four-dimensional feature which accounts for a large proportion of variation in the stress index.

Note that the first SI principal components aren't necessarily the best predictors of yield. However, LASSO – a penalized least squares variable selection method – in fact selects these same four principal components as the best four (Hastie et al., 2009). This choice of feature also has a natural biophysical interpretation. For instance, a large and positive regression coefficient for the loadings corresponding to principal component 3 would imply that a reduction in stress in early April is highly connected with increased crop yield. By using this approach, the explained variance of the regression model increases from 60.56% from averaging SI over the growing season to 70.06%. In addition, as discussed above, the inclusion of principal components allows the user to gain intuition about the effect different seasonal patterns in the stress index will have on crop yield in a way averaging across the season cannot. Using these principal component loadings, our new model is

$$y_{j,t} = \beta_{0,j} + \beta_{1,j}t + \beta_{2,j}PC1_{j,t} + \cdots + \beta_{5,j}PC4_{j,t} + \epsilon_{j,t}. \quad (3)$$

where $PC1_{j,t}$ indicates the loading for principal component 1 in region j and year t.

2.1.2. Alternative bases and levels of sparsity

Because of their widely documented ability to model complex nonlinear signals while maintaining sparsity, we briefly explore wavelet bases as an alternative to principal components (Mallat, 2009). Specifically, we examine a variety of different wavelet bases and levels of sparsity both in terms of cross-validated prediction error as well as R^2. Fig. 4 plots R^2 of the yield model for various bases and levels of sparsity. From this plot we see that principal components dominate in terms of model fit. While R^2 measures how well a model fits to data, it is not a good indicator of a model's prediction abilities. As such, Fig. 5 plots cross-validation root mean squared error (in bushels per acre) for each basis and sparsity level. Once again we observe that principal components outperform wavelets. From these figures we conclude that principal components lead to a model with better fit and prediction performance. This example highlights the need to be selective in the choice of basis to represent stress index and other variables in such a model. While wavelets excel at representing piece-wise smooth models in a very sparse way (requiring the storage of only 1 vector – the mother wavelet – as well as a series of indices), this is also their

downfall in some circumstance such as this one which require a richer representation.

2.2. Incorporating temperature

Temperature affects a plant's development and growth in a variety of ways, in particular its photosynthesis and respiration. In general, temperature affects plant functioning through its action on enzymatic reactions. At low temperatures, enzyme proteins are not sufficiently flexible to complete the conformation necessary for enzymatic reaction. Conversely, high temperatures can coagulate the enzyme leading to similar barriers to the reaction. Alongside a minimum and maximum temperature to allow growth, most plants have an optimum temperature to encourage growth. For instance, Ritchie and NeSmith (1991) conclude that the minimum and optimum temperatures for wheat are respectively 0 and 20–25 °C. As a result of temperature's influence on plant development, we suspect that its inclusion into the model will result in prediction performance gains. In addition, by directly including temperature effects interpreting impacts of climate on yield is made more straightforward.

2.2.1. Growing degree day

While temperature could go directly into the model, its measurement in hourly or smaller increments creates a considerable amount of data. As a result, some dimension reduction is needed to limit the number of explanatory variables. One could do this using just the maximum and minimum daily temperatures or better still, a one dimensional summary that combines the two. Thus 'growing degree day' (GDD) measures the heat accumulation in a region based on local weather by taking an average of the daily minimum and maximum and subtracting a base temperature as follows:

$$\mathrm{GDD} = \max\left(0, \frac{T_{max} + T_{min}}{2} - T_{base}\right).$$

Thus the GDD measures the daily average temperature but in a way that reflects the extremes more sensitively. The base temperature represents the physiological temperature below which development would be zero.

A day with a high and low of 30 and 15 °C and a base temperature of 10 degrees would have a GDD value of 12.5 °C. Thus GDD is a simple, single-dimensional summary for describing the plant's exposure to heat. While GDD is a simple heuristic, it is commonly used by horticulturists to estimate the stages of a plant's growth. As an example, the maturation of wheat corresponds to about 1600 GDDs (Dolan et al., 2006). Thus GDD provides us with a simple low-dimension summary of temperature, allowing for comparison of the thermal time available in different climatic zones.

While SI gives scientific insight into the moisture available for plant growth, it says little directly about the heat available to the crop. Thus to improve our model we can also include GDD, which up until now has been used primarily in this context for tuning the explanatory variables (Potgieter et al., 2006). Like SI, GDD is a daily value, and hence can be treated similarly. Thus through the correlations plotted in Fig. 6 we look at the time of season where GDD is most correlated with yield. This figure tells us that an appropriate window would be the one bounded by days 50 through 160. Using a cumulative average over the whole season, the explained variation in yield increases from 70.06% to 73.20%, with the shortened window performing similarly. As emphasized by others (see, for instance, Potgieter et al., 2006), including GDD accounts for the biophysical phenology of the crop as well as improves interpretability of the model. Hence while the prediction improvements are minimal, the variable's inclusion is an important step in the development of a crop yield model. In addition to averaging over the whole season or a shorter window, we can also use principal

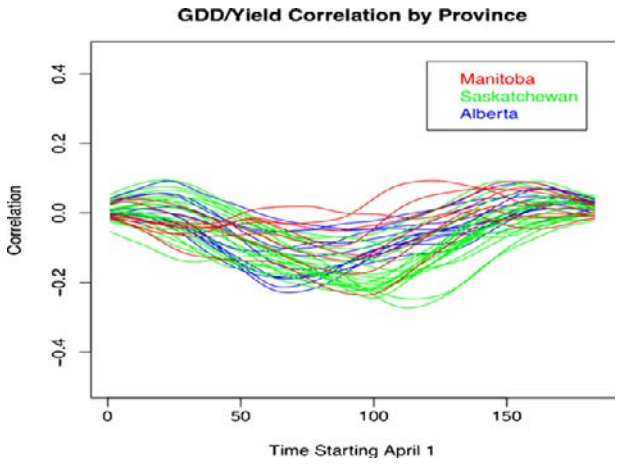

Fig. 6. Correlation of GDD and yield over time. Smoothed with lowess smoothing. From this we see that a reduced window average may be appropriate.

components as we did for SI above. While using the first 4 principal components only increases this to 76.48%, the additional 120 variables result in reduced cross-validation prediction performance, hence we prefer using just the windowed average. We emphasize that this is a user and case-specific choice, and for alternate purposes different choices may be preferred. The expanded LS model (3) then becomes

$$y_{j,t} = \beta_{0,j} + \beta_{1,j}t + \beta_{2,j}PC1_{j,t} + \cdots + \beta_{5,j}PC4_{j,t} + \beta_{6,j}\overline{GDD}_{j,t} + \epsilon_{j,t}, \tag{4}$$

where $\overline{GDD}_{j,t}$ is the windowed average of GDD in region j, year t. It is worth noting that temperature is a component of SI; however, the addition of GDD into the model improves both model fit and prediction, thereby eliminating concerns about the deleterious effects that collinearity between the two covariates might introduce.

We compare the previous models as well as those developed later in the paper in Table 1, showing the features and performance of each successive model. The traditional regression models represented in Table 1, fitted for each region separately, ignore a considerable amount of information. Specifically, because of the close spatial proximity of the regions, considerable strength may be gained by exploiting the correlation among regions. For instance, use of neighbouring SI values can help stabilize predictions based on SI values, since the latter come from a small set of regional monitoring stations and hence can be fairly noisy. The amount of borrowed strength can be considerable when the correlation between stations is high. In addition, modelling all stations jointly while incorporating spatial information allows us to continue to make predictions even in the presence of missing or noisy data. If a measuring station goes out of operation temporarily, its missing values may be inferred from data collected at nearby regions

Table 1
Features of various models.

Model	Parameters	Effective parameters	R^2	CV RMSE
1: Single LS	3	3	.33	6.83
2: LS with SI	120	120	.61	5.79
3: LS with PCA	240	240	.70	5.72
4: LS with PCA +GDD	280	280	.73	5.69
5: Bayes	283	139	.70	5.35

We see that while model 4 has the best fit to the data ($R^2 = .73$), the Bayesian model gives the best prediction performance in terms of cross-validated root mean squared error (in bushels per acre). Effective parameters is defined as $tr(S)$, where $\hat{y} = Sy$, and may be considered a measure of model complexity (Hastie et al., 2009).

to yield accurate forecasts. This idea leads into our next section, which focuses on spatial models that look at all regions together in a unified manner.

2.3. A context-specific spatial Bayesian approach

Classical regression methods rely on the assumption that their model residuals are uncorrelated. Indeed violation of that assumption can have very serious deleterious effects on parameter estimates compared, for example, to violations of the assumption that those residuals have a Gaussian distribution (Day, 1965). In our case the residuals are most certainly spatially dependent and thus the actual amount of information in the data can be much less than the assumptions underlying (1) would suggest. The unwary analyst would then be led to make overconfident forecasts with parameter estimates which vary considerably from one region to the next, yet have unduly small standard errors.

One work-around would model the regions separately. However, this wastes the benefits spatial dependence provides by borrowing strength, telegraphing information across the regions through the wires of correlation for the mutual improvement of all their forecasts. This progression naturally leads us to a Bayesian framework for handling this problem, one which jointly models all regions simultaneously while accounting for their spatial dependence. Thus we move from the frequency paradigm of classical statistics to the Bayesian paradigm of modern statistics.

These two paradigms, which tend to give similar inferences at least for fairly large datasets, are very different in concept. Frequentists see data as being generated by a system governed by some true but unknown parameters. They commonly seek to estimate these true parameters well in some sense, for a variety of inferential purposes such as forecasting. The central tenet of their theory is repeated sampling—in the long run the parameters can be estimated to arbitrarily high levels of precision if the system producing the data were unperturbed. However, Bayesian statisticians reject the notion of repeated sampling as a fundamental construct in their theory, recognizing realistically that most systems cannot remain unperturbed and pump out replicate data over an extended sequence of trials. Although their models involve uncertain parameters, these parameters like all uncertain objects such as future data values, are characterized by a probability distribution. Initially that distribution, called a prior, simply reflects the Bayesian's own knowledge. An abundance of such knowledge would mean a prior concentrated around a single point and a state of near certainty. The information in the data adds to the state of knowledge through the celebrated Bayes theorem. The latter relies on the likelihood function of the uncertain parameters which captures all the information in the data. A likelihood tightly concentrated around a single value would mean the data has eliminated much of the uncertainty about the parameters. However generally, Bayes rule needs to be applied to get the combined effect of data and prior knowledge; this yields the Bayesian's updated prior, or the so-called posterior distribution. Due to its adaptability and ease of use, Bayesian inference has become a prominent fixture in modern spatial statistics, and in particular the modelling of random spatio-temporal fields (Banerjee et al., 2004; Le and Zidek, 2006).

2.3.1. Available prior information

Consider, for example, the spatial structure discussed above. Even before estimating the parameters in Eq. (3), we expect parameters in adjacent regions to be similar. Thus we would be surprised if the parameters relating GDD to yield had completely opposite signs in two neighbouring regions. This reflects our prior beliefs about those parameters, namely that knowledge of one would tell us something about the other. More simply, we would see them as stochastically dependent in the language of the probability distribution that characterizes our beliefs about them. We might even have some idea of their approximate magnitudes. For instance, a magnitude of 100 (bushels per acre/degree celsius) for the coefficients $\beta_{6,j}$ for GDD would be completely untenable, since it would mean that changing one cold day to a warm one (adding, say, 10 GDD over the entire cumulative season), would increase the yield by roughly 10 bushels per acre. Thus even without formalizing our beliefs in a prior distribution, loose bounds on parameters are almost always apparent.

Application of the Bayesian approach starts by characterizing our beliefs about the parameters in the form of a prior distribution. In the regression models introduced above, this would amount to a joint prior distribution on each β to account for our belief in their dependence (similarity) for adjoining regions. For simplicity, stack all of the coefficients into a vector $\boldsymbol{\beta}$, the first 7 coefficients being for all variables in region 1, the next 7 for region 2, and so on. Assuming a Gaussian distribution as a convenient prior form, we can explicitly write the prior as follows:

$$\boldsymbol{\beta} \sim N(0,\ \Sigma_0 \otimes g\Omega). \tag{5}$$

By using such a Kronecker structure, Σ_0 models the correlation within a given coefficient across space, while $g\Omega$ corresponds to Zellner's g-prior (Zellner, 1986) with Ω the 7×7 empirical covariance between explanatory variables. As such, this choice of prior fits within the empirical Bayes paradigm. While specifying the coefficients (particularly the intercept) to have zero-mean seems restrictive, we note that a priori it does not seem unreasonable to assume that in the presence of full stress (signaling the complete absence of water) the crop yield would be zero. We now specify Σ_0, the correlation between regions, as

$$\Sigma_0 = \exp\left(\frac{-D}{\phi}\right), \tag{6}$$

with a slight abuse of notation where D is the matrix with element (i, j) the Euclidean distance between regions i and j (as measured from the center of the region). Here ϕ is a parameter controlling the rate of decay of correlation as distance increases. In this way, ϕ controls how spatially smooth the coefficients are, while g controls how tight around zero the coefficients are. While we are not convinced that wheat is planted in more than the southern section of the three northern-most regions, including the region centers rather than some more southerly geographic location is conservative, as the true geographic center is further removed from adjacent regions, and therefore the correlation expressed through Σ_0 is decreased. Others have proposed more complex spatially-varying models which rely on Markov chain Monte Carlo for inference (e.g. Gelfand et al., 2003; Banerjee et al., 2004); however, our goal of an online implementation restricts us to models with analytic tractability.

While we suspect neighbouring regions to be similar, Fig. 2 highlights the differences between provinces. While one could include an indicator variable to allow for provincial effects, accounting for provincially-varying coefficients would involve a considerable number of interaction terms. In fact, the varying irrigation and technology policies in each province result in a sharp boundary between provinces for several of the mean parameters. As such, it is not entirely logical to use a stationary prior (Cressie, 1993) which assigns correlation between regions solely based on distance without any respect for political boundaries. As a result, we adjust our prior distribution to have reduced correlation between regions in different provinces. While the obvious approach is to scale down the prior correlation between regions in different provinces with a constant value, this may lead to non-positive definiteness of Σ_0; alternative methods which do not suffer from this problem are therefore needed. We accomplish this task by deforming the

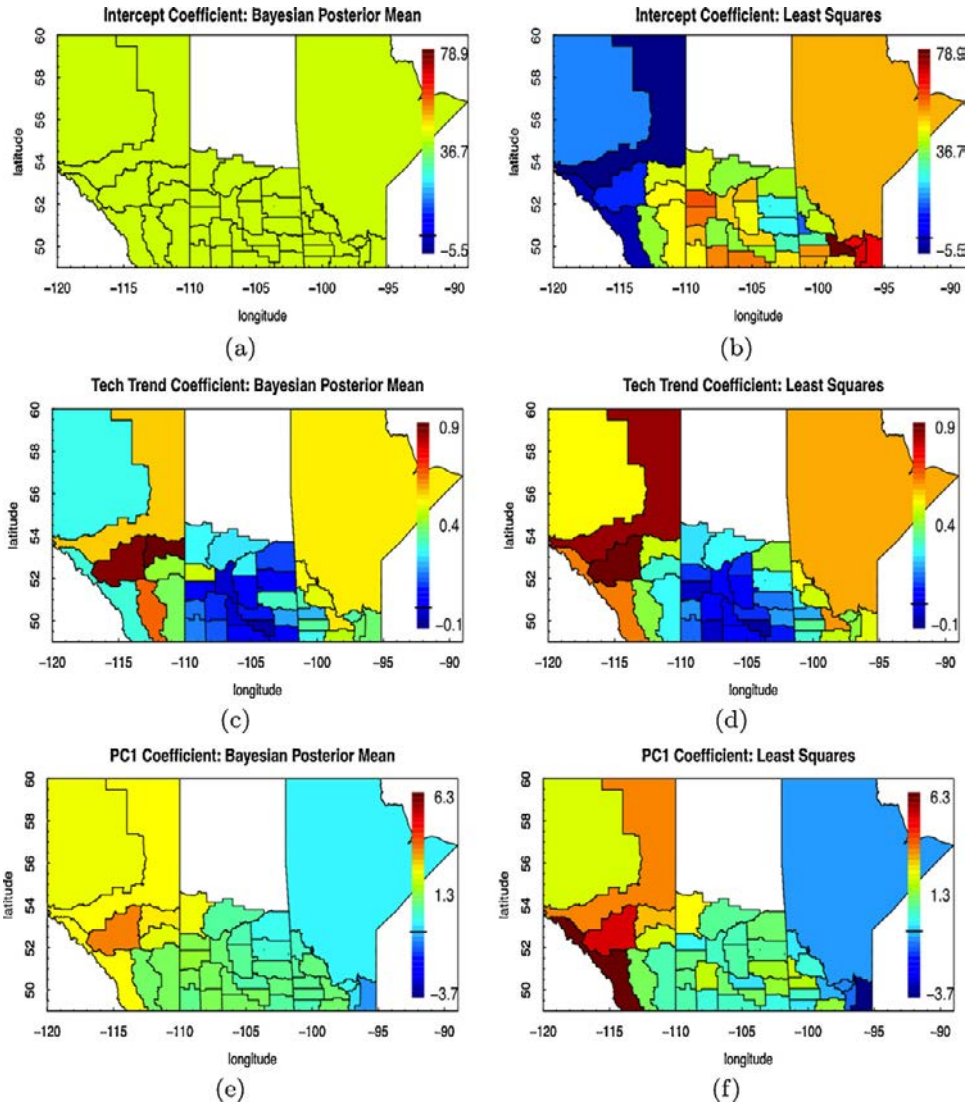

Fig. 7. Coefficient surfaces for intercept, technology trend, and PC1. Other coefficients are similarly smoothed.

physical space, in effect pushing neighbouring provinces apart. Motivated by Sampson and Guttorp (1992), this artificial distortion of the space results in a stationary prior in the deformed space, yet a nonstationary one in the original space. The distance d (measured in degrees latitude/longitude) by which the provinces are pushed apart in the artificial space is selected through cross-validation. Searching over the integers from 1 to 10, we find $d=4$ to give the best prediction performance (CV RMSE of 5.35 vs. 5.39 for $d=0$), intuitively meaning that Alberta and Manitoba are pushed respectively west and east from Saskatchewan by 4 degrees longitude in the artificial space. The end result is a reduction in the off-diagonal elements of Σ_0 corresponding to between-province regions while maintaining positive definiteness. Note that the prior parameters ϕ, g, and d result in an additional 3 parameters in the Bayesian model, as reflected in Table 1.

2.3.2. Likelihood and posterior distributions

We begin by employing the likelihood corresponding to (4), namely

$$y_{j,t} \sim N(\beta_{0,j} + \beta_{1,j}t + \beta_{2,j}PC1_{j,t} + \cdots + \beta_{5,j}PC4_{j,t} + \beta_{6,j}\overline{GDD}_{j,t}, \sigma^2). \tag{7}$$

In keeping with common practice, we also assign an Inverse-Gamma prior distribution on σ^2 with shape and scale parameters a and b set to be highly noninformative. Before proceeding, we introduce the notation y, the column vector of stacked y_j, and X, the $(31\times 40)\times 240$ block-diagonal matrix of explanatory variables. Using Bayes theorem to combine our initial knowledge (in the form of prior distributions) and the information provided by the data (in the form of the likelihood), we can obtain the posterior distribution of the parameters. Specifically, for the regression coefficients $\boldsymbol{\beta}$, the marginal posterior is obtained using Bayes Theorem as follows:

$$\pi(\boldsymbol{\beta}|X,y) \propto \int \pi(y|X,\boldsymbol{\beta},\Sigma)\pi(\boldsymbol{\beta}|\Sigma)\pi(\Sigma)d\Sigma. \tag{8}$$

Due to the conjugate nature of the prior and likelihood, we are able to analytically complete this integral. The resulting distribution is a multivariate Student-T,

$$\boldsymbol{\beta} \sim T(\boldsymbol{\beta}_f, \Psi, n+2a) \tag{9}$$

where $\boldsymbol{\beta}_f = (X^TX + (\Sigma_0 \otimes g\Omega)^{-1})^{-1}(X^Ty)$, $\Psi = (X^TX + (\Sigma_0 \otimes g\Omega)^{-1})(SS+2b)/(n+2a)$, $SS = y^Ty - \boldsymbol{\beta}_f^T(X^TX + (\Sigma_0 \otimes g\Omega)^{-1})\boldsymbol{\beta}_f^T$.

From this last expression, we get the posterior mean $\boldsymbol{\beta}_f$, which may be used as a simple estimator for $\boldsymbol{\beta}$. In fact, comparing $\boldsymbol{\beta}_f = (X^TX + (\Sigma_0 \otimes g\Omega)^{-1})^{-1}(X^Ty)$ to the LS estimate $(X^TX)^{-1}(X^Ty)$, we

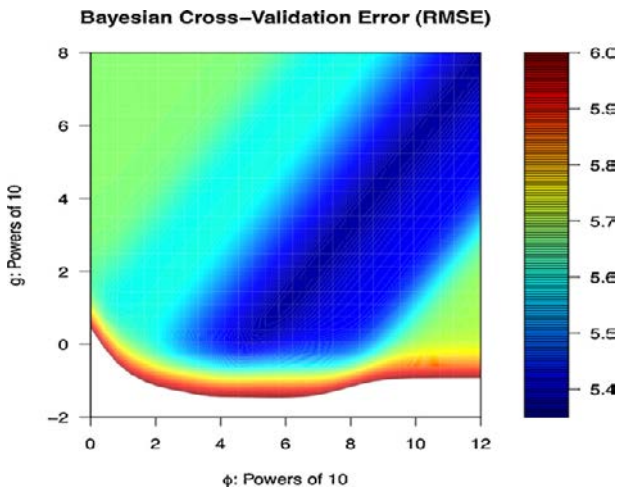

Fig. 8. Cross-validation errors using Bayesian posterior mean. For comparison, the least squares error is 5.69. From this, we observe a ridge of excellent prediction. Hence there is some tradeoff between the two parameters to be tuned.

readily see how the prior covariance affects the parameter estimates. In particular, a diffuse prior distribution adjusts the estimate little, whereas an informative prior distribution – one that is fairly tightly concentrated around zero – shrinks the posterior estimate considerably.

Setting $g = 10$ and $\phi = 10^6$, we obtain coefficient estimates as shown in Fig. 7, which also shows the corresponding least squares estimate using (4). We see that the spatial information used in the Bayesian model causes the coefficients to be more correlated across space. In addition, the zero-mean prior distribution leads to some shrinkage in the coefficient estimates. Interestingly, we notice little shrinkage in the estimated coefficient for technology trend, suggesting that the data contains considerable information on this quantity.

3. Results

We proceed by comparing the prediction performance of the least squares and Bayesian methods. To accomplish this we use leave-one-out cross-validation, removing years one at a time in succession to compare each model's predictive ability. More specifically, we successively remove each year in turn, using the

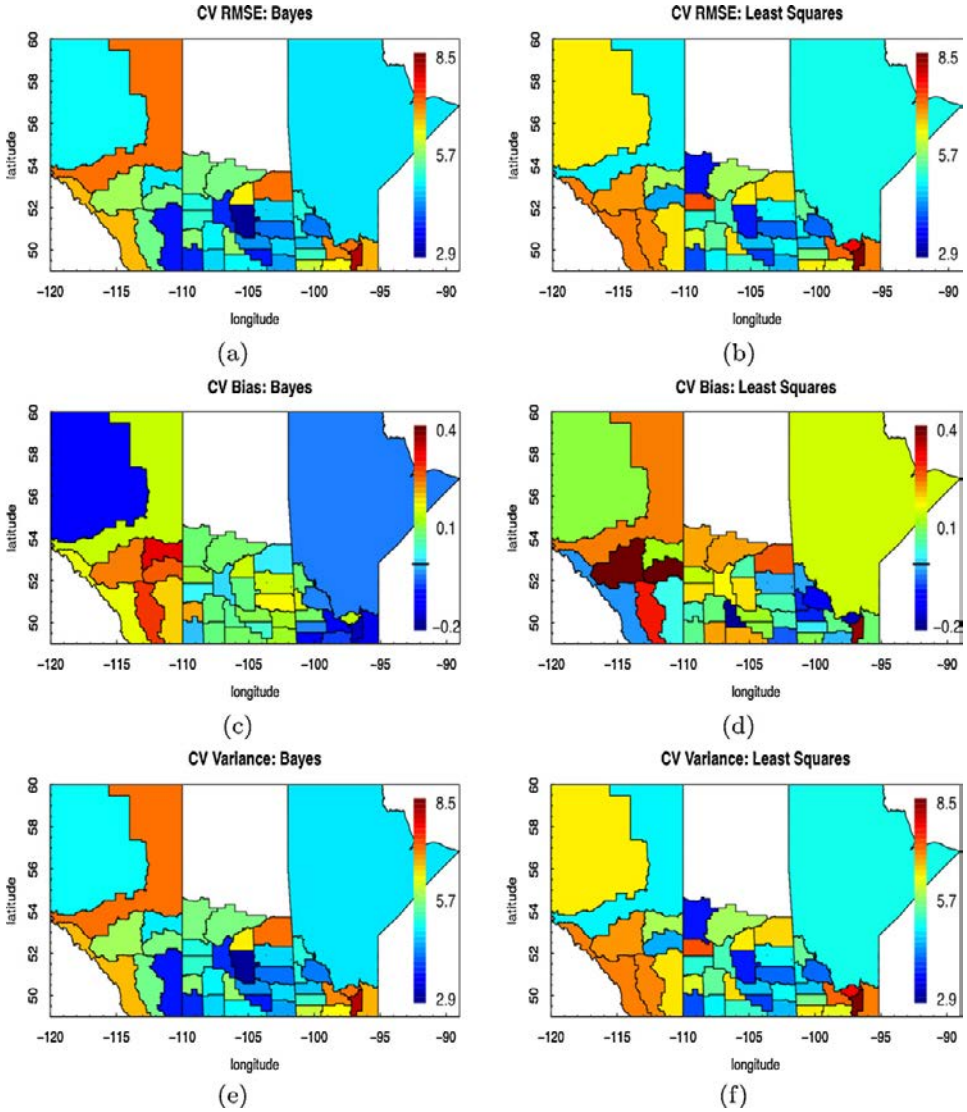

Fig. 9. Cross-validation results by region. The Bayesian model improves prediction by all standards in the majority of regions. We plot root mean squared error (RMSE) as well as the breakdown to bias and variance for the models.

remaining years to find the posterior mean, notated $\hat{\boldsymbol{\beta}}^i$ if year i is removed. This posterior mean is then used to perform prediction on the removed year. From this the root mean squared error (RMSE) is calculated as the square root of the sum of squared prediction errors for each year and region.

$$\text{RMSE} = \sqrt{\sum_{i=1}^{31}\sum_{j=1}^{40}(y_{i,j} - X_{i,j}\hat{\boldsymbol{\beta}}^i)^2/(31 \times 40)}. \quad (10)$$

Fig. 8 shows the cross-validation root mean squared error (RMSE) of the posterior mean estimate for various settings of g and ϕ. As $g \to \infty$ and $\phi \to 0$, the Bayesian model converges to the least squares solution, as evidenced by converging cross-validation errors. However, if g is too small, the prior on the regression coefficients is too informative towards zero, and hence the resulting posterior means are overly shrunken, resulting in poor prediction (RMSE >6). While one could assign prior distributions to these parameters, we prefer finding them through cross-validation for computational efficiency. Specifically, given the optimal parameters, the model is conjugate, and hence sequential updating and prediction is analytic and therefore nearly instant. It is very interesting to note that the optimal prediction error for the Bayesian model is less than for the least squares model, indicating that prediction is improved with regularization (provided by the zero-mean prior and/or correlation). The area of lowest prediction error occurs along a diagonal of g and ϕ and has value approximately 5.35. This is likely due to the fact that an increase in g results in a more diffuse posterior which regularizes less, while increases in ϕ result in increased correlation between regions and hence more regularization. Hence the optimal prediction seems to occur for moderate amounts of regularization.

The cross-validation RMSE can also be calculated for each region by summing only over years. In this way we can gain an improved perspective on the model's prediction performance. However, while cross-validation RMSE gives an idea of the prediction performance of a model, it does little to tell of a model's bias. To do this we decompose the RMSE into the model's prediction bias and variance. Doing this for each region, we obtain Fig. 9 detailing the prediction RMSE, bias, and variance of the Bayesian and LS models in each region. From this figure we observe that, with the exception of one or two individual regions, the Bayesian model improves RMSE in all areas except for southern Manitoba. Digging deeper, we see a negative bias in this area. Thus the regularization of the model is perhaps not useful in this region due to some systematic differences in this area. Specifically, this section of southern Manitoba is known to use significant irrigation (Gaia Consulting Limited, 2007). As a result, further model development might be explored in this area to account for irrigation.

4. Conclusion

In this paper we have examined the role of SI in predicting crop yields, emphasizing the need to create a judicious low-dimensional summary in order to improve prediction. Simply averaging SI over the entire season is inefficient, as yield may be insensitive to stress in certain parts of the summer. The traditional solution to this problem is to average over a reduced window of data, hence cutting out those areas lacking in sensitivity from the analysis. However, this one-dimensional feature is not particularly sensitive to changes in stress indices within that window. For example, a region which has low SI in June but high SI in July might ultimately have the same averaged value as another region which had just the opposite trend. To address this issue, we have implemented principal components analysis to create a set of flexible summary statistics which better describe the variations in SI, and as a result improve prediction considerably. We also demonstrated principal components' improved performance over wavelet bases.

We have also shown the importance of incorporating spatial correlation into crop yield models; ignoring this information can lead to bias both in model identification and prediction. Specifically, we observed that a common least squares fit of crop yield on some explanatory variables over the entire region resulted in biased residual errors, and hence violated the assumptions of the model. To avoid this problem, we could fit each agricultural region with its own model. The problem, however, is that this ignores information between crop regions, and as such we observed reduced prediction power and model identifiability. We addressed this issue through the use of a Bayesian model which modelled all regions together, yet accounted for spatial correlation. This model smooths and stabilizes prediction and also allows for analytic and therefore efficient updating and prediction. In addition, we created a non-stationary prior distribution to address the issue of province to province variability resulting from provincial differences in policy, management, and other factors affecting yield. Through cross-validation, we demonstrated this model to achieve improved prediction performance in modelling Canadian wheat yield over the least squares model which ignores spatial dependence, and hope that others will attempt to replicate our findings in other contexts based on the promise seen in this application.

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