Author Response on "Can river temperature models be transferred between catchments?" by Faye L. Jackson et al.

Dear Markus,

We are pleased to see that the reviewers find the revised manuscript to be much improved and that consider that we have responded in a thorough and detailed manner. We have made further revisions to the manuscript based on these latest comments and hope that you now agree the paper is suitable for publication.

Regards, Faye, Iain, Rob and David.

Anonymous Referee #2

I appreciate that the authors have responded to the reviewers' comments in a thorough and detailed manner. In relation to my comments, the authors have placed their study much more effectively into the context of previous literature, which highlights the specific contributions of this study and the ongoing limitations of and potential for improvement of empirical stream temperature models I do not fully agree with all statements made by the authors in their responses to reviewers' comments or their revisions, but I do not see any value in quibbling over details. I do, however, have a couple of suggestions the authors should consider prior to submitting a final version of this manuscript.

We thank the reviewer for their additional comments. We are pleased that the Reviewer considers that we have responded to their comments in a thorough and detailed manner and that they feel the manuscript now better highlights the study contribution. We can see that there remain some differences of perspective, but are pleased that reviewer does not consider these to be worth "quibbling" over.

1. In presenting the models, it appears that the authors are using R formula syntax. It would be useful for readers who are not R users for the authors to acknowledge this point and to clarify that an intercept term is included by default.

We have refined our text to reflect the style of the model equations. The text now reads:
A 'full' model was first fitted which included all the available covariates from the reduced dataset and a river network smoother (RNS) (see below). The model can be conveniently written in R formula syntax as:

$$Tw_{max} \sim s(covariate_1) + \ldots + s(covariate_n) + RNS$$

where, n is the number of covariates (n = 5, 6 for LS, LS_Ta models respectively), s(covariate$_i$) denotes that covariate i was fitted as a smoother, and an intercept is included by default.

2. One point on which I continue to disagree with the authors is their confounding of spatial versus temporal relations between Tw and Ta, especially when the spatial relation is for a single metric. In the paragraph beginning "Many studies have shown …" on p. 26, I recommend that the authors edit the passage to clarify which relations are temporal and which are spatial.

We appreciate that Reviewer 2 and 4 continue to have problems with this aspect of the manuscript although we note that we provided a detailed explanation of this thinking in our previous 14 page response letter.

However, following reviewer 2's specific request, we have now updated the referencing in the aforementioned paragraph. Specifically we have removed the references to "spatial" (static) Tw~Ta models and replaced them with references to papers that (1) model relationships between Tw~Ta using within-year (temporal) data and then (2) assess how those Tw~Ta relationships vary with catchment or landcape characteristics. We feel that the use of these references should further clarify our main arguments. Specifically:

- Temporal Tw~Ta relationships (specifically the slope and intercept of Tw~Ta relationships or other model coefficients in case of logistic models) vary between sites and catchments in response to regional, landscape and hydrological controls.
- Where the spatial variability in Tw~Ta relationships is random across a catchment, this could make it difficult to detect a common static "spatial" Tw~Ta relationship
- Where there is systematic spatial variability in temporal Tw~Ta relationships within or between catchments, this could result in spatial biases when models are transferred
- Given the potential for these differences it is perhaps not too surprising that a single Ta coefficient (i.e. a single Tw~Ta) is not a good predictor of Tw across space in static "spatial" models to Tw
- Ta may provide better predictions if it was permitted to interact with other covariates that affect "temporal" Tw~Ta relationships e.g. hydrogeology, woodland etc.

The revised paragraph now reads:

Many studies have shown that within year temporal relationships between Tw and Ta (often termed thermal or climate sensitivity) can be highly variable between sites and catchments, and importantly that this variability relates to regional, hydrological and landscape controls (Tague, et al., 2007; Kelleher et al., 2012; Krider et al., 2013; Chang and Psaris, 2013; Hilderbrand et al., 2014; Segura et al., 2015; Mauger et al., 2016). For example, Fellman et al. (2014) observed slopes of between -0.180 and 1.282 across 9 watersheds in Alaska depending on glacial influence, while Mauger et al., 2016

observed slopes of between 0.32 and 1.51 across 48 non-glacial streams in Alaska which related to mean elevation and catchment area. Similarly, Tague et al., (2007) observed systematic regional differences in Tw~Ta relationships in Western Oregon that depended on local hydrogeology and concluded that under such circumstances air temperature alone (i.e. consistent with a single air temperature coefficient) would be unlikely to explain spatial variation in river temperatures. Given the reported spatial variability in Tw~Ta relationships and importantly, that these relationships can vary systematically within and between catchments depending on other controls (e.g. hydrogeology), it is unsurprising that models containing Ta_{max} do not substantially improve predictions of the spatial variability in Tw_{max} than models containing landscape variables alone, and that transferred models result in biased Tw predictions. If Ta is to substantially improve predictions of Tw in static spatial models (such as those presented in this study), then it is likely that they would need to include greater model complexity e.g. allowing for interactions between Ta_{max} and landscape covariates (e.g. Mayer, 2012).

Anonymous Referee #4

I've read the revision by Jackson and colleagues and think it's improved over the previous draft.

We are pleased that the reviewer considers the paper has improved.

Overall, I'm left with the impression that the models transferred surprisingly well (with the exception of Bladnoch) despite many things changing to make the transfer process less consistent than it would have to be. For example, each model had a different set of covariates, use of a RNS varied, and functional relationships estimated from GAMs would be somewhat idiosyncratic to individual catchments.

The performance of the models is detailed in the paper. The fact that the catchment specific models varied just emphasises the difficulties of transferring models between catchments (as was the purpose of the the paper). Of course the RNS cannot be transferred, so does not affect between catchment predictions. This is also a critical point we make in the paper. The only relationships that varied significantly in the multi-catchment model were those associated with Ta (which were linear). There was a smoothed response to UCA in the multi-catchment model that was common across catchments.

If these factors had been held constant and linear models used instead of GAMs, transferability would probably increase further.

The only relationships that varied significantly in the multi-catchment model were those associated with Ta (which were linear). There was a smoothed response to UCA in the multi-catchment model that was common across catchments. We therefore fail to see how imposing linear models would improve predictions. We note that it was our deliberate intention to

allow the models to vary between catchments as only this provides a genuine test of model transferability i.e. you are transferring a model to a new area with no prior knowledge of that area.

One point of concern I do have is the conclusion drawn regarding the poor transferability of the air temperature relationship. Examination of the data plot for Bladnoch in Figure 3d suggests the two temperature observations with the largest catchment area (& lowest elevation, warmest air temperature?) were so cold that they resulted in the GAM relationship being strongly nonlinear. Figure 2 also describes the negative relationship between air temp and stream temp of -0.22 in this catchment (difficult to see in the scatterplot). Because this is also a small dataset of n = 19, the estimated relationships are easily affected by individual observations, so it's important to know what's going on at those two sites.

We believe that the relationship is being influenced by two sites with very low UCA, intermediate Ta and low Tw. Neverthless it is not only the Tw~Ta relationship at the Bladnoch that is the issue. The relationships at the other sites are also very different and the models containing Ta are consistently worse in predicting Tw in new catchments. We have therefore revised the discussion to further emphasise these points as follows:

In contrast to the LS models, one LS_Ta model included a physically implausible relationship that would not be expected to transfer well (Smith et al., 2016). Specifically, an inverse modal relationship between Tw_{max} and Ta_{max} in the Bladnoch model. This relationship could have arisen because of spatial variability in local (temporal) $Tw_{max} \sim Ta_{max}$ relationships due to controls that were not captured by our covariates, coupled with a relatively small air temperature range (1.7°C) and sample size (19 sites).Nevertheless, even where the relationships between Tw_{max} and Ta_{max} were plausible, they were inconsistent between catchments in terms of effect size and direction, as indicated by the varying responses in the single catchment models and the interaction with Catchment in the multi-catchment model. For example, in the latter, the relationships were positive in the Dee and Tweed and negative in the Spey and Bladnoch (where the relationship simplifies to linear).

Perhaps there were local inputs of coldwater springs, or a deep reservoir, or other factor creating a local temperature anomaly?

We agree that other factors could be affecting this Tw~Ta response and indeed our text states this. Specifically we identify that static "spatial" Tw~Ta responses will be affected by local variability in "temporal" Tw~Ta relationships which vary with catchment characteristics (see response above)

Regardless, the authors should be careful about drawing general conclusions about this portion of the analysis as two observations may be driving it.

We think that the conclusions are well founded based on the differing responses across all the catchments, not just the Bladnoch as detailed above. We are conscious that the previous manuscript may have over emphasised the role of the Bladnoch, but we have now revised the manuscript to refer to the varying responses across all the catchments and to highlight that the Ta models generally gave poorer predictions when transferred, regardless of the catchment being considered.

Another point that warrants mention is that the way air temperature is used to explain variation in this model, it's representing a spatially static landscape pattern rather than something that's temporally dynamic (based on the description in Table 1). That distinction is important because different processes are involved and several of the studies and models cited by the authors are not using air temperature to represent a spatial pattern, but temporal dynamics instead.

See response above and revisions to referencing and text where we explain the potential influence of temporal Tw~Ta responses on spatial Tw~Ta responses.

Can spatial statistical river temperature models be transferred between catchments?

Faye.L.Jackson[12], Robert.J.Fryer[3], David.M.Hannah[1], Iain.A.Malcolm[2]

[1] School of Geography, Earth and Environmental Science, University of Birmingham, Birmingham, B15 2TT, UK
[2] Marine Scotland Science, Scottish Government, Freshwater Laboratory, Faskally, Pitlochry, PH16 5LB, UK
[3] Marine Scotland, Marine Laboratory, 375 Victoria Road, Aberdeen, AB11 9DB, UK

Correspondence to: F. L. Jackson, F.Jackson@marlab.ac.uk

Abstract. There has been increasing use of spatial statistical models to understand and predict river temperature (Tw) from landscape covariates. However, it is not financially or logistically feasible to monitor all rivers and the transferability of such models has not been explored. This paper uses Tw data from four river catchments collected in August 2015 to assess how well spatial regression models predict the maximum 7 day rolling mean of daily maximum Tw (Tw_{max}) within and between catchments. Models were fitted for each catchment separately using (1) landscape covariates only (LS models) and (2) landscape covariates and an air temperature (Ta) metric (LS_Ta models). All the LS models included upstream catchment area and three included a river network smoother (RNS) that accounted for unexplained spatial structure. The LS models transferred reasonably to other catchments, at least when predicting relative levels of Tw_{max}. However, the predictions were biased when mean Tw_{max} differed between catchments. The RNS was needed to characterise and predict finer scale spatially correlated variation. Because the RNS was unique to each catchment and thus non-transferable, predictions were better within catchments than between catchments. A single model fitted to all catchments found no interactions between the landscape covariates and catchment, suggesting that the landscape relationships were transferable. The LS_Ta models transferred less well, with particularly poor performance when the relationship with the Ta metric was physically implausible or required extrapolation outside the range of the data. A single model fitted to all catchments found catchment-specific relationships between Tw_{max} and the Ta metric, indicating that the Ta metric was not transferable. These findings improve our understanding of the transferability of spatial statistical river temperature models and provide a foundation for developing new approaches for predicting Tw at unmonitored locations across multiple catchments and larger spatial scales.

Key words: transferability, water temperature, landscape controls, spatial statistical models, spatial variability, air temperature, Scotland

1 Introduction

River temperature (Tw) is a key control on the health of aquatic systems (Webb et al., 2008) and is particularly important for the growth, survival and demographic characteristics of cold water adapted species such as salmonids (Elliott and Elliott, 2010; Gurney et al., 2008; Jonsson and Jonsson, 2009; McCullough et al., 2001). Rising Tw will influence fish populations by altering the thermal suitability of rivers (Comte et al., 2013; Isaak et al., 2010, 2012). Thus models that can; 1) identify

areas most affected by thermal extremes, 2) improve understanding of spatio-temporal variability of thermal regimes, 3) predict the potential effects of climate change and 4) illustrate opportunities for thermal moderation, such as riparian tree planting (Hannah et al., 2008; Hrachowitz et al., 2010), are important for fisheries management. Large-scale models are required to provide information at the spatial scales appropriate to management decisions i.e. catchment (Chang and Psaris, 2013; Hrachowitz et al., 2010; Imholt et al., 2011, 2013; Jackson et al., 2017; Steel et al., 2016), regional (Hill et al., 2013; Isaak et al., 2012; Ruesch et al., 2012) and national scales.

Although process based models provide important mechanistic understanding at small spatial scales, their intensive data requirements prohibit their use at larger scales (Jackson et al., 2016). In contrast, empirical models of Tw rely on Tw observations and explanatory covariates (e.g. altitude or air temperature) which can often be derived remotely at relatively low cost. The development of affordable, reliable, accurate Tw dataloggers has led to a rapid increase in Tw monitoring (Sowder and Steel, 2012), to the point that staff time, data storage and quality control are often now the greatest limitations on data collection (Jackson et al., 2016). At the same time, there have been substantial developments in spatial statistical modelling approaches (Ver Hoef et al., 2006, 2014; Ver Hoef and Peterson, 2010; Isaak et al., 2014; Jackson et al., 2017; O'Donnell et al., 2014; Peterson et al., 2013; Rushworth et al., 2015), monitoring network design (Dobbie et al., 2008; Jackson et al., 2016; Som et al., 2014), spatial datasets (e.g. shapefiles incorporating covariates such as in "The National Stream Internet Project" (Isaak et al., 2011) or gridded air temperature datasets (Perry and Hollis, 2005a, b)) and spatial analysis tools (Isaak et al., 2011, 2014; Peterson et al., 2013; Peterson and Ver Hoef, 2014).

While continuous river temperature data are routinely collected in some areas, resulting in large regional temperature datasets and associated models (e.g. Wehrly et al. 2009; Moore et al. 2013), this is far from universal. In many cases financial and logistical considerations limit data collection making it impractical to monitor all rivers. For example, in Scotland there are 16006 river catchments (unique rivers running to the sea), including 629 catchments >10km^2, but there was no systematic nationwide quality controlled river temperature data collection until 2015 (Jackson et al. 2016). For management purposes, it is therefore often necessary to predict Tw at unmonitored locations, both within (Hrachowitz et al., 2010; Jackson et al., 2017; Peterson and Urquhart, 2006) and between catchments (Isaak et al., 2014). In recent years, it has become increasingly common to develop and apply spatial statistical river network models that incorporate network covariance structure to predict spatial variability in river temperature (e.g. Isaak et al., 2014; Jackson et al., 2017). It is widely acknowledged that these models can dramatically improve predictions of river temperature where sufficient observational data exist, but the covariance component of the predictions cannot typically be transferred between catchments. Despite these important issues, there has not yet been an assessment of the transferability of spatial statistical Tw models between catchments; i.e. the ability of a model developed in one catchment to predict Tw in another. This paper investigates the ability of spatial statistical Tw models to predict Tw at unmonitored locations within and between catchments.

The principles explored in this paper are likely to be relevant to other water temperature metrics so, for brevity, this study focuses on maximum summer temperature, a metric which is prevalent in the recent literature, reflecting its importance

for the survival of cold water adapted fish (Chang and Psaris, 2013; Hrachowitz et al., 2010; Jackson et al., 2017; Malcolm et al., 2008; Marine and Cech, 2004).

Models are fitted using two sets of covariates. The first set contains landscape covariates which can be generated from readily available spatial datasets and have been the focus of many previous studies of spatial variability in river temperature (e.g. Hrachowitz et al., 2010). Due to increasing interest in the use of air temperature (Ta) to predict spatial variability in water temperature (e.g. Jonkers & Sharkey, 2016), the second set contains a metric of air temperature in addition to landscape covariates.

The paper addresses the following objectives:

1. Develop statistical models for predicting maximum summer water temperature from landscape covariates in four separate river catchments.
2. Determine whether models containing an air temperature metric explain more of the variation in maximum summer water temperature than those only containing landscape covariates.
3. Assess the transferability of models containing only landscape covariates or both landscape and air temperature covariates between catchments
4. Produce single models of maximum summer water temperature for all four catchments using both sets of covariates and consider their potential for transferability at larger (e.g. national) scales.

2 Methodology

2.1 Water temperature data and metric

Tw data were obtained from monitoring sites in four catchments; the Bladnoch in Western Scotland and the Dee (Aberdeenshire), Spey and Tweed in Eastern Scotland (Fig.1). These catchments are Special Areas of Conservation for Atlantic salmon and form part of the Scotland River Temperature Monitoring Network (SRTMN) (Jackson et al., 2016). Details of the network, including design and quality control procedures, are given in Jackson et al. (2016). The catchments all contain an adequate numbers of Tw dataloggers to develop Tw models on a single catchment basis with 59, 34, 25 and 19 sites in the Dee, Tweed, Spey and Bladnoch, respectively. The choice of catchments ensured a broad geographic coverage across Scotland with a wide environmental range of landscape covariates (Jackson et al., 2016).

Data were collected at 15 minute intervals throughout August 2015. The maximum temperature was calculated for each day and used to produce a 7 day rolling mean of maximum temperatures. The metric of maximum temperatures used in this study (Tw_{max}) was the maximum value of this 7 day rolling mean. This metric was preferred to a single observation of Tw as it characterises the occurrence of sustained high temperatures which are thought to be most ecologically damaging.

2.2 Model covariates

Detailed discussion of the landscape covariates and their calculation can be found in (Jackson et al., 2016). In brief, the covariates were: elevation (Elevation), upstream catchment area (UCA), percentage riparian woodland (%RW), hillshading / channel illumination (HS), channel width (Width), channel gradient (Gradient), channel orientation (Orientation), distance to coast (DC) and distance to the sea along the river (RDS). Table 1 summarises how the covariates were calculated. Before model fitting, Gradient, UCA and Width were log transformed to reduce skewness and HS was centred by subtracting the median value from all observations.

An air temperature metric (Ta_{max}) was calculated for each site from the gridded UKCP09 Ta dataset (available from the UK MET Office). See Perry and Hollis (2005a, 2005b) for details of this dataset. Analogous to the calculation of Tw_{max}, Ta_{max} was given by the maximum of the 7 day rolling mean of daily maximum air temperatures in August 2015.

Figure 2 illustrates the distribution and correlation among covariates included in the single or multi-catchment models (excluding strongly correlated (> 0.8) covariate pairs, see below for details) for each of the four catchments and for the global (four catchment) dataset.

2.3 Modelling

Ten models of Tw_{max} were developed: two models for each of the four river catchments using either 1) landscape covariates only (LS models) or 2) landscape covariates and Ta_{max} (LS_Ta models) and two models for all four catchments combined, again using either 1) landscape covariates only (multi-catchment LS model) or 2) landscape covariates and Ta_{max} (multi-catchment LS_Ta model). The modelling process differs slightly between the single and multi-catchment models and these are described in turn. All analysis was done in R version 3.2.3 (R Core Team, 2015).

2.3.1 Single catchment models

The set of covariates was first reduced to avoid problems of collinearity. If two covariates were strongly correlated (Pearson correlation coefficient >0.8) in any one catchment, one of the covariates was dropped from the set available for modelling for all catchments. This ensured all the LS models were based on a common set of covariates (UCA, %RW, HS, Orientation, DC) as were the LS_Ta models (Ta_{max}, UCA, %RW, HS, Orientation, DC).

The relationship between Tw_{max} and the covariates was explored using generalised additive models (GAMs) with Gaussian errors and an identity link (Wood, 2001). A 'full' model was first fitted which included all the available covariates from the reduced dataset and a river network smoother (RNS) (see below). The model can be conveniently written in R formula syntax as:

$$Tw_{max} \sim s(covariate_1) + \ldots + s(covariate_n) + RNS$$

~~Here~~where, n is the number of covariates (n = 5, 6 for LS, LS_Ta models respectively)~~, and~~ s(covariate$_i$) denotes that covariate i was fitted as a smoother, and an intercept is included by default. The amount of smoothing was estimated from the data (Wood, 2001), with each smoother constrained to have at most 2 degrees of freedom (df) based on the expected simplicity of Tw_{max} responses to the covariates. The RNS is included to account for spatial structure in the data that cannot be explained by the covariates. The RNS is a modified version of that developed by O'Donnell et al. (2014), with the amount of smoothness at a confluence controlled by the proportional influence of upstream tributaries weighted by Strahler river order (Strahler, 1957) and fitted using a set of 'reduced rank' basis functions. See Jackson et al. (2017) for full details. The RNS was allowed up to 7 df based on knowledge of RNS complexity for the Spey (Jackson et al., 2017). To ensure the RNS did not account for variability that would otherwise be explained by covariates, RNS basis functions were excluded if they were strongly correlated (>0.8) with any of the covariates. Thus, base 1 was removed from the Spey and Dee RNSs due to correlations with DC. In the LS_Ta models, base 2 was also removed from the Spey RNS due to correlation with Ta_{max}. The model was fitted by maximum likelihood using the "mgcv" package (Wood, 2016) in R.

All possible subsets of the full model were then fitted. The final model was that with the lowest Bayesian Information Criterion (BIC) or Akaike Information Criterion corrected for small sample size (AICc) that contained no terms significant at the 5% level. The choice of Information Criterion was based on the desire to penalise more complex models that would be unlikely to transfer well (Millidine et al., 2016). Thus, BIC was used for the Dee and Tweed where there were more sites and AICc was used for the Bladnoch and Spey where there were fewer sites. Terms in the final model with 1 df were replaced by linear terms.

In common with similar modelling studies (Hrachowitz et al., 2010; Imholt et al., 2011; Jackson et al., 2017; Ruesch et al., 2012), no interactions were considered between covariates due to data constraints.

2.3.2 Multi-catchment models

Covariates were excluded if they were strongly correlated (>0.8) across the entire multi-catchment dataset. The reduced set of covariates was Elevation, UCA, %RW, HS, Gradient and Orientation for the LS model, and Ta_{max}, UCA, %RW, HS, Gradient and Orientation for the LS_Ta model. The RNS basis functions were the same as those included in the single catchment models.

A 'starting' model was fitted of the form:

$$Tw_{max} \sim \text{Catchment} + s(\text{covariate}_1) + \ldots + s(\text{covariate}_n) + \text{RNS:Catchment}$$

where Catchment is a categorical variable allowing a different mean level for each catchment and RNS:Catchment denotes a separate RNS for each catchment. The covariate smoothers were given a maximum of 2 df and the RNS a maximum of 7 df for each catchment. The model was then refined in a backwards and forwards stepwise procedure which considered a) replacing smooth covariate effects by linear terms and then dropping them altogether; b) dropping the RNS by Catchment

term altogether; c) adding interactions between the covariates (either linear or smoothed) and Catchment. An interaction between a covariate and Catchment would indicate inter-catchment differences in the relationship between Tw_{max} and the covariate, suggesting that the model might not transfer well to new catchments. Interactions between the covariates were not considered. Model selection was based on BIC. Finally, any non-significant terms ($p > 0.05$) in the final model were removed.

2.3.4 Model performance and transferability of single-catchment models

The ability of single-catchment models to predict Tw_{max} within the catchment they were developed (the donor catchment) was assessed using Leave-One-Out-Cross-Validation. Each site was removed in turn, the final model was refitted, and then Tw_{max} was predicted at the missing site using a) using all model terms (i.e. the covariates and the RNS if present) and b) only covariates (i.e. excluding the columns in the model matrix relating to the RNS). The prediction using all model terms should outperform that using only covariates because it incorporates the extra information about spatial structure that is captured by the RNS. However, a RNS from one catchment cannot be used to predict in another because the river networks will differ. The prediction using only covariates therefore provides a benchmark for assessing the transferability of models between catchments, since it measures how well a model will transfer to a catchment that is identical in all but its river network.

Transferability to another catchment (the target catchment) was assessed by using the model from the donor catchment to predict Tw_{max} at the monitoring sites in the target catchment. As RNSs cannot be transferred, only covariates were used in the predictions (i.e. the columns in the model matrix due to the RNS were ignored).

Three performance metrics were calculated: Root Mean Square Error (RMSE) (Eq.1), which measures overall performance (accuracy), Standard Deviation (SD) (Eq.2), which measures how well a model can predict within-catchment spatial variability (precision), and Bias (Eq.3).

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{s=1}^{n}(\hat{x}_s - x_s)^2} \tag{1}$$

$$\mathrm{SD} = \sqrt{\frac{1}{n}\sum_{s=1}^{n}((\hat{x}_s - \bar{\hat{x}}) - (x_s - \bar{x}))^2} \tag{2}$$

$$\mathrm{Bias} = \bar{\hat{x}} - \bar{x} \tag{3}$$

where x_s and $\hat{x}_s$ are the observed and predicted Tw_{max} at site s, $\bar{x}$ and $\bar{\hat{x}}$ are the mean observed and predicted Tw_{max} in the catchment, and $_n$ is the number of sites in the catchment. Standard deviation was used rather than variance, so that all three metrics are on the same scale and can be compared. Model performance was also illustrated by plotting observed Tw_{max} against predicted values and comparing this to a 1:1 line. Points close to the 1:1 line indicate precise unbiased predictions,

points consistently displaced above or below the line indicate biased predictions, and high scatter about the line indicates imprecise predictions. The consequences of predicting outside of the environmental range of a given model was shown by coding sites as "in" or "out" of range.

3 Results

Across Scotland, August 2015 was wetter than the 1981-2010 mean (MET Office, 2016) and this was reflected in relatively low Tw. Rainfall in Eastern Scotland (which covers the Spey, Dee and Tweed) was 107% of the 1981-2010 mean, whereas rainfall in Western Scotland (which covers the Bladnoch) was only 98% of the 1981-2010 mean (MET Office, 2016). Maximum air temperature was the same in Eastern Scotland as the 1981-2010 mean maximum and 0.2°C cooler in Western Scotland over the same period (MET Office, 2016).

Figure 1 shows the spatial variability in Tw_{max} across the four catchments and Figure 2 summarises the distribution of Tw_{max} by catchment (bottom left diagonal panel). Median Tw_{max} in the Dee (15.1°C), Tweed (15.6°C) and Spey (15.6°C) were broadly similar, but median Tw_{max} in the Bladnoch (16.4°C) was ca. 1°C higher (Fig. 2). The range of Tw_{max} was 5.7, 5.9, 6.0 and 5.5°C in the Bladnoch, Dee, Spey and Tweed, respectively (Fig. 2).

3.1 Single catchment models

All four LS models were simple (Table 2), explained much of the variance in Tw_{max} (76.6-85.6%) and contained similar positive relationships between Tw_{max} and UCA (Fig. 3). This relationship was near linear until ca. 100km^2 and then levelled off in the Bladnoch (Fig. 3d), smooth, but near-linear in the Spey and the Tweed (Fig. 3b, c) and linear in the Dee (Fig. 3a). The magnitude of the effect was similar across catchments at ca. 4°C. Three models contained a RNS, which explained much of the variance; 61.7, 13.9 and 63.7% in the Dee, Tweed and Spey respectively (Table 2). The Tweed model also had a negative linear effect of %RW.

The LS_Ta models always had a better BIC / AICc than the corresponding LS models, but were typically more complex, always required more df, and only explained a greater % variance in the Bladnoch and the Tweed (Table 2). For the Tweed, the LS_Ta model used only covariates, whereas the LS model required a RNS to account for unexplained spatial structure. For the Bladnoch, the LS_Ta model included UCA and Ta_{max}, whereas the LS model only included UCA.

In common with the LS models, UCA was in all the LS_Ta models (Table 2) and the direction, shape and magnitude of the effects were consistent with the LS models (Fig. 4, top row). Ta_{max} was in all the LS_Ta models except the Spey (Table 2). There was a positive linear relationship between Tw_{max} and Ta_{max} in the Dee and Tweed (Figure 4e, f) and a U shaped response in the Bladnoch which is physically implausible, increasingly so when extended beyond the range of Ta_{max} observed in the Bladnoch (Fig. 4g). Orientation had a small positive effect on Tw_{max} in both the Dee and Tweed (Fig. 4h, i) with higher temperatures for a N-S orientation than an E-W orientation. There was also a negative linear effect of %RW and a positive smoothed effect of HS in the Tweed, and a positive linear effect of DC in the Spey (Fig. 4j, k, l, respectively).

3.2 Transferability of single catchment models

The transferability of the LS and LS_Ta models is summarised by their RMSE, bias and standard deviation in Table 3 and illustrated in Figs. 5 and 6 respectively. All the models performed well within catchments (i.e. in the catchments where they were developed) when all model terms (i.e. both covariates and the RNS) were used in the predictions, with a bias of < 0.1°C in absolute value and a RMSE of < 1°C. The LS_Ta models always had a lower RMSE than the LS_models. As expected, within-catchment predictions were poorer when only the covariates were used (excluding RNS), with a median RMSE of 1.2°C and a maximum RMSE of 1.8°C.

The rest of this section focusses on the predictions, both within and between catchments, using only the covariates. For the catchments in Eastern Scotland (Dee, Tweed and Spey), the RMSE, bias and standard deviation of any model was broadly similar whether it was used to predict for the donor catchment or to the other two target catchments. The RMSE of the LS models tended to be lower than that of the LS_Ta models (median 1.3 and 1.7°C respectively). The LS and LS_Ta models both had median absolute biases of 0.3°C and median standard deviations of 1.1 and 1.4°C respectively. RMSE is a combination of bias and standard deviation, so the RMSE of both sets of models was generally dominated by the standard deviation.

Predictions involving the Bladnoch, either as donor or target catchment, tended to be poor. The Bladnoch is in Western Scotland and was warmer than the other catchments (Fig. 2). The Bladnoch models always over-predicted Tw_{max} in the other catchments and the Dee, Tweed and Spey models all under-predicted Tw_{max} in the Bladnoch (Fig. 5, 6). This often led to substantial bias and hence RMSE. The Bladnoch LS_Ta model had the largest biases, which were also due to the implausible relationship with Ta_{max} (Figure 4g). The Dee, Tweed and Spey had reasonable standard deviations when transferred to the Bladnoch (median 1.0 and 1.1°C for the LS and LS_Ta models respectively) which suggests that, despite having poor RMSE, the models still could be used to predict areas of relatively high or low Tw_{max} within the Bladnoch (rather than absolute values of Tw_{max}). The same is true of the Bladnoch LS models when transferred to the Dee, Tweed and Spey (median standard deviation 1.3°C). However, the Bladnoch LS_Ta model had a high standard deviation (median 3.3°C) when transferred to the Dee, Tweed and Spey, again due to the implausible relationship with Ta_{max}.

3.3 Multi-catchment models

The multi-catchment LS model included Catchment, UCA, %RW, Elevation and a RNS for each catchment (Table 4). By fitting a single model to all four catchments it was possible to assess whether covariate effects were consistent across catchments and thus transferable to new catchments or regions. None of the covariates interacted with catchment. The Catchment effect indicates inter-catchment differences in mean Tw_{max} having accounted for the landscape covariates; in particular, higher Tw_{max} in the Bladnoch (Figure 7d). In common with the single catchment LS models, there was a positive smooth relationship between Tw_{max} and UCA with an effect size of ca. 3°C (Figure 7a). There was also a negative linear relationship between Tw_{max} and both %RW and Elevation, with effect sizes of ca. 1°C and 2°C respectively. The model

explained 84.4% of the variance, comparable to the single catchment LS models. The RNSs explain less of the variance than in the single catchment models (Tables 3, 4).

The multi-catchment LS_Ta model explained 83.2% of the variance and contained Catchment, UCA, %RW, Ta_{max} and a RNS for each catchment (Table 4, Figure 8). None of the landscape covariates interacted with catchment. However, the Ta_{max} relationship did interact with catchment, (Fig. 8a-d), with positive relationships in the Dee and Tweed and negative (albeit non-significant) relationships in the Spey and Bladnoch. This suggests that relationships with Ta_{max} are non-transferable and Ta_{max} would not be a good predictor of Tw_{max} in new catchments.

4.0 Discussion

Even with the introduction of relatively cheap and accurate dataloggers it is not financially or logistically possible to monitor everywhere. Consequently, there is a need to develop models to understand and predict river temperatures at large spatial scales to inform evidence based management of rivers and fisheries even where extensive local temperature data collection does not exist. Spatial statistical models offer great promise in this respect. However, to date, the transferability of these models has not been considered. This study fitted separate models of Tw_{max} to data from four catchments and transferred these models between catchments. Models containing only landscape covariates typically contained similar covariates and covariate responses, and performed better than models containing Ta_{max} when transferred between catchments. A physically implausible model transferred particularly poorly. The covariates alone often explained much less of the spatial temperature variability than when a RNS was added, but provided the only means of predicting temperature in new catchments with no or limited data (a minimum of 19 loggers was required to fit the full models including covariates and RNS). A single model fitted to all four catchments suggested common responses to landscape covariates, but inter-catchment differences in mean temperature and in the relationships between Tw_{max} and Ta_{max}. These findings are discussed in more detail below.

4.1 Tw_{max} responses to landscape covariates

The single catchment LS models contained similar covariates with comparable effect sizes and response shapes which suggested that transferability between catchments could be reasonably successful. This was confirmed by the lack of significant interactions with Catchment in the multi-catchment model. However, when there are inter-catchment differences in mean temperature, the models might only be good predictors of relative values of Tw_{max} within a new catchment (i.e. areas of higher or lower Tw_{max}) rather than absolute values. It is also unclear how well the models would perform in years with differing hydro-climatic characteristics. This study was conducted in a single year with relatively low temperatures and high flows. In a hotter, drier year it might be expected that between site differences would be greater. Under such circumstances the current models may not provide accurate predictions of absolute temperatures or inter-site differences without refitting.

All of the Tw_{max} responses to landscape covariates (across all models) were physically plausible and hence broadly transferable (Smith et al., 2016). UCA (which was in all the models) is a proxy for discharge, water volume and thermal capacity (Chang and Psaris, 2013; Hannah et al., 2008). Higher UCAs are generally associated with larger water volumes which have a greater thermal capacity, taking longer to warm but also retaining heat for longer (Chang and Psaris, 2013; Imholt et al., 2011). Elevation reflects adiabatic lapse rates which reduces temperatures with increasing altitude (Hrachowitz et al., 2010, Jackson et al 2017). The negative relationship between Tw_{max} and %RW woodland occurs because riparian shading reduces the amount of incident shortwave radiation reaching the river during daylight hours (Garner et al., 2014; Hannah et al., 2008; Moore et al., 2005). The positive relationship between Tw and HS is consistent with greater Tw in locations with lower shading effects and greater direct shortwave contributions (illumination). Tw was greatest in channels characterised by a north/south orientation which typically experience maximum exposure to incoming radiation (Malcolm et al., 2004). Increasing Tw with distance from the coast, reflected continentality and the differing specific heat capacities of land and sea, specifically thermal buffering of relatively cooler sea during summer months (Chang and Psaris, 2013; Hrachowitz et al., 2010).

4.2 Tw ~ Ta relationships

In contrast to the LS models, one LS_Ta model included a physically implausible relationship that would not be expected to transfer well (Smith et al., 2016). Specifically, an inverse modal relationship between Tw_{max} and Ta_{max} in the Bladnoch model. This relationship could have arisen ~~due to~~ because of spatial variability in local (temporal) Tw_{max} ~ Ta_{max} relationships due to controls that were not captured by our covariates, coupled with a relatively small air temperature range (1.7°C) and sample size (19 sites). ~~the relatively small air temperature range (1.7°C) observed in the Bladnoch which provided only limited contrast between sites. However, it is also possible that this reflected systematic spatial variability in other controls (described by our covariates or otherwise) that influence local Tw_{max} ~ Ta_{max} relationships e.g. hydrogeology or landuse.~~ Nevertheless, even where the relationships between Tw_{max} and Ta_{max} ~~relationships~~ were plausible, they were inconsistent between catchments in terms of effect size and direction, as indicated by the varying responses in the single catchment models and the interaction with Catchment in the multi-catchment model. For example, in the latter, the relationships were positive in the Dee and Tweed and negative in the Spey and Bladnoch (where the relationship simplifies to linear).

Given the number of previous studies that have predicted Tw from Ta~~, both~~ within sites over time (temporal models), ~~and~~ between sites (spatial models) or both (e.g. two stage spatio-temporal models), it may appear surprising that models containing Ta_{max} ~~was such a poor predictor~~ gave poorer predictions of between-catchment temperature variability than those containing landscape covariates alone in this study. However, previous spatial models of Tw incorporating air temperature as a predictor (e.g. Wehrly et al., 2009; Moore et al., 2013) have focussed on the ability of these models to predict within the data space (interpolate), while this study investigated the ability of models to predict outside of the data space (extrapolate). Indeed, within our multi-catchment model it would have been possible to force a single Tw_{max} ~ Ta_{max}

relationship that reflected an average response across catchments. However, this would result in biased estimates of Tw_{max} within individual catchments.

The ability of Ta_{max} to predict spatial variability in Tw_{max} is likely to degrade where the temporal relationships between Tw and Ta vary spatially, within and between catchments (Kelleher et al., 2012; Segura et al., 2015). It is expected that within catchment (between site) variability in the temporal relationships between Tw and Ta would add noise to any spatial relationships making them harder to detect and reducing the overall precision of any predictions. Systematic differences in Tw~Ta relationships between catchments would result in biased predictions when models are transferred between rivers or regions.

Many studies have shown that within year temporal relationships between Tw and Ta (often termed thermal or climate sensitivity) can be highly variable between sites and catchments, and importantly that this variability relates to ~~(Arismendi et al., 2014; Arora et al., 2016; Fellman et al., 2014; Luce et al. 2014; Mayer, 2012; Tague, 2007) across a range of spatial scales depending on~~ regional, hydrological and landscape controls (Tague, et al., 2007; Kelleher et al., 2012; Krider et al., 2013; Chang and Psaris, 2013; Hilderbrand et al., 2014; Segura et al., 2015; Mauger et al., 201~~6~~7). For example, ~~Arismendi et al. (2014) investigated Tw~Ta relationships at 25 sites across the Western US using linear regression and reported that the slope of the relationship varied between 0.32 and 1.01, while~~ Fellman et al. (2014) observed slopes of between -0.180 and 1.282 across 9 watersheds in Alaska depending on glacial influence, while Mauger et al., 201~~6~~7 observed slopes of between 0.32 and 1.51 across 48 non-glacial streams in Alaska which related to mean elevation and catchment area. Similarly, Tague et al., (2007) observed systematic regional differences in Tw~Ta relationships in Western Oregon that depended on local hydrogeology and concluded that under such circumstances air temperature alone (i.e. consistent with a single air temperature coefficient) would be unlikely to explain spatial variation in river temperature~~variability~~. Given the reported spatial variability in Tw~Ta relationships and importantly, that these relationships can vary systematically within and between catchments depending on other controls (e.g. hydrogeology), it is unsurprising that models containing Ta_{max} do~~es~~ not substantially improve predictions of the spatial variability in Tw_{max} than models containing landscape variables alone, and that transferred models result in biased Tw predictions. If ~~models including~~ Ta is to ~~are to provide~~ substantially ~~better~~improve predictions of Tw in static spatial models (such as those presented in this study), then it is likely that they would need to include greater model complexity e.g. allowing for interactions between Ta_{max} and landscape covariates (e.g. Mayer, 2012).

4.34 The importance of RNS

The performance of the single catchment LS and LS_Ta models in this study compared favourably to regional models of Tw_{max} (Moore et al. 2013; Roberts et al. 2013; Wehrly, et al. 2009) when predictions were made for the catchment in which the models were developed (i.e. interpolation). For the models that included a RNS, RMSE (0.7-0.9 °C) was approximately half that reported by previous studies, although it should be noted that these studies were conducted at considerably larger

spatial scales (Moore et al. 2013; Roberts et al. 2013; Wehrly, et al. 2009). The RMSE of models without a RNS (0.9-1.8 °C) was generally similar or slightly better than reported by other studies.

The landscape covariates included in the models in this study explained large (catchment) scale trends in Tw_{max}, but were less successful at explaining variability at finer spatial scales. For example, the ca. 20% variance explained by UCA in the Spey and Dee models is consistent with the 18-25% of Tw variability explained by discharge in Arora et al. (2016). Smaller scale variability tends to reflect drivers such as water residence time (and heat advection), water sources (Brown et al., 2006; Brown and Hannah, 2008), channel incision, gradient (Jackson et al., 2017) and land use (Imholt et al., 2013) which are harder to accurately characterise from spatial datasets. In the absence of accurate local scale characterisation of landscape controls, smaller scale spatial variability is modelled by the RNS. However, whilst the RNS improves predictions within catchments, it is not transferable so does nothing to help predictions between catchments.

4.45 Extending predictions

The inclusion of the Catchment main effect in both multi-catchment models showed differences in mean Tw_{max} between catchments (that were not accounted for by the covariates). This sometimes led to substantial bias when transferring single catchment models to new catchments. Accounting for between-catchment differences in mean Tw will be necessary to improve between-catchment predictions of Tw. The multi-catchment models in this study used a simple categorical variable to allow the intercept (and hence mean Tw_{max}) to differ between catchments. However, to predict to new catchments, it would be necessary to extend the modelling approach so that the intercept can be predicted from surrounding catchments. One approach could be to allow the intercept to vary smoothly between catchments using a Gaussian Markov Random Field (Cressie, 1993), so the intercept in unmonitored catchments could be estimated from nearby monitored catchments. This approach has been developed in other contexts (Millar et al., 2015, 2016) and offers promise in the context of large-scale Tw modelling.

An alternative approach could involve modelling Tw as a function of Ta over shorter time periods (days or weeks) and then allowing this relationship to interact with landscape covariates or location. Such an approach could have additional benefits, allowing the inclusion of temporally incomplete data (e.g. Letcher et al., 2016) or data from temporally inconsistent locations. Where sufficient resources were available it may be possible to supplement the existing network with sites that are monitored for shorter time periods to expand spatial coverage although the consequences of such deployments for assessing inter-annual temperature variability would need to be investigated. Finally, the development of spatio-temporal models, where temporal variability was driven by Ta or discharge, could potentially allow for fore- or hind-casting of river temperature which wasn't possible using the approaches presented in this paper.

5 Conclusions and future work

This study demonstrated that landscape covariates can explain broad scale patterns in Tw_{max} and that such relationships are transferable between catchments, at least to predict relative levels of Tw_{max}. It was necessary to use a RNS to characterise and predict finer scale spatially correlated variation, so predictions of spatial temperature variability were better within catchments than between catchments. Ta_{max} was not a transferable predictor of Tw_{max} and could result in poor predictions when the relationship was implausible or transferred outside the range observed in the donor catchment. It would be unwise to use a Tw~Ta relationship to predict spatial variability in Tw without also including meaningful (process relevant) interactions between Ta and landscape covariates, something that was not possible in this study due to data constraints.

Mean Tw_{max} also varied between catchments (having adjusted for the landscape covariates). Future work that looks to predict to new catchments should investigate how to understand and predict these between catchment differences. A large scale correlated spatial smoother (e.g. regional effect) offers potential in this respect. Finally, some of the local scale processes represented in this study (e.g. effect of riparian shading) may benefit from improved characterisation using finer scale spatial datasets or remotely sensed data. Improved process representation could lead to both better within and between catchment model predictions.

Data availability

Some map features are based on digital spatial data licensed from the Centre of Ecology and Hydrology, NERC © Crown Copyright and database right (2016), all rights reserved, Ordnance Survey License number 100024655. Catchment boundaries were from SEPA (2009). The digitised river network is from the CEH and includes Scottish Environmental Protection Agency (SEPA) coding. Catchment boundaries were from SEPA (2009) and Salmon rivers from Marine Scotland (2008). The gridded Ta dataset was from UKCP09: Daily gridded air temperature dataset (2015) UK MET Office. Summary Tw data used in the study will be made available on the Marine Scotland Science webpages, upon acceptance of the article.

Author contributions

I.A.Malcolm and D.M.Hannah secured funding for the project. The authors conceived the study. F.L.Jackson, carried out the data analysis with support from I.A.Malcom and R.J.Fryer. F.L.Jackson, I.A.Malcolm, R.J.Fryer and D.M.Hannah interpreted the results and prepared the manuscript.

Competing interests

The authors declare that they have no conflict of interest

Acknowledgements

This project is part of Marine Scotland Science (MSS) Freshwater Fisheries Laboratories Service Level Agreement FW02G and it is supported by a NERC Open CASE studentship (University of Birmingham and MSS) awarded to Faye Jackson; grant reference NE/K007238/1. The authors also thank the Scotland River Temperature Monitoring Network collaborators for their contribution to data collection (http://www.gov.scot/Topics/ marine/Salmon-Trout-Coarse/Freshwater/Monitoring/temperature/Collaborating).

References

Anon: Sun or Moon Altitude/Azimuth Table, Data Serv. Washington, DC U.S. Nav. Obs. Astron. Appl. Dep. [online] Available from: http://aa.usno.navy.mil/data/docs/AltAz.php (Accessed 26 March 2014), 2001.

~~Arismendi, I., Safeeq, M., Dunham, J. B. and Johnson, S. L.: Can air temperature be used to project influences of climate change on stream temperature?, Environ. Res. Lett., 9, doi:10.1088/1748-9326/9/8/084015, 2014.~~

Arora, R., Tockner, K. and Venohr, M.: Changing river temperatures in Northern Germany: trends and drivers of change, Hydrol. Process., 30, 3084–3096, doi:10.1002/hyp.10849, 2016.

Bivand, R. and Rundel, C.: rgeos: Interface to Geometry Engine - Open Source (GEOS). R package version 0.3-17., [online] Available from: https://cran.r-project.org/package=rgeos, 2016.

Brown, L. E. and Hannah, D. M.: Spatial heterogeneity of water temperature across an alpine river basin, Hydrol. Process., 22, 954–967, doi:10.1002/hyp, 2008.

Brown, L. E., Hannah, D. M., Milner, A. M., Soulsby, C., Hodson, A. J. and Brewer, M. J.: Water source dynamics in a glacierized alpine river basin (Taillon-Gabiétous, French Pyrénées), Water Resour. Res., 42(8), doi:10.1029/2005WR004268, 2006.

Chang, H. and Psaris, M.: Local landscape predictors of maximum stream temperature and thermal sensitivity in the Columbia River Basin, USA., Sci. Total Environ., 461–462, 587–600, doi:10.1016/j.scitotenv.2013.05.033, 2013.

Comte, L., Buisson, L., Daufresne, M. and Grenouillet, G.: Climate-induced changes in the distribution of freshwater fish: Observed and predicted trends, Freshw. Biol., 58(4), 625–639, doi:10.1111/fwb.12081, 2013.

Cressie, N.: Statistics for spatial data:Wiley series in probability and statistics, Wiley-Interscience, New York., 1993.

Csardi, G. and Nepusz, T.: The igraph software package for complex network research, InterJournal, Complex Sy, 1695 [online] Available from: http://igraph.org, 2006.

Dobbie, M. J., Henderson, B. L. and Stevens, D. L.: Sparse sampling: Spatial design for monitoring stream networks, Stat. Surv., 2, 113–153, doi:10.1214/07-SS032, 2008.

Elliott, J. M. and Elliott, J. A.: Temperature requirements of Atlantic salmon Salmo salar, brown trout Salmo trutta and Arctic charr Salvelinus alpinus: Predicting the effects of climate change, J. Fish Biol., 77(8), 1793–1817, doi:10.1111/j.1095-8649.2010.02762.x, 2010.

Fellman, J. B. J., Nagorski, S., Pyare, S., Vermilyea, A. W., Scott, D. and Hood, E.: Stream temperature response to variable glacier coverage in coastal watersheds of Southeast Alaska, Hydrol. Process., 28, 2062–2073, doi:10.1002/hyp.9742, 2014.

Garner, G., Malcolm, I. A., Sadler, J. P. and Hannah, D. M.: What causes cooling water temperature gradients in a forested stream reach?, Hydrol. Earth Syst. Sci., 18, 5361–5376, doi:10.5194/hess-18-5361-2014, 2014.

Gurney, W. S. C., Bacon, P. J., Tyldesley, G. and Youngson, A. F.: Process-based modelling of decadal trends in growth, survival, and smolting of wild salmon (Salmo salar) parr in a Scottish upland stream, Can. J. Fish. Aquat. Sci., 65, 2606–2622, doi:10.1139/F08-149, 2008.

Hannah, D. M., Malcolm, I. A., Soulsby, C. and Youngson, A. F.: A comparison of forest and moorland stream microclimate, heat exchanges and thermal dynamics, Hydrol. Process., 22(7), 919–940, doi:10.1002/hyp, 2008.

Hijmans, R. J.: raster: Geographic Data Analysis and Modeling. R package version 2.5-2., [online] Available from: https://cran.r-project.org/package=raster, 2015.

Hilderbrand, R. H., Kashiwagi, M. T., and Prochaska, A. P., 2014. Regional and Local Scale Modeling of Stream Temperatures and Spatio-Temporal Variation in Thermal Sensitivities. Environ. Manage. 54, 14–22. doi:10.1007/s00267-014-0272-4

Hill, R. A., Hawkins, C. P. and Carlisle, D. M.: Predicting thermal reference conditions for USA streams and rivers, Freshw. Sci., 32(1), 39–55, doi:10.1899/12-009.1, 2013.

Ver Hoef, J. M. and Peterson, E. E.: A Moving Average Approach for Spatial Statistical Models of Stream Networks, J. Am. Stat. Assoc., 105(489), 6–18, doi:10.1198/jasa.2009.ap08248, 2010.

Ver Hoef, J. M., Peterson, E. E., Clifford, D. and Shah, R.: SNN: An R package for spatial statistical modeling on stream networks, J. Stat. Softw., 56(3), 2014.

Ver Hoef, J. M., Peterson, E. and Theobald, D.: Spatial statistical models that use flow and stream distance, Environ. Ecol. Stat., 13, 449–464, doi:10.1007/s10651-006-0022-8, 2006.

Hrachowitz, M., Soulsby, C., Imholt, C., Malcolm, I. A. and Tetzlaff, D.: Thermal regimes in a large upland salmon river: a simple model to identify the influence of landscape controls and climate change on maximum temperatures, Hydrol. Process., 24(23), 3374–3391, doi:10.1002/hyp.7756, 2010.

Imholt, C., Soulsby, C., Malcolm, I. A. and Gibbins, C. N.: Influence of contrasting riparian forest cover on stream temperature dynamics in salmonid spawning and nursery streams, Ecohydrology, 6(3), 380–392, doi:10.1002/eco.1291, 2013.

Imholt, C., Soulsby, C., Malcolm, I. A., Hrachowitz, M., Gibbins, C. N., Langan, S. and Tetzlaff, D.: Influence of scale on thermal characteristics in a large montane river basin, River Res. Appl., 29(4), 403–419, doi:10.1002/rra, 2011.

Isaak, D. J., Luce, C. H., Rieman, B. E., Nagel, D. E., Peterson, E. E., Horan, D. L., Parkes, S. and Chandler, G. L.: Effects of climate change and wildfire on stream temperatures and salmonid thermal habitat in a mountain river network, Ecol. Appl., 20(5), 1350–1371, 2010.

Isaak, D. J., Peterson, E. E., Ver Hoef, J. M., Wenger, S. J., Falke, J. A., Torgersen, C. E., Sowder, C., Steel, A. E., Fortin, M.-J., Jordan, C. E., Ruesch, A. S., Som, N. and Monestiez, P.: Applications of spatial statistical network models to stream data, WIREs Water, 1(3), 227–294, doi:10.1002/wat2.1023, 2014.

Isaak, D. J., Wenger, S. J., Peterson, E. E., Hoef, J. M. Ver, Hostetler, S., Luce, C. H., Dunham, J. B., Kershner, J., Roper, B. B., Nagel, D., Horan, D., Chandler, G., Parkes, S. and Wollrab., S.: NorWeST: An interagency stream temperature database and model for the Northwest United States. U.S. Fish and Wildlife Service, Great Northern Landscape Conservation Cooperative Grant. www.fs.fed.us/rm/boise/AWAE/projects/NorWeST.html., 2011.

Isaak, D. J., Wollrab, S., Horan, D. and Chandler, G.: Climate change effects on stream and river temperatures across the northwest U.S. from 1980–2009 and implications for salmonid fishes, Clim. Change, 113(2), 499–524, doi:10.1007/s10584-011-0326-z, 2012.

Jackson, F. L., Hannah, D. M., Fryer, R. J., Millar, C. P. and Malcolm, I. A.: Development of spatial regression models for predicting summer river temperatures from landscape characteristics: implications for land and fisheries management, Hydrol. Process., 31, 1225-1238, doi:10.1002/hyp.11087, 2017.

Jackson, F. L., Malcolm, I. A. and Hannah, D. M.: A novel approach for designing large-scale river temperature monitoring networks, Hydrol. Res., 47(3), 569–590, doi:10.2166/nh.2015.106, 2016.

Jonkers, A. R. T. and Sharkey, K. J.: The Differential Warming Response of Britain's Rivers (1982–2011), PLoS One, 11(11), e0166247, doi:10.1371/journal.pone.0166247, 2016.

Jonsson, B. and Jonsson, N.: A review of the likely effects of climate change on anadromous Atlantic salmon Salmo salar and brown trout Salmo trutta, with particular reference to water temperature and flow, J. Fish Biol., 75(10), 2381–2447, doi:10.1111/j.1095-8649.2009.02380.x, 2009.

Kelleher, C., Wagener, T., Gooseff, M., McGlynn, B., McGuire, K., and Marshall, L., 2012. Investigating controls on the thermal sensitivity of Pennsylvania streams. Hydrol. Process. 26. doi:10.1002/hyp.8186

Krider, L. A., Magner, J. A., Perry, J., Vondracek, B., and Ferrington, L.C., 2013. Air-Water Temperature Relationships in the Trout Streams of Southeastern Minnesota's Carbonate-Sandstone Landscape. J. Am. Water Resour. Assoc. 49, 896–907. doi:10.1111/jawr.12046

Letcher, B. H, Hocking, D. J, O'Neil, K, Whiteley, A.R, Nislow, K.H, O'Donnell, M.J.: A hierarchical model of daily stream temperature using air-water temperature synchronization, autocorrelation, and time lags. PeerJ, 4:e1727, https://doi.org/10.7717/peerj.1727, 2016

~~Luce, C., Staab, B., Kramer, M., Wenger, S., Isaak, D. and McConnell, C.: Sensitivity of Summer Stream Temperatures to Climate Variability in the Pacific Northwest, Water Resour. Res., 50(4), 3428–3443, doi:10.1002/2013/WR014329, 2014.~~

Malcolm, I. A., Hannah, D. M., Donaghy, M. J., Soulsby, C. and Youngson, A. F.: The influence of riparian woodland on the spatial and temporal variability of stream water temperatures in an upland salmon stream, Hydrol. Earth Syst. Sci., 8(3), 449–459, doi:10.5194/hess-8-449-2004, 2004.

Malcolm, I. A., Soulsby, C., Hannah, D. M., Bacon, P. J., Youngson, A. F. and Tetzlaff, D.: The influence of riparian woodland on stream temperatures: implications for the performance of juvenile salmonids, Hydrol. Process., 22(7), 968–979, doi:10.1002/hyp, 2008.

Marine, K. R. and Cech, J. J. J.: Effects of High Water Temperature on Growth , Smoltification , and Predator Avoidance in Juvenile Sacramento RiverChinook Salmon, North Am. J. Fish. Manag., 24(1), 198–210, doi:10.1577/M02-142, 2004.

Mauger, S., Shaftel, R., Leppi, J., and Rinella, D., 2017. Summer temperature regimes in southcentral Alaska streams: watershed drivers of variation and potential implications for Pacific salmon. Can. J. Fish. Aquat. Sci. 74, 702–715. doi:10.1139/cjfas-2016-0076

Mayer, T. D.: Controls of summer stream temperature in the Pacific Northwest, J. Hydrol., 475, 323–335, doi:10.1016/j.jhydrol.2012.10.012, 2012.

McCullough, D., Spalding, S., Sturdevant, D. and Hicks, M.: Summary of Technical Literature Examining the Physiological Effects of Temperature on Salmonids., 2001.

MET Office: Regional values - August 2015, [online] Available from: http://www.metoffice.gov.uk/climate/uk/summaries/2015/august/regional-values (Accessed 20 October 2016), 2016.

Millar, C. ., Millidine, K. ., Middlemass, S. . and Malcolm, I. .: Development of a Model for Predicting Large Scale Spatio-Temporal Variability in Juvenile Fish Abundance from Electrofishing Data, Scottish Mar. Freshw. Sci. Rep., 6(6), 33, doi:10.7489/1616-1, 2015.

Millar, C. P., Fryer, R. J., Millidine, K. J. and Malcolm, I. A.: Modelling capture probability of Atlantic salmon (Salmo salar) from a diverse national electrofishing dataset: Implications for the estimation of abundance, Fish. Res., 177, 1–12, doi:10.1016/j.fishres.2016.01.001, 2016.

Millidine, K. J., Malcolm, I. A. and Fryer, R. J.: Assessing the transferability of hydraulic habitat models for juvenile Atlantic salmon, Ecol. Indic., 69, 434–445, doi:10.1016/j.ecolind.2016.05.012, 2016.

Moore, R. D., Nelitz, M. and Parkinson, E.: Empirical modelling of maximum weekly average stream temperature in British Columbia, Canada, to support assessment of fish habitat suitability, Can. Water Resour. J., 38(2), 135–147, doi:10.1080/07011784.2013.794992, 2013.

Moore, R. D., Sutherland, P., Gomi, T. and Dhakal, A.: Thermal regime of a headwater stream within a clear-cut, coastal British Columbia, Canada, Hydrol. Process., 19(13), 2591–2608, doi:10.1002/hyp.5733, 2005.

O'Donnell, D., Rushworth, A., Bowman, A. W., Scott, M. E. and Hallard, M.: Flexible regression models over river networks, J. R. Stat. Soc. Ser. C (Applied Stat., 63(1), 47–63, doi:10.1111/rssc.12024, 2014.

Pebesma, E. J. and Bivand, R. S.: Classes and methods for spatial data in R., [online] Available from: http://cran.r-project.org/doc/Rnews/, 2005.

Perry, M. and Hollis, D.: The development of a new set of long-term climate averages for the UK, Int. J. Climatol., 25(8), 1023–1039, doi:10.1002/joc.1160, 2005a.

Perry, M. and Hollis, D.: The generation of monthly gridded datasets for a range of climatic variables over the UK, Int. J. Climatol., 25(8), 1041–1054, doi:10.1002/joc.1161, 2005b.

Peterson, E. E. and Ver Hoef, J. M.: STARS: An ArcGIS Toolset Used to Calculate the Spatial Information Needed to Fit Statistical Models to Stream Network Data, J. Stat. Softw., 56(2), 2014.

Peterson, E. E. and Urquhart, N. S.: Predicting water quality impaired stream segments using landscape-scale data and a regional geostatistical model: a case study in Maryland., Environ. Monit. Assess., 121(1–3), 615–38, doi:10.1007/s10661-005-9163-8, 2006.

Peterson, E., Ver Hoef, J. and Scopel, C.: SSN and STARS : Tools for Spatial Statistical Modeling on Stream Networks, , 2–4, 2013.

R Core Team, ..: R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria., [online] Available from: http://www.r-project.org/, 2015.

Roberts, J. J., Fausch, K. D., Peterson, D. P. and Hooten, M. B.: Fragmentation and thermal risks from climate change interact to affect persistence of native trout in the Colorado River basin. Glob Change Biol, 19, 1383–1398. doi:10.1111/gcb.12136, 2013

Ruesch, A. S., Torgersen, C. E., Lawler, J. J., Olden, J. D., Peterson, E. E., Volk, C. J. and Lawrence, D. J.: Projected Climate-Induced Habitat Loss for Salmonids in the John Day River Network, Oregon, U.S.A., Conserv. Biol., 26(5), 873–882, doi:10.1111/j.1523-1739.2012.01897.x, 2012.

Rushworth, A. M., Peterson, E. E., Ver Hoef, J. M. and Bowman, A. W.: Validation and comparison of geostatistical and spline models for spatial stream networks, Environmetrics, (26.5), 327–338, doi:10.1002/env.2340, 2015.

Segura, C., Caldwell, P., Sun, G., McNulty, S., and Zhang, Y., 2015. A Model to Predict Stream Water Temperature across the Conterminous USA. Hydrol. Process. 29, 2178–2195. doi:10.1002/hyp.10357

Smith, T., Hayes, K., Marshall, L., McGlynn, B. and Jencso, K.: Diagnostic calibration and cross-catchment assessment of a simple process-consistent hydrologic model, Hydrol. Process., doi:10.1002/hyp.10955, 2016.

Som, N. A., Monestiez, P., Ver Hoef, J. M., Zimmerman, D. L. and Peterson, E. E.: Spatial sampling on streams: principles for inference on aquatic networks, Environmetrics, doi:10.1002/env.2284, 2014.

Sowder, C. and Steel, E. A.: A note on the collection and cleaning of water temperature data, Water, 4, 597–606, doi:10.3390/w4030597, 2012.

Steel, E. A., Sowder, C. and Peterson, E. E.: Spatial and Temporal Variation of Water Temperature Regimes on the Snoqualmie River Network, JAWRA J. Am. Water Resour. Assoc., 1–19, doi:10.1111/1752-1688.12423, 2016.

Strahler, A.: Quantitative analysis of watershed geomorphology, Trans. Am. Geophys. Union, 38, 913–920, 1957.

Tague, C., Farrell, M., Grant, G., Lewis, S. and Rey, S.: Hydrogeologic controls on summer stream temperatures in the McKenzie River basin, Oregon, Hydrol. Process., 21, 3288–3300, doi:10.1002/hyp, 2007.

Webb, B. W., Hannah, D. M., Moore, R. D., Brown, L. E. and Nobilis, F.: Recent advances in stream and river temperature research, Hydrol. Process., 22(7), 902–918, doi:10.1002/hyp, 2008.

Wehrly, K. E., Brenden, T. O. and Wang, L.: A Comparison of Statistical Approaches for Predicting Stream Temperatures Across Heterogeneous Landscapes, JAWRA J. Am. Water Resour. Assoc., 45(4), 986–997, doi:10.1111/j.1752-1688.2009.00341.x, 2009.

Wood, S. N.: mgcv: GAMs and generalized ridge regression for R., R-News, 1(2), 20–25, 2001.

Wood, S. N.: Mixed GAM Computation Vehicle with GCV/AIC/REML Smoothness Estimation, , 1–273 [online] Available from: https://cran.r-project.org/web/packages/mgcv/mgcv.pdf, 2016.

Table 1 Covariate calculations. All calculations were in R, version 3.2.3 (R Core Team, 2015) except where specified.

Covariate	Process and associated packages	Datasets
Elevation	'extract' function in the 'raster' package (Hijmans, 2015)	OS. Terrain 10m DTM, CEH DRN
Gradient	'extract' function in the 'raster' package (Hijmans, 2015) to get elevations of the node and a location 1km upstream. The difference in these elevations divided by the length between the two nodes provided Gradient. The length upstream was calculated using 'SpatialLinesLengths' from 'sp' (Pebesma and Bivand, 2005)	OS. Terrain 10m DTM, CEH DRN
Orientation	Standard trigonometry based on the x and y locations of the node and associated upstream points 1km upstream lengths. The lengths upstream was calculated using 'SpatialLinesLengths' from 'sp' (Pebesma and Bivand, 2005)	CEH DRN
Upstream Catchment Area (UCA)	Arc Hydro Tools (ArcGIS 10.2.1) was used to 'burn in' the DRN to the DTM and then calculate an UCA raster.	OS. Terrain 10m Digital Terrain Model, DTM; CEH DRN
Hillshading/ Illumination (HS)	'terrain' and 'hillShade' functions in the 'raster' package (Hijmans, 2015) were used to create a hillshade layer for every hour the sun was above the horizon. These layers were then summed to create a single layer of maximum potential exposure. HS values for the nodes were an average of the raster grid cells in the 1km river polygon. Raster grid cells were weighted by the proportion of the cell within the buffer.	CEH DRN , OS. Terrain 10m DTM; Solar azimuth and altitude values from the U.S. Naval Observatory Astronomical Applications Department (Anon, 2001)
Percentage riparian woodland (%RW)	The percentage of woodland in a buffer 50m wide and 1km long (upstream) provided %RW. Areas were calculated using 'gArea' from 'rgeos' (Bivand and Rundel, 2016) and lengths the 'SpatialLinesLengths' from 'sp' (Pebesma and Bivand, 2005).	OS MasterMap, CEH DRN
Width	Width was calculated by finding the area classified as water within the 1km upstream and dividing this by the distance upstream. Areas were calculated using 'gArea' from 'rgeos' (Bivand and Rundel, 2016) and lengths the 'SpatialLinesLengths' from 'sp' (Pebesma and Bivand, 2005).	OS MasterMap, CEH DRN
Distance to coast (DC)	gDistance' from the 'rgeos' R package (Bivand and Rundel, 2016).	CEH DRN, OS Panorama coastline
River distance to sea (RDS)	"shortest.paths" function from the igraph R package (Csardi and Nepusz, 2006)	CEH DRN, OS Panorama coastline
Highest 7-day average maximum August Ta (Ta_{max})	Take the Ta value, from daily maximum predicted Ta matrix, for each cell containing a SRTMN site. Use these daily values to calculate rolling averages then select the highest, for each site.	Gridded UKCP09 predicted Ta dataset (UK MET Office)

5

Table 2 LS model and LS_Ta model for each catchment, with the % variance explained by the model (all terms) and the same model but with the RNS omitted (covariates).

Catchment	Model	AICc / BIC	df	% variance	
				all terms	covariates
LS model					
Dee	UCA + RNS	137.0	8.8	80.0	18.3
Tweed	s(UCA) + %RW + RNS	100.1	7.6	85.6	71.7
Spey	s(UCA) + RNS	69.8	6.8	85.5	21.8
Bladnoch	s(UCA)	55.5	2.9	76.6	76.6
LS_Ta model					
Dee	Ta_{max} + UCA + s(Orientation) + RNS	131.8	11.7	85.1	19.9
Tweed	Ta_{max} + s(UCA) + %RW + s(HS) + Orientation	98.5	7.7	85.3	85.3
Spey	UCA + DC + RNS	69.3	7.4	85.1	19.9
Bladnoch	Ta_{max} + UCA	53.9	4.8	85.9	85.9

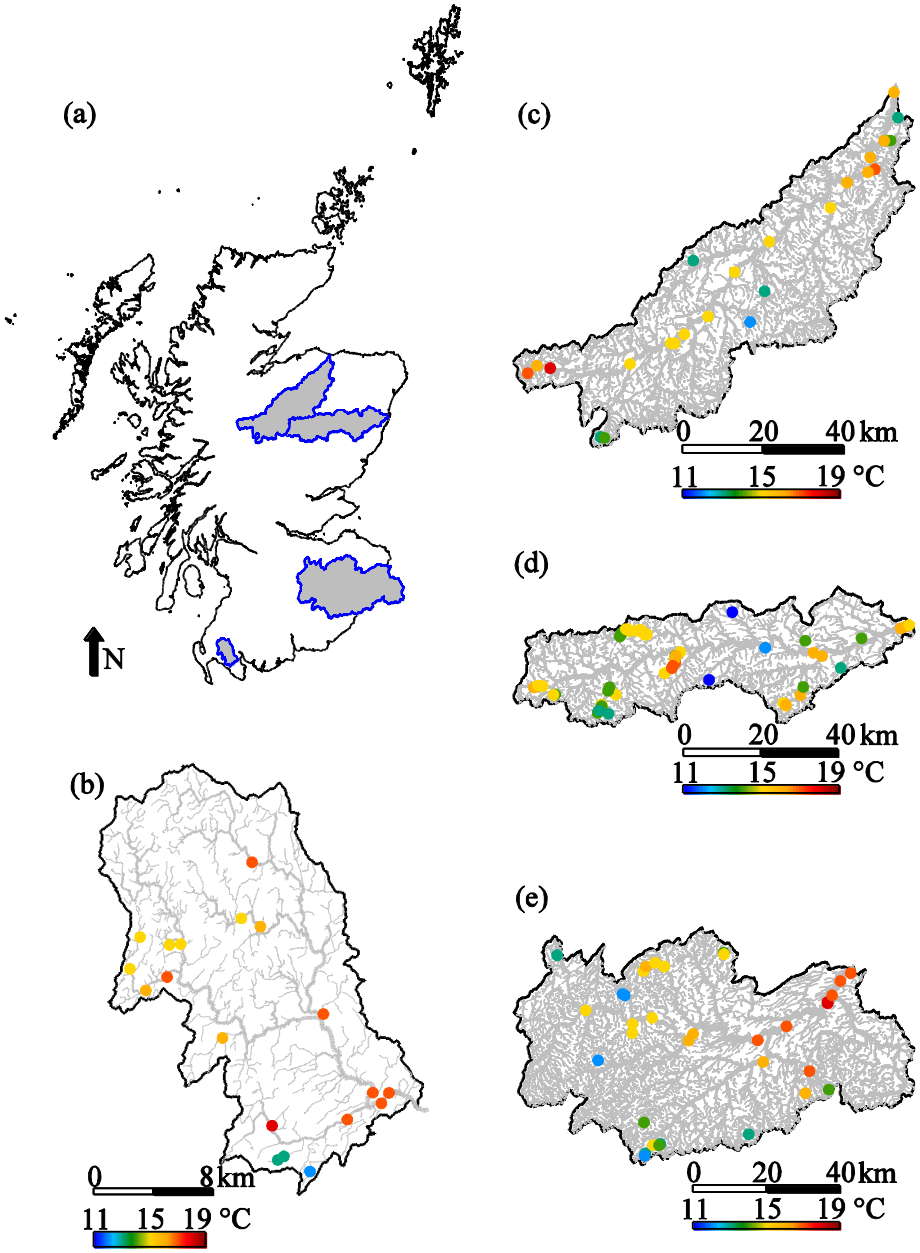
Table 3 Transferability of LS and LS_Ta models. The values in normal font are for predictions using only covariates (any RNS information is ignored). The values in italics are for predictions when the target and donor catchments are the same and all model terms are used (both covariates and the RNS).

	Donor catchment	Target catchment			
		Dee	Tweed	Spey	Bladnoch
LS models					
RMSE	Dee	1.3 *(0.8)*	1.2	1.3	2.3
	Tweed	1.1	1.1 *(0.9)*	1.3	1.9
	Spey	1.3	1.3	1.4 *(0.9)*	2.5
	Bladnoch	2.2	1.9	2.4	0.9 *(0.9)*
Bias	Dee	-0.6 *(0.1)*	-0.6	-0.1	-2.0
	Tweed	0.2	-0.1 (*0.0)*	0.3	-1.7
	Spey	-0.6	-0.8	-0.2 *(-0.0)*	-2.3
	Bladnoch	1.9	1.4	2.0	0.0 *(0.0)*
Standard Deviation	Dee	0.8 *(0.8)*	1.1	1.3	1.2
	Tweed	1.1	1.0 *(0.9)*	1.2	1.0
	Spey	1.1	1.1	1.4 *(0.9)*	1.0
	Bladnoch	1.1	1.3	1.3	0.9 *(0.9)*
LS_Ta models					
RMSE	Dee	1.7 *(0.7)*	0.9	1.9	1.9
	Tweed	1.2	0.9 *(0.9)*	2.3	1.5
	Spey	1.5	2.0	1.8 *(0.8)*	4.2
	Bladnoch	8.4	4.2	5.2	0.9 *(0.9)*
Bias	Dee	-1.1 *(0.1)*	-0.3	0.0	-1.4
	Tweed	-0.7	-0.0 *(-0.0)*	-0.1	-1.0
	Spey	-0.1	-1.4	-0.7 *(0.0)*	-4.1
	Bladnoch	7.6	3.2	4.1	-0.1 *(-0.1)*
Standard deviation	Dee	1.3 *(0.7)*	0.9	1.9	1.2
	Tweed	1.0	0.9 *(0.9)*	2.3	1.1
	Spey	1.5	1.4	1.6 *(0.8)*	1.1
	Bladnoch	3.7	2.7	3.3	0.9 *(0.9)*

Table 4 Multi-catchment LS and LS_Ta model, with the % variance explained by the model (all terms) and when the RNS is omitted (covariates).

Model	BIC	df	% variance	
			all terms	covariates
Multi-catchment LS model				
Catchment + s(UCA) + %RW + Elevation + RNS:Catchment	379.3	24.8	84.4	51.9
Multi-catchment LS_Ta model				
Catchment + Ta_{max}:Catchment + s(UCA) + %RW + RNS:Catchment	395.4	25.7	83.2	57.2

Figure 1. Study catchments and spatial patterns of Twmax for August 2015 a) Catchment positions in Scotland b) River Bladnoch catchment, c) River Spey catchment, d) River Dee catchment, e) River Tweed catchment



5

Figure 2 Distributions and inter-relationships between Tw_{max} and covariates. Scatter plots of the relationships are shown below the diagonal, kernel density plots of the individual covariates in the diagonal (scaled to have the same maximum value) and correlation coefficients above the diagonal. Numbers in black indicate the correlation coefficients where data is pooled across all catchments.

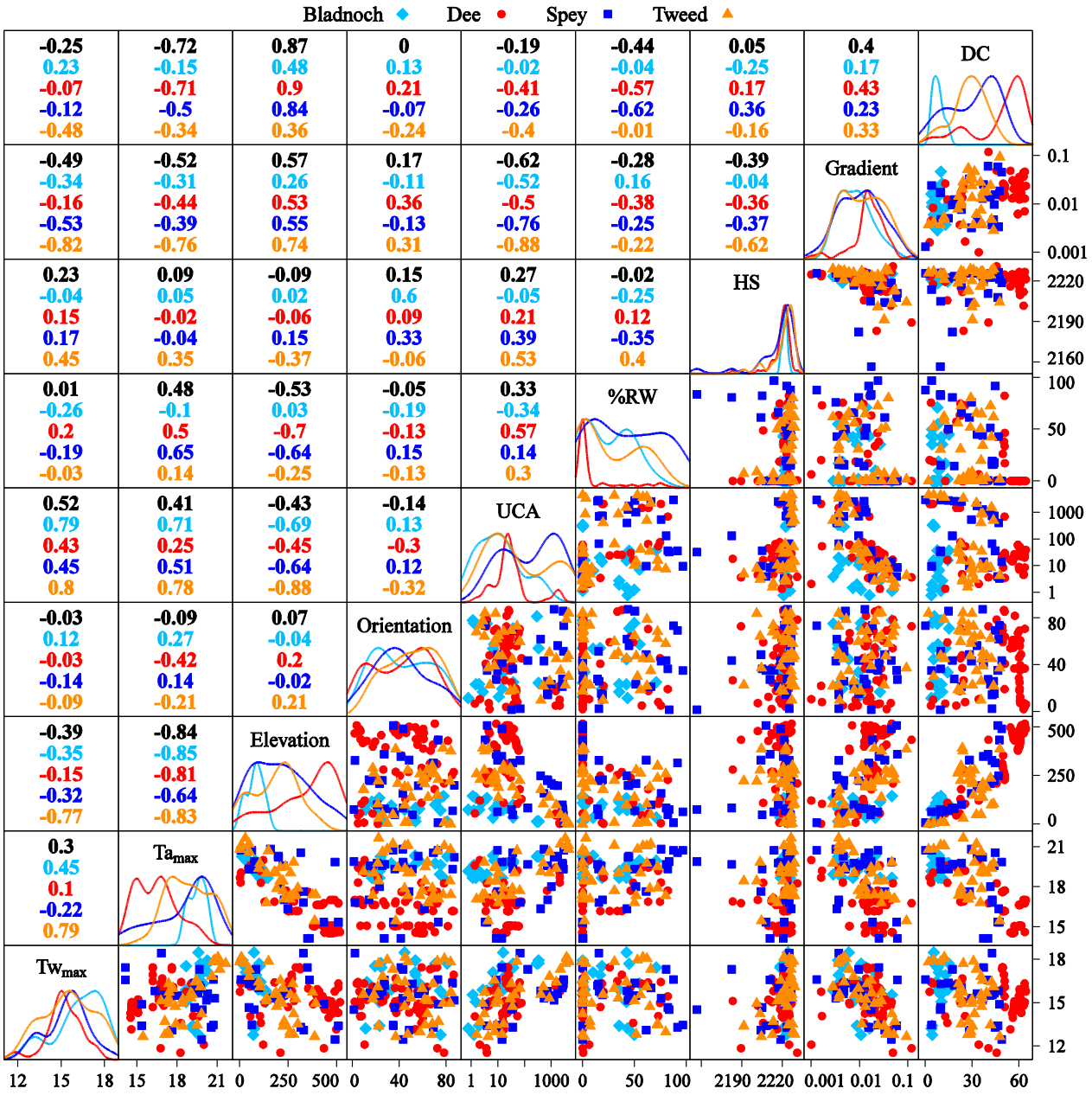


Figure 3. LS model effects with pointwise 95% confidence bands: a) Dee UCA, b) Tweed UCA, c) Spey UCA, d) Bladnoch UCA, e) Tweed %RW.

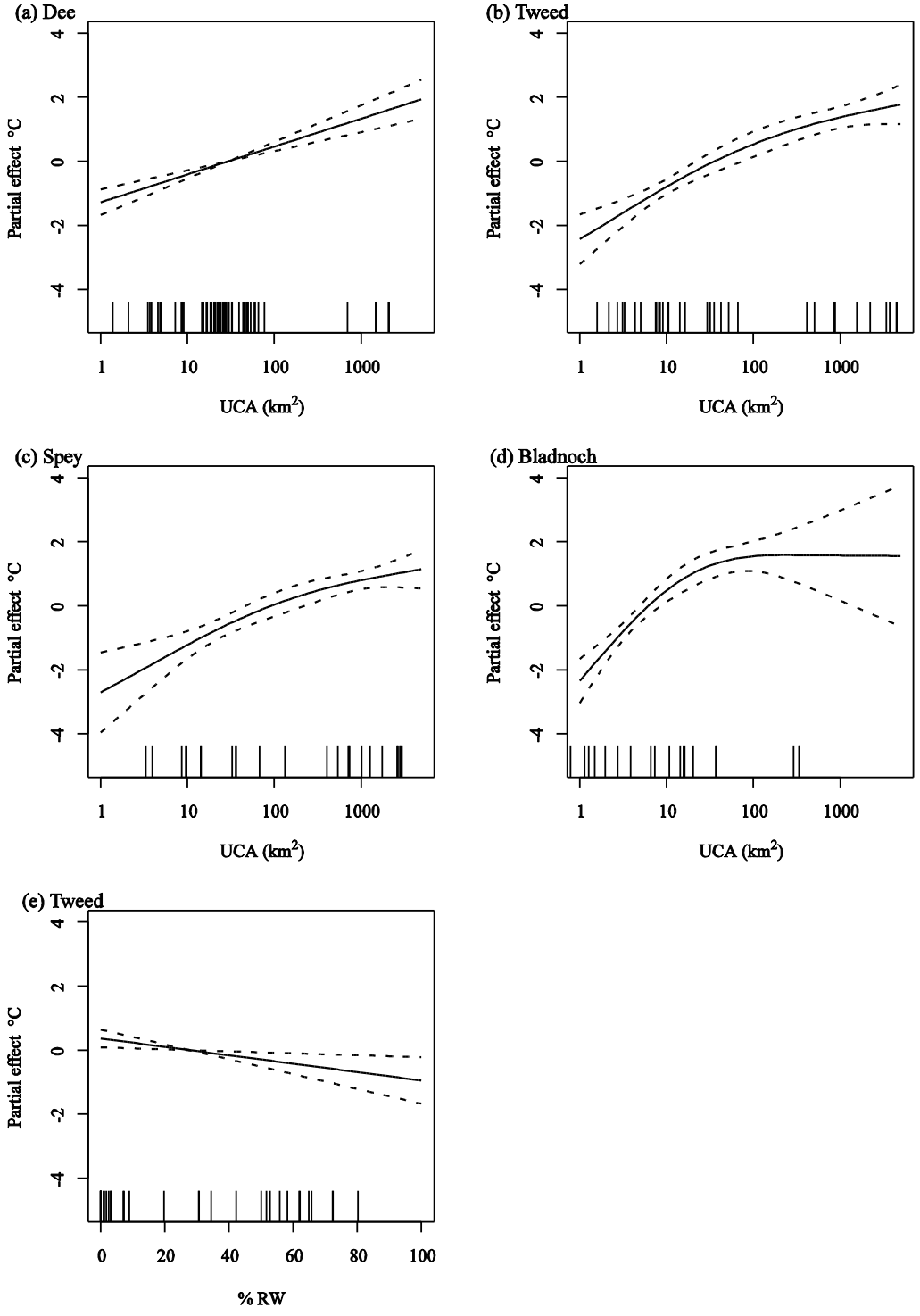


Figure 4. LS_Ta model effects with pointwise 95% confidence bands. Each column corresponds to a catchment and each row to a covariate. a) Dee UCA, b) Tweed UCA, c) Spey UCA, d) Bladnoch UCA, e) Dee Ta_{max}, f) Tweed Ta_{max}, g) Bladnoch Ta_{max}, h) Dee Orientation, i) Tweed orientation, j) Tweed %RW, k) Tweed hillshading, l) Spey DC.

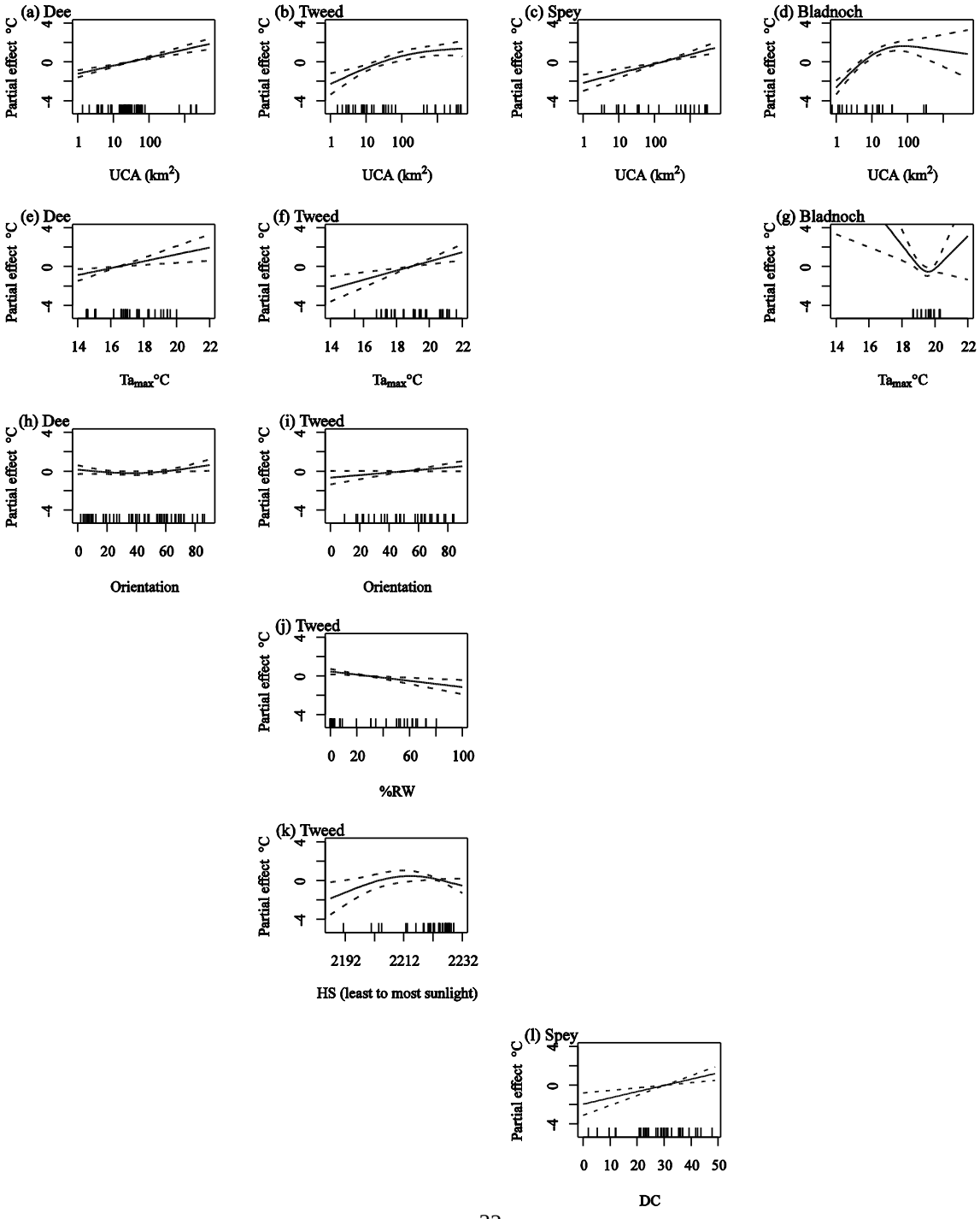


Figure 5. LS model transferability. Panels a, b, c, d show predicted Tw_{max} when the target catchment is the Dee, Tweed, Spey and Bladnoch respectively. The colours and symbols indicate the donor catchment: Dee (red circles), Tweed (orange triangles), Spey (dark blue squares) and Bladnoch (light blue diamonds). Filled (open) symbols indicate sites in (out) of the environmental range of the donor catchment. When the target and donor catchments are the same, the coloured points are based on predictions using only covariates; the grey symbols show the corresponding predictions based on the covariates and the RNS. The dashed lines are robust regression lines of observed against predicted values. Models which transfer well have points falling close to the 1:1 line.

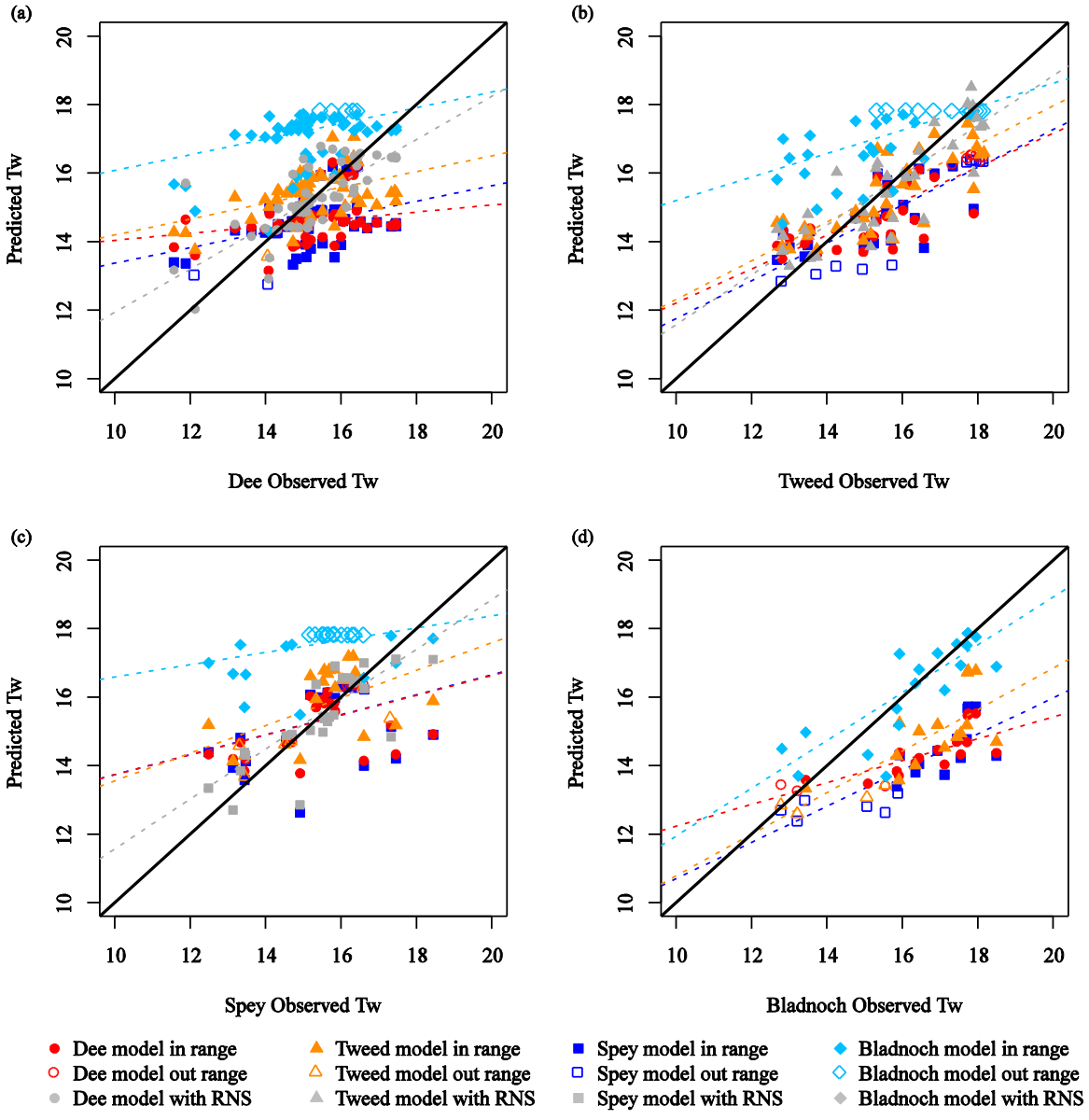


Figure 6. LS_Ta model transferability. Panels a, b, c, d show predicted Tw_{max} when the target catchment is the Dee, Tweed, Spey and Bladnoch respectively. The colours and symbols indicate the donor catchment: Dee (red circles), Tweed (orange triangles), Spey (dark blue squares) and Bladnoch (light blue diamonds). Filled (open) symbols indicate sites in (out) of the environmental range of the donor catchment. When the target and donor catchments are the same, the coloured points are based on predictions using only covariates; the grey symbols show the corresponding predictions based on the covariates and the RNS. The dashed lines are robust regression lines of observed against predicted values. Models which transfer well have points falling close to the 1:1 line.

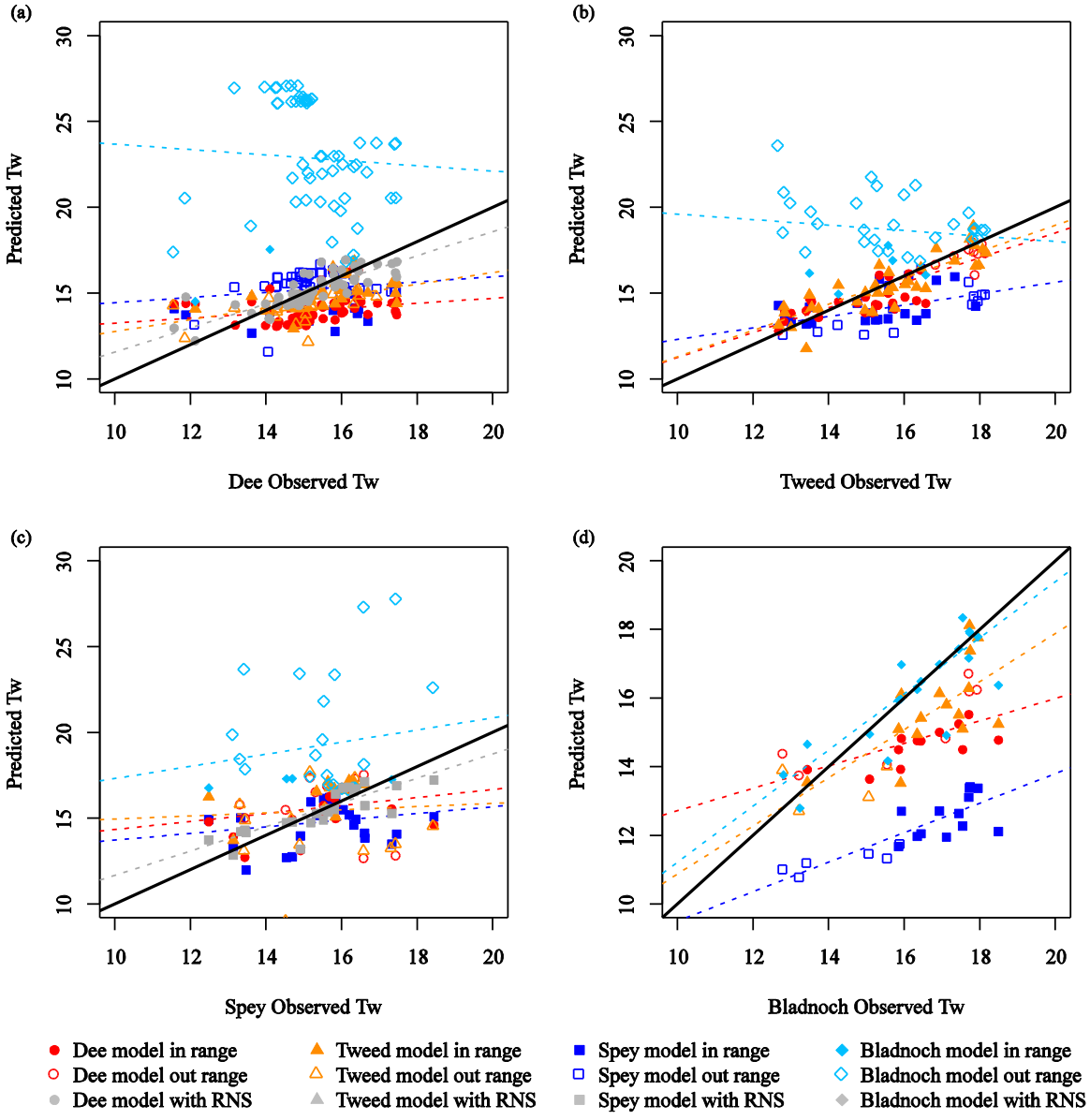


Figure 7. Multi-catchment LS model effects with pointwise 95% confidence bands: a) UCA, b) %RW, c) Elevation, d) Catchment.

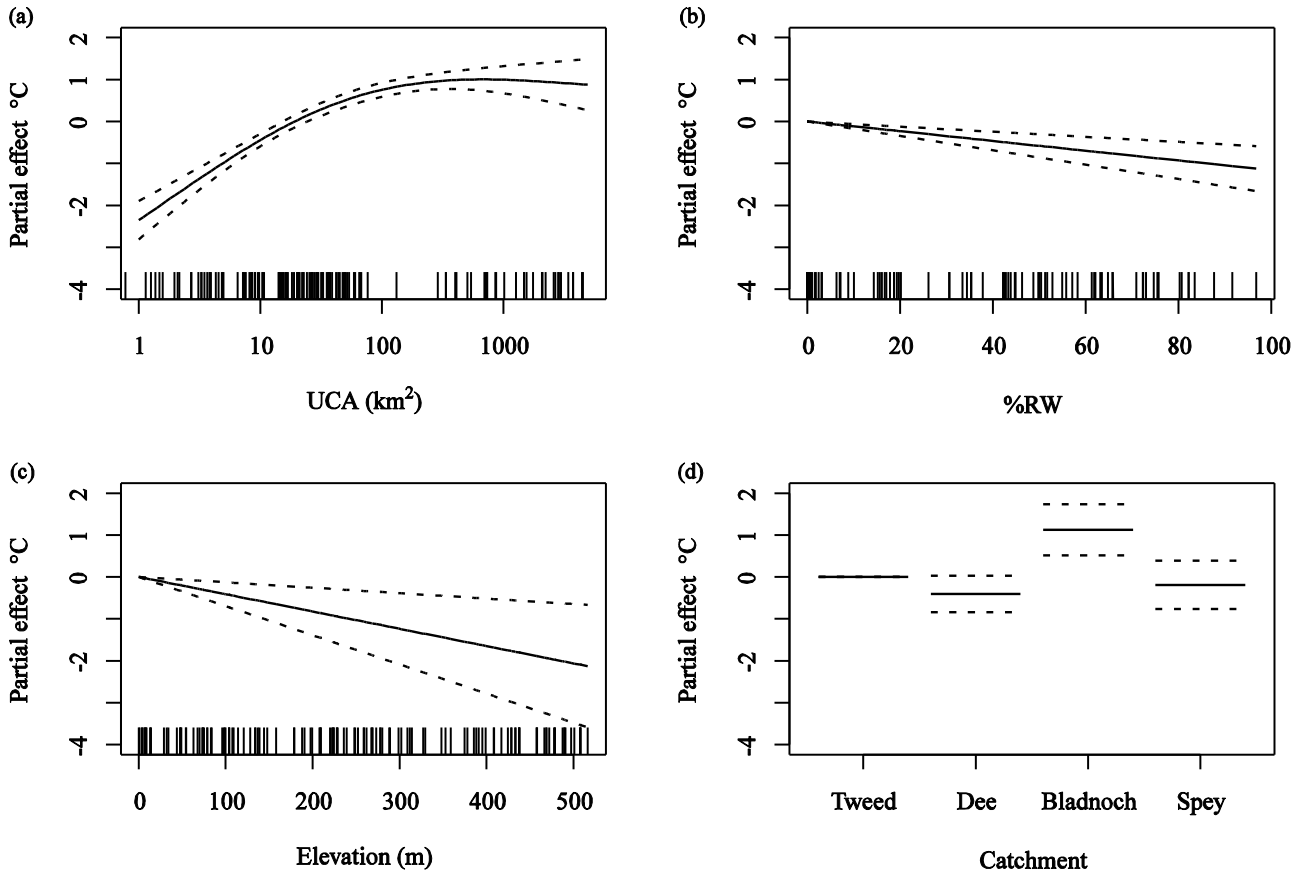
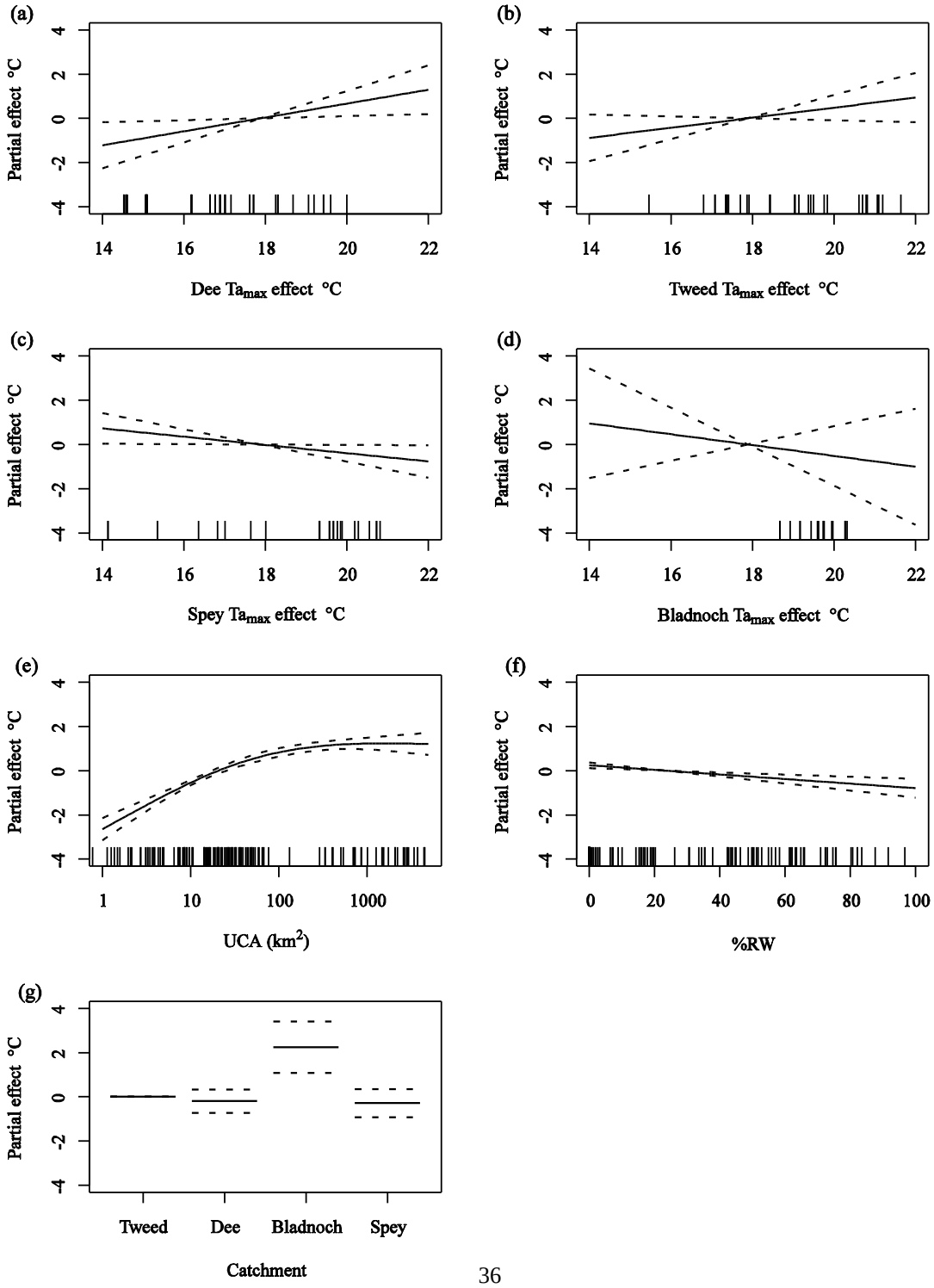



Figure 8. Multi-catchment LS_Ta model effects with pointwise 95% confidence bands: a) Dee Ta_{max}, b) Tweed Ta_{max}, c) Spey Ta_{max}, d) Bladnoch Ta_{max}, e) UCA, f) %RW, g) Catchment.