1	Uncertainty propagation in observational references to climate model scales
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ABSTRACT

Climate model simulations and observational references of the Earth's climate are the two 21 primary sources of information used for climate related decision-making. While uncertain-22 ties in climate models and observational references have been assessed thoroughly, it has 23 remained difficult to integrate these, partly because of the lack of formal concepts on how 24 to consider observational uncertainties in model-observation comparison. One of the dif-25 ficulties dealing with observational uncertainty is its propagation to the space-time scales 26 represented by the models. This is a challenge due to the correlation of observational errors 27 in space and time. Here we present an approximation which allows to derive propagation 28 factors to different model scales and apply these to uncertainty estimates provided by the 29 Climate Change Initiative (CCI) sea-surface temperature (SST) dataset. The propagated un-30 certainty in SST observations is found to systematically lower seasonal forecast skill and 31 to increase the uncertainty in verification of seasonal forecasts, an aspect that remains cur-32 rently overlooked. Uncertainty in forecast quality assessment is dominated by the shortness 33 of the satellite record. Expanding the record length of these datasets might hence reduce the 34 verification uncertainties more than the efforts to reduce the observational uncertainties. 35

1. Introduction

The scientific community is taking action to confront the challenge of climate variability and change by understanding the physical basis and by providing estimates of the present and future climate. Climate model simulations and observational references are the two resulting sources of information that support stakeholders and policymakers. The quantification of uncertainties in both sources of information is crucial and large efforts are devoted quantifying these (Flato et al. 2013; Hartmann et al. 2013).

Climate model uncertainties are typically assessed by comparing simulated and observed con-43 ditions of the past climate (Reichler and Kim 2008). The agreement between models and ob-44 servations is instrumental in gaining confidence into simulated climates which have not yet been 45 observed (Knutti 2008). This holds particularly for near-term climate predictions such as sub-46 seasonal to seasonal predictions where retrospective predictions can be verified (Doblas-Reyes 47 et al. 2013). Accurate observational references of the Earth's climate are therefore indispens-48 able to quantify model uncertainties, yet observations are subject to uncertainties as well. While 49 the uncertainties related to the limited statistical sample in model-observation comparison is usu-50 ally reported (e.g. for seasonal forecasting Doblas-Reves et al. 2013; Ferro 2014; Scaife et al. 51 2014; Siegert et al. 2016b) uncertainties in the observational references remain weakly explored. 52 This tendency pertains to the climate modelling community in general (as highlighted in Gómez-53 Navarro et al. 2012; Addor and Fischer 2015; Massonnet et al. 2016; Mudryk et al. 2017) despite 54 the large efforts that have gone into quantifying uncertainties in observational references (Kennedy 55 2014; Povey and Grainger 2015; Merchant et al. 2017) 56

Like climate models, observational references rely on a number of structural and parametric choices in the design and calibration of the algorithm used to generate the data sets (Thorne et al.

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2005; Liu et al. 2015) and are therefore an approximation of the theoretical true climate (Mas-59 sonnet et al. 2016). Data sets report the resulting uncertainties typically by characterizing the 60 dispersion of the error distribution between the measured and the theoretical true value (Merchant 61 et al. 2014; Liu et al. 2015). One of the challenges in including these uncertainty estimates in 62 the assessment of model simulations is the aggregation to the space-time averages, motivated by 63 the mismatch in observational and model grids and data frequency. Measurement errors are cor-64 related in time and space due to for instance the background atmospheric or oceanic conditions 65 that prevail locally in time and in space (Povey and Grainger 2015). Therefore, the information 66 about uncertainty has to be propagated taking into account the expected correlation structure of 67 the observational errors. The lack of knowledge of correlation length scales but also the missing 68 methodological concepts to efficiently propagate uncertainties remain key obstacles to estimating 69 uncertainties at model scales. Past studies have therefore used alternative data sets to estimate ob-70 servational uncertainties (Stoffelen 1998; Reichler and Kim 2008), however, this approach ignores 71 the uncertainty estimates actually reported in the data sets. Providing methodologies of uncer-72 tainty propagation to climate model scales is therefore an opportunity to bridge the modelling and 73 observational data communities. 74

The European Space Agency (ESA) Climate Change Initiative (CCI) has placed a special focus 75 on estimating uncertainties in climate data records (Merchant et al. 2017). This is an important 76 contribution towards mutual uncertainty assessment of models and observations. This study aims 77 to support this practice by illustrating simple ways to propagate uncertainties to scales used in 78 seasonal forecast verification of the El Niño Southern Oscillation (ENSO) relying on the CCI sea-79 surface temperature (SST) gap-free analysis (L4 product) (Merchant et al. 2014). The propagated 80 observational uncertainties are subsequently confronted to two other uncertainties present in the 81 context of forecast verification: the limited ensemble size and the limited record length of the 82

datasets. The comparison allows to understand how important the observational uncertainty is in the practice of seasonal forecast verification. Finally, an estimate of the systematic reduction in seasonal forecast skill due to observational uncertainty is provided, highlighting the fact that current practice underestimates the deterministic skill of forecasting systems.

87 2. Methods

⁸⁸ a. Observational references and seasonal forecast verification

The role of observational uncertainty is explored in this study using the SST CCI gap-free anal-89 ysis v1.1 (Merchant et al. 2014) and three alternative SST data sets which use different data and 90 techniques to represent observed SSTs namely: the Hadley Centre Global Sea Ice and Sea Sur-91 face Temperature (HadISST) data set v.1.1 (Rayner et al. 2003), the ERA-Interim re-analysis 92 (Dee et al. 2011), and the Extended Reconstructed Sea Surface Temperature (ERSST) v.4 data 93 set (Huang et al. 2015). The observational references are hereafter called ORs. HadISST uses 94 in-situ data (Met Office Marine Data Bank (MDB) and Comprehensive Ocean-Atmosphere Data 95 Set (ICOADS) release 2.5 and satellite data from Advanced Very High Resolution Radiometers 96 (AVHRR) data. ERA-Interim is an atmospheric re-analysis product and uses SST data from dif-97 ferent sources as described in Dee et al. (2011) which include both in-situe and satellite remotely 98 sensed data. ERSST4 relies exclusively on in-situ (ICOADS) data. Finally, SST CCI relies on 99 satellite remotely sensed data only blended from AVHRR and (A)ATSR (Advanced Along-Track 100 Scanning Radiometers including ATSR1 and ATSR2). SST CCI and ERA-Interim (from 2009 on-101 wards) use data from the near-realtime Operational Sea Surface Temperature and Sea Ice Analysis 102 (OSTIA) system (Donlon et al. 2012). The SST CCI product is the only OR that is both daily 103 and provides an estimate of the observational uncertainty at its native resolution. Note that the un-104

certainty in the SST CCI gap-free product comprises of the observational error plus the error that
 arises from interpolation in space and time expressed as one standard deviation. In this study, we
 use the SST-CCI observational record, because a gap-free observational record appears to be most
 suitable for comparison with climate model data, which is typically gridded and without gaps.
 Other products, such as ERSSTv4, have uncertainty estimates which are however not explored in
 this study.

The observed SSTs are compared to seasonal coupled climate model predictions from the Eu-111 ropean Centre for Medium-range Weather Forecasts (ECMWF) forecasting system 4 (S4, Molteni 112 et al. 2011). The hindcast considered spans the period 1981 - 2010 using 51 ensemble members 113 with a horizontal resolution of ~ 80 km in the atmosphere (T255) and with 1 degree resolution 114 in the ocean. We focus on the El Niño Southern Oscillation (ENSO), which is the process that 115 contributes most to seasonal predictability across the globe (Latif et al. 1998). The variability of 116 ENSO is computed as the SST anomaly (with respect to the climatology 1981 - 2010) over the 117 Niño3.4 region (170W - 120W; 5S - 5N, black box in Fig.1b). S4 is initialized every month and 118 simulates the consecutive 7 months. Here, we only consider the prediction of summer months of 119 the Northern Hemisphere (June-July-August, JJA) as they are the most difficult to predict from the 120 predictions initialized in May (Barnston et al. 2012). The analysis is extended to global SSTs at a 121 final stage. 122

Seasonal forecast skill is computed using the Pearson correlation of the ensemble mean prediction with the observations. Probabilistic properties that could be derived from the ensemble are omitted. The correlation is a popular skill metric of seasonal forecast quality (Doblas-Reyes et al. 2013; Scaife et al. 2014). It measures the linear relationship between the prediction and the observation across forecasts initialized at different dates and its square is equivalent to the re-calibrated mean square skill score (MSSS, Siegert et al. 2016a). This study focuses on the correlation coefficient only, keeping in mind that the observational uncertainty is equally relevant in probabilistic
verification (Jolliffe 2017).

¹³¹ b. Propagation of uncertainties to climate model scales

The SST CCI analysis provides an estimate of the uncertainty at the resolution of the data (1/20 132 degree ~ 6 km). This uncertainty at the grid point level has to be propagated to space-time averages 133 used in the verification of seasonal predictions (typically monthly means and regional averages or 134 coarser grid scales). In this study we are interested in the observational uncertainty of the average 135 SST in the Niño3.4 region over a 30-day period. Since we can not expect observational errors to be 136 uncorrelated in space and time, the usual formula to calculate the standard error of the mean does 137 not apply. Instead, we have to take into account the finite correlation length (λ) and correlation 138 time scale (τ) of the observational error. 139

Say we have an OR of the variable *x* with an accompanying observational uncertainty σ_x on a regular grid with grid spacing of Δx and Δt in space and time, respectively. We are consequently interested in the uncertainty $\sigma_{\overline{x}}$ of the space-time mean \overline{x} in a configuration consisting of a domain with dimensions of *M* times *N* grid points and *T* time instances. We assume that the observational error $\varepsilon_{i,j,t}$ has an exponential correlation function

$$cor(\varepsilon_{i,j,t},\varepsilon_{i',j',t'}) = exp\left(-\frac{\Delta x\sqrt{(i'-i)^2 + (j'-j)^2}}{\lambda} - \frac{\Delta t|t'-t|}{\tau}\right)$$
(1)

while i < M, j < N, t < T are indices of the data, such that the distances in space $\Delta x \sqrt{(i'-i)^2 + (j'-j)^2}$ and time $\Delta t |t'-t|$ are scaled by the correlation lengths (Cressie 2015). The exponential function can be expanded for all possible distances (all possible values for *i*, *j*, and *t*) to form the covariance matrix Σ with dimension of all points in space and time (*MNT*). The uncertainty of \bar{x} is consequently defined as,

$$\sigma_{\overline{x}} = \sqrt{w^T \Sigma w} \tag{2}$$

where w is the averaging vector with length of MNT values of $\frac{1}{MNT}$ or additional weighting val-150 ues to account for the effective area of the grid points. The calculation of this expression requires 151 enumeration over all pairs of grid points. The computational complexity of such an approach is 152 $\mathcal{O}(M^2N^2T^2)$, which makes the calculation computationally unfeasible even for moderate domain 153 sizes and time periods. To overcome the complexity, it is useful to assume a constant observational 154 uncertainty within the domain ($\hat{\sigma}_x$). Since many points in space and time share the same distances 155 (in space and time) one can formulate the following analytical solution (following the derivations 156 described in Appendix A), 157

$$\sigma_{\overline{x}} = \frac{\hat{\sigma}_x}{MNT} \sqrt{(T+2S_T)(MN+2NS_M+2MS_N+4S_{MN})}$$
(3)

where the S terms describe the exponential decay in all dimensions,

$$S_{M} = \sum_{i=1}^{M-1} (M-i)e^{\frac{-i\Delta x}{\lambda}}$$
$$S_{N} = \sum_{j=1}^{N-1} (N-j)e^{\frac{-j\Delta x}{\lambda}}$$
$$S_{T} = \sum_{t=1}^{T-1} (T-t)e^{\frac{-t\Delta t}{\tau}}$$
$$S_{MN} = \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} (M-i)(N-j)e^{\frac{-\Delta x\sqrt{i^{2}+j^{2}}}{\lambda}}$$

The computational complexity is only $\mathcal{O}(M + N + T + MN)$ which allows us to efficiently propagate uncertainty to different length scales. An alternative approach is presented in Appendix B in case the assumption of a constant σ_x is weakly justified due to continental boundaries or strong inhomogeneity of σ_x in the space-time domain. The approach relies on generating random fields ¹⁶³ from Σ which are averaged for the space-time domain using a Monte Carlo approach. This solu-¹⁶⁴ tion is also sufficiently efficient to propagate observational uncertainty and explore the uncertainty ¹⁶⁵ related to the length and time scales. Note that the Monte-Carlo approach is orders of magnitude ¹⁶⁶ faster than the enumeration in equation 2 due to efficient algorithms based on Fourier transforma-¹⁶⁷ tions (Schlather et al. 2015).

It is useful to elaborate on equation 3 using practical examples for better understanding. Obser-168 vational errors are traditionally classified into random and systematic errors (Povey and Grainger 169 2015). Errors such as sensor noise, which are uncorrelated in time and space, reduce with averag-170 ing with the square root of the sample size (\sqrt{MNT}) following the law of large numbers. Random 171 errors are analogous to zero correlation scales ($\lambda = \tau = 0$) which yields zero for the S terms below 172 the square root in equation 3 leaving \sqrt{MNT} in the denominator. For locally systematic errors due 173 to e.g. weather systems ($\lambda, \tau > 0$) the S-terms grow and therefore can be understood as the correc-174 tion factor of the law of large numbers. If the errors are globally systematic due to e.g. errors in the 175 retrieval algorithm, the length scales become infinitely large ($\lambda = \tau = \infty$) and the expression below 176 square becomes $M^2 N^2 T^2$. The uncertainty does in this case not decrease $\sigma_{\bar{x}} = \hat{\sigma}_x$. The SST CCI 177 provides the differentiated uncertainty components for non-gap filled data products (L3 products) 178 with an accompanying tool for the propagation. In the gap-filled (L4) product these uncertainties 179 can no longer be retained as the correlation structure is unknown after interpolation. In this case 180 approximate length scales have to be used. 181

¹⁸² c. Inference of uncertainty from different observational references

An alternative way to determine the uncertainty in ORs is to infer it from the spread between available ORs for a given space-time mean (Martin et al. 2012). This can be done by assuming that different ORs are equally probable. This assumption is known to be flawed given that the

quality of ORs differ (Massonnet et al. 2016). Martin et al. (2012) find that using ensembles 186 of different SST products the resulting uncertainty is not robust (underestimated by a third in 187 their analysis). However, this approach has been and remains the most adopted practice in the 188 modelling community (e.g. Bellprat et al. 2012; Gómez-Navarro et al. 2012; Sunyer Pinya et al. 189 2013; Reichler and Kim 2008). It is therefore important to bridge to this practice. An advantage 190 of the approach is that an ensemble of structurally different ORs allows to account for structural 191 uncertainties in the retrieval algorithms (Thorne et al. 2005). The different ORs can consequently 192 be understood as an ensemble of opportunity from which $\sigma_{\overline{x}}$ can be estimated. This approach fits 193 naturally with data sets that systematically explore parameter choices using an ensemble approach 194 (Morice et al. 2012). More sophisticated inference methods include parameters that account for 195 structural differences in the ORs and estimate $\sigma_{\overline{x}}$ using the triple-collocation approach (Stoffelen 196 1998; Gruber et al. 2016) or Bayesian inference (Siegert et al. 2016b). In this study we use only 197 the standard deviation between different ORs as a comparison for the uncertainty propagation. 198

199 3. Results

²⁰⁰ a. Uncertainty in the observed El Niño Southern Oscillation

The seasonal forecast capability of ECMWF S4 and the different ORs are summarized in figure 1. The time-series show the evolution of Niño3.4 SSTs for both the ensemble mean forecast (from which the correlation skill is determined) and the individual members. The time series length is constrained by the length of SST CCI, which spans the period 1992-2010. S4 has a high ensemble mean forecast skill shown here for the month of June (~ 0.9 correlation) and the ensemble range usually encompasses the estimates from the ORs. The ORs cluster and are closer to each other than to the model result, yet discrepancies between the ORs are visible.

The lower panel of figure 1 shows the observational uncertainty (σ_x) provided by SST CCI at 208 a specific time instance (1st of June 2000). The variability of the spatial σ_x reaches one order of 209 magnitude globally (not shown). Daily variations are negligible during the summer months but 210 the uncertainty within the Niño3.4 region varies with a factor of three as denoted by the black box 211 in figure 1b. Assuming constant uncertainty yields $\hat{\sigma}_x=0.22$ with a low standard deviation in space 212 and time (\pm 0.001 K) due to the temporal stability. The implications of the notable changes in the 213 OR uncertainty in Niño3.4 is explored later in this section. In order to know $\sigma_{\overline{x}}$ for the monthly 214 and spatial SST average in the Niño3.4 domain, we need to propagate $\hat{\sigma}_x$ to its space-time average. 215 The assumption of constant observational uncertainty greatly facilitates the propagation and 216 allows to formulate the analytical solution as in equation 3. The solution suggests that the un-217 certainty propagates as a function of the ratio between the size of the space-time domain and 218 the correlation length, independently of the data spacing $(\Delta x, \Delta t)$, and the number of data points 219 (MNT). This allows to present the propagation as a look-up graph (Fig.2) that is independent of 220 the application. To describe this ratio we define spatial and temporal degrees of freedom (d.o.f) as 221 the number of times that the correlation scale fits into the domain size. The spatial d.o.f is defined 222 as $\frac{MN\Delta x^2}{\lambda^2}$ and the temporal d.o.f. as $\frac{T\Delta t}{\tau}$. A correlation time scale of 5 days is in this sense equal to 223 6 temporal d.o.f for a monthly average, while a length scale of 100 km would correspond to 100 224 d.o.f for a region of 1000km by 1000 km. The reader will note that spatial or temporal d.o.f should 225 not be misinterpreted as effective sample sizes with which the standard deviation can be scaled. 226 As shown in equation 3 the correction term is more complicated. To make the propagation general 227 in the physical space, the graph is further shown for unit observational uncertainty ($\sigma_x = 1$). The 228 resulting standard deviation of the space-time mean (y-axis) can consequently be understood as 229 the propagation factor with which the average observational uncertainty ($\hat{\sigma}_x$) of the data needs to 230 be multiplied. 231

The SST CCI reports correlation lengths for errors of 100 km in space and a time scale of one day 232 for the locally systematic errors in single sensor L3 products. These represent scales associated 233 with small synoptic systems and the coverage of the satellite (revisiting the same location every 234 two days). We take here this estimate as a first guess, bearing in mind that these length scales do 235 not take into account the uncertainty introduced from the interpolation in space and time. Taking 236 the case of the monthly Niño3.4 domain the scales are equivalent to 30 temporal d.o.f. and 320 237 spatial d.o.f (the Niño3.4 regions covers 4000 km x 800 km). The resulting standard deviation of 238 the space-time mean yields $\sigma_{\rm x}$ = 0.007 K (the propagation factor is 0.03). This estimate is arguably 239 too small and indicates that systematic uncertainties operating at larger scales are present. We 240 consider therefore additionally scales associated with large synoptic systems of $\lambda = 1000$ km and 241 τ = 10 days. The resulting estimate yields $\sigma_{\overline{x}} = 0.076$ K. 242

The two estimates of monthly Niño3.4 SST uncertainties are compared in figure 3 with the 243 standard deviations obtained from the four different ORs. The standard deviation from a sample 244 of four points is highly uncertain and hence a distribution obtained from all individual years and 245 the months (May-August) are shown as a histogram in figure 3. The propagated uncertainties from 246 SST CCI are at the lower tail of uncertainty estimates, yet the estimate using large synoptic scales 247 is consistent with the comparison of the different ORs for summer Niño3.4 SSTs (approximately 248 $\sigma_{\overline{x}} = 0.1$ K). Differences between ORs can be substantially larger as seen in figure 3. Note that 249 the two alternative estimates do not represent the same quantity as discussed in section 2c and are 250 therefore not expected to agree entirely. The former is a self-consistent estimate of uncertainty 251 in the SST CCI product, the latter is an estimate of the uncertainty collectively among the ORs. 252 However, the comparison indicates that correlation scales associated with larger synoptic scales 253 are reflecting the uncertainty of the Niño3.4 SSTs more realistically and might still underestimate 254 the uncertainty Martin et al. (2012). 255

The propagated estimate assumes that the uncertainty is constant in space and time over the 256 domain of interest, and that the spatial and temporal correlations decay exponentially with con-257 stant decorrelation parameters. The correlation function needs not necessarily to be exponential. 258 The exponential function in equation 1 can be replaced by a different correlation function that is 259 separable into the product of a temporal component and an isotropic spatial component with con-260 stant parameters. The assumption of constant observational variance used in figure 2 appears very 261 restrictive, and seems to defeat the purpose of an observational data set that aims to resolve obser-262 vational uncertainty in space and time. However, we have found by producing large samples from 263 known distributions that the error due to the constant variance assumption is very small as long as 264 the observational variance does not change too much over space and time in the domain of interest. 265 In particular, we have analysed the observational error of Nino3.4 monthly average SST by sam-266 pling 1000 error fields 1) using the spatially and temporally varying observational error standard 267 deviations provided in the data set (with much reduced spatial resolution), and 2) replacing all 268 error standard deviations by their space-time mean, i.e. simulating under a constant error variance 269 assumption. The analytical expression yields an observational error standard deviation of 0.0767 270 K. The 1000 simulated error fields with varying variances have standard deviation of 0.0766 K 271 and the 1000 simulated error fields with constant variances have standard deviation of 0.0765 K. 272 This result shows that analytical and simulated results agree when using 1000 Monte-Carlo simu-273 lations, and that the difference between varying and constant error variances is negligible (at least 274 in this example). 275

²⁷⁶ b. Observational uncertainty in verification of seasonal sea-surface temperature forecasts

Having assessed the uncertainty in observed Niño3.4 SSTs, it is crucial to understand how important the uncertainty is in practice compared to other sources of uncertainty in forecast veri-

fication. There are three sources of uncertainties when dealing with the assessment of seasonal 279 forecast skill: (1) a sample uncertainty due to the limited number of retrospective predictions 280 or limited OR record length over which the skill is evaluated, (2) a sample uncertainty due to a 281 limited ensemble size used to compute the ensemble-mean forecast often constrained by limited 282 computational resources, (3) and an uncertainty due to the uncertainties in OR itself. Note that 283 other uncertainties in the comparison of models and observations such as the unpredictable inter-284 nal variability or the uncertainty due to model inadequacy (Notz 2015) are not uncertainties of the 285 prediction skill, but part of the forecast error that the skill itself aims at measuring. 286

While uncertainties from (1) and (2) are commonly assessed (Ferro 2014; Scaife et al. 2014; 287 Siegert et al. 2016b) the observational uncertainty remains an overlooked problem and formal 288 concepts to include observational uncertainty in deterministic verification metrics are lacking (for 289 probabilistic metrics approaches, different have been presented; Candille and Talagrand 2008; 290 Jolliffe 2017). Here we explore impact of OR uncertainty on the correlation by generating an 291 ensemble of observations. This is far from trivial (Povey and Grainger 2015) and proper ensemble 292 generation is only possible at the level of the algorithm used to generate an ORs. However, at 293 the user level the uncertainty estimate provided by CCI can be used to perturb the analysis using 294 Gaussian random noise or using the different ORs as an ensemble of opportunity by resampling 295 the ORs in each specific year. 296

The impact of the observational uncertainty on the correlation skill of Niño3.4 SSTs is illustrated in figure 4 in comparison to the sampling uncertainties. The sample uncertainties are assessed by resampling the ensemble members of the forecast prior to computing the model ensemble mean and resampling the years in the verification period, both with replacement. An ensemble size of 10 members is used, which represents the typical ensemble size used in non-operational climate prediction hindcasts (Doblas-Reves et al. 2013). The total uncertainty is estimated by sampling jointly all sources (1-3) using the alternative ORs as an estimate of the observational uncertainty.
 Note that the seamingly increased skill in July in comparison to June is an artifact of the limited
 period considered (1992 - 2010). For longer periods the forecast skill decreases monotonically as
 the model departs from the initialization date (May 1st).

The observational uncertainty (green area) contributes about 20% in the summer months and 307 50% in the first month after the initialisation with similar amplitudes for both observational en-308 semble approaches considered. The observational ensemble using the CCI uncertainty estimate 309 tends to reduce the skill since adding observational error reduces the correlation (Massonnet et al. 310 2016). The total source of uncertainty increases with time and reaches a range of 0.7 - 0.95 cor-311 relation. The ensemble size uncertainty (orange area) remains overall small with 10 members as 312 each member retains a strong signal over the Niño3.4 region. The record length of SST CCI is 313 overall the largest source of uncertainty (blue area). Expanding the record length of SST CCI 314 beyond the current 20 years might hence reduce the verification uncertainties more efficiently than 315 current efforts to reduce the observational uncertainties for the Niño3.4 region. The sum of all 316 three sources of uncertainties is clearly larger than the total uncertainty obtained by jointly sam-317 pling the uncertainty due to non-linear interactions of the terms. In the supplementary information 318 (Fig. S1) we show that the qualitative conclusions drawn are also valid for varying ensemble sizes 319 and record lengths. 320

The example gives a regionally limited perspective and the focus is expanded to a global view in figure 5 for the month of August by comparing the relative contribution of each uncertainty source with respect to the sum of all sources. The uncertainty related to the length of the SST record dominates almost everywhere except in the poles. The record length uncertainty is particularly large in regions of high interannual variability. The observational uncertainty, sampled using the CCI uncertainty estimate, is the dominant source of uncertainty over the polar regions and ³²⁷ contributes also in various other regions up to 40%. The ensemble size uncertainty is the largest ³²⁸ over the extratropical North Pacific and North Atlantic. The SSTs over these regions are primarily ³²⁹ forced by the atmospheric flow at seasonal time scales (Cayan 1992) and therefore subject to the ³³⁰ atmospheric internal variability which is large in the extratropical Northern Hemisphere. A large ³³¹ ensemble size is therefore required in this region to reduce the effect of the internal variability in ³³² the ensemble mean in this region (Scaife et al. 2014).

Finally, it is important to take into account that observational errors not only increase the verification uncertainty but also have systematic effects on the prediction skill. Uncertainties in a reference lower the correlation skill (Massonnet et al. 2016), similarly as a limited ensemble size leads to systematically lower correlation (Ferro 2014; Scaife et al. 2014). This reduction in correlation skill can be estimated by dividing the sample correlation by the correction for attenuation (Spearman 1904),

$$R = \frac{\sigma_o^2 - \sigma_x^2}{\sigma_o^2},\tag{4}$$

where σ_o is the total interannual standard deviation of the ORs and σ_x the observational un-339 certainty. The reference variability is hence attenuated for the observational uncertainty without 340 altering the co-variance between the model and the reference. Corrections for probabilistic mea-341 sures have also recently been proposed (Ferro 2017). The resulting increase in the correlation skill 342 of ECMWF S4 global SSTs is shown in figure 6. The skill increases in many regions up to 0.2 and 343 beyond, in agreement with the regions where the uncertainty increases most (figure 5, first panel). 344 In the poles and also regions in the southern Ocean the observational uncertainty is larger than the 345 interannual variability of the OR and hence no attenuation can be calculated. 346

347 4. Discussion and conclusions

Just like climate model predictions, observational references (ORs) are subject to uncertainties. 348 These uncertainties are usually disregarded in the verification of seasonal forecasts or the evalua-349 tion of climate models in general. The common assumption that limitations of the models dom-350 inate the observational uncertainty persists and the role of OR limitations is therefore often seen 351 as minor. These assumptions are rarely assessed and individual studies suggest that observational 352 uncertainties might be larger than anticipated (e.g. Addor and Fischer 2015; Prodhomme et al. 353 2016; Massonnet et al. 2016). Formal concepts of how to account for observational uncertainties 354 provided by ORs in climate model evaluation are, however, still scarce. 355

In this study, we present a step forward to narrow this gap by presenting simple ways to prop-356 agate observational uncertainties to space-time means, a necessary step in forecast verification 357 where the model and OR spatial and temporal resolution do not match each other. The solution 358 described is independent of the data structure and is illustrated as a "look-up" graph from which 359 propagated uncertainties can be readily estimated. The solution assumes a constant observational 360 uncertainty in the region and under the period considered for the space-time average and an al-36 ternative Monte-Carlo simulation approach is suggested if this assumption is weakly justified. 362 Propagated observational uncertainties from the SST CCI product are consistent with differences 363 in different ORs over the Niño3.4 region, yet the latter tends to be larger. Using the different ORs 364 as complementary estimates and the propagated SST CCI uncertainty we find that the observa-365 tional uncertainty contributes fundamentally to the forecast skill assessment of seasonal predic-366 tions of SSTs. Particularly at high latitudes, the observational uncertainty can dominate over other 367 sources of verification uncertainties. However, over most regions, the largest uncertainty in sea-368 sonal forecast quality originates from the limited period over which the hindcasts are evaluated. 369

The observational uncertainty is also shown to systematically reduce the correlation skill by up to 0.2 correlation and beyond. Accounting for the increased verification uncertainty and systematic underestimation of skill should become a future practice in order to fully understand the utility of a seasonal forecasts.

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FIG. 1. a) June observations (solid lines) and seasonal forecast of ECMWF System 4 initialized in 1st May (dashed line shows the ensemble mean, gray lines the individual members) of Niño3.4 sea-surface temperature (SST) anomalies with respect to the climatology of 1992 - 2010. The time-series are shown only for the period where ESA SST CCIs is available. (b) Observational uncertainty (one standard deviation) of SST in the Niño3.4 region for the 1st June 2000.

Observational uncertainty Niño3.4 SST



FIG. 2. Uncertainty propagation to space-time averages as a function of the correlation scales in space (x-axis) 529 and time (different lines) for unit observational uncertainty $\sigma_x=1$. The correlation scales are expressed as degrees 530 of freedom (d.o.f.) by computing the number of times the correlation scale fits in the space-time domain. The 531 propagation is consequently independent of the data spacing and the number of data points. The aspect ratio of 532 the spatial domain impacts the propagation. The mean distance between all possible pair of points in a square is 533 smaller than in a strongly rectangular region as for instance the Niño3.4 region with aspect ratio of region of 1:5. 534 The observational uncertainty therefore decreases stronger in non-rectangular regions as denoted by the different 535 aspect ratios. The standard deviation of the space-time average serves as a propagation factor with which the 536 observational uncertainty provided by the OR has to be multiplied. For example for 5 spatial and temporal d.o.f. 537 the observational uncertainty reduces by a factor of 0.5. Mind the logarithmic scales of the axes. 538



FIG. 3. Observational uncertainty of monthly Niño3.4 SSTs as propagated from SST CCI uncertainty estimates using the approach depicted in figure 2 and length scales associated with small (dashed line) and large (solid line) synoptic scales. The histogram shows the standard deviation between the four ORs in all years of the period 1981-2010 (only three ORs prior to 1992) during the months May - August as a comparison of observational uncertainty inferred from the data itself.

ENSO Prediction (Observational uncertainty)

ENSO Prediction (Sampling Uncertainty)



FIG. 4. Sub-seasonal to seasonal forecast skill of ECMWF S4 (10 members) with respect to SST CCI (dashed line). The areas show the 5-95% percentile range of the bootstrapped (10⁶ samples) uncertainty sources around the sample correlation skill for (a) the uncertainty in the observations assessed using the SST CCI propagated uncertainty ($\lambda = 1000$ km and $\tau = 10$ days) and the ensemble of different ORs and for (b) the sample uncertainty due to a limited ensemble size and record length of the SST CCI dataset. The grey area shows the total uncertainty obtained by resampling all sources at the same time.



FIG. 5. Relative contribution of each source of uncertainty with respect to the sum of all sources. The relative contribution is calculated by the variance of the correlation after resampling one source divided by the sum of variances of all sources (instead of the total uncertainy due to interaction of the individual terms).



Lost skill due to observational uncertainty

FIG. 6. Reduction of correlation skill in ECMWF S4 due to the observational uncertainty for the prediction of the month of August (initialized in 1st of May) estimated using the correction for attenuation (Spearman 1904). The observational uncertainty is estimated by propagating SST CCI uncertainties to monthly means in each grid-point. Grid-points in gray denote areas where the observational uncertainty is larger than the interannual variability of the SST CCI and where as a consequence no correction for attenuation can be calculated.