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Understanding and forecasting polar stratospheric variability with statistical models

C. Blume[1,2,*] **and K. Matthes**[1,2,*]

[1]Helmholtz Centre Potsdam, German Research Centre for Geosciences (GFZ), Potsdam, Germany
[2]Institute for Meteorology, Free University of Berlin (FUB), Berlin, Germany
[*]now at: Helmholtz Centre for Ocean Research Kiel (GEOMAR), Kiel, Germany

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Correspondence to: C. Blume (christian.blume@met.fu-berlin.de)

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Abstract

The variability of the north-polar stratospheric vortex is a prominent aspect of the middle atmosphere. This work investigates a wide class of statistical models with respect to their ability to model geopotential and temperature anomalies, representing variability in the polar stratosphere. Four partly nonstationary, nonlinear models are assessed: linear discriminant analysis (LDA); a cluster method based on finite elements (FEM-VARX); a neural network, namely a multi-layer perceptron (MLP); and support vector regression (SVR). These methods model time series by incorporating all significant external factors simultaneously, including ENSO, QBO, the solar cycle, volcanoes, etc., to then quantify their statistical importance. We show that variability in reanalysis data from 1980 to 2005 is successfully modeled. FEM-VARX and MLP even satisfactorily forecast the period from 2005 to 2011. However, internal variability remains that cannot be statistically forecasted, such as the unexpected major warming in January 2009. Finally, the statistical model with the best generalization performance is used to predict a vortex breakdown in late January, early February 2012.

1 Introduction

The variability of the north-polar stratospheric vortex (Baldwin and Holton, 1988) is a key dynamical feature of the middle atmosphere. Every two years on average it breaks down during winter resulting in a sudden stratospheric warming (Labitzke and Naujokat, 2000) tremendously increasing temperatures within a few days. A large number of these extreme warming events in the stratosphere have been found to propagate downward to the troposphere (Baldwin and Dunkerton, 2001) influencing the weather.

There are external variability factors that influence the dynamics of the polar stratosphere. These factors include, the Quasi-Biennial Oscillation (QBO) (e.g., Baldwin et al., 2001), the El Niño-Southern Oscillation (ENSO) (e.g., Manzini et al., 2006), the 11-year solar cycle (e.g., Gray et al., 2010), and high impact volcanic eruptions

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(Robock, 2000). These external factors (or forcings) also interact with each other, resulting in a complex and nonlinear dynamical response (e.g., Calvo et al., 2009; Richter et al., 2011).

Previous efforts investigated the impact of these factors. Holton and Tan (1980, 1982) showed that the QBO east phase leads to a generally warmer, more disturbed polar vortex and vice versa for QBO west. This so-called Holton-Tan relationship was later shown to be present during solar minimum but significantly weaker during solar maximum (e.g., Labitzke, 1987; Labitzke and van Loon, 1988). They showed that sudden stratospheric warmings are most likely to happen during solar maximum (minimum) and QBO west (east) phase. Accordingly, the work made by Camp and Tung (2007a) found the least-perturbed vortex state to take place during solar minimum and QBO west conditions. Recent studies have shown that positive ENSO phases (El Niño) lead to a more disturbed polar vortex as opposed to negative ENSO phases (La Niña) where the vortex is less disturbed (Camp and Tung, 2007b; Mitchell et al., 2011). The least understood forcing factor are aerosols injected into the stratosphere by very strong but rare volcanic eruptions (Robock, 2000) leading to nonlinear feedbacks with other forcings (e.g., Garfinkel and Hartmann, 2007).

When making polar stratospheric forecasts, general circulation model runs consisting of multiple observation constrained ensemble members are performed. These forecasts are reliable on a daily scale but, on a seasonal scale, they quickly become computationally very expensive and loose their forecast skill (Gerber et al., 2009; Kuroda, 2010). This work investigates statistical models that are mathematically much simpler and demand significantly less computer power, and even though they do not simulate physical processes explicitly, one can learn about underlying relationships. A wide class of statistical models is considered with respect to their ability to model and seasonally forecast geopotential and temperature anomalies representing variability in the polar middle stratosphere from 10 hPa to 30 hPa.

Common statistical methods analyzing polar stratospheric variability are linear (e.g., Camp and Tung, 2007b; Crooks and Gray, 2005) and do not consider more than a few

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atmospheric forcing factors at the same time. In this work, the statistical methods used are partly nonstationary and nonlinear, incorporating all external forcings simultaneously. The statistical models are trained for the time period from 07/01/1980 through 06/31/2005 and used for forecasting for the period from 07/1/2005 to 04/30/2011. The impact of each forcing factor on the statistical response will be quantified. While making reasonable assumptions about the external factors, the statistical model with the best generalization performance is used to predict the winter 2011/12.

2 Data

This work makes use of two reanalysis data sets resolving the stratosphere, available up to 0.1 hPa from 1979 to present. These data sets are the ERA-Interim reanalysis (Simmons et al., 2006) and the MERRA reanalysis (Rienecker et al., 2011), both considered from 7/1/1980 through 6/31/2011. ERA will be used to train the statistical models, and MERRA to validate the final results.

Two daily target geopotential and temperature time series are computed so as to represent the variability in the polar middle stratosphere. Anomalies of the area-weighted average on the polar cap (60° N–90° N) are computed at 10, 20, and 30 hPa. A subsequent principal component analysis (Jolliffe, 2002) of the three time series reveals that the first principal component (P1) explains more than 90 % of the overall variance in both ERA and MERRA. Therefore, only P1 was retained for both geopotential (P1Z) and temperature (P1T). P1Z and P1T are both positive for weak and warm vortex events and negative for strong and cold vortex conditions. A polar cap average of geopotential anomalies is equivalent to the Northern Annual Mode (NAM) (Baldwin and Dunkerton, 2001), only reversed in sign. The NAM is the leading principal component of geopotential anomalies north of 20° N. We decided to use the polar cap method as it is simpler and the resulting time series for geopotential and temperature are positively correlated ($R = 0.8$) (Baldwin and Tompson, 2009), pointing in the same direction during extreme vortex events. P1Z and P1T are physically closely correlated.

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A lead-lag correlation analysis between P1Z and P1T reveals that there is a correlation of approx. 0.7 when lagging P1T with 10 days whereas lagging P1Z leads to only 0.3. Therefore, the temperature anomaly usually appears first and the actual vortex breakdown a few days later. A prominent example of that is the major stratospheric warming in January 2009. In addition, P1T reflects the strong stratospheric cooling (overturning) proceeding most major warmings. For simplicity, P1Z is referred to hereafter as *geopotential* and P1T as *temperature*.

This analysis makes use of nine physical *external factors* which describe large-scale phenomena important for the polar stratosphere. Their purpose on the one hand is to improve model variability, and on the other to obtain insight into relationships and impacts of the various forcings. The factors representing variability in sea surface temperatures (SSTs) are the Nino3.4 index (Trenberth, 1997), the Pacific Decadal Oscillation (PDO) (MacDonald and Case, 2005), and the Atlantic Multidecadal Oscillation (AMO) (Delworth and Mann, 2000). Furthermore, the first two principal components of equatorial stratospheric zonal wind anomalies (QBO1 and QBO2) (Wallace et al., 1993) are included. Factors representing tropospheric high-latitude blockings (Martius et al., 2009; Woollings and Hoskins, 2008) are the first two principal components of geopotential anomalies between 35° N and 85° N at 500 hPa (TROP1 and TROP2). TROP1, as the leading principal component, is equivalent to the NAM in 500 hPa. Moreover, the F10.7 cm radio flux representing solar variability (SFL; ftp://ftp.ngdc.noaa.gov/STP/SOLAR_DATA) and the aerosol optical depth (AOD; http://data.giss.nasa.gov/modelforce/strataer) representing volcanic eruptions are included. Additionally, three baseline factors representing the seasonal cycle (one sine and one cosine with a period of one year) and a linear trend term are included. Since the different external factors have different magnitudes and physical units, they are normalized on the full period from 1980 to 2011, such that the minimum is at −1 and the maximum at +1.

In order to improve regression results, optimal time lags of each of the nine physical external factors were calculated using a lead-lag correlation analysis. Every external

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factor was correlated with geopotential (temperature) for different lags from 0 to 365 days. The largest statistically significant correlation on this period indicates the optimal lag. We obtain zero lags for PDO, TROP1, TROP2, and AOD for both, geopotential and temperature. For Nino3.4 we computed 96 (82) days; for AMO 8 (185) days; for QBO1 173 (137) days; for QBO2 0 (264) days; and for SFL 0 (50) days, for geopotential and temperature, respectively. To reduce short-term fluctuations and extreme values, the daily external factors are sent through a low-pass filter, calculating the 5-day running mean.

3 Statistical models

This work assesses and compares four statistical models with respect to their ability to model geopotential and temperature. These models have been chosen as they make different assumptions about the underlying data. The model intercomparison is similar to that in Blume et al. (2012) but, as opposed to classification, now for regression problems including an additional nonstationary method. A statistical method is nonstationary if its response depends on the event number and, therefore, on time when dealing with time series. The four models are:

1. Linear discriminant analysis (LDA) (Montgomery et al., 2001), also known as multiple linear regression, which is a linear and stationary model. LDA is one of the most common statistical tools to analyze stratospheric variability (e.g., SPARC CCMVal, 2010; Randel et al., 2009; Crooks and Gray, 2005). LDA models data by finding the coefficients to a linear combination of external factors using the method of least-squares. The simplicity and robustness of LDA make it a popular method. LDA does not have free tuning parameters.

2. A cluster method based on finite elements (FEM-VARX) (Horenko, 2010, 2011), which is locally linear in the determined clusters, but nonstationary since the switching process between clusters is time dependent. FEM-VARX models data

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by (a) Finding persistent clusters in the time series given the external factors using a finite element method (FEM); and (b) Linearly modeling the data corresponding to each cluster by incorporating the external factors using a VARX (vector autoregression with external factors) approach. In this work, autoregressive processes are not considered for simplicity so that VARX boils down to a simple linear combination. FEM-VARX has two tuning parameters in this work: The number of clusters K and the persistency threshold C which limits the maximum transitions from a given cluster to any other cluster.

3. The multi-layer perceptron (MLP) (Zhang et al., 1998), a fully-connected, feed-forward neural network which is a stationary but nonlinear model. Approximation and generalization performance of the MLP stem from the nonlinear transfer function (sigmoid) and the numerous connections within the hidden layers (Bishop, 1995). This analysis is restricted to two hidden layers since it was shown that an MLP with two hidden layers and sigmoidal transfer function can approximate any continuous function (Kurkova, 1992). MLP is trained using back-propagation (Avriel, 2003) which iteratively adjusts weights and biases. A weight is given at each synapse (connection between two neurons) and a bias at each neuron. In this work, MLP has two tuning parameters: the number of neurons in the first hidden layer $L_1 > 0$ and the number of neurons in the second hidden layer $L_2 \geq 0$.

4. The support vector regression (SVR) (Basak et al., 2007), which is also stationary but nonlinear. SVR is a support vector machine (Vapnik, 1995) adjusted to solve regression problems. Approximation and generalization performance of a support vector machine stem from the nonlinear kernel that is used to transform the feature space into a higher dimensional space. In this work, the popular radial basis kernel is used. This kernel was shown to be the most efficient while being very simple and including the linear case (Keerthi and Lin, 2003). SVR has two tuning parameters: The scaling parameter γ in the radial basis kernel and the parameter δ controlling the trade-off between approximating the training data and

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generalizing to unseen data.

It is worth noting that LDA and FEM-VARX can in principle also be used in a nonlinear fashion by transforming the external factors with a nonlinear function (e.g., higher order polynomials, cross-products of different factors, etc.) in a first step. However, this has not been done here since the corresponding functions are unknown a priori. The nonlinearity in MLP and SVR stems from the nonlinear transfer function and the nonlinear kernel in MLP and SVR, respectively.

As previously indicated, all models but LDA have free tuning parameters that need to be determined which is then called the model architecture. The optimal model architecture (combination of tuning parameters) aims at meeting the principle of Occam's Razor (Ariew, 1976) stating that the simplest model is the preferred if it contains just as much information as any of the more complicated models. There are two major branches found in the literature of information theory (Burnham and Anderson, 2002) aiming at selecting the optimal model which are information criteria and cross-validation. The approach to be used depends on the statistical method and the specific application.

For FEM-VARX, the optimal architecture was determined with the use of the Akaike information criterion (Akaike, 1974; Horenko, 2011) where the parameter setting leading to the smallest criterion is preferred. For MLP and SVR, a 5-fold cross-validation (Kohavi, 1995) was conducted in which the training data were partitioned into 5 equally-sized contiguous subsets (folds). The model architecture with the largest correlation calculated from the tested subsets has been selected. In the following, the optimal values are given in parentheses, for geopotential and temperature, respectively. For FEM-VARX, K (5, 5) denotes the number of clusters and C (146, 112) the persistency threshold. For MLP, L_1 (8, 3) and L_2 (5, 0) denote the number of neurons in the first and second hidden layer, respectively. For SVR, γ (0.2, 1) denotes the radial scaling parameter and δ (0.3, 0.3) the trade-off parameter.

LDA and SVR only lead to global solutions, whereas FEM-VARX and MLP might run into local minima during training. In order to reduce this effect, a total of 30 models were trained for FEM-VARX and MLP. For FEM-VARX, K is fixed and values of C were

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chosen slightly different from the optimal value. For MLP, those pairs of L_1 and L_2 were chosen that were ranked highest according to the cross-validation. The regression and forecast results are the average across these realizations.

4 Results for training and forecast period

The statistical models are trained with data from the training period (1980–2005) while being set up with optimal model architectures as described above. After being trained, the models are used to forecast the period from 2005 through 2011 ("Hindcasting"), meaning that the models are evaluated with the available external factors from this period. The result of this procedure is presented for geopotential in Fig. 1, where the truth is shown in gray. The correlation coefficient between each model and truth is given in parentheses. The training period is modeled well ($R \approx 0.9$) by all models except LDA ($R \approx 0.3$). FEM-VARX possesses the highest explanatory power over the training period. Please note that all external factors are used in a resolution of a few days. For the forecast period a large drop in correlation is observed for all methods, largest for SVR. Only FEM-VARX ($R = 0.34$) and MLP ($R = 0.42$) lead to satisfactory results on the forecast period. They are able to approximate most anomalies and forecast the general behavior in 5 out of 6 winters. Looking more closely, significant differences between truth and forecast become evident. The most obvious is the sudden stratospheric warming in January 2009. This is a very extraordinary strong warming (Labitzke and Kunze, 2009b) during solar minimum and QBO west which was not expected according to the Solar-QBO relationships by Labitzke and Kunze (2009a) and Camp and Tung (2007a). This is an example of variability that cannot be explained using statistical methods reflecting the chaotic nature of the system.

The temperature results (not shown) are similar to the geopotential results with slightly smaller correlations. For the training period, correlations of 0.25 (LDA), 0.53 (SVR), 0.86 (MLP), and 0.92 (FEM-VARX) are obtained. For the forecast period, correlations of 0.22 (LDA), 0.16 (SVR), 0.25 (MLP), and 0.24 (FEM-VARX) are computed

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for temperature. These correlations, except for SVR, are statistically indistinguishable. However, we still obtain the same ranking of the different models as for geopotential.

It can be seen that it is possible to statistically model and forecast polar stratospheric variability. The MERRA reanalysis is utilized to validate the regression results which leads to very similar results (not shown). We conclude that the ERA results can be considered as robust and trustworthy.

5 Impact of external factors

Next, the statistical importance (or *impact*) of each of the external factors on the statistical models is calculated. The impact I_k is the standard deviation of the difference between model responses so that $I_k = \sigma(Y - Y^{(k)})$, where Y is the original model response and $Y^{(k)}$ is the model response for external factor k held constant at its median. The relative impact is then simply I_k divided by the sum of all impacts for one statistical model. This is shown in Fig. 2 for geopotential and temperature along with a weighted average over all four models. The weights were determined from the correlation coefficients for the training period, meaning that FEM-VARX is given the largest weight and LDA the smallest. It is observed that the impacts of FEM-VARX, MLP, and SVR are very similar, whereas LDA misinterprets the importance of factors, such as the impact of high-latitude blockings (TROP1) on the geopotential or of the solar term (SFL) on the temperature. LDA assumes linear and stationary relationships which is not valid for the polar stratosphere (e.g., Calvo et al., 2009; Richter et al., 2011).

Apart from LDA, the impacts in geopotential and temperature are very similar across the different models. A large impact of the QBO terms and a medium impact of SFL are observed in agreement with e.g., Holton and Tan (1982), Labitzke and Kunze (2009a) and Camp and Tung (2007a). QBO1 is more important than QBO2 for geopotential and vice versa for temperature. The ENSO impact is moderate as also found by Camp and Tung (2007b) and Mitchell et al. (2011). The AMO and PDO impacts are of similar magnitude. There are only two sufficiently powerful volcanic eruptions (El Chichón in

1982 and Mt. Pinatubo in 1991) (Robock, 2000). Therefore, the impact of the aerosol optical depth (AOD) index is very small for this period. It is worth noting that the AOD impacts vary significantly across the four models reflecting a large uncertainty for this forcing. Surprisingly, the two factors representing tropospheric high-latitude blockings (TROP1/2) show a relatively small importance. Especially for the modeling of temperature, they can be most certainly omitted. However, the TROP1 impact on geopotential is of the same order as the SFL impact and need to be accounted for. However, as stressed by Woollings and Hoskins (2008), TROP1 represents high-latitude blockings in both the Atlantic and Pacific sectors and cannot be used as a proxy for all blocking situations. The sine and cosine terms largely influence the model response, which reflects the strong seasonal dependence of the dynamics in the polar stratosphere. The linear trend term was also found to be relatively strong ($\approx 10\%$).

6 The winter 2011/12

MLP performs best over the forecast period (see Fig. 1) and is therefore used to predict the winter 2011/12. As this winter lies in the future, we need to make assumptions about the external factors while taking into account the optimal lags from Section 2. For SST variability along with SFL, we used predictions from the NOAA climate prediction center (http://www.cpc.ncep.noaa.gov). We obtain −0.5 for Nino3.4, 0 for AMO, −0.3 for PDO, and −0.5 for SFL. Please note that the external factors are normalized between −1 and +1 for the period from 1980 to 2011. TROP2 has a very small impact (see Fig. 2) which is why it is set to zero. AOD is held at −1, as future volcanic eruptions that might affect the stratosphere are unknown. The trend term is held at one (its value in 2011), as an approximate value for the extension of only one winter. We selected 0.8 for QBO1 and 0 for QBO2 by extending the corresponding oscillations with a period of 28 months.

Figure 3 shows the resulting MLP forecast for the winter 2011/12 by only varying the sine and cosine terms, for geopotential and temperature and for three different

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conditions of TROP1. A value of −1 represents extremely pronounced high-latitude blocking situations (Woollings and Hoskins, 2008), whereas +1 represents no high-latitude blockings at all. For moderate values of TROP1, the synoptic situation remains unclear and regional blocking situations may still occur. It is shown in Fig. 3 that the geopotential forecast changes significantly with varying TROP1. However, for minimum and average TROP1 conditions, the geopotential forecast is well above one standard deviation. This also holds for the temperature forecast, which is almost unaffected by TROP1 changes, indicating the small statistical importance of TROP1 on the temperature response (see Fig. 2). To summarize, both forecasts tend to be positive and well above one sigma, indicating a warm stratospheric winter with a weak stratospheric vortex. Since the anomalies in Fig. 3 are quite large, a sudden stratospheric warming is likely to take place in late January, early February 2012. The temperature anomaly leads and is proceeded by the geopotential anomaly.

The winter 2011/12 will most probably coincide with a westerly QBO in 50 hPa and weak solar activity (NOAA). Hence, our finding contrasts the Solar-QBO relationship found by Labitzke and Kunze (2009a), which predicts a cold and undisturbed polar stratosphere under these conditions. Correspondingly, Camp and Tung (2007a) found that solar minimum conditions and a westerly QBO point to the least disturbed vortex state. Moreover, work made by e.g., Camp and Tung (2007b) and Mitchell et al. (2011) indicates that a warm and disturbed polar stratosphere is more likely to take place during warm ENSO phases (El Niño) than during cold ENSO phases (La Niña). This is also in contrast to our forecast, since the Nino3.4 index is most likely to be moderately negative for the winter 2011/12 according to the NOAA predictions. However, since the impacts of the individual external factors do not add up linearly, a nonlinear statistical method is certainly more appropriate. Our analysis, in addition to being nonlinear, incorporates all the significant external factors simultaneously.

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7 Conclusions

We have presented a novel statistical treatment of variabilities in the polar middle stratosphere, making use of four independent and different statistical models. For the first time, partly nonstationary and nonlinear statistical methods were trained with polar stratospheric geopotential and temperature anomalies incorporating all significant external factors simultaneously. It was shown that, with the help of external factors, FEM-VARX and MLP are able to model and satisfactorily forecast the variabilities. However, a degree of internal chaotic variability, seen e.g. in the sudden stratospheric warming of January 2009, remains that cannot be forecasted using statistical models.

The statistical impact of each of the external factors on the statistical models was computed. It was shown that the QBO factors, the seasonal terms, and the trend term show the greatest impact. The solar cycle and the SST variabilities have a medium impact along with high-latitude large-scale blockings (TROP1). Volcanic eruptions (AOD) only point to a small but more uncertain statistical importance. It was observed that relative impacts of external factors are very similar for FEM-VARX, MLP, and SVR, whereas those of LDA differ significantly from the model-averaged impact.

The multi-layer perceptron (MLP) showed the best generalization performance. Hence, it was used to predict the winter 2011/12 under reasonable assumptions about the external factors. It predicts a disturbed and warm polar stratosphere, with a sudden stratospheric warming likely to take place during late January, early February 2012. This is in contrast to previous studies which expect a cold and less disturbed polar stratosphere given the same external factors (weak solar, QBO west, La Niña). However, standard analysis is based on linear models and does not consider more than a few external factors at the same time. Our prediction is based on a nonlinear statistical method incorporating all significant external factors simultaneously.

There are several improvements that could be made to this analysis. There may exist other currently unknown external factors to improve the statistical modeling of polar stratospheric variability. Instead of a linear lag correlation analysis, the lags should

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be computed separately for each statistical model, with a grid search technique using cross-validation or information criteria. Unfortunately, these lag calculations would be computationally extremely expensive. It will also be interesting to decrease the temporal resolution of the considered time series to see if the modeling improves. Additionally, we will further investigate the nonlinear interrelationships between external factors using the introduced methods.

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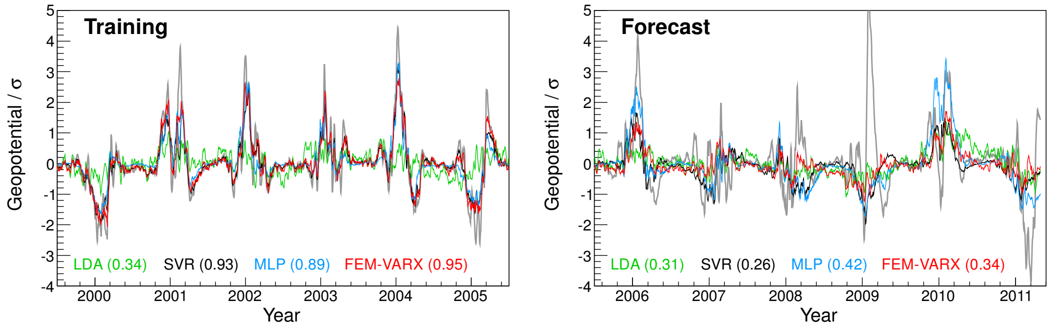

Fig. 1. Geopotential results for the training period (left) and the forecast period (right) for each of the statistical models together with the correlation coefficient *R* (in parentheses) calculated between the particular model and truth (gray). The forecast is shown for the full forecast period whereas the training results are only shown for a representative period (last six years). Labeled is the first of January of the particular year. The 95 % confidence interval of the correlation factors are ±0.02 for the training and ±0.04 for the forecast period.

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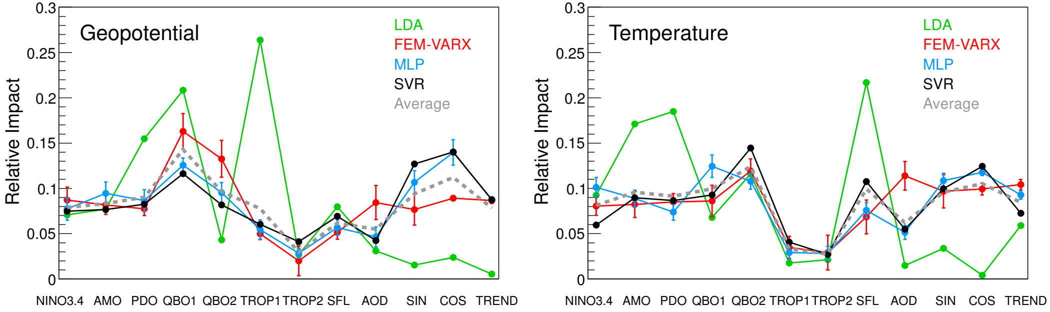

Fig. 2. Relative impact of the external factors on each of the statistical models for geopotential (left) and temperature (right). The average impact (gray) is calculated as a weighted mean over the different models where the weights are calculated from the correlation coefficients (see left panel of Fig. 1) on the training period. The impacts are presented for ENSO (NINO3.4), the Atlantic Multidecadal Oscillation (AMO), the Pacific Decadal Oscillation (PDO), the Quasi-Biennial Oscillation (QBO1, QBO2), high-latitude blockings (TROP1, TROP2), the solar signal (SFL), volcanoes (AOD), seasonal dependency (SIN, COS), and a linear trend (TREND).

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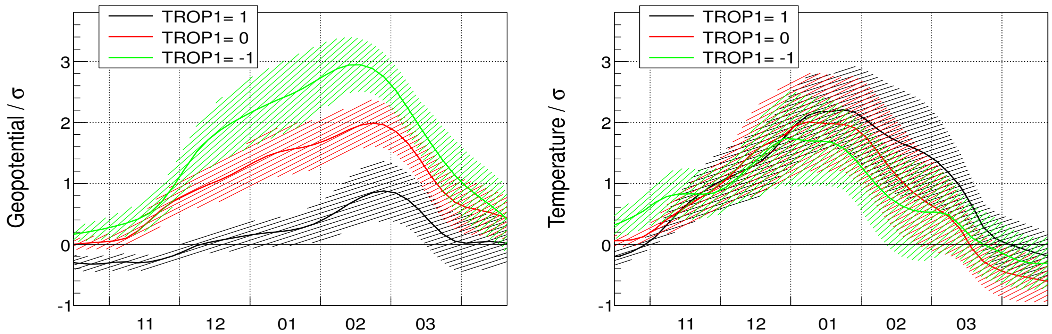

Fig. 3. MLP forecast for the winter 2011/12, holding the external factors constant and varying only the sine and cosine terms. The assumptions about the external factors are partly received from predictions made by the NOAA and partly from scientific reasoning (see text). The forecast is shown for geopotential (left) and temperature (right) for three different conditions of TROP1 (high-latitude blockings). The hatched area denotes the 95% confidence interval calculated from the 30 model realizations. Please note the additional uncertainty imposed by the only moderate hindcasting performance (see right panel of Fig. 1).

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