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Causal discovery of drivers of surface ozone variability in Antarctica using a deep learning algorithm

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Abstract

The discovery of causal structures behind a phenomenon under investigation has been at the heart of scientific inquiry since the beginning. Randomized control trials, the gold standard for causal analysis, may not always be feasible, such as in the domain of climate sciences. In the absence of interventional data, we are forced to depend only on observational data. This study demonstrates the application of one such causal discovery algorithm using a neural network for identifying the drivers of surface ozone variability in Antarctica. The analyses reveal the overarching influence of the stratosphere on the surface ozone variability in Antarctica, buttressed by the southern annular mode and tropospheric wave forcing in mid-latitudes. We find no significant and robust evidence for the influence of tropical teleconnection on the ground-level ozone in Antarctica. As the field of atmospheric science is now replete with a massive stock of observational data, both satellite and ground-based, this tool for automated causal structure discovery might prove to be invaluable for scientific investigation and flawless decision making.

Introduction

Ubiquitous throughout the troposphere and stratosphere, ozone plays a significant role in atmospheric radiative forcing, atmospheric chemistry, and air quality. Considered an atmospheric cleanser, Ozone in the stratosphere (90% of total amount) saves life on Earth by filtering harmful UV radiation. Stratospheric ozone throughout the globe has been on a downward trend, as indicated by the analysis of both satellite and ground-based measurements of total column ozone (TCO) due to a steady increase in anthropogenic emissions of the reactive chlorofluorocarbons (CFCs). However, the stratospheric ozone hole is on a recovery path in response to the Montreal Protocol and its subsequent amendments. Nonetheless, the precise causes of the observed changes in stratospheric ozone are complicated to isolate. They remain uncertain due to the inability of existing chemistry-climate models (CCMs) to reproduce the observations.
In contrast, tropospheric ozone is a prominent air pollutant and greenhouse gas despite being only 10% of the total column amount. The accurate assessment of tropospheric ozone trends is far more challenging due to the complicated interplay of many simultaneous processes with significant temporal and spatial variations. Ground-level ozone concentration at a given location is affected by photochemical reactions, atmospheric transport, atmospheric diffusion, topography, and emission sources of the primary pollutants [such as nitrogen oxides (NO$_x$) and non-methane volatile organic compounds (NMVOCs)]. The inter-annual variability of ozone concentration is governed by changes in emission of photochemical precursors, various favorable/unfavorable weather conditions, or a combined effect of all these. Favorable meteorological conditions for high ozone episodes include high temperature, intense sunlight, and light wind. On the other hand, dry deposition, dissolution into the seawater, and photolysis reactions involving nitrogen oxides (NOx) are the most prominent sinks of tropospheric ozone.

A variety of methods has been applied to date for the analysis of ground-level ozone that ranges from simple statistical models like multiple linear regression (MLR) to sophisticated chemistry-climate models (CCMs) such as GEOS-Chem. However, these models face difficulty in dealing with complicated cause-effect relationships among meteorology and air pollutants. Multiple regression models are limited in their interpretability as these are based on cross-correlation, which might be highly biased due to autocorrelation effects or spurious correlations arising from an unaccounted third process or a common driver. Apart from these, they lack insights into the directionality of relationships. Therefore, CCMs are used to investigate the impact of changes in emissions and meteorology using controlled perturbation of the system, allowing interpretation of simulation results as causal effects forced by the interventions. Nonetheless, the ability of CCMs in resolving essential processes such as land–biosphere interactions, stratosphere-troposphere transport (STT), and detailed atmospheric dynamics remain questionable, restricting their interpretability and conclusions.

Causality is a fundamental scientific notion and is indispensable for accurate forecasting, flawless explanation, and decision making. Discovering causal relations from observational data has drawn much attention recently as the traditional way of causal analysis using interventions or randomized control trials might be impractical, infeasible, or outright unethical. For example, causal discovery methods relying solely on observational data have been used recently to study
ocean-atmosphere interactions,⁸ the Walker circulation,⁹ and the mid-latitude winter circulation in the northern hemisphere.⁷ With methodologies based on conditional independence tests, heuristic scoring, or deep learning, we can identify causal linkages in observational data using the premise that causes temporally precede their effects in time series. In this paper, we use one such causal model based on a deep neural network to discover the potential drivers of surface ozone variability over Antarctica. This method overcomes the pitfalls of common statistical approaches, i.e., spurious correlations arising from the presence of common drivers, autocorrelation, or indirect effects using a carefully designed causal discovery algorithm.

Results

Fig. 1 shows the daily time series of surface ozone measurements at all five stations considered in this study, i.e., Arrival Heights, Marambio, Neumayer, South Pole, and Syowa. As shown in the figure, surface ozone has a marked seasonal cycle with the highest concentration during winter (June-July-August; JJA) and the lowest during summer (December-January-February; DJF); consistent with the remoteness of the Antarctic continent. However, there are a few noticeable differences in surface ozone seasonal cycle among various stations. There is a clear secondary peak (up to 50 ppbv) during spring (September-October-November; SON) at South Pole station recurring every year and have concentrations equivalent or higher than those during the primary peak (JJA). In contrast, secondary peaks at all other stations are sporadic and rarely exceed those during the primary peak. The occurrence of the secondary peak in Antarctica has been attributed to enhancement episodes due to NOₓ emission from snowpack¹³ and photolysis of remote PAN formed above continental source regions upon descent within the Antarctic region.³⁰ Notwithstanding, these peaks might also result from the transport of photochemically produced ozone in the planetary boundary layer (PBL) over the Antarctic plateau to other parts of Antarctica due to katabatic flow prevalent apart from the direct transport of airmass from UTLS enriched in ozone.

We identify the ozone enhancement events [OEE] at all stations included in this study using the methodology adopted by Cristofanelli et al. 2018.³¹ OEEs identified at all stations in Antarctica are shown in Fig. 1 in magenta color. To identify the OEE, we first fit an annual sinusoidal curve (green curve in the top panel of Fig. 1) to the daily surface ozone dataset, followed by estimation
of gaussian PDF of residual (grey curve in the top panel of Fig. 1) from sinusoidal fit. We fit another Gaussian distribution to all points lying beyond one $\sigma$ of the last PDF. The intersection of these two PDFs (vertical dash line in the bottom panel of Fig. 1) shows the threshold value for an OEE event. Analyses suggest that OEEs primarily occur during late spring and early summer (November-December-January) at all stations with the highest frequency during December month at the South Pole (up to 80%) and November month at coastal stations (60%, 70%, and 65% at Arrival Heights, Neumayer, and Syowa respectively) as shown in Fig. S1. On an annual basis, OEE frequency ranges from 2% at Arrival Heights to 25% at the South Pole. OEE frequency has been increasing at South Pole, Arrival Heights, and Neumayer since 1990, whereas it has been decreasing at Syowa.

**Potential drivers of ozone variability**

Several studies have attributed the changes in surface ozone to short-range and long-range air mass transport and stratosphere-troposphere exchange (STE). Atmospheric waves propagating from the troposphere to the stratosphere control the variation in STE, which is in turn modulated by the meridional circulation driven by momentum imparted by the waves. Fig. 2 (top panel) shows the time series of inter-annual variation in STT at all five stations in Antarctica. As shown, STT contributes up to ~15% of the airmass transport at surface level in Antarctica, with a considerable variation across different stations. STT is the highest during March (Autumn) at all stations. There is enhanced STT contribution during the summer and autumn seasons as compared to winter and spring. The South Pole receives the highest proportion of air mass transport from the stratosphere as it is situated on the Antarctic Plateau, and Marambio receives the least. Arrival Heights receives the highest amount of STT among coastal stations due to the influence of katabatic winds blowing from the high-altitude plateau region, consistent with previous studies. As shown in Fig. 2, the contribution of STT increased during 1980–2000 and is decreasing since then.

We now investigate the influence of descending air mass transport from the UTLS on OEE variability in Antarctica. Fig. 2 (b and c) shows the interannual variation in the frequency of OEEs during the spring and summer seasons (the seasons with the highest number of OEEs in a year). The frequency of OEEs during these two seasons had an increasing trend during the 1990s. However, this increasing trend has been disrupted during recent years and has turned to
decreasing trend during summer. Fig. 2 (d and e) shows the interannual variation in the
frequency of the fraction of 15 days back-trajectories coming from the upper troposphere
corresponding to OEEs. It shows a high contribution (40–100% of OEEs) of air mass coming
from the upper troposphere (with pressure less than 500 hPa). Downward transport to the lower
troposphere from UTLS is driven by residual mean flow due to Rossby wave forcing on the
poleward side of the jet stream, facilitating a secondary circulation from the vortex edge to the
inner vortex observed over the South Pole and Arrival Heights. 37,38

A close analysis of OEEs during summer suggests the evident influence of southern annular
mode (SAM) on the occurrence of OEEs, as shown in Fig. 2 (c). The frequency of OEEs across
all stations in Antarctica seems to follow the variation in the SAM index. After 1997, there is a
clear increasing trend in OEEs during the period in which the SAM index has been decreasing
and vice-versa. We estimate the $R^2$ between SAM index and OEEs during 1997–2015 summer
across all stations. OEEs at Marambio, South Pole, and Arrival Heights have very strong
influence from SAM. It explains ~93%, ~68%, and ~61% of OEEs variance at these stations,
respectively. Similarly, it explains ~27% and ~20% of OEEs variance at Neumayer and Syowa,
respectively. SAM drives changes in mid-latitude jet, which modulates the lower tropospheric
circulation, causing variations in surface ozone concentration. As the variation in SAM and
southern mid-latitude jet position has been previously shown to be driven by stratospheric ozone
hole in Antarctica, 4 it demonstrates the clear impact of the stratospheric ozone hole and
stratosphere-troposphere coupling on summertime OEE variation. This pattern in OEE variation
is consistent with previous studies wherein stratospheric cooling associated with ozone loss in
the stratosphere and increasing greenhouse gases were found to shift the tropopause altitude and
transport ozone to the troposphere with a lag of about a month. 39,40 As the polar vortex
strengthened due to increased ozone loss in the stratosphere and global warming, it caused
enhanced transport from UTLS to the lower troposphere resulting in an increase in the frequency
of occurrence of OEEs.

Furthermore, atmospheric transport over the Antarctic continent is controlled by several
synoptic-scale pressure patterns. For example, Amundsen–Bellingshausen Seas low (ABSL) has
substantial control over the tropospheric circulation in the Ross Sea region. 37 Similarly, lows
over the drake passage, Amundsen, Bellingshausen, Weddell Seas, and the ridge over the
peninsular region drive the air transport over the Antarctic Peninsula. These are influenced by
SAM and El Niño and southern oscillation (ENSO) in turn.\textsuperscript{41} Moreover, meridional circulation is
also influenced by ENSO and Quasi-biennial oscillation (QBO). It can make substantial
contributions to the transport of ozone from the stratosphere to the troposphere. Therefore, we
include different factors that are known to control ozone variability in the troposphere,\textsuperscript{42,43} i.e.,
solar flux (SF) at 10.7 cm wavelength, heat flux (HF) at 200 hPa (averaged over 45°–75°S)
accounting for the changes in meridional circulation, potential vorticity (PV) at 200 hPa
accounting for variation in the strength of polar vortex and STT, and aerosol optical depth
(AOD) at 550 nm (averaged over 45°–75°S) which represents aerosol loading in the atmosphere
and volcanic eruptions in addition to the SAM index, multivariate ENSO index (MEI) and the
equatorial winds at 30 and 50 hPa which represent QBO.

Table S2 shows the maximum cross-correlation of selected proxies with surface ozone at various
stations. As is clear from the table, the selected proxies are highly correlated with surface ozone
and thus should be able to explain the surface ozone variability. The MLR fit with these proxies
at all stations is performed to find out the usefulness of selected proxies for explaining the
surface ozone variability and are shown in Fig. 3 (without seasonal harmonics) and Fig. S2 (with
seasonal harmonics). MLR suggests that selected variables can explain the variations in the
surface ozone reasonably well (with $R^2_{adj}$ ranging from 0.9 in the case of the South Pole to 0.96
for Neumayer and Syowa).

The LASSO fit for surface ozone at Neumayer is shown in Fig. S5, and they show a good fit
with $R^2$ of 0.58 at Neumayer. The estimated regression coefficients for all proxies suggest that
PV, HF, AAO, SF, and MEI are the only important factors for explaining the surface ozone
variability, with PV being the most crucial factor accounting for the majority of variations. While
LASSO regression allows discovering active variables, it does not deal well with the strong
inter-dependencies due to the spatio-temporal nature of the variables. Multiple regression models
based on cross correlation (both MLR and LASSO) can be strongly biased by autocorrelation
effects, indirect linkages via a third process, or a shared driver leading to noncausal, false
correlations that restrict their interpretability. Furthermore, it does not provide any information
on the direction of the link, making it inadequate for studying causal effects.
Causal Discovery of the drivers

Having identified the inadequacies of MLR and LASSO, we now apply our proposed TCDF framework to identify the causal drivers of surface variability and compare it with the same done using causal effect network (CEN) analysis using PCMCI. Herein, we examine whether the surface ozone variability is driven by stratospheric variability and teleconnections with various climate modes such as ENSO, QBO, and AAO. The usage of TCDF for surface ozone at Neumayer station is illustrated in Fig. S6. In brief, TCDF tries to identify the causal drivers of surface ozone variability by regressing it with the included proxies (shown in Fig. S6 left column) using attention based 1-D Temporal CNN. The identified potential drivers are then subject to further validation by using PIVM to identify the true causes. Then a causal network graph is generated, as shown in Fig. S6 right panel.

Discovered causal relationships for all four stations are shown in Fig. 4. Our analyses suggest that surface ozone is influenced by changes in stratosphere and Brewer-Dobson circulation through changes in PV at 200 hPa. Although, no indication of dependence of surface ozone on tropical teleconnections is found. SAM has significant control over the surface ozone at all four stations. Similarly, we do not find any influence of the solar cycle on surface ozone variability. To confirm the discovery made by TCDF, we fit another MLR on surface ozone using the discovered causal drivers only, and the MLR fit for the same is shown in Fig. S3. It clearly shows that we can achieve the same fit (shown by $R^2$) as done before without using other non-causal variables, suggesting the irrelevance of using non-causal variables in explaining ozone variability. We tried another MLR analysis (Figure S4) using non-casual variables, and it shows a considerable reduction in $R^2$.

Having discovered the causal parents of surface ozone, we now estimate their causal effect on surface ozone variability by calculating their average causal effect (ACE) on surface ozone at all stations. ACE consists of both direct and indirect effects of causes on surface ozone. ACE has been estimated using gAIPW in the framework of the potential outcomes, and are shown in Table 1. The ACE can be interpreted as the changes in surface ozone with the corresponding change of 1 standard deviation (sd) in the geophysical driver under investigation. PV (0.58–0.93) and HF (0.12–0.24) have a positive relationship with surface ozone at all stations included in this
study. In contrast, AAO (0.13–0.32) and AOD (2.51–3.75) have a negative impact on surface ozone in Antarctica.

To validate the causal relationships discovered by TCDF, we perform another causal discovery using causal effect network (CEN) analysis with a different algorithm. CEN uses PCMCI to detect causal relationships by forming networks between variables under consideration at different time lags. It evaluates the partial correlation between different combinations of variables iteratively conditioning for other variables and their parents. Those found significant even after accounting for other variables are retained. The identified causal links (at 95% confidence interval) for surface ozone variability at different stations are shown in Fig. 5. Here, a significant positive causal relation is shown with a red arrow, whereas the blue arrows show a negative correlation. Links without the arrows show a strong correlation, but the causal relationship cannot be determined with the given information because of coarser sampling. In contrast to TCDF, the CEN analyses reveal that all tested geophysical drivers are causally correlated with surface ozone at 95% confidence interval either directly or indirectly but at different time lags. The discovered relationships are consistent across the stations except for solar flux, which has a significant negative causal relationship with surface ozone only at Neumayer.

Discussion

This study uses PCMCI and a deep learning-based causal discovery framework, TCDF, to diagnose the causal drivers of surface ozone variability in Antarctica. Causal effects of discovered drivers using TCDF have been estimated using a doubly robust estimator based on the potential outcome framework. Our analyses indicate that the surface ozone variability at all four Antarctic stations is driven primarily by stratospheric variability (PV and HF at 200 hPa). The surface ozone is bereaved of teleconnections with tropical climate variabilities such as ENSO and QBO, although a strong influence with AAO is found. Similarly, the solar cycle does not seem to have any influence over the surface ozone variabilities. The relationship of PV with surface ozone is confounded by HF, or PV mediates the influence of HF on surface ozone. Likewise, the relationship of AOD with ground-level ozone is confounded by AAO. The causal
The stratospheric control of surface ozone variabilities in Antarctica mediated by the heat flux in the UTLS region is consistent with our understanding of the influence of stratospheric variability inside polar vortex over the surface climate, which in turn affect the surface ozone variations. For example, Boljka et al. found that a weakened tropospheric zonal flow tends to be preceded by stratospheric warmings forced by tropospheric wave sources (both near the tropopause and the surface), which in turn might drive the surface ozone variability. Similarly, Wang et al. 2021 reported a robust association between Antarctic sea ice and stratospheric polar vortex variability in both observations and model simulations, mediated by Amundsen Sea low and surface winds changes. Among the climate modes considered, only AAO seems to have a significant impact on surface ozone. Our analyses reveal the coupling between ENSO, AAO, and QBO, consistent with previous studies, where a similar interaction between ENSO, AAO, and QBO is observed. For example, Pohl et al. and Carvalho et al. suggest that El Niño corresponds to negative AAO phase, as observed in both TCDF and CEN analyses at the South Pole, whereas Taguchi et al. present the evidence of co-variation of QBO and ENSO.

Our results are consistent with Lu et al., wherein they analysed the tropospheric ozone variability in the southern hemisphere (SH) using GEOS-Chem. They reported the poleward expansion of the SH Hadley circulation (SHHC) to be responsible for the tropospheric ozone increase. As shown by various studies, poleward expansion of SHHC is synonymous with the increasing trend in AAO as the AAO confounds the latitudinal position, width, and strength of mid-latitude jet.

While the causal graphs generated by TCDF are sparse and interpretable, they are not entirely devoid of modeling errors and require domain knowledge to identify discrepancies. For example, the interactions among ENSO, AAO, and QBO vary across different stations as analysed using TCDF. In contrast, they are same across all stations as analysed using PCMCI. These caveats might be handled better using a more advanced causal discovery algorithm that leverages shared dynamics across different causal graphs and robustly deals with hidden confounders to discover causal links from time-series data like Amortized Causal Discovery.
In summary, we perform the causal analysis of surface ozone variability in Antarctica using a state-of-the-art causal discovery framework based on a deep temporal convolutional network. This framework avoids the drawbacks of common multivariate regression methods and generates a causal graph that is sparse and interpretable. The generated causal graphs were found to be consistent with the existing knowledge. With exponential growth in the amount of observational data from both satellite and ground-based measurements, causal discovery methods might provide novel insights across various domains of atmospheric and climate sciences, which can aid knowledge discovery and guide robust policymaking.

Methods

Data

In this study, ground-based surface ozone measurements from 5 Antarctic stations, namely Arrival Heights, Marambio, Neumayer, South Pole, and Syowa, are used (see Table S1 for details). While surface ozone measurements at Arrival Heights and Syowa start from 1997, those at the South Pole and Neumayer start much earlier. However, there was an instrument change at Neumayer during 1992, which produced a marked difference in surface ozone measurements. Therefore, we have taken 1993 as the starting year for this study. Surface ozone measurements at different stations have data gaps, i.e., the South Pole measurements have gaps during September–December 2016 and August–December 2017. Similarly, Arrival Heights station data has missing data during October–December 2016 and December 2017. Henceforth, we have used monthly surface ozone during 1997-2015 for causal discovery to circumvent the data gaps. As the measurements at Marambio started late, we do not consider Marambio measurements for causal discovery and inference.

Estimation of stratosphere-troposphere transport

We use a lagrangian transport model HySPLIT using meteorological data from National Center for Environmental Prediction (NCEP) (2.5° latitude-longitude grids) and Global Data Assimilation System (GDAS) (1° latitude-longitude grids) to generate 15 days backward trajectories on a daily basis at 500m above the ground level [agl]. Both meteorological datasets
have been used widely in several studies concerned with the airmass transport in Antarctica. They can capture the meteorological variability in the Antarctic region reasonably well.\textsuperscript{10-13}

Generated backward trajectories have been discretized to $1^\circ \times 1^\circ$ latitude-longitude grids. After that, we use NCEP tropopause data to identify the trajectories coming from the stratosphere. Any trajectory with endpoints with corresponding pressure lower than the associated grid tropopause pressure is marked as being influenced by stratospheric transport and is counted over each month to estimate the monthly frequency of stratosphere-troposphere transport (STT).

**Causal Discovery**

The goal of causal discovery is to uncover causal relationships using observational data. Before finding causal relationships between distinct combinations of drivers at different time delays, causal discovery methods must overcome numerous hurdles provided by the causative process or the sampling process generating observational data. Because the cause typically occurs before the effect, utilising the concept of time aids in the determination of the directionality of a causal link. Causal links are the relationships found to be significant even after accounting for the influences of other drivers (observed or hidden) or auto-correlations.

**Granger Causality**

Testing time-lagged causal connections in the framework of Granger causality (GC) is a popular method to causal discovery. A widely used approach to identify the drivers of atmospheric ozone variability utilizing a linear GC framework is to use an autoregressive regression model.\textsuperscript{14-17} The generalized regression models (e.g. MLR) assume a linear relationship between the quantity under investigation and selected exogenous quantities (predictors). Mathematically, one such MLR model for surface ozone variability in Antarctica can be represented as follows:

$$Y_t = c + x_t + \sum_{n=1}^{4} (a_n \cos(n\omega t) + b_n \sin(n\omega t)) + \sum_i q_i F_i + \epsilon_t \quad (1)$$

where $\omega = 2\pi/12$ for surface ozone observations sampled monthly.

This MLR model has the following components: a constant mean level (represented by regression coefficient $c$) and a linear trend ($x$), seasonal effects ($a_n$ and $b_n$), components to describe the influence of external forcings ($F$), and noise ($\epsilon$) with autoregressive correlation. It
includes an autoregressive noise factor to account for irregular cycles, long-range dependencies, and the impacts of various driving mechanisms that a model overlooks. The parameters of the model are estimated by performing least-square minimization.\textsuperscript{18}

If the predictor variables are highly correlated, multicollinearity can become a problem during MLR fitting, causing the coefficient estimates of the model to be unreliable and have high variance. The least absolute shrinkage and selection operator (LASSO) regression overcomes this issue by adding a penalty term to the traditional MLR model objective. It produces a sparse model with only a subset of the input predictor variables, enhancing the prediction accuracy and interpretability of the resulting statistical model.\textsuperscript{19} Mathematically, the minimization objective of a LASSO model, i.e., penalized residual sum of squares (PRSS), can be represented as follows:

\begin{equation}
PRSS(\beta) = MLR_{obj} + \lambda \sum_i |\beta_i| \quad (2)
\end{equation}

where $\beta_i$ represents regression coefficients, i.e., a, b, and q in MLR and $\lambda$ represents the lasso penalty ($\lambda \geq 0$).

**Pearl Causality**

Linear Granger causal methods like lasso regression can only identify causal relationships with observed data. In practise, however, not all key parameters may be observed, and GC is unable to appropriately deal with unmeasured time series, including hidden confounders. Low detection power of linear GCs can be accentuated using a constraint-based approach that uses a series of independence tests to identify causal links, including hidden confounders. PCMCI is one such method, the most widely used causal discovery algorithm in climate sciences.\textsuperscript{7,20–23} The PCMCI algorithm (working within the premises of Pearl causality (PC)) consists of two steps:

1. Identification of parents of each driver using Peter Spirtes and Clark Glymour (PC)-algorithm based condition selection which performs iterative conditional independence test by calculating the partial correlation between two time series conditioning on other available time-series at different lags.
2. Evaluation of the significance of causal links by determining p-values using momentum conditional independence (MCI) test followed by calculating the strength of causal links using MLR.

PCMCI algorithm has two free parameters, which have to be chosen by the user: maximum time delay ($\tau_{\text{max}}$) and significance threshold ($\alpha$). Further details about the PCMCI can be found in Runge et al. 2015.\textsuperscript{24}

**Temporal Causal Discovery Framework (TCDF)**

Despite the high detection power of PCMCI, it cannot detect the contemporaneous links and is suited for assessing linear relationships only. In addition, it requires constraining pre-conditions rarely satisfied in climate sciences like stationarity. However, several novel causal discovery methods have been proposed recently circumventing these requirements. For example, Neural Additive Vector Autoregression (NAVAR) extends the popular Vector Autoregression (VAR) of GC framework to nonlinear additive relationships modeling\textsuperscript{25} and uses a deep neural network (DNN) to do the same. Tank et al. 2021\textsuperscript{26} extended the LASSO regression in order to perform non-linear causal discovery with the help of a neural network based on Multi-layer perceptron (MLP) and Long-short term memory (LSTM) using convex group-lasso penalties. However, these methods based on GC and PC framework struggle with the presence of hidden confounders.

Nauta et al. 2019\textsuperscript{27} proposed a novel causal discovery framework called Temporal Causal Discovery Framework (TCDF), which uses attention-based temporal convolutional networks (TCNs) for identifying non-causal links, including the hidden confounders. TCDF performs the causal discovery in three stages:

1. **Identification of potential causes:** TCDF uses multiple one-dimensional convolutional networks (CNNs) called Attention-based Dilated Depth-wise Separable Temporal Convolutional Networks (AD-DSTCNs) to identify the potential causes. Herein, multiple layers of TCN control the allowable temporal lags among input time series.

2. **Causal Validation and Delay Discovery:** Discovered potential causes in the first stage are validated using Permutation Importance Validation Method (PIVM), i.e., original time
series is intervened by random permutation, and the resulting loss is compared with the loss estimated using original time series to isolate the true causes.

3. **Construction of causal graph:** Finally, TCDF interprets the internal parameters of TCNs and summarises the discovered causal linkages between input time series and relevant time delays by constructing a causal graph.

TCDF has a few hyperparameters such as the number of epochs, number of hidden layers, kernel size, dilation coefficient, loss function, significance level for intervention loss, and learning rate.

Here, we perform the causal discovery using TCDF due to its simplicity and the ability to deal with the hidden confounders. Our causal discovery method utilizing the TCDF framework is different from that of Nauta et al. 2019\(^\text{27}\) in the sense that the algorithm is not constrained to look for the cutoff attention score (\(τ_j\)) in the first half during the attention interpretation stage as it would restrict the number of potential causes to just half of all time series included in the study. Discovered causal graphs from TCDF are compared with the same derived using PCMCI to ascertain its robustness. We have also performed the MLR and lasso regression to identify the inadequacies of these traditional statistical techniques for causal discovery.

We include various proxies (\(F_i\)) representing exogenous processes that drive the changes in surface ozone in Antarctica. As surface ozone has substantial seasonal variability, we include regression parameters expressed by a cosine and sine harmonic expansion utilising four harmonics, i.e., 12 months (\(n = 1\)), 6 months (\(n = 2\)), 4 months (\(n = 3\)), and 3 months (\(n = 4\)) in eq. 1. All data are rescaled to [-0.5, 0.5] before use for modeling. Since we are interested in determining the drivers of surface ozone variability, we also estimate the adjusted coefficients of determination (\(R^2_{adj}\)) for MLR as it gives a measure of improvement in model fit when a parameter is added to the model.\(^{17}\)

We test for the stationarity of our datasets using Kwiatkowski–Phillips–Schmidt–Shin (KPSS) test and Augmented Dickey-Fuller (ADF) unit root test before performing causal discovery using PCMCI and stationarise the dataset by first order differencing as required. We take six months as \(τ_{max}\) to account for tropical teleconnections to the polar region, and \(α\) is taken as 0.05.
Estimation of causal effects

We estimate the average causal effect (ACE) following the framework of potential outcomes. The causal effect is defined as the difference between two potential outcomes. Here, the first potential outcome concerns the treatment group and the other with the intervention or control group.\(^9\) Analytically, ACE is defined as:

\[
ACE(x_1, x_2) = E[Y|do(X = x_1)] - E[Y|do(X = x_2)] \quad (3)
\]

where \(do(X = x)\) represents an intervention that sets \(X\) to \(x\).

As both potential outcomes cannot be observed simultaneously, the strong ignorability assumption is required to identify causal effects. Since the causal graph must be known (existence and absence of links) for causal effect estimation, we use the causal graphs discovered using TCDF in this study. Assuming the relationships to be linear with no interactions, the dependence of \(Y\) on \(X\) and confounders \(C\) can be expressed mathematically as:

\[
E[Y|do(X = x), C = c] = \alpha X + \beta C + \gamma \quad (4)
\]

Here, we use a doubly robust nonparametric estimator based on the theory of influence functions called generalized augmented inverse probability weighted (gAIPW) estimator.\(^{28,29}\) We present ACE along with its 95% confidence interval estimated using 500 bootstrap samples.

Data availability

The surface ozone data are available from GAW-WDCRG (http://ebas.nilu.no). The data for solar flux, MEI and AAO index are taken from (www.esrl.noaa.gov/psd/data/climateindices/list/). QBO data is taken from (https://www.geo.fu-berlin.de/met/ag/strat/produkte/qbo/qbo.dat). Heat flux is calculated using ERA-Interim meteorological reanalyses from European Centre for Medium-Range Weather Forecasts (ECMWF) and the AOD data is from Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2) reanalyses.
Acknowledgement

We thank the Head CORAL, the Director of Indian Institute of Technology Kharagpur (IIT KGP), and the Ministry of Education (MoE) for facilitating the study. PK acknowledges the support from MoE and IIT KGP. We thank the data managers and the scientists who worked hard for making available ground-based surface ozone and all other data for this study.

Author contributions

PK conceived the idea, designed the research and performed the data analyses. PK wrote the first draft, which was subsequently revised with inputs from JK and AM. JK supervised the research at IIT KGP.

Competing interests

The authors declare no conflict of interest.

Supplementary information

Supplementary table and figures are available in the attached supplementary document.

References


**Table 1:** Causal Effects (the proportion of changes in surface ozone with the change of 1 standard deviation (sd) of the geophysical driver under investigation) of various causal relations discovered by TCDF estimated using generalized augmented inverse probability weighting (gAIPW). Here average causal effect (ACE) is shown along with its 95% confidence interval estimated by drawing 500 bootstrap samples.

<table>
<thead>
<tr>
<th>Arrival Heights</th>
<th>Neumayer</th>
<th>South Pole</th>
<th>Syowa</th>
</tr>
</thead>
<tbody>
<tr>
<td>PV</td>
<td>0.93 [0.84, 1.04]</td>
<td>0.58 [0.53, 0.66]</td>
<td>0.77 [0.70, 0.86]</td>
</tr>
<tr>
<td>AAO</td>
<td>-0.18 [-0.35, 0.01]</td>
<td>-0.13 [-0.29, 0.04]</td>
<td>-0.14 [-0.29, -0.01]</td>
</tr>
<tr>
<td>HF</td>
<td>0.14 [-0.06, 0.36]</td>
<td>0.17 [0.02, 0.35]</td>
<td>0.12 [-0.03, 0.28]</td>
</tr>
<tr>
<td>AOD</td>
<td>-2.51 [-4.26, -0.58]</td>
<td>-2.85 [-4.54, -1.26]</td>
<td>2.50 [0.71, 4.42]</td>
</tr>
</tbody>
</table>
Figure 1: Daily time-series of surface ozone at various stations in Antarctica. Here, points in magenta color show the identified enhanced ozone events (OEEs) using the methodology described in the text.
Figure 2: Inter-annual variation in the frequency of OEEs and associated back-trajectories altitude. a) Timeseries for OEEs during Spring. b) OEEs occurring during Summer. Here, the fraction of trajectories coming from UTLS (crossing 500 hPa) simulated using c) GDAS and d) NCEP meteorological reanalyses corresponding to OEEs is also shown.
Figure 3: MLR fit for Surface Ozone at different stations in Antarctica. Here, the goodness of fit is represented with $R^2$ and adjusted $R^2$ ($R_{adj}^2$).
Figure 4: TCDF Causal Graph for Surface Ozone at all four stations (Neumayer, Syowa, Arrival Heights, and the South Pole) in Antarctica. Here, numbers in the middle of the detected links represent the optimal lag between cause and effect.
Figure 5: Causal graph for surface ozone at all four stations (Neumayer, Syowa, Arrival Heights and South Pole) considered in this study generated using PCMCII at 5% significance level. Here, the color of nodes shows the autocorrelation, whereas the color of the detected links represents the conditional cross-correlation between concerned nodes. The numbers in the middle of the detected links represent the detected lags between cause and effect.
Figure 1

Daily time-series of surface ozone at various stations in Antarctica. Here, points in magenta color show the identified enhanced ozone events (OEEs) using the methodology described in the text.
Figure 2

Inter-annual variation in the frequency of OEEs and associated back-trajectories altitude. a) Timeseries for OEEs during Spring. b) OEEs occurring during Summer. Here, the fraction of trajectories coming from UTLS (crossing 500 hPa) simulated using c) GDAS and d) NCEP meteorological reanalyses corresponding to OEEs is also shown.
Figure 3

MLR fit for Surface Ozone at different stations in Antarctica. Here, the goodness of fit is represented with $R^2$ and adjusted $R^2$. 

- $R^2_{ArrivalHeights} = 0.730 (0.719)$
- $R^2_{SouthPole} = 0.667 (0.652)$
- $R^2_{Neumayer} = 0.701 (0.688)$
- $R^2_{Syowa} = 0.707 (0.694)$
Figure 4

TCDF Causal Graph for Surface Ozone at all four stations (Neumayer, Syowa, Arrival Heights, and the South Pole) in Antarctica. Here, numbers in the middle of the detected links represent the optimal lag between cause and effect.
Figure 5

Causal graph for surface ozone at all four stations (Neumayer, Syowa, Arrival Heights and South Pole) considered in this study generated using PCMI at 5% significance level. Here, the color of nodes shows the autocorrelation, whereas the color of the detected links represents the conditional cross-correlation between concerned nodes. The numbers in the middle of the detected links represent the detected lags between cause and effect.

Supplementary Files

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