An Automated Geostatistical Toolkit for Mapping Stable Isotope Ratios of Precipitation over Space and Time

TONGLIN ZHANG[a], ZHONGFANG LIU[a], AJAY KALANGI[a], HYOJEONG LEE[a], CHRIS MILLER[a], JASON WEST[b], LAN ZHAO[a], GABRIEL BOWEN[a]

[a]Purdue University, West Lafayette, Indiana, USA

[b] Texas A&M University, College Station, Texas, USA

1 Introduction

We have developed a hierarchical statistical approach to interpolate the stable isotopic composition of precipitation at continental to global scales using a flexible array of ancillary variables, and applied it to estimate the past climate variables. The statistical model is composed of a function of independent variables and a spatiotemporally dependent error term. Based on AIC (Akaike information criterion) and CV (cross validation), maximum likelihood estimation, and numerical computation methods, the research develops an automatic model selection procedure of the best model for δ^{18}O, a statistical model estimation and testing procedure, and a universal kriging prediction procedure. It found that the best model for δ^{18}O contained the linear term of altitude and the linear and quadratic term of latitude, with a significant spatial correlated effects, which is consistent with the model developed by [1]. In order to investigate the robustness, we used the model selection methods to find the best hierarchical model for global temperature variations and applied it to reconstruct the past climate. The statistical toolkit has been implemented in the IsoMAP portal, allowing users to explore new models for particular regions and times using a range of different independent variables.

2 Statistical Method

2.1 Notation and Tasks

- Let $\mathcal{S} = \{\mathbf{s}_1, \cdots, \mathbf{s}_n\}$ be the location of observations.
- Let $T(\mathbf{s})$, $\delta(\mathbf{s})$, $l_o(\mathbf{s})$, $l_a(\mathbf{s})$, and $a(\mathbf{s})$ be the longterm average temperature, longterm average δ^{18}O, longitude, latitude, and altitude at $\mathbf{s}$.
- Let $T(\mathbf{s}_i)$, $\delta(\mathbf{s}_i)$, $l_o(\mathbf{s}_i)$, $l_a(\mathbf{s}_i)$, and $a(\mathbf{s}_i)$ be the corresponding observed values at i-th station.
- Let $T = (T(\mathbf{s}_1), T(\mathbf{s}_2), \cdots, T(\mathbf{s}_n))$, $\delta = (\delta(\mathbf{s}_1), \delta(\mathbf{s}_2), \cdots, \delta(\mathbf{s}_n))$, $l_o = (l_o(\mathbf{s}_1), l_o(\mathbf{s}_2), \cdots, l_o(\mathbf{s}_n))$, $l_a = (l_a(\mathbf{s}_1), l_a(\mathbf{s}_2), \cdots, l_a(\mathbf{s}_n))$ and $a = (a(\mathbf{s}_1), a(\mathbf{s}_2), \cdots, a(\mathbf{s}_n))$ be the vector of observed values respectively.
- Statistical tasks include
  - to propose a hierarchical mdoel which includes a model for δ^{18}O by using geographical variables, and a model for temperature by using δ^{18}O and geographical variables.
  - to develop estimation and model selection procedures.
  - to compute the universal kriging predictions.
  - to apply the methods to reconstruct the past temperature.

2.2 Hierarchical model for δ^{18}O and temperature

We jointly model δ^{18}O and temperature. For δ^{18}O, we propose the model

$$\delta(\mathbf{s}) = \mu_\delta(l_a(\mathbf{s}), a(\mathbf{s})) + \epsilon_\delta(\mathbf{s}),$$

where μ_δ is the mean function and ϵ_δ is the error term. For temperature, we propose the model

$$T(\mathbf{s}) = \mu_T(\delta(\mathbf{s}), l_a(\mathbf{s}), a(\mathbf{s})) + \epsilon_T(\mathbf{s}),$$

where μ_T is the mean function and ϵ_T is the error term.
We assume both $\epsilon_\delta(\mathbf{s})$ and $\epsilon_T(\mathbf{s})$ are spatially correlated, with the form of the covariance function given by

$$c(\tau) = \sigma^2 \rho_\theta(\tau)$$

We model the correlation function $\rho_\theta(\tau)$ by the Matérn correlation function defined by

$$\rho_\theta(\tau) = \frac{\theta_1}{2^{\theta_3 - 1}\Gamma(\alpha)} (\frac{\tau}{\theta_2})^{\theta_3} K_{\theta_3}(\frac{\tau}{\theta_2}),\ \tau > 0$$

where τ is the distance, $0 \le \theta_1 < 1$, $\theta_2 > 0$, $\theta_3 \ge 0$ are unknown parameters, and K_{θ_3} is the modified Bessel function.

2.3 Geostatistical Modeling

Suppose μ_δ and μ_T are modeled parametrically by a linear function of independent variables, which may include the higher order main and interaction effects. Then, they can be generally expressed by a general geostatistical model as

$$Y = X\beta + \epsilon$$

with the covariance matrix of the error term ϵ as

$$\Sigma = \sigma^2 R_\theta = \sigma^2 \begin{pmatrix} \rho_\theta(d_{11}) & \rho_\theta(d_{12}) & \cdots & \rho_\theta(d_{1n}) \\ \rho_\theta(d_{21}) & \rho_\theta(d_{22}) & \cdots & \rho_\theta(d_{2n}) \\ \vdots & \vdots & \ddots & \vdots \\ \rho_\theta(d_{n1}) & \rho_\theta(d_{n2}) & \cdots & \rho_\theta(d_{nn}) \end{pmatrix},$$

where d_{ij} is the spheric distance between sites i and j.
Let $\ell(\beta, \sigma^2, \theta)$ be the loglikelihood function. Then,

$$\ell(\beta, \sigma^2, \theta) = -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log(\sigma^2) - \frac{1}{2}\log|\det(R_\theta)| - \frac{1}{2\sigma^2}[(Y - X\beta)^t R_\theta^{-1}(Y - X\beta)].$$

The maximum likelihood estimates $\hat\beta$, $\hat\sigma^2$ and $\hat\theta$ can be derived by maximizing $\ell(\beta, \sigma^2, \theta)$. Let p be the dimension of β. Then, the Akaike information criterion (AIC) is

$$AIC = 2p - 2\ell(\hat\beta, \hat\sigma^2, \hat\theta).$$

The best model is the model with the minimum AIC value.

2.4 Universal Kriging Prediction

Let s_0 be an unobserved site for response variable. Let x_0 be the vector of independent variables at s_0. Then, the universal kriging prediction of $Y_0 = Y(\mathbf{s}_0)$ is

$$\hat Y_0 = x_0^t\hat\beta + c_0^t R^{-1}(Y - X\hat\beta)$$

where $c_0 = c_0(\hat\theta)$ is the correlation between Y_0 and Y and $R = R_{\hat\theta}$. The variance of the universal kriging prediction is

$$V(\hat Y_0 - Y_0) = \sigma^2[1 + x_0^t(X^tR^{-1}X)^{-1}x_0 - c_0^tR^{-1}X(X^tR^{-1}X)^{-1}X^tR^{-1}c_0].$$

The universal kriging prediction can be used to derive the cross validation according to $CV_2 = \sum_{i=1}^n(\hat Y_{(i)} - Y_i)^2/n$ or $CV_1 = \sum_{i=1}^n|\hat Y_{(i)} - Y_i|/n$, where $\hat Y_{(i)}$ is the univerisal kriging prediction of Y_i when Y_i is excluded from the analysis.
The best model is the model with the minimum CV_2 or CV_1 value.

2.5 Test for Spatial Dependence

If $\theta_1 = 0$, then ϵ are spatially independent and the model reduces to a linear regression model. Let $\tilde\beta$ and $\tilde\sigma^2$ be the MLE of the regression model. Then, we can use the likelihood ratio test based on

$$\Lambda = 2[\ell(\hat\beta, \hat\sigma^2, \hat\theta) - \ell_{\theta_1 = 0}(\tilde\beta, \tilde\sigma^2)].$$

The spatial dependence is significant if Λ is large. We can approximately compare it with the χ_3^2 distribution to find the p-value.

2.6 Autmoatic Model Selection Method

Based on AIC, CV_2 and CV_1, We use the backward elimination methods starting from the mean functions

$$\mu_\delta(\mathbf{s}) = \gamma_0 + \gamma_{l_a}|l_a(\mathbf{s})| + \gamma_a a(\mathbf{s}) + \gamma_{l_a a}|l_a(\mathbf{s})|a(\mathbf{s}) + \gamma_{l_a^2} l_a^2(\mathbf{s}) + \gamma_{a^2} a^2(\mathbf{s})$$

and

$$\mu_T(\mathbf{s}) = \beta_0 + \beta_\delta\delta(\mathbf{s}) + \beta_{l_a}|l_a(\mathbf{s})| + \beta_A a(\mathbf{s}) + \beta_{\delta^2}\delta^2(\mathbf{s}) + \beta_{l_a^2} l_a^2(\mathbf{s}) + \beta_{a^2}a^2(\mathbf{s}) + \beta_{\delta l_a}\delta(\mathbf{s})|l_a(\mathbf{s})| + \beta_{\delta a}\delta(\mathbf{s})a(\mathbf{s}) + \beta_{l_a a}|l_a(\mathbf{s})|a(\mathbf{s}) + \epsilon_T(\mathbf{s}).$$

Candidate models are derived by removing a few terms from the mean functions. Based on the AIC and CV values of all the candidate models, we can derive the best one among them.

2.7 Results of Model Selection

The best models for δ^{18}O has the mean function of

$$\mu_\delta(\mathbf{s}) = -3.6632 + 0.1214|l_a(\mathbf{s})| - 0.0040 l_a^2(\mathbf{s}) - 0.0016a(\mathbf{s})$$

and the covariance function of $\hat c_\delta(\tau) = 9.567\hat\rho(\tau)$ with

$$\hat\rho(\tau) = \frac{0.7728}{2^{-0.5913}\Gamma(0.4087)}(\frac{\tau}{1349.243})^{0.4087}K_{0.4087}(\frac{\tau}{1349.243}),\ \tau > 0.$$

The best model for temperature has the mean function of

$$\mu_T(\mathbf{s}) = 31.0713 + 0.9612\delta(\mathbf{s}) - 0.2066|l_a(\mathbf{s})| - 0.4389 l_a^2(\mathbf{s}) - 0.0038a(\mathbf{s}) - 0.0002\delta(\mathbf{s})a(\mathbf{s})$$

and the covariance function of $\hat c(\tau) = 20.16\hat\rho(\tau)$ with

$$\hat\rho(\tau) = \frac{0.6384}{2^{-0.5913}\Gamma(-0.8218)}(\frac{\tau}{9381.37})^{0.1782}K_{0.1782}(\frac{\tau}{9381.37}),\ \tau > 0.$$

2.8 Model for Past Temperature

Let $T_\eta(\mathbf{s})$ be the temperature and $\delta_\eta(\mathbf{s})$ be the δ^{18}O at site $\mathbf{s}$, η years ago. Past temperature $T_\eta(\mathbf{s})$ can be estimated by using the observations of δ^{18}O from ice cores. Let $\delta_0(\mathbf{s})$ be the most recent δ^{18}O value in an ice core. Let

$$d_\delta(\mathbf{s}) = \delta_\eta(\mathbf{s}) - \delta_0(\mathbf{s})$$

be difference of δ^{18}O between the most recent value and the value of η years ago. Then, the temporal variation of δ^{18}O is modeled by

$$d_\eta(\mathbf{s}) = f(\eta) + \epsilon_\eta(\mathbf{s}),$$

where $f(\eta)$ is the mean function and $\epsilon_\eta(\mathbf{s})$ is a white noise error term. After $f(\eta)$ has been estimated by $\hat f(\eta)$, we can use this model combined with previous model to reconstruct the past temperature.

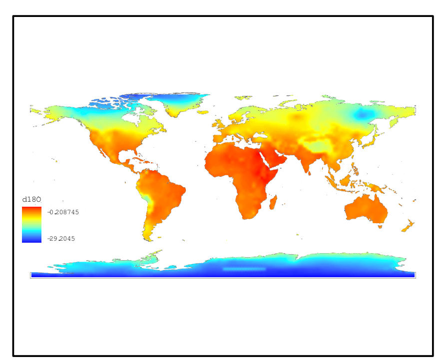
3 Results

3.1 Model Selection for δ^{18}O

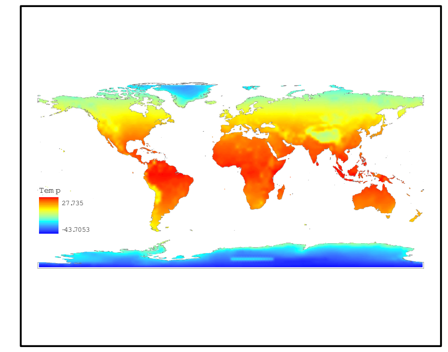
$\mu_\delta(l_a(s), a(s))$	Spatial Model AIC	Spatial Model CV	Regression AIC	Regression CV	Λ
$(l_a(\mathbf{s}), a(\mathbf{s}))$	28.646	0.159	225.67	3.30	425.75
$(l_a(\mathbf{s}), l_a^2(\mathbf{s}), a(\mathbf{s}))$	0.000	0.000	17.45	0.20	246.18
$(l_a(\mathbf{s}), a(\mathbf{s}), a^2(\mathbf{s}))$	29.146	0.171	198.51	2.76	398.10
$(l_a(\mathbf{s}), a(\mathbf{s}), l_a(\mathbf{s})a(\mathbf{s}))$	30.629	0.017	195.16	2.69	393.27
$(l_a(\mathbf{s}), l_a^2(\mathbf{s}), a(\mathbf{s}), a^2(\mathbf{s}))$	0.542	0.013	0.00	0.00	228.19
$(l_a(\mathbf{s}), l_a^2(\mathbf{s}), a(\mathbf{s}), l_a(\mathbf{s})a(\mathbf{s}))$	1.814	0.008	18.95	0.23	245.87
$(l_a(\mathbf{s}), a(\mathbf{s}), a^2(\mathbf{s}), l_a(\mathbf{s})a(\mathbf{s}))$	30.787	0.176	185.54	2.55	383.48
$(l_a(\mathbf{s}), l_a^2(\mathbf{s}), a(\mathbf{s}), a^2(\mathbf{s}), l_a(\mathbf{s})a(\mathbf{s}))$	1.713	0.015	0.67	0.02	227.69

Note: AIC and CV are given by the difference to the minimum values. The p-values of Λ are all 0.

3.2 Global Variation of δ^{18}O

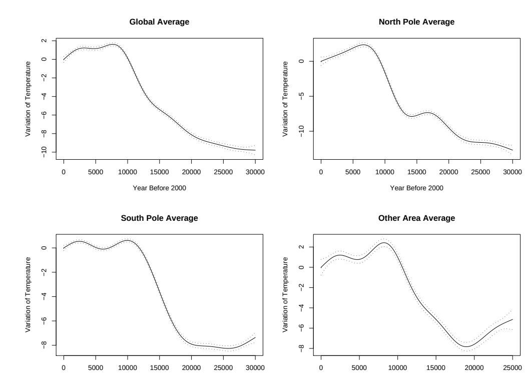


3.3 Global Variation of Current Temperature



3.4 Past Temperature Reconstruction

Based on the δ^{18}O records of ice cores from North Pole to South Pole available at *http://www.ncdc.noaa.gov/paleo/icecore.html*, we derived the estimates of past temperature variations.



4 Conclusion

- δ^{18}O can be predicted by the quadratic term of latitude and a linear term of altitude, with significant interaction effects.
- Temperature can be predicted by the linear term of δ^{18}O, the quadratic term of latitude, and a linear term of altitude, with signifiant interaction effects between δ^{18}O and altitude, which indicates the slope of δ^{18}O decreases as altitude increases.
- Spatial dependence cannot be ignored for both δ^{18}O and temperature.
- Using spatial statistical model can locally reconstruct past climate.

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