Spatiotemporal modeling of European paleoclimate using doubly sparse Gaussian processes

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Summary

Goal Probabilistic consensus model conditioned on multiple data sources that inform paleoclimate

Target users Practitioners from e.g., anthropology and archaeology

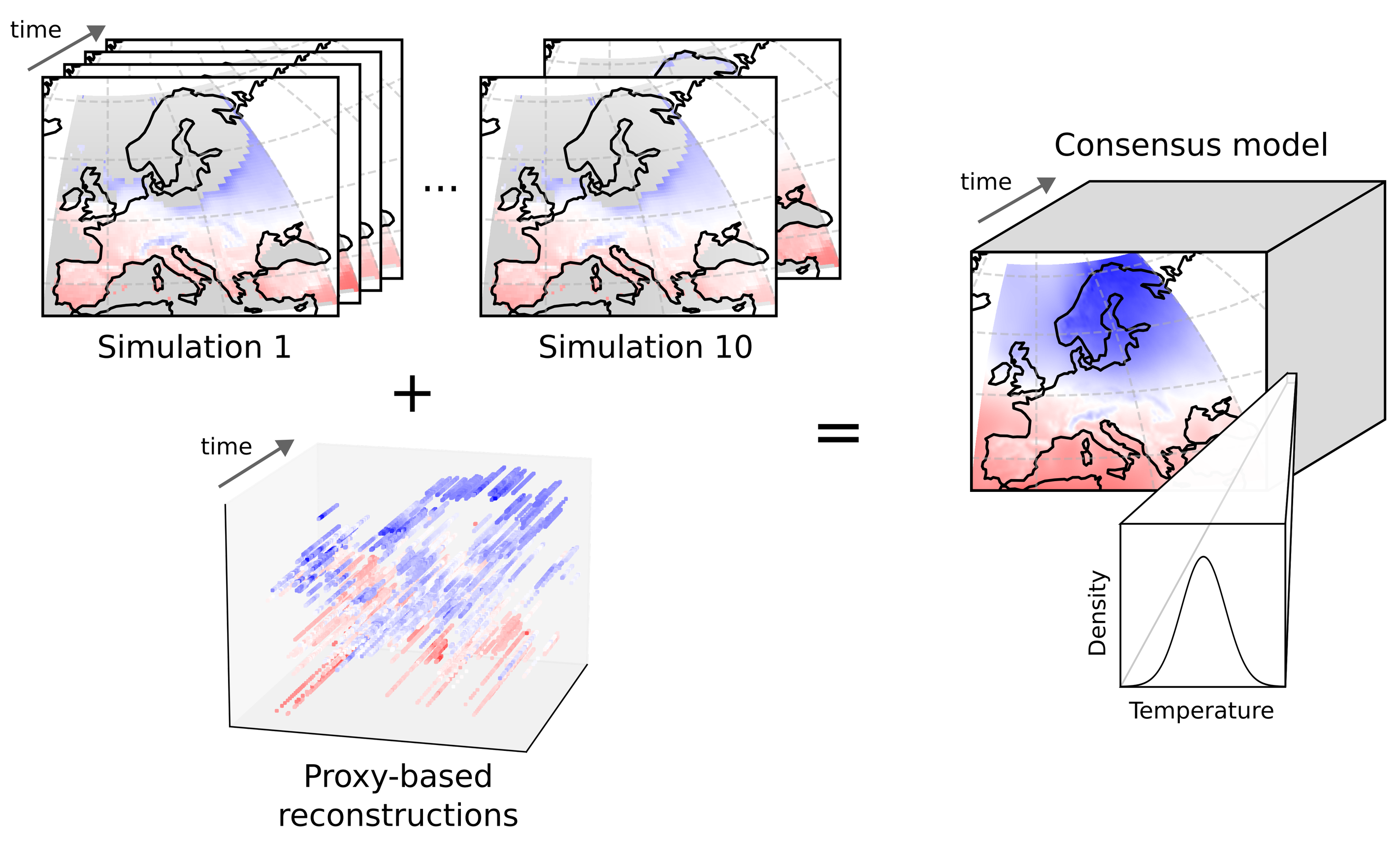
Data Mixed gridded and point data:
1. paleoclimate simulations
2. proxy data (from fossilized pollen)

Model Spatiotemporal Gaussian process (GP)

Approximate inference Doubly sparse GP
1. temporal part as **state-space model**
2. **inducing points** in space and time

Results Continuous spatiotemporal posterior for European paleoclimate from 21 to 6 ka

Integrating paleoclimate models and proxies



Data about paleoclimate

Simulations outputs of physical models, at unaligned grids in space/time

Proxy data reconstructions from e.g. fossilized pollen

Problem

There is no **consensus model** of grid and point evidence with uncertainty

Gaussian process spatiotemporal model

Scope European mean annual temperature (MAT) between 21ka and 6ka i.e., from the Last Glacial Maximum (LGM) to the mid-Holocene (MH)

$$\begin{aligned}
m(x)&: \text{near-modern reference climate (spatial interpolation)}\\
C(x,t)&: \text{climate variable at coordinates } x \text{ and time } t\\
Y_{s,p}&: \text{simulation or reconstruction at coordinates } x_s \text{ and time } t_p\\
k_x(x,x')&: \text{anisotropic Matérn 3/2 kernel}\\
k_t(t,t')&: \text{Ornstein-Uhlenbeck kernel}\\
\overline{C}(x,t) = C(x,t) - m(x)&: \text{modeled anomaly}\\
\overline{Y}_{s,p} = Y_{s,p} - m(x_s)&: \text{anomaly data}\\
\overline{C}(x,t) \sim \mathcal{GP}(0, k_x(x,x')k_t(t,t'))&: \text{prior}\\
\overline{Y}_{s,p} | \overline{C}(x_s,t_p) \sim \mathcal{N}(\overline{C}(x_s,t_p), \sigma)&: \text{likelihood}
\end{aligned}$$

$\mathcal{O}(10^6)$ data points is too many to perform exact inference.

Approximate inference

Doubly sparse GPs [1,2]

- Spatially and temporally sparse, variational GP (S²CVI) posterior q in `markovflow` [3]
- S²CVI combines **inducing point methods** with the **state-space representation** of GPs using separate spatial and temporal inducing points.
- Variational objective computational complexity scales as

$$\mathcal{O}((M_t + N)(M_s d)^3)$$

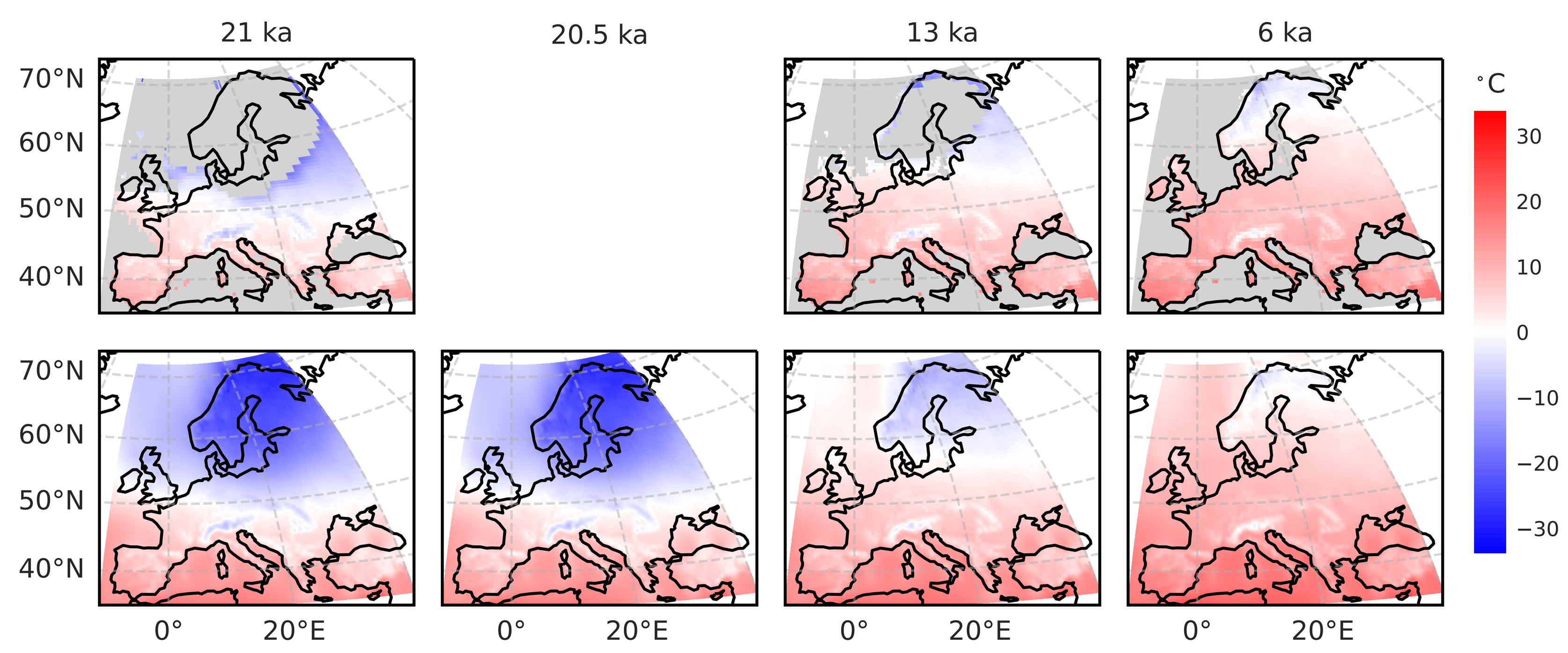
We used $M_s = 100$ spatial inducing points, $M_t = 6$ temporal inducing points, a state-space dimension $d = 1$ for k_t, and a batch size $N_b = 1000$.

Training

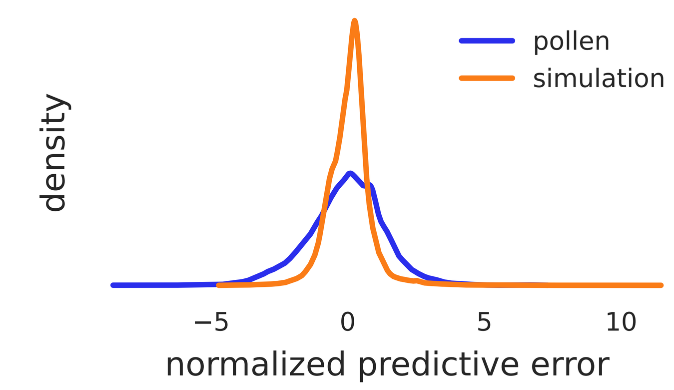
- Hyperparameters include length scales of k_x and k_t, scale of combined kernel, likelihood variance σ, and spatial inducing points.
- Alternate updates of variational parameters using natural gradients and hyperparameters using Adam.
- Trained for 30 epochs (36h on an NVIDIA V100 GPU).

Results

The model produces high quality spatial and temporal interpolations



MAT from a single simulation (Y; top) vs posterior mean ($\mathbb{E}_{C\sim q}[C(x,t)]$; bottom).



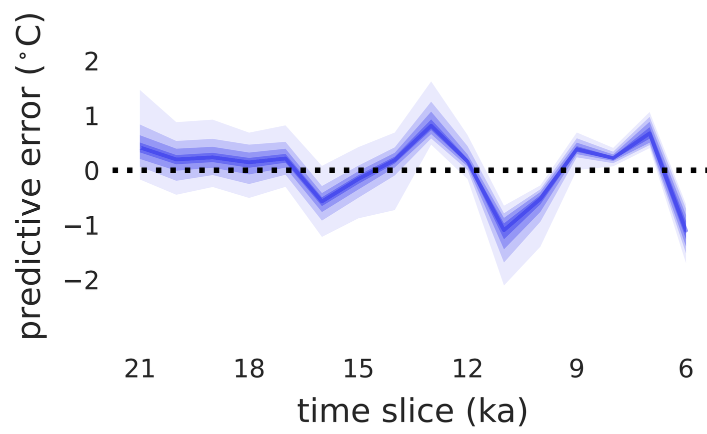
KDE of posterior predictive (PP) error distribution.

Error

$$E = \frac{C(x_s,t_p) - Y_{s,p}}{\sqrt{\sigma^2 + \mathrm{Var}_{\overline{C}\sim q}[C(x_s,t_p)]}}.$$

98.9% of all data falls within 3 standard deviations of the PP mean

Leave-one-time-slice-out cross-validation



Validation error

$$E_{\text{val}} = \mathbb{E}_{\overline{C}\sim q}[C(x_s,t_p)] - Y_{s,p}.$$

Shown are 80%, 60%, 40%, 20% intervals centered about the median (line).
Mean error: 0.05°C
Mean absolute error: 0.7°C

Planned Improvements

- use a parametric mean function for the GP prior
- set informative priors for optimized hyperparameters
- use non-i.i.d. likelihoods for the data
- jointly model MAT and total annual precipitation (multi-output GP)
- incorporate proxy dating uncertainty
- apply the model to other continents

References

[1] William Wilkinson, Arno Solin, Vincent Adam. *Sparse algorithms for Markovian Gaussian processes*, AISTATS 2021.

[2] Vincent Adam, Stefanos Eleftheriadis, Nicolas Durrande, Artem Artemev, James Hensman. *Doubly sparse variational Gaussian processes*, AISTATS 2020.

[3] Vincent Adam et al. *Markovflow*, commit: `fc82c0a`. `https://github.com/secondmind-labs/markovflow`.

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