Spatio-Temporal Local Interpolation for Quantifying Global Ocean Heat Transport from Autonomous Observations

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 $\label{eq:constraint} \begin{array}{l} \textbf{Temperature} \times \textbf{Velocity} \text{ integrated w.r.t. depth} \\ \text{across Latitude (Meridional) or Longitude (Zonal)} \end{array}$

OHT(\boldsymbol{x} , t) at $\boldsymbol{x} = (x, y)$ where longitude x, latitude y, and time t:

$$OHT(\boldsymbol{x}, t) = C_{p} \int \frac{\theta(\boldsymbol{x}, t, p) \cdot \mathbf{v}(\boldsymbol{x}, t, p)}{g(\boldsymbol{x}, p)} dp$$
$$\propto \int \underbrace{\theta(\boldsymbol{x}, t, p)}_{\text{Temperature}} \cdot \underbrace{\mathbf{v}(\boldsymbol{x}, t, p)}_{\text{Velocity}} dp$$

where g: gravitational acceleration, C_p : specific heat content.

OHT can be estimated from various data sources



Research Vessel

Underwater Probe

Satellite altimetry

Argo samples nearly uniform $3^{\circ} \times 3^{\circ} \times 10$ days





$$OHT(\boldsymbol{x},t) \propto \int \underbrace{\boldsymbol{\theta}(\boldsymbol{x},t,\boldsymbol{p})}_{\text{Temperature}} \cdot \underbrace{\mathbf{v}(\boldsymbol{x},t,\boldsymbol{p})}_{\text{Velocity}} d\boldsymbol{p}$$

- Both are globally non-stationary spatio-temporal field
- Capture local structures from the sparse observation
- Computationally feasible method to handle massive in-situ data

Geostrophic Velocity ${\bf v}$

For fixed pressure p^* , relative velocity

$$\mathbf{v}_{\mathrm{rel}}(\boldsymbol{
ho}^*) := \mathbf{v}(\boldsymbol{
ho}^*) - \mathbf{v}_{\mathrm{ref}}(\boldsymbol{
ho}_0) = rac{1}{f}\mathbf{k} imes
abla_{\boldsymbol{x}} \Psi(\boldsymbol{
ho}^*)$$

where f: Coriolis parameter, Ψ : dynamic height anomaly $\left(\int_{p^*}^{p_{ref}} \frac{1}{\rho} d\rho\right)$



Consider an additive model of $\{\Psi(\mathbf{x}, t)\}$ indexed by location $\mathbf{x} = (x, y)$ where latitude *x*, longitude *y* in degrees, and time *t* in days.

$$\Psi_{p^*}(\boldsymbol{x}, t) = \underbrace{m_{p^*}(\boldsymbol{x}, t)}_{\text{Mean Field}} + \underbrace{a_{p^*}(\boldsymbol{x}, t)}_{\text{Anomaly Field}} + \underbrace{\epsilon(\boldsymbol{x}, t)}_{\text{Nugget Effect}}$$
(1)

where $\mathbb{E}\Psi(\mathbf{x}, t) = m(\mathbf{x}, t)$, and $a(\mathbf{x}, t)$ is zero-mean, second-order stationary random field.

Modelling Ψ : Local Semiparametric Regression¹

Within a small spatial window $\mathcal{W}(\boldsymbol{x}^*) = \{\boldsymbol{x} : \|\boldsymbol{x} - \boldsymbol{x}^*\| \le \lambda_{\boldsymbol{x}}\},\$ $m(\boldsymbol{x}, t) = \beta_0 + [\text{1st- and 2nd-order linear terms of } \boldsymbol{x} \text{ and } \boldsymbol{y}]$ $+ \sum_{i=1}^{L} \left[\beta_{c_i} \cos\left(\frac{2\pi l}{365}t\right) + \beta_{s_i} \sin\left(\frac{2\pi l}{365}t\right) \right], \quad \forall \boldsymbol{x} \in \mathcal{W}(\boldsymbol{x}^*)$



¹ Ridgway, K. R., Dunn, J. R., & Wilkin, J. L. (2002). Ocean interpolation by four-dimensional weighted least squares—Application to the waters around Australasia. *Journal of Atmospheric and Oceanic Technology*, 19(9), 1357–1375.

Modelling Ψ : Local Semiparametric Regression²

Within a small spatiotemporal window $\widetilde{\mathcal{W}}(\mathbf{x}^*, t^*) = \mathcal{W}(\mathbf{x}^*) \times [t^* \pm \lambda_t]$,

 $a_i \stackrel{\mathrm{iid}}{\sim} \mathsf{GP}\left(0, k\left((\boldsymbol{x}_1, t_1), (\boldsymbol{x}_2, t_2); \boldsymbol{\xi}\right)\right), \qquad ext{ year } i = 1, \cdots, I$

for observations $j = 1, ..., J_i$ within $\widetilde{\mathcal{W}}(\mathbf{x}^*, t^*)$, where $k(\cdot; \boldsymbol{\xi})$ is an space-time Matern covariance function depending on parameters $\boldsymbol{\xi}$.



²Kuusela, M., & Stein, M. L. (2018). Locally stationary spatio-temporal interpolation of Argo profiling float data. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Science, 474(2220)

Geostrophic velocity where the yearday time *t* is in year *i*:

$$\mathbf{v}_{\rm rel}(\boldsymbol{x},t) = \frac{\mathbf{k} \times [\nabla_{\boldsymbol{x}} \Psi(\boldsymbol{x},t) \mid \Psi_i, \beta, \boldsymbol{\xi}, \sigma]}{f(\boldsymbol{y}) g(\boldsymbol{x})}$$
(2)

Joint process $[a_i, \nabla_x a_i]$ is a multivariate Gaussian Process for year *i*:

$$\begin{bmatrix} a_i \\ \nabla_{\boldsymbol{x}} a_i \end{bmatrix} \stackrel{\textit{iid}}{\sim} \mathsf{GP}\left(\boldsymbol{0}, \begin{bmatrix} k(\boldsymbol{s}, \boldsymbol{s}) & \nabla_{\boldsymbol{x}^*} k(\boldsymbol{s}, \boldsymbol{s}^*)^\top \\ \nabla_{\boldsymbol{x}} k(\boldsymbol{s}, \boldsymbol{s}^*) & \nabla_{\boldsymbol{x}} \nabla_{\boldsymbol{x}^*} k(\boldsymbol{s}, \boldsymbol{s}^*) \end{bmatrix}\right)$$

implies the Gaussian predictive distribution of $\nabla_{\mathbf{x}} \Psi$ with

$$\mathbb{E}(\nabla_{\boldsymbol{x}} \Psi^{\star} | \Psi_{i}, \beta, \boldsymbol{\xi}, \sigma) = \beta(\boldsymbol{x}^{\star}) + \nabla_{\boldsymbol{x}} \boldsymbol{k}_{i}^{\star}(\boldsymbol{\xi})^{\top} (\boldsymbol{K}_{i}(\boldsymbol{\xi}) + \sigma^{2} \boldsymbol{I})^{-1} [\boldsymbol{\Psi} - \boldsymbol{m}]_{i}$$

under the Gaussian nugget $\epsilon_{ij} \sim N(0, \sigma^2)$.

Parameter Estimation: EM procedure

For spatio-temporal grid points $\{(\textbf{\textit{x}}^*,t^*): \textbf{\textit{x}}^* \in \mathcal{X}, t^* \in [0,365]\},\$

$$\log \mathcal{L}(\boldsymbol{\beta}(\boldsymbol{x}^*), \boldsymbol{\xi}(\boldsymbol{x}^*, t^*)) = \sum_{i=1}^{l} \log \mathsf{N}(\boldsymbol{\Psi}_i; \tilde{\boldsymbol{\eta}}_{i\cdot}^\top \boldsymbol{\beta}, \boldsymbol{K}_i(\boldsymbol{\xi}))$$

where $\tilde{\eta}_{ij}$ is the $\sum_{l=1}^{i-1} n_l + j$ th column of the design matrix.

For iteration $\tau = 0, 1, \ldots$,

$$\begin{split} \beta^{(\tau+1)} &= \operatorname{argmax}_{\beta} \log \tilde{\mathcal{L}}(\beta | \boldsymbol{\xi}^{(\tau)}), \quad (\mathsf{E step}) \\ \boldsymbol{\xi}^{(\tau+1)} &= \operatorname{argmax}_{\boldsymbol{\xi}} \log \mathcal{L}(\boldsymbol{\xi} | \beta^{(\tau+1)}), \quad (\mathsf{M step}) \end{split}$$

where $\tilde{\mathcal{L}}$ is an approximated likelihood of \mathcal{L} with Vecchia approximation

Debiasing Mean-field Misspecification

Suppose the mean-field *m* is mis-specified: the anomaly field includes systematic bias $B(\mathbf{x}) = \mathbb{E}[a(\mathbf{x}, t)] \neq 0$

$$\Psi(\boldsymbol{x},t) = [m(\boldsymbol{x},t) + B(\boldsymbol{x})] + [a(\boldsymbol{x},t) - B(\boldsymbol{x})] + \epsilon$$

We may estimate *B* from the conditional mean of predictive Ψ ,

$$\mathbb{E}[\boldsymbol{a}(\boldsymbol{x}^{\star},t^{\star})] \stackrel{\rho}{\leftarrow} \frac{1}{I} \sum_{i=1}^{I} \hat{a}_{i}(\boldsymbol{x}^{\star},t^{\star}) \approx \frac{1}{I} \sum_{i=1}^{I} \left[\frac{1}{J_{i}} \sum_{j=1}^{J_{i}} \hat{a}_{i}(\boldsymbol{x}^{\star},t_{ij}^{\star}) \right] := \widehat{B}(\boldsymbol{x}^{\star})$$

Consequently,

$$\nabla_{\boldsymbol{x}}\widehat{\boldsymbol{B}}(\boldsymbol{x}^{\star}) = \frac{1}{I}\sum_{i=1}^{I} \left[\frac{1}{J_{i}}\sum_{j=1}^{J_{i}}\nabla_{\boldsymbol{x}}\boldsymbol{k}_{i}^{\star}(\boldsymbol{\xi}_{(j)})^{\top}(\boldsymbol{K}_{i}(\boldsymbol{\xi}_{(j)}) + \sigma_{(j)}^{2}\boldsymbol{I})^{-1}[\boldsymbol{\Psi} - \hat{\boldsymbol{m}}]_{ij}\right]$$



NATIONAL CENTER FOR ATMOSPHERIC RESEARCH



5.34-petaflops, High Performance Cluster with 145,152 Intel Xeon processors (36 cores/node)

Local model constructs the velocity field from sparse observations

(East / West) Zonal velocity



(Surface)

Argo

(10 m, Debiased)



Debiasing procedure captures higher-order features

(North / South) Meridional Velocity at 10 m



Argo provides velocity field at multiple depths



Argo provides in-situ temperature at multiple depths



OHT Field is mapped by Local Regression with plug-in estimator

Estimated OHT at any given location \mathbf{x}_{ij} and time t_{ij} :

$$\begin{split} \operatorname{OHT}(\boldsymbol{x}_{ij}, t_{ij}) &\propto \int \theta_{ij}(\boldsymbol{p}) \cdot \mathbf{v}_{ij}(\boldsymbol{p}) \, \mathrm{d}\boldsymbol{p} \\ & \cong \int \theta_{ij}(\boldsymbol{p}) \cdot \hat{\mathbf{v}}_{ij}(\boldsymbol{p}) \, \mathrm{d}\boldsymbol{p} \\ & \cong \sum_{k=0}^{N_{\mathrm{int}}} \widetilde{\theta} \widetilde{\mathbf{v}}(\boldsymbol{x}_{ij}, t_{ij}, \boldsymbol{p}_k) \Delta_{\boldsymbol{p}_k} := \widetilde{\operatorname{OHT}}(\boldsymbol{x}_{ij}, t_{ij}) \end{split}$$

where $\widetilde{\theta \mathbf{\hat{v}}}$ is the piecewise cubic Hermite interpolant (PCHIP).

We map the OHT field again with Local Semiparametric Regression:

$$\widetilde{OHT}(\boldsymbol{x}_{ij}, t_{ij}) = \underbrace{\widetilde{m}(\boldsymbol{x}_{ij}, t_{ij})}_{\text{Mean Field}} + \underbrace{\widetilde{a}_i(\boldsymbol{x}_{ij}, t_{ij})}_{\text{Anomaly Field}} + \underbrace{\epsilon_{ij}}_{\text{Nugget Effect}}$$

Upper-Ocean[†] Heat Transport mean field

† Upper Ocean: 10 to 900 dbar



Zonal



Upper-Ocean[†] mean Meridional Heat Transport driven by Geostrophy



Anomalous Heat Transport has connection to the anomalous climate phenomena, i.e., El Niño.







Discussion

Statistical Aspects

- Parameter Tuning
 - Seasonal cycle harmonics
 - Bandwidth selection for spatio-temporal windows
- Uncertainty Quantification
 - Incorporate $\mathbb{V}(\mathbf{v}|\boldsymbol{\Psi}_i, \hat{\beta}, \hat{\theta}, \hat{\sigma})$ to the 2nd stage regression
 - Global confidence band for Two-stage estimate
- Relaxing the assumptions
 - Mapping the vertical dimension (4D map)
 - Multivariate joint process (θ, \mathbf{v})
 - Beyond Gaussian field

Oceanographic / Climatological Aspects

- Ocean contribution to Meridional Heat Transport
 - Other sources of heat transport, i.e., Ekman
 - Impact of Ageostrophic transport

Thank You



Autonomous Underwater Observations



Argo float

Spray glider



 1 Woods Hole Oceanographic Institution

Gliders fill under-coverage along the US East Coast



¹Todd, Robert E. and Locke-Wynn, Lea (2017). Underwater Glider Observations and the Representation of Western Boundary Currents in Numerical Models. *Oceanography*, 30(2), 88-89

Spray profiles correct under-estimated velocity of Gulf Stream



Figure: Mean velocity differences (Debiased) at 15 dbar



Spray profiles correct under-estimated Heat Transport of Gulf Stream



Figure: Mean absolute heat transport differences over 10 to 900 dbar



Spray profiles correct under-estimated Meridional Heat Transport of Gulf Stream





Earth's Radiation Balance



¹L. Bryden, H., & Imawaki, S. (2001). Chapter 6.1 Ocean heat transport., International Geophysics (pp. 455–474).

Choice of GP Kernel

Matèrn covariance function with smoothing parameter $\nu = 3/2$

$$k((\mathbf{x}_{1}, t_{1}), (\mathbf{x}_{2}, t_{2}); \boldsymbol{\xi}) = \phi\left(1 + \sqrt{3}d\right) \exp\left(-\sqrt{3}d\right),$$

$$d((\mathbf{x}_{1}, t_{1}), (\mathbf{x}_{2}, t_{2})) = \|(\mathbf{x}_{1}, t_{1}) - (\mathbf{x}_{2}, t_{2})\|_{\text{diag}(1/\boldsymbol{\xi})}$$

The partial derivative and hessian of the covariance function is given as

$$\frac{\partial k(\boldsymbol{x}^*, \boldsymbol{x}_i)}{\partial \boldsymbol{x}^*} = \frac{-3\phi}{\xi_x^2} (\boldsymbol{x}^* - \boldsymbol{x}_i) \exp\left(-\sqrt{3}d\right)$$
$$\frac{\partial k(\boldsymbol{x}^*, \boldsymbol{x}_i)}{\partial \boldsymbol{y}^*} = \frac{-3\phi}{\xi_y^2} (\boldsymbol{y}^* - \boldsymbol{y}_i) \exp\left(-\sqrt{3}d\right)$$
$$\frac{\partial^2}{\partial \boldsymbol{x}_1 \partial \boldsymbol{x}_2} k(\boldsymbol{x}_1, \boldsymbol{x}_2) = \frac{3\phi}{\xi_x^2} \left(1 - \sqrt{3}\frac{\Delta_x^2}{d\xi_x^2}\right) \exp(-\sqrt{3}d)$$

where $\Delta_x = x_1 - x_2$

Surface Geostrophic Velocity from Satellite Altimetry



Sub-surface mean Zonal Velocity field at 10 dbar



Geostrophic Velocity from Satellite Altimetry



Upper-Ocean[†] mean Zonal Heat Transport field

† Upper Ocean: 10 to 900 dbar



Initial:



Upper-Ocean[†] mean Meridional Heat Transport field

† Upper Ocean: 10 to 900 dbar



Initial:



PCHIP Interpolation

Fritsch, F. N. and Carlson, R. E. (1980). Monotone Piecewise Cubic Interpolation. *SIAM Journal on Numerical Analysis*, 17(2):238–246

Let $\theta \hat{\mathbf{v}} = \tilde{q}$

$$egin{aligned} \widetilde{Q}(x_i,y_i,t_i) &= \int_{
ho_L}^{
ho_U} [heta \widehat{\mathbf{v}}](x_i,y_i,t_i,m{
ho}) \mathrm{d}m{
ho} \ &\cong \sum_{k=0}^{N_{\mathrm{int}}} \left[\widetilde{q}(p_k) H_1(p_k^*) + \widetilde{q}(p_{k+1}) H_2(p_k^*)
ight. \ &+ \partial_{
ho} \widetilde{q}(p_k) H_3(p_k^*) + \partial_{
ho} \widetilde{q}(p_{k+1}) H_4(p_k^*)
ight] \Delta_{
ho_k} \end{aligned}$$

where $p_k^* \in [p_k, p_{k+1}]$, $\Delta_{p_k} = p_{k+1} - p_k$, and $H_l(p)$ are the cubic Hermite basis functions for which interval $[p_k, p_{k+1}]$:

$$\begin{aligned} & H_1(\boldsymbol{p}) = \phi\left(\frac{p_{k+1}-p}{\Delta_{p_k}}\right), \, H_2 = \phi\left(\frac{p-p_k}{\Delta_{p_k}}\right), \, H_3(\boldsymbol{p}) = -\Delta_{p_k}\psi\left(\frac{p_{k+1}-p}{\Delta_{p_k}}\right), \\ & H_4(\boldsymbol{p}) = \Delta_{p_k}\psi\left(\frac{p-p_k}{h_k}\right) \text{ where } \phi(\boldsymbol{p}) = 3\boldsymbol{p}^2 - 2\boldsymbol{p}^3, \, \psi(\boldsymbol{p}) = \boldsymbol{p}^3 - \boldsymbol{p}^2. \end{aligned}$$

Anomalous Heat Transport has connection to the unexplained ocean climate fluctuations.



45[°]E 90[°]E 135[°]E 180[°]E 225[°]E 270[°]E 315[°]E 360[°]E



Equatorial subsurface temperature anomalies (May 1-5, 2016)

Map Area

Spray Profile Statistics

Out of 10,577 availabe profiles, only 2,791 profiles (26.4%) have measurements down to 800dbar.



Figure: Number of profiles in $1^{\circ} \times 1^{\circ}$ grid at 15 dbar

Mean Velocity field from Argo profiles



Figure: Mean velocity (Debiased) at 15 dbar



Mean Velocity field from Aggregated Spray and Argo



Figure: Mean velocity (Debiased) at 15 dbar



Mean Heat Transport field from Argo profiles



Figure: Mean absolute heat transport over 10 to 900 dbar

Mean Field Difference

Mean Heat Transport field from Aggregated profiles



Figure: Mean absolute heat transport over 10 to 900 dbar



Upper-Ocean mean Meridional Heat Transport in North Atlantic basin from Argo



Upper-Ocean mean Meridional Heat Transport in North Atlantic basin from Aggregated Spray and Argo



