The Fast and the Fourier-ous

Non-parametric autocovariance modelling with spline kernels

Lachlan Astfalck, The University of Western Australia, ARC ITRH TIDE

Modelling Non-linear Processes with Linear Models

Non-parametric autocovariance modelling with spline kernels

Lachlan Astfalck, The University of Western Australia, ARC ITRH TIDE

Man, I love a GP…

Non-parametric autocovariance modelling with spline kernels

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ARAFURA SEA
PAPUA NEW GUINEA
CORAL SEA
CORAL SEA ISLANDS TERRITORY
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NORTHERN TERRITORY
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Mount Isa
QUEENSLAND
AUSTRALIA
Mackay
Alice Springs
Rockhampton
Gladstone
Tropic of Capricorn
WESTERN AUSTRALIA
Bundaberg
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SOUTH AUSTRALIA
Toowoomba
Gold Coast
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NEW SOUTH WALES
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Gosford
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Queanbeyan
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AUSTRALIAN CAPITAL TERRITORY
Mount Gambier
Melbourne
Warrnambool
Geelong
VICTORIA
INDIAN OCEAN
TASMAN SEA
Devonport
TASMANIA
Hobart
0 150 300 mi
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What we know about the internal waves that may have sunk Indonesia's submarine

By science reporter **Gemma Conroy**

ABC Science | Oceans and Reefs

Sat 1 May 2021

SCIENCE

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What Is An 'Internal Wave'? It Might Explain The Loss Of An Indonesian Submarine

APRIL 30, 2021 · 2:02 PM ET

By Scott Neuman

What Killed the Thresher?

By Norman Polmar

April 2023 | Naval History

FEATURED ARTICLE | VIEW ISSUE

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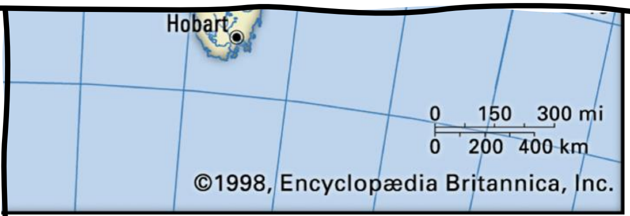
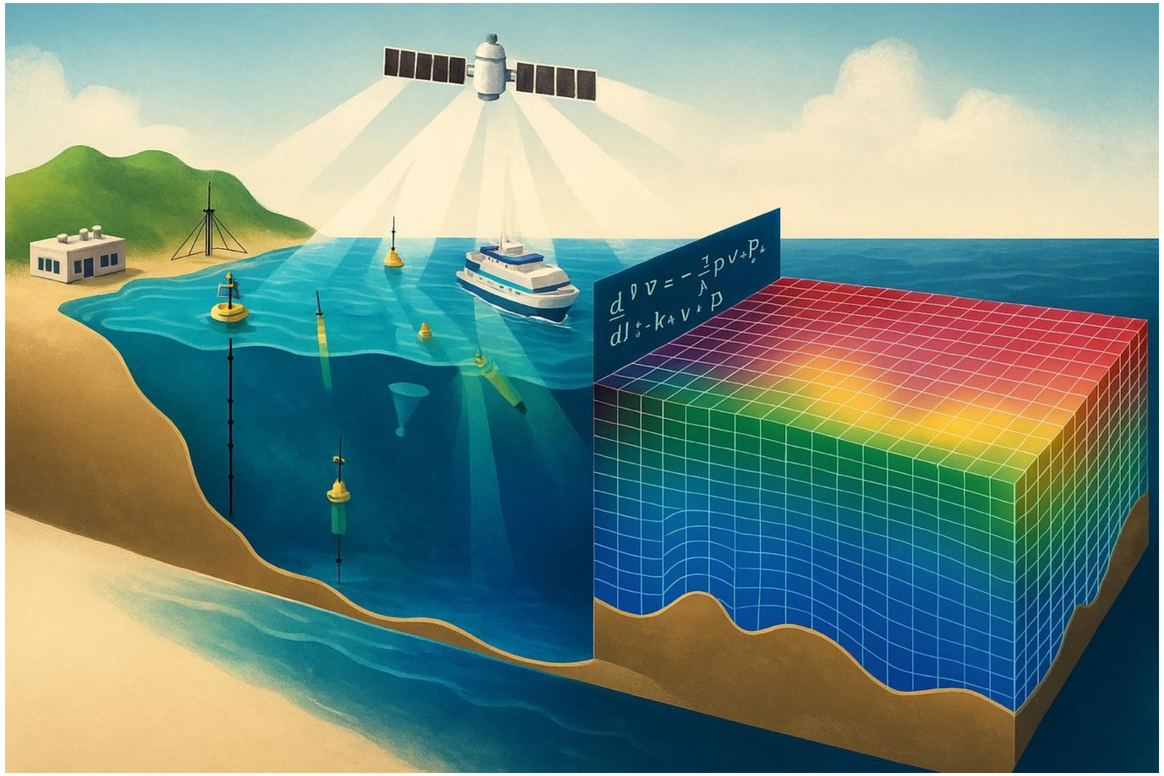
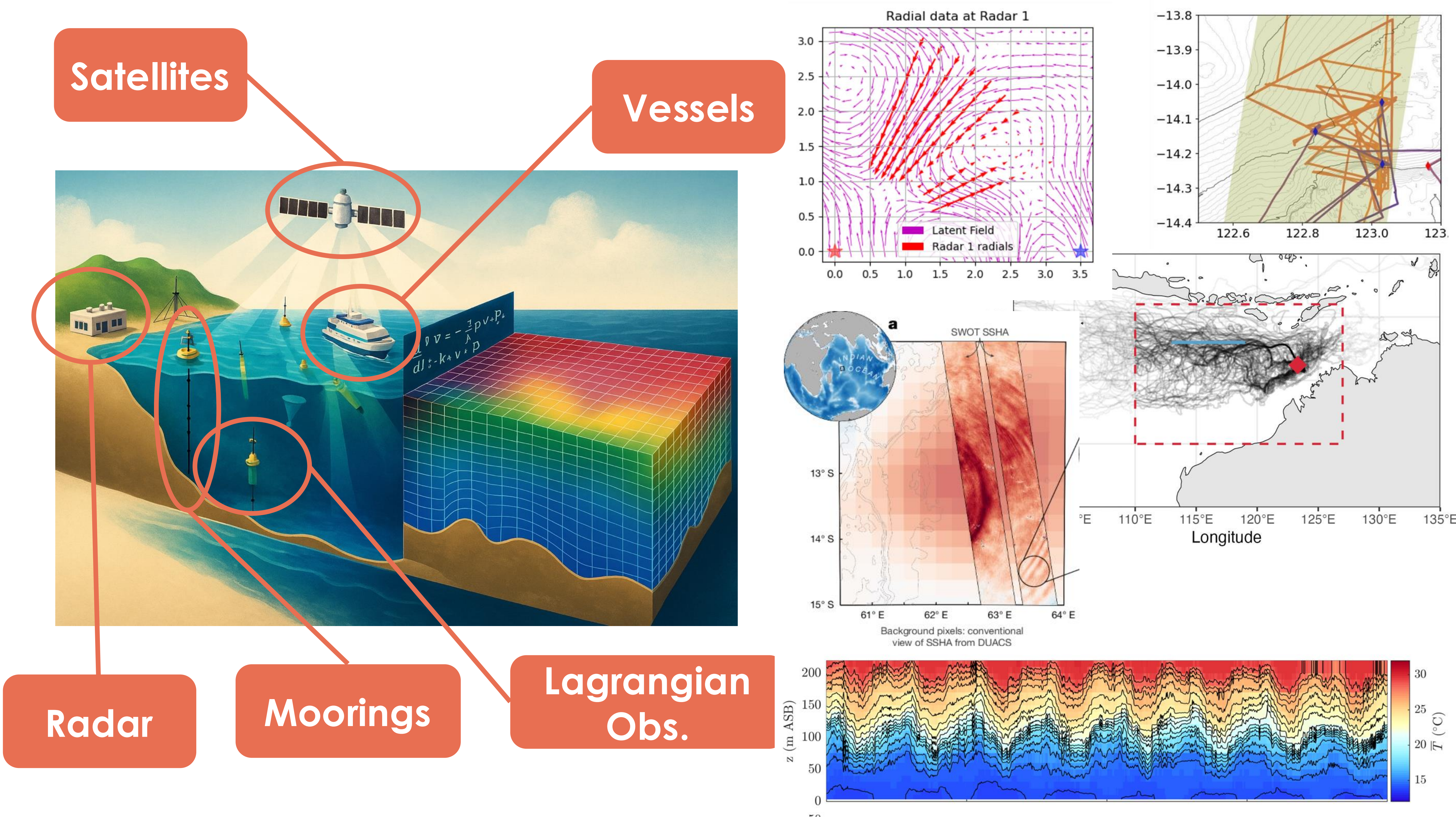
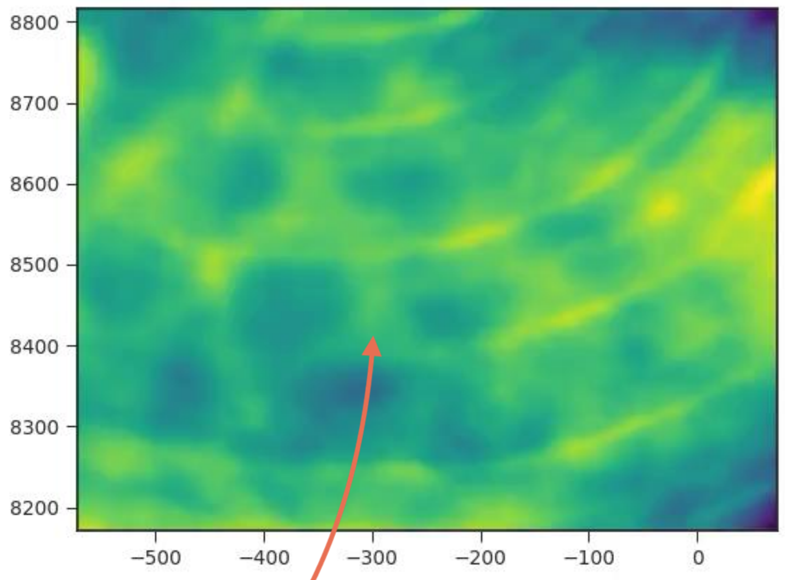
The USS *Thresher* (SSN-593), which sank 60 years ago this April, was the world's first nuclear-powered submarine to be lost at sea. Amid the public shock over the tragedy, the U.S. Navy grappled for an answer as to what went wrong. Even today, rival theories seek to explain the mystery.



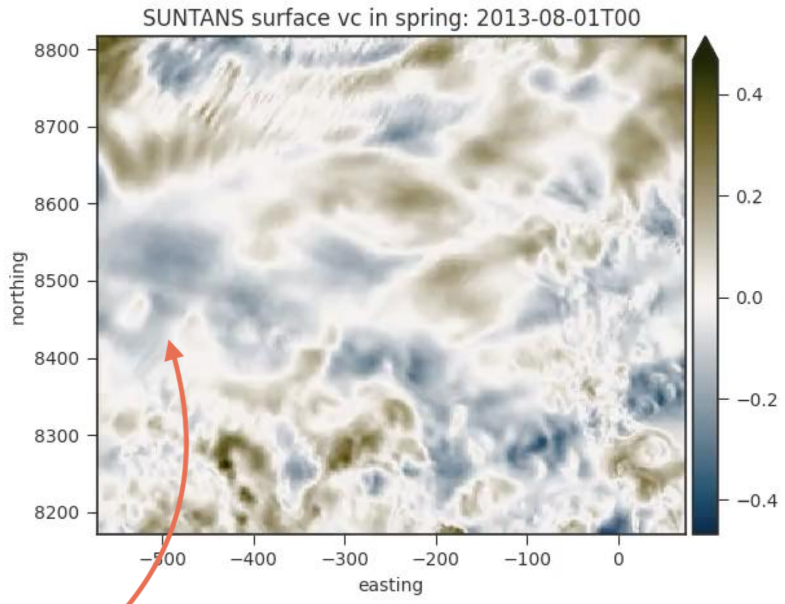


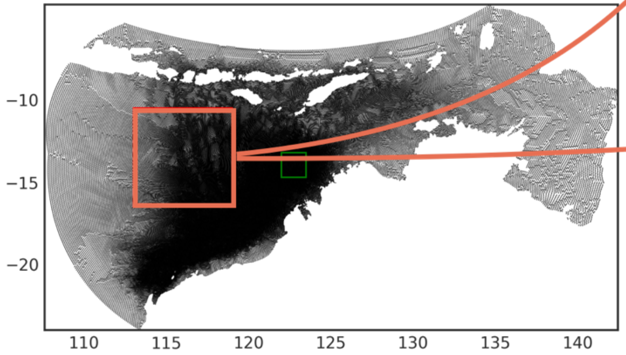

Satellites
Vessels
Radar
Moorings
Lagrangian Obs.
Radial data at Radar 1
Latent Field
Radar 1 radials
INDIAN OCEAN
a
SWOT SSHA
13° S
14° S
15° S
61° E
62° E
63° E
64° E
Background pixels: conventional view of SSHA from DUACS
110°E
115°E
120°E
125°E
130°E
135°E
Longitude
z (m ASB)
$\overline{T}$ (°C)

Sea-surface height



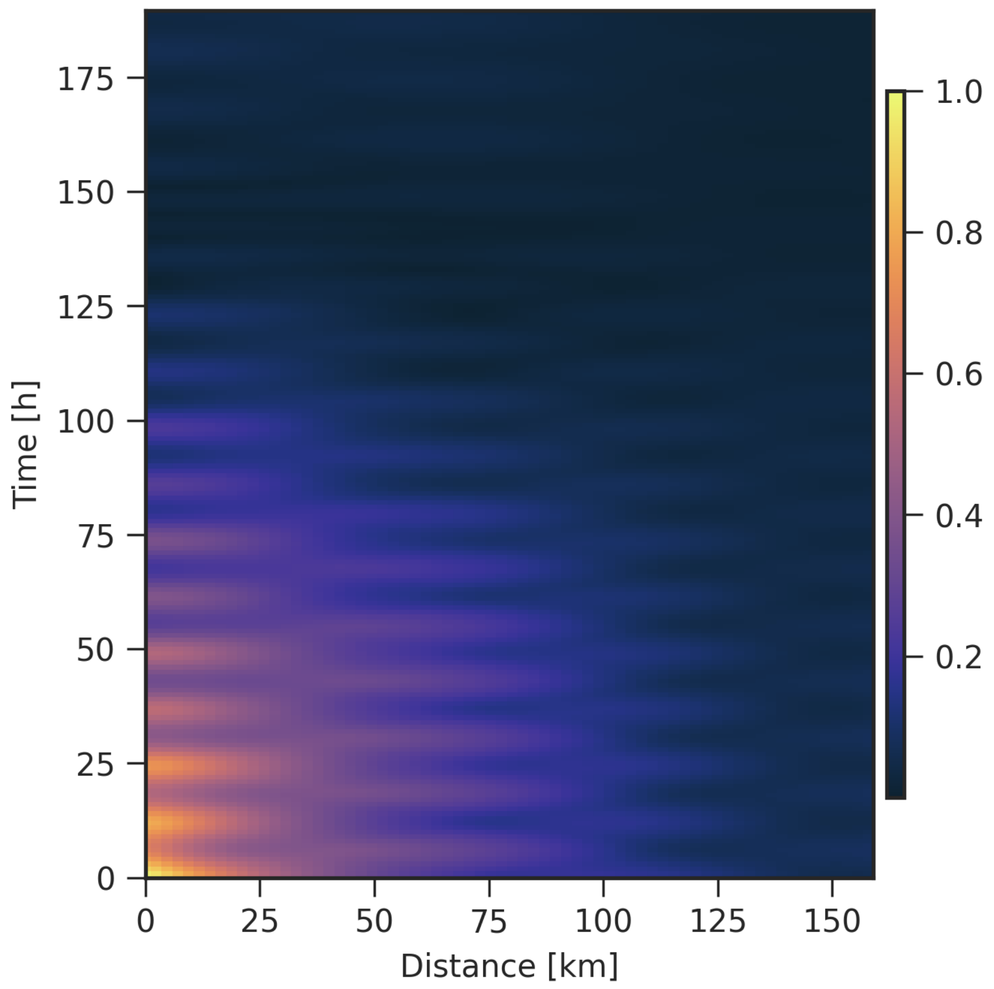
Meridional Velocity



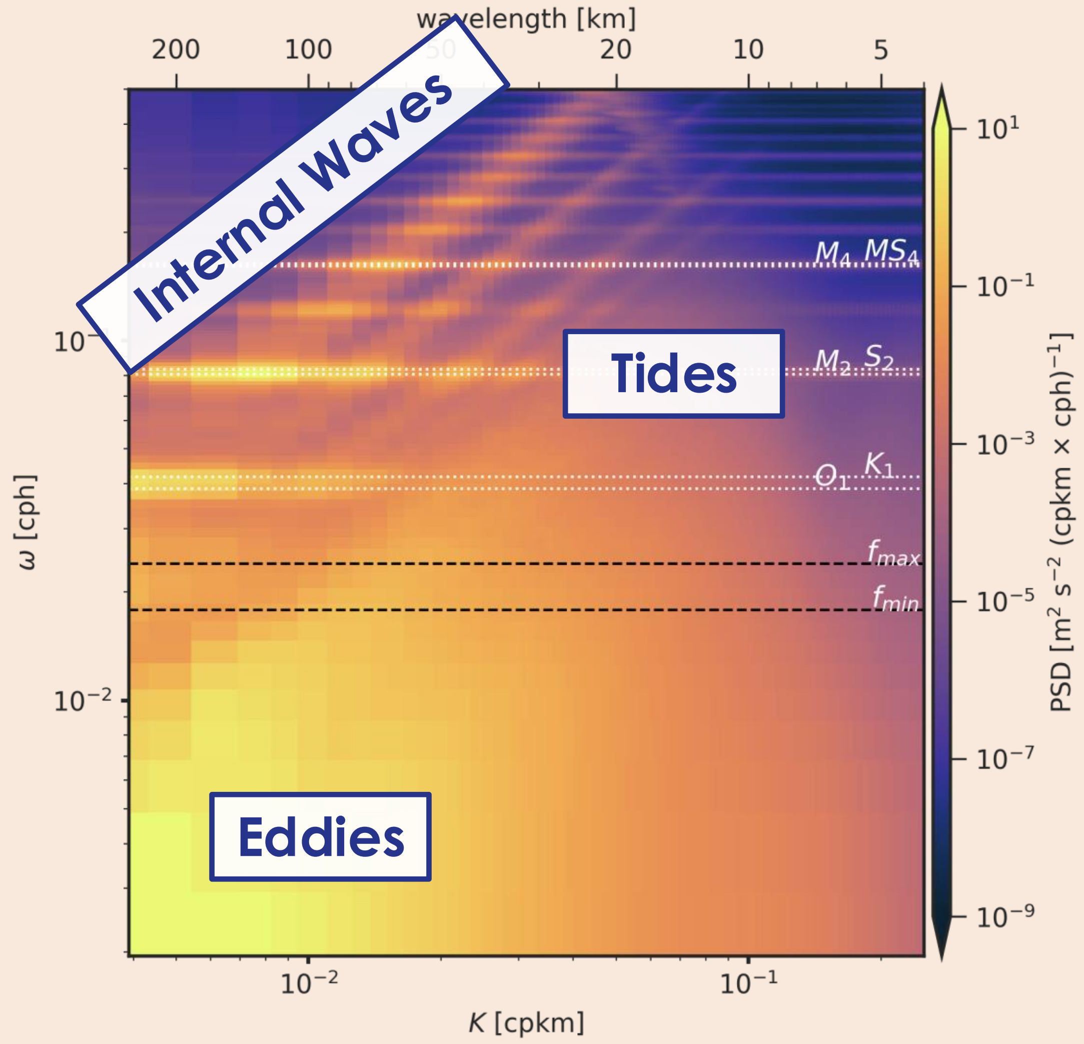


MD Rayson, LC Astfalck, ALS Ponte, AP Zulberti, NL Jones. (2024). 'Characteristic velocity and timescales of non-phase-locked internal tides in a mesoscale eddy field'. JGR Oceans.

Auto-Correlation

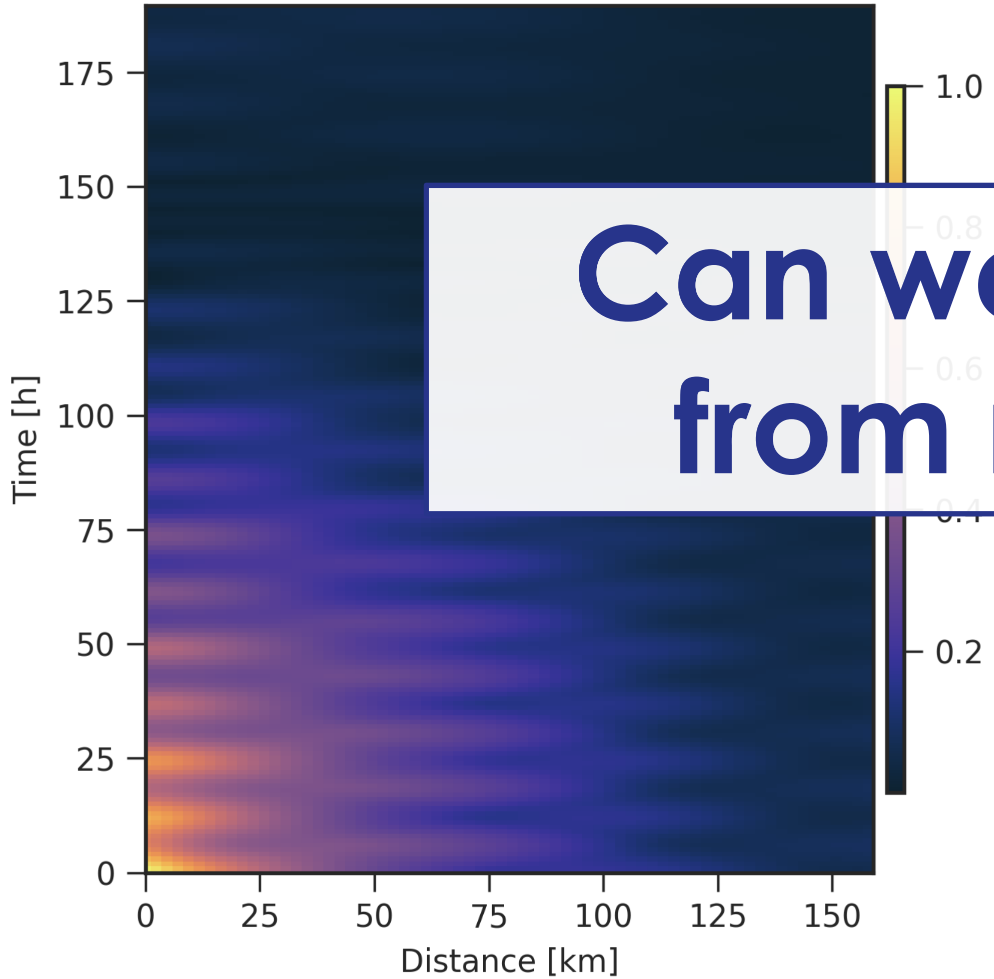


Spectral Density

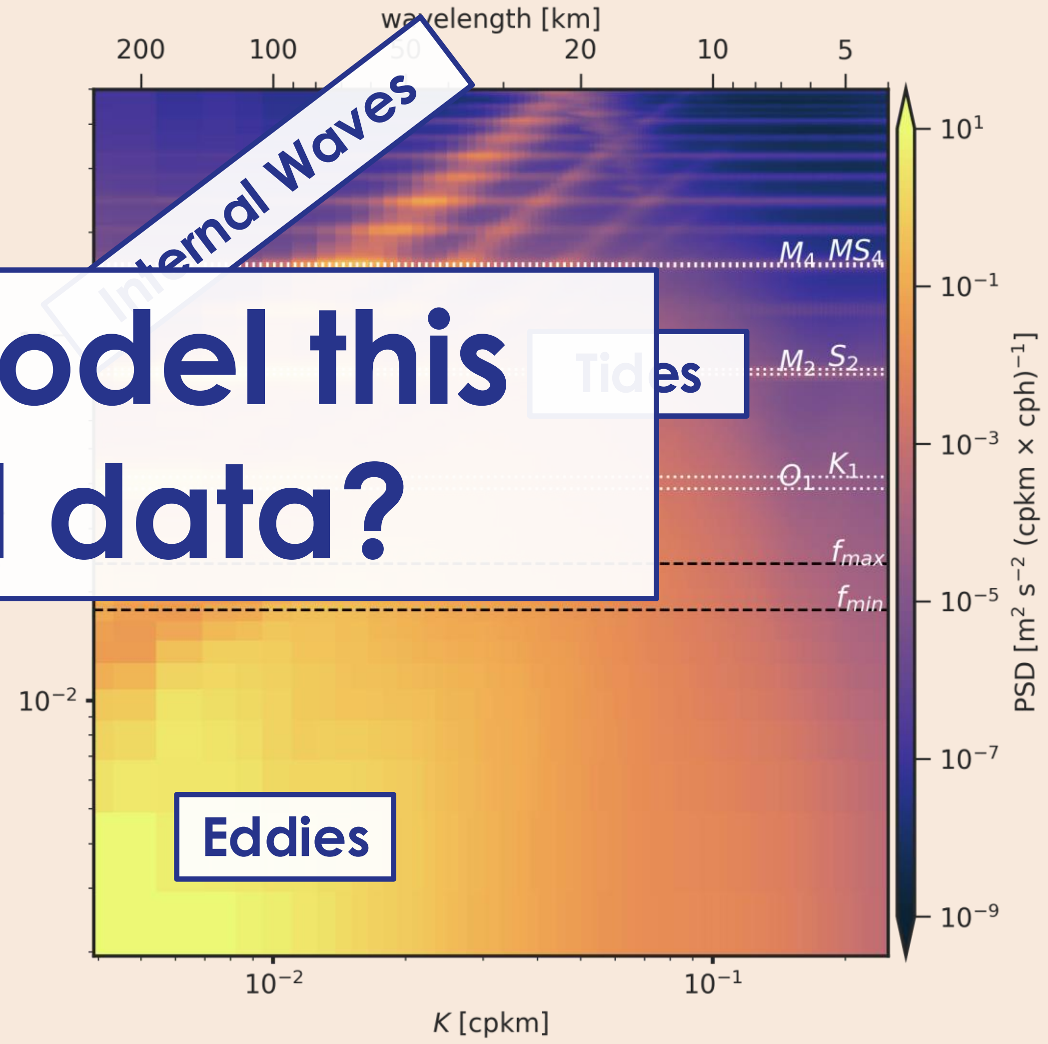


WC Edge, MD Rayson, NL Jones, AP Zulberti, LC Astfalck. Uncovering involute spatiotemporal dynamics of surface currents in the ocean. 2024 Ocean Modelling and Observations Workshop.

Auto-Correlation



Spectral Density



Can we model this from real data?

WC Edge, MD Rayson, NL Jones, AP Zulberti, LC Astfalck. Uncovering involute spatiotemporal dynamics of surface currents in the ocean. 2024 Ocean Modelling and Observations Workshop.

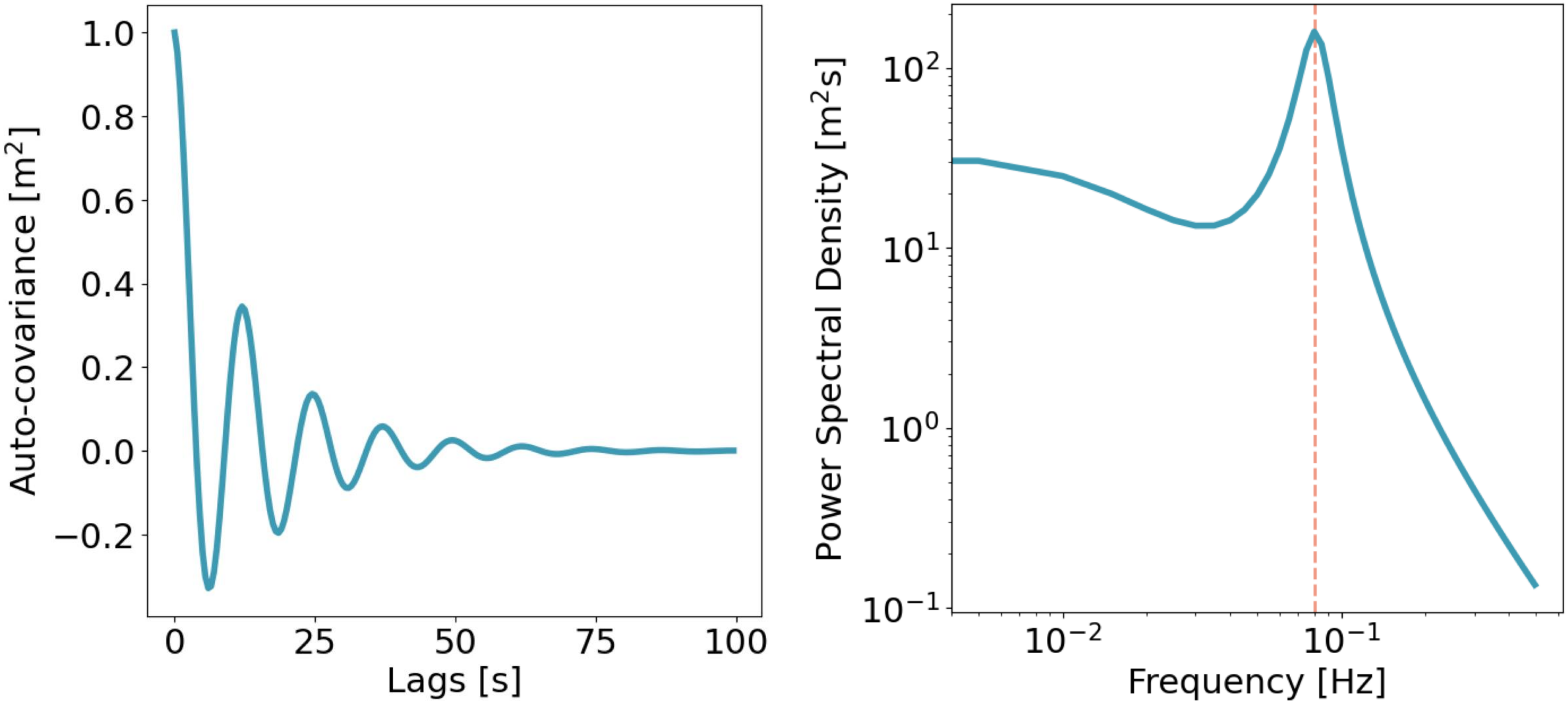
Wiener-Khinchin's Theorem

There is a remarkable result called Wiener-Khinchin's theorem that states if $X(t)$ is a stochastic process described with an auto-covariance function $\gamma_X(\tau)$, and $S_X(\omega)$ is its power spectral density,

$$S_X(\omega) = \mathcal{F}\{\gamma_X(\tau)\} = \int_{-\infty}^{\infty} \gamma_X(\tau) e^{-2\pi i \omega \tau} \, \mathrm{d}\tau.$$

As Fourier transforms are one-to-one, we may describe the behaviour of a process either, and equivalently, by its ACF or PSD.

Bochner's Theorem tells us if the PSD is positive the ACF is positive semi-definite!


Auto-covariance [m²]
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
0
25
50
75
100
Lags [s]
Power Spectral Density [m²s]
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-1}
Frequency [Hz]

What is the Gap in the Market?

$\Rightarrow$ **The gap**: a closed-form nonparametric family of ACFs that are

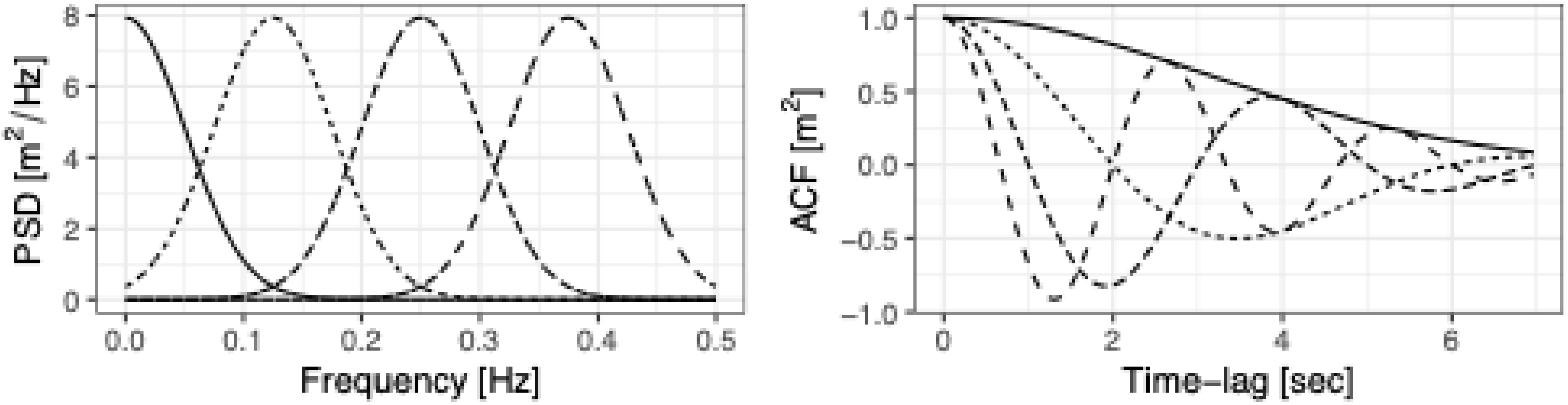
- provably dense (including in higher dimensions)
- efficient functional approximators
- defined over irregular coordinates

$\Rightarrow$ **Highlight**: this implies a general, closed-form, method to handle non-separability.

Spectral Kernels

⇒ **Wilson & Adams (2013)** use the Gaussian–Gaussian Fourier pairing to define the *Spectral Mixture Kernel*

Problem: Not provably dense in dimensions > 1; infinitely smooth; annoying to fit.



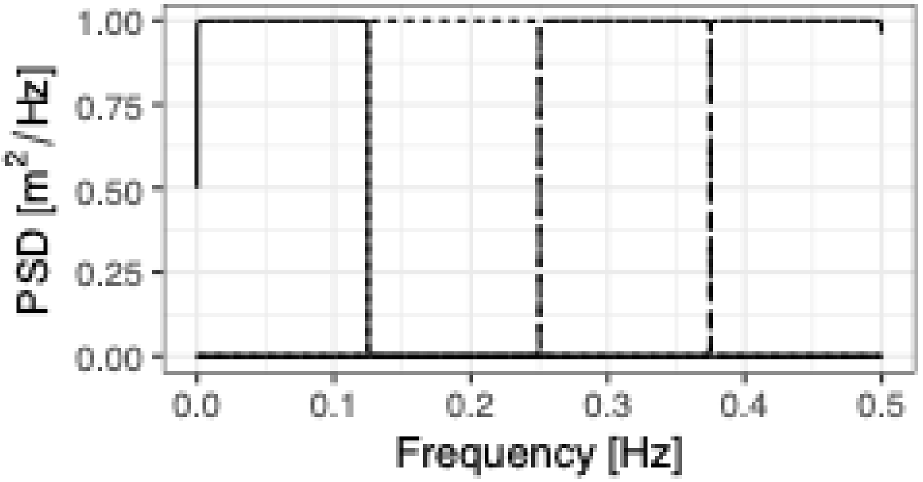
$$f(\omega) = \sum_i c_i f_i(\omega) \qquad \rho(\tau) = \sum_i c_i \rho_i(\tau)$$

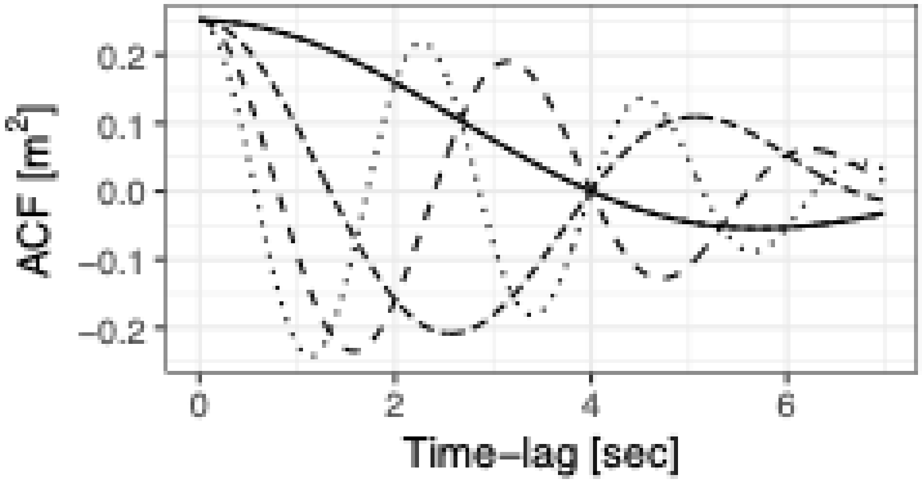
Spectral Kernels

$\Rightarrow$ **Tobar (2019)** uses the Sinc–Rectangular Fourier pairing to define the *Sinc Kernel*

Problem: Rectangles are inefficient function approximators.

$$\text{Rectangles} = \mathcal{O}(m^{-1}) \qquad \text{Simpson's Rule} = \mathcal{O}(m^{-4})$$
$$\text{Trapezoids} = \mathcal{O}(m^{-2}) \qquad \text{Gaussian Quadrature} = \mathcal{O}(c^{-2m}),\ c > 1$$





Introducing: The Spline Kernel

Paraphrased Theorem 1. *Let* $\{B_{i,k}(\omega)\}_{i=0}^{m-1}$ *denote a B-spline basis of degree* k *with knots* $\mathcal{K} = \{\kappa_0, \ldots, \kappa_{m+k}\}$. *Define* $\rho_{i,k}(\tau)$ *as the inverse Fourier transform of* $B_{i,k}(\omega)$. *Assume suitable* `[assumptions]`.

The ACF associated with $B_{i,k}$ *admits the closed-form expression*

$$\rho_{i,k}(\tau) = \frac{(-1)^k k!}{(2\pi\iota\tau)^{k+1}} \sum_{j=i}^{i+k} \alpha_j e^{2\pi\iota\kappa_j\tau} \left(e^{2\pi\iota\kappa_{\mathrm{w},j}\tau} \sum_{l=0}^{k} \frac{(-2\pi\iota\kappa_{\mathrm{w},j}\tau)^l}{l!} - 1 \right),$$

where $\kappa_{\mathrm{w},j} := \kappa_{i+k+1} - \kappa_j$, *and the* α_j *are known coefficients.*

Theorems also available for approximation efficiency and in higher dimensions.

LC Astfalck. (2025). Universal approximation of auto-covariance functions via spline kernels. Submitted to JASA

Why B-Splines?

B-splines form a basis for the space of piecewise polynomial splines ("B" for basis). That is, span$\{B_{i,k}(\omega)\} = \mathcal{S}_{k,\mathcal{K}}$. They are

- compactly supported,
- able to represent polynomials of arbitrary degree,
- locally adaptive,
- a familiar first stop in non-parametric approximation, and
- can achieve geometric convergence.

A Jackson-type Inequality

Paraphrased Theorem 2. *Let $f \in \mathcal{W}^{k,p}(\mathbb{R})$, the Sobolev space of k-times weakly differentiable functions in $L^p(\mathbb{R})$, for some $1 \leq p \leq 2$, and* `[some other assumptions].` *Let $\{\kappa_0 < \cdots < \kappa_{m+k}\}$ be a knot sequence with maximum knot distance $h_{\max} = \max_i\{\kappa_i - \kappa_{i-1}\}$.*

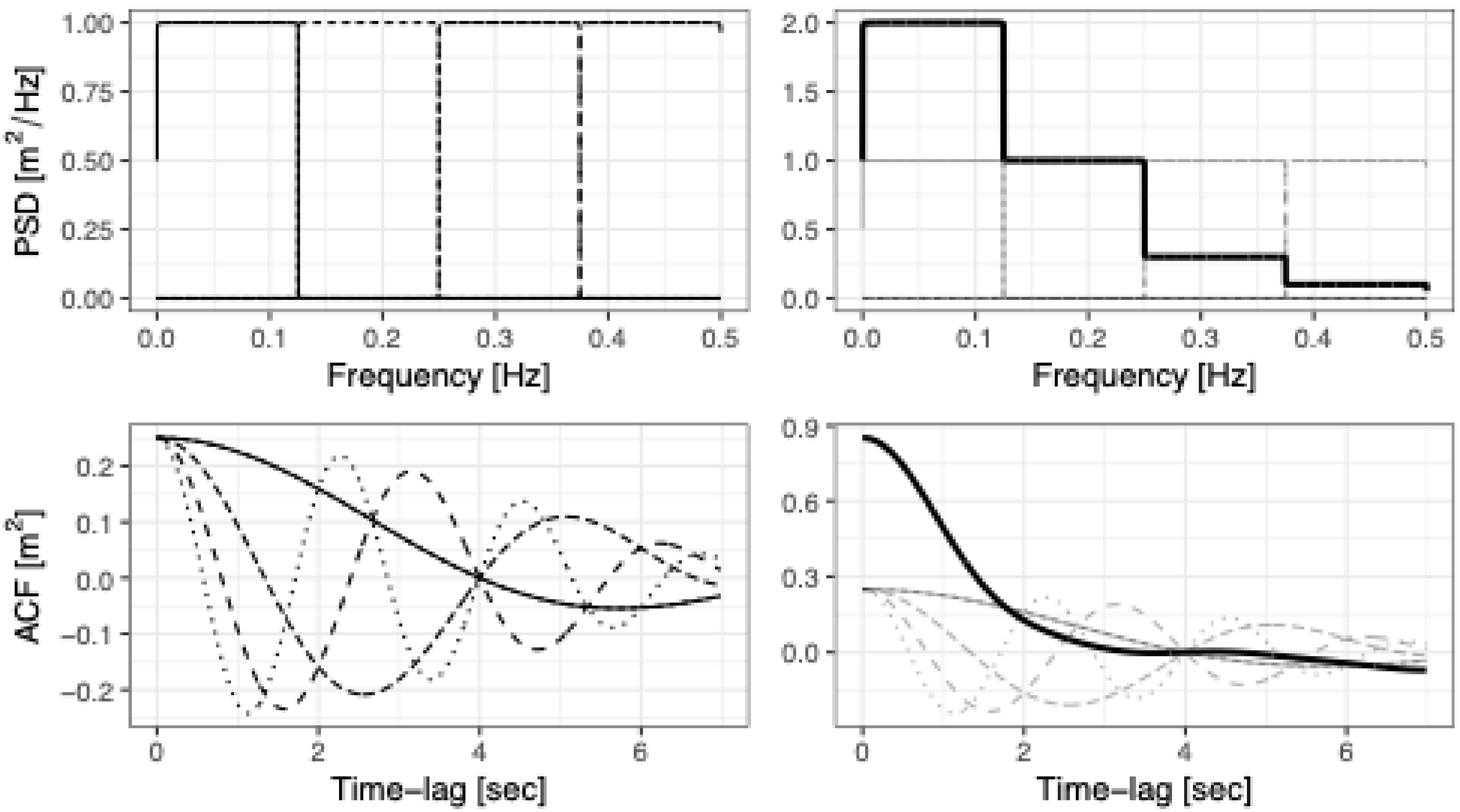
There exists a spline approximation $\hat{f}_k$ such that the autocovariance function $\gamma(\tau)$ and its spline-based approximation $\hat{\gamma}_k(\tau)$, from Theorem 1, satisfy

$$\|\gamma - \hat{\gamma}_k\|_{L^q} \leq C_j h_{\max}^{k+1} \|f^{(k)}\|_{L^p} \quad \text{for} \quad \frac{1}{p} + \frac{1}{q} = 1,$$

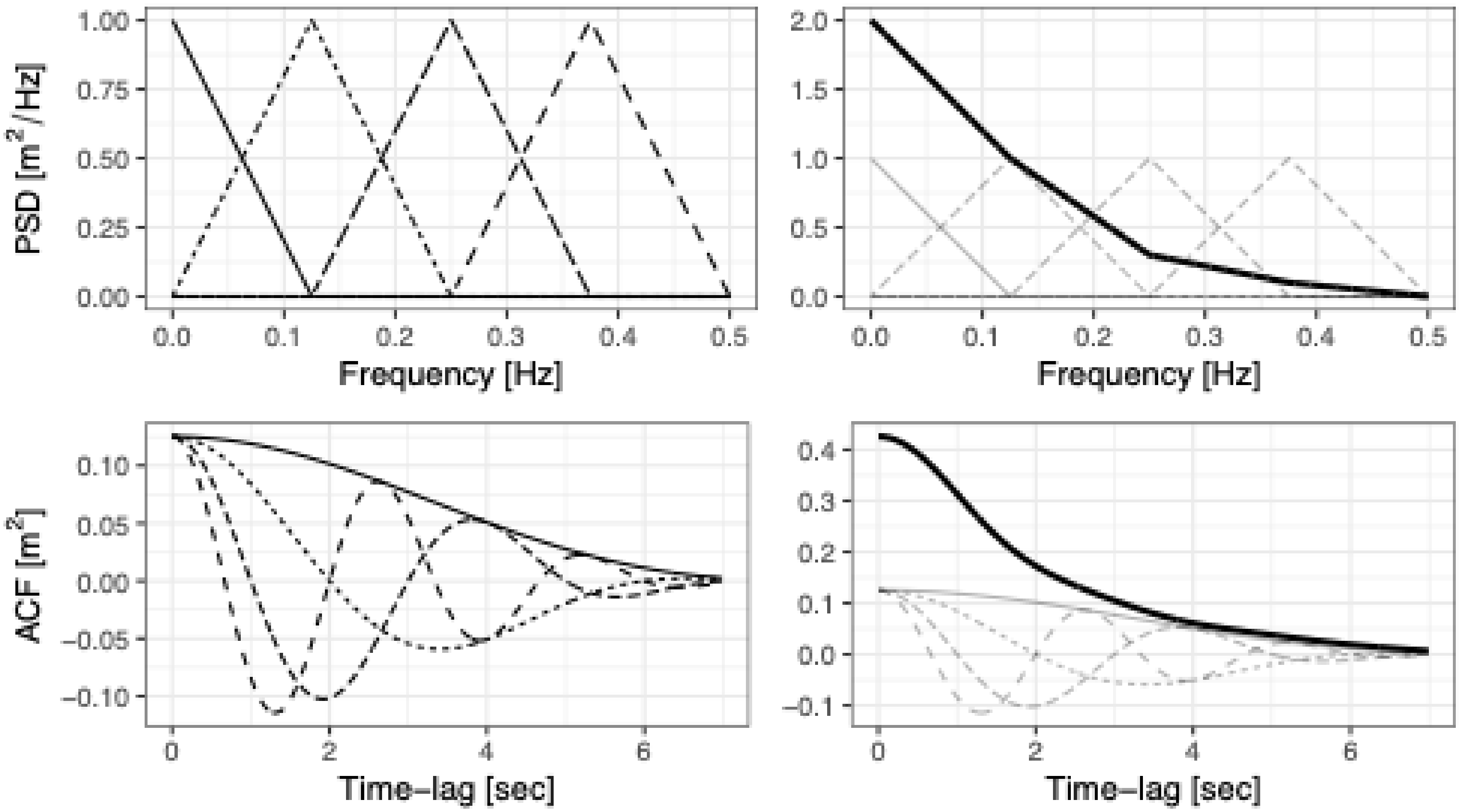
where $f^{(k)}$ is the kth derivative of f. Consequently, the class of spline-based ACFs is dense in the image of $\mathcal{W}^{k,p}(\mathbb{R})$ under the inverse Fourier transform, with convergence in $L^q(\mathbb{R})$.

LC Astfalck. (2025). Universal approximation of auto-covariance functions via spline kernels. Submitted to JASA

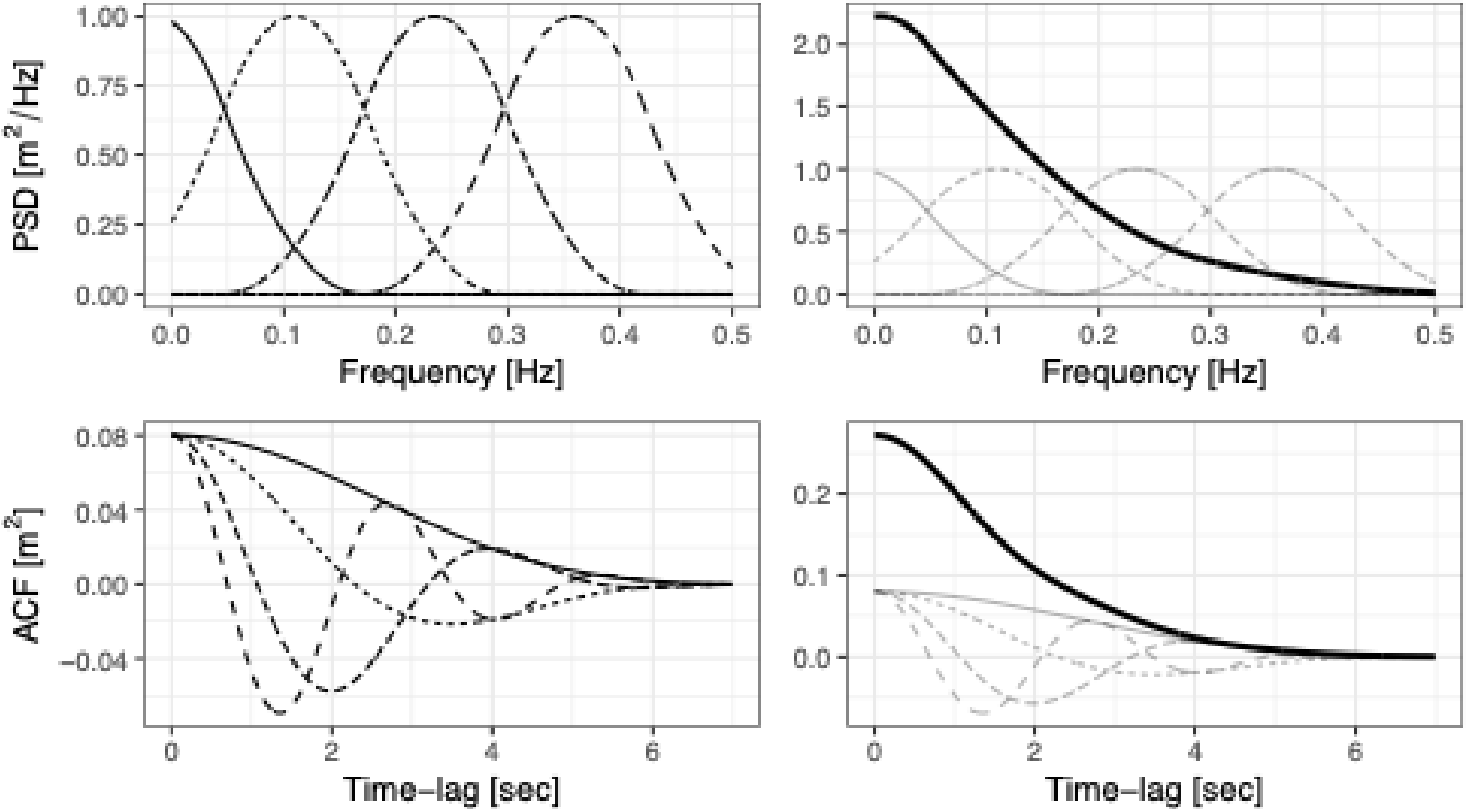
A Simple Example (k = 0)



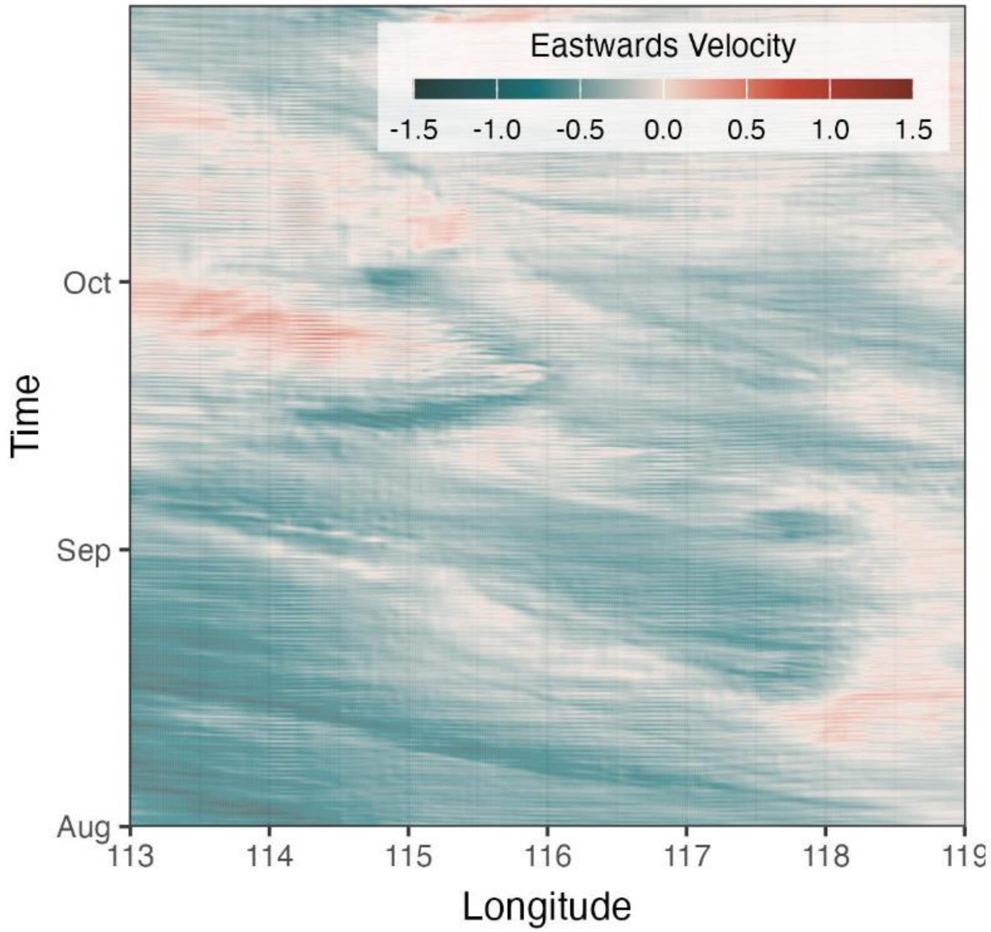
A Simple Example (k = 1)



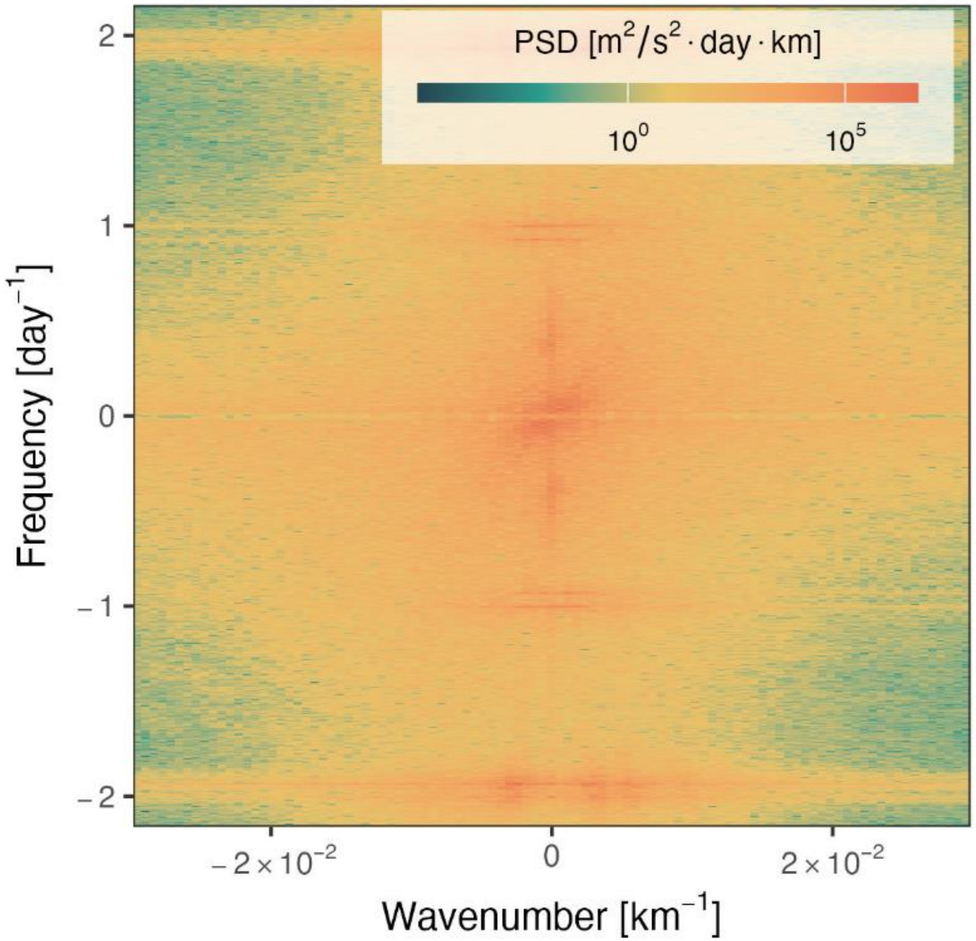
A Simple Example (k = 2)



Numerical Oceanographic Model

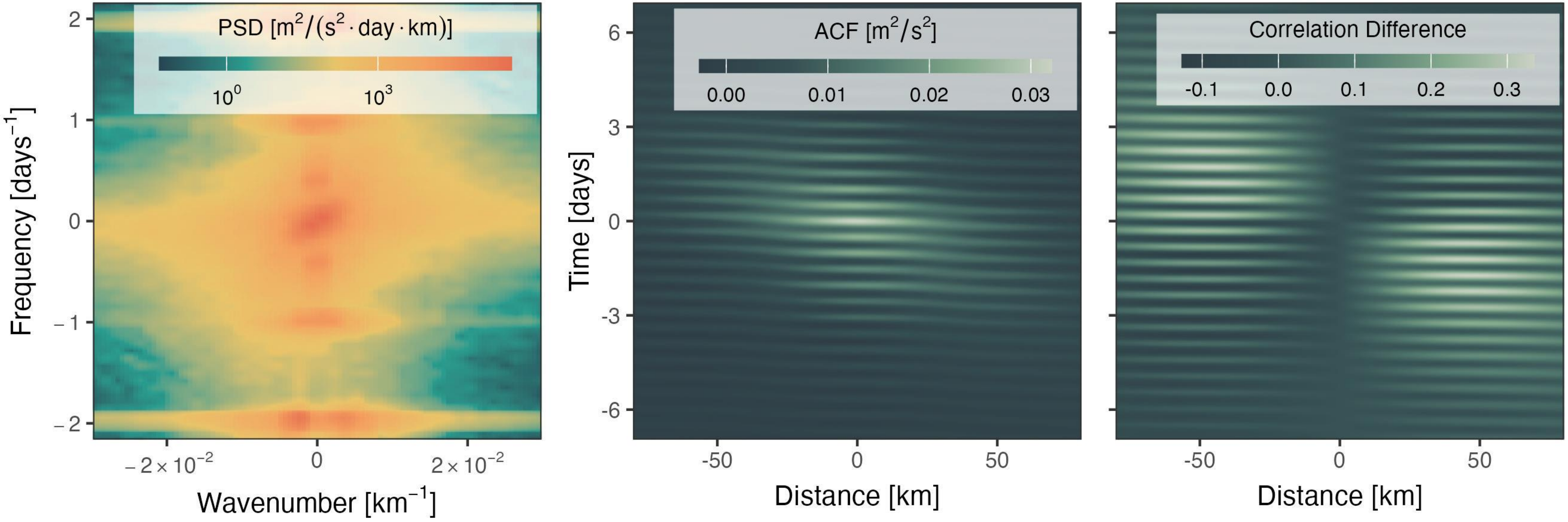


SUNTANS Numerical Model; Longitudinal Slice



2D Periodogram of SUNTANS slice

Closed-form, Non-parametric Fit



Universal Modelling of Autocovariance Functions via Spline Kernels

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[1]*School of Physics, Mathematics & Computing, The University of Western Australia, Australia*

June 30, 2025

Abstract

Flexible modelling of the autocovariance function (ACF) is central to time-series, spatial, and spatio-temporal analysis. Modern applications often demand flexibility beyond classical parametric models, motivating non-parametric descriptions of the ACF. Bochner's Theorem guarantees that any positive spectral measure yields a valid ACF via the inverse Fourier transform; however, existing non-parametric approaches in the spectral domain rarely return closed-form expressions for the ACF itself. We develop a flexible, closed-form class of non-parametric ACFs by deriving the inverse Fourier transform of B-spline spectral bases with arbitrary degree and knot placement. This yields a general class of ACF with three key features: (i) it is provably dense, under an L^1 metric, in the space of weakly stationary, mean-square continuous ACFs with mild regularity conditions; (ii) it accommodates univariate, multivariate, and multidimensional processes; and (iii) it naturally supports non-separable structure without requiring explicit imposition. Jackson-type approximation bounds establish convergence rates, and empirical results on simulated and real-world data demonstrate accurate process recovery. The method provides a practical and theoretically grounded approach for constructing a non-parametric class of ACF.

Keywords: autocovariance function, spline basis, non-parametric modelling, non-separability, Gaussian processes

An Honest Appraisal

bskernel

lifecycle experimental license MIT

This package provides flexible auto-covariance kernel construction via inverse Fourier transforms of B-spline bases, as well as some handy tools for optimisation. Please note, if you have found yourself in the GitHub repo, please navigate here for the pkgdown page.

What we do have

- ✓ A framework for non-parametric modelling of the ACF
- ✓ Support for multivariate and multidimensional processes (e.g. multivariate spactial processes)
- ✓ Theoretical results and empirical validations
- ✓ An `R` package (an autodiffed `python` implementation in `GPJax` is en-route)
- ✓ Demonstration on some simpler oceanographic datasets

`astfalckl.github.io`

An Honest Appraisal

What we need

- ★ For target problem, only applied to numerical data with Whittle-based inference
- ★ Much work remains on efficient inference in complex problems (fast solutions for regular data + unknown knots; variational methods; amortised inference)
- ★ Pragmatic solutions for trans-dimensional estimation
- ★ Extensions to non-stationary descriptions

`astfalckl.github.io`