Novelty Assessment Report

Paper: Revisiting Nonstationary Kernel Design for Multi-Output Gaussian Processes

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Abstract

Multi-output Gaussian processes (MOGPs) provide a Bayesian framework for modeling non-linear functions with multiple outputs, in which nonstationary kernels are essential for capturing input-dependent variations in observations. However, from a spectral (dual) perspective, existing nonstationary kernels inherit the inflexibility and over-parameterization of their spectral densities due to the restrictive spectral–kernel duality. To overcome this, we establish a generalized spectral–kernel duality that enables fully flexible matrix-valued spectral densities — albeit at the cost of quadratic parameter growth in the number of outputs. To achieve linear scaling while retaining sufficient expressiveness, we propose the multi-output low-rank nonstationary (MO-LRN) kernel: by modeling the spectral density through a low-rank matrix whose rows are independently parameterized by bivariate Gaussian mixtures. Experiments on synthetic and real-world datasets demonstrate that MO-LRN consistently outperforms existing MOGP kernels in regression, missing-data interpolation, and imputation tasks.

Core Task Landscape

This paper addresses: **Nonstationary Kernel Design for Multi-Output Gaussian Processes**

A total of **24 papers** were analyzed and organized into a taxonomy with **15 categories**.

Taxonomy Overview

The research landscape has been organized into the following main categories:

- **Kernel Design and Covariance Structures**
- **Scalability and Computational Efficiency**
- **Specialized Multi-Output Modeling Frameworks**
- **Spatiotemporal and Temporal Modeling**
- **Applications and Domain-Specific Implementations**
- **General Frameworks and Surveys**

Complete Taxonomy Tree

- Nonstationary Kernel Design for Multi-Output Gaussian Processes Survey Taxonomy
- Kernel Design and Covariance Structures
  - Spectral and Frequency-Domain Kernel Methods ★ (3 papers)
  - [0] Revisiting Nonstationary Kernel Design for Multi-Output Gaussian Processes (Anon et al., 2026) View paper
  - [12] Nonstationary multi-output gaussian processes via harmonizable spectral mixtures (Altamirano, 2021) View paper
  - [23] Spectral mixture kernels for Multi-Output Gaussian processes (Gabriel Parra, 2017) View paper
  - Convolution-Based Multi-Output Kernels (2 papers)
  - [13] Computationally efficient convolved multiple output Gaussian processes (Mauricio A. Ãlvarez, 2011) View paper
  - [24] Sparse Convolved Multiple Output Gaussian Processes (Ãlvarez, 2009) View paper
  - Advanced Nonstationary Kernel Architectures (2 papers)
  - [1] Advanced stationary and nonstationary kernel designs for domain-aware gaussian processes (Marcus M. Noack, 2022) View paper
  - [7] Modelling non-stationary functions with Gaussian processes (Sami Remes, 2019) View paper
  - Nonparametric Operator Learning with Kernels (1 papers)
  - [10] Learning Nonparametric Volterra Kernels with Gaussian Processes (Magnus Ross, 2021) View paper
- Scalability and Computational Efficiency
  - Variational Sparse Approximations (2 papers)
  - [6] Collaborative nonstationary multivariate gaussian process model (Rui Meng, 2021) View paper
  - [17] Large Linear Multi-output Gaussian Process Learning (Vladimir Feinberg, 2017) View paper
  - Local and Adaptive Approximation Methods (3 papers)
  - [2] Multi-output local Gaussian process regression: Applications to uncertainty quantification (Ilias Bilionis, 2012) View paper
  - [5] Adaptive multioutput gradient RBF tracker for nonlinear and nonstationary regression (Tong Liu, 2023) View paper
  - [15] Efficient adaptive deep gradient RBF network for multi-output nonlinear and nonstationary industrial processes (Tong Liu, 2023) View paper
- Specialized Multi-Output Modeling Frameworks
  - Sparse Correlation and Transfer Learning (2 papers)
  - [4] Non-stationary and Sparsely-correlated Multi-output Gaussian Process with Spike-and-Slab Prior (Xin-Ming Wang, 2024) View paper
  - [14] Multi-Output Selective Ensemble Identification of Nonlinear and Nonstationary Industrial Processes. (Tong Liu, 2022) View paper

- Deep and Hierarchical Gaussian Process Extensions (1 papers)
- [20] Conditional Deep Gaussian Processes: multi-fidelity kernel learning (Chi-Ken Lu, 2020) View paper

- Spatiotemporal and Temporal Modeling
  - Temporal Evolution of Spatial Dependence (1 papers)
  - [21] Learning Temporal Evolution of Spatial Dependence with Generalized Spatiotemporal Gaussian Process Models (Lan Shiwei, 2019) View paper
  - Multivariate Spatial Nonparametric Models (1 papers)
  - [19] Multivariate spatial nonparametric modelling via kernel processes mixing (Montserrat Fuentes, 2013) View paper
  - Time-Varying Coefficient Models for Time Series (1 papers)
  - [22] A Stratified Penalized Kernel Method for Semiparametric Variable Labeling and Estimation of Multi-Output Time-Varying Coefficient Models for Nonstationary Time Series (Ting Zhang, 2021) View paper
- Applications and Domain-Specific Implementations
  - System Identification and Parameter Estimation (1 papers)
  - [9] UAV parameter estimation with multi-output local and global Gaussian process approximations (Prasad Hemakumara, 2013) View paper
  - Healthcare and Academic Analytics (2 papers)
  - [8] A Novel Gaussian Process Approach for Prediction of University Academic Evaluation (Daohua Yu, 2025) View paper
  - [16] Nonstationary multivariate Gaussian processes for electronic health records. (Rui Meng, 2021) View paper
  - Remote Sensing and Spatial Enhancement (2 papers)
  - [11] Autonomous Intelligence Measurements and Sensor Systems (AIMS): Gaussian Processes in Remote Sensing: Literature Review (Peter Fuhr, 2024) View paper
  - [18] Non-stationary Multi-output Gaussian Processes for Enhancing Resolution over Diffusion Tensor Fields (Jhon F. Cuellar-Fierro, 2018) View paper
- General Frameworks and Surveys (1 papers)
  - [3] Gaussian Processes (Yashaswini Mittal, 2023) View paper

Narrative

Core task: nonstationary kernel design for multi-output Gaussian processes. The field addresses how to model complex dependencies across multiple outputs when the underlying statistical properties vary over input space or time. The taxonomy reveals several complementary research directions. Kernel Design and Covariance Structures focuses on constructing flexible covariance functions, including spectral and frequency-domain methods that capture nonstationarity through modulated basis representations. Scalability and Computational Efficiency tackles the computational burden of multi-output GPs through sparse approximations and efficient linear algebra. Specialized Multi-Output Modeling Frameworks explores convolution-based constructions and latent process formulations that share information across outputs. Spatiotemporal and Temporal Modeling emphasizes settings where inputs have explicit spatial or temporal structure, while Applications and Domain-Specific Implementations demonstrate how these methods solve real-world problems in remote sensing, healthcare, and engineering. General Frameworks and Surveys provide overarching perspectives on the landscape.

Within Kernel Design and Covariance Structures, spectral and frequency-domain approaches have emerged as a particularly active line of work for handling nonstationarity. Harmonizable Spectral Mixtures[12] and Spectral Mixture Kernels[23] exemplify how frequency-domain representations can flexibly model varying correlation patterns, offering an alternative to purely spatial constructions. Nonstationary Kernel Design[0] sits naturally within this spectral branch, emphasizing frequency-domain techniques for multi-output settings where standard stationary assumptions break down. Compared to Harmonizable Spectral Mixtures[12], which focuses on harmonizable processes, and Spectral Mixture Kernels[23], which popularized spectral mixtures for single-output cases, the original work extends these ideas to the multi-output regime with explicit nonstationary mechanisms. Meanwhile, other branches such as Specialized Multi-Output Modeling Frameworks pursue convolution-based methods like Convolved Multiple Output GP[13] and Sparse Convolved GP[24], trading spectral flexibility for interpretable latent process structures. The interplay between spectral expressiveness and computational tractability remains a central open question across these directions.

Related Works in Same Category

The following **2 sibling papers** share the same taxonomy leaf node with the original paper:

1. Nonstationary multi-output gaussian processes via harmonizable spectral mixtures

Authors: Altamirano, Matias, MatÃas Altamirano, Tobar, Felipe, et al. (7 authors total) | **Year/Venue**: 2021 | **URL**: View paper

Abstract

Kernel design for Multi-output Gaussian Processes (MOGP) has received increased attention recently. In particular, the Multi-Output Spectral Mixture kernel (MOSM) arXiv:1709.01298 approach has been praised as a general model in the sense that it extends other approaches such as Linear Model of Corregionalization, Intrinsic Corregionalization Model and Cross-Spectral Mixture. MOSM relies on Cram\'er's theorem to parametrise the power spectral densities (PSD) as a Gaussian mixture, thus, having a ...

Relationship Analysis

Both papers belong to the Spectral and Frequency-Domain Kernel Methods category, using spectral representations and harmonizable processes for nonstationary multi-output GP kernel design. The candidate paper (MOHSM) proposes a two-level mixture spectral density based on Kakihara's theorem with localized stationary regimes, while the original paper (MO-LRN) introduces an advanced Kakihara theorem that removes conventional restrictions and proposes a low-rank spectral density with independent bivariate Gaussian mixture factors. The original paper explicitly critiques MOHSM's limitations (inflexibility, over-parameterization) and demonstrates superior performance with linear parameter scaling versus MOHSM's quadratic growth.

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2. Spectral mixture kernels for Multi-Output Gaussian processes

Authors: Gabriel Parra, Tobar, Felipe, Felipe Tobar, Felipe A. Tobar | **Year/Venue**: 2017 | **URL**: View paper

Abstract

Early approaches to multiple-output Gaussian processes (MOGPs) relied on linear combinations of independent, latent, single-output Gaussian processes (GPs). This resulted in cross-covariance functions with limited parametric interpretation, thus conflicting with the ability of single-output GPs to understand lengthscales, frequencies and magnitudes to name a few. On the contrary, current approaches to MOGP are able to better interpret the relationship between different channels by directly model...

Relationship Analysis

Both papers belong to the Spectral and Frequency-Domain Kernel Methods category, utilizing spectral representations and frequency-domain parameterizations for constructing nonstationary multi-output Gaussian process kernels. They overlap in addressing the design of expressive spectral densities for MOGPs through spectral mixture approaches, with both leveraging Cramér's theorem (or related spectral duality results) to map spectral densities to kernel space. The key difference is that the original paper (MO-LRN) proposes a low-rank factorization of the spectral density with independent bivariate Gaussian mixture components to achieve linear parameter scaling, while the candidate paper (MOSM) focuses on complex-valued square-exponential cross-spectral densities without the low-rank constraint, resulting in different expressiveness-efficiency trade-offs.

Contributions Analysis

Overall novelty summary. The paper proposes a generalized spectral–kernel duality and a multi-output low-rank nonstationary (MO-LRN) kernel for multi-output Gaussian processes. It resides in the 'Spectral and Frequency-Domain Kernel Methods' leaf, which contains three papers total. This leaf sits within the broader 'Kernel Design and Covariance Structures' branch, indicating a moderately populated research direction focused on frequency-domain parameterizations. The taxonomy shows this is an active but not overcrowded area, with sibling papers exploring harmonizable processes and spectral mixture approaches for capturing nonstationarity.

The taxonomy reveals several neighboring research directions. The 'Convolution-Based Multi-Output Kernels' leaf (two papers) pursues latent function interpretations rather than spectral representations, while 'Advanced Nonstationary Kernel Architectures' (two papers) explores domain-aware and input-dependent covariances without frequency-domain constraints. The 'Scalability and Computational Efficiency' branch addresses computational bottlenecks through sparse approximations, a concern orthogonal to kernel expressiveness. The scope notes clarify that spectral methods exclude purely spatial-domain convolution approaches, positioning this work within a distinct methodological paradigm that emphasizes frequency-domain flexibility over latent process interpretability.

Among 18 candidates examined, the generalized spectral–kernel duality contribution shows one refutable candidate out of seven examined, suggesting some prior work addresses similar duality concepts within the limited search scope. The MO-LRN kernel contribution examined one candidate with no refutations, indicating less direct overlap in the specific low-rank spectral density parameterization. The experimental validation contribution examined ten candidates with no refutations, though this reflects the limited search scale rather than exhaustive coverage. The statistics suggest the duality framework has more substantial prior work, while the specific low-rank construction and empirical demonstrations appear more distinctive within the examined literature.

Based on the top-18 semantic matches examined, the work appears to offer meaningful contributions in low-rank spectral density design and empirical validation, though the generalized duality framework shows some overlap with existing spectral approaches. The analysis covers a focused subset of the literature and does not claim exhaustive coverage of all relevant prior work in multi-output Gaussian process kernel design or spectral methods more broadly.

This paper presents **3 main contributions**, each analyzed against relevant prior work:

Contribution 1: Generalized spectral–kernel duality for multi-output Gaussian processes

Description: The authors introduce an advanced version of Kakihara's theorem that relaxes structural constraints on spectral densities, allowing fully flexible matrix-valued spectral densities for multi-output Gaussian processes, though at the cost of quadratic parameter growth in the number of outputs.

This contribution was assessed against **7 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

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1. Modelling non-stationary functions with Gaussian processes

URL: View paper

Brief Assessment

Modelling Nonstationary Functions[7] focuses on non-stationary kernel design for single-output and multi-output GPs using spectral mixture approaches, but does not present a generalized spectral-kernel duality that relaxes structural constraints on matrix-valued spectral densities in the same manner as the original paper's advanced Kakihara theorem.

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2. Spectral mixture kernels for Multi-Output Gaussian processes

URL: View paper

Prior Art Analysis

Spectral Mixture Kernels[23] demonstrates that prior work exists on spectral-kernel duality for multi-output Gaussian processes with flexible matrix-valued spectral densities. The candidate paper presents Cramér's theorem as the foundation for constructing multi-output spectral mixture kernels through spectral density design, predating the original paper's claimed generalization of Kakihara's theorem. Both papers address the same fundamental problem of designing matrix-valued spectral densities for MOGPs, though they employ different theoretical frameworks and parameterizations.

Evidence

Evidence 1 - **Rationale**: Both papers establish spectral-kernel duality theorems for multi-output GPs. The candidate presents Cramér's theorem as the foundation for flexible matrix-valued spectral densities, while the original claims to establish a 'generalized' version. This shows prior work existed on this theoretical framework. - **Original**: we establish a generalized spectral-kernel duality that enables fully flexible matrix-valued spectral densities - albeit at the cost of quadratic parameter growth in the number of outputs. - **Candidate**: theorem 2.1(cramér's theorem [5, 6]) a family{kij(τ)}m i,j=1 of complex-valued functions are the covariance functions of a weakly-stationary multivariate stochastic process if and only if they (i) admit the representation kij(τ) = ∫ rn eιω⊤τ dμfij(ω) ∀i,j ∈{1,...,m } where each fij is a complex-valu...

Evidence 2 - **Rationale**: The candidate explicitly states its purpose is to enable flexible spectral densities for MOGPs using Cramér's theorem, demonstrating that the concept of flexible matrix-valued spectral densities for multi-output GPs was already established in prior work. - **Original**: to overcome this, we establish a generalized spectral-kernel duality that enables fully flexible matrix-valued spectral densities - **Candidate**: the main purpose of this work is to extend the spectral mixture concept to mogps: we rely on cramér's theorem [5, 6], the multivariate version of bochner's theorem, to propose an expressive family of complex-valued square-exponential cross-spectral densities

Evidence 3 - **Rationale**: Both papers use Gaussian mixture parameterizations in the spectral domain to construct flexible kernels. The candidate demonstrates that bivariate Gaussian spectral densities for multi-output kernels were already established, refuting the novelty of using such parameterizations. - **Original**: by specifying the spectral density as a mixture of bivariate gaussians, i.e., p(ω1, ω2) =pq q=1 αqsq(ω1, ω2), where each sq(ω1, ω2) is a bivariate gaussian component, the ng-sm kernel can be derived via eq. (1). - **Candidate**: by making use of the preceding formula withλ = 1 2 σ-1 ij , b = -1 2 (σ-1 ij μij + ι(τ + θij)) and c= -1 2 μ⊤ ijς-1 ij μij + ιφij, we get kij(τ) = αij exp (1 2 (σ-1 ij μij + ι(τ + θij))⊤ σij (σ-1 ij μij + ι(τ + θij)) -1 2 μ⊤ ijς-1 ij μ⊤ ijς-1 ij μij + ιφij)

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3. Symplectic spectrum gaussian processes: Learning hamiltonians from noisy and sparse data

URL: View paper

Brief Assessment

Symplectic Spectrum GP[36] focuses on Hamiltonian mechanics and symplectic structures for physical systems, not on general multi-output GP kernel design or spectral-kernel duality theory.

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4. Multi-Output Convolution Spectral Mixture for Gaussian Processes

URL: View paper

Brief Assessment

Convolution Spectral Mixture[38] focuses on constructing multi-output kernels through convolution in the spectral domain, not on establishing a generalized spectral-kernel duality that relaxes structural constraints on spectral densities.

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5. MOGPTK: The multi-output Gaussian process toolkit

URL: View paper

Brief Assessment

MOGPTK[35] is a software toolkit for multi-output Gaussian processes. The provided context only mentions spectral Gaussian means/variances for parameter initialization, with no discussion of spectral-kernel duality theory or relaxing structural constraints on spectral densities.

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6. Multi-Output Gaussian Process Toolkit with sparse formulation for spectral kernels

URL: View paper

Brief Assessment

Sparse Spectral Kernels[39] focuses on sparse approximations and toolkit implementation for the MOSM kernel, not on establishing new spectral-kernel duality theorems. The candidate does not present theoretical work on relaxing structural constraints on spectral densities or establishing generalized duality results.

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7. The Generalised Gaussian Process Convolution Model

URL: View paper

Brief Assessment

The Generalised GP Convolution[37] candidate paper's provided context contains only the title page and declaration, with no technical content about spectral-kernel duality or multi-output Gaussian processes. Cannot assess novelty refutation without access to the paper's methodology sections.

Contribution 2: Multi-output low-rank nonstationary (MO-LRN) kernel

Description: The authors design a novel nonstationary kernel for multi-output Gaussian processes that uses a low-rank spectral density parameterized by independent bivariate Gaussian mixtures. This design achieves linear parameter scaling in the number of outputs while maintaining sufficient expressiveness for modeling complex patterns.

This contribution was assessed against **1 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

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1. Non-stationary Multi-output Gaussian Processes for Enhancing Resolution over Diffusion Tensor Fields

URL: View paper

Brief Assessment

Diffusion Tensor Fields[18] focuses on enhancing resolution over diffusion tensor fields using non-stationary multi-output Gaussian processes, which is a different application domain. The candidate's limited context does not provide sufficient technical detail about kernel parameterization or low-rank spectral density design to challenge the original paper's novelty claim about linear parameter scaling through independent bivariate Gaussian mixtures.

Contribution 3: Experimental validation across multiple tasks

Description: The authors conduct comprehensive experiments on synthetic and real-world datasets for regression, interpolation, and imputation tasks, demonstrating that their MO-LRN kernel consistently outperforms existing multi-output Gaussian process kernels.

This contribution was assessed against **10 related papers** from the literature. Papers with potential prior art are analyzed in detail with textual evidence; others receive brief assessments.

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1. Remarks on multi-output Gaussian process regression

URL: View paper

Brief Assessment

Multi-Output GP Remarks[25] provides only a brief abstract fragment mentioning multi-output regression problems and MOGPs. No experimental details, datasets, or task descriptions are provided that would allow comparison with the original paper's comprehensive experiments on regression, interpolation, and imputation tasks across synthetic and real-world datasets.

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2. Multi-output Gaussian processes for multi-population longevity modelling

URL: View paper

Brief Assessment

Longevity Modelling[26] focuses on multi-population longevity modeling using mortality data, not general regression/interpolation/imputation tasks on synthetic and real-world datasets as in the original paper.

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3. Multi-output Gaussian processes for crowdsourced trafï¬c data imputation

URL: View paper

Brief Assessment

Traffic Data Imputation[31] focuses on crowdsourced traffic data imputation using multi-output Gaussian processes, which is a specific application domain. Without access to the candidate's full text, I cannot assess whether it demonstrates prior work on the general experimental methodology (regression, interpolation, and imputation tasks) claimed by the original paper.

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4. Accurate and uncertainty-aware multi-task prediction of HEA properties using prior-guided deep Gaussian processes

URL: View paper

Brief Assessment

HEA Property Prediction[33] focuses on predicting high-entropy alloy properties using deep Gaussian processes, not on multi-output Gaussian process kernel design for general regression/interpolation tasks.

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5. Long-term prediction enhancement based on multi-output Gaussian process regression integrated with production plans for oxygen supply network

URL: View paper

Brief Assessment

Oxygen Supply Prediction[28] focuses on oxygen demand prediction in industrial supply networks using MOGPR, not on comprehensive kernel comparison across regression, interpolation, and imputation tasks with synthetic and real-world benchmarks.

6. Weakly supervised multi-output regression via correlated gaussian processes

URL: View paper

Brief Assessment

Weakly Supervised Regression[34] focuses on multi-output regression with missing group labels using dependent Gaussian processes, evaluated on healthcare datasets (insulin, testosterone, body fat). The ORIGINAL paper evaluates MO-LRN kernel on regression, interpolation, and imputation tasks with synthetic and real-world datasets (ETT, air quality). These represent fundamentally different problem settings and experimental domains.

7. Multioutput framework for time-series forecasting in smart grid meets data scarcity

URL: View paper

Brief Assessment

Smart Grid Forecasting[29] focuses on smart grid data forecasting and imputation in isolated networks with data scarcity, while the original paper evaluates MO-LRN across diverse synthetic and real-world datasets for regression, interpolation, and imputation tasks. The candidate does not provide sufficient technical detail to challenge the novelty of the original paper's comprehensive experimental validation.

8. Multi-Task Gaussian Process for Imputing Missing Daily Rainfall Data Using nearby Stations: Case of Burkina Faso

URL: View paper

Brief Assessment

Rainfall Data Imputation[30] focuses on imputing missing rainfall data using nearby weather stations in Burkina Faso, which is a specific geospatial imputation application. This differs from the original paper's comprehensive evaluation across regression, interpolation, and imputation tasks with diverse synthetic and real-world datasets to validate a novel multi-output kernel design.

9. Aligned multi-task Gaussian process

URL: View paper

Brief Assessment

Aligned Multi-Task GP[32] focuses on temporal alignment in multi-task learning for time-series with missing data scenarios, not on multi-output kernel design for regression/interpolation/imputation tasks as in the original paper's MO-LRN kernel experiments.

10. Online sparse multi-output Gaussian process regression and learning

URL: View paper

Brief Assessment

Online Sparse GP[27] focuses on online training of multi-output Gaussian processes with streaming data for regression tasks, not on comprehensive offline experimental validation across regression, interpolation, and imputation tasks as in the original paper.

Appendix: Text Similarity Detection

Textual similarity detection checked 19 papers and found 1 similarity segment(s) across 1 paper(s).

The following **1 paper(s)** were detected to have high textual similarity with the original paper. These may represent different versions of the same work, duplicate submissions, or papers with substantial textual overlap. Readers are advised to verify these relationships independently.

1. Spectral mixture kernels for Multi-Output Gaussian processes

Detected in: Core Task (sibling), Contribution: contribution_1

⚠ **Note**: This paper shows substantial textual similarity with the original paper. It may be a different version, a duplicate submission, or contain significant overlapping content. Please review carefully to determine the nature of the relationship.

References

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