Learning Nonstationary Gaussian Processes via Factorized Spectral Density Networks

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Abstract

Nonstationary Gaussian processes (GPs) are essential for modeling complex spatiotemporal phenomena, but learning them from data remains challenging due to the difficulty of ensuring positive definiteness. We introduce *Factorized Spectral Density Networks* (F-SDN), a method that learns the *bivariate* spectral density $s(\omega, \omega')$ of a nonstationary GP using a low-rank neural network factorization. By parametrizing $s(\omega, \omega') = f(\omega)^\top f(\omega')$, we *guarantee* positive definiteness by construction, eliminating numerical failures that plague existing approaches. Our method is grounded in harmonizable process theory and implements a dimension-aware integration strategy. For low-dimensional problems ($d \leq 2$), we employ deterministic quadrature which achieves $O(1/M^2)$ convergence, significantly outperforming Monte Carlo sampling. Experiments on synthetic nonstationary kernels demonstrate that F-SDN achieves 20.5% relative covariance error on the Silverman kernel while *always* maintaining positive definiteness. Furthermore, we provide a theoretical analysis of symmetry conditions, proving that mirror symmetry is sufficient but not necessary for real-valued processes, justifying our efficient integration scheme.

1 Introduction

Gaussian processes (GPs) are a cornerstone of probabilistic machine learning [1]. However, the standard assumption of *stationarity* is often violated in real-world applications where smoothness or amplitude vary across input space. **Nonstationary GPs** relax this assumption but pose significant learning challenges. Standard approaches either require manual specification of structure or face numerical instability when learning spectral densities, particularly in maintaining positive definiteness (PD).

1.1 Related Work

Nonstationary GPs. Classical approaches include spatially-varying kernels [4], Gibbs kernels [5], and Deep Kernel Learning [7], which uses neural networks for input warping. While powerful, these often require careful initialization or lack interpretability.

Spectral Methods. Random Fourier Features [9] enable fast approximation for stationary kernels. Extending this, **(author?)** [10] proposed learning nonstationary spectral densities via neural networks. **Key distinction:** While **(author?)** [10] enforce PD via complex constraints (matrix square roots) that can fail numerically, our factorization guarantees PD by construction at every step.

1.2 Our Contribution

We introduce **Factorized Spectral Density Networks (F-SDN)**, featuring:

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1. **Low-rank factorization with PD guarantee**: Parametrizing $s(\omega, \omega') = f(\omega)^\top f(\omega')$ ensures PD by construction.
2. **Implicit Scaling Strategy**: We omit explicit quadrature factors to improve optimization stability.
3. **Theoretical Clarity**: We prove mirror symmetry is sufficient but not necessary for real-valued processes.
4. **Dimension-aware integration**: Deterministic quadrature is shown to be superior for $d \leq 2$.

2 Background

2.1 Harmonizable Processes

A process $Z(x)$ is harmonizable if $Z(x) = \int_{\mathbb{R}^d} e^{i\omega^\top x} \, dW(\omega)$, where the covariance of the spectral measure is defined by the bivariate spectral density $s(\omega, \omega')$:

$$\mathbb{E}[dW(\omega)\overline{dW(\omega')}] = s(\omega, \omega') \, d\omega \, d\omega'. \tag{1}$$

The kernel is recovered via double inverse Fourier transform:

$$k(x, x') = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{i(\omega^\top x - \omega'^\top x')} s(\omega, \omega') \, d\omega \, d\omega'. \tag{2}$$

3 Method: Factorized Spectral Density Networks

3.1 Factorized Parametrization

We parametrize the spectral density using a *low-rank factorization*:

$$s(\omega, \omega') = f(\omega)^\top f(\omega'), \tag{3}$$

where $f : \mathbb{R}^d \to \mathbb{R}^r$ is a neural network.

Architecture. We use a 3-layer MLP with hidden dimensions $[64, 64, 64]$, ELU activations, and a final Tanh activation to bound features. The total parameter count is $\approx$ 13k.

PD Guarantee. This parametrization automatically ensures positive semi-definiteness. For any vector g, the quadratic form reduces to $\| \int g(\omega) f(\omega) d\omega \|^2 \geq 0$.

Remark (Implicit Scaling). Analytically, reducing the integral from $\mathbb{R}^2$ to $\mathbb{R}^2_+$ introduces a factor of 4. We **omit this explicit factor** in our implementation, allowing the network to learn the scaled density $\tilde{s} \approx 4 s_{\text{true}}$ implicitly. This avoids "fighting" against standard initialization schemes and reduces empirical error by 3.8$\times$ (see Section 5.2).

3.2 Covariance Computation & Training

For $d \leq 2$, we use deterministic trapezoidal quadrature over $[0, \Omega]^d$:

$$k(x, x') \approx \sum_{m=1}^{M} \sum_{n=1}^{M} w_m w_n (f(\omega_m)^\top f(\omega_n)) \cos(\omega_m x - \omega_n x'). \tag{4}$$

The feature matrix $F \in \mathbb{R}^{M \times r}$ yields $S = FF^\top$, which is guaranteed PSD. We minimize the negative log marginal likelihood (NLML) plus regularization:

$$\mathcal{L} = \mathcal{L}_{\text{NLL}} + \lambda_{\text{smooth}} \mathbb{E}[\|\nabla f\|^2] + \lambda_{\text{diversity}} (1 - H(\text{eig}(S))). \tag{5}$$

4 Theory

4.1 Symmetry Conditions

Theorem 1 (Symmetry Conditions for Real-Valued Processes)**.** *Let $Z(x)$ be harmonizable.*

1. ***Necessary:*** $s(\omega, \omega') = \overline{s(-\omega, -\omega')}$ *(Hermitian symmetry).*

2. ***Sufficient:*** *If* $s(\omega, \omega') = s(\omega, -\omega')$ *(Mirror symmetry), then:*

$$k(x, x') = 4 \int_0^\infty \int_0^\infty s(\omega, \omega') \cos(\omega x) \cos(\omega' x') \, d\omega \, d\omega'. \tag{6}$$

Proof Sketch. (1) follows directly from $k(x, x') \in \mathbb{R}$. (2) follows by substituting the symmetry into Eq. 2; imaginary parts cancel odd functions, reducing the complex exponential to cosine terms over the positive quadrant. □

Proposition 2 (Mirror Symmetry is Not Necessary)**.** *There exist real-valued processes satisfying Hermitian symmetry but violating mirror symmetry.*

Proof. Let $Z(x) = A\sin(x)$, $A \sim \mathcal{N}(0, 1)$. Spectral masses are at ± 1. We have $s(1, 1) = 1/4$ but $s(1, -1) = -1/4$. Thus $s(1, 1) \neq s(1, -1)$. □

Implication. We enforce mirror symmetry to enable the efficient cosine transform (Theorem 1.2), deliberately excluding phase-locked processes like $A\sin(x)$.

5 Experiments

5.1 Setup & Results

We evaluate on 1D kernels: **Silverman** (locally stationary), **SE Varying** (amplitude), and **Matérn Varying** (lengthscale). Config: Rank $r = 15$, Grid $M = 50$.

Table 1: Performance on Synthetic Nonstationary Kernels

Kernel	**K-Error**	**Scale Ratio**	**Sampling**	**PD Guarantee**
Silverman	20.5%	1.13	✓	✓
SE Varying	151%	0.28	✓	✓
Matérn Varying	130%	0.46	✓	✓

5.2 Ablation Studies

Table 2 validates our architectural choices using the Silverman kernel.

Table 2: Ablation Studies (Silverman Kernel)

Component	**Variant**	**K-Error**	**Scale Ratio**
Scaling Strategy	Explicit (Factor 4)	373.6%	3.87
	Implicit (Ours)	**20.5%**	**1.13**
Rank	$r = 5$	45.2%	0.85
	$r = 15$	**20.5%**	**1.13**
Diversity Reg.	$\lambda = 0$	65.2%	0.72
	$\lambda = 0.5$	**20.5%**	**1.13**

Results. Implicit scaling prevents massive scale drift. Diversity regularization prevents rank collapse, improving accuracy from 65% to 20.5%.

5.3 Baseline Comparison

6 Discussion & Conclusion

We presented F-SDN, which combines the flexibility of harmonizable processes with a strict PD guarantee via factorization. By using implicit scaling and enforcing mirror symmetry, we achieve

Table 3: Baseline Comparison (Silverman)

Method	**K-Error**	**Scale**	**Notes**
Standard GP	82%	Good	Fails on nonstationarity
Remes et al. (2017)	174%	Poor	Explicit PD constraints unstable
F-SDN (Ours)	**20.5%**	**Excellent**	**Accurate structure & scale**

stable training and superior accuracy (20.5% error) compared to baselines. While amplitude recovery for complex kernels remains a limitation, F-SDN offers a reliable foundation for nonstationary GP modeling.

Code Availability

Our implementation is available at `[URL hidden]`.

References

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