
Learning Nonstationary Gaussian Processes via Factorized Spectral Density Networks

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Abstract

1 Nonstationary Gaussian processes (GPs) are essential for modeling complex spa-
2 tiotemporal phenomena, but learning them from data remains challenging due to
3 the difficulty of ensuring positive definiteness. We introduce *Factorized Spectral*
4 *Density Networks* (F-SDN), a method that learns the *bivariate* spectral density
5 $s(\omega, \omega')$ of a nonstationary GP using a low-rank neural network factorization.
6 By parametrizing $s(\omega, \omega') = f(\omega)^\top f(\omega')$, we *guarantee* positive definiteness by
7 construction, eliminating numerical failures that plague existing approaches. Our
8 method is grounded in harmonizable process theory and implements a dimension-
9 aware integration strategy. For low-dimensional problems ($d \leq 2$), we employ
10 deterministic quadrature which achieves $O(1/M^2)$ convergence, significantly out-
11 performing Monte Carlo sampling. Experiments on synthetic nonstationary kernels
12 demonstrate that F-SDN achieves 20.5% relative covariance error on the Silverman
13 kernel while *always* maintaining positive definiteness. Furthermore, we provide a
14 theoretical analysis of symmetry conditions, proving that mirror symmetry is suffi-
15 cient but not necessary for real-valued processes, justifying our efficient integration
16 scheme.

17 1 Introduction

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

24 1.1 Related Work

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

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

32 1.2 Our Contribution

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

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

41 2 Background

42 2.1 Harmonizable Processes

43 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
 44 measure is defined by the bivariate spectral density $s(\omega, \omega')$:

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

45 The kernel is recovered via double inverse Fourier transform:

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

46 3 Method: Factorized Spectral Density Networks

47 3.1 Factorized Parametrization

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

$$s(\omega, \omega') = f(\omega)^\top f(\omega'), \quad (3)$$

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

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

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

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

58 3.2 Covariance Computation & Training

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

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

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

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

62 4 Theory

63 4.1 Symmetry Conditions

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

Algorithm 1 Training F-SDN (Deterministic Regime for $d \leq 2$)

```
1: Input: Data  $\{(x_i, y_i)\}_{i=1}^n$ , rank  $r$ , grid size  $M$ , learning rate  $\eta$ 
2: Initialize: Neural network  $f_\theta : \mathbb{R}^d \rightarrow \mathbb{R}^r$  (Xavier init)
3: Precompute: Fixed frequency grid  $\{\omega_m\}_{m=1}^M \subset [0, \Omega]^d$ 
4: while not converged do
5:   1. Spectral Features (Implicit Scaling)
6:   Compute features:  $v_{mi} \leftarrow f_\theta(\omega_m)_i$  // Network learns magnitude
7:   Construct spectral matrix:  $S \leftarrow VV^\top$  // Guaranteed PSD
8:   2. Covariance Synthesis
9:   Compute cosine basis  $B$  on grid  $\omega$  and inputs  $x$ 
10:   $K \leftarrow B \cdot S \cdot B^\top \cdot \Delta\omega^2$  // Trapezoidal rule
11:   $K \leftarrow K + \sigma^2 I$ 
12:  3. Optimization
13:   $L \leftarrow \text{Cholesky}(K)$  // Never fails
14:   $\mathcal{L}_{\text{NLL}} \leftarrow \frac{1}{2} y^\top K^{-1} y + \sum \log L_{ii}$ 
15:   $\mathcal{L}_{\text{reg}} \leftarrow \lambda_{\text{div}}(1 - H(\text{eig}(S))) + \lambda_{\text{smooth}} \|\nabla_\omega f\|^2$ 
16:  Update  $\theta \leftarrow \theta - \eta \nabla_\theta (\mathcal{L}_{\text{NLL}} + \mathcal{L}_{\text{reg}})$ 
17: end while
```

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

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

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

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

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

72 *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
73 $s(1, -1) = -1/4$. Thus $s(1, 1) \neq s(1, -1)$. \square

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

76 5 Experiments

77 5.1 Setup & Results

78 We evaluate on 1D kernels: **Silverman** (locally stationary), **SE Varying** (amplitude), and **Matérn**
79 **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	✓	✓

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

5.2 Ablation Studies

Table 2 validates our architectural choices using the Silverman kernel.

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

5.3 Baseline Comparison

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

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 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].

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