Supplement S6: Numerical Methods

Algorithms, Implementation, and Validation

GIFT Framework v2.1
Geometric Information Field Theory

Abstract

This supplement documents the computational framework, algorithms, and validation procedures used in GIFT numerical calculations. We present the complete software stack, core algorithms for observable computation, statistical validation methods, K_7 metric reconstruction using neural networks, and comprehensive testing procedures. All code is open-source and reproducible.

Keywords: Numerical methods, machine learning, validation, reproducibility, open-source

Contents

1 Computational Framework

1.1 Software Stack

The GIFT computational framework relies on standard scientific Python libraries:

```
# Core numerical libraries
numpy>=1.24.0      # Array operations
scipy>=1.10.0      # Scientific computing
sympy>=1.11.0      # Symbolic mathematics

# Machine learning
torch>=2.0.0       # Neural networks for K7 metric

# Visualization
matplotlib>=3.7.0  # Plotting
plotly>=5.14.0     # Interactive 3D

# Statistical analysis
pandas>=2.0.0      # Data manipulation
statsmodels>=0.14  # Statistical models
```

1.2 Hardware Requirements

Minimum configuration:

- CPU: 8 cores
- RAM: 32 GB
- Storage: 100 GB SSD

Recommended for ML training:

- GPU: NVIDIA A100 (40GB) or equivalent
- RAM: 128 GB
- Storage: 1 TB NVMe

1.3 Installation

```
# Clone repository
git clone https://github.com/gift-framework/GIFT.git
cd GIFT

# Create virtual environment
python -m venv venv
source venv/bin/activate

# Install dependencies
pip install -r requirements.txt
```

2 Core Algorithms

2.1 Topological Parameter Computation

All topological parameters are computed exactly from integer arithmetic:

```
import numpy as np

# E8 parameters
dim_E8 = 248
rank_E8 = 8

# K7 cohomology
b2_K7 = 21
b3_K7 = 77
H_star = b2_K7 + b3_K7 + 1  # = 99

# G2 parameters
dim_G2 = 14
dim_K7 = 7

# Derived parameters
p2 = dim_G2 / dim_K7  # = 2 (exact)
Wf = 5  # Weyl factor

# Base coupling
beta_0 = np.pi / rank_E8
xi = (Wf / p2) * beta_0  # = 5*pi/16
```

2.2 Observable Computation

Example: Computing gauge couplings

```python
def compute_gauge_couplings():
    """Compute the three gauge coupling constants."""

    # Fine structure constant inverse
    alpha_inv = (dim_E8 + rank_E8) / 2  # = 128

    # Weinberg angle
    zeta_3 = 1.2020569031595943  # Apery's constant
    gamma_euler = 0.5772156649015329
    M2 = 3  # Second Mersenne prime
    sin2_theta_W = zeta_3 * gamma_euler / M2

    # Strong coupling
    W_G2 = 12  # |W(G2)| Weyl group order
    alpha_s = np.sqrt(2) / W_G2

    return {
        'alpha_inv_MZ': alpha_inv,
        'sin2_theta_W': sin2_theta_W,
        'alpha_s_MZ': alpha_s
    }
```

2.3 Neutrino Mixing Angles

```
def compute_neutrino_mixing():
    """Compute PMNS mixing parameters."""

    # Reactor angle (exact)
    theta_13 = np.pi / b2_K7  # = pi/21

    # Atmospheric angle
    theta_23_rad = (rank_E8 + b3_K7) / H_star  # = 85/99
    theta_23 = np.degrees(theta_23_rad)

    # Solar angle
    delta = 2 * np.pi / (Wf ** 2)  # = 2pi/25
    gamma_GIFT = 511 / 884
    theta_12 = np.degrees(
        np.arctan(np.sqrt(delta / gamma_GIFT))
    )

    # CP phase (exact)
    delta_CP = dim_K7 * dim_G2 + H_star  # = 197 degrees

    return {
        'theta_12': theta_12,
        'theta_13': np.degrees(theta_13),
        'theta_23': theta_23,
        'delta_CP': delta_CP
    }
```

2.4 Heat Kernel Coefficient

The GIFT heat kernel coefficient γ_{GIFT} is computed as:

```
def compute_gamma_GIFT():
    """Compute heat kernel coefficient gamma_GIFT."""
    numerator = 2 * rank_E8 + 5 * H_star
    denominator = 10 * dim_G2 + 3 * dim_E8
    return numerator / denominator  # = 511/884

# Verification
gamma_GIFT = 511 / 884
gamma_euler = 0.5772156649015329
print(f"gamma_GIFT = {gamma_GIFT:.16f}")
print(f"gamma_Euler = {gamma_euler:.16f}")
print(f"Difference = {abs(gamma_GIFT - gamma_euler):.6f}")
# Difference = 0.000839 (0.145%)
```

3 Statistical Validation

3.1 Monte Carlo Uncertainty Propagation

```python
def monte_carlo_validation(n_samples=1_000_000):
    """
    Monte Carlo propagation of experimental uncertainties.
    """
    import numpy as np

    # Experimental values with uncertainties
    exp_values = {
        'alpha_inv': (127.955, 0.016),
        'sin2_theta_W': (0.23122, 0.00004),
        'alpha_s': (0.1179, 0.0010)
    }

    results = {}
    for name, (mean, sigma) in exp_values.items():
        # Sample from Gaussian distribution
        samples = np.random.normal(mean, sigma, n_samples)

        # Compute statistics
        results[name] = {
            'mean': np.mean(samples),
            'std': np.std(samples),
            'median': np.median(samples),
            'percentile_16': np.percentile(samples, 16),
            'percentile_84': np.percentile(samples, 84)
        }

    return results
```

3.2 Chi-Square Analysis

```python
def chi_square_test(gift_values, exp_values,
                    exp_uncertainties):
    """
    Compute chi-square statistic for GIFT predictions.
    """
    chi2 = 0
    n_obs = len(gift_values)

    for obs in gift_values:
        gift = gift_values[obs]
        exp = exp_values[obs]
        sigma = exp_uncertainties[obs]
        chi2 += ((gift - exp) / sigma) ** 2

    dof = n_obs - 3  # 3 free parameters
    p_value = 1 - scipy.stats.chi2.cdf(chi2, dof)

    return chi2, dof, p_value
```

3.3 Sobol Sensitivity Analysis

Global sensitivity analysis identifies which parameters most affect predictions:

```python
from SALib.sample import sobol as sobol_sample
from SALib.analyze import sobol as sobol_analyze

def sobol_analysis():
    """
    Sobol global sensitivity analysis for GIFT parameters.
    """
    problem = {
        'num_vars': 3,
        'names': ['p2', 'rank_E8', 'Wf'],
        'bounds': [[1.9, 2.1], [7.9, 8.1], [4.9, 5.1]]
    }

    # Generate samples
    param_values = sobol_sample.sample(problem, 2048)

    # Evaluate model at each sample point
    Y = np.array([evaluate_model(p) for p in param_values])

    # Analyze sensitivity
    Si = sobol_analyze.analyze(problem, Y)

    return Si
```

4 K_7 Metric Computation

4.1 Neural Network Architecture

The K_7 metric is approximated using neural networks:

```python
import torch
import torch.nn as nn

class K7MetricNetwork(nn.Module):
    """Neural network for K7 metric tensor components."""

    def __init__(self, hidden_dim=256):
        super().__init__()
        self.net = nn.Sequential(
            nn.Linear(7, hidden_dim),
            nn.GELU(),
            nn.Linear(hidden_dim, hidden_dim),
            nn.GELU(),
            nn.Linear(hidden_dim, hidden_dim),
            nn.GELU(),
            nn.Linear(hidden_dim, 28)  # 7x7 symmetric
        )

    def forward(self, x):
        """
        Args:
            x: Coordinates on K7, shape (batch, 7)
        Returns:
            Metric tensor components, shape (batch, 28)
        """
        return self.net(x)

    def get_metric(self, x):
        """Reconstruct full metric tensor."""
        components = self.forward(x)
        # Unpack to symmetric 7x7 matrix
        metric = torch.zeros(x.shape[0], 7, 7)
        idx = 0
        for i in range(7):
            for j in range(i, 7):
                metric[:, i, j] = components[:, idx]
                metric[:, j, i] = components[:, idx]
                idx += 1
        return metric
```

4.2 Training Procedure

```python
def train_k7_metric(model, dataloader, epochs=1000):
    """Train K7 metric network with G2 holonomy."""

    optimizer = torch.optim.Adam(
        model.parameters(), lr=1e-4
    )

    for epoch in range(epochs):
        for batch in dataloader:
            coords = batch['coordinates']

            # Get predicted metric
            g = model.get_metric(coords)

            # Loss 1: Ricci-flat condition
            loss_ricci = compute_ricci_loss(g, coords)

            # Loss 2: G2 holonomy constraint
            loss_g2 = compute_g2_loss(g, coords)

            # Loss 3: Determinant = p2 = 2
            det_g = torch.det(g)
            loss_det = ((det_g - 2.0) ** 2).mean()

            # Total loss
            loss = loss_ricci + 0.1 * loss_g2 + 0.01 * loss_det

            optimizer.zero_grad()
            loss.backward()
            optimizer.step()
```

4.3 Harmonic Form Extraction

```python
def extract_harmonic_forms(metric_network, n_points=10000):
    """
    Extract harmonic 2-forms and 3-forms from trained metric.

    Returns:
        h2: Array of shape (21, n_points, 21) for b2=21
        h3: Array of shape (77, n_points, 35) for b3=77
    """
    # Sample points on K7
    coords = sample_k7_manifold(n_points)

    # Get metric at each point
    g = metric_network.get_metric(coords)

    # Compute Hodge star operator
    hodge = compute_hodge_star(g)

    # Solve eigenvalue problem for harmonic forms
    # Laplacian eigenvalue = 0 for harmonic forms

    # 2-forms: 21 harmonic forms
    h2 = solve_harmonic_eigenvalue(
        hodge, degree=2, n_forms=21
    )

    # 3-forms: 77 harmonic forms
    h3 = solve_harmonic_eigenvalue(
        hodge, degree=3, n_forms=77
    )

    return h2, h3
```

5 Validation Suite

5.1 Unit Tests

```python
import pytest

class TestTopologicalConstants:
    """Unit tests for topological constants."""

    def test_betti_numbers(self):
        assert b2_K7 == 21
        assert b3_K7 == 77
        assert b2_K7 + b3_K7 == 98

    def test_dimensions(self):
        assert dim_E8 == 248
        assert rank_E8 == 8
        assert dim_G2 == 14
        assert dim_K7 == 7

    def test_p2_dual_origin(self):
        p2_local = dim_G2 / dim_K7
        p2_global = 496 / 248
        assert p2_local == 2
        assert p2_global == 2
        assert p2_local == p2_global

    def test_generation_number(self):
        N_gen = 168 / 56
        assert N_gen == 3
```

```python
class TestExactRelations:
    """Unit tests for exact topological relations."""

    def test_tau_electron_ratio(self):
        ratio = 7 + 10*248 + 10*99
        assert ratio == 3477

    def test_strange_down_ratio(self):
        ratio = 4 * 5  # p2^2 * Wf
        assert ratio == 20

    def test_koide_parameter(self):
        Q = 14 / 21
        assert Q == pytest.approx(2/3, rel=1e-10)

    def test_cp_phase(self):
        delta_CP = 7 * 14 + 99
        assert delta_CP == 197
```

5.2 Integration Tests

```python
class TestFullPipeline:
    """Integration tests for complete pipeline."""

    def test_gauge_sector(self):
        results = compute_gauge_couplings()
        assert results['alpha_inv_MZ'] == 128
        assert abs(results['sin2_theta_W'] - 0.23122) < 0.001
        assert abs(results['alpha_s_MZ'] - 0.1179) < 0.001

    def test_neutrino_sector(self):
        results = compute_neutrino_mixing()
        assert abs(results['theta_12'] - 33.44) < 0.5
        assert abs(results['theta_13'] - 8.57) < 0.1
        assert abs(results['theta_23'] - 49.2) < 0.5
        assert results['delta_CP'] == 197

    def test_all_observables(self):
        """Verify all 37 observables compute without error."""
        results = compute_all_observables()
        assert len(results) == 37
        for name, value in results.items():
            assert np.isfinite(value), f"{name} not finite"
```

5.3 Numerical Stability

```python
def test_numerical_stability():
    """Test numerical stability across precisions."""

    # Single precision
    result_32 = compute_observables(dtype=np.float32)

    # Double precision
    result_64 = compute_observables(dtype=np.float64)

    # Extended precision (if available)
    result_128 = compute_observables(dtype=np.float128)

    # Check consistency
    for obs in result_64:
        rel_diff = abs(result_64[obs] - result_128[obs])
        rel_diff /= result_128[obs]
        assert rel_diff < 1e-10, f"{obs} unstable"
```

6 Performance Benchmarks

6.1 Computation Times

Operation	Time (ms)	Notes
Topological constants	< 0.1	Integer arithmetic
Gauge couplings	< 1	Simple formulas
All 37 observables	< 10	Full computation
Monte Carlo (10^6)	~ 5000	Statistical validation
K_7 metric training	$\sim 3{,}600{,}000$	1 hour on A100

Table 1: Computation time benchmarks

6.2 Memory Usage

Dataset	Memory (MB)
Topological parameters	< 1
Full observable set	< 10
K_7 metric network	~ 100
Training batch	~ 1000

Table 2: Memory usage

6.3 Scaling

The Monte Carlo validation scales linearly with sample size:

- 10^4 samples: 50 ms
- 10^5 samples: 500 ms
- 10^6 samples: 5 s
- 10^7 samples: 50 s

7 Reproducibility

7.1 Random Seed Management

```python
def set_reproducibility(seed=42):
    """Set all random seeds for reproducibility."""
    import random
    import numpy as np
    import torch

    random.seed(seed)
    np.random.seed(seed)
    torch.manual_seed(seed)
    if torch.cuda.is_available():
        torch.cuda.manual_seed_all(seed)
        torch.backends.cudnn.deterministic = True
        torch.backends.cudnn.benchmark = False
```

7.2 Version Control

All numerical results are tagged with:

- Git commit hash
- Python version
- Library versions
- Hardware specification
- Timestamp

7.3 Result Caching

```
import hashlib
import json

def cache_result(params, result, cache_dir='./cache'):
    """Cache computation result with parameter hash."""
    param_hash = hashlib.md5(
        json.dumps(params, sort_keys=True).encode()
    ).hexdigest()

    cache_file = f"{cache_dir}/{param_hash}.json"
    with open(cache_file, 'w') as f:
        json.dump({'params': params, 'result': result}, f)
```

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