A Study of TaBPFN as Surrogate Model in Bayesian Optimization

By: Ocean Wang
Supervised by: Professor E. Raponi
Leiden Institute of Advanced Computer Science (LIACS)
April 24, 2025

Outline

- Research Background
- Bayesian Optimization
- Traditional Surrogate Model GP
- TabPFN: A New Approach
- Research Question
- Methodology
- Current Progress
- Next Steps
- Questions

Research Background

•**Bayesian Optimization (BO)**: A machine learning-based approach for optimizing expensive black-box functions

•**Key Applications**:
•Hyperparameter tuning in ML algorithms
•Experimental design
•Simulator calibration
•Materials discovery

•**Current Limitation**: Traditional surrogate models have drawbacks

•**Opportunity**: Exploring alternative surrogate models with improved properties

Bayesian Optimization

- Sequential strategy for global optimization of black-box functions
- Components:
- **Surrogate model**: Approximates the objective function
- **Acquisition function**: Determines next evaluation point
- Particularly effective for expensive-to-evaluate functions

Traditional Surrogate Model GP

Gaussian Process (GP) Regression:

- Currently the standard approach in BO
- **Advantages**:
  - Provides uncertainty estimates
  - Works well with limited data
- **Limitations**:
  - Struggles with non-stationary functions
  - Poor scaling to high dimensions
  - Requires careful kernel design

TabPFN: A New Approach

Tabular Prior-Data Fitted Network:

- Recent breakthrough in tabular learning
- Pre-trained transformer that uses in-context learning
- Single forward pass approximates Bayesian inference
- Updated version (2024) supports:
  - Up to 10,000 samples
  - Up to 500 features
  - Regression tasks

TabPFN: Key Features

- **Dual-attention mechanism**:
- One for feature interactions
- One for sample relationships

- **Advanced prior**:
- Combines principles from Structural Causal Models
- Incorporates Bayesian Neural Networks

- **Fast inference**: No training required for each new dataset

Research Question:

How effectively does TabPFN perform as a surrogate model for Bayesian Optimization in regression tasks when evaluated on standardized benchmarks?

Focus areas:

- Performance across different objective function landscapes from BBOB
- Computational efficiency
- Scaling with increasing problem dimensionality

Methodology

Three-phase approach:

1. **Implementation**:
    1. Setup TabPFN as surrogate model in BO framework
    2. Define evaluation metrics
2. **Experimentation**:
    1. Benchmark using BBOB test suite in COCO environment
    2. Measure key performance metrics
3. **Analysis**:
    1. Statistical comparison with existing methods
    2. Evaluate effectiveness and efficiency

BBOB Test Suite

Black-Box Optimization Benchmarking (BBOB):

- Standardized framework for gradient-free optimization
- 24 noiseless test functions with different properties:
  - Separable functions
  - Functions with low/moderate conditioning
  - Unimodal functions
  - Multi-modal functions
  - Weak/strong global structure

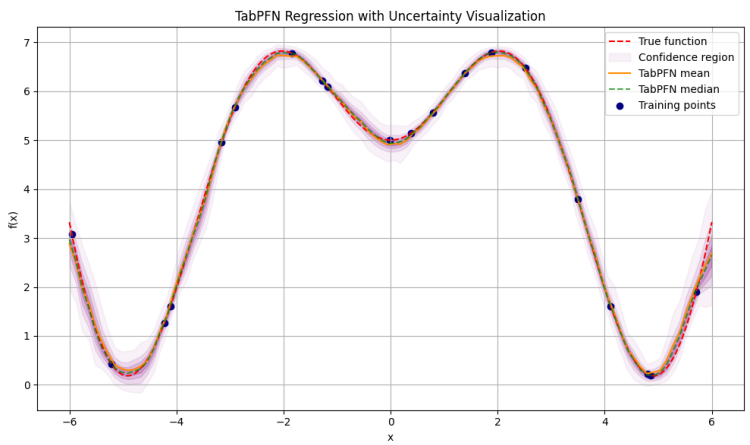
Current Progress

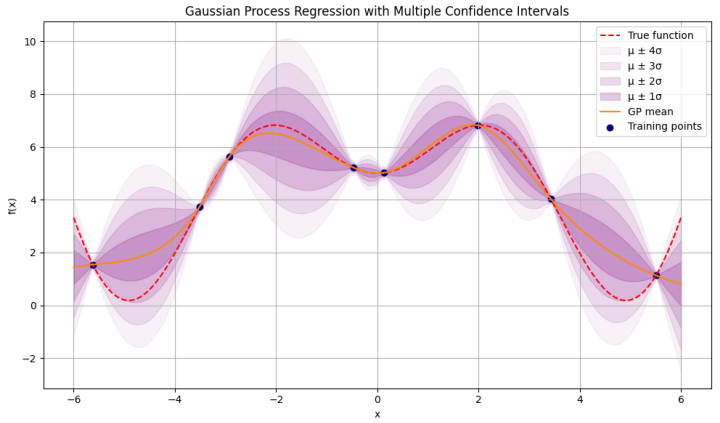
- Preliminary literature review
- Established development environment using Bo-Torch implementation
- Created visualization framework for surrogate model comparison
- Implemented comparative code for:
  - Standard GP regression with Matern kernel
  - TabPFN regression with uncertainty visualization
  - Surrogate model performance on BBOB test functions

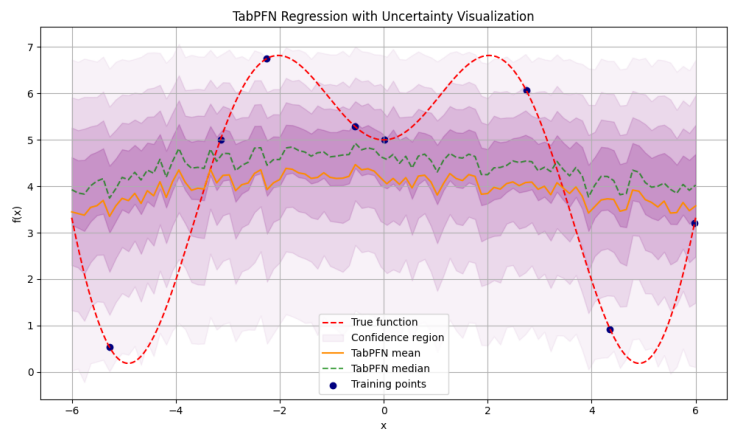
Visualization: GP vs TabPFN

- Generated "sausage plots" for both surrogate models:
  - Confidence intervals with multiple uncertainty bands
  - Performance on 1D test functions
- Implemented Bayesian optimization process visualization:
  - Surrogate model updates during optimization
  - Acquisition function behavior at each iteration
  - Sampling point selection strategy

Surrogate Model Comparison

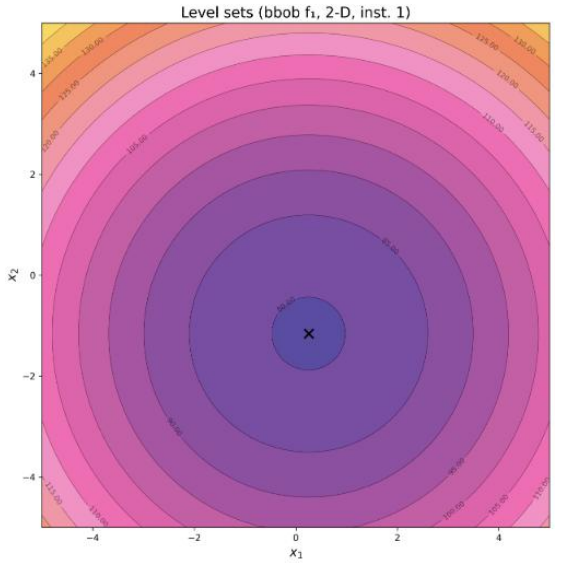


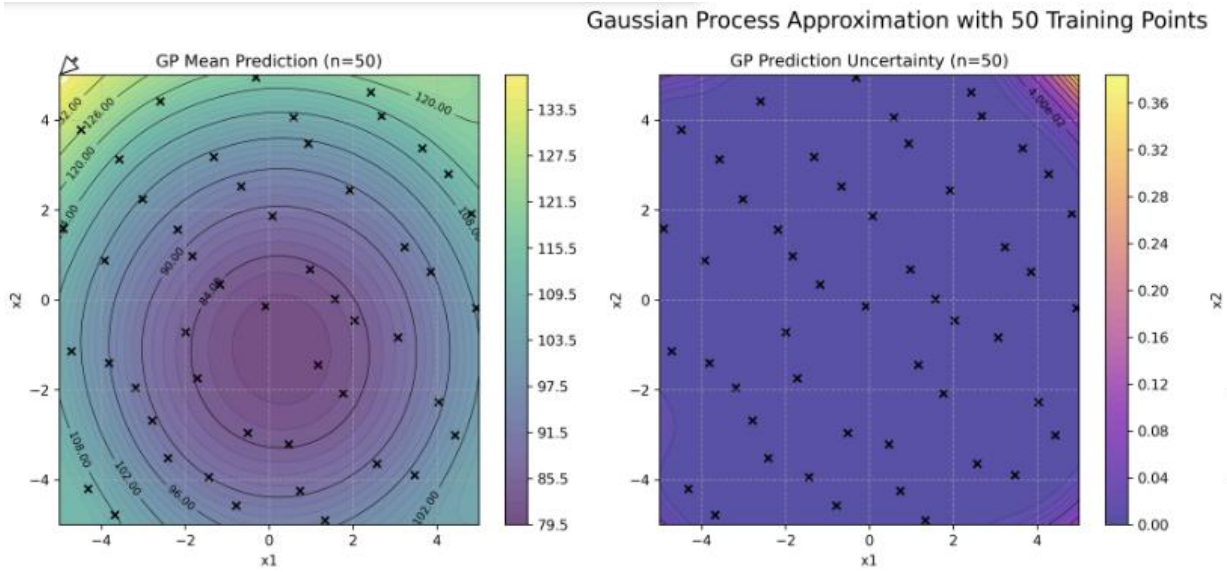


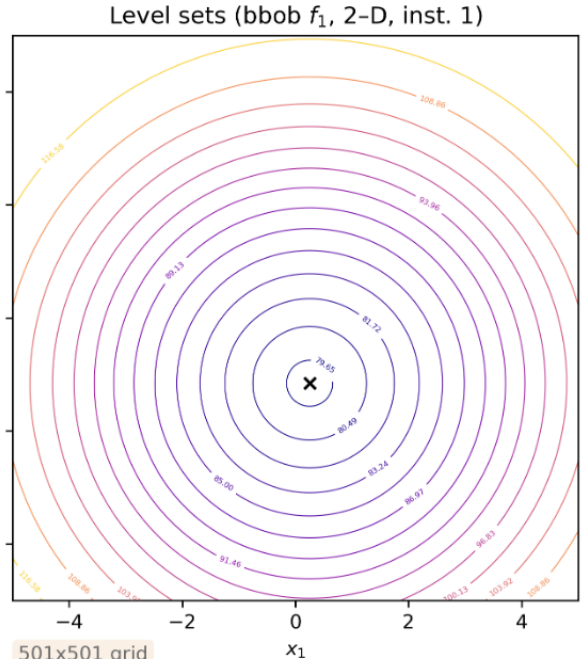


BBOB Test Function Analysis

- Created 2D contour plots of BBOB test functions
- Implemented GP surrogate fitting with various sample sizes (10-1000)
- Generated visualizations of:
  - Mean predictions
  - Prediction uncertainty
  - Absolute error compared to true function







Next Steps

- Replace GPR with TabPFN in BO and run on BBOB test suite
- Analyze performance across different problem dimensions
- Compare computational efficiency against traditional surrogate models
- Complete thesis writing with comprehensive analysis

Thank you!

Questions?

- Ocean Wang
  Bachelor Computer Science & Datascience and Artificial Intelligence
  Leiden Institute of Advanced Computer Science (LIACS)