Predicting from Strings:

Language Model Embeddings for Bayesian Optimization

Yilong Chen

Department of Statistics, University of Chicago

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1. Preliminaries
2. Regressor
3. Pretraining and Inference
4. Attention Mechanism
5. Experiment

Blackbox Optimization Problem

Goal: Maximize a real-valued function f over a search space $\mathcal{X}$:

$$x^* = \arg\max_{x \in \mathcal{X}} f(x) \tag{1}$$

Challenges:

- f is a blackbox function, i.e., no analytical expression or gradients.
- Evaluation of f is expensive or limited.
- Requires balance between **exploration** and **exploitation**.

Definition of a Regressor

Regressor: A prediction model that outputs the distribution of $f(\cdot)$ values over a query point x, given the history of evaluations:

$$\{(x_s, y_s)\}_{s=1}^{t}$$

where $y_s = f(x_s)$ for $s = 1, 2, \ldots, t$.

Key Properties:

- *Learnability:* The regressor can be trained using offline or online data.
- *Distributional Output:* Provides mean and uncertainty estimates for predictions.

Acquisition Function for Exploration and Exploitation

Definition: The regressor is transformed into an acquisition function:

$$a_{t+1}(x) : \mathcal{X} \to \mathbb{R}$$

which guides the optimization process.

Next Proposal:

$$x_{t+1} = \arg\max_{x \in \mathcal{X}} a_{t+1}(x) \tag{2}$$

Acquisition Optimizer:

- Samples $x \in \mathcal{X}$ efficiently, using zeroth-order or evolutionary algorithms.
- Balances exploration (high uncertainty) and exploitation (high mean).

Bayesian Optimization Loop

Procedure:

1. Initialize a set of observations $\{(x_s, y_s)\}_{s=1}^{t}$.
2. Train a regressor on the given data.
3. Compute the acquisition function $a_{t+1}(x)$ based on the regressor's predictions.
4. Find the next proposal:

$$x_{t+1} = \arg\max_{x \in \mathcal{X}} a_{t+1}(x)$$

5. Evaluate $f(x_{t+1})$ and update the history.
6. Repeat until a stopping criterion is met.

Outcome: Approximate the global maximum of $f(x)$.

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Embedding-Based Regressor: Concept

Purpose: Convert input $x \in \mathcal{X}$ into a fixed-length representation for regression.

Embedding Process:

- The embedder $\phi : \mathcal{X} \to \mathbb{R}^d$ maps x to a vector $\bar{x} \in \mathbb{R}^d$.
- Input x is represented as a **string**, which is processed by a language model (e.g., T5 encoder).
- A forward pass through the model produces token logits in $\mathbb{R}^{L \times d}$.

Insert Graph: Diagram of embedding process:

- Input string $\rightarrow$ Tokenization $\rightarrow$ Language Model $\rightarrow$ Average Pooling $\rightarrow$ $\bar{x}$.

Embedding-Based Regressor: Final Representation

Final Step:

- Perform **average pooling** across the token axis to generate a fixed-length embedding in $\mathbb{R}^d$.
- Output: $\bar{x} \in \mathbb{R}^d$.

Benefits:

- Handles arbitrary input types (e.g., JSON, categorical).
- Generates consistent, fixed-length feature vectors for regression tasks.

In-context Regression Transformer: Input Sequence

Input Sequence:

$$(\bar{x}_1 \oplus \bar{y}_1), \ldots, (\bar{x}_t \oplus \bar{y}_t) \tag{3}$$

where:

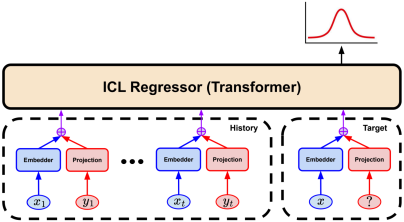
- $\bar{x}_i \in \mathbb{R}^d$: Embedding of trial x_i.
- $\bar{y}_i \in \mathbb{R}^d$: Feature representation of observed value y_i, obtained via a trainable projection.
- $\oplus$: Concatenation operator.

In-context Regression Transformer: Prediction

Prediction Process:

- Append query $(\bar{x} \oplus \bar{0})$, where $\bar{0}$ is a placeholder.
- Perform a forward pass through the Transformer.
- The output feature corresponding to $t + 1$ predicts:

$$\mathcal{N}(\mu_{t+1}(x), \sigma^2_{t+1}(x)) \tag{4}$$



Additional Techniques

Parallel Predictions:

- Simultaneously predict over a set of k target points:

$$(\bar{x}_{t+1} \oplus \bar{0}), \ldots, (\bar{x}_{t+k} \oplus \bar{0}) \tag{5}$$

- Custom attention pattern allows tokens to attend to history but not to targets.

Additional Techniques

y-Normalization:

- Shift objectives to have zero mean and scale by standard deviation.
- Transform y values into $[0, 1]$ for numerical stability.

Encoding Metadata:

- Include task-specific metadata m as part of input:

$$\bar{x} \to (\bar{x} \oplus m) \tag{6}$$

- Useful for providing additional context about the objective or search space.

Pretraining and Inference: Overview

Task Definition:

- A task $\mathcal{T} = (f, \mathcal{X})$ represents a specific objective function f over a search space $\mathcal{X}$.

Pretraining:

- Assumes a collection of offline **training tasks** $\{\mathcal{T}_1, \mathcal{T}_2, \dots\}$.
- Each task has its own evaluated trials $\{(x_s, y_s)\}_{s=1}^{T}$.
- T: Offline trajectory length (task-specific).

Purpose:

- Learn from historical offline data to generalize across tasks.

Pretraining: Loss Function

Frozen Embedder:

- During pretraining, the weights θ of the ICL regression Transformer are optimized.
- The embedder remains **frozen**.

Training Example:

- History: $\{(x_s, y_s)\}_{s=1}^{t'}$ for some $t' \in [0, T]$.
- Targets: $\{(x_{t'+i}, y_{t'+i})\}_{i=1}^{T-t'}$.

Loss Function:

$$\sum_{i=1}^{T-t'} \ell_\theta(x_{t'+i}, y_{t'+i}; \{(x_s, y_s)\}_{s=1}^{t'}), \tag{7}$$

where:

- ℓ_θ is the negative log-likelihood of the Gaussian distribution.

Inference: Overview

At Inference:

- The Transformer predicts the mean $\mu_{t+1}(x)$ and standard deviation $\sigma_{t+1}(x)$ for the target.
- The acquisition function is defined as:

$$a_{t+1}(x) = \mu_{t+1}(x) + \sqrt{\beta} \cdot \sigma_{t+1}(x), \tag{8}$$

where $\sqrt{\beta}$ is a problem-dependent constant.

Optimization:

- Uses a zeroth-order optimizer (e.g., evolutionary search) to maximize $a_{t+1}(x)$.
- Requires only **forward passes** (no gradient-based optimization).

Handling Distributional Shifts

Challenges:

- Distributional shifts may occur between pretraining and inference.

Solutions:

- **Data Augmentation:** Randomize parameter names during pretraining.
- **Search Space Transformation:** Adjust search space at inference to align with pretraining conditions.

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Attention in Transformer for $\bar{x} \oplus \bar{0}$

Goal: Predict a distribution $\mathcal{N}(\mu_{t+1}(\bar{x}), \sigma^2_{t+1}(\bar{x}))$ for a query point $\bar{x} \oplus \bar{0}$.

Input Sequence:

$$\mathcal{S} = \{(\bar{x}_1 \oplus \bar{y}_1), (\bar{x}_2 \oplus \bar{y}_2), \ldots, (\bar{x}_t \oplus \bar{y}_t), (\bar{x} \oplus \bar{0})\}$$

Attention Formula:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right) V$$

Key Idea: Query $\bar{x} \oplus \bar{0}$ computes attention weights over historical points $\{(\bar{x}_i \oplus \bar{y}_i)\}_{i=1}^t$.

How Attention Works for $\bar{x} \oplus \bar{0}$

Steps:

- Compute attention weights:

$$\alpha_{t+1,i} = \mathrm{softmax}\left(\frac{K(\bar{x} \oplus \bar{0}) \cdot Q(\bar{x}_i \oplus \bar{y}_i)}{\sqrt{d_k}}\right)$$

- Aggregate historical information:

$$z_{t+1} = \sum_{i=1}^{t} \alpha_{t+1,i} V_i(\bar{x}_i \oplus \bar{y}_i)$$

  where V_i is the value vector of $(\bar{x}_i \oplus \bar{y}_i)$.

- Use z_{t+1} to predict $\mu_{t+1}(\bar{x})$ and $\sigma^2_{t+1}(\bar{x})$.

Output:

$$\mathcal{N}(\mu_{t+1}(\bar{x}), \sigma^2_{t+1}(\bar{x}))$$

Synthetic Optimization: Overview

Definition:

- In common optimization scenarios, the search space is modeled as a flat Cartesian product of:
  - **Float parameters**: Continuous-valued parameters.
  - **Categorical parameters**: Discrete-valued parameters.
- The goal is to evaluate the performance of **Embed-then-Regress** on such tasks.

Key Representation:

- Each x (input) is represented as a *JSON string*.
- Example:

$$\{"p0" : 0.3, "p1" : 4\}$$

- Where:
  - $p0$: Continuous parameter.
  - $p1$: Integer parameter.

Benchmark: Blackbox Optimization Benchmarking (BBOB)

Setup:

- Uses the **BBOB suite** (ElHara et al., 2019), one of the most widely used synthetic function benchmarks.
- Contains 24 objectives over **continuous search spaces**.

Training-Test Split:

- Original functions are divided into **training** and **test sets**.
- Apply transformations (e.g., shifting, rotating, discretizing, etc.) to generate diverse functions.
- Induce non-continuous search spaces with categorical parameters.

Goal: Evaluate the generalization of the trained model on unseen tasks.

Comparison with GP-Bandit

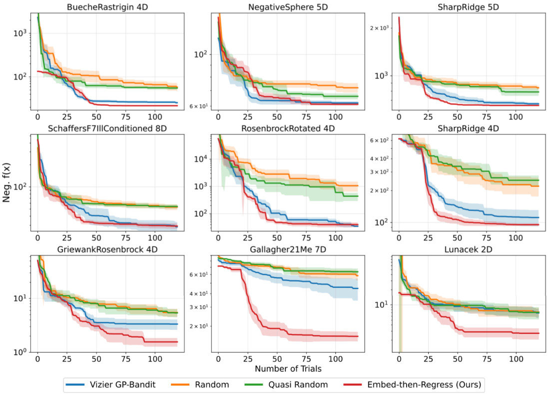
Baseline:

- The traditional baseline is **GP-Bandit** (Song et al., 2024c), a UCB-based Bayesian Optimization method.
- Uses the same acquisition optimizer (**Firefly**) as Embed-then-Regress.

Findings:

- Embed-then-Regress is generally **comparable** to GP-Bandit in performance.
- In some cases, it **significantly outperforms** GP-Bandit, especially on:
  - Non-continuous search spaces.
  - Test functions requiring task generalization.

Performance



Thank You