Semi-Parametric Deep Neural Networks in Linear Time and Memory

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Abstract

Recent advances in deep learning have been driven by large-scale parametric models, which can be computationally expensive and lack interpretability. Semi-parametric methods query the training set at inference time and can be more compact, although they typically have quadratic computational complexity. Here, we introduce SPIN, a general-purpose semi-parametric neural architecture whose computational cost is linear in the size and dimensionality of the data. Our architecture is inspired by inducing point methods and relies on a novel application of cross-attention between datapoints. At inference time, its computational cost is constant in the training set size as the data gets distilled into a fixed number of inducing points. We find that our method reduces the computational requirements of existing semi-parametric models by up to an order of magnitude across a range of datasets and improves state-of-the-art performance on an important practical problem, genotype imputation.

1 Introduction

Recent advances in deep learning have been driven by large-scale parametric models, which can be computationally expensive and lack interpretability. Semi-parametric methods query the training set at inference time and can be more compact, although they typically have quadratic computational complexity. Here, we introduce SPIN, a general-purpose semi-parametric neural architecture whose computational cost is linear in the size and dimensionality of the data. Our architecture is inspired by inducing point methods and relies on a novel application of cross-attention between datapoints. At inference time, its computational cost is constant in the training set size as the data gets distilled into a fixed number of inducing points. We find that our method reduces the computational requirements of existing semi-parametric models by up to an order of magnitude across a range of datasets and improves state-of-the-art performance on an important practical problem, genotype imputation.

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Figure 1: Genotype imputation is a natural candidate for semi-parametric approaches due to the biological principle of recombination.

scales linearly in the size of the training set $D_{\text{train}}$ and the dimensionality of $x$. Our architecture is inspired by inducing point approximations for kernel methods [46] [63] and relies on a novel application of attention called cross-attention between datapoints [43]. Our approach also learns a compact encoding $H_{\text{train}}$ that replaces $D_{\text{train}}$ at inference time in downstream applications, resulting in a computational complexity that is constant in $D_{\text{train}}$ at inference time.

We evaluate our method on a wide range of standard supervised learning benchmarks as well as a motivating real-world application in computational genomics—genotype imputation [48]. We find that our method yields performance improvements, while reducing computation and memory requirements by up to an order of magnitude. In the genomics setting, our approach outperforms one of the highly engineered state-of-the-art software package - Beagle, widely used within commercial genomics pipelines [11], indicating that our technique has the potential to impact real-world systems.

Contributions In summary, we introduce a semi-parametric neural architecture inspired by inducing point methods whose key component is a novel cross-attention mechanism between data and inducing points. It’s the first general-purpose semi-parametric architecture with the following characteristics:

1. Linear time and space complexity in the size and the dimension of the data during training.
2. The ability to learn a compact encoding of the training set for downstream applications. As a result, at inference time, computational complexity does not depend on training set size.

2 Background

Parametric and Semi-Parametric Machine Learning Most supervised methods in deep learning are parametric. Formally, given a training set $D_{\text{train}} = \{(x^{(i)}, y^{(i)})\}_{i=1}^{n}$ with features $x \in \mathcal{X}$ and labels $y \in \mathcal{Y}$, we seek to learn the parameters $\theta \in \Theta$ of a mapping $y = f_{\theta}(x)$ using supervised learning. Crucially, the learning signal from $D_{\text{train}}$ is fully contained in the parameters $\theta$, whose dimension stays fixed.

In contrast, non-parametric approaches learn a mapping $y = f_{\theta}(x \mid D_{\text{train}})$ that can query the training set $D_{\text{train}}$ at inference time; when the mapping $f_{\theta}$ has parameters, the approach is called semi-parametric. Many deep learning algorithms—including memory-augmented architectures [29] [59], retrieval-based language models [54] [31] [28], and non-parametric transformers [43]—are instances of this approach. Semi-parametric approaches are often specialized to specific tasks, and their computation scales superlinearly in the size of the training set [43]. This paper develops domain-agnostic semi-parametric methods that are computationally efficient.

A Motivating Application: Genotype Imputation A specific motivating example for developing efficient semi-parametric methods is the problem of genotype imputation (Figure 1). Consider the problem of determining the genomic sequence $y \in \{A, T, C, G\}^k$ of an individual; rather than directly measuring $y$, it is common to use an inexpensive microarray device to measure a small subset of genomic positions $x \in \{A, T, C, G\}^p$, where $p \ll k$. Genotype imputation is
the task of determining $y$ from $x$ via statistical methods and a dataset $D_{\text{train}} = \{x^{(i)}, y^{(i)}\}_{i=1}^n$ of fully-sequenced individuals [48].

Imputation is part of most standard genome analysis workflows. It is also a natural candidate for semi-parametric approaches [47]; a query genome $y$ can normally be represented as a combination of sequences $y^{(i)}$ from $D_{\text{train}}$ because of the biological principle of recombination [41], as shown in Figure 1. Additionally, the problem is a poor fit for parametric models: $k$ can be as high as $10^9$ and there is little correlation across non-proximal parts of $y$. Thus, we need an unwieldy number of parametric models (one for a subset of $y$), whereas a single semi-parametric model can run imputation across the genome.

**Attention Mechanisms** Our approach for designing semi-parametric models relies on modern attention mechanisms [60], specifically dot-product attention $\text{Att}(Q, K, V)$, which combines a query matrix $Q \in \mathbb{R}^{d_q \times e_q}$ with key and value matrices $K \in \mathbb{R}^{d_k \times e_k}$, $V \in \mathbb{R}^{d_v \times e_v}$ as

$$\text{Att}(Q, K, V) = \text{softmax}(QK^T / \sqrt{e_q})V.$$ 

To attend to different aspects of the keys and values, multi-head attention (MHA) extends this mechanism via $e_h$ attention heads:

$$\text{MHA}(Q, K, V) = \text{concat}(O_1, ..., O_{e_h})W^O \quad O_j = \text{Att}(QW_j^Q, KW_j^K, VW_j^K)$$

Each attention head projects $Q, K, V$ into a lower-dimensional space using learnable projection matrices $W_j^Q, W_j^K \in \mathbb{R}^{e_q \times e_h}$, $W_j^K \in \mathbb{R}^{e_k \times e_h}$ and mixes the outputs of the heads using $W^O \in \mathbb{R}^{e_h \times e_q}$. As is commonly done, we assume that $e_{qh} = e_v/e_h$, $e_{qh} = e_q/e_h$, and $e_a = e_q$.

Given two matrices $X, H \in \mathbb{R}^{d \times e}$, a multi-head attention block (MAB) wraps MHA together with layer normalization and a fully connected layer:

$$\text{MAB}(X, H) = O + \text{FF}(\text{LayerNorm}(O)) \quad O = X + \text{MHA}(\text{LayerNorm}(X), H, H)$$

Previous applications of multi-head attention to semi-parametric models [43] scale quadratically in the dataset size; our work is inspired by efficient attention architectures [48, 46] and develops scalable semi-parametric models with linear computational complexity.

### 3 Method

#### 3.1 A Framework for Semi-Parametric Learning Based on Neural Inducing Points

A key challenge posed by semi-parametric methods—one affecting both classical kernel methods [32] as well as recent attention-based approaches [43]—is the $O(n^2)$ computational cost per gradient update at training time, due to pairwise comparisons between training set points. Our work introduces methods that reduce this cost to $O(hn)$—where $h \ll n$ is a hyper-parameter—without sacrificing performance.

**Neural Inducing Points** Our approach is based on *inducing points*, a technique popular in approximate kernel methods [46, 63]. A set of inducing points $\mathcal{H} = \{h^{(j)}\}_{j=1}^h$ can be thought of as a “virtual” set of training instances that can replace the training set $D_{\text{train}}$. Intuitively, when $D_{\text{train}}$ is large, many datapoints are redundant—for example, groups of similar $x^{(i)}$ can be replaced with a single inducing point $h^{(j)}$ with little loss of information.

The key challenge in developing inducing point methods is finding a good set $\mathcal{H}$. While classical approaches rely on optimization techniques [63], we use an *attention mechanism* to produce $\mathcal{H}$. Each inducing point $h^{(j)} \in \mathcal{H}$ attends over the training set $D_{\text{train}}$ to select its relevant “neighbors” and updates itself based on them. We implement attention between $\mathcal{H}$ and $D_{\text{train}}$ in $O(hn)$ time.

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2 We use the pre-norm parameterization for residual connections and omit details such as dropout, see Nguyen and Salazar [52] for the full parameterization.

3 By default we use gradient descent instead of stochastic gradient descent, which has the benefit that a query point gets to attend to all the training points rather than a subset only. In Section 4.4 we will introduce a batching setting where each gradient update is approximated using a subset of the training set.
where \( d \) with a sequence of input features \( x \) with linear-time complexity.

The encoder consists of a sequence of layers, each of which takes as input \( D \) to make predictions and measure loss on a set of \( D \) while querying the inducing points \( H \).

**3.2 Semi-Parametric Inducing Point Networks**

Next, we describe semi-parametric inducing point networks (SPIN), a domain-agnostic architecture with linear-time complexity.

**Notation and Data Embedding** The SPIN model relies on a training set \( D_{\text{train}} = \{ (x^{(i)}, y^{(i)}) \}_{i=1}^n \) with a sequence of input features \( x^{(i)} \in X \subseteq V_x^p \) and a sequence of labels \( y^{(i)} \in Y \subseteq V_y^k \) where \( V_x \) and \( V_y \) are input and output vocabulary respectively.

We embed each dimension (each attribute) of \( x \) and \( y \) into an \( e \)-dimensional embedding and represent \( D_{\text{train}} \) as a tensor of embeddings \( D \in \mathbb{R}^{n \times d \times e} \), where \( d = p + k \) is obtained from concatenating the sequence of embeddings for each \( x^{(i)} \) and \( y^{(i)} \). The set \( D_{\text{train}} \) is used to learn inducing points \( H = \{ h^{(j)} \}_{j=1}^b \); similarly, we represent \( H \) via a tensor \( H \in \mathbb{R}^{b \times f \times e} \) of \( b \) inducing points, each being a sequence of \( f \leq d \) embeddings of size \( e \).

To make predictions and measure loss on a set of \( b \) examples \( D_{\text{query}} = \{ (x^{(i)}, y^{(i)}) \}_{i=1}^b \), we use the same embedding procedure to obtain a tensor of input embeddings \( X_{\text{query}} \in \mathbb{R}^{b \times f \times e} \) by embedding \( \{ (x^{(i)}, 0) \}_{i=1}^b \), in which the labels have been masked with zeros. We also use a tensor \( Y_{\text{gold}} \in \mathbb{R}^{b \times d} \) to store the ground truth labels and inputs (the objective function we use requires the model to make predictions on masked input elements as well, see below for details).

**High-Level Model Structure** [Figure 2] presents an overview of SPIN modules. At a high level, there are two components: (1) an Encoder module, which takes as input \( D_{\text{train}} \) and returns a tensor of inducing points \( H \); and (2) a Predictor module, which is a fully parametric model that outputs logits \( Y_{\text{query}} \) from \( H \) and \( X_{\text{query}} \).

\[
H = \text{Encoder}(D_{\text{train}}) \quad \quad \quad \quad Y_{\text{query}} = \text{Predictor}(X_{\text{query}}, H)
\]

The encoder consists of a sequence of layers, each of which takes as input \( D \in \mathbb{R}^{n \times d \times e} \) and two tensors \( H_A \in \mathbb{R}^{n \times f \times e} \) and \( H_D \in \mathbb{R}^{n \times f \times e} \) and output updated versions of \( H_A, H_D \) for the next layer. Each layer consists of a sequence of up to three cross-attention layers described below. The final output \( H \) of the encoder is the \( H_D \) produced by the last layer.

**3.2.1 Encoder Architecture**

Each layer of the encoder consists of three sublayers denoted as XABA, XABD, ABLA:

\[
H'_A = \text{XABA}(H_A, D) \quad H'_D = \text{XABD}(H_D, H'_A) \quad H_A = \text{ABLA}(H'_A) \quad H_D = \text{ABLA}(H'_D)
\]

\(^\text{Here we consider the case where both input and output are discrete, but our approach is easily generalizable to continuous input and output spaces.}\)
Cross-Attention Between Attributes (XABA) An XABA layer captures the dependencies among attributes via cross-attention between the sequence of latent encodings in $H$ and the sequence of datapoint features in $D$.

$$XABA(H_A, D) = MAB(H_A, D)$$

This updates the features of each datapoint in $H_A$ to be a combination of the features of the corresponding datapoints in $D$. In effect, this reduces the dimensionality of the datapoints (from $n \times d \times e$ to $n \times f \times e$). The time complexity of this layer is $O(ndfe)$, where $f$ is the dimensionality of the reduced tensor.

Cross-Attention Between Datapoints (XABD) The XABD layer is the key module that takes into account the entire training set to generate inducing points. First, it reshapes (“unfolds”) its input tensors $H_A' \in \mathbb{R}^{n \times f \times e}$ and $H_D \in \mathbb{R}^{h \times f \times e}$ into ones of dimensions $(1 \times n \times f \times e)$ and $(1 \times h \times f \times e)$ respectively. It then performs cross-attention between the two unfolded tensors. The output of cross-attention has dimension $(1 \times h \times f \times e)$; it is reshaped (“folded”) into an output tensor of size $(h \times f \times e)$.

$$XABD(H_D, H_A') = fold(MAB(unfold(H_D), unfold(H_A')))$$

This layer produces inducing points. Each inducing point in $H_D$ attends to dimensionality-reduced datapoints in $H_A'$ and uses its selected datapoints to update its own representation. The computational complexity of this operation is $O(nhfe)$, which is linear in training set size $n$.

Self-Attention Between Latent Attributes (ABLA) The third type of layer further captures dependencies among attributes by computing regular self-attention across attributes:

$$ABLA(H_A') = MAB(H_A', H_A')$$

$$ABLA(H_D') = MAB(H_D', H_D')$$

This enables the inducing points to refine their internal representations.

The dataset encoder consists of a sequence of the above layers [Figure 3](#). The ABLA layers are optional based on validation performance. The input $H_D$ to the first layer is part of the learned model parameters; the initial $H_A$ is a linear projection of $D$. The output of the encoder is the output $H_D$ of the final layer.

3.2.2 Predictor Architecture

The predictor is a parametric model that maps an input tensor $X_{query}$ to an output tensor of logits $Y_{query}$. The predictor can use any parametric model; we propose an architecture based on a simple cross-attention operation followed by a linear projection to the vocabulary size as shown in [Figure 3](#):

$$\text{Predict}(X_{query}, H) = FF(MAB(X_{query}, H_D))$$
Figure 4: Left: Overview of genotype imputation on a target genome using a reference dataset. Right: Existing non-parametric method for genomic imputation [47].

3.3 Objective Function

To train the model, we use maximum likelihood estimation and maximize the log probability of generating the label part of $Y_{\text{gold}}$ under the predicted logits $Y_{\text{query}}$. Denote this loss term as $L_{\text{labels}}$. In addition, following prior works [19, 26, 43], we randomly mask out a subset of input attributes in $X_{\text{query}}$ and ask the model to reconstruct these masked attributes and denote this loss term $L_{\text{attributes}}$. The overall training loss is a weighted combination of the loss over label predictions and over the predictions of the masked attributes.

$$L_{\text{SPIN}} = (1 - \lambda)L_{\text{labels}} + \lambda L_{\text{attributes}}$$

Following previous work NPT [43], we start with a weight $\lambda$ of 0.5 and anneal it to lean towards the loss for predicting labels.

4 Experiments

4.1 Genotype Imputation Experiments

Genotype imputation (Figure 4 left) is the task of inferring the sequence $y$ of an entire genome via statistical methods from a small subset of positions $x$—usually obtained from an inexpensive DNA microarray device [48]—and a dataset $D_{\text{train}} = \{x^{(i)}, y^{(i)}\}_{i=1}^n$ of fully-sequenced individuals [48]. Imputation is part of most standard workflows in genomics [49] and involves mature imputation software (Figure 4 right) [58, 10] that benefits from over a decade of engineering [47]. These systems are fully non-parametric and match genomes in $D_{\text{train}}$ to $x, y$; their scalability to modern datasets of up to millions of individuals is a known problem in the field [50]. Improved imputation holds the potential to reduce sequencing costs and improve workflows in medicine and agriculture.

**Experiment Setup** We compare against one of the state-of-the-art packages, Beagle [10] on the 1000 Genomes dataset [14] following the methodology described in [58]. We use 5008 complete sequences $y$ that we divide into train/val/test split of 0.86, 0.12, and 0.02 respectively. We construct inputs $x$ by masking positions that do not appear on the Illumina Omni2.5 array [67]. Our experiments focus on five sections of the genome for chromosome 20 and we pre-process the input into sequences of $K$-mers for all methods (see Appendix A.1). The performance of this task is measured with Pearson correlation coefficient $R^2$ between the imputed SNP and the actual value of SNP at a particular position.

We additionally compare against NPTs, Set Transformers, and classical machine learning methods. NPT-16, SPIN-16 and Set Transformer-16 refer to embedding dimension 16, model depth 4, attention head 1, while NPT-64, SPIN-64 and Set Transformer-64 refer to embedding dimension 64, model depth 4, and attention heads 4. SPIN uses 10 inducing points for datapoints and for each attribute
A batch size of 256 is used for Transformer methods and we train using the lookahead Lamb optimizer [71].

Table 1: Performance Summary on Genomic Sequence Imputation. A difference of 0.5% is statistically significant at p-value 0.05.

| Approach         | Parametric | Pearson $R^2\uparrow$ | Param Count↓ | Complexity     |
|------------------|------------|------------------------|--------------|----------------|
| Gradient Boosting| True       | 87.63                  | -            | -              |
| Traditional ML   | True       | 95.31                  | 65M          | -              |
| KNN              | False      | 89.70                  | -            | -              |
| Bio Software     | Beagle     | False                  | 95.64        | $O(n^2)$       |
| Transformer      | NPT-16     | False                  | 95.87        | 16.7M          |
| Set Transformer  | True       | 95.90                  | 33.4M        | $O(hn)$        |
| SPIN-16          | False      | 96.04                  | 8.1M         | $O(hn)$        |

Results. Table 1 presents the main results for genotype imputation. Compared to the previous state-of-the-art commercial software Beagle, which is specialized in this task, all Transformer-based methods achieve strong performance, despite making fewer assumptions and being more general. Among the Transformer-based approaches, SPIN achieves the highest Pearson $R^2$, at a fraction of other methods’ number of parameters. Among traditional ML approaches, MLP performs the best. However, all the traditional ML methods are trained using one model per output position (per component of y); the hyper-parameters of each model are also tuned separately. As a result, this process is not scalable and requires a very high number of parameters. We provide memory requirements (Peak GPU Memory usage in GB), average train time per epoch, and details on hyper-parameter tuning in Appendix A.1.

4.2 UCI Experiments

We present experimental results for 6 standard UCI benchmarks, namely Yacht, Concrete, Boston-Housing (regression datasets), Kick, Income, and Breast Cancer (classification datasets). We evaluate SPIN with relevant transformer baselines such as NPT [44] and a baseline we developed by incorporating inducing set point blocks (ISAB) introduced by Set Transformer [46] as a drop-in replacement for the multi-head attention blocks used in NPT. We also evaluate against Gradient Boosting [23], MLP [34, 27], KNN [2]. Following Kossen et al. [43] we measure the average ranking of methods and standard deviation based on these tasks. To show the memory efficiency of our approach we also report the Peak GPU Memory usage and standard deviation as a fraction of GPU Mem used by NPT for different splits of the test dataset in Table 2.

Table 2: Performance Summary on UCI Datasets.

| Approach         | Average Ranking order $\downarrow$ | Peak GPU Mem (relative to NPT)$\downarrow$ |
|------------------|------------------------------------|------------------------------------------|
| Traditional ML   | Gradient Boosting                  | 3.00 ± 2.00                             | -                                         |
|                  | MLP                                | 3.83 ± 1.94                             | -                                         |
|                  | KNN                                | 5.33 ± 1.21                             | -                                         |
| Transformer      | NPT                                | 2.83 ± 1.47                             | 1.0x                                      |
|                  | Set Transformer                    | 3.00 ± 1.22                             | 1.67 ± 0.51x                             |
|                  | SPIN                               | 2.83 ± 1.33                             | 0.52 ± 0.21x                             |

Results. SPIN and NPT achieve the best average ranking order on UCI datasets, but SPIN uses half the GPU memory compared to NPT. We provide detailed results on each of the datasets and hyperparameter details in Appendix A.2. Additionally, SPIN uses one-third of the parameters at inference time, for instance on the Yacht dataset, NPT has 42.7M parameters during training and inference, SPIN has 33.1M parameters during training but the SPIN modules used at inference have only 10.0M parameters since we can directly use learned latent instead of the training data.
4.3 Ablation Analysis

To evaluate the effectiveness of each module we introduced, we perform ablation analysis by gradually removing components from SPIN. Both SPIN-16 and SPIN-64 consist of 2 layers each of XABA, XABD, and ABLA for a model depth of 4. We remove components one at a time and compare the performance with default modules. In Table 3 we observe that for both SPIN-64 and SPIN-16, XABD (cross-attention between datapoints) is a crucial component, and incorporating ABLA (self-attention between latents) can sometimes help as in the case of SPIN-16.

| Model  | Approach                        | Pearson $R^2$ |
|--------|---------------------------------|---------------|
| SPIN-64| SPIN (XABA+XABD+ABLA)          | 94.01         |
|        | - XABD                         | 93.33         |
|        | - ABLA                         | 94.24         |
|        | - XABA - ABLA                  | 94.07         |
| SPIN-16| SPIN (XABA+XABD+ABLA)          | 94.26         |
|        | - XABD                         | 88.47         |
|        | - ABLA                         | 94.09         |
|        | - XABA - ABLA                  | 94.31         |

4.4 Effect of Batching

One way to alleviate the memory and computational burden of scaling non-parametric Transformers to large datasets is batching, where the train/val/test datasets are split into multiple slices, and gradients are only estimated on one slice at a time [43]. While batching allows for scaling to large datasets, the training time per epoch increases as the batch size goes down. In Appendix A.3, we show that on the UCI dataset Kick, while NPT with batching gets a comparable classification accuracy, our approach SPIN uses 5x less GPU memory, 3x fewer parameters, and 2x less average training time per epoch. On the genomics dataset, Table 4 shows the comparison between different batching regimes for both NPT and SPIN. We observe that SPIN consumes half the memory and training time per epoch. The computational efficiency of SPIN is orthogonal to the strategy of batching.

| Approach | Batch Size | Pearson $R^2$ | Peak GPU Mem (GB) | Avg. Train time/epoch(s) |
|----------|------------|---------------|-------------------|-------------------------|
| NPT      | No Batching | 96.84         | 18.21             | 1.03                    |
|          | 2048       | 96.74         | 10.49             | 1.34                    |
|          | 1024       | 96.83         | 9.24              | 1.73                    |
|          | 256        | 96.85         | 8.12              | 4.39                    |
| SPIN     | No Batching | 97.06         | 6.08              | 0.52                    |
|          | 2048       | 97.01         | 3.86              | 0.86                    |
|          | 1024       | 97.04         | 3.44              | 1.22                    |
|          | 256        | 97.07         | 2.97              | 3.64                    |

4.5 Compute Resources

For all the experiments, we use one 24GB NVIDIA GeForce RTX 3090 GPU. We do not use multi-GPU training or other memory-saving techniques such as gradient checkpointing, pruning, mixed precision training, etc. but note that these are orthogonal to our approach and can be used to further reduce the computational complexity.
5 Related Work

Non-Parametric and Semi-Parametric Methods Non-parametric methods have a long history in machine learning, starting from nearest neighbors approaches [21, 3] and density estimation [24], and including more recent approaches based on kernels [17], such as Gaussian processes [57] and support vector machines [32]. Kernel methods are a classical example of non-parametric approaches with quadratic complexity [4], which motivates a long line of approximate methods based on random projections [1], Fourier analysis [55], and inducing point methods [64]. Inducing points have been widely applied in kernel machines [51], Gaussian processes classification [36], regression [12], semi-supervised learning [18], and more [33]. Our work combines non-parametric inducing points methods with deep learning and attention.

Deep Semi-Parametric Models Deep Gaussian Processes [16], Deep Kernel Learning [65], and Neural Processes [25] build upon classical methods. Deep GPs rely on sophisticated variational inference methods [62], making them challenging to implement, while Neural Processes and their attentive versions [42] rely on multiple samples of datasets, not unlike in meta-learning [20]. Retrieval augmented transformers [8] use attention to query external datasets in specific domains such as language modeling [28] and question answering [69], and in a way that is similar to earlier memory-augmented models [29]. Non-Parametric Transformers (NPTs) [44] use a domain-agnostic architecture based on attention that runs in $O(n^2d^2)$ at training time and $O(nd^2)$ at inference time; NPTs are closest to our work. We leverage their idea of attention over data and improve its scalability to $O(nd)$ at training time and $O(d)$ at inference time.

Attention Mechanisms The quadratic cost of self-attention [60] can be reduced using efficient architectures such as sparse attention [6], Set Transformers [46], the Performer [13], the Nystromer [68], Long Ranger [30], Big Bird [70], the Perceiver [38, 37], and others [40, 61]. Our work most closely resembles the Set Transformer [46] and Perceiver [38, 37] mechanisms—we extend these mechanisms to cross-attention between datapoints and use them to attend to datapoints, similarly to Non-Parametric Transformers [44].

6 Limitations

The SPIN model achieves linear complexity via advanced self-attention mechanisms; This also introduces additional hyper-parameters into the model, potentially increasing tuning time. The resulting architecture remains overparametrized even after with small numbers of inducing points $h, f$ and may overfit.

The primary source of expressivity is attention between datapoints, which has a query dimension $he$. Highly expressive models may learn to ignore the training set and operate in a fully-parametric mode; this failure mode is best avoided via regularization and large datasets. Interestingly, our approach benefits from big data, while classical non-parametric models work best on small datasets due to their computational complexity. Regularization via small $h, f$, dropout, and feature masking control overfitting; we will explore more compact architectures in future work.

7 Conclusion

In this paper, we introduce a domain-agnostic general-purpose architecture, the semi-parametric inducing point network (SPIN). Unlike previous semi-parametric approaches whose computational cost grows quadratically with the size of the dataset, our approach scales linearly in the size and dimensionality of the data by leveraging a cross attention mechanism between datapoints and induced latents, allowing it to scale to large datasets.

We present empirical results on six UCI datasets and a real-world important task in genomics, genotype imputation, and show that SPIN can achieve competitive, if not better, performance relative to state-of-the-art methods at a fraction of the computational cost. Furthermore, our approach allows the use of a compact encoding of training dataset at inference time, which is potentially useful for privacy-preserving applications or where retrieving from training data at inference is cost-prohibitive.
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Appendix: Semi-Parametric Deep Neural Networks in Linear Time and Memory

A Experimental Details

A.1 Genomic Sequence Imputation

Imputation is performed on single-nucleotide polymorphisms (SNPs) with a corresponding marker panel specifying the microarray. We randomly sample five sections of the genome for chromosome 20 for conducting experiments. Each section is selected with 100 SNPs to be predicted and 150 closest SNPs are obtained. For compact encoding of SNPs, we form $K$-mers, which are commonly used in various genomics applications [15], where $K$ is a hyper-parameter that controls the granularity of tokenization (how many nucleotides are treated as a single token). This now becomes a $2^K$-way classification task. We set $K$ to 5 for all the genomics experiments, so that there are 20 (100/5) target SNPs to be imputed and 30 (150/5) attributes per sampled section. We report Pearson $R^2$ for each of the five sections in Table 5. For computational load, we report peak GPU memory usage in GB where applicable, an average of train time per epoch in seconds and parameter count per method.

Hyper-parameters for tuning We provide the list of hyper-parameters that were grid searched for different methods in Table 6. Beagle is a specialized software using dynamic programming and does not require any hyper-parameters from the user.
| Approach         | Pearson $R^2$ | Peak GPU Mem (GB) | Params Count | Avg. Train time/epoch(s) |
|------------------|--------------|-------------------|--------------|--------------------------|
| **Genomics Dataset (SNPs 68300-68400)** |
| Traditional ML   | 81.12        | -                 | -            | -                        |
| Gradient Boosting|              |                   |              |                          |
| MLP              | 97.63        | -                 | -            | -                        |
| KNN              | 86.96        | -                 | -            | -                        |
| Bio Software     | 98.07        | -                 | -            | -                        |
| Beagle           |              |                   |              |                          |
| Transformer      | NPT          | 96.91             | 0.45         | 16.7M                    | 2.22 |
|                  | Set Transformer | 96.73       | 0.76         | 33.4M                    | 2.93 |
|                  | SPIN         | 97.21             | 0.28         | 8.0M                     | 2.23 |
| **Genomics Dataset (SNPs 169500-169600)** |
| Traditional ML   | 91.53        | -                 | -            | -                        |
| Gradient Boosting|              |                   |              |                          |
| MLP              | 97.19        | -                 | -            | -                        |
| KNN              | 95.65        | -                 | -            | -                        |
| Bio Software     | 97.87        | -                 | -            | -                        |
| Beagle           |              |                   |              |                          |
| Transformer      | NPT          | 97.46             | 0.45         | 16.7M                    | 1.98 |
|                  | Set Transformer | 97.39       | 0.76         | 33.4M                    | 2.99 |
|                  | SPIN         | 97.46             | 0.28         | 8.0M                     | 2.76 |
| **Genomics Dataset (SNPs 287600-287700)** |
| Traditional ML   | 82.77        | -                 | -            | -                        |
| Gradient Boosting|              |                   |              |                          |
| MLP              | 96.20        | -                 | -            | -                        |
| KNN              | 95.56        | -                 | -            | -                        |
| Bio Software     | 92.62        | -                 | -            | -                        |
| Beagle           |              |                   |              |                          |
| Transformer      | NPT          | 97.10             | 0.45         | 16.7M                    | 2.24 |
|                  | Set Transformer | 97.15       | 0.76         | 33.4M                    | 2.99 |
|                  | SPIN         | 97.15             | 0.28         | 8.0M                     | 2.60 |
| **Genomics Dataset (SNPs 424600-424700)** |
| Traditional ML   | 82.77        | -                 | -            | -                        |
| Gradient Boosting|              |                   |              |                          |
| MLP              | 91.98        | -                 | -            | -                        |
| KNN              | 84.39        | -                 | -            | -                        |
| Bio Software     | 93.72        | -                 | -            | -                        |
| Beagle           |              |                   |              |                          |
| Transformer      | NPT          | 94.12             | 0.45         | 16.7M                    | 2.23 |
|                  | Set Transformer | 94.02       | 0.76         | 33.4M                    | 2.90 |
|                  | SPIN         | 94.26             | 0.28         | 8.0M                     | 2.21 |
| **Genomics Dataset (SNPs 543000-543100)** |
| Traditional ML   | 72.66        | -                 | -            | -                        |
| Gradient Boosting|              |                   |              |                          |
| MLP              | 89.56        | -                 | -            | -                        |
| KNN              | 78.22        | -                 | -            | -                        |
| Bio Software     | 94.58        | -                 | -            | -                        |
| Beagle           |              |                   |              |                          |
| Transformer      | NPT          | 89.69             | 0.45         | 16.7M                    | 1.95 |
|                  | Set Transformer | 92.12       | 0.76         | 33.4M                    | 2.52 |
|                  | SPIN         | 91.50             | 0.28         | 8.0M                     | 2.28 |
### Table 6: Hyperparameters for Genomics Dataset

| Model                  | Hyperparameter       | Setting                                      |
|------------------------|----------------------|----------------------------------------------|
| **NPT, SPIN, Set Transformer** | Embedding Dimension | [16, 128]                                    |
|                        | Depth                | [2, 8]                                       |
|                        | Label Masking        | [0, 0.5]                                     |
|                        | Target Masking       | [0.3]                                        |
|                        | Learning rate        | [1e − 5, 1e − 2]                             |
|                        | Dropout              | [0.4, 0.6]                                   |
|                        | Batch Size           | [256, 5008 (No Batching)]                    |
| **Gradient Boosting**  | Max Depth            | [5, 10]                                      |
|                        | n_estimators         | [100]                                        |
|                        | Learning rate        | [1e − 2]                                     |
| **MLP**                | Hidden Layer Sizes   | [(500, 500, 500)]                            |
|                        | Batch Size           | [128, 256]                                   |
|                        | L2 regularization    | [0, 1e − 2]                                  |
|                        | Learning rate init   | [1e − 4, 1e − 2]                             |
| **KNN**                | n_neighbors          | [2, 1000]                                    |
|                        | weights              | [distance]                                   |
|                        | algorithm            | [auto]                                       |
|                        | Leaf Size            | [10, 100]                                    |
| **Bio Software**       | None                 | None                                         |

### A.2 UCI Regression Tasks

In Table 7 we report performance and computational requirements for 10 cv splits for Yacht dataset, 3 cv splits for Boston Housing and 6 cv splits for Concrete dataset. The lower number of cv splits for Boston-Housing and Concrete are due to computational load requirements for these datasets. **Yacht** dataset consists of 308 instances, 5 categorical features and 1 continuous target. **Boston Housing** dataset consists of 506 instances, 13 continuous features and 1 continuous target. **Concrete** consists of 1030 instances, 8 continuous features and 1 continuous target.
| Approach       | RMSE ↓ | Peak GPU Mem (GB) ↓ | Params Count ↓ | Avg. Train time/epoch(s) ↓ |
|---------------|--------|---------------------|----------------|--------------------------|
| **Boston-Housing** |        |                     |                |                          |
| Gradient Boosting | 2.60 ± 0.38 | -                   | -              | -                        |
| Traditional ML MLP | 2.78 ± 0.28 | -                   | -              | -                        |
| KNN            | 3.79 ± 0.68 | -                   | -              | -                        |
| Transformer NPT | 2.46 ± 0.27 | 8.2                 | 168.0M         | 1.43                     |
| Set Transformer | 2.40 ± 0.21 | 16.5                | 336.0M         | 1.62                     |
| SPIN           | 2.54 ± 0.25 | 6.2                 | 168.0M         | 1.43                     |
| **Yacht**      |        |                     |                |                          |
| Gradient Boosting | 0.87 ± 0.37 | -                   | -              | -                        |
| Traditional ML MLP | 0.83 ± 0.18 | -                   | -              | -                        |
| KNN            | 11.97 ± 2.06 | -                   | -              | -                        |
| Transformer NPT | 1.42 ± 0.64 | 2.1                 | 42.7M          | 0.10                     |
| Set Transformer | 1.29 ± 0.34 | 4.1                 | 85.4M          | 0.19                     |
| SPIN           | 1.28 ± 0.66 | 1.6                 | 32.2M          | 0.07                     |
| **Concrete**   |        |                     |                |                          |
| Gradient Boosting | 4.61 ± 0.72 | -                   | -              | -                        |
| Traditional ML MLP | 5.29 ± 0.74 | -                   | -              | -                        |
| KNN            | 6.62 ± 0.77 | -                   | -              | -                        |
| Transformer NPT | 5.43 ± 0.61 | 3.4                 | 69.9M          | 0.13                     |
| Set Transformer | 5.35 ± 0.80 | 6.8                 | 139.9M         | 0.21                     |
| SPIN           | 5.99 ± 0.33 | 1.9                 | 38.3M          | 0.13                     |

### A.3 UCI Classification Tasks

In Table 8, we report mean and std dev for classification accuracy over 10 cv splits for Breast Cancer. We report results for 1 cv split for Kick and Income dataset because of computational load. Breast Cancer dataset consists of 569 instances, 30 continuous features and 1 categorical target. Kick dataset consists of 72,983 instances, 14 continuous, 17 categorical features and 1 categorical target. Income consists of 299,285 instances, 6 continuous, 35 categorical features and 1 categorical target. We provide hyperparameters grid searched for UCI datasets in Table 9. Additionally, we provide average ranking separated by Regression and Classification tasks in Table 10 and Table 11 respectively.\(^1\)

\(^1\)NPT reports a mean of 1.27 on this task that we could not reproduce. However, we emphasize that for UCI experiments, all the model parameters are kept same for all the transformer methods.
| Approach                          | Accuracy       | Peak GPU Mem (GB) | Params Count | Avg. Train time/epoch(s) |
|----------------------------------|----------------|-------------------|--------------|--------------------------|
| **Breast Cancer**                |                |                   |              |                          |
| Gradient Boosting                | 94.03±2.74     | -                 | -            | -                        |
| Traditional ML MLP              | 94.03±3.05     | -                 | -            | -                        |
| KNN                              | 95.26±2.48     | -                 | -            | -                        |
| Transformer                      |                |                   |              |                          |
| NPT                              | 95.79±1.22     | 2.6               | 51.3M        | 0.15                     |
| Set Transformer                  | 94.91±1.53     | 5.2               | 102.6M       | 0.21                     |
| SPIN                             | 95.61±2.22     | 0.9               | 16.7M        | 0.16                     |
| **Kick**                         |                |                   |              |                          |
| Gradient Boosting                | 90.20          | -                 | -            | -                        |
| Traditional ML MLP              | 89.96          | -                 | -            | -                        |
| KNN                              | 87.71          | -                 | -            | -                        |
| Transformer                      |                |                   |              |                          |
| NPT                              | 90.04          | 14.9              | 232.6M       | 56.22                    |
| Set Transformer                  | 90.03          | 15.0              | 465.0M       | 52.35                    |
| SPIN                             | 90.06          | 3.6               | 73.7M        | 27.76                    |
| **Income**                       |                |                   |              |                          |
| Gradient Boosting                | 95.8           | -                 | -            | -                        |
| Traditional ML MLP              | 95.4           | -                 | -            | -                        |
| KNN                              | 94.8           | -                 | -            | -                        |
| Transformer                      |                |                   |              |                          |
| NPT                              | 95.6           | 24                | 1504M        | -                        |
| Set Transformer                  | -              | OOM               | OOM          | -                        |
| SPIN                             | 95.6           | 11.5              | 418.9M       | 68.02                    |
Table 9: Hyperparameters for UCI Dataset

| Model                        | Hyperparameter          | Setting                      |
|------------------------------|-------------------------|------------------------------|
| NPT, SPIN, Set Transformer   | Embedding Dimension     | [16, 128]                    |
|                              | Depth                   | [8]                          |
|                              | Label Masking           | [0, 0.5]                     |
|                              | Target Masking          | [0.3]                        |
|                              | Learning rate           | [1e−5, 1e−2]                 |
|                              | Dropout                 | [0.4, 0.6]                   |
|                              | Batch Size              | [2048, No Batching]          |
| Gradient Boosting            | Max Depth               | [3, 10]                      |
|                              | n_estimators            | [50, 1000]                   |
|                              | Learning rate           | [1e−3, 0.3]                  |
| MLP (Boston Housing, Breast Cancer, Concrete, and Yacht) | Hidden Layer Sizes | [(25) – (500), (25, 25) – (500, 500), (25, 25, 25) – (500, 500, 500)] |
|                              | Batch Size              | [32, 256]                    |
|                              | L2 regularization       | [0, 1]                       |
|                              | Learning rate           | [constant, invscaling, adaptive] |
|                              | Learning rate init      | [1e−5, 1e−1]                 |
| MLP (Kick, Income)           | Hidden Layer Sizes      | [(25, 25, 25) – (500, 500, 500)] |
|                              | Batch Size              | [128, 256]                   |
|                              | L2 regularization       | [0, 1e−2]                    |
|                              | Learning rate           | [constant, invscaling, adaptive] |
|                              | Learning rate init      | [1e−5, 1e−1]                 |
| KNN (Boston Housing, Breast Cancer, Concrete, and Yacht) | n_neighbors | [2, 100]                     |
|                              | weights                 | [uniform, distance]          |
|                              | algorithm               | [ball_tree, kd_tree, brute]  |
|                              | Leaf Size               | [10, 100]                    |
| KNN (Kick, Income)           | n_neighbors             | [2, 1000]                    |
|                              | weights                 | [distance]                   |
|                              | algorithm               | [auto]                       |
|                              | Leaf Size               | [10, 100]                    |

Table 10: Average Ranking on UCI Regression Dataset (Yacht, Boston Housing, Concrete) based on RMSE

| Approach          | Average Ranking order | Peak GPU Mem (relative to NPT) |
|-------------------|-----------------------|---------------------------------|
| Traditional ML    |                       |                                 |
| Gradient Boosting | 2.33 ± 1.53           | -                               |
| MLP               | 2.67 ± 1.53           | -                               |
| KNN               | 6.00 ± 0.00           | -                               |
| Transformer       |                       |                                 |
| NPT               | 3.67 ± 1.53           | 1.0x                            |
| Set Transformer   | 2.67 ± 1.53           | 1.99 ± 0.03x                    |
| SPIN              | 3.67 ± 1.15           | 0.69 ± 0.12x                    |
| Approach       | Average Ranking order | Peak GPU Mem (relative to NPT) |
|----------------|-----------------------|---------------------------------|
| Traditional ML|                       |                                 |
| Gradient Boosting | 4.33 ± 1.53          | -                               |
| MLP             | 5.00 ± 1.00           | -                               |
| KNN             | 4.67 ± 1.53           | -                               |
| Transformer     |                       |                                 |
| NPT             | 2.00 ± 1.00           | 1.0x                            |
| Set Transformer | 3.50 ± 0.70           | 1.67 ± 0.51x                    |
| SPIN            | 2.00 ± 1.00           | 0.52 ± 0.21x                    |