Kriging Convolutional Networks

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Abstract

Spatial interpolation is a class of estimation problems where locations with known values are used to estimate values at other locations, with an emphasis on harnessing spatial locality and trends. Traditional Kriging methods have strong Gaussian assumptions, and as a result, often fail to capture complexities within the data. Inspired by the recent progress of graph neural networks, we introduce Kriging Convolutional Networks (KCN), a method of combining advantages of Graph Convolutional Networks (GCN) and Kriging. Compared to standard GCNs, KCNs make direct use of neighboring observations when generating predictions. KCNs also contain the Kriging method as a specific configuration. We further improve the model’s performance by adding attention. Empirically, we show that this model outperforms GCNs and Kriging in several applications. The implementation of KCN using PyTorch is publicized at the GitHub repository[1] 

Spatial data is ubiquitous in a wide variety of fields such as ecology (Fink et al. 2010), economics (Gao and Liu 2014), and meteorology (Xingjian et al. 2015). A common task within these fields is to estimate values at target locations from nearby known values. Improving these estimations should provide clear benefits for these applications. Estimation techniques tailored to spatial data must leverage the fact that every data point is associated with a location. Most importantly, these techniques should be able to capture the spatial correlation among these locations.

In many fields, the most prevalent method for spatial data modeling is kriging (Cressie 1991). The fundamental assumption of kriging is that observations at locations are from an underlying Gaussian process. After estimating the variogram, which is essentially the strength of spatial correlations between data points, kriging uses a linear interpolation of observed values to predict the value at a new location. The kriging prediction is the best linear unbiased estimator for spatial points given its Gaussian assumption. However, this assumption is quite constrictive, as data in many applications are not from a Gaussian distribution. For example, we will show in our experiments that this assumption leads to poor performance when estimating integer counts that contain a significant fraction of zeros.

Researchers also use flexible machine learning algorithms (Hengl et al. 2018) for spatial data modeling. Given the huge success of GNNs and the similarity between spatial data and graph data, researchers have started to apply Graph Neural Networks (GNN) (Wu et al. 2019) to spatial data (Li et al. 2017; Yu, Yin, and Zhu 2017; Zhu and Liu 2018; Yan et al. 2019). GNNs were first developed for explicit graph data, but can model any data that can be transformed into a graph either by their spatial vicinity or their physical connections (e.g. routes). The main idea is to propagate information along graph edges, so graph nodes can share information during the learning process. GNNs are relatively generic, and can find nonlinear relationships between the inputs, hidden layers, and neighborhood information of each node. By design, GNNs are more flexible than kriging.

However, kriging has an advantage over GNNs: kriging directly uses observed training labels to predict the label of a new data point. In comparison, there is no straightforward way to feed training labels as input to a GNN. It is not feasible to directly feed training labels as part of the input because the GNN will directly output the given label of a training data point and learn nothing. Furthermore, spatial data modeling requires inductive learning – the model needs to be able to make predictions for new locations that are not in the graph formed by training data. While kriging is intrinsically inductive, only a few GNNs such as GraphSAGE (Hamilton, Ying, and Leskovec 2017) can work inductively.

Inspired by these two observations, we develop a new model, the Kriging Convolutional Network (KCN), as an improvement to GNNs. The KCN is still a type of GNN. However, it does not form a single large graph over all data points. Every time a KCN fits the label of a data point (call it the center), it forms a small graph over the center and its neighboring training data points. These neighbors are the $K$ nearest neighbors according to a distance metric. In the input to the KCN, we hide the label of the center node. The input

1Equal contribution. The first two authors are arranged by the alphabet order
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[1] This is a new implementation updated in 2023 using PyTorch, so the performance values are slightly different with those reported in the paper.
consists of feature vectors for all nodes in the graph \((K + 1)\) nodes), as well as the labels of the neighbors. The KCN also needs the adjacency matrix of the graph, which is defined to be the spatial kernel matrix or a normalized version of that. The target value of the KCN is the label of the center node. We iterate over all of the training data, treating each node as the center to train the KCN model. The KCN uses the same structure to predict the label of a new data point.

The KCN combines the best parts of both models. In comparison to the GNN, it is able to directly leverage training labels in prediction, and no re-training is necessary when new data points are introduced. In contrast to kriging, the KCN is more versatile. On a large dataset where overfitting is not an issue, the KCN has a clear advantage over kriging. Even though the KCN’s underlying mechanisms are very different from kriging, our theoretical analysis reveals a deep connection between the two models. In fact, with a special configuration, the KCN can emulate kriging.

In summary, this work has three contributions:

- the development of the KCN, which is a GNN that directly uses training labels for prediction;
- the theoretical result showing that the KCN approximately recovers local universal kriging; and
- empirical studies indicating the KCN’s advantage over baseline models.

Related Work

Kriging (Cressie 1991) has been widely used in spatial data modeling. Using Kriging to model non-Gaussian data is often accomplished through careful transformation of labels (Sauto and Goovaerts 2000). However, it is not always feasible to transform a variable to be Gaussian (Dance 2018). One direction of exploration is to weaken the Gaussian assumption of kriging models (Wallin and Bolin 2015), but these methods are often specially designed for their respective applications.

GNNs are neural networks that work on graph data (Gori, Monfardini, and Scarselli 2005), (Wu et al. 2019) and Zhou et al. (2018) have done extensive surveys of this topic. A GNN typically consists of a few layers, each of which has a non-linear transformation of the hidden vectors and a step of information propagation between nodes. GNN architectures differ by how they propagate information among graph nodes (Kipf and Welling 2016, Atwood and Towsley 2016, Hamilton, Ying, and Leskovec 2017, Velickovic et al. 2018). When a GNN is applied to spatial data (Wu et al. 2019, Yan et al. 2019), one first builds a graph over data points in the spatial area and then runs the GNN on the graph. To the best of our knowledge, all of these methods feed features as the input and fit labels by the output of the network. In this work, we develop our KCN model based on the Graph Convolutional Network (GCN) (Kipf and Welling 2016) and Graph Attention Network (GAT) (Velickovic et al. 2018).

Background

Suppose there are \(N\) spatial data points, \((s, X, y) = (s_i, x_i, y_i)_{i=1}^{N}\), where \(s_i\), \(x_i\), and \(y_i\) are respectively the location, the feature vector, and the label of data point \(i\). Usually a location \(s_i\) is a GPS coordinate, \(s_i \in \mathbb{R}^2\). There are \(d\) features in a feature vector \(x_i \in \mathbb{R}^d\). The domain of the target value \(y_i\) is application-dependent. For example, \(y_i \in \mathbb{N}\) when \(y_i\) is a count, and \(y_i \in \mathbb{R}^+\) when \(y_i\) represents the precipitation level. One important task of spatial data modeling is to predict or estimate the value \(y_i\) for a new location \(s_\ast\) with a feature vector \(x_\ast\). Let \(\hat{y}_\ast\) denote the prediction.

Kriging

There are many variants of kriging, of which universal kriging is the most appropriate for the setting above. Universal kriging has the following model assumption (Eq. 3.4.2 in (Cressie 1991)).

\[
y_i = \beta^T x_i + \epsilon(s_i), \quad i = 1, \ldots, n , \ast
\]  

Here \(\beta\) is the coefficient vector. \(\epsilon(\cdot)\) is a zero-mean random process with variogram \(2\gamma(\cdot)\). The variogram \(2\gamma(\cdot)\), which specifies the spatial correlation between data points, is a function of spatial distance: \(2\gamma(||s_i - s_j||) = \mathbb{E}[(\epsilon(s_i) - \epsilon(s_j))^2]\). The variogram often takes a special function form with its parameters estimated from the data. With this model assumption, kriging minimizes the expected squared error, \(\mathbb{E}[\epsilon] = (\hat{y}_\ast - y_\ast)^2, \) in closed form. Then the prediction \(y_\ast\) of universal kriging is \(\hat{y}_\ast^{\text{kriging}} = \lambda^T (y - \mu)\) with

\[
\lambda = \Gamma^{-1} (\gamma - B^TX^T\Gamma^{-1}\gamma + Bx_\ast),
\]

with \(B = X(X^T\Gamma^{-1}X)^{-1}, \Gamma = [\gamma(||s_i - s_j||)]_{i,j=1}^n, \) and \(\gamma = [\gamma(||s_i - s_j||)]_{i,j=1}^n\).

Note that kriging uses known training labels as well as all features as the input to make the prediction. Despite its complex form, kriging has a subtle relation with the KCN model proposed later.

Graph Convolutional Networks

Suppose we have a graph \(G = (V, E)\), where \(V = \{1, \ldots, M\}\) is set of data points, and \(E\) is the edge set. Each data point \(i \in V\) has a feature vector \(x_i\) and a label \(y_i\). Later, we will collectively denote \((X, y)\) as a stack of all features and labels for notational convenience. Let \(A\) denote the adjacency matrix of the graph, and \(\hat{A}\) denote the normalized adjacency matrix,

\[
\hat{A} = D^{-\frac{1}{2}} (A + I) D^{-\frac{1}{2}},
\]

with \(D = \text{diag}(A + 1)\) being the degree matrix plus one. Then a GCN (Kipf and Welling 2016) takes \(\hat{A}\) and \(\hat{X}\) as the input and fits known labels in \(y\) as the target. The GCN consists of \(L\) GCN layers. Each GCN layer \(\ell\) takes an input \(H_{\ell-1} \in \mathbb{R}^{n \times d_{\ell-1}}\) and outputs a matrix \(H_{\ell} \in \mathbb{R}^{n \times d_{\ell}}\). The layer is parameterized by a matrix \(W^\ell\) with size \(d_{\ell-1} \times d_{\ell}\). Formally, the GCN is defined by

\[
H^0 = \hat{X},
\]

\[
H^\ell = \sigma (\hat{A} H^{\ell-1} W^\ell), \quad \ell = 1, \ldots, L
\]

\[
\hat{y} = H^L.
\]

Here \(\sigma(\cdot)\) is a non-linear activation function.
Kriging Convolution Network

In this work, we develop a new learning model that directly use training labels as the input for predictions. We call this model a Kriging Convolution Network (KCN).

Let’s first demonstrate how a KCN model can be used for prediction. To predict a scalar for a graph node, the last layer $H^L$ has only $d_L = 1$ column, and its entry corresponding to the new data point $(s_i, x_i)$ is the prediction $\hat{y}_i$. In practice, a two-layer GCN with $L = 2$ is often sufficient. A GCN considers a semi-supervised task, in which only part of the labels $\hat{y}$ are observed. A GCN then defines its training loss based on the known labels, and aims to predict unknown labels. To apply a GCN to the previous task, we form a graph for $(s_i, x_i)$, and put all features to the graph nodes. When predicting a scalar for a graph node, the last layer $H^L$ has only $d_L = 1$ column, and its entry corresponding to the new data point $(s_i, x_i)$ is the prediction $\hat{y}_i$.

Then the KCN model is defined to be a GCN followed by a dense layer. The KCN is formally defined as

$$\text{Algorithm 1: The training algorithm of KCN}$$

$$\text{Input: (s, X, y), K}$$

$$\text{Output: } \theta = (W^1, \ldots, W^L, w_{\text{den}})$$

$$\text{for } i \leftarrow 0 \text{ to } N \text{ do}$$

$$\beta_i = \{K\text{ nearest neighbors of } s_i \text{ and } i\};$$

$$\text{Compute } A \text{ from } s_{\alpha_i} \text{ by (9);}$$

$$\text{Prepare } H^0 \text{ from } (x_i, X_{\alpha_i}, y_{\alpha_i}) \text{ by (10);}$$

$$\text{end}$$

$$\text{for } \text{iter} \leftarrow 0 \text{ to } \text{num training iter} \text{ do}$$

$$i = \text{iter}\%N;$$

$$H^L = \text{GCN}(A, H^0, W^1, \ldots, W^L);$$

$$\hat{y}_i = \sigma\left(e^\top H^L w_{\text{den}}\right);$$

$$\text{Compute loss}(y_i, \hat{y}_i) \text{ and its derivative;}$$

$$\text{Update weights } \theta = W^1, \ldots, W^L, w_{\text{den}}$$

$$\text{end}$$

Here $\phi$ is the kernel length, which is a hyperparameter. In this graph, the edge $(j, k)$ has a large weight when $j$ and $k$ are near each other and vice versa.

Next we define the feature input to the GCN. The input should include features $x_i$ and $X_{\alpha_i}$, and neighboring labels $y_{\alpha_i}$. Incorporating this information into a matrix will require a bit of care. We place $y_{\alpha_i}$ and a zero in place of $y_i$ into a vector with length $(k+1)$, so the model has no access to $y_i$. We also use an indicator vector $e$ to indicate that the instance $i$ is the one to be predicted. Then the GCN input is expressed by a matrix $H^0$ with size $(k+1) \times (2+d)$.

$$H^0 = \begin{bmatrix} 0 & 1 & x_i^\top \\ y_{\alpha_i} & 0 & X_{\alpha_i} \end{bmatrix}.$$ (10)

The locations $s_{\beta_i}$ can be included in the feature matrix $X$ as features if there is reason to suspect spatial trends.

Then the KCN model is defined to be a GCN followed by a dense layer. The KCN is formally defined as

$$H^L = \text{GCN}(A, H^0),$$ (11)

$$\hat{y}_i = \sigma \left( e^\top H^L w_{\text{den}} \right).$$ (12)

Here $A$ and $H^0$ are the adjacency matrix and the input feature matrix constructed from the neighborhood of $i$. Note that every data point $i$ gets its own $A$ and $H^0$, whose index $i$ is omitted for notational simplicity. The vector $e$ is the indicator vector for $i$: it takes the first vector of $H^L$, corresponding to $i$, as the input to the dense layer. The dense layer allows for a final transformation of the data without interference from neighbors.

The KCN parameters are all weight matrices, $\theta = \{W^1, \ldots, W^L, w_{\text{den}}\}$. We train the KCN model by minimizing the loss in (9). Then we can predict the label of a new data point using its features and neighbors in the training set. Algorithm 1 summarizes the training procedure of the KCN.

Compared to local kriging, which only uses nearest neighbors for kriging, the KCN uses the same input. However, the KCN is much more flexible. When the training set is large enough such that the overfitting issue is less of a concern, the KCN model has clear advantages.
Compared to the direct application of a GCN on spatial data, a KCN is able to use labels from neighbors directly. Furthermore, a KCN does not need to use the test data points to form the graph. Therefore, it does not need to re-train the model when there is a new batch of test data points.

The KCN is also similar to the KNN classifier but is much more powerful: while the KNN simply averages the labels of neighbors, the KCN uses a neural network as the predictive function.

**KCN with Graph Attention**

The recent success of attention mechanism on GNNs inspires us to try the Graph Attention network (GAT) (Velicković et al. 2018) as the predicting model. The original GAT model computes attention weights with a neural network; it also requires that the attention weights of a node’s neighbors sum up to 1. Here we use the dot-product self-attention (Vaswani et al. 2017) so that the model has a choice to fall back on the GCN model.

Suppose the input feature at the ℓ-th layer of the GCN is $H^{ℓ−1}$, then we compute an attention matrix $U$ by

$$P = H^{ℓ−1}W_{att}, \quad M = \sigma(PP^\top),$$

$$\Lambda = \text{diag}(M), \quad U = \Lambda^{-\frac{1}{2}}MA^{-\frac{1}{2}}.$$  \hspace{1cm} (13)

Here $W_{att}$ is the weight matrix for the attention mechanism. It projects input features into a new space. Then the attention weights are decided by inner products between features in this new space. We normalize the attention matrix so that the diagonal elements of $U$ are always one.

In each layer $ℓ$, we get an attention matrix $U_ℓ$ as above. Then we use $A^{att}_ℓ = A \odot U_ℓ$ as the new adjacency matrix used in layer $ℓ$. The actual computation is

$$H^{ℓ} = \sigma (A^{att}_ℓH^{ℓ−1}W^ℓ), \quad ℓ = 1, \ldots, L \hspace{1cm} (14)$$

We call this new model the KCN-att. When the matrix $W_{att}$ has small weights, then $U$ approaches a matrix with all entries being one. In this case, the KCN-att becomes similar to the KCN. When the matrix $W_{att}$ has large weights, then $U$ tends to approach the identity matrix, and then the KCN-att tends to reduce neighbors’ influence.

**KCN based GraphSAGE**

We also use GraphSAGE (Hamilton, Ying, and Leskovec 2017) as the predictive model of the KCN given that GraphSAGE performs well on several node classification tasks. GraphSAGE cannot use a weighted graph, so we treat the graph over the neighborhood of $i$ as a complete graph. Let $H^{ℓ−1}_k = \{h^{ℓ−1}_k \mid k \in \beta_i \}$ be the input to the GraphSAGE layer $ℓ$, then the layer computes its output $H^ℓ$ as follows.

$$g^ℓ_j = \text{AGG} (\{h^{ℓ−1}_k \mid k \in \beta_i, k \neq j \}), \quad \forall j \in \beta_i \hspace{1cm} (15)$$

$$h^ℓ_j = \sigma (W^ℓ_jh^{ℓ−1}_j + W^ℓ_jg^ℓ_j), \quad \forall j \in \beta_i \hspace{1cm} (16)$$

$$H^ℓ = \{h^ℓ_j \mid \|h^ℓ_j\|_2 : \forall j \in \beta_i \} \hspace{1cm} (17)$$

The function $\text{AGG}()$ aggregates a list of vectors into one. We use the max-pooling aggregator, one the three aggregators proposed in the original work (Hamilton, Ying, and Leskovec 2017).

$$\text{AGG}(H^{ℓ−1}_{β_i \setminus j}) = \max(\sigma(W_{pool}h^{ℓ−1}_k + b), k \in β_i, k \neq j)$$

Here $\max$ takes the element-wise max values over a list of vectors. We refer to this model as the KCN-sage.

**Analysis**

**Computation Complexity**

The time complexity of KCN and the two variants includes nearest-neighbor search and network training. In order to find the $K$ nearest neighbors we utilize a KD tree, which takes $O(N \log(N))$ time to build. Here we treat the dimensionality of spatial coordinates as a constant because it usually a small number (2 or 3). Querying a single data point in the tree takes time $O(K \log(N))$, and searching neighbors for all data points takes a total of $O(NK \log(N))$ time.

When we train the model on a single instance, the computation of the adjacency matrix takes time $O(K^2)$. The computation within each layer takes time $O(K^2d_{max})$, with $d_{max}$ being the largest dimensionality of hidden layers. The forward computation and backpropagation for one instance takes time $O(K^2Ld_{max})$, and one training epoch takes time $O(NK^2Ld_{max})$.

**Relation to Kriging**

KCN is a flexible model and approximately includes local kriging as a special case. This fact is shown by the following theorem.

**Theorem 1**: Assume the variogram of a kriging model satisfies $2γ(0) > 0$. Also assume $X = [x_*, X^\top_{α*}]^\top$ has full column rank. Then there exists a set of special parameters and activations with which a KCN makes the same prediction as the kriging prediction, i.e. $y^*_α = \hat{y}^*_α^{\text{invg}}$.

**Proof sketch**: Let $\hat{\Gamma}$ be the covariance matrix corresponding to the new data point and training data point.

$$\hat{\Gamma} = \begin{bmatrix} 0 & \gamma^\top & \gamma \\ \gamma & \Gamma & \Gamma \end{bmatrix}. \hspace{1cm} (18)$$

Here $\gamma$ and $\Gamma$ are semivariograms defined in the same way as kriging. To approximate kriging, we set the KCN to have one convolutional layer and a dense layer. We set

$$\hat{\Lambda} = \hat{\Gamma}^{-1} + \hat{\Gamma}^{-1}X(X^\top \hat{\Gamma}^{-1}X)^{-1}X^\top \hat{\Gamma}^{-1}$$

as the “normalized adjacency matrix” and directly use it to multiply the hidden input. We consider a 1-layer GCN with a special activation function $σ_{\text{div}}()$. The first row of the GCN output is $e^\top \hat{H}^0 = σ_{\text{div}}(eA\hat{H}^0W^1)$. In the Appendix we show $e\hat{A} = \begin{bmatrix} z^\top, -z^\top \lambda^\top \end{bmatrix}$, then

$$e\hat{A}h^0 = \begin{bmatrix} -z^\top \lambda^\top y_{α*}, z^\top, -z^\top (x_∗ - \lambda^\top X_{α*}) \end{bmatrix}.$$\footnote{The value $2γ(0)$ is called the nugget of the variogram, which is usually greater than zero.}

Here $z$ is a scalar, and $\lambda$ is the kriging coefficient defined in (2). Let $W^1$ be the matrix taking the first two elements
of the vector, then $e^\mathbf{AH}^0\mathbf{W}^1 = [-z^{-1}\lambda^\top y_{\alpha,}, z^{-1}]$. Denote it as $u$. Define the activation function to be $\sigma_{\text{elu}}(u) = [-u_1/u_2, 0]$, set $w_{\text{den}} = [1, 0]$, and set the activation of the fully connected layer to be identity, then the KCN predicts $\hat{y}_s^{\text{KCN}} = \lambda^\top y_{\alpha,}$, which is exactly the same as kriging prediction $\hat{y}_s^{\text{kriging}}$.

In the real implementation, we use normal activation functions such as ReLU. The combination of the first two rows of $\mathbf{W}^1$, the GCN activation, and the dense layer can be viewed as two-layer feedforward network applied to $u$. If the two-layer neural network can emulate the function $-u_1/u_2$, then a normal setting of the network can also approximate kriging well.

This theorem and its proof have strong implications for our model development. First, if the KCN uses $\mathbf{A}$ defined above as the normalized Laplacian, then the KCN has a straightforward way to discover kriging solutions. Since $\mathbf{A}$ has a small size, $(K + 1) \times (K + 1)$, the computation of $\mathbf{A}$ is affordable. Second, the matrix $\mathbf{A}$ indicates that we should introduce the feature matrix into the computation of the “normalized Laplacian”. Otherwise, the KCN may need complicated computations to recover kriging results. This is one main motivation behind our usage of graph attention in KCN-att.

Experiment
We evaluate our methods on three tasks: bird count modeling, restaurant rating regression, and precipitation regression. We use Kriging, Random Forest, Graph Convolution Network, and Graph SAmple and aggreGatE as baselines.

Experiment setup
Kriging: we use the implementation of Kriging within Automap (Hiemstra et al. 2008). Automap essentially automates the process of Kriging, by automatically fitting variograms, and testing several different models. In all of our experiments Automap tests spherical, exponential, gaussian, matern, and stein variograms and picks the best one based on the smallest residual sum of squares. Since all of the datasets have a large number of data points, we use local kriging and only consider the closest 100 points.

Random Forest: Hengl et al. (2018) use Random Forest to make predictions for spatial data. For each data point, the algorithm calculates the distances between that point and all training points. These distances are then used as the feature vector of that data point. This algorithm does not scale to very large datasets, so we downsample the training set to a size of 1000. We use the implementation of Random Forest (Wright and Ziegler 2017), and method of tuning (Probst, Wright, and Boulesteix 2018) used by the authors of Hengl et al. (2018). The implementation tunes four hyperparameters of Random Forest: the number of trees to use, the number of variables to consider at a node split, the minimal node size, and the sample fraction when training each tree.

GCN: we modify Kipf’s implementation of (Kipf and Welling 2016) for regression problems. Before we run the GCN on spatial data, we first build a undirected graph over data points: we connect two data points if one is among the other’s $K$ nearest neighbors. We only consider a GCN with two hidden layers. We tune the hyper-parameters of the GCN in the same way as we tune the KCN and the KCN-att below.

GraphSAGE: we implement GraphSAGE with the Spektral graph deep learning library. For each experiment, we build an undirected graph in the same way as the GCN. Then we train a two hidden layer GraphSAGE, with hyperparameters are tuned as below.

KCN & KCN-att & KCN-sage: the three models use two hidden layers respectively. We tune the following hyperparameters: hidden sizes $\epsilon \in (20, 10), (10, 5), (5, 3)$), dropout rate $\epsilon \in (0, 0.25, 0.5)$, and kernel length $\epsilon \in (1, .5, .1, .05)$. Note that GraphSAGE and KCN-sage do not consider weighted adjacency matrix, so there is no need to tune kernel length for them. We also employed early stopping to decide the number epochs.

Bird count modeling
One application of our KCN models is modeling bird count data from the eBird project (Fink et al. 2010), which contains over one billion of records of bird observation events. Modeling bird data from the eBird project provides an opportunity to deepen our understanding of birds as part of the ecosystem. In this experiment, we model the distribution of wood thrush in June, which is of great interest to ornithologists (Johnston et al. 2019). Figure 1 shows a picture of a wood thrush and the distribution of observed counts over the eastern US.

We restrict our data to a subset of records of wood thrushes observed in June 2014. Each record has a GPS location, a count of wood thrushes observed, and a list of features such as observation time, count type (stationary count, traveling count, etc.), effort hours, and effort area. After removing 583 records with uncertain counts or counts over 10, we get 107,246 records to form our dataset. Bird counts in this dataset are highly sparse: only 11,468 records (fraction of 0.11) have positive counts. We split the dataset into a training set and a test set by 1:1.

When we test our models and baselines, we consider two evaluation metrics. The first one is mean squared error (MSE), so we have a fair comparison with Kriging, the minimization objective of which is the mean squared error. The second one is negative log-likelihood. We use a zero-inflated Poisson distribution (Lambert 1992) as the predictive distri-
In the KCN models, a data point has \( K \) nearest neighbors. The message propagation between two test points is not defined, since the number of neighbors is zero. A test point might only connect to another test data point, which means that the neighbors are small in the construction of the graph. In this case, the performance of the GCN is poor, since it is only able to use a small number of neighbors. The KCN models achieve similar performances. The KCN and the KCN-att achieve similar performances, while the KCN-sage performs slightly better than the KCN because the KCN-att is able to use observational features to decide whether a neighboring count is from the same situation or not.

**Restaurant rating regression**

Yelp is a popular rating website, which allows users to rate and provide information about businesses. They have hosted a large collection of these business ratings and attributes for download. In this experiment, we only consider the restaurants within that dataset. Each restaurant has a GPS location and an average rating rounded to the nearest .5, from 0 to 5. Additionally, we choose 13 related attributes from the dataset, all but one of which is categorical. We turn these categorical covariates into 30 indicator variables. These indicators give information about restaurant attributes such as whether it serves alcohol, and whether or not it takes credit card. After we drop any rows where the ratings, coordinates, or number of reviews is NA, we obtain 188,586 restaurants. We then split the data 1:1 to form a training and test set.

Table 2 shows the experiment results on this dataset. The KCN, the KCN-att, and the KCN-sage improve the performance of their corresponding baseline models. The KCN, the KCN-att, the KCN-sage, and the GraphSAGE outperform baseline models by a large margin. The regression task on this dataset is a hard one. The features seem to not be very useful. It is actually hard to overfit the labels with a normal feedforward neural network. However, there are some weak spatial effect. The average rating over the entire dataset achieves a mean squared error of 1.01 while the average of the nearest 35 neighbors results in a mean squared error of 0.93. This is understandable, since it is normal that good restaurants and bad restaurants mix in the area. In this experiment, we find that Kriging is very stable when features are discrete and sparse. We add a small amount of noise to the feature matrix to avoid numerical issues.

**Precipitation regression**

The National Oceanic and Atmospheric Administration keeps detailed records of precipitation levels across the United States. One such dataset provides monthly average precipitation in inches from 1981 to 2010 across the US. We average the precipitation level in May for 8,832 stations. We then take the log of these average precipitation values as target values for the regression task. Essentially, we assume a log-normal distribution of precipitation levels. Finally we have a target value, coordinates of each station, and one feature (the elevation) of each station. Data are split with portion 1:1 as a training and testing. Figure 3 shows the data
distribution over the US.

Table 3 summarizes the experimental results using the mean squared error. The target values in the log-scale are more likely to be from a Gaussian distribution than the previous two datasets, so Kriging performs relatively well compared to others. The Random Forest method only outperforms generative models in supervised learning tasks.

### Appendix: Detailed Proof of Theorem 1

We need to derive \( \mathbf{u} = \mathbf{e}^\top \mathbf{A} \mathbf{X} \), where \( \mathbf{e} = [1, 0] \). \( \mathbf{A} \) is “normalized adjacency matrix” defined in [19], and \( \mathbf{X} = [\mathbf{x}_s, \mathbf{x}_t] \) are feature vectors. We create the following shorthands notations to facilitate our derivation.

\[
t = -\gamma^\top \Gamma^{-1} \gamma, \quad \mathbf{a} = -\Gamma^{-1} \gamma, \quad \mathbf{c} = \mathbf{x}_s + \mathbf{X}^\top \mathbf{a},
\]

\[
\mathbf{T} = \mathbf{X}^\top \Gamma^{-1} \mathbf{X}, \quad \mathbf{B} = \mathbf{X} \mathbf{T}^{-1}, \quad r = \mathbf{c}^\top \mathbf{T}^{-1} \mathbf{c}
\]

We will show that the first row of \( \bar{\mathbf{A}} \) is

\[
\mathbf{e}^\top \bar{\mathbf{A}} = \begin{bmatrix} z^{-1}, -z^{-1} \lambda \end{bmatrix},
\]

\[
z = -\gamma^\top \Gamma^{-1} \gamma + \gamma^\top \Gamma^{-1} \mathbf{X} \mathbf{T}^{-1} \mathbf{X}^\top \Gamma^{-1} \gamma.
\]

By checking [19], we first compute theinverse \( \bar{\Gamma}^{-1} \) is

\[
\bar{\Gamma}^{-1} = \begin{bmatrix} t^{-1} & t^{-2} \mathbf{a}^\top \\ t^{-2} \mathbf{a} & \Gamma^{-1} + t^{-1} \mathbf{a} \mathbf{a}^\top \end{bmatrix}.
\]

Denote \( \mathbf{v}_1 = \mathbf{e} \bar{\mathbf{A}}^{-1} = t^{-1}[1, \mathbf{a}^\top] \).

We then consider the second term in (19). We have

\[
\mathbf{X}^\top \bar{\Gamma}^{-1} = t^{-1} \mathbf{c}[1, \mathbf{a}^\top] + [0, \mathbf{X} \Gamma^{-1}]
\]

\[
= [t^{-1} \mathbf{c}, t^{-1} \mathbf{c} \mathbf{a}^\top + \mathbf{X} \Gamma^{-1}].
\]

Denote \( \mathbf{S} = (\mathbf{X}^\top \bar{\Gamma}^{-1} \mathbf{X})^{-1} \),

\[
\mathbf{S} = (t^{-1} \mathbf{c} \mathbf{c}^\top + \mathbf{T}^{-1})^{-1}
\]

\[
= \mathbf{T}^{-1} - \mathbf{T}^{-1} \mathbf{c}(t + \mathbf{c} \mathbf{c}^\top \mathbf{T}^{-1} \mathbf{c})^{-1} \mathbf{c}^\top \mathbf{T}^{-1}.
\]

The first line is from the equation \( [1, \mathbf{a}^\top] \mathbf{X} = \mathbf{c}^\top \).

Denote \( \mathbf{v}_2 = \mathbf{e} \bar{\Gamma} \mathbf{X} \mathbf{S} \mathbf{X}^\top \bar{\Gamma}^{-1} \). Insert the expansion of \( \mathbf{X}^\top \bar{\Gamma}^{-1} \), we have

\[
\mathbf{v}_2 = t^{-1} \mathbf{c}^\top \mathbf{S} [t^{-1} \mathbf{c}, t^{-1} \mathbf{c} \mathbf{a}^\top + \mathbf{X} \Gamma^{-1}].
\]

By \( \mathbf{c}^\top \mathbf{S} = t(t+r)^{-1} \mathbf{c} \mathbf{T}^{-1} \) and \( w = \mathbf{c}^\top \mathbf{S} \mathbf{c} = rt(t+r)^{-1} \), we have

\[
\mathbf{v}_2 = (t+r)^{-1} t \mathbf{c} \mathbf{T}^{-1} - t \mathbf{r} - t \mathbf{r} \mathbf{a}^\top + \mathbf{c} \mathbf{c}^\top \mathbf{T}^{-1} \mathbf{X} \Gamma^{-1}.
\]

Since \( t^{-1} - (t+r)^{-1} = (t+r)^{-1} \), we have

\[
\mathbf{e}^\top \bar{\mathbf{A}} = \mathbf{v}_1 - \mathbf{v}_2
\]

\[
= (t+r)^{-1} [1, \mathbf{a}^\top - \mathbf{c} \mathbf{c}^\top \mathbf{T}^{-1} \mathbf{X} \Gamma^{-1}].
\]
Then we expand $a$ and $c$ to get

$$ e^T \mathbf{A} = (t + r)^{-1} [1, -((\gamma + \mathbf{Bx}) - \mathbf{Bx}\Gamma^{-1}\gamma)\Gamma^{-1}] $$

$$ = z^{-1} [1, -\lambda^T] $$

Here $z = t + r$.

Since $\mathbf{A}$ are computed from normal matrix operations, its entries are bounded. Therefore, $z \neq 0$.

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