Refining Coarse-Grained Spatial Data Using Auxiliary Spatial Data Sets with Various Granularities

Yusuke Tanaka,1,3 Tomoharu Iwata,2 Toshiyuki Tanaka,3 Takeshi Kurashima,1 Maya Okawa,1 Hiroyuki Toda1
1NTT Service Evolution Laboratories, NTT Corporation
2NTT Communication Science Laboratories, NTT Corporation
3Graduate School of Informatics, Kyoto University
{tanaka.y, iwata.tomoharu, kurashima.takeshi, okawa.maya, toda.hiroyuki}@lab.ntt.co.jp, tt@i.kyoto-u.ac.jp

Abstract

We propose a probabilistic model for refining coarse-grained spatial data by utilizing auxiliary spatial data sets. Existing methods require that the spatial granularities of the auxiliary data sets are the same as the desired granularity of target data. The proposed model can effectively make use of auxiliary data sets with various granularities by hierarchically incorporating Gaussian processes. With the proposed model, a distribution for each auxiliary data set on the continuous space is modeled using a Gaussian process, where the representation of uncertainty considers the levels of granularity. The fine-grained target data are modeled by another Gaussian process that considers both the spatial correlation and the auxiliary data sets with their uncertainty. We integrate the Gaussian process with a spatial aggregation process that transforms the fine-grained target data into the coarse-grained target data, by which we can infer the fine-grained target Gaussian process from the coarse-grained data. Our model is designed such that the inference of model parameters based on the exact marginal likelihood is possible, in which the variables of fine-grained target and auxiliary data are analytically integrated out. Our experiments on real-world spatial data sets demonstrate the effectiveness of the proposed model.

1 Introduction

Many cities around the world are now collecting large amounts of spatial data from a wide range of sources. Governments and other organizations are releasing data on items such as poverty rate, air pollution, traffic flow, energy consumption and crime (?, ?, ?). Analyzing such spatial data is of critical importance in improving the life quality of citizens in many fields such as socio-economics (?, ?, ?), public health (?), public security (?, ?) and urban planning (?). For example, knowing the spatial distribution of poverty enables us to optimize allocation of resources for remedial action. Likewise, the spatial distribution of air pollution is useful in creating policies that can control air quality and thus protect human health.

Naturally, information at fine spatial granularity is preferred because it allows us to identify key regions that require intervention to improve city environments efficiently.

Copyright © 2019, Association for the Advancement of Artificial Intelligence (www.aaai.org). All rights reserved.
grained target data via the effective use of auxiliary data sets with various granularities. An important characteristic is discerning the usefulness of each auxiliary data set which depends on not only the strength of relationship with the target data but also the level of spatial granularity. For example, consider the case of two auxiliary data sets that have the same strength of relationship with the target data, but different granularities. In that case, the finer-grained one is seen as more helpful for refining the coarse-grained target data.

With the proposed model, the fine-grained target data are assumed to follow a Gaussian process (GP) \( \mathcal{GP} \) whose mean function is modeled by a linear regression of the auxiliary data sets. This GP-based modeling allows us to consider the spatial correlation in the target data and the auxiliary data sets simultaneously. Since the target data are observed not at fine granularity but at coarse granularity, we model a spatial aggregation process to transform the fine-grained target data into the coarse-grained target data. Furthermore, to handle auxiliary data sets with various granularities, we apply GP regression to each auxiliary data set to derive a predictive distribution defined on the continuous space; this conceptually corresponds to spatial interpolation. A key idea is that it hierarchically incorporates the predictive distributions into the model; that is, it does not use point estimates. This enables us to consider uncertainty in the prediction of auxiliary data sets. The uncertainty is governed by several factors, one of which is sample density, i.e., spatial granularity of the auxiliary data; the finer the granularity is, the lower the uncertainty is. Incorporating the uncertainty leads to effectively learning the usefulness of the auxiliary data with consideration of the levels of spatial granularity; this allows our model to accurately refine the coarse-grained target data. We predict the fine-grained target data via a Bayesian inference procedure. The proposed model is designed such that the estimation of model parameters based on the exact marginal likelihood is possible: By analytically integrating out the variables of fine-grained target and auxiliary data, we can estimate the parameters without explicitly obtaining these variables. We construct the predictive distribution of the fine-grained target data by using the estimated parameters.

2 Related Work

The problem of refining coarse-grained spatial data has been studied in various fields such as socio-economics \( (?; ?) \), agricultural economics \( (?; ?) \), epidemiology \( (?; ?) \), meteorology \( (?; ?) \) and geographical information system (GIS) \( (?; ?) \). This problem is also called statistical downscaling, spatial disaggregation, and areal interpolation. The previous works can be categorized into two cases in terms of target data availability.

In the first case, in which a large amount of coarse- and fine-grained target data are available, we can predict the fine-grained target data by using a mapping function from coarse-to fine-grained data. The mapping function can be learnt by using various machine learning methods including linear regression models \( (?; ?) \), neural networks \( (?; ?) \) and support vector machines \( (?; ?) \). Recently, super-resolution techniques based on deep neural networks have been applied for refining coarse-grained spatial data \( (?; ?) \). The super-resolution techniques aim to learn a mapping function from low- to high-resolution images \( (?; ?) \). The method by \( (?; ?) \) is based on the analogy between gridded spatial data and images; values at grid cells are regarded as values at pixels. The large amount of fine-grained data needed for training are, however, not available in many cases (e.g., poverty survey), and often only coarse-grained data are available. These methods are not applicable in such situations.

In the second case, in which only coarse-grained target data are available, many regression-based methods have been proposed that use auxiliary spatial data sets to refine coarse-grained target data \( (?; ?; ?; ?; ?) \). Regression models (linear and non-linear) are used for estimating the relationships between target data and auxiliary data sets. A few methods can construct the regression models under the spatial aggregation constraints \( (?; ?) \). The constraints state that a value associated with a coarse-grained region is a linear average of their constituent values in a fine-grained partition. In order to satisfy the spatial aggregation constraints, the regression residuals at the coarse-grained regions are allocated to the fine-grained regions by using the spatial interpolation method, i.e., kriging \( (?; ?) \). These methods, however, assume that the auxiliary data sets have spatial granularities equivalent to that of fine-grained target data to be estimated. This assumption makes it difficult to utilize multiple auxiliary data sets with various granularities.

Several regression methods have been developed for estimating relationships between multi-scale spatial data sets \( (?; ?; ?; ?; ?) \). These methods predict the target data with the same granularity as that of the training data by utilizing multi-scale auxiliary data sets. They do not, however, consider the spatial aggregation constraint, which is a critical factor in refining the coarse-scale target data.

There have been several hierarchical Bayesian models to predict fine-grained target data using fine-grained auxiliary data sets. Although they introduce a fully Bayesian inference \( (?; ?; ?) \) or a variational inference \( (?; ?) \) for model parameters, the uncertainty in the prediction of auxiliary data sets is ignored: They cannot discern the usefulness of each auxiliary data set considering their levels of spatial granularity.

Different from prior works, the proposed model can effectively make use of auxiliary data sets with various granularities by hierarchically incorporating Gaussian processes. This hierarchical modeling allows us to effectively learn the usefulness of each auxiliary data set considering the levels of spatial granularity. Our model also considers the spatial aggregation constraints by integrating the Gaussian processes with a spatial aggregation process to transform the fine-grained target data into the coarse-grained target data.

3 Problem Formulation

In this section, we describe the spatial data this study focuses on, and define our problem of refining coarse-grained spatial data by using, for the same region, auxiliary spatial data sets with various granularities. Assume that we have a target spatial data set with coarse granularity, and we would like to obtain a fine-grained version. Let \( S \) be the collection
of indices of auxiliary data sets. The notations used in this paper are listed in Table 1.

**Partition:** Let $X$ be a total region of a city, and $x \in X$ be a location point represented by its coordinates (e.g., latitude and longitude). Partition $P$ of $X$ is a collection of disjoint subsets, called regions, of $X$, whose union is equal to $X$. Let $|P|$ denote the number of regions in $P$. We can consider several partitions of $X$ as follows. Let $P_{\text{coar}}$ be the coarse-grained partition, i.e., that of the coarse-grained target data. Let $P_{\text{fine}}$ be the fine-grained partition, of the desired fine-grained target data. For $s \in S$, let $P_s$ be the partition of the $s$th auxiliary data set.

**Spatial data:** Let $\mathbf{x} = (a_1, \ldots, a_{|P_{\text{coar}}|})^T$ be a $|P_{\text{coar}}|$-dimensional vector consisting of the coarse-grained target values, where $a_i \in \mathbb{R}$ is the value associated with region $i \in P_{\text{coar}}$. For $s \in S$, let $y_s = (y_{s,1}, \ldots, y_{s,|P_s|})^T$ be a $|P_s|$-dimensional vector consisting of the $s$th auxiliary data values, where $y_{s,p} \in \mathbb{R}$ is the value associated with region $p \in P_s$ of the $s$th auxiliary data set.

**Problem:** Suppose that we have coarse-grained target data $\mathbf{a}$ whose partition is $P_{\text{coar}}$, auxiliary data sets with the respective partitions $\{(P_s, y_s) \mid s \in S\}$, and the desired fine-grained partition $P_{\text{fine}}$, we wish to estimate a $|P_{\text{fine}}|$-dimensional vector $\mathbf{z} = (z_1, \ldots, z_{|P_{\text{fine}}|})^T$ consisting of the fine-grained target values, where $z_j \in \mathbb{R}$ is the value associated with region $j \in P_{\text{fine}}$. Here, the values $a_i$, $y_{s,p}$, and $z_j$ are assumed to be intensive quantities such as ratios; that is, they are independent of the area scale of the respective regions. When the values are extensive quantities such as population, they can be transformed into intensive quantities by dividing them with the areas of regions.

### 4 Proposed Model

We propose a probabilistic model that allows auxiliary spatial data sets with various granularities to be used in refining coarse-grained spatial data. Our model is based on Gaussian process (GP) (9), which is a flexible non-parametric model for non-linear functions in a continuous domain. We model the generative process for coarse-grained target data $\mathbf{a}$, given the auxiliary data sets with known partitions $\{(P_s, y_s) \mid s \in S\}$, coarse-grained partition $P_{\text{coar}}$, and fine-grained partition $P_{\text{fine}}$. In other words, we model the conditional probability $p(\mathbf{a} \mid \{y_s\}_{s \in S})$ instead of the joint probability of $\mathbf{a}$ and $\{y_s\}_{s \in S}$. It enables us to adopt two-step inference approach described in Section 5, which is advantageous in the computational cost for learning model parameters.

The generative process (given three auxiliary data sets) is illustrated schematically in Figure 2, where darker hues represent regions with higher values. This process contains the following three steps: (a) Deriving the predictive distribution over continuous space for each auxiliary data set $\mathbf{y}_s$ via GP regression, which corresponds to spatial interpolation; (b) generating the fine-grained target data $\mathbf{z}$ via a GP whose mean function is modeled as the linear regression of the continuous predictive distributions of the auxiliary data sets; (c) generating the coarse-grained target data $\mathbf{a}$ by spatially aggregating the constituent values in a fine-grained partition.

In our problem, each value is associated with a region in a partition rather than a single location point in $X$; this prevents us from directly applying GP. We thus associate each region in a partition with its centroid, and regard each value as being associated with the centroid of that region. This assumption, while significantly simplifying computations involved, might worsen the fit of the GP to the data set, which however is appropriately taken into account in the following steps as increased uncertainty of the GPs for both the respective auxiliary data sets (described in (5)) and the target data (described in (6)). For $s \in S$, let $X_s = (x_{s,1}, \ldots, x_{s,|P_s|})$ be the set of the centroids in partition $P_s$, where $x_{s,p}$ is the centroid of region $p \in P_s$. Similarly, for fine-grained parti-
tion $P^\text{fine}$, let $X^\text{fine} = (x_1, \ldots, x_{|P^\text{fine}|})$ be the set of centroids in $P^\text{fine}$. Thus, our problem is now reformulated as estimating $z = (z_1, \ldots, z_{|P^\text{fine}|})^\top$, where $z_j \in \mathbb{R}$ is a target value at the centroid of region $j \in P^\text{fine}$, as indicated by the auxiliary spatial data sets $\{(X_s, y_s) \mid s \in S\}$.

(a) Deriving predictive distributions of auxiliary spatial data sets: In order to handle auxiliary spatial data sets with various granularities, we use GP regression to derive a posterior Gaussian process for a latent continuous random function on $X$; this conceptually corresponds to spatial interpolation of each auxiliary spatial data set. We then evaluate the predictive distribution on the basis of the posterior Gaussian process. Let $f_s(x)$ be a noise-free latent function for the $s$th auxiliary data set at location $x$. We assume that $f_s(x)$ follows a Gaussian process, $f_s(x) \sim GP(0, k_s(x, x'))$, with mean zero and a covariance function $k_s(x, x')$. Though our model does not depend on any particular choice of the covariance function, for simplicity we consider the well-known covariance function, i.e., squared-exponential kernel, which is widely used for measuring the similarity between function values in spatial coordinates (7). The squared-exponential kernel is defined as

$$k_s(x, x') = \alpha_s^2 \exp\left(-\frac{1}{2\gamma_s^2}\|x - x'\|^2\right),$$

where $\gamma_s$ is the scale parameter, $\alpha_s^2$ is a signal variance that controls the magnitude of the covariance, and $\| \cdot \|$ is the Euclidean norm. We assume that the $s$th auxiliary data set $y_s$ is generated with an additive Gaussian noise with noise variance $\sigma_s^2$. Defining $f^*_s(x_p)$ as the prediction of the $s$th auxiliary data set for the centroid $x_p$ of the fine-grained partition, the predictive distribution of $f^*_s = (f^*_s(x_1), \ldots, f^*_s(x_{|P^\text{fine}|}))^\top$ is as follows:

$$p(f^*_s) = \mathcal{N}(f^*_s \mid \bar{f}^*_s, \Sigma^*_s),$$

where $\bar{f}^*_s = K^*_s(x_{\text{centroids}} + \Sigma^*_s I)^{-1}y_s$, is the predictive means, and $\Sigma^*_s = K^*_s - K^*_s(x_{\text{centroids}} + \Sigma^*_s I)^{-1}K^*_s$ is the covariance matrix, whose diagonal elements represent the uncertainties in the prediction at the test points $X^\text{fine}$. Incorporation of the predictive distributions (2) is expected to allow the usefulness of auxiliary data to be effectively learnt as it allows consideration of the uncertainty in the prediction. Details are given in (7) in Section 5. Here, $K^*_s$ is a $|P^s| \times |P^s|$ covariance matrix whose entries are covariances between training points $X_s$. $K_{ss}$ is a $|P^s| \times |P^\text{fine}|$ covariance matrix whose entries are covariances between training points $X_s$ and test points $X^\text{fine}$. $K_{ss}$ is a $|P^\text{fine}| \times |P^\text{fine}|$ covariance matrix whose entries are covariances between test points $X^\text{fine}$.

(b) Generative process of fine-grained target data: We model a generative process for the fine-grained target data $z$. Let $z(x)$ be a noise-free latent function for the fine-grained target data at location $x$. We assume that $z(x)$ follows a Gaussian process, $z(x) \sim GP(m(x), k(x, x'))$, with mean function $m(x) = \sum_{s \in S} w_s f_s(x) + w_0$, where $w_s \in \mathbb{R}$ and $w_0 \in \mathbb{R}$ are the regression coefficient of the $s$th auxiliary data set and the bias parameter, respectively. The covariance function $k(x, x')$ is a squared-exponential kernel with the scale parameter $\gamma$ and signal variance $\alpha^2$. Given the predictive distributions for the auxiliary data sets from (2), the conditional distribution of $z$ at the centroids $X^\text{fine}$ is given by

$$p(z \mid F^* ) = \mathcal{N}(z \mid F^* w, K),$$

where $w = (w_0, \ldots, w_{|S|})^\top$ and $K$ is a $|P^\text{fine}| \times |P^\text{fine}|$ covariance matrix defined by $k(x, x')$. Here, we let $|S|$ be the number of auxiliary data sets. We define the augmented matrix as the $|P^\text{fine}| \times (|S| + 1)$ matrix $F^* = (f^*_1, \ldots, f^*_{|S|}, 1)$, in which 1 is a column vector of 1’s. This GP-based modeling enables us to consider the spatial correlation in the target data and the auxiliary data sets simultaneously.

(c) Generative process of coarse-grained target data: We design a spatial aggregation process to transform the fine-grained target data $z$ into the coarse-grained target data $a$, in order to encourage consistency between $z$, which is to be estimated, and the available coarse-grained target data $a$. In the spatial aggregation process, a value associated with one region in the coarse-grained partition is obtained by aggregating the values in the fine-grained regions contained in the coarse-grained region (see the upper part of Figure 2). Then, $a$ is generated from the following conditional distribution given $z$,

$$p(a \mid z) = \mathcal{N}(a \mid H z, \sigma^2 I),$$

where $\sigma^2$ is the noise variance for the coarse-grained target data, and $H$ is a $|P^\text{coar}| \times |P^\text{fine}|$ aggregation matrix, whose entries are nonnegative weighting coefficients; the row sum of $H$ should equal 1. We set the coefficients in accordance with the property of the target data. For example, in cases where target data are incidences of disease, then the $(i, j)$-entry $H(i, j)$ of $H$ would be proportional to the population in the intersection of the coarse-grained region $i$ and the fine-grained region $j$. In the following, for simplicity, we consider a simple aggregation matrix, in which entry $H(i,j)$ is 1/|$P^\text{fine}$| if the fine-grained region $j$ is contained in the coarse-grained region $i$, and zero otherwise. Here, $P^\text{fine}$ is a subset of $P^\text{coar}$, all the elements of which are contained in the coarse-grained region $i \in P^\text{coar}$.

5 Inference

Given the coarse-grained target data $a$, the auxiliary spatial data sets with centroids $\{(X_s, y_s) \mid s \in S\}$, the centroids of fine-grained partition $X^\text{fine}$ and the aggregation matrix $H$, we aim to predict the fine-grained target data $z$ via a Bayesian inference procedure. In order to calculate the predictive distribution of $z$, we need to estimate the model parameters. The problem of estimating the model parameters can be divided into two steps: 1) Estimate hyperparameters $\alpha_s, \gamma_s, \sigma_s$ for each auxiliary data set and 2) estimate regression coefficient $w$ and hyperparameters $\alpha, \gamma, \sigma$ for the target data. Although one could also opt for estimating all the model parameters simultaneously (i.e., one-step inference), it will increase the computational cost of inference drastically; we adopt the efficient two-step inference as described in the following paragraphs. We finally construct the predictive distribution of $z$ by using the estimated parameters. Details of the inference procedure are shown in Algorithm 1.
Algorithm 1: Bayesian inference procedure of the fine-grained target data $z$

**Input:** $a, \{X_s, y_s\} \mid s \in S$, $X_{\text{fine}}$, $H$

**Output:** Predictive distribution of $z$

1. Initialize model parameters, $\{\alpha_s \mid s \in S\}, \{\gamma_s \mid s \in S\}$, $\{\sigma_s \mid s \in S\}$, $w, \alpha, \gamma, \sigma$
2. /* first inference step */
3. for $s \in S$
4. Estimate $\alpha_s, \gamma_s, \sigma_s$ by maximizing the logarithm of (5)
5. end for
6. /* second inference step */
7. Estimate $w, \alpha, \gamma, \sigma$ by maximizing the logarithm of (6)
8. Construct predictive distribution of $z$ by (8) using the estimated model parameters

The first inference step: Given the $s$th auxiliary spatial data set with centroids $(X_s, y_s)$, the marginal likelihood of $y_s$ is given by

$$p(y_s | \alpha_s, \gamma_s, \sigma_s) = N(y_s | 0, K_s + \sigma_s^2 I).$$

(5)

The hyperparameters $\alpha_s, \gamma_s, \sigma_s$ are estimated by maximizing the logarithm of (5). We solve the optimization problem through the use of the BFGS method (7). By solving the optimization problem for each auxiliary data set independently, we obtain the set of the estimated hyperparameters for all auxiliary data sets. The predictive distribution of $f^*_s$ corresponding to (2) is obtained using the estimated hyperparameters.

The second inference step: Given the coarse-grained target data $a$ and the centroids of fine-grained partition $X_{\text{fine}}$, the marginal likelihood of $a$ is given by

$$p(a | w, \alpha, \gamma, \sigma) = \int \int p(a | z) p(z | F^*) \prod_{s \in S} p(f^*_s) dF^* dz$$

$= \int \int N(a | Hz, \sigma^2 I) N(z | F^* w, K) \prod_{s \in S} N(f^*_s | f^*_s, \Sigma^*_s) dF^* dz$

$$= N(a | H \tilde{F}^* w, \Lambda),$$

(6)

where $\tilde{F}^* = (f^*_{1}, \ldots, f^*_{|S|})$ is a $|P_{\text{fine}}| \times (|S| + 1)$ matrix, and we analytically integrate out the latent variables $F^*$ and $z$ with the help of the conjugacy of the distributions (2), (3), and (4). $\Lambda$ is a $|P_{\text{coar}}| \times |P_{\text{coar}}|$ covariance matrix represented by $\Lambda = \sigma^2 I + \Omega \Lambda^{-1} \Omega^\top$, where $\Omega = K + \sum_{s \in S} w^2 \Sigma^*_s$. The $(i, i')$-entry $\Lambda(i, i')$ of $\Lambda$ is shown in (7). Here, $\delta_{\bullet, \bullet}$ in (7) represents Kronecker delta; $\delta_{A, B} = 1$ if $A = B$, and $\delta_{A, B} = 0$ otherwise. The residual variance term in (7) represents the residual variance in the regression of $z(x_j)$. This term contains the uncertainty in the prediction of $f_s(x_j)$, i.e., $\Sigma^*_s(j, j')$, which is weighted by $w^2$. The spatial correlation term in (7) represents the strength of spatial correlation between $z(x_j)$ and $z(x_{j'})$. This term contains the covariance between $f_s(x_j)$ and $f_s(x_{j'})$, i.e., $\Sigma^*_s(j, j')$, which is weighted by $w^2$. On the basis of the marginal likelihood (6) with this covariance matrix $\Lambda$, our model can effectively learn the regression coefficient $w$ while taking into consideration the prediction uncertainties and the spatial correlations from the auxiliary data sets with various granularities, simultaneously. The parameter $w$ and the hyperparameters $\alpha, \gamma, \sigma$ are estimated by maximizing the logarithm of (6). We solve the optimization problem by using the BFGS method (7). The derivatives of the logarithm of (6) with respect to $w_s, \alpha, \gamma, \sigma$ are described in Appendix A.

Predictive distribution of fine-grained target data: Using the estimated model parameters, the predictive distribution of the fine-grained target data $z$ is given by

$$p(z^*) = N(z^* | \bar{z}^*, \text{cov}(z^*)),$$

(8)

where $\bar{z}^* = \tilde{F}^* w + \Omega \Lambda^{-1} (\alpha - \tilde{F}^* w)$ is the predictive means, and where $\text{cov}(z^*) = \Omega - \Omega \Lambda^{-1} \Omega^\top$ is the covariance matrix. We can obtain the refinement results, i.e., the estimated fine-grained target data, by using the predictive means $\bar{z}^*$. By analyzing the covariance matrix $\text{cov}(z^*)$, we can also evaluate the confidence of the refinement results.
Table 2: MAPE $L$ and standard errors for the predictions of the fine-grained target data.

<table>
<thead>
<tr>
<th></th>
<th>PM2.5</th>
<th>Ozone</th>
<th>Formaldehyde</th>
<th>Benzene</th>
<th>Elemental carbon</th>
<th>Poverty rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proposed model</td>
<td>0.038 ± 0.005*</td>
<td>0.030 ± 0.005*</td>
<td>0.078 ± 0.010**</td>
<td>0.138 ± 0.021</td>
<td>0.100 ± 0.012*</td>
<td>0.202 ± 0.024**</td>
</tr>
<tr>
<td>2-stage SD</td>
<td>0.052 ± 0.007</td>
<td>0.035 ± 0.007</td>
<td>0.101 ± 0.013</td>
<td>0.181 ± 0.032</td>
<td>0.123 ± 0.016</td>
<td>0.228 ± 0.028</td>
</tr>
<tr>
<td>LR-based method</td>
<td>0.056 ± 0.007</td>
<td>0.040 ± 0.007</td>
<td>0.108 ± 0.013</td>
<td>0.185 ± 0.031</td>
<td>0.123 ± 0.016</td>
<td>0.234 ± 0.028</td>
</tr>
<tr>
<td>GPR</td>
<td>0.072 ± 0.010</td>
<td>0.062 ± 0.011</td>
<td>0.191 ± 0.020</td>
<td>0.267 ± 0.029</td>
<td>0.195 ± 0.019</td>
<td>0.344 ± 0.046</td>
</tr>
</tbody>
</table>

Figure 3: Comparison of the predicted fine-grained target data for PM2.5 data set.

<table>
<thead>
<tr>
<th>Proposed model</th>
<th>2-stage SD</th>
</tr>
</thead>
<tbody>
<tr>
<td>w_{a}</td>
<td>w_{j}</td>
</tr>
<tr>
<td>1. Fire incident (Zip code) 0.173</td>
<td>1-2 fam. bldg (Comm.) -0.088</td>
</tr>
<tr>
<td>2. Taxi dropoff (Taxi zone) 0.139</td>
<td>Hospital (Comm.) 0.069</td>
</tr>
<tr>
<td>3. 311 call (Zip code) 0.135</td>
<td>Public school (Comm.) 0.069</td>
</tr>
<tr>
<td>4. Public telephone (Zip code) 0.114</td>
<td>Lots of vacant (Comm.) -0.067</td>
</tr>
<tr>
<td>5. Natural gas (Zip code) 0.109</td>
<td>Crime (Police precinct) 0.064</td>
</tr>
<tr>
<td>6. Mean commute (Comm.) -0.109</td>
<td>Unemployment (Comm.) 0.063</td>
</tr>
<tr>
<td>7. 1-2 fam. bldg (Comm.) -0.089</td>
<td>Pct. served parks (Comm.) 0.062</td>
</tr>
<tr>
<td>8. Pct. served park (Comm.) 0.075</td>
<td>Library (Comm.) ± 0.061</td>
</tr>
<tr>
<td>9. GHG emission (Zip code) 0.068</td>
<td>Fire incident (Zip code) 0.059</td>
</tr>
<tr>
<td>10. Population (Comm.) 0.062</td>
<td>Park (Comm.) 0.058</td>
</tr>
</tbody>
</table>

Figure 4: Comparison of the predicted fine-grained target data for Form 1.

6 Experiments

Data description: We evaluated the proposed model using real-world spatial data sets from NYC Open Data. There are 44 data sets that contain a variety of categories such as social indicators, land use, air quality and taxi traffic. Each data set is associated with one of six geographical partitions, i.e., school district (32), UHF42 (42), community district (59), police precinct (77), zip code (186) and taxi zone (249), where each number in parenthesis denotes the number of regions in the corresponding partition. In our experiments, we try to refine the poverty rate data set and the five air pollution data sets (i.e., PM2.5, ozone, formaldehyde, benzene, elemental carbon). The experimental setting is as follows: 1) Given the poverty rate data set with the borough partition ($|P| = 5$), we would like to refine the data into the community district partition ($|P_{fine}| = 59$), and 2) given each air pollution data set with the borough partition ($|P| = 5$), we aim to refine the data into the UHF42 partition ($|P_{fine}| = 42$). Appendix B details the data sets and the experimental settings.

Baselines: The existing methods can be applied to auxiliary data sets with various granularities if pre-processing is applied, i.e., spatial interpolation, so that the granularities of the auxiliary data sets match with that of the fine-grained target data. Accordingly, we first performed spatial interpolation of each auxiliary data set $y_{a}$ by using GP regression; we then obtained the predictive values $f_{a}^*$ at the centroids $X_{fine}$ of the target fine-grained partition so that the spatial granularities of all auxiliary data sets equaled that of the fine-grained target data. We compared the proposed model with three baselines: GP regression (GPR) (2), Linear regression-based method (LR-based method) (2) and Two-stage statistical downscaling method (2-stage SD) (2). Here, GPR is a simple spatial interpolation, namely, it predicts the fine-grained target data $z$ by using only the coarse-grained target data $a$. Details of these baselines are given in Appendix C.

Fine-grained target data prediction: We evaluated our model in terms of its performance in predicting fine-grained target data $z$. The evaluation metric is the mean absolute percentage error (MAPE) in fine-grained target values: $L = \frac{1}{|P_{fine}|} \sum_{j \in P_{fine}} \left| \frac{z_{j}^{true} - z_{j}^{pred}}{z_{j}^{true}} \right|$, where $z_{j}^{true}$ is the true value associated with region $j$ in the target fine-grained partition; $z_{j}^{pred}$ is its predicted value. Table 2 shows the MAPE and the standard error of absolute percentage error for the proposed model, 2-stage SD, LR-based method and GPR. For all data sets, our model performed better than the baselines, and the differences between our model and the baselines are statistically significant (Student’s t-test). In Table 2, the single star (*) and the double star (**) indicate significant differences at the levels of $P < 0.05$ and $P < 0.01$, respectively. We found similar results using other evaluation metrics (e.g., MAE, RMSE, RMSPE). These results show that our model well utilized the auxiliary data sets with various granularities to accurately predict the fine-grained target data.

Figures 3 and 4 visualize the predicted fine-grained target...
Figure 4: Comparison of the predicted fine-grained target data for poverty rate data set.

Figure 5: Top-2 auxiliary data sets ranked by the proposed model for PM2.5 data set.

Figure 6: Top-2 auxiliary data sets ranked by the 2-stage SD for PM2.5 data set.

data \( z \) for the PM2.5 data set and for the poverty rate data set, respectively. We illustrate the true fine-grained data on the left in Figures 3 and 4, and the predictions made by the proposed model, 2-stage SD and LR-based method on the right. Here, the predictive values of each method were normalized to the range \([0, 1]\), and darker hues represent regions with higher values. As shown in these figures, our model refined the coarse-grained data more precisely than the other methods. In particular, in both data sets, our model achieved significant improvement in the north part of the map (i.e., Manhattan). Such visualization results are useful for finding key regions, e.g., the poorest regions of a city.

Evaluation of auxiliary spatial data sets: Table 3 shows the top ten relevant auxiliary data sets as determined by our model and 2-stage SD for the PM2.5 data set. These auxiliary data sets are arranged in descending order of the absolute values of the estimated regression coefficient \( w \), each of which is listed in the “\( w_s \)” columns of Table 3. By comparing the sorted list of the auxiliary data sets created by the proposed model with that yielded by 2-stage SD, we can confirm that the proposed model assigned relatively large regression coefficients to the auxiliary data sets with finer-grained partitions (i.e., Zip code and Taxi zone).

Figures 5 and 6 visualize the top two relevant auxiliary data sets as estimated by our model and 2-stage SD for the PM2.5 data set, respectively. Comparing these visualizations with that of the true target data in Figure 3(a) shows that our model emphasized the most useful auxiliary data sets, i.e., those that are both strongly related with the target data and have fine granularities; 2-stage SD evaluated the usefulness of auxiliary data sets only in terms of the strength of relationships between the target data and the auxiliary data sets in the coarse-grained partition.

Figure 7 shows the relation between the regression coefficient and the uncertainty in the prediction of auxiliary data sets estimated by the proposed model for the PM2.5 data set. In this figure, each auxiliary data set is depicted by a dot whose color indicates its partition. The horizontal axis shows the averages of the variances in the predicted values of each auxiliary data set; for the \( s \)th auxiliary data set, the average of variances was calculated by 
\[
\frac{1}{|P^{fine}|} \sum_{j \in P^{fine}} \Sigma_s(j, j),
\]
which is the degree of uncertainty in predicting the \( s \)th auxiliary data set; the vertical axis shows the absolute values of the estimated coefficients. As shown, the absolute coefficient values estimated by our model were likely to be higher for the auxiliary data sets that had lower degrees of uncertainty. These results indicate that our model can effectively learn the usefulness of each auxiliary data set by considering the uncertainty in the prediction of auxiliary data sets. Consequently, the proposed model can precisely refine the coarse-grained target data by effectively utilizing auxiliary data sets with various granularities.

7 Conclusion
This paper has proposed a probabilistic model for refining coarse-grained spatial data by utilizing auxiliary spatial data sets with various granularities on the same region. Our model can effectively make use of auxiliary data sets with various granularities by hierarchically incorporating Gaussian processes. Our model also has the advantage of allowing the inference of model parameters based on the exact marginal likelihood, in which the variables of fine-grained target and auxiliary data are analytically integrated out. Using multiple real-world spatial data sets in New York City,
we confirmed that our model can predict the fine-grained target data more precisely compared with the baselines.

Our future work is to consider shapes of regions as in the previous study (7). The assumption of using the centroid of each region allows for GP-based formulations and significantly simplifying computations involved; meanwhile, it might worsen the fit of the GP to the exotic shaped regions (e.g., extremely elongated). Another future work is to incorporate fully Bayesian treatment for model parameters. It can be expected to provide the better results.

### A Derivatives of model parameters

The log-marginal likelihood of \( a \) is given by

\[
\log p(a \mid w, \alpha, \gamma, \sigma) = -\frac{1}{2} (a - \text{HF}^* w)^\top \Lambda^{-1} (a - \text{HF}^* w) \\
- \frac{1}{2} \log(\det(\Lambda)) - \frac{1}{2} \log 2\pi. \tag{9}
\]

We describe the first derivatives of (9) with respect to \( w_s, \alpha, \gamma, \sigma \), which is required for estimating the parameter based on the BFGS method. The derivative of (9) with respect to \( w_s \) is given by

\[
\frac{\partial}{\partial w_s} \log p(a \mid w, \alpha, \gamma, \sigma) = \frac{\partial (a - \text{HF}^* w)}{\partial w_s} p + \frac{1}{2} \text{tr} \left( (pp^\top - \Lambda^{-1}) \frac{\partial \Lambda}{\partial w_s} \right), \tag{10}
\]

where \( p = \Lambda^{-1} (a - \text{HF}^* w) \) and \( \partial \Lambda/\partial w_s \) is a matrix of elementwise derivatives. The derivative of the element \( \Lambda(i, i') \) (7) is obtained by

\[
\frac{\partial \Lambda(i, i')}{\partial w_s} = \frac{1}{|P_{i}^{\text{fine}}||P_{i'}^{\text{fine}}|} \sum_{j \in P_{i}^{\text{fine}}} \sum_{j' \in P_{i'}^{\text{fine}}} 2w_s \Sigma_s(j, j'). \tag{11}
\]

Denoting \( \theta \in \{\alpha, \gamma, \sigma\} \), the derivative of (9) with respect to \( \theta \) is given by

\[
\frac{\partial}{\partial \theta} \log p(a \mid w, \alpha, \gamma, \sigma) = \frac{1}{2} \text{tr} \left( (pp^\top - \Lambda^{-1}) \frac{\partial \Lambda}{\partial \theta} \right). \tag{12}
\]

The matrix of elementwise derivatives \( \partial \Lambda/\partial \theta \) is trivial. The derivative of the element \( \Lambda(i, i') \) (7) with respect to each hyperparameter is as follows:

\[
\frac{\partial \Lambda(i, i')}{\partial \alpha} = \frac{1}{|P_{i}^{\text{fine}}||P_{i'}^{\text{fine}}|} \sum_{j \in P_{i}^{\text{fine}}} \sum_{j' \in P_{i'}^{\text{fine}}} 2\alpha \exp \left( -\frac{1}{2\gamma^2} \|x_j - x_{j'}\|^2 \right),
\]

\[
\frac{\partial \Lambda(i, i')}{\partial \gamma} = \frac{1}{|P_{i}^{\text{fine}}||P_{i'}^{\text{fine}}|} \sum_{j \in P_{i}^{\text{fine}}} \sum_{j' \in P_{i'}^{\text{fine}}} \gamma^2 \left( -\frac{1}{2\gamma^2} \|x_j - x_{j'}\|^2 \right) \times \exp \left( -\frac{1}{2\gamma^2} \|x_j - x_{j'}\|^2 \right),
\]

\[
\frac{\partial \Lambda(i, i')}{\partial \sigma} = 2\sigma \delta_{i,i'}. \tag{15}
\]

### B Description of real-world spatial data sets

We used the real-world spatial data sets from NYC Open Data 2\(^\text{nd}\) for evaluating the proposed model. The data sets were collected and released for improving the urban environment in New York City, and contain a variety of categories such as social indicators, land use, air quality and taxi traffic. Details of the data sets are listed in Table 4. There are multiple data sets in each category, with the total number of data sets being 44. Each data set is associated with one of six geographical partitions, i.e., school district, UHF42, community district, police precinct, zip code and taxi zone. These partitions have various spatial granularities; the number of regions in each partition is shown in Table 4. These data sets are gathered once a year using the time ranges shown in Table 4; the values of data are divided by the number of observation times. When the values of data are extensive quantities (i.e., proportional to the scale of areas, e.g., population), the values are divided by the areas of respective regions; the resulting values are intensive quantities (i.e., independent of area scale, e.g., population density).

In our experiments, we try to refine the poverty rate data set in the social indicator category and the five air pollution data sets in the air quality category. The poverty rate data set contains the values of poverty rates associated with each region in the community district partition as visualized in Figure 1(a). The air pollution data sets contain the average concentrations of pollutants (i.e., PM2.5, ozone, formaldehyde, benzene, elemental carbon) associated with each region in the UHF42 partition. In order to evaluate the performance in refining coarse-grained data, we used the data that were aggregated into a coarser-grained partition, i.e., borough partition, via spatial averaging, where the borough partition has five regions as illustrated in Figure 1(b). The experimental setting is as follows: 1) Given the poverty rate data set with borough partition (\(|P_{\text{coar}}| = 5\)), we would like to refine the data into the community district partition (\(|P_{\text{fine}}| = 59\)), and 2) given each air pollution data set with the borough partition, we aim to refine the data into the UHF42

\(^2\)https://opendata.cityofnewyork.us
Table 4: Spatial data sets.

<table>
<thead>
<tr>
<th>Category/Name</th>
<th>#data sets</th>
<th>Partition</th>
<th>#regions</th>
<th>Time range</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Education</td>
<td>3</td>
<td>School district</td>
<td>32</td>
<td>2010</td>
<td>Class size, ratio of #pupils to #teachers, SAT score</td>
</tr>
<tr>
<td>Air quality</td>
<td>8</td>
<td>UHF42</td>
<td>42</td>
<td>2009–2010</td>
<td>Average concentration of pollutants</td>
</tr>
<tr>
<td>Social indicator</td>
<td>13</td>
<td>Community district</td>
<td>59</td>
<td>2009–2013</td>
<td>Poverty rate, population, mean commute time, etc.</td>
</tr>
<tr>
<td>Land use</td>
<td>11</td>
<td>Community district</td>
<td>59</td>
<td>2009–2013</td>
<td>Area percentage for commercial office, parking, etc.</td>
</tr>
<tr>
<td>Crime</td>
<td>1</td>
<td>Police precinct</td>
<td>77</td>
<td>2010–2016</td>
<td>Number of crimes</td>
</tr>
<tr>
<td>Incident</td>
<td>2</td>
<td>Zip code</td>
<td>186</td>
<td>2010–2016</td>
<td>#311 calls, #fire incidents</td>
</tr>
<tr>
<td>Telecommunication</td>
<td>2</td>
<td>Zip code</td>
<td>186</td>
<td>2016</td>
<td>#public telephones, #free Wi-Fi hotspots</td>
</tr>
<tr>
<td>Consumption</td>
<td>2</td>
<td>Zip code</td>
<td>186</td>
<td>2010–2014</td>
<td>GHG emission, natural gas consumption</td>
</tr>
<tr>
<td>Taxi traffic</td>
<td>2</td>
<td>Taxi zone</td>
<td>249</td>
<td>2014–2016</td>
<td>#taxi pick-up and drop-off events</td>
</tr>
</tbody>
</table>

C Baselines description

For GPR, we predict the fine-grained target data \( z \) based only on the coarse-grained target data \( a \). For LR-based method and 2-stage SD, given the coarse-grained target data \( a \) and the predictive values of all auxiliary data sets \( F^* \), we predict the fine-grained target data \( z \). Details of these baselines are given below.

**Gaussian process regression (GPR):** We compared our proposed model with a simple spatial interpolation (i.e., GPR) of the coarse-grained spatial data \( a \). This baseline assumes that the target data are explained by only the spatial correlation. Given \( a \) and the set of centroids of the coarse-grained partition \( P^\text{coar} \), we predicted the fine-grained target data \( z \) by using the predictive distribution. Note that this baseline does not use the auxiliary spatial data sets.

**Linear regression-based method (LR-based method):** We used a linear regression-based method that has been applied in various studies \((?, ?)\). The linear regression model is used for estimating the relationships between the coarse-grained target data and the auxiliary data sets. The procedure in the training phase is as follows: 1) aggregate all auxiliary data sets into the coarse-grained partition of target data via spatial averaging; 2) estimate the regression coefficients \( \mathbf{w} \) of the respective auxiliary data sets by using the coarse-grained target data and the auxiliary data sets aggregated via spatial averaging. In the prediction phase, generate unknown values \( z \) for the target fine-grained partition by applying the estimated relationships to the predictive values of auxiliary data sets \( F^* \) as follows: \( z = F^* \hat{\mathbf{w}} \), where \( \hat{\mathbf{w}} \) is the estimated regression coefficient.

**Two-stage statistical downscaling method (2-stage SD):** We used the statistical downscaling method proposed in \((?)\). This method assumes that coarse-grained target data \( a \) can be decomposed into linear regression terms and residual terms. The downscaling procedure is divided into two stages. In the first stage, we obtain the regression coefficients \( \mathbf{w} \) in a manner similar to the training phase of the LR-based method. In the second stage, given the estimated coefficient \( \hat{\mathbf{w}} \), the fine-grained target data \( z \) are estimated to be those that satisfy the following relation:

\[
a_i = \hat{w}_0 + \sum_{s \in S} \hat{w}_s \left[ \frac{1}{|P^\text{fine}_i|} \sum_{j \in P^\text{fine}_i} f_s(x_j) \right] + R^\text{coar}_i
\]

linear regression term

\[
= \frac{1}{|P^\text{fine}_i|} \sum_{j \in P^\text{fine}_i} \left[ \hat{w}_0 + \sum_{s \in S} \hat{w}_s f_s(x_j) + R^\text{fine}_j \right]
\]

residual term

\[
= \frac{1}{|P^\text{fine}_i|} \sum_{j \in P^\text{fine}_i} z_j.
\]

This relation expresses the spatial aggregation constraint, i.e., the assumption that value \( a_i \) associated with coarse-grained region \( i \) is the linear average of the constituent values in the fine-grained partition. Here, \( R^\text{coar}_i \) and \( R^\text{fine}_i \) are the residuals in the coarse-grained and fine-grained partitions, respectively. To obtain the fine-grained target data \( z \), the residual value \( R^\text{fine}_i \) in the fine-grained partition must be determined. Since the linear regression terms have already been fixed in the first stage, \( R^\text{coar}_i \) is obtained from (16); the residuals in the fine-grained partition are predicted by applying the spatial interpolation method, i.e., simple kriging \((?)\), to the residuals \( R^\text{coar}_i \) in the coarse-grained partition.