

Visual Bandwidth Selection for Kernel Density Maps

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Summary: Within this paper we investigate the challenge to find an appropriate bandwidth in kernel density estimation. Kernel density estimation methods can be used in visualizing and analyzing spatial data, with the objective of understanding and potentially predicting event patterns. Our aim is to provide a computational tool to visually select the bandwidth parameter and to visually investigate the effect of different parameters within the kernel density calculations. With this tool the user is able to visually find the most appropriate bandwidth for the particular dataset and scale. The slider-tool includes a graphical user interface and can read point datasets. A specific number of kernel density maps are generated by using a range of bandwidths. In the graphical interface these kernel density maps can be drawn near real-time while the user changes the respective bandwidth using a slider tool. This helps to determine which bandwidth setting fits the needs and provide an appropriate visualization of a particular point dataset.

Zusammenfassung: *Visuelle Radius Festlegung für Kernel Dichte Abschätzungen.* In dieser Arbeit untersuchen wir die Möglichkeiten, um einen angemessenen Radius in der Kernel-Dichte Schätzung zu erhalten. Kernel-Dichte Schätzung Methoden können in der Visualisierung und Analyse räumlicher Daten zum Verständnis und zur Vorhersage von räumlichen Mustern dienen. Unser Ziel ist es, ein Computer-Werkzeug zur visuellen Parameter Bestimmung zu entwickeln. Die Radien verschiedener Kernel werden visuell geprüft und können experimentell untersucht werden. Mit diesem Werkzeug kann der Anwender den am besten geeigneten Radius für den jeweiligen Datensatz bestimmen. Das Schieberegler-Werkzeug beinhaltet eine grafische Benutzeroberfläche und kann Punktdatensätze einladen. Anhand statistischer Parameter des verwendeten Punktdatensatzes wird eine bestimmte Anzahl der Kernel Dichte Karten mit verschiedenen Radien vorbereitet. In der grafischen Benutzeroberfläche lassen sich diese Kernel-Dichte-Karten „in real-time“ darstellen. Der Benutzer selektiert verschiedene Radien mit einem Slider-Tool, wobei die jeweiligen Kernel Dichte Karten nacheinander abgebildet werden. Dadurch lässt sich der optimale Radius zur zweckdienlichen Visualisierung von einem bestimmten Datensatz finden.

1 Introduction

Geographic information systems use different methods to display spatial information, and within this paper we investigate new tools to enhance the visual clustering of data. On a general level the aim is to detect spatial patterns in data and formulate hypotheses based on the clusters of point data. Therefore we need to link numerical and graphical procedures with a map. We try to identify where

specific clusters are located on the map and visualize alternatives to visually cluster spatial data.

From a theoretical perspective, this relates to the concept of Geovisualization, which provides theory, additionally methods and tools for the visual exploration, analysis, synthesis and presentation of data that contain geographic information (MACÉACHREN & KRAAK 2001). From a broader perspective it includes the concept of exploratory spatial data analysis to detect spatial

properties of data. There are different types of users who use geovisualization systems differently and bring different knowledge to the decision-making process. The use of these tools should support the interaction between different actors, e. g., decision-makers, the public and experts. The communication between these actors supports the development of models and the creation of task-specific maps. Visualization is a key point in the mediation of content and decisions. Therefore, the choice of visualization methods, the orientation of the visualization on the geographic area, as well as the selection of the geographic area is of high importance. The overall goal is an adequate communication for example to gain political support for a certain decision and enhance communication between experts from various fields. It is essential to provide visualization techniques as a means of exploring spatial data in order to detect features of interest contained in them as suggested by HEARNshaw & UNWIN (1994). As VIRRANTaus et al. (2009) state, the impact of the visualization on knowledge acquisition (does the map present unknown information, or is it used to display and confirm previously known information?), its role as an investigative tool (is the map for private study, or is it part of a more public decision making process?), and its didactic capabilities (is the map being used interactively or is being read passively?) can be researched through models of visualization. In this paper the density map is regarded as a tool to confirm and depict previously known information.

Point densities can be displayed as isarithmic maps. An isarithmic map is created by interpolating a set of isolines between sample points of known values (SLOCUM et al. 2001, SLOCUM et al. 2005). In the special case of handling the locations of events as true point data the term isometric map is used. *Kernel density estimation* (KDE) can supply point densities from a set of point locations. For that reason we choose to display point densities as isometric maps using *kernel density estimation* (KDE) method. In these isometric maps the isolines show a curve in which the point density value is constant. Within this paper we investigate kernel density estimation methods which are included in a variety of applications: point data smoothing; creation of continuous surfaces from point data in order to combine these with other data-

sets that are continuous/in raster form; probability distribution estimation; interpolation or hot spot detection. It is important to understand visualization techniques as a means to explore geographic data and to detect correlations in spatial data. Methods for kernel density estimates have a wide variety of applications. These include the estimation of probability distributions and the interpolation of point data for hot spot detection. Kernel density estimation can also be used in the visualization and analysis of temporal patterns, such as crime events at different times of day and / or over different time periods. The goal is an understanding and prediction of potential patterns in the available data point. Previous research includes work done by LEVINE (2004), who provides an excellent discussion of the various techniques and options, including alternative methods for bandwidth selection (CHIU 1991), together with examples from crime analysis, health research, urban development and ecology (LEVINE 2004, SMITH et al. 2008). Research by KRISP & ŠPATENKOVÁ (2009) investigated the possibility to visually review the significance of a bandwidth selection for the fire & rescue services resource planning. Bandwidth selection, as explained in the following, is often more of an art than a science as suggested by SMITH et al. (2008).

Historically, Point Pattern Analysis was introduced for scientific applications in the early 1920s. GLEASON (1920) and SVEDBERG (1922) used Point Pattern Analysis (PPA) to statistically describe their botanical and ecological work. Since then many different science fields such as epidemiology, criminology, archaeology or seismology use PPA. For instance, one can conduct a "Hot spot" analysis to have a better understanding of locations of crime. A Hot Spot is a concentration of point events within a limited area. This can help the police, for example, to make decisions where to intensify daily patrols. Point Pattern Analysis involves the ability to compare and describe point patterns and test whether there is a significant difference to a random spatial point pattern. A point pattern is a set of locations of point events (O'SULLIVAN & UNWIN 2003). There are three main types of point patterns which can be analyzed, clustered, evenly spaced and random spatial point patterns. In a clustered

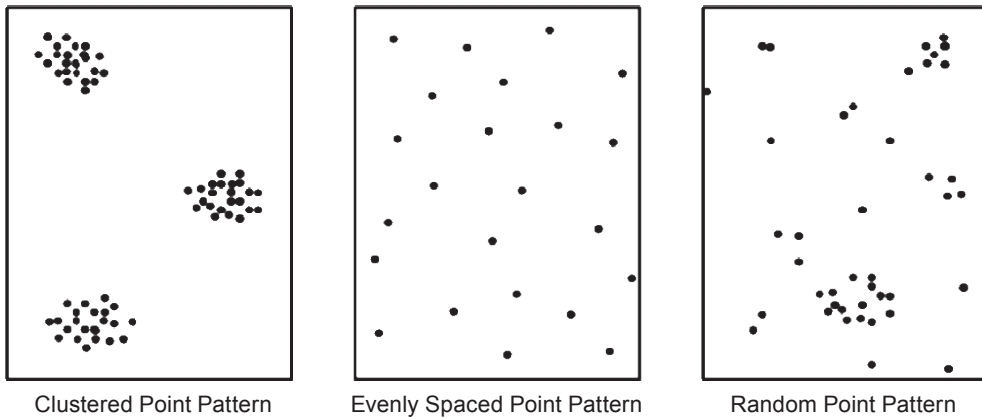


Fig. 1: Types of Point Patterns in practice.

point pattern the events are grouped in regions of the study area. Because of the spatial dependency in a clustered pattern one can speak of a positive auto-correlation. An evenly spaced point pattern is a point pattern with approximately equal distances between neighboring points. A point's neighbor is the nearest other point located to itself. Approximately equal distances of all neighboring points imply that the pattern is negatively correlated. The random spatial point pattern is used as a theoretical point pattern to be compared with an empirical point pattern. The events in a random spatial point pattern are normally distributed. There is no interaction between the points and they are therefore not auto-correlated. One way to define an independently and uniformly set of points is using a homogeneous *Poisson* distribution.

Many different analyzing methods have been developed in the past. A popular PPA method is kernel density estimation. For kernel density estimation a series of estimations are made over a grid which is placed on the entire point pattern. Every estimation shows the intensity at a certain location. Therefore kernel density estimation detects the highs and lows of point densities of the pattern and is useful for detecting hot spots. To make a kernel density estimation the user has to select the kernel function and a bandwidth for the estimation. Of a number of different kernel functions the normal distribution function is the most commonly used (DIGGLE 2003). Quite logically, the function weighs closer points more than distant points. The normal distribu-

tion function extends then in all directions to infinity. This gives the advantage of a throughout covered study area that shows the intensity at all locations. Generally it is difficult to compare point density values in different datasets, because the number of points and the size of the study area may differ greatly. This influences the results of the calculations. The definition of “high” and “low” point densities needs to be considered because those values differ greatly depending on the dataset, the scale of the map and the object to be studied.

2 Problem Statement and Aim

We suggest that looking at a point dataset as a continuous surface by using kernel density enhances the identification of clusters is of particular importance. The choice of the bandwidth affects the kernel density estimation strongly. When the kernel density estimation is carried out with a small bandwidth, the estimation interacts with individual events. For this reason a user has to experiment with different bandwidths to visually find out which results make most sense. A smaller bandwidth will produce a finer density estimate with all little peaks and valleys. A larger bandwidth will result into a smoother distribution of point densities (cf. Fig. 2). There are only few rules considered how to choose a bandwidth by other methods than by visual rating (VENABLES & RIPLEY 1997).

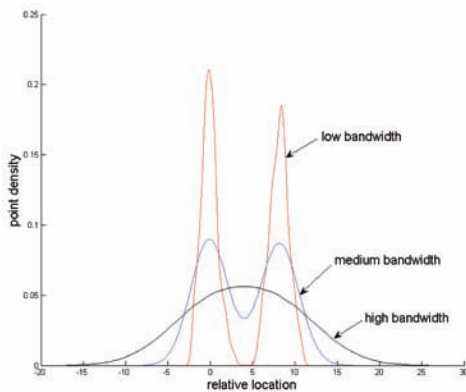


Fig. 2: Kernel Density with different bandwidths.

In many cases a domain-expert has specific knowledge about the issue at hand. The expert has a certain idea of a density surface in mind and intends to depict this surface in a density map. The expert's knowledge can be utilized to determine the optimal parameters for a density calculation. The challenge is to find an appropriate bandwidth in KDE. For every KDE and its resulting kernel density map two parameters are fundamental and have to be specified: cell size and bandwidth. In existing research publications the choice of bandwidth is taken predominantly as the result of experimental studies by visually comparing different bandwidth setting, e. g., in WOLFF & ASCHE (2009). However, the lack of rules and standards concerning bandwidth parameterisation prompts SMITH et al. (2006). Our aim is to provide a computational tool to visually select the bandwidth parameter and to visually investigate different parameters within the kernel density calculations. This will help to determine which bandwidth settings would fit the needs and provide an appropriate visualization of a particular point dataset. Therefore a computational tool is needed to display the density map based on a dynamically changing bandwidth and output grid size.

3 Applied Method and Test Data

The flowchart in Fig. 3 shows the methodological steps to visually determine the kernel

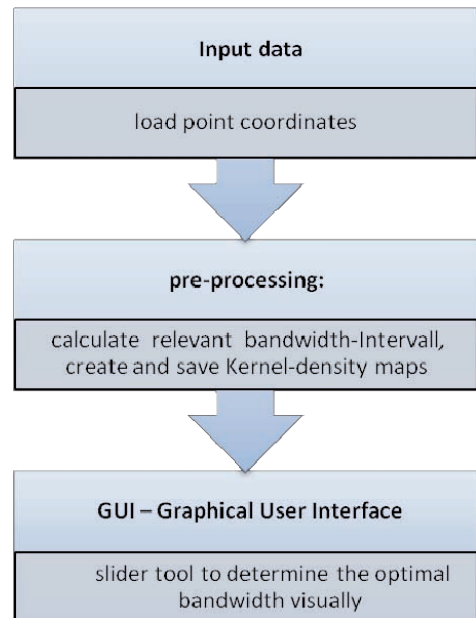


Fig. 3: Flowchart to visually determine the kernel density bandwidth.

density bandwidth for density estimation for an exemplary point dataset.

Input Data

As a study area we have selected an area in the centre of Munich, Germany, containing 1412 points in an area roughly 1 km × 1.5 km. The exemplary dataset includes points representing vegetation locations, for example for trees and bushes. This is a partly artificial point dataset for a showcase purpose. It does serve the purpose of studying the process to find an optimal bandwidth and acquire the most favorable density map for this study area. The entire data set is used for input. O'SULLIVAN & UNWIN (2003) stated that it is required to include a complete data set and not a sample data set to analyze point patterns.

Pre-Processing & Determining the Relevant Bandwidth Interval

To provide a reasonable performance while using the slider-tool, a pre-processing of the kernel density maps is required. On the one hand a range of relevant bandwidth recording to the input data set has to be calculated. From each determined bandwidth then different

kernel density maps with different resolutions were processed and saved as .png image files. This pre-processing is required, because the calculation of kernel density is very time-consuming in case of large dataset, especially on demand of a large bandwidth and high resolution for the output map. For example, a resolution of 400 × 400 pixel the processing of a kernel density-map containing circa 2000 points requires around 15 minutes computing time (Standard Windows PC: 16 GB RAM, CPU 2 × 1.87 GHz). In contrast to this, the pre-processed maps can be loaded and drawn on the screen near real time. Eventually technological improvements may make this aspect of the application work obsolete in the near future as the maps may be computed on-the-fly.

Which bandwidths are relevant for varying point datasets? Which are the minimal and maximal bandwidths to determine the optimal one by visual observation of the kernel density maps? These questions were discussed in this work. In existing research literature of kernel density estimation, SILVERMAN worked on the issue of determining the optimal bandwidth for a certain case, before making the actual density computation. He suggested the calculation formulated in the following equation 1 (SILVERMAN 1986).

Formula based on (SILVERMAN 1986):

$$bw_optimal = 1.06 \cdot \min\left(\sqrt{\text{var}(P)}, \frac{\text{IQR}(P)}{1.34}\right) \cdot n^{\frac{1}{5}} \quad (1)$$

With:

- $bw_optimal$ = optimal bandwidth
- P = dataset: point coordinates
- $\text{IQR}(P)$ = interquartile range (the distance between the 1st and 3rd quartile) of P
- $\text{var}(P)$ = variance of P
- n = number of points (length of P)

SILVERMAN’S formula for calculating an optimal bandwidth has two outcomes, one optimal radius for the x-coordinates and another one for the y-coordinates. Thereby it takes either the variance (var) or the interquartile range (IQR) of the coordinates to the basis, depending on which one is smaller.

For a visual determination of the kernel bandwidth SILVERMAN’S calculation could be used as a starting point for defining a relevant bandwidth interval. But this idea does not consider the point distribution or their distance to the closest neighbor.

In some cases the majority of the points are located densely in one or only some small sectors of the area of investigation. The remaining points are sparsely distributed. The calculation based on SILVERMAN (1986) gives a good solution for areas with densely distributed points. Alternatively an adaptive kernel can be applied. The following Fig. 4 outlines the main steps of determining the relevant bandwidth-interval:

The nearest neighbor distance turned out to be an adequate parameter to determine the bandwidth. First the nearest neighbor distance (spherical) of each point was calculated (nnd).

In the next step the amount of all these calculated distances was classified in 50 clusters using the k-means-algorithm. K-mean-clustering was used, because it takes the value-differences into account. The resulting 50 values represent the range of the relevant kernel bandwidths. Additionally the value half of the minimal bandwidth was added to consider a smaller bandwidth than the minimal nearest neighbor distance, for the case of evenly spaced points. Furthermore the value quarter of the maximum nearest neighbor distance was added, to consider a bandwidth larger

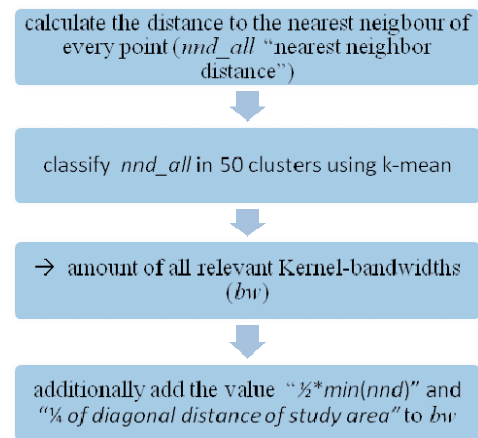


Fig. 4: Flowchart showing the calculation of relevant bandwidth-interval.

than the maximum nearest neighbor distance, for the case of clustered points in only one section of the study area. This gives the possibility of a wider range for the relevant kernel bandwidth shown in equation 2.

Formula to calculate the amount of the relevant kernel bandwidth:

$$[bw] = \left[\frac{1}{2} \min(nnd), \left[k_mean(nnd) \right], \max(nnd), \frac{1}{4} dist \right] \quad (2)$$

With:

bw = bandwidth

nnd = nearest neighbor distance

k_mean = 50 values resulting from a k-mean clustering of all nnd-values

dist = diagonal distance of study area

Kernel Density Map Output and Classification

The calculation of the pixel kernel density values is based on a bimodal Gaussian distribution. The density value for every pixel results from the addition of all kernels laying over this particular pixel. The estimation is shown in equation 3 based on SCOTT (1992):

Formula based on (SCOTT 1992):

$$\hat{f}_h(x) = \frac{1}{N \cdot h} \sum_{i=1}^N K(u) \quad \text{with} \quad u = \frac{x - x_i}{h},$$

$$\text{Gaussian-Kernel: } K_G = \frac{1}{\sqrt{2\pi}} \cdot \exp\left(-\frac{1}{2}u^2\right) \quad (3)$$

With:

$\hat{f}_h(x)$ = general Kernel density function

KG = standard Gaussian function

h = smoothing parameter (bandwidth)

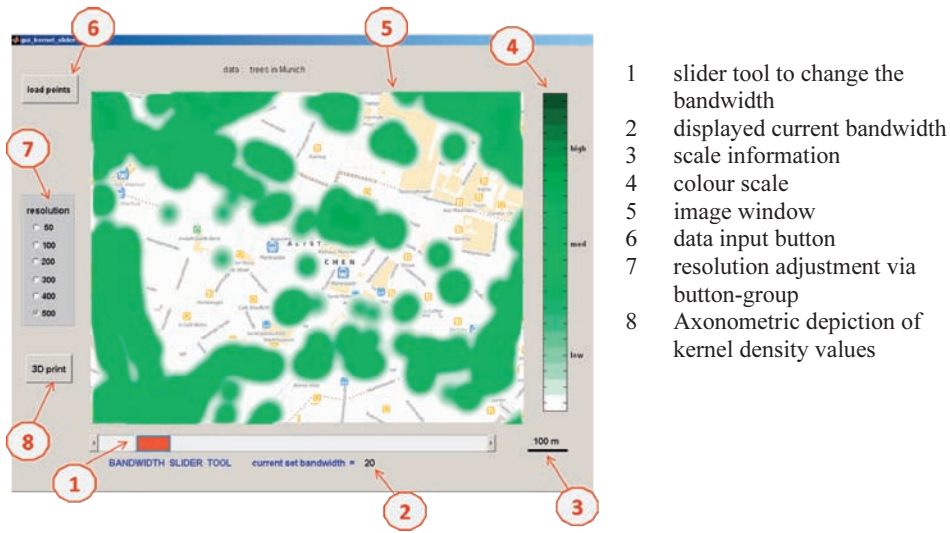
x_1, x_2, \dots, x_N = points, placed within the kernel radius h

Input values of this function are the point coordinates resolution and the kernel bandwidth. The function performs a bivariate Gaussian kernel estimation. The result is a kernel density map stored in a raster image which can be classified differently according to the values in each raster cell. Image classifications (clustering) are based on feature characteristics, for

example color or shape. Image classifications basically differ depending on parametric or non-parametric, hard or soft, pixel by pixel, section by section; monitored or unsupervised classification. Parametric classification methods assume a parameterized data distribution, for example a Gaussian-distribution. In case of unsupervised classification methods the user merely determines the number of the classes in which the data have to be divided. There is no need for samples. The cluster algorithms lead to the separation of classes based on statistical parameters. The assignment of spectral classes to information classes results after the classification. The conditional intervention often leads to undesirable overlap between the information classes. In case of unsupervised classification methods the user determines the number of the classes as well as their spectral occurrence in the multispectral feature space. Thereby an analysis of samples leads to pre-determined features. The separation of these spectral classes is done on the basis of spectral-geometric or statistical classifiers. Based on the definition of the spectral classes before the classification, an automated assignment by the classification algorithm is done (KÖHN 1996).

There are numerous methods and algorithms for image classifications. One simple method to separate a raster image into regions is the use of a grey-tone histogram for determining the regions (ALBERTZ & WIGGENHAGEN 2008). For the assignment of the different grey-scales different algorithms are used, among others the natural-breaks algorithm (also referred to as Jenks classification), the Quantile- algorithm or the separation into equal intervals.

An approved algorithm for image classification is the k-means clustering. But there is a number of other classification methods like Maximum-Likelihood classification, the Group-average clustering or the classification method based on the minimum distance. More detailed information is given by JÄHNE (2002). Which classification method is finally chosen depends on the purpose to be achieved and on the characteristics of the data. There is no "right" or "correct" decision for choosing a certain method. With every of the 52 pre-defined kernel bandwidths in each case 5 kernel



- 1 slider tool to change the bandwidth
- 2 displayed current bandwidth
- 3 scale information
- 4 colour scale
- 5 image window
- 6 data input button
- 7 resolution adjustment via button-group
- 8 Axonometric depiction of kernel density values

Fig. 5: Graphical User-Interface: kernel-slider-tool.

density maps with different resolutions were processed and saved, altogether 260 maps. The lowest resolution is 50×50 pixel, whereby 1 pixel refers to 22 m. The following contains 100×100 pixel, then 200×200 pixel, 300×300 pixel up to the maximum of 400×400 pixel, whereby 1 pixel refers to 2.75 m. 20 colour-classes were used for the colour-classification of the created kernel density maps. A green colour scale was applied. Dark green pixels refer to very high density values and light-green coloured pixel stand for low density values.

density estimation can be demonstrated clearly and an appropriate bandwidth can be determined visually. In the case of our test data in the background of the kernel density map an Open-Street-map of the associated area was drawn. The kernel density map was shown in the same screen-frame for each resolution. Furthermore the color range and the scale information are shown in the interactive user interface.

Additionally in Fig. 5 a “3D-print” button is to see on the top-left corner. It activates an axonometric depiction of kernel density values using the current settings of bandwidth and

4 Resulting Tool for Visual Determination of an Adequate Kernel Bandwidth

A visual determination of an adequate kernel bandwidth for kernel density estimations can be done best using a Slider-tool. In this work a slider-tool was developed using Matlab GUI (graphical user interface) as shown in Fig. 5. By changing the bandwidth slider interactively the related pre-processed kernel density map will be drawn on the image-window. Likewise the resolution can be changed using the resolution-button-group, while the kernel density map will be actualized. This way the influence of the kernel bandwidth to the kernel

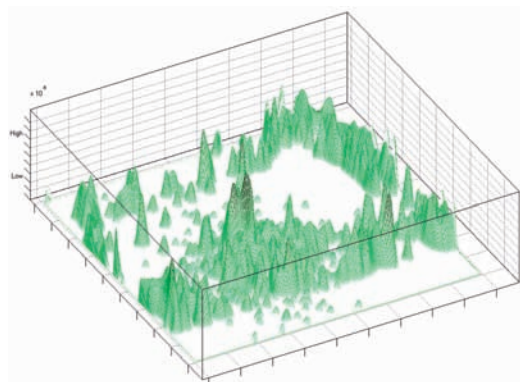


Fig. 6: Axonometric depiction of kernel density values.

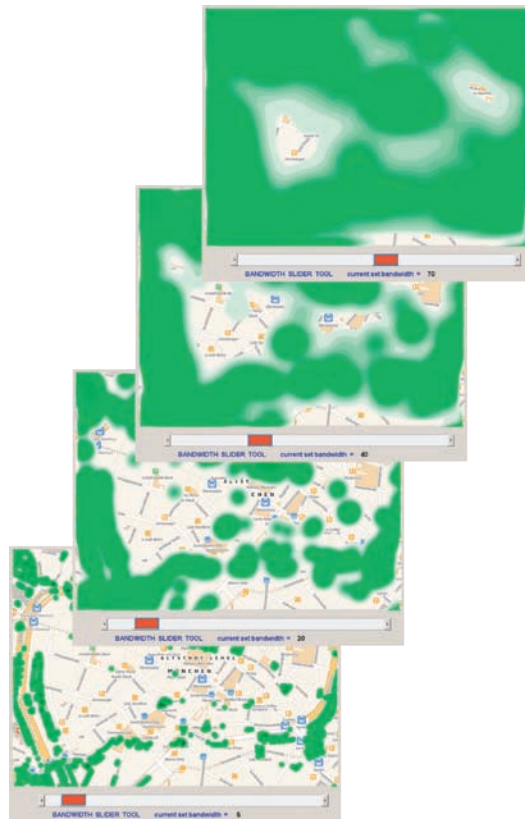


Fig. 7: Screenshots-series with different bandwidth-settings in the slider-tool.

resolution for the slider-tool. The plot is shown in Fig. 6.

An interactive zoom and navigation tool allows the user to study the three dimensional kernel density map from different perspectives. Hence the 2D- and the 3D-visualisation of the kernel density map can be drawn side by side and compared directly with each other. Fig. 7 illustrates the advantage of the direct interactively print output by changing the bandwidth using a slider. So the different resulting maps can be compared easily and the appropriate bandwidth can be chosen visually better.

An advantage for using resolutions under 100×100 pixel is the short image processing time. But for an adequate kernel density a map resolution higher than 300×300 pixel is necessary. For values over 500×500 pixel no visible differences can be recognized in the resulting map. It is to add on that the kernel density map was shown in the same screen-frame

for each resolution. For very small bandwidths a rough structure results in the kernel density map. On the other side a quite strong smoothing can be seen in the kernel density maps by using a large bandwidth.

5 Discussion and Conclusions

Kernel Density Estimations are well established in the visual analysis of point densities. To find an appropriate bandwidth does take experience with the point data at hand or experimentation is required to achieve a satisfactory output. Therefore the bandwidth slider tool lets the user select and browse through a large number of pre-processed density computations, significantly eases the process of finding an appropriate bandwidth setting.

The choice of the size of the bandwidth plays a decisive role for the kernel density es-

timation. In some references the bandwidth is also called smoothing-parameter, meaning when the bandwidth is set too large, important information may be lost. In case of a small bandwidth local data information has a more significant impact on the kernel density estimation map. The kernel slider tool supports the interactive process to select the optimal bandwidth.

Modifications on the bandwidth slider tool may include an adapted zoom tool to change the scale of the map window and a pan tool to move the map in the display area. However, the idea is to keep the tool as simple as possible and to let the user focus on the bandwidth finding process.

6 Further Research

The bandwidth slider tool will be evaluated further and further research will include test on users from specific domains. In many cases the bandwidth setting for a specific point dataset is not clear. By visually identifying the optimal bandwidth setting for a more specific dataset and scale, for example mobile phone base stations in the centre of Munich, we may draw more general conclusions on a most advantageous KDE bandwidth setting. An alternative method to modify the visual output of the estimation is to use an adaptive rather than a fixed bandwidth, meaning a dynamic search radius with a fixed amount of points included.

The current tool uses a rather time consuming pre-processing stage. This pre-processing may be computed faster by an alternative KDE algorithm or by advanced hardware. We suggest that future developments in more powerful hardware technology will make the pre-processing time for the bandwidth selection tools significantly faster or obsolete.

In this work the colors from light green to dark green were used to represent the corresponding densities of trees. These selected colors are quite appropriate for our specified case, as the representation can reflect the natural phenomenon quite well. However, this set of colors is not suitable for representing other densities, e. g., the density of street lamps. In the nearest future, the matching between different color sets, transparencies and different

kinds of densities will be investigated, so that the representation can give users a good visual impression. Additionally further research will explore the possibility to use an asynchrony kernel to calculate densities for dynamic point data. The visual analysis of these moving points, for example individual mobile phone locations, will require research into advanced dynamic visual clustering methods.

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