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Case Study



Analysing and visualising bike-sharing demand with outliers

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Abstract

Bike-sharing is a popular component of sustainable urban mobility. It requires anticipatory planning, e.g. of station locations and inventory, to balance expected demand and capacity. However, external factors such as extreme weather or glitches in public transport, can cause demand to deviate from baseline levels. Identifying such outliers keeps historic data reliable and improves forecasts. In this paper we show how outliers can be identified by clustering stations and applying a functional depth analysis. We apply our analysis techniques to the Washington D.C. Capital Bikeshare data set as the running example throughout the paper, but our methodology is general by design. Furthermore, we offer an array of meaningful visualisations to communicate findings and highlight patterns in demand. Last but not least, we formulate managerial recommendations on how to use both the demand forecast and the identified outliers in the bike-sharing planning process.

Keywords Analytics · Forecasting · Outlier detection · Data visualisation

1 Introduction and background

As a component of sustainable urban mobility, bike-sharing is on the rise in cities around the world. Empirical research as exemplified by Teixeira et al. [1] and Blazanin et al. [2] has been dedicated to highlighting requirements and beneficial impacts of the related modal shifts in urban transport. As pointed out in the related references, careful planning is required to make so-called shared micromobility systems more attractive than less environmentally friendly alternatives, such as cars. While the concept of shared micromobility also includes e-scooters and dockless bike-shares, here, we focus on systems that rely on a set of dedicated stations. As, for example, Luo et al. [3] point out, while dockless systems offer more convenience and equity to users, their CO2 footprint is significantly higher due to the reduced lifespan of vehicles. On the other hand, station-based sharing systems require carefully planned station locations and well-balanced inventory levels to ensure adequate service provision. When, for example, a station is mostly used to pick-up bikes, re-balancing ensures a steady supply and avoids service denials.

Planning for bike-sharing operations means determining, for example, the best distribution of stations across the service area, Neumann-Saavedra et al. [4], the best distribution of bikes across stations [5], and the best path for truck drivers to take when re-distributing bikes each day [6]. When taking a pro-active approach to planning, optimisation procedures that determine stock levels per station rely on predicted demand. When taking a re-active approach, quick online decision-making is crucial to maintain a good service level. Since inefficient re-balancing operations are a major

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cost driver for operators [6], identifying demand outliers to improve efficiency in bike-sharing systems is highly important. Unaccounted-for outliers can affect bike-sharing systems in two ways: (i) outliers in historic data contaminate the forecasts used in future inventory management, and (ii) on the day demand levels may indicate that the schedule is non-optimal for the current day and drivers should be re-routed.

Therefore, identification of outlier demand has several potential benefits for bike-sharing forecasting and planning: (1) Detecting outliers early in the day, through online analysis as proposed in [7], allows for rapid interventions to better re-allocate bikes on a given day; (2) Removing any detected outliers from training data for demand forecasting would improve results on predicting reference demand curves; (3) If outliers can be attributed to specific events previously unknown, extending future forecast models to include such events can improve forecasts; (4) Even when explanatory factors for outliers cannot be determined, if such outliers are concentrated spatio-temporally in certain stations, this knowledge can better support planning decisions; and (5) Identifying changes in the underlying reference model when patterns in the detected outliers are observed can trigger a review of the current forecasting method.

We define outlier demand as a short-term change in demand, resulting in usage levels which deviate from regular usage. Note that, to count as an outlier, a demand shift has to exceed the general degree of random variation observed in demand over time. In this paper, we focus on demand observed at bike-sharing stations, as these are the target of inventory rebalancing efforts. In contrast to other classical mobility problems, such as those related to buses or trains, bike-sharing capacity is on the vertices of the transport network, rather than on the edges.

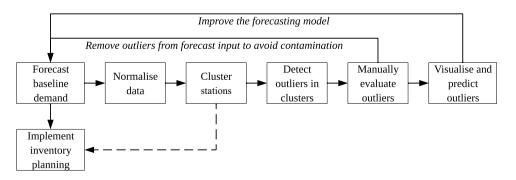
As an example of existing work in this area [8], discuss the problem of variability in bike-sharing demand and propose a rule-based method to adjust the redistribution plan when demand differs from the forecast. In a simulation study, they show that service levels can be improved when adjustments are made to the optimal redistribution plan. Wider literature on outlier detection in transport planning is scarce—e.g. Rennie et al. [9], consider identifying and correcting for outliers in revenue management systems in railways.

Talvitie and Kirshner [10] find that outliers can have a substantial effect on the predictions of usage of different urban transport modes, but only apply a simplistic trimming method to identify outliers. In the road traffic domain, Guo et al. [11], suggest a procedure for identifying outliers in real time based on the conditional variance of predictions, and determine that incorporating information on such outliers into future predictions increases the systems performance.

Furthermore, as indicated, e.g., in Basole et al. [12], to account for demand outliers and adjust planning, experts require meaningful visualisations. Therefore, we propose a set of visualisations to help identify and analyse spatial and temporal patterns in the detected outliers. For example, given shifts in the availability of urban infrastructure, a subset of stations may be predisposed to outliers and as such, this area would be a good target for a temporary "pop-up" station. Throughout this paper, we assume that bike-sharing companies employ analysts who are in charge of strategic decisions, such as where to locate stations, tactical decisions, such as what number of bikes should be available on any given day at those stations, and operational decisions, such as on-the-fly rebalancing of bikes. In that, we follow previous research, such as Wang et al. [13], who expect analysts to evaluate bike share programs and station locations, or Ma et al. [14], who consider analysts or dispatchers to be in charge of rebalancing operations.

To combine automated outlier detection, manual analysis, demand forecasts, and planning, we suggest the following process for analysing bike-sharing demand data (see Fig. 1): First, a baseline demand forecast supports anticipative planning, e.g. of inventory levels. Second, this baseline can be used to normalise observed usage data. Using the resulting observations, analysts can cluster stations with similar usage patterns to support both planning adjustments and outlier detection. When detecting outliers in a cluster's usage patterns, these are visualised to enable manual outlier evaluation. Insights from this analysis can be used to both clean the data that underlies the baseline forecast and to extend the baseline forecasting model.

Fig. 1 Flowchart of process for analysing bike-sharing demand data. Figure adapted from Rennie [15]





In this paper, we analyse the Capital Bikeshare data set, which is publicly available at [16]. This data set is commonly used to test forecasting approaches for bike-sharing [17, 18], yet these methods typically do not account for outliers. In Sect. 2, we introduce the data set and perform an exploratory analysis. Sections 3 and 4 then model the temporal and spatial patterns in demand for bike-sharing. In Sect. 5, we provide a methodology for identifying outlying demand for bike-sharing services. The results of applying the outlier detection method to the Capital Bikeshare data are then discussed in Sect. 6.

In summary, this paper contributes (i) an in-depth analysis of temporal patterns in usage of Capital Bikeshare services; (ii) a method for spatial clustering of bike-sharing stations based on geographic proximity and similarity of usage patterns; (iii) an investigation of temporal trends in detected outliers and the factors that may cause them; and (iv) an analysis of spatial patterns of the outliers detected. Our methodology is data-driven and general by design, and not tailored to specifics related to Washington D.C., and can thus be readily applied to all bike-sharing data sets around the world.

2 Capital Bikeshare data

The Capital Bikeshare data set spans a three year period, from January 1 2017 to December 31 2019. It describes every recorded trip by its time of pick-up, time of drop-off, pick-up station location, and drop-off station location. The data set features only those 578 stations that recorded at least one pick-up or drop-off within the recorded time frame.

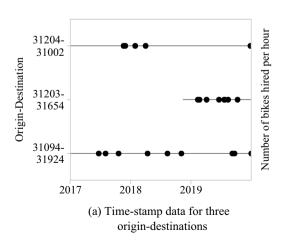
Out of a potential 334,084 unique origin—destination (O–D) pairs, the data set records 105,735 O–D pairs that customers completed based on pick-ups and drop-offs. As examples, the times of bike rentals for three different O–D pairs are shown in Fig. 2a, with each dot representing one journey. Note that station 31654 opened in November 2018, and so data is only available from that date onward for O–D pair 31203–31654.

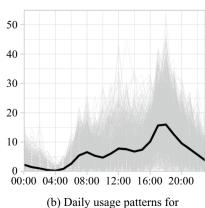
Data cleansing If the first use of a station in the data set was not January 1st 2017, we check historical data from 2016 for any usage to determine if the station was open. If there are no earlier bookings, we consider the station as newly opened from the time of its first recorded trip. Capital Bikeshare pre-process the data to remove trips that are made by staff for system maintenance and any trips with a journey time of less than 60 s (as these may be false starts).

Data aggregation Given the large number of O–D pairs, very few journeys are recorded per unique pair on average. This makes it difficult to detect meaningful patterns, or any deviation from such a pattern, on the O–D level. When numbers are this small, noise dominates over any trend, as also pointed out in related research on forecasting slow-moving retail products [19]. To alleviate the problem of small numbers, we aggregate trips as pick-up and drop-off events, considering usage per station rather than O–D pairs. To further reduce the problem of sparse observations, and to make observations comparable over time, we aggregate usage by hour of day [20]. Specifically, we define the daily usage pattern to be a time series of the number of times per hour that a station is used, either pick-up or drop-off—see Fig. 2b. When considering pick-ups and drop-offs separately, we differentiate the daily pick-up pattern and the daily drop-off pattern.

Exploratory analysis: Spatial variation The total usage varies greatly across stations, with those closer to the centre of Washington D.C. being more popular on average. Figure 3a visualises this idea by indicating the mean annual usage per station across the region. The most popular stations observe more than 130,000 uses per year, whereas the least

Fig. 2 Origin–destination (O–D) level data and aggregated daily usage patterns, with mean usage pattern indicated in **b**. Figure adapted from Rennie [15]





station 31203



popular stations observe less than one on average. Over half of the stations (51%) recorded fewer than 5000 pick-up or drop-off events per year. To indicate the distribution, Fig. 3b provides the mean annual usage per station in a histogram.

Exploratory analysis: Temporal variation In addition to daily usage patterns varying across space, there is also significant temporal variation. Figure 4 that there are significantly different mean usage patterns and inter-daily variance for different days, months, and, to some extent, years. Here, we define inter-daily variance as the daily variability in the usage at a station at a given hour of the day. We present results here for only a single station as these mean and variance patterns can vary across stations, though similar differences between, e.g. days are observed across most stations. This variation in patterns across stations motivates the functional regression model described in Sect. 3.2.

3 Modelling baseline temporal usage patterns

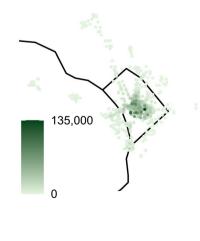
As discussed in Sect. 2, usage patterns vary across time and space. If we do not first remove temporal patterns observed in baseline demand, any outlier detection procedure will likely simply detect baseline trend characteristics as outliers. For example, there is a much higher level of variability in demand on weekends in summer. If we failed to account for this before performing the outlier detection procedure, many of the detected outliers would occur on Saturdays in the summer months. By first accounting for known temporal patterns, the detected outliers are more likely to be genuine outliers rather than explainable patterns already known to analysts.

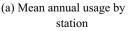
Similarly, if we do not account for spatial baseline variability and instead aggregate data across all stations then we will simply detect unused or extremely busy stations as outliers. Conversely, if we assume all stations behave independently, then the increased noise makes it more difficult to detect outlying usage patterns. As such, before implementing the outlier detection procedure outlined later in Sect. 5, we carry out a two-step process to (i) remove known temporal patterns; and (ii) spatially cluster stations which behave similarly. These two steps are key in identifying meaningful outliers, as we shall show.

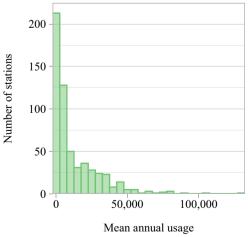
3.1 Background: bike-sharing demand forecasting

Within the bike-sharing literature, a range of techniques have been considered to predict demand, both spatially and temporally. Zhou et al. [21] apply a Markov Chain based model to predict daily pick-ups and drop-offs at each station within the Zhongshan City bike-sharing system. The problem of predicting demand in the presence of spatial heterogeneity is further considered by Gao et al. [22] who estimate a distance decay function and then use multiple linear regression to predict temporal demand in the dockless bike-sharing system in Shanghai. Dockless bike-sharing systems are also discussed by Xu et al. [23], who use long short-term memory neural networks to predict demand, and capture the spatial and temporal imbalance in usage. Sohrabi and Ermagun [24] use a combination of pattern

Fig. 3 Mean annual usage per station with **a** indicating higher usage nearer the city centre, and **b** showing a histogram of number of stations under varying levels of usage, in intervals of 5000. Figure adapted from Rennie [15]



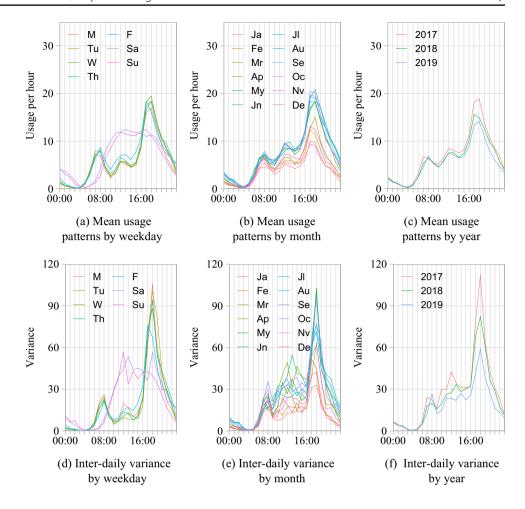




(b) Histogram of mean annual usage of stations



Fig. 4 Mean usage patterns and inter-daily variance for station 31203 by hour of day, which is a representative pattern as seen across the network. Figure originally included in Rennie [15]



recognition on historic data traffic patterns and *K*-nearest neighbours to make spatiotemporal demand predictions over short time horizons (between 15 min and 4 h), for the Capital Bikeshare data.

The choice of forecasting approach will likely affect the outcome of outlier detection. In the following, we discuss and apply two methods of predicting the baseline temporal patterns in the data: (i) functional regression to account for changes in mean; and (ii) temporal partitioning to account for changes in variance.

Beyond the model presented here, alternative approaches could be used to account for trend and seasonality, and establishing a baseline for bike-sharing demand. In general, any forecasting or modelling approach from which residuals can be obtained could be used instead. After the temporal patterns have been accounted for and the residuals obtained, we are then able to analyse the spatial correlations to group together stations which deviate from the baseline demand forecast in a similar way, as we shall discuss later in Sect. 4.

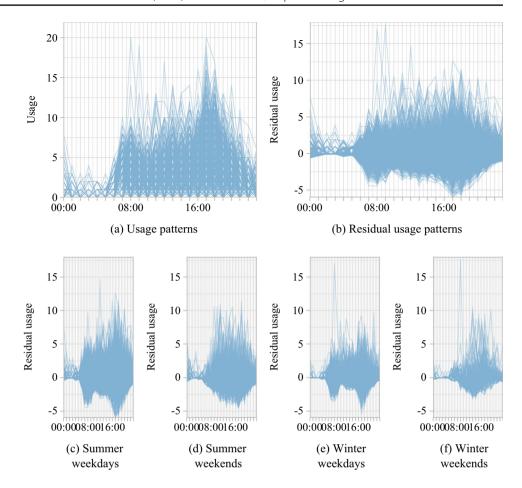
3.2 Functional regression

Mean daily usage patterns differ systematically across days of the week, months, and years. We apply a functional regression model [25] to remove the different mean patterns. We will demonstrate this process on the daily usage patterns of station 31005 as shown in Fig. 5a.

Let $x_{ns}(t)$ be the usage pattern for day n for station s. We implement the following functional regression model:



Fig. 5 Residual usage patterns for station 31005. Figure originally included in Rennie [15]



$$x_{n,s}(t) = \beta_{0,s}(t) + \beta_{1,s}(t)\mathbb{1}_{Mon_n} + \beta_{2,s}(t)\mathbb{1}_{Tue_n} + \beta_{3,s}(t)\mathbb{1}_{Wed_n} + \underbrace{\beta_{4,s}(t)\mathbb{1}_{Thu_n} + \beta_{5,s}(t)\mathbb{1}_{Fri_n} + \beta_{6,s}(t)\mathbb{1}_{Sat_n}}_{\text{Day}} + \beta_{7,s}(t)\mathbb{1}_{Jan_n} + \beta_{8,s}(t)\mathbb{1}_{Feb_n} + \beta_{9,s}(t)\mathbb{1}_{Mar_n} + \beta_{10,s}(t)\mathbb{1}_{Apr_n} + \beta_{11,s}(t)\mathbb{1}_{May_n} + \beta_{12,s}(t)\mathbb{1}_{Jun_n} + \beta_{13,s}(t)\mathbb{1}_{Jul_n} + \beta_{14,s}(t)\mathbb{1}_{Aug_{nl}} + \beta_{15,s}(t)\mathbb{1}_{Sep_n} + \underbrace{\beta_{16,s}(t)\mathbb{1}_{Oct_n} + \beta_{17,s}(t)\mathbb{1}_{Nov_n}}_{\text{Month}} + \underbrace{\beta_{18,s}(t)\mathbb{1}_{2017_n} + \beta_{19,s}(t)\mathbb{1}_{2018_n}}_{\text{Year}} + e_{n,s}(t).$$

$$(1)$$

where e.g., $\mathbb{1}_{Mon_n} = 1$ if day n relates to a Monday, 0 otherwise. Here, $\beta_{0,s}(t)$ represents the mean usage pattern for a Sunday in December 2019. Appendix 9.1.2 contains details of the model selection process where we consider the significance of each of the factors (day, month, year) for a range of stations. The vast majority of stations select the full model containing all three factors as the best-fitting model.

As Fig. 5b indicates, the core of the distribution of residuals is symmetric around 0 as desired. The majority of "spikes" in usage are caused by increased demand, resulting in a slight positive skew to the residual patterns. We note that the variance of these residuals is clearly not constant over time and we shall discuss this shortly. Further discussion of the residual distribution is included in Appendix 9.1.3. Other features of the usage patterns including positive skew, and inter-daily correlation are discussed in Appendices 9.1.4 and 9.1.5.



3.3 Temporal partitioning

Our functional regression approach accounts for different mean usage patterns, but it does not account for the differing inter-daily variances. The simplest option to obtain a data set with homogeneous inter-daily variance is to temporally partition the full data set. While we could partition based on each weekday, month, and year, this would result in around 4 observations per partition—an insufficient number to inform outlier detection. In deciding how to partition the data, there is a trade-off between having reasonably constant inter-daily variance within each group and ensuring there is enough data within each group in order to establish patterns. Therefore, we group together days, months, and years where the inter-daily variances are sufficiently similar.

From Fig. 4, it is clear that weekdays (Mon–Fri) are similar to each other, and weekends (Sat–Sun) are also similar to each other. The differences between the inter-daily variance across different months is less clear. Defining *summer* as April through to October, then months within summer exhibit similar inter-daily variance patterns, as do months within winter (November to March). Further analysis of the variance in Appendix 9.1.1 supports this partitioning. All years are grouped together. This results in four partitions: (i) summer weekdays, (ii) winter weekdays, (iii) summer weekends, and (iv) winter weekends, as displayed in Fig. 5c–f. Note that we do not attempt to remove the *intra*-daily variability of these residuals with further parametric modelling, as instead we turn to functional data analysis to detect outlying curves from these residual daily usage patterns.

The choice of partition is important and should reflect the choices made in the planning process, e.g. with regard to inventory redistribution. If the increased inter-daily variance on weekends, for example, is already known and accounted for in planning, such that there are different schedules for redistribution, then partitioning as we propose would be appropriate. However, if the general planning process (including demand forecast and inventory optimisation) assumes uniformity across all days of the week, it would then be informative to do the same in the outlier detection to flag the weekend effect when it occurs.

4 Clustering stations by spatial usage patterns

When outlier demand is driven by factors such as regional events or weather, we expect it to affect more than a single, isolated station. At the same time, we cannot assume that all stations experience outlier demand at the same time and in the same way. Therefore, we first cluster the stations such that those in the same cluster are likely to experience similar effects from demand outliers.

We propose a two-stage process to determine which stations should be clustered. First, we construct a graph based on the geographic co-ordinates of the stations to determine which stations are permitted to be in the same cluster based on geographic distance. Secondly, we follow an idea from Zahn [26] who suggests the removal of edges from a graph's minimum spanning tree (MST) as a method of finding clusters of nodes.

The first step of constructing the graph is non-trivial. Graph construction in the bike-sharing setting is more open-ended than in situations where mobility networks rely on established legs, as, e.g., in the railway application studied in Rennie [15]. For bike-sharing, direct journeys between any two stations are possible, so that in theory, all stations could be vertices in a fully connected graph. Although we could simply add edges between every node i.e. a complete graph, there are two reasons for not doing so: (i) For the purposes of aiding planning, we do not want two stations which are geographically far apart to be in the same cluster if no stations in between are similar to both. (ii) The algorithm used to compute the MST is slowed down by an increased number of edges, and due to the greedy nature of it, we are more likely to end up at a non-optimal solution if we add in extraneous edges.

4.1 Graph construction from geographical distance

We first construct a graph where the nodes represent the stations and the edges indicate which stations are permitted to be in the same cluster. This approach implicitly assumes that similarity of usage is driven by the stations' geographical proximity. That is, if two stations are close together, potential customers are more likely to treat them as interchangeable, causing similar usage patterns.



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In the Capital Bikeshare data set, stations are more densely distributed in the centre of D.C., so that customers can choose from a large variety of stations. We expect this to render them more sensitive to distance, such that they are less willing to travel to a more distant station. Therefore, we use different criteria to add an edge between stations depending on how close to the centre of D.C. those stations are.

To identify the dense city-centre, we establish a circle around the centre of D.C. of radius R, with the median coordinates of all stations as the centre, as shown in Fig. 6a with $R = 5000 \,\mathrm{m}$. We add an edge between stations i and j if: (i) both stations lie inside the radius, and are less than D_{inner} apart; or (ii) one or both stations lie outside the radius R, and are less than D_{outer} apart.

Not all stations that are geographically close exhibit similar usage patterns e.g. due to proximity to railway stations. Therefore, to quantify how similar the usage patterns of two stations are, we add weights to the edges of the graph. For each edge between stations i and j, we also compute an edge weight representing the dissimilarity between the usage patterns for those stations. The edge weights are given by:

$$w(i,j) = 1 - \rho(i,j), \tag{2}$$

where $\rho(i,j)$ is the average functional dynamical correlation [27] between the daily usage patterns for stations i and j. Here, the average correlation is based on the correlations between daily usage patterns across the entire time period considered (2017–2019), as there is no evidence of the clusters changing over time. However, if the correlations (and therefore clusters) are changing over time, a moving window approach could be used to update the average correlation and clusters over time.

4.2 Minimum spanning tree clustering

We apply a minimum spanning tree approach to cluster stations that are connected in the geographical proximity graph. A graph's spanning tree is a subgraph that includes all vertices in the original graph and a minimum number of edges, such that the spanning tree is connected. If the original graph is disconnected, we compute a spanning tree for each component—termed a spanning forest. A minimum spanning tree (MST) is the spanning tree with the minimum sum of edge weights. Since the graph is weighted, we use Prim's algorithm [28] to calculate the MST.

To obtain the clusters from the MST, we set a threshold, ρ_{τ} , for the correlation and remove all edges with weights above $1 - \rho_{\tau}$.

4.3 Clustering results: daily usage patterns

Figure 7 visualises the outcome from four different values of ρ_{τ} .

These values of ρ_{τ} are chosen to illustrate the clustering for two reasons: (i) $\rho_{\tau} = -1$ indicates that all initially connected edges stay in place. In fact, the minimum correlation observed is -0.57, and any threshold between -1 and -0.57 results in all edges of the MST remaining in place. (ii) 90% of the observed correlations lie between 0

Fig. 6 Graph construction when $R = 5000 \,\mathrm{m}$, $D_{inner} = 500 \,\mathrm{m}$, and $D_{outer} = 1000 \,\mathrm{m}$. Figure originally included in Rennie [15]

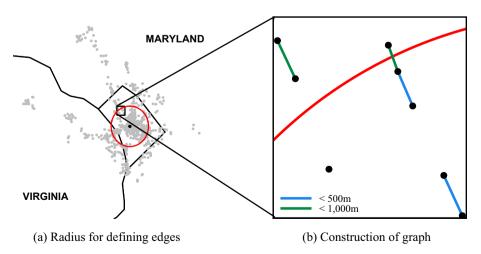
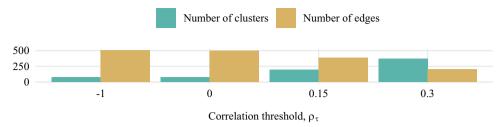
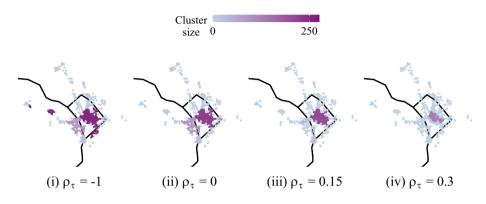




Fig. 7 Clustering of stations under different values of ρ_{τ} . Figure adapted from Rennie [15]



(a) Number of clusters and edges for different thresholds



(b) Cluster sizes for different thresholds

and 0.3, therefore the values of ρ_{τ} = 0, 0.15, and 0.3 demonstrate the clustering when the threshold is close to the minimum, mean, and maximum correlations.

Figure 7 can be used by analysts to determine the most appropriate threshold, depending on which aspect of planning they are considering. Figure 7a shows how the number of clusters (and edges) changes with the choice of clustering threshold—with little difference seen between a threshold of -1 and 0. By inspecting which stations are clustered together, if an analyst has expert knowledge regarding which stations are likely to behave similarly, they can cross-check with the clustering and choose the threshold which supports this decision. Figure 7b visualises the sizes the clusters that each station belongs to, demonstrating the non-uniform distribution of cluster size across the geographic area. This can also be used to determine an appropriate threshold. For example, if an analyst is interested in the general demand patterns of central D.C., they can choose a threshold that highlights all of central D.C. in a single large cluster e.g. ρ_{τ} =0. In contrast, if the analyst is more interested in obtaining clusters of similar size, Fig. 7b(iv) would guide them towards a higher threshold.

Across all thresholds, the stations closer to the centre of D.C. form a larger cluster, with those further away from the centre branching into smaller clusters. Clearly, the choice of threshold values ρ_{τ} impacts the precise clustering results.

The distance parameters, $\{R, D_{inner}, D_{outer}\}$, also affect clustering. The number of clusters increases as ρ_{τ} or R is increased, whereas increasing D_{inner} or D_{outer} has the opposite effect. There is an inverse relationship between the number of clusters and the uniformity of cluster size. As the number of clusters increases, individual stations tend to split off to form their own cluster whilst the majority of stations remain in the large central cluster, resulting in decreased uniformity of cluster size. For decision-making, clusters of similar sizes are often more informative (compared to a large cluster consisting of most stations, and the remaining stations each in their own cluster).

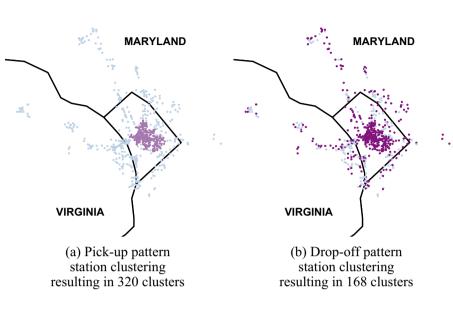
We leave the choice of parameters to analyst input, such that analysts may use their expertise to select appropriate values based on the visualisation and their business case [29]. For the remainder of this paper, unless otherwise specified, we set the parameter values as $\rho_r = 0.15$, R = 5000 m, $D_{inner} = 500$ m, and $D_{outer} = 1000$ m. These values are chosen to balance the number of clusters with more similar cluster sizes. Appendix 9.2.1 includes further details on the reasoning for these choices.



Cluster

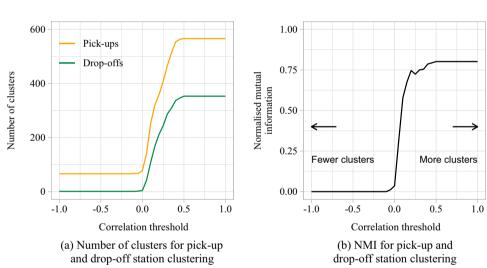
size 0

Fig. 8 Comparison of clustering stations based on pick-up and drop-off patterns for ρ_{τ} = 0.15, R = 5000 m, D_{inner} = 500 m, and D_{outer} = 1000 m. Figure adapted from Rennie [15]



100 200 300 400

Fig. 9 Comparison of pick-up and drop-off station clustering. Figure adapted from Rennie [15]



4.4 Clustering results: daily pick-up and drop-off patterns

So far, we have focused on clustering stations based on the similarity of their daily usage patterns. However, when considering forecasting for inventory rebalancing, differentiating pick-ups and drop-offs is highly important. Depending on the aggregation level of forecasting, it may be desirable to consider separate clusterings for drop-off and pick-up patterns. Figure 8 shows that drop-off patterns tend to be more homogeneous, in comparison to pick-up patterns, resulting in fewer clusters for the same correlation threshold.

Figure 9a shows that this increased homogeneity of drop-off patterns is consistent across all values of the correlation threshold, ρ_{τ} . Although the number of clusters resulting from both pick-up and drop-off station clustering follows a similar relationship with the correlation threshold—increasing steeply between 0 and 0.4—the drop-off clustering consistently results in fewer clusters.

To formally compare the output of these two clusterings, we use the normalised mutual information (NMI) [30]. The NMI is 1 if two clusterings are identical, and 0 if they are completely different (see Appendix 9.2.2 for details). Figure 9b shows that the similarity of the pick-up and drop-off clusterings are highly dependent on the correlation



threshold. When a low threshold is used, the clusterings are completely different. However, as the correlation threshold increases above 0.25, the clusterings become more similar, achieving an NMI of around 0.75.

This evidence that pick-ups and drop-offs are not spatially homogeneous motivates the need for separate forecasting of the two. The differences across the varying threshold also indicates that the need for separate forecasting is more critical when considering a larger area i.e. when considering total demand, but is less critical over smaller areas closer to the station level. Monitoring the difference in the number of clusters and the similarity of the two clusterings can help analysts to decide on the level of forecasting. Analysts could also examine changes in the NMI over time for a given correlation threshold. For example, if the pick-up and drop-off clusterings are becoming more similar to each other over time, this could indicate increasing levels of homogeneity in pick-up patterns.

5 Detecting outliers within a cluster of stations

To demonstrate the outlier detection procedure, we focus on one of the resulting clusters. The nine stations in the cluster we consider are highlighted in green in Fig. 10.

Figure 10 demonstrates how the currently analysed cluster may be highlighted for analysts. On the one hand, the location of the cluster within the D.C. area can provide contextual information for analysts in the search for an explanation of outlier demand. On the other hand, the zoomed in section on the right shows how the stations relate to one another within the cluster. This could be useful if the outlier demand is not detected in all stations. For example, all but one of the green cluster stations lie in a relatively straight line. If the station which lies to the North East of the main group of stations in the cluster behaves differently, analysts can look to nearby clusters for further information.

To identify outlier demand in usage patterns, we use the notion of *statistical depth*. In statistics, depth provides an ordering of observations, where those near the centre of the distribution have higher depth and those far from the centre have lower depth. In the case where each observation is a time series of usage throughout the day, the *functional depth* can measure how close to the central trajectory, i.e. median usage pattern, each daily usage pattern is. Therefore, to measure the outlyingness of each daily usage pattern, we calculate its functional depth (with respect to other daily usage patterns that lie in the same partition of data). Days whose usage pattern has lower functional depth are more outlying. In particular, if the depth is below some threshold, we classify the day as an outlier.

For each partition of data, p, and for each station s, we calculate a threshold, $C_{s,p}$, for the functional depth as per Febrero et al. [31]. To calculate the threshold, we (i) resample the daily usage patterns with probability proportional to their functional depths (such that any usage patterns affected by outlier demand are less likely to be resampled), (ii) smooth the resampled patterns, and (iii) sets the threshold $C_{s,p}$ as the median of the 1^{st} percentile of the functional depths of the resampled patterns.

Let $d_{n,s,p}$ be the functional depth for day n (which occurs in partition p) for station s. We then transform the functional depths to lie between 0 and 1 such that they are comparable between different stations and aggregated over the different partitions of data. Define $z_{n,s}$ to be the normalised functional depth on day n for station s:

Fig. 10 Cluster chosen for further investigation. Figure adapted from Rennie [15]

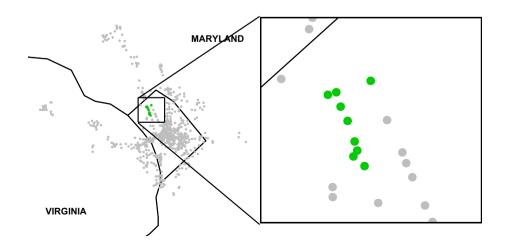
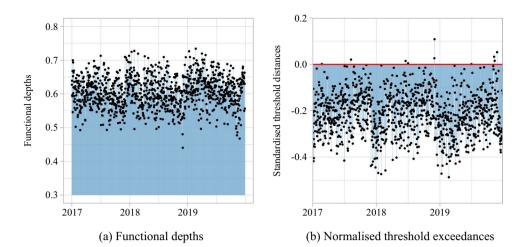




Fig. 11 Normalisation of the functional depths, exemplified for station 31316 where there are two partitions of data (summer/winter). Figure originally included in Rennie [15]



$$z_{n,s} = \sum_{p=1}^{P} \left(\mathbb{1}_{n \in p} \left(\frac{C_{s,p} - d_{n,s,p}}{C_{s,p}} \right) \right).$$
 (3)

The functional depths for station 31303 are shown in Fig. 11a, and their normalised counterparts in Fig. 11b. Figure 11a provides a way to check for unaccounted for trend and seasonality in the usage patterns. However, much like univariate regression residuals which can be used to visually identify residuals patterns, the functional depths should appear random with no obvious patterns. If an analyst can identify a pattern in the functional depths, this would suggest that the forecasting model may need to be reconsidered. Weekdays could be highlighted in different colours to help identify temporal patterns on a smaller scale. Figure 11b can also be used by analysts to check how many non-outlier days are close to, but do not exceed, the threshold. Analysts can use this information to manually vary the threshold to detect further outliers they perceive to be false negatives.

We then define the sum of threshold exceedances across all S stations in the cluster to be:

$$z_n = \sum_{s=1}^{S} z_{n,s} \mathbb{1}_{\{z_{ns} > 0\}}.$$
 (4)

The values of z_n for this cluster are shown in Fig. 12. The value of z_n is only positive for days which have been classified as an outlier.

Fig. 12 Sum of threshold exceedances, z_n . Figure originally included in Rennie [15]

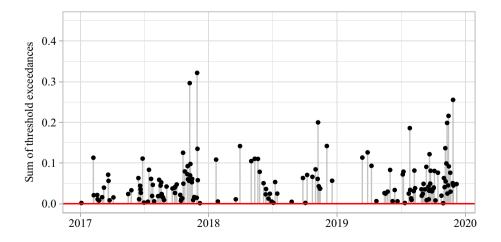
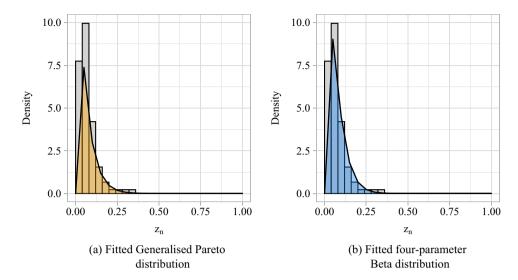




Fig. 13 Comparison of fitted distributions. Figure originally included in Rennie [15]



5.1 Computing outlier severity

Although the values of z_n give an indication of how severe the outlier is (with z_n being larger if the magnitude of the outlier demand is larger, or if it affects a larger number of stations), we wish to make the severity easier to interpret across different clusters. Therefore, we fit a distribution to the sum of threshold exceedances and use the non-exceedance probability given by the CDF of the distribution as a measure of severity.

In contrast to Rennie et al. [9] who fit a generalised Pareto distribution (GPD) to the sum of threshold exceedances, here we fit a four-parameter Beta distribution [32]. For a GPD, assuming the shape parameter is non-negative, the support has no upper bound. In this application the upper bound is finite and known to be equal to the number of stations within the cluster. Since $z_{n,s}$ lies between 0 and 1, the sum across S stations must lie between 0 and S. Therefore, a four parameter Beta distribution, bounded on (0, S) is likely to provide a better fit—see Fig. 13.

The severity of an outlier on day n, θ_n , is therefore given by the CDF of the four parameter Beta distribution:

$$\theta_n = F_{(\alpha, \beta, a, c)}(z_n) = \int_{0}^{z_n} \frac{(q)^{\alpha - 1} (S - q)^{\beta - 1}}{B(\alpha, \beta) S^{\alpha + \beta + 1}} dq,$$
(5)

Table 1 Examples of outlier severities for different days, where arrows indicate positive or negative outliers

Date	Cluster 1	Cluster 2	Cluster 3	
11/01/2017	0.033↓	-	_	
12/01/2017	0.852↑	0.720↑	-	
:	:	:	:	٠.

Table 2 Example of ranked alert list for 30/03/2018

Rank	Severity	Direction of change	Cluster
1	0.892	↑	31104, 31115, 31129, 31217, 31219, 31222,
2	0.828	↑	 32008, 32048
3	0.347	<u>†</u>	31000, 31001, 31002, 31003, 31004, 31005,
:	:	:	:



where $B(\alpha, \beta)$ is the Beta function. This results in an outlier severity, between 0 and 1, for each cluster on each day, as exemplified in Table 1.

We differentiate *positive* and *negative* outliers. Positive outliers are primarily caused by increased usage i.e. where the sum of the functional residual is greater than zero, whereas negative outliers indicate a shortfall in usage.

5.2 Visualising detected outliers for analysts

There are multiple different visualisations that could be used to present the information from Table 1 to analysts. To support on-the-day forecast adjustments, the simplest approach is as a ranked *alert list*, as exemplified by Table 2. By presenting the alert list as a table rather than a visualisation, this gives a clear, prioritised list of tasks to complete. Here, different font styles show where the outlier was detected: Italic indicating the stations where the outlier was detected, and bold indicating other stations in the same cluster likely to be affected. By displaying the severity alongside the ranking, analysts are better able to prioritise their adjustments. For example, an analyst may choose to only adjust the forecasts for the top two outliers in Table 2, as the third has a much lower severity in comparison.

To give a wider view of how outliers have occurred and to account for them in the historic data, the severity per cluster can be visualised in a spatiotemporal heatmap as exemplified in Fig. 14. This figure shows the severity of detected outliers over time for every cluster, where clusters are arranged from left to right by nearest to furthest from the centre of Washington D.C. The order of the clusters along the x-axis could also be arranged to highlight further spatial patterns e.g. from North to South. This type of visualisation can help to identify large-scale patterns in the outliers. For example, knowing for which times of year or days of the week outliers are more likely to be detected can help to steer the attention of analysts. Similarly, dedicated analysts may be assigned to monitor dedicated clusters, and this helps to identify which clusters may need more manual adjustments.

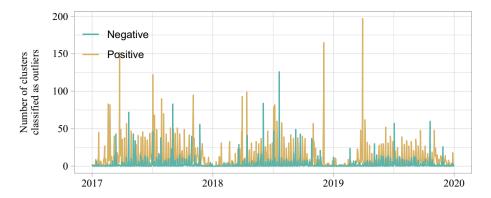
In addition to identifying patterns in Fig. 14, analysts could utilise this figure to find changes in the outlier patterns. For example, changes in the distribution of outliers along the x-axis would suggest a change in the spatial demand pattern, and could indicate a refresh of the clustering process is required. Changes in the distribution of outliers along the y-axis may indicate more or fewer outliers over time or, if the new pattern is regular, suggest that a variable is missing from the demand forecast. Changes in the colour of points may indicate that outliers are becoming more (or less) severe, i.e. demand is becoming less (or more) predictable, which could prompt a review of the forecasting and optimisation approached. For example, it could indicate that a more robust approach to optimisation is required if outliers are occurring more frequently or with higher severity.

Fig. 14 Outlier severity for each cluster between 2017 and 2019. Figure originally included in Rennie [15]





Fig. 15 Positive and negative outliers. Figure originally included in Rennie [15]



6 Discussion

In this section, we discuss patterns in the outliers detected in the Capital Bikeshare data, and suggest potential explanations for their causes.

Figure 15 visualises the number of positive and negative outliers over the days of the time span recorded in the data set. By visualising the positive and negative outliers jointly, analysts can immediately see that (i) negative outliers typically affect far fewer clusters than positive outliers; (ii) the spikes where outlier demand affects a large number of clusters do not occur at the same time for positive and negative outliers; and (iii) the seasonal patterns in the detected outliers are not the same for positive and negative outliers. This can aid analysts in their predictions of outliers: though positive outliers are always more common, the proportion of outliers that are negative changes throughout the year. Though the largest negative outliers occur in summer, the transition between summer and winter seems particularly affected by negative outliers, with May and October exhibiting the highest proportion of negative outliers at around 33%.

The increased occurrence of positive outliers can be explained by the fact that demand is bounded below by zero, and in many cases the mean usage pattern is close to zero, such that negative demand is unobservable. This may motivate a transformation of the data before outlier detection is performed—see Appendix 9.1.4 for further details.

Outliers occur independently in different clusters. In fact, only four days observe outliers in more than 125 of the 195 clusters—one negative and three positive. The three positive outliers occur on 25 March 2017, 3 December 2018, and 30 March 2019. Explanations from events arise for two of these dates: 3 December 2018 relates to the funeral of George H. W. Bush, and a NATO protest occurred in Washington D.C. on 30 March 2019. 25 March 2017 and 30 March 2019 were both warm days, and the last Saturday in March—perhaps suggesting that the definition of *summer* should be from the last Saturday in March, rather than April 1.

IT is interesting to note that the next most widespread positive outlier relates to Independence Day in 2017. Independence Day was detected as a positive outlier in 123, 80, and 35 clusters in 2017, 2018, and 2019. However it was detected as a negative outlier in 46, 47, and 57 stations respectively. The date of the widespread negative outlier is 21 July 2018 which relates to one of the worst storms Washington D.C. has seen. Further discussion of how weather is related to outliers can be found in Sect. 6.2.

6.1 Spatiotemporal patterns in detected outliers

In this section, we analyse the detected outliers and consider spatial and temporal patterns within the outliers.

Temporal patterns Even after accounting for the lower means and reduced inter-daily variance of the winter months, we detect fewer outliers in winter (indicated by the two horizontal white bars in Fig. 14). Otherwise, we find no clear systematic temporal patterns to the detected outliers. Appendix 9.3.1 provides additional discussion on the temporal aspects of the detected outliers, including the visible temporal patterns in the outliers when we fail to account for temporal patterns in the forecasting step.

However, Fig. 16 shows that although outliers can sometimes occur as one-off events, they are also quite likely to occur in temporal clusters. Therefore, once an outlier has been identified, the information can be used to support adjustments to planning in the subsequent days.



Fig. 16 Exemplified severity for outliers detected in one cluster, showing temporal clustering of outliers with each colour representing one of nine clusters, and the potential temporal range of the outlier highlighted in grey. Figure adapted from Rennie [15]

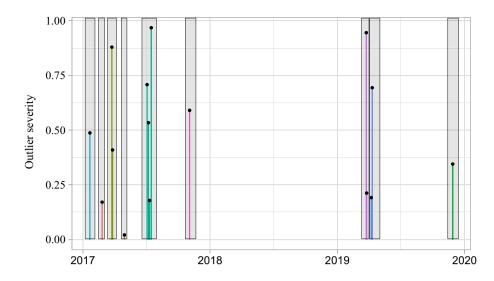


Fig. 17 Two (non-central D.C.) clusters which exhibit higher numbers of outliers. Figure originally included in Rennie [15]

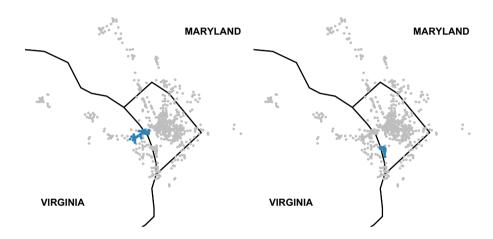
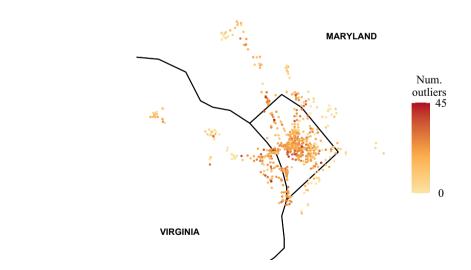


Fig. 18 Number of days each station was classified as an outlier between 2017 and 2019. Figure originally included in Rennie [15]



Spatial patterns Next, we discuss spatial patterns in the detected outliers and consider the relationship between outliers in pick-up and drop-off usage patterns. Figure 14 shows that the cluster which is formed around the centre of Washington D.C. (indicated by the first column on the left) experiences more frequent and higher probability outliers. Otherwise, there is little geographic pattern to how often outliers occur in terms of distance from the centre.



Two other clusters besides the central D.C. cluster exhibit a higher number of outliers with higher severity than other clusters. Figure 14 indicates these by darker vertical lines. These clusters are highlighted in Fig. 17. These clusters are both fairly close to the centre of Washington D.C., and are close by the two main bridges across the Potomac River into the centre. The stations in these clusters are also situated close to The Pentagon, Arlington National Cemetery, and Ronald Reagan Washington National Airport. Therefore these clusters are likely to experience business commuter demand, tourist demand, and potentially also airport travellers i.e. have multiple sources of outlier demand.

We also consider the frequency of outliers on the station level. Figure 18 shows the number of days that each individual station was classified as an outlier between 2017 and 2019. Stations where no outliers were detected are not shown. Outliers are more commonly detected in stations nearer the centre of D.C.

We analyse the differences in the spatial patterns of the outliers detected in pick-up and drop-off usage patterns. For this, we use the clustering based on the overall usage patterns as it allows direct comparison of outliers in different clusters. Subsequently, we apply the outlier detection procedure separately to the pick-up and drop-off usage patterns. This enables us to isolate how the detected outliers and their severities change when the stations in each cluster remain constant. Additional discussion of the spatiotemporal patterns of the outliers can be found in Appendix 9.3, including further visualisations that analysts may use to identify such patterns to aid in decision-making.

To formally compare the output of the outlier detection procedure for pick-up and drop-off usage patterns, we use cosine similarity [33]. That is, the cosine of the angle between two vectors, where 0 represents complete dissimilarity, and 1 complete similarity. Figure 19a provides the cosine similarity between clusters i.e. the cosine similarity of the vector of outlier severities for those detected in pick-up stations over the three year period, and that for drop-off stations.

Figure 19a shows that outliers detected in pick-up and drop-off stations are fairly similar, although this changes depending on the correlation threshold used in the clustering step. As the correlation threshold ranges from 0 to 0.3, the average cosine similarity ranges from 0.69 to 0.44. As the correlation threshold increases, the number of clusters increases. Therefore, when we look at outliers on a small cluster or station level, there is less similarity between pick-ups and drop-offs. However, when the clusters are larger and the outliers aggregated, there is a clearer pattern between pick-ups and drop-offs. Further, this similarity is not uniform across the different clusters - those closer to the centre of D.C. have a higher cosine similarity. That is, the closer a cluster is to the centre of D.C., the more likely it is that if a day is a pick-up station cluster outlier, it will also be a corresponding drop-off station cluster outlier. We did not find any temporal patterns in the comparison of pick-up and drop-off outliers.

6.2 Weather as an explanatory factor for demand outliers

It is widely acknowledged that weather can be used as a predictor for average bike-sharing demand [34]. Therefore, we examine whether extreme temperature or rainfall drive extreme changes in demand i.e. outliers. To that end, we analyse weather data obtained from Visual Crossing [35] and investigate whether weather can be used to explain and eventually predict the outliers in demand. The data is included in Appendix 9.3.2.

Figure 20a shows the proportion of days in each temperature range that have a maximum outlier severity within each severity range. Higher temperatures (between 70 and 90 °F) result in higher severity outliers, indicated by the red region in the top right of Fig. 20a. The red region in the bottom left shows that a high proportion of days with a very low average daily temperatures (\leq 25 °F) are classified as outliers. However, these outliers typically have a low severity. This

Fig. 19 Cosine similarity between outliers detected in pick-up and drop-off usage patterns under different correlation thresholds. Figure originally included in Rennie [15]

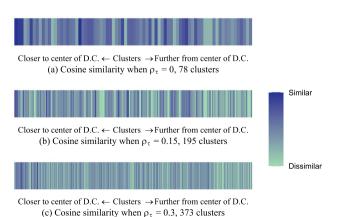
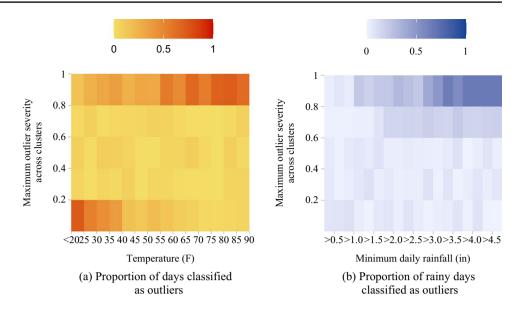




Fig. 20 Severity of outliers at different temperatures and precipitation levels. Figure originally included in [15]



can be explained by these outliers being negative demand outliers—and low temperatures typically occur in winter, when demand is already low.

In addition to temperature, we also expect precipitation levels to affect demand for bike-sharing. As we expect increased rainfall to have a negative impact of usage, we consider only the severity of negative demand outliers here. Figure 20b shows the proportion of days with a minimal level of precipitation which were classified as outliers with some severity. Higher rainfall generally results in higher likelihood of the day being classed as a negative demand outlier. When precipitation levels are especially high, the outliers that are detected also tend to have higher severities.

There are likely many other factors which cause and influence outlier demand in the Capital Bikeshare network. For example, Ma et al. [17] have previously linked usage of bike-sharing stations to usage of Metrorail services. We anticipate that cancellations, or short-term changes to Metrorail services may also generate outlier demand for bike-sharing. However, due to lack of available of data on such cancellations, we leave this to future research.

7 Conclusion

In this paper, we identified temporal patterns in the Capital Bikeshare data set and applied a combination of functional regression and temporal partitioning to remove such trends and obtain a homogeneous data set. We also accounted for spatial patterns in temporal usage by clustering together similar stations. By basing our clustering algorithm on a combination of geographical knowledge, and similarity of usage patterns, we were able to identify how usage changes as stations get further away from the city centre. Throughout this paper, we have presented visualisations to illustrate our findings and provided detailed descriptions of how such visualisations may be used by analysts to aid in their decision making.

Our in-depth study of detected outliers showed that not all stations are equally prone to outliers—those closest to the centre of D.C. exhibit far more outlying demand. This is also true for known outlier days e.g. national holidays such as July 4, where some clusters of stations exhibit increased demand and others decreased. For forecasting and planning purposes, this knowledge is highly important since outlier demand changes not only the magnitude of demand, but also the spatial distribution of where customers go. In terms of rebalancing bikes at stations, this could have a large impact on the efficiency of the schedule. Further, we also showed that outliers are more likely to occur in the summer months (even after accounting for increased usage and usage variability), suggesting rebalancing needs to be more reactive in the summer months.

Our analysis of weather patterns showed that outliers are more likely to occur when the weather conditions are more extreme. Both temperature and precipitation were found to have an impact on demand—with excessively high precipitation or very low temperatures causing negative demand outliers, and high temperatures causing positive demand outliers.



Further research is needed to evaluate the effects that identifying and correcting for outliers may have on revenue and planning in the bike-sharing domain. This could include considering the impact of forecast accuracy on re-allocation and revenue, and the cost-benefit relationship that may result from making a change to the forecast to account for outlier demand. The method outlined in this paper could be used to generate an outlier *alert*, to notify Capital Bikeshare when the rebalancing policy for a given day is non-optimal. Online detection of outlier demand would allow re-allocation of bikes during the day and, as such, further analysis of how these alerts could be deployed in an automated system, and how they may affect the complexity of the routing problem, is needed.

A further extension could consider how outlier detection may be applied to dockless bike-sharing systems—where users may pick-up or drop-off a bike anywhere rather than at dedicated stations. Similar methodology could be applied in this case, though an additional pre-processing step would be required—where regions are defined. All pick-ups or drop-offs within a single region would then be treated in the same way as a single station. These regions may be defined based on knowledge of the underlying city geography, or by applying spatial clustering methods.

Author contributions All authors discussed the manuscript idea and research decisions. NR performed the data analysis documented in the text. NR wrote the main manuscript text and prepared the figures. All authors reviewed and edited the manuscript. All authors jointly worked on the revision, with NR focusing on the figures and data analysis. All authors read and approved the final manuscript.

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Data availability The datasets analysed during this study are available from Capital Bikeshare in a public repository that does not issue datasets with DOIs at s3.amazonaws.com/capitalbikeshare-data/index.html. Further information on any pre-processing performed by Capital Bikeshare is available at ride.capitalbikeshare.com/system-data, and the license agreement at ride.capitalbikeshare.com/data-license-agreement. The paper at hand was included as Chapter 4 in the doctoral thesis [15]. The figures within this paper are also included in, or adapted from Rennie [15].

Declarations

Competing interests The authors declare no competing interests.

Appendix

Forecasting baseline demand

Temporal partitioning

In Sect. 3, for the purposes of temporal partitioning of data, we define summer to be the months April through October. Winter is therefore November through March. The partitioning is chosen to give constant variance within a partition whilst also ensuring there is a sufficient number of observations within each partition to make outlier detection feasible. Figure 21 shows the rolling daily variance for station 31203, with the summer months highlighted.

The variance of winter is not constant, being slightly higher in the months that border the summer season. Further partitioning could be carried out e.g. partition by month. However, this results in much less data within each partition, which then makes outlier detection more difficult. When applying binary segmentation changepoint detection [36] to identify the partitions with different levels of variance, the algorithm returns 8 changepoints: 24 March 2017,

Fig. 21 Variance of usage patterns with summer months highlighted in green. Figure originally included in Rennie [15]

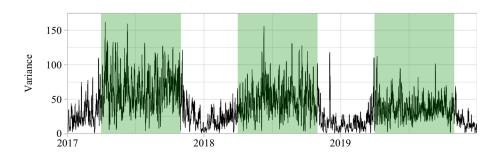
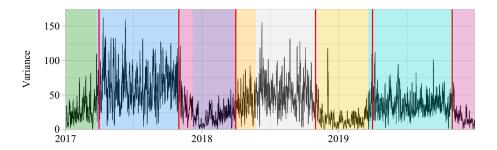




Fig. 22 Changepoints in variance of usage patterns. Figure originally included in Rennie [15]



4 Nov 2017, 6 Dec 2017, 31 Mar 2018, 24 May 2018, 4 Nov 2018, 20 Mar 2019, and 4 Nov 2019. These are highlighted in Fig. 22. These are relatively close to our pre-defined summer and winter partitions (indicated by red vertical lines in Fig. 22.

If there are already pre-defined seasons in use for planning purposes, these may be more appropriate.

Functional regression model comparison

In this section, we perform model comparison for the functional regression model used to account for different daily trends as detailed in Sect. 3, Eq. 1.

We use the *Cross-Validated Mean Integrated Squared Error* (CV-MSE) to determine the best-fitting model. The CV-MSE is given by:

$$CV - MSE = \frac{1}{N} \sum_{n=1}^{N} \int (x_{n,s}(t) - \hat{x}_{n,s}(t)) dt,$$
(6)

where $\hat{x}_{n,s}(t)$ is the prediction for the nth daily rental pattern at the station s, under the model fitted to all but the nth rental pattern. The model which produces the lowest CV-MSE is chosen as the best fitting. Unlike other model selection criterion such AIC, CV-MSE does not take into account the number of parameters. The CV-MSE for each of the 8 models considered is shown in Table 3, for the stations in the cluster discussed in Sect. 5.

In most cases, the model which achieves the minimum mean squared error is model 8, which includes all three factors (day, week, and year). However, model 5 (day and month) also produces very similar results.

Distribution of residuals

Figure 23 shows the distribution of the residuals for each hour of the day for station 31005—see also Fig. 5. The core of the distribution is symmetric around zero, but the tails of the distribution are positively skewed.

Table 3 Cross validated mean square error for functional regression model comparison applied to unpartitioned data, with bold text highlighting best performing model

Model	Factors		Station Number									
	Day	Month	Year	31303	31308	31309	31315	31316	31317	31319	32014	32040
1				135.90	72.98	16.04	25.80	15.29	27.96	34.27	52.42	22.75
2	✓			120.38	60.17	16.04	25.64	14.29	27.71	33.43	50.80	22.78
3		1		98.01	59.65	12.67	18.82	11.93	19.57	25.78	37.97	17.09
4			✓	133.96	71.89	15.49	25.70	14.86	28.03	33.97	48.01	22.63
5	✓	1		82.40	46.50	12.61	18.65	10.83	19.20	24.80	36.07	17.01
6		1	✓	96.59	58.52	12.07	18.79	11.52	19.61	25.44	33.34	16.95
7	✓		✓	119.04	59.02	15.47	25.63	13.87	27.77	33.13	46.28	22.66
8	✓	1	✓	80.85	45.29	12.00	18.62	10.39	19.23	24.46	31.32	16.87



Fig. 23 Distribution of residual usage for each hour of the day for station 31005

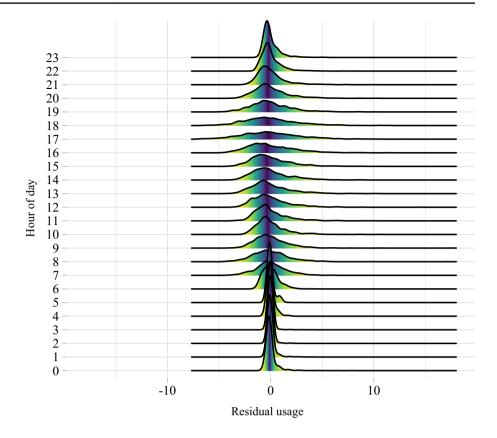


Fig. 24 Distribution of skewness of distributions of total daily usage across all stations

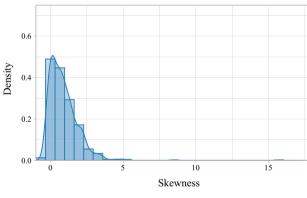


Fig. 25 Distribution of total daily usage for station 31235. Figure originally included in Rennie [15]

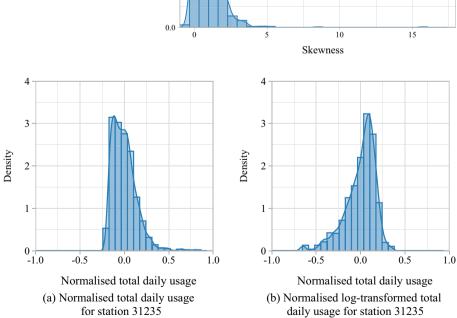
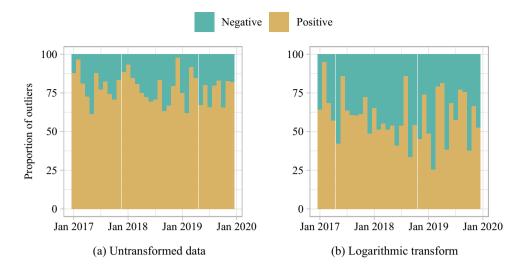




Fig. 26 Fraction of outliers that are positive and negative, before and after applying a logarithmic transformation. Figure originally included in Rennie [15]



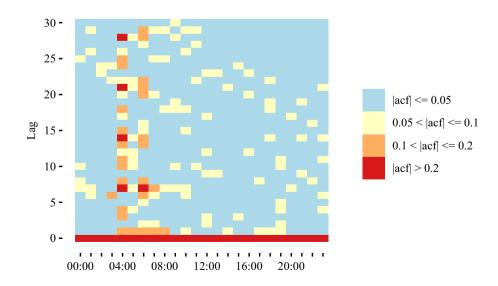
Accounting for skewness

Figure 25a shows the distribution of the normalised total daily usage for station 31235, which exhibits positive skew. Not all stations exhibit such positively skewed distributions—see Fig. 24.

The distributions of total daily usage have a skewness lying between – 0.4 and 15.8, with the median skewness across all stations being 0.71. Larger positive skew is more common in stations where mean usage is very low, and since demand is bounded below by zero, only increases in demand are observed. This results in more *positive* outliers than *negative* (see Sect. 6). Given that most stations exhibit slight positive skew, it may be desirable to transform the data before perfroming outlier detection. To account for the skew, the rental patterns can first be transformed e.g. with a logarithmic transform. However, this is not applicable to all stations (as some are already negatively skewed) and can result in a negatively skewed distribution—Fig. 25b.

When applying the outlier detection procedure to the untransformed data, the fraction of positive outliers is consistently higher than the fraction of negative outliers. On average, 78% of outliers are positive. That is, outliers are more likely to be caused by increased demand than decreased. This is easily explained by the fact that demand is bounded below by zero, and in many cases the mean usage pattern is close to zero, such that negative demand is unobservable. Applying a logarithmic transformation before carrying out the outlier detection results in around 60% of outliers being positive (Fig. 26).

Fig. 27 Inter-daily autocorrelations of residuals for station 31005. Figure originally included in [15]





Inter-daily autocorrelation

Figure 27 shows the inter-daily autocorrelations between the residual patterns for different days, at each hour. The early hours of the morning—especially at 04:00 and 06:00—exhibit some autocorrelation of lag 7 i.e. weekly. A functional ARIMA model could be fitted to remove the autocorrelation. However, as it only affects a so few hours of the day, we do not investigate this further here.

Using spatial patterns to cluster stations

Effect of parameter choices on clustering

Our clustering method is tuned using four parameters: the correlation threshold ρ , as well as distance metrics introduced in Sect. 4. We now evaluate the sensitivity of changing these parameters on (i) the number of clusters obtained, and (ii) the standard deviation in cluster sizes (SDCS) [37]. The SDCS is given by:

$$SDCS = \sqrt{\frac{1}{K-1} \sum_{k=1}^{K} \left(S_k - \frac{S}{K} \right)^2},\tag{7}$$

where S is the number of stations, K is the number of clusters, S_k is the number of stations in cluster k. The SDCS quantifies a measure of the balance of the different cluster sizes. We do not seek to minimise nor maximise the SDCS—since choosing extreme parameter values trivially creates clusters of size 1 or one giant cluster.

Figure 28 shows the change in number of clusters and SDCS as we vary parameter values. There is an inverse relationship between the number of clusters and the SDCS across all four variables. While an increase in either correlation

Fig. 28 Cluster sensitivity to parameter changes when other parameters remain fixed at ρ_r =0.15, R = 5000 m, D_{imner} = 500 m, and D_{outer} = 1000 m. Figure originally included in Rennie [15]

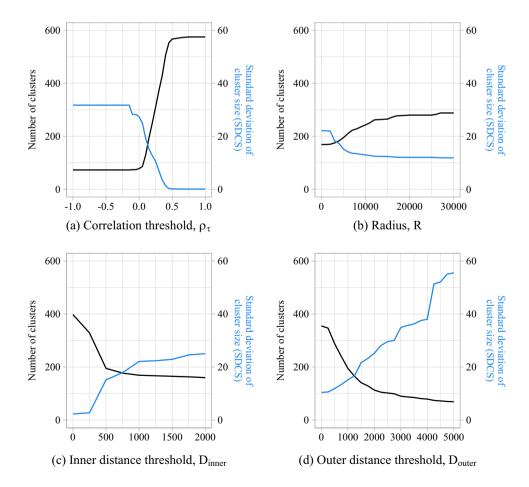
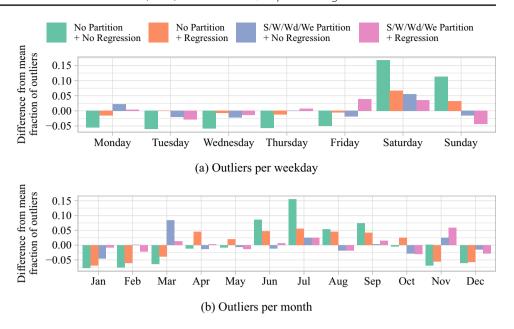




Fig. 29 Fraction of outliers occurring on each day of the week and month of the year, with and without applying functional regression model. Figure originally included in Rennie [15]



threshold or radius results in a decrease of SDCS, increasing either of the distance thresholds increases the SDCS. In order to achieve a balance between number of clusters and SDCS, we choose parameter values close to the intersection of the two lines. This results in a correlation threshold of between 0 and 0.4; a radius between 5000 m and 10,000 m; an inner distance threshold between 500 m and 1000 m, and an outer distance threshold of approximately 1000 m.

Normalised mutual information

For a graph containing M stations, the mutual information between two clusterings \mathscr{A} and \mathscr{B} of the M nodes in the graph is defined as:

$$I(\mathcal{A}, \mathcal{B}) = \sum_{a=1}^{|\mathcal{A}|} \sum_{b=1}^{|\mathcal{B}|} \frac{|\mathcal{A} \cap \mathcal{B}|}{M} \log \left(|\mathcal{A} \cap \mathcal{B}| \frac{M}{M_a M_b} \right), \tag{8}$$

where M_a is the number of nodes in the a^{th} cluster of clustering \mathscr{A} , and similarly for M_b . The normalised mutual information (NMI) between two clusterings is defined as [30]:

$$NMI(\mathscr{A},\mathscr{B}) = \frac{2I(\mathscr{A},\mathscr{B})}{H(\mathscr{A}) + H(\mathscr{B})},\tag{9}$$

where $H(\mathcal{A})$ is the entropy (a measure of uncertainty) defined as:

$$H(\mathscr{A}) = -\sum_{a=1}^{|\mathscr{A}|} \frac{M_a}{M} \log\left(\frac{M_a}{M}\right). \tag{10}$$

 $NMI(\mathcal{A}, \mathcal{B}) = 1$ if \mathcal{A} and \mathcal{B} are identical, and 0 if they are completely different.

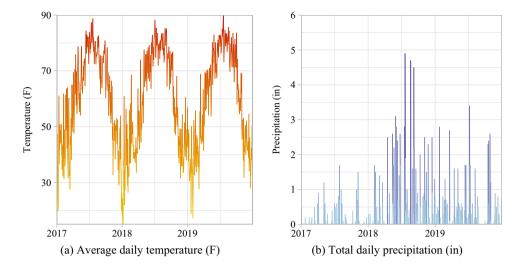
Additional discussion

Effects of data temporal patterns on outlier detection

In Sect. 3, we outlined two steps (functional regression and temporal partitioning) that could be undertaken to account for different patterns in the data. Here, we consider how the inclusion of these steps affects the outcome of the outlier detection. For a homogeneous data set, we would expect approximately equal numbers of outliers detected on each day of the week, and month of the year. Figure 29 shows the difference between the mean fraction of outliers per day (or month) and fraction of outliers which are observed on each day of the week (or month).



Fig. 30 Weather data obtained from Visual Crossing for 2017–2019. Figure originally included in Rennie [15]



The results are shown for the case where the (i) there is no accounting for temporal patterns; (ii) the regression model is applied with no partitioning; (iii) only partitioning is applied with no regression, and (iv) both regression and partitioning is applied. When we do not account for temporal patterns in the data, we detect far more outliers on weekends and in the summer months. Including the regression step (without partitioning) improves this imbalance somewhat. When the data has been partitioned, regression makes little difference to the proportion of outliers detected on each day or month. Although we partition the data to account for different variance, this implicitly takes care of differences in mean between the same groups. As there is little difference in mean trend between days or months in the same groups. partitioning with or without regression gives similar results.

Weather as an explanatory factor for demand outliers

Figure 30 shows the weather data used for analysis in Sect. 6.2.

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