Data Analysis with the Morse-Smale Complex: 
The msr Package for R

Samuel Gerber
SCI Institute, University of Utah

Kristin Potter
SCI Institute, University of Utah

Abstract

In many areas, scientists deal with increasingly high-dimensional data sets. An important aspect for these scientists is to gain a qualitative understanding of the process or system from which the data is gathered. Often, both input variables and an outcome are observed and the data can be characterized as a sample from a high-dimensional scalar function. This work presents the R package msr for exploratory data analysis of multivariate scalar functions based on the Morse-Smale complex. The Morse-Smale complex provides a topologically meaningful decomposition of the domain. The msr package implements a discrete approximation of the Morse-Smale complex for data sets. In previous work this approximation has been exploited for visualization and partition-based regression, which are both supported in the msr package. The visualization combines the Morse-Smale complex with dimension-reduction techniques for a visual summary representation that serves as a guide for interactive exploration of the high-dimensional function. In a similar fashion, the regression employs a combination of linear models based on the Morse-Smale decomposition of the domain. This regression approach yields topologically accurate estimates and facilitates interpretation of general trends and statistical comparisons between partitions. In this manner, the msr package supports high-dimensional data understanding and exploration through the Morse-Smale complex.

Keywords: Morse-Smale complex, visualization, exploratory data analysis, regression, high-dimensional data.

1. Introduction

Recent advances in computational topology have led to a multitude of algorithms to estimate the topological properties of a function from a finite sample (van Kreveld et al. 1997; Edelsbrunner et al. 2003; Carr et al. 2003; Gyulassy et al. 2007). These algorithms led to the analysis of data sets based on their topological properties and have shown promising re-
sults in a wide variety of applications, including combustion simulations (Bremer et al. 2010; Mascarenhas et al. 2010), fluid dynamics (Laney et al. 2006), climate simulations (Gerber et al. 2010), protein folding (Weber et al. 2007) and molecular shape analysis (Cazals et al. 2003).

This paper describes the R (R Development Core Team 2010) package msr (Gerber et al. 2011a) for data analysis with the Morse-Smale complex. The Morse-Smale complex provides a topologically meaningful decomposition of the domain of a scalar function. The basic functionality of this package rests on the computation of the Morse-Smale complex from unorganized scattered data. The domain decomposition induced by the Morse-Smale complex is used to build the exploratory visualization technique described in (Gerber et al. 2010) and the regression approach in (Gerber et al. 2011b).

Gerber et al. (2010) exploit the Morse-Smale complex decomposition to form abstract two-dimensional representations of high dimensional scalar functions. These representations present high-level summaries of the salient features of the functions and form the scaffolding for an exploratory data analysis tool. In regression, domain decompositions have been used successfully to build flexible non-parametric models such as regression trees (Breiman et al. 1984), MARS (Friedman 1991) and variations on those approaches (Chaudhuri et al. 1994; Alexander and Grimshaw 1996). These partition-based regression methods split the domain recursively into smaller partitions with low-order parametric models in each partition. The recursive partitioning is based on splitting rules that typically measure the quality of the resulting fit. In a similar fashion, Gerber et al. (2011b) use the domain of the Morse-Smale complex as the splitting rule for a partition-based regression scheme.

To take full advantage of the package presented in this paper, a high-level understanding of the properties of the Morse-Smale complex is necessary. Thus, a brief overview of the Morse-Smale complex, and some issues involving its discrete approximation, is included in this paper. For completeness, the visualization and regression techniques in Gerber et al. (2010) and Gerber et al. (2011b) are summarized.

2. The Morse-Smale complex

In Morse theory, the Morse-Smale complex provides a tool to examine the topology of a manifold $M$ based on the critical points of a function $f$ defined on $M$. Here, the interest is not on the topology of $M$ but on the exploitation of the Morse-Smale complex to glean information about the geometry of the function $f$ itself.

Informally, the Morse-Smale complex partitions the domain of a function $f$ based on the critical points of $f$. The interior of each partition is a monotonic region, i.e. contains no critical points, with a single local minimum and maximum on the boundary, as illustrated in Figure 1.

2.1. Formal definition

Let $M$ be a smooth, compact, $p$-dimensional manifold. A smooth function $f : M \rightarrow \mathbb{R}$ is Morse if, for all critical points $x$ of $f$, the Hessian matrix $Hf(x)$ is not singular. An integral line, $\lambda : \mathbb{R} \rightarrow M$, is a curve in $M$ with $\frac{d\lambda}{ds}(s) = \nabla f(\lambda(s))$, with $\alpha(\lambda) = \lim_{s \to -\infty} \lambda(s)$ and $\omega(\lambda) = \lim_{s \to \infty} \lambda(s)$. Note, $\alpha(\lambda)$ and $\omega(\lambda)$ are both, by definition, critical points of $f$. Define the ascending and descending, also referred to as stable and unstable, manifolds of a critical
Figure 1: A two-dimensional scalar function (a) and the corresponding Morse-Smale complex (b). The Morse-Smale complex induces a segmentation of the function into monotonic regions using gradient flows with a single local minimum and maximum.

point $x$ as $A(x) = \{\lambda : \alpha(\lambda) = x\}$ and $D(x) = \{\lambda : \omega(\lambda) = x\}$. A Morse function $f$ is Morse-Smale if the ascending and descending manifolds only intersect transversely. The Morse-Smale complex is the set of intersections, $A(x_i) \cap D(x_j)$, over all combinations of critical points $(x_i, x_j)$. The Morse-Smale complex includes regions (i.e., sub-manifolds of $M$) of dimensions 0 through $p$ and partitions $\mathcal{M}$. The 0 through $p-1$ dimensional components of the Morse-Smale complex delineate the boundaries of the $p$-dimensional regions.

2.2. Persistence

The Morse-Smale complex introduces a measure of the significance of each extremal point, called persistence. Persistence is a measure of the amount of change in the function $f$ required to remove a critical point, and thus, to merge two or more partitions. Note, persistence describes the significance of an extremal point in geometric terms and not in the statistical sense of a hypothesis test. Figure 2 illustrates the concept of persistence simplification on a one-dimensional function.

**Definition** Let $x_i$ be the critical points of $f$. Define $s(x_i)$ as the set of critical points that have a direct integral line connecting to $x_i$. Let $n(x_i) = \arg\min_{x_j \in s(x_i)} ||f(x_i) - f(x_j)||$, the persistence of a critical point $x_i$ is then defined as $p(x_i) = ||f(x_i) - f(n(x_i))||$. This definition is motivated by the amount of change of $f$ in $L_{\infty}$ required such that the critical point pair $(x_i, n(x_i))$ is either canceled or merged into a single critical point. Recursively removing the critical point with minimal persistence leads to a nested series of successively simplified Morse-Smale complicies, also called a filtration (Edelsbrunner et al. 2006; Chazal et al. 2009). At each level, some of the partitions induced by the Morse-Smale complex are merged into a single partition until the Morse-Smale partitioning consists of only a single partition (i.e., the
The sequential simplification by persistence leads to a hierarchy of Morse-Smale complexes. At the highest persistence level, the Morse-Smale complex only consists of the highest maximum and lowest minimum, and the segmentation corresponds to the entire domain. With decreasing persistence levels, more extremal points and corresponding partitions are introduced in order of their persistence level. Thus, persistence introduces a notion of scale at which the Morse-Smale complex of $f$ is considered.

### 2.3. Morse-Smale complex approximation

The definition of the Morse-Smale complex, in terms of ascending and descending manifolds, leads to a direct algorithm. Given a set of observations $O = \{y_i, x_i\}_{i=1}^N$ with $y_i = f(x_i)$, determine, for each data point $x_i$, its $\alpha$- and $\omega$-limit and corresponding partition by following the gradient at $x_i$. A direct approach would require the estimation of the gradient at $x_i$, and to trace the integral line that passes through it. This would require essentially an estimate of $f$. However, the only information required to partition the domain is the $\alpha$- and $\omega$-limit of the integral line, which is computed using a discrete approximation of the integral line without having to first estimate $f$.

Note, that the 0 through $p - 1$ dimensional components have measure zero. Thus, in practice, the points of a data set are, with probability one, part of the $p$-dimensional components of the Morse-Smale complex with integral lines ending in local minima and maxima.

In *Gerber et al. (2010)*, the domain is approximated via a $k$ nearest-neighbor graph. The algorithm follows paths of steepest ascent and descent based on the connectivity of the graph; essentially a variant of the quick shift algorithm (*Vedaldi and Soatto 2008*). For such an algorithm, let the adjacencies of point $x_i$ be $\text{adj}(x_i) = \{x_j : x_i \in \text{knn}(x_j), x_j \in \text{knn}(x_i)\}$. Then the approximate integral line is traced out by following the path of steepest ascent $p_a(x_i) = \arg\max_{x_j \in \text{adj}(x_i)} f(x_j) - f(x_i)$ and descent $p_d(x_i) = \arg\max_{x_j \in \text{adj}(x_i)} f(x_i) - f(x_j)$, with $p_a(x_i) = x_i$ and $p_d(x_i) = x_i$ if all neighbors have lower/higher function value (i.e., a local maxima/minima). This assigns each point to a $p$-dimensional component, identified
by local minima/maxima association, of the Morse-Smale complex. Hence, the Morse-Smale approximation results in a partition \( C = \{C_1, \ldots, C_n\} \), with \( C_i \) the set of points for partition \( i \), such that \( \bigcup_i C_i = \{x_i\}^n \) and \( C_j \cap C_i = \emptyset \forall i \neq j \).

For computing the persistence-based hierarchy of the Morse-Smale complex, an approximation of saddle point values between neighboring partitions is required. Let \( s(p_a, p_b) \) be the set of edges \( (x_i, x_j) \) such that \( x_i \) is assigned to partition \( p_a \) and \( x_j \) to \( p_b \). Then, the persistence of the minima \( a_{\text{min}} \) of partition \( p_a \) is defined as \( \min_{k \in P(X)} \min_{e \in s(p_a, p_k)} \max_{x_i \in e} \|a_{\text{min}} - x_i\| \). Again, as in the continuous case, this is recursively applied with \( \overline{P}(X) \), the minimal persistence extrema, removed.

Depending on the number of nearest neighbors and sampling density, artificial extremal points can be introduced or true extremal points can be removed. Artificial extremal points are introduced if the k-nearest neighbors of a point connect only to points with lower function values. True maxima (or minima) can be removed if the k-nearest neighbors graph introduce a monotonous steepest ascent (or descent) path\(^1\) to another maxima (minima) point. This arises mostly in the case of a large number of nearest neighbors, and/or a sparse sample of the domain.

### 2.4. Partition prediction

The Morse-Smale complex approximation provides the partition assignments, or labels, for the input data, but not the complete domain. In Gerber et al. (2011b), two approaches to extend this partitioning to the complete domain are considered.

The first approach estimates the probability distribution \( P(X|C = C_i) \) with a kernel density estimator over the observations \( s \) in partition \( i \):

\[
p_i(x) = \frac{1}{\|C_i\|} \sum_{s \in C_i} K(x, s).
\]

From this, Bayes Theorem yields the partition probabilities \( P(C = C_i|X = x) = \frac{p_i(x)P(C=C_i)}{\sum_j p_j(x)P(C=C_j)} \) with \( P(C = C_i) = \frac{\|C_i\|}{\sum_j \|C_j\|} \).

The second approach employs a support vector machine (SVM) to build a multi-class classifier using the one-against-one approach described in Hsu and Lin (2002). The SVM is trained on the partition assignments of the Morse-Smale complex. To estimate partition probabilities from the classifier, a logistic regression is fit to the decision values of the SVM as described in Platt (1999).

### 3. The Morse-Smale complex for scalar function visualization

In Gerber et al. (2010) the Morse-Smale complex is used to build a summary representation of the high-dimensional scalar function \( f : \Omega \rightarrow \mathbb{R} \), with \( \Omega \) a compact connected subset of \( \mathbb{R}^n \). Each partition \( C_i \) of the Morse-Smale complex is summarized by an inverse regression curve, \( r_i(y) = E[X \in C_i|Y = y] \). The regression estimates approximate a graph of curves connecting the minima and maxima as identified by the Morse-Smale segmentation; essentially

\(^1\)strictly positive or negative difference between neighboring points along the path
a compressed representation of the domain. For visualization, the extremal points are projected, using principal components, into two-dimensions (2D). Then, each regression curve is separately projected into 2D, again using principal components. Finally, the projected curves are affine-transformed such that the end points match the corresponding projected extremal points. This concept is illustrated in Figure 3.

The visualization created by this method can help to gain a qualitative understanding of higher dimensional functions. In Gerber et al. (2010) this exploratory analysis approach is demonstrated on

- climate simulations outcomes.
- chemical compositions in combustion simulations.
- concrete mixture strengths.
- socio-economic variables in relation to crime rates.

![Figure 3: Schematic illustration of the visualization: the two-dimensional scalar function is decomposed into piecewise monotonic partitions by the Morse-Smale complex. The function is then represented by a network of regression curves. Each curve summarizes the domain of a partition with \( r_i = E[X \in C_i | y = y] \). For visualization of higher dimensional functions, this network is embedded into 2D.](image)

The approach consists of three steps to arrive at a 2D representation for visualization of the high-dimensional scalar function:

1. **Morse-Smale approximation**: Compute a segmentation using the Morse-Smale approximation of \( f \).
2. **Geometric summaries**: Construct regression curves \( r_i \) with kernel regression.
3. **Dimension reduction**: Embed the regression curves in 2D using a three-step dimension-reduction approach:
i. Project extremal points onto its first two principal components.

ii. Project each regression curve onto its first two principal components.

iii. Affine-transform projected curves to match the corresponding projected extremal points.

4. Morse-Smale regression

The idea presented in Gerber et al. (2011b) is to use the Morse-Smale complex induced segmentation of the domain of a function $f : \Omega \rightarrow \mathbb{R}$ to combine simple linear models within each partition to approximate the underlying function $f$. Two approaches are considered. First, a piecewise linear model

$$\hat{f}_l(x) = a_j + b_j x \quad \text{if } x \in C_j, \ j=1, \ldots, k.$$  

(2)

Second, a sum of weighted linear models, with weights based on the probabilistic interpretation of the segmentation induced by the Morse-Smale complex, i.e., a soft assignment of each point based on the partition probabilities.

$$\hat{f}_w(x) = \sum_{j=1}^{k} w_j(x)(a_j + b_j x)$$  

(3)

with $w_j(x) = P(C = C_i|X = x)$ estimated as described in Section 2.4.

5. Package description

The methods for approximating the Morse-Smale complex from a sample of a scalar function form the basis of the msr package (Gerber et al. 2011a). The regression and visualization approaches are built on this basic functionality. This section gives a brief overview of the package. Detailed descriptions of the available methods are in the manual pages contained in the package.

5.1. Morse-Smale complex approximation

The main functions for the Morse-Smale approximation is msc.nn. The functions msc.nn.kd and msc.nn.svm add predictive capacity to msc.nn by estimating the partition probabilities with the kernel density estimation or a multi-class SVM, respectively (see Section 2.4). All these methods return a basic Morse-Smale complex object msc.nn (potentially supplemented with predictive capabilities), which is the basic input for the regression and visualization methods.

The nearest neighbor graph is computed using the approximate nearest neighbor library ANN (Mount and Arya 2010). For performance, the kernel density estimation is implemented in C with an interface to R. For the SVM multi-class classifier the R package e1071 (Dimitriadou et al. 2010) is used, which provides an interface to the C++ library libsvm (Chang and Lin 2001).
For both `msc.nn.kd` and `msc.nn.svm`, the generic R method `predict` is implemented and returns a matrix with partition probabilities for each point, either of the original data `x` or, if the argument `newdata` is specified, for the locations of the new observations. Two additional utility functions are supplied:

- `msc.level.ind` extracts the indices into the original, supplied data `x` for a given partition index, Morse-Smale complex, and persistence level.
- `msc.sublevels` extracts a subset of the hierarchy of Morse-Smale complexes.

### 5.2. Visualization

The visualization functionality is accessed through `plot.msc`. This function takes in an `msc.nn` object, computes the necessary geometry for the plots, and creates the visualization. The package `rgl` Adler and Murdoch (2010) is used for three-dimensional display, and user interaction through mouse clicks bring up detailed 2D plots of the inverse regression curves. The plotting function returns an object that allows the user to modify what is displayed in the `rgl` device, such as the optional display of the standard deviation tubes, or the 3D axis.

![Figure 4: Visual summary representation from 2000 observations of the function in Figure 1. The regression curves for each partition are projected into 2D with the 3rd dimension encoding the function value. The function value is redundantly encoded using a colormap. The standard deviation of the regression curve is displayed by the opaque tube surrounding the curve.](image)

The visualization displays the graph of the regression curves in 3D. The regression curves are projected into 2D and the 3rd dimension is used to encode the function value, also redundantly encoded with a colormap. While color provides a quick overview of the location of minima and maxima, the 3rd dimension can be used to better perceive quantitative differences in minima and maxima and helps to visualize the function as a height field over the graph representation of the domain.
Opaque tubes surrounding the curves encode the standard deviation of the regression curves by mapping to the radius of the tubes. The standard deviation provides information about the shape of a partition, i.e. the extent of the level sets.

Figure 4 shows the use of the 3rd dimension as well as the standard deviation tubes, which can be turned on or off through a user parameter. In addition, the user can inspect the behavior of the independent variables in each partition by clicking on the corresponding regression curve which then highlights that curve in an identifying color in a corresponding 2D graph, as shown in Figure 5, left. A separate graphics device is then opened, and plots the regression curve \( r_i(y) = E[X \in C_i | Y = y] \) with \( d \) graphs of \( y \) as a function of \( r_i(y) \) for each dependent variable in \( X \) (Figure 5, right). To compare various partitions simultaneously, the user can select multiple curves, which are displayed in the same plot using the matching color from the main display.

![Figure 5: The interactive visualization of the data set from Figure 1. (Left) The user is presented with the visual summary and can select curves of interest (highlighted in red, green, purple and blue). (Right) These curves, representing independent variables, are then plotted side-by-side.](image)

### 5.3. Regression

The piecewise linear model for the Morse-Smale regression is implemented in the two methods:

- msc.lm: The piecewise linear model.
- msc.elnet: The piecewise linear model with \( L_1 \) regularization using the package glmnet (Friedman et al. 2010).

and for the weighted linear model:

- msc.slm: The weighted linear model.
- msc.slm.elnet: The weighted linear model with \( L_1 \) regularization using the package glmnet (Friedman et al. 2010).
The methods take as input a Morse-Smale complex object and additional parameters that influence the fitting.

6. A complete tour

This section gives a complete tour of the package on a simple 2D function, for which it is easy to show visual results for all aspects of the package. The tour is based on the 2D function shown in Figure 1, which is defined by

\[
f(x) = \frac{1}{2} \left( e^{-\left(x_1 - \frac{1}{4}\right)^2/0.3^2} + e^{-\left(x_2 - \frac{1}{4}\right)^2/0.3^2} + e^{-\left(x_1 - \frac{3}{4}\right)^2/0.1^2} + e^{-\left(x_2 - \frac{3}{4}\right)^2/0.1^2} \right) .
\]

6.1. Morse-Smale complex construction and partition prediction

Create 2000 observations from \( f \), uniformly distributed on \([0, 1]^2\) (scaled to \([0, 1]\) for color-mapping).

```R
R> library(msr)
R> data(fourpeaks)
R> d <- fourpeaks(2000)
R> d[, 1] <- (d[, 1] - min(d[, 1]))/(max(d[, 1]) - min(d[, 1]))
```

and compute the Morse-Smale complex at persistence level 0.1 with 15 nearest neighbors.

```R
R> ms <- msc.nn(y = d[, 1], x = d[, 2:3], pLevel = 0.1, knn = 15)
R> summary(ms)
```

Plot the function and the segmentation induced by the Morse-Smale complex in 2D.

```R
R> par(mfcol = c(1, 2))
R> fancy <- c("#0066CC", "#CCCC00", "#D22905")
R> colormap = colorRamp(fancy, interpolate = "linear", bias = 0.5)
R> colors <- rgb(colormap(d[, 1]), maxColorValue = 255)
R> par(mar = c(8, 5, 5, 4))
R> plot(d[, 2], d[, 3], type = "p", xlab = "", ylab = "", col = colors,
+     pch = 19, cex.axis = 2.5)
R> pal <- brewer.pal(9, "Set1")
R> pal <- colorRampPalette(pal)
R> pal <- pal(length(ms$level[[1]]$mins))
R> colors <- pal[ms$level[[1]]$partition]
R> par(mar = c(8, 5, 5, 4))
R> plot(d[, 2], d[, 3], col = colors, type = "p", xlab = "", ylab = "",
+     pch = 19, cex.axis = 2.5)
```
Show the number of extrema as a function of persistence.

```r
c> np <- length(ms$persistence)
c> ms$persistence[np] <- 1
c> par(mar = c(6, 4, 4, 4) + 3)
c> plot(ms$persistence, np:1 + 1, xlab = "Persistence Percentage",
c>       ylab = "Extrema", cex = 2, cex.lab = 2, cex.axis = 2, type = "p",
c>       pch = 19)
```

The persistence is expressed as a percentage of the function range. Note, that `persistence` always contains the complete persistence hierarchy, even if only a subset of the complete Morse-Smale complex persistence hierarchy is computed.

In the above example, the Morse-Smale complex was computed for a fixed persistence level. Alternatively, compute the first 15 persistence levels of the Morse-Smale complex.

```r
c> ms <- msc.nn(y = d[, 1], x = d[, 2:3], nLevels = 15, knn = 15)
```

and access individual levels.
At this point, the Morse-Smale complex has no prediction capabilities. Compute a Morse-Smale complex that supports partition prediction by SVM.

```r
R> ms.svm <- msc.nn.svm(y = d[, 1], x = d[, 2:3], nLevels = 15,
+ knn = 15, cost = 1, precompute = TRUE)
```

The `precompute` flag indicates that the SVM at each persistence level is computed and stored for later use. If set to `FALSE`, the SVM is computed on demand, which saves storage space, but can be time consuming if multiple predictions at different levels are made.

Alternatively, construct a Morse-Smale complex with partition prediction by kernel density estimation for two different bandwidths.

```r
R> ms.kd1 <- msc.nn.kd(y = d[, 1], x = d[, 2:3], nLevels = 15, knn = 15,
+ bw = 0.05)
R> ms.kd2 <- msc.nn.kd(y = d[, 1], x = d[, 2:3], nLevels = 15, knn = 15,
+ bw = 0.15)
```

Create a test data set and predict partition probabilities at level 12.

```r
R> test <- fourpeaks(2000)
R> ms.svm$predictLevel <- 12
R> psvm <- predict(ms.svm, newdata = test)
R> ms.kd1$predictLevel <- 12
R> pkd1 <- predict(ms.kd1, newdata = test)
R> ms.kd2$predictLevel <- 12
R> pkd2 <- predict(ms.kd2, newdata = test)
```

For both visualization and regression, `predictLevel` determines the level of the current Morse-Smale hierarchy at which prediction or visualization is performed.

Now plot the partition probabilities for partition index 8.

```r
R> par(mfcol = c(1, 4))
R> pId <- ms.svm$level[[12]]$partition == 8
R> colors <- vector(length = length(ms.svm$y))
R> colors[] = fancy[1]
R> colors[pId] = fancy[3]
```
6.2. Visualization

Using the Morse-Smale complex from the previous section show visualizations at level 2, 7, and 12.

R> ms$predictLevel <- 2
R> plot(ms, span = 0.9)
R> ms$predictLevel <- 7
R> plot(ms)
R> ms$predictLevel <- 12
R> plot(ms)
As for the partition prediction, the `predictLevel` defines at which persistence level the visualization is performed.

### 6.3. Regression

The regression is invoked directly on the Morse-Smale complex object. Construct Morse-Smale complex with SVM prediction and fit a piecewise linear model with a cross-validation for choosing the prediction level.

```r
R> ms.svm$predictLevel <- 1
R> msr.lm <- msc.lm(ms.svm)
R> summary(msr.lm)
```

```
  Length Class Mode
lms  14 -none- list
ms   9 msc.svm list
blend 1 -none- logical
```

```r
R> pLevel <- msr.lm$ms$predictLevel
R> print(pLevel)

[1] 12
```

```r
R> print(msr.lm$lms[[pLevel]]$cv)

[1] 0.001967322
```

This constructs a hierarchy of linear models and the `msr$ms$predictLevel` designates the model used for prediction. Predict the test data and print the mean squared error.

```r
R> p <- predict(msr.lm, newdata = test)
R> print(mean((p - test[, 1])^2))

[1] 0.003848764
```
Instead of the piecewise linear model, fit a sum of weighted linear models. The persistence level is, as for the piecewise linear model, selected automatically with cross-validation.

```r
R> mslm <- msc.slm(ms.svm)
R> print(msslm$slm[[pLevel]]$cv)
[1] 0.001460281
```

Predict at different levels and plot the corresponding models.

```r
R> mslm$ms$predictLevel = 1
R> p1 <- predict(mslms, newdata = test)
R> print(mean((p1 - test[, 1])^2))
[1] 0.03675813
```

```r
R> mslm$ms$predictLevel = 7
R> p2 <- predict(mslms, newdata = test)
R> print(mean((p2 - test[, 1])^2))
[1] 0.01178318
```

```r
R> mslm$ms$predictLevel = 12
R> p3 <- predict(mslms, newdata = test)
R> print(mean((p3 - test[, 1])^2))
[1] 0.003329688
```

```r
R> par(mfcol = c(1, 3))
R> ps <- p1
R> ps[ps > 1] <- 1
R> ps[ps < 0] <- 0
R> colors <- rgb(colormap(ps), maxColorValue = 255)
R> plot(test[, 2], test[, 3], type = "p", xlab = "", ylab = "", + col = colors, pch = 19, cex.axis = 2.5, cex = 1)
R> ps <- p2
R> ps[ps > 1] <- 1
R> ps[ps < 0] <- 0
R> colors <- rgb(colormap(ps), maxColorValue = 255)
R> plot(test[, 2], test[, 3], type = "p", xlab = "", ylab = "", + col = colors, pch = 19, cex.axis = 2.5, cex = 1)
R> ps <- p3
R> ps[ps > 1] <- 1
R> ps[ps < 0] <- 0
R> colors <- rgb(colormap(ps), maxColorValue = 255)
R> plot(test[, 2], test[, 3], type = "p", xlab = "", ylab = "", + col = colors, pch = 19, cex.axis = 2.5, cex = 1)
```
7. Visualizing the UCI crime data

The communities and crime data set from the UCI machine learning repository\(^2\) combines socio-economic data from the 1990 US Census, law enforcement data from the 1990 US LEMAS survey, and crime data from the 1995 FBI UCR. The original data set contains 1,994 observations (communities) with 128 attributes. This analysis uses a reduced data set, with attributes that have missing entries removed, and investigates the crime rate in relation to 99 socio-economic variables.

```r
R> data(uci_crime_subset)
```

First, construct the Morse-Smale complex and plot the persistences.

```r
R> ms <- msc.nn(y = crimes[, 100], x = crimes[, 1:99], knn = 120,
+               nLevels = 5)
R> np <- length(ms$persistence)
R> ms$persistence[np] <- 1
R> par(mar = c(5, 4, 4, 2) + 3)
R> plot(ms$persistence, np:1 + 1, xlab = "Persistence Percentage",
+       ylab = "Extrema", cex = 2.5, cex.lab = 2, cex.axis = 2, type = "p",
+       pch = 19)
```

\(^2\)http://archive.ics.uci.edu/ml/datasets/Communities+and+Crime
This shows that the Morse-Smale complex with 4 extrema requires a function change of 26 percent of the function range to introduce an additional extrema. This indicates that the Morse-Smale complex at this level is relatively stable and the extremal points are not very likely artifacts from noisy observations.

Now plot the Morse-Smale based summary representation of the function at persistence level 3 (see Figure 6).

R> ms$predictLevel = 3
R> obj <- plot(ms)

This visualization is interactive and allows for deeper investigation of the function. By clicking on a regression curve, representing one partition of the Morse-Smale complex, a window with the inverse regression curves per variable is shown for that curve. In the case of the crime data, this opens multiple device windows to show the 99 variables of the domain. This can
be cumbersome to analyze. To restrict attention to variables of interest, a `plotList` on the object is created which allows the user to select specific variables for plotting.

```r
R> obj$plotList <- c(1, 12, 27, 20, 32, 33, 97)
R> names <- colnames(crimes)[obj$plotList]
R> print(names)
R> plot(obj)
```

This allows for the easy comparison of user selected variables of interest. For example, the selected variables show that two peak crime rate configurations involve a large percentage of urban population, while the third high crime rate peak concerns rural areas. One peak crime rate is related to high unemployment rates while the other two have relatively low unemployment. This illustrates how the proposed visualization can be used to build hypotheses for further examination.

### 8. A Morse-Smale regression example

This example is based on the energy/objective function of a camera estimation problem.

```r
R> data(camera_estimation)
R> energy$E <- (energy$E - min(energy$E))/(max(energy$E) - min(energy$E))
R> train <- energy[1:2000, ]
R> test <- energy[8001:10000, ]
```

Create a Morse-Smale complex object with kernel density based partition prediction.

```r
R> ms <- msc.nn.kd(y = train$E, x = train[, 2:10], knn = 40, nLevels = 17,
+                 bw = 0.3)
```

The piecewise linear model

```r
R> ms.lm <- msc.lm(ms)
```

at level

```r
R> pLevel <- ms.lm$ms$predictLevel
R> print(pLevel)
```

```
[1] 8
```

has the lowest cross-validation error. Plot the cross validation error as a function of the number of extrema.

```r
R> cv <- c()
R> for (i in 1:ms.lm$ms$nLevels) {
+   cv[i] <- ms.lm$ms$predictLevel[i]cv
+ }
R> par(mar = c(5, 4, 4, 2) + 3)
R> plot(1:ms.lm$ms$nLevels, cv, xlab = "Persistence Level", ylab = "CV error",
+     pch = 19, cex = 2.5, cex.lab = 2, cex.axis = 2)
```
The segmentation from the Morse-Smale complex can be used to compute an ANOVA with the partition id as factor.

```r
R> df <- data.frame(test, pID = as.factor(ms$level[[pLevel]]$partition))
R> lm1 <- lm(E ~ . * pID, data = df)
```

Here, the different partitions are, except for a few (visible with `summary(lm1)`, not shown), not significantly different. However, in general, this illustrates how the partition based regression can be used to detect different regions of the parameter space where the function shows different behaviours.

Next, extract a single persistence level Morse-Smale complex and estimate a piecewise linear model with an $L_1$ regularization

```r
R> ms15 <- msc.sublevels(ms, pLevel)
R> ms.l1 <- msc.elnet(ms15)
```

and show coefficients for partition 1 and 5

```r
R> b1 <- as.vector(ms.l1$elnet[[1]]$lm[[1]]$beta)
R> b5 <- as.vector(ms.l1$elnet[[1]]$lm[[5]]$beta)
R> print(cbind(b1, b5))
```

```
           b1         b5
[1,] 0.137135930 0.06078743
[2,] 0.055223674 0.05719516
[3,] 0.037854162 -0.13567797
[4,] 0.000000000 -0.07790446
[5,] 0.441683899 0.44336507
[6,] 0.003399937 -0.01622836
[7,] -0.042798237  0.11095513
[8,] 0.099981109  0.13525573
[9,] 0.200526643  0.18097927
```
to compare differences between the partitions.
Alternatively, employ a forward stepwise approach for a sparse regression estimate.

R> ms.lm1 <- msc.lm(ms15, modelSelect = T)

Next, construct a weighted additive.

R> ms.slm <- msc.slm(ms)

The cross validation selected persistence level

R> print(ms.slm$ms$predictLevel)

[1] 12

with a mean squared test error of

R> penergy <- predict(ms.slm, test)
R> mean((test$E - penergy)^2)

[1] 0.002840482

Note, that due to the averaging of different linear models the additive weighted approach is not suitable for interpretation, but typically yields better function approximations than the piecewise linear approach.

9. Conclusion

This paper described the R package msr for exploratory data analysis based on the Morse-
Smale complex approximation of a function. The package is built in a modular fashion with the Morse-Smale complex approximation as the fundamental building block. A visualization and a regression approach are implemented on top of the Morse-Smale approximation. The regression and visualization facilitate a qualitative understanding of high-dimensional functions. However, the modular design enables to harness the Morse-Smale complex for data analysis approaches other than the two methods presented here.

Acknowledgements

We thank Oliver Rübel for early tests and many bug reports as well as helpful discussions on the design of the package. We thank Peter G. Lindstrom for providing us with the optimization data set.

This work was funded by the National Institute of Health grants U54-EB005149 and 2-P41-
RR12553-08, NSF grant CCF-073222 and CNS-0615194, and Award No. KUS-C1-016-04, made by King Abdullah University of Science and Technology (KAUST).

References
Adler D, Murdoch D (2010). rgl: 3D visualization device system (OpenGL). R package version 0.92.794, URL http://CRAN.R-project.org/package=rgl.

Alexander WP, Grimshaw SD (1996). “Treed Regression.” Journal of Computational and Graphical Statistics, 5(2), 156–175.

Breiman L, Friedman J, Stone CJ, Olshen RA (1984). Classification and Regression Trees. 1 edition. Chapman and Hall/CRC.

Bremer PT, Weber G, Pascucci V, Day M, Bell J (2010). “Analyzing and Tracking Burning Structures in Lean Premixed Hydrogen Flames.” IEEE Trans. on Vis. and Comp. Graphics, 16(2), 248–260.

Carr H, Snoeyink J, Axen U (2003). “Computing contour trees in all dimensions.” Comput. Geom. Theory Appl., 24(3), 75–94.

Cazals F, Cazal F, Lewiner T (2003). “Molecular shape analysis based upon Morse-Smale complex and the connolly function.” In Proc. ACM Symposium on Computational Geometry (SOCG), pp. 351–360.

Chang CC, Lin CJ (2001). LIBSVM: a library for support vector machines. URL http://www.csie.ntu.edu.tw/~cjlin/libsvm.

Chaudhuri P, ching Huang M, yin Loh W, Yao R (1994). “Piecewise-polynomial regression trees.” Statistica Sinica, 4, 143–167.

Chazal F, Guibas L, Oudot S, Skraba P (2009). “Analysis of scalar fields over point cloud data.” In SODA ’09: Proceedings of the twentieth Annual ACM-SIAM Symposium on Discrete Algorithms, pp. 1021–1030.

Dimitriadou E, Hornik K, Leisch F, Meyer D, Weingessel A (2010). e1071: Misc Functions of the Department of Statistics (e1071), TU Wien. R package version 1.5-24, URL http://CRAN.R-project.org/package=e1071.

Edelsbrunner H, Harer J, Natarajan V, Pascucci V (2003). “Morse-Smale Complexes for Piecewise Linear 3-Manifolds.” In Proc. 19th Sympos. Comput. Geom., pp. 361–370.

Edelsbrunner H, Morozov D, Pascucci V (2006). “Persistence-sensitive simplification of functions on 2-manifolds.” In Proc. ACM Symposium on Computational Geometry (SOCG), pp. 127–134.

Friedman J, Hastie T, Tibshirani R (2010). “Regularization Paths for Generalized Linear Models via Coordinate Descent.” Journal of Statistical Software, 33(1), 1–22. URL http://www.jstatsoft.org/v33/i01/.

Friedman JH (1991). “Multivariate adaptive regression splines.” Ann. Statist., 19(1), 1–141. With discussion and a rejoinder by the author.

Gerber S, Bremer PT, Pascucci V, Whitaker R (2010). “Visual Exploration of High Dimensional Scalar Functions.” IEEE Transactions on Visualization and Computer Graphics, 16(6), 1271–1280.
Gerber S, Potter K, Ruebel O (2011a). *msr*: Morse-Smale approximation, regression and visualization. R package version 0.1, URL http://CRAN.R-project.org/package=msr.

Gerber S, Rübel O, Bremer PT, Pascucci V, Whitaker R (2011b). “Morse-Smale Regression.” *Journal of Computational and Graphical Statistics*, p. (submitted).

Gyulassy A, Natarajan V, Pascucci V, Hamann B (2007). “Efficient Computation of Morse-Smale Complexes for Three-dimensional Scalar Functions.” *IEEE TVCG*, 13(6), 1440–1447.

Hsu CW, Lin CJ (2002). “A Comparison of Methods for Multiclass Support Vector Machines.” *IEEE Transaction on Neural Networks*, 13(2), 415–425.

Laney D, Bremer PT, Mascarenhas A, Miller P, Pascucci V (2006). “Understanding the Structure of the Turbulent Mixing Layer in Hydrodynamic Instabilities.” *IEEE TVCG*, 12(5), 1052–1060.

Mascarenhas A, Grout RW, Bremer PT, Hawkes ER, Pascucci V, Chen J (2010). Topological feature extraction for comparison of terascale combustion simulation data. Mathematics and Visualization. Springer. To appear.

Mount DM, Arya S (2010). Approximate nearest neighbors (ANN)library.

Platt JC (1999). “Probabilities for SV Machines.” *Advances in Large Margin Classifiers*, pp. 61–74.

R Development Core Team (2010). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0, URL http://www.R-project.org/.

van Kreveld MJ, van Oostrum R, Bajaj CL, Pascucci V, Schikore D (1997). “Contour Trees and Small Seed Sets for Isosurface Traversal.” In *Symposium on Computational Geometry*, pp. 212–220.

Vedaldi A, Soatto S (2008). “Quick Shift and Kernel Methods for Mode Seeking.” In *Proc. European Conf. on Computer Vision*, pp. 705–718.

Weber G, Bremer PT, Pascucci V (2007). “Topological Landscapes: A Terrain Metaphor for Scientific Data.” *IEEE Trans. on Vis. and Comp. Graphics*, 13(6), 1077–2626.
Affiliation:

Samuel Gerber
Scientific Computing and Imaging Institute
University of Utah
72 S Central Campus Drive, Room 3750
Salt Lake City, UT 84112
E-mail: sgerber@cs.utah.edu
URL: http://www.cs.utah.edu/~sgerber/