Piece-wise quadratic lego set for constructing arbitrary error potentials and their fast optimization

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Abstract

Most of machine learning approaches have stemmed from the application of minimizing the mean squared distance principle, based on the computationally efficient quadratic optimization methods. However, when faced with high-dimensional and noisy data, the quadratic error functionals demonstrate many weaknesses including high sensitivity to contaminating factors and dimensionality curse. Therefore, a lot of recent applications in machine learning exploited the properties of non-quadratic error functionals based on L1 norm or even sub-linear potentials corresponding to fractional norms. The back side of these approaches is tremendous increase in computational cost for optimization. Till so far, no approaches have been suggested to deal with arbitrary error functionals, in a flexible and computationally efficient framework. In this paper, we develop the theory and basic universal data approximation algorithms (\(k\)-means, principal components, principal manifolds and graphs), based on piece-wise quadratic error potentials of subquadratic growth (PQSQ potentials). We develop a new and universal framework to minimize arbitrary sub-quadratic error potentials using an algorithm with guaranteed fast convergence to the local or global error minimum. The approach can be applied in most of existing machine learning methods, including methods of data approximation and regularized regression, leading to the improvement in the computational cost/accuracy trade-off.

Keywords: data approximation, nonquadratic potential, principal components, clustering

1. Introduction

Modern machine learning and artificial intelligence methods are revolutionizing many fields of science today, such as medicine, biology, engineering, high-energy physics and sociology, where large amounts of data have been collected due to the emergence of new high-throughput computerized technologies. Historically and methodologically speaking, many machine learning algorithms have been based on minimizing the mean squared error potential, which can be explained by tractable properties of normal distribution and existence of computationally efficient methods for quadratic optimization. However, most of the real-life datasets are characterized by strong noise, long-tailed distributions, presence of contaminating factors, large dimensions. Using quadratic potentials can be drastically compromised by all these circumstances: therefore, a lot of practical and theoretical efforts have been made in order to exploit the properties of non-quadratic error potentials which can be more appropriate in certain contexts. For example, methods of regularized regression such as lasso and elastic net based on the properties of L1 metrics\textsuperscript{[1, 2]}, found numerous applications in bioinformatics\textsuperscript{[3]}, and L1 norm-based methods of dimension reduction are of great use in automated image analysis\textsuperscript{[4]}. Not surprisingly, these approaches comes with drastically increased computational cost, for example, connected with applying linear programming optimization techniques which are substantially more expensive compared to mean squared error-based methods.

In practical applications of machine learning, it
would be very attractive to be able to deal with arbitrary error potentials, including those based on L1 or fractional norm, in a computationally efficient and scalable way. There is a need in developing methods allowing to tune the computational cost/accuracy of optimization trade-off accordingly to various contexts.

In this paper, we suggest such a universal framework able to deal with a large family of error potentials. We exploit the fact that finding a minimum of a piece-wise quadratic function, or, in other words, a function which is the minorant of a set of quadratic functionals, can be almost as computationally efficient as optimizing the standard quadratic potential. Therefore, if a given arbitrary potential (such as L1-based or fractional norm-based) can be approximated by a piece-wise quadratic function, this should lead to relatively efficient and simple optimization algorithms. It appears that only potentials of quadratic or subquadratic growth are possible in this approach: however, these are the most useful ones in data analysis. We introduce a rich family of piece-wise quadratic potentials of sub-quadratic growth (PQSQ-potentials), suggest general approach for their optimization and prove convergence of a simple iterative algorithm in the most general case. We focus on the most used methods of data dimension reduction: however, potential applications of the approach can be much wider.

Data dimension reduction by constructing explicit low-dimensional approximators of a finite set of vectors is one of the most fundamental approach in data analysis. Starting from the classical data approximators such as k-means and linear principal components (PCA), multiple generalizations have been suggested in the last decades (self-organizing maps, principal curves, principal manifolds, principal graphs, principal trees, etc.) in order to make the data approximators more flexible and suitable for complex data structures.

We solve the problem of approximating a finite set of vectors \( \vec{x}_i \in \mathbb{R}^m, i = 1...N \) (data set) by a simpler object \( L \) embedded into the data space, such that for each point \( \vec{x}_i \) an approximation error \( \text{err}(\vec{x}_i, L) \) function can be defined. We assume this function in the form

\[
\text{err}(\vec{x}_i, L) = \min_{y \in L} \sum_k u(x^k_i - y^k),
\]

where the upper \( k = 1...m \) stands for the coordinate index, and \( u(x) \) is a monotonously growing symmetrical function, which we will be calling the error potential. By data approximation we mean that the embedding of \( L \) in the data space minimizes the error

\[
\sum_i \text{err}(\vec{x}_i, L) \to \min.
\]

Note that our definition of error function is coordinate-wise (it is a sum of error potential over all coordinates).

The simplest form of the error potential is quadratic \( u(x) = x^2 \), which leads to the most known data approximators: mean point (L is a point), principal points (L is a set of points) \([5]\), principal components (L is a line or a hyperplane) \([6]\). In more advanced cases, L can posses some regular properties leading to principal curves (L is a smooth line or spline) \([10]\), principal manifolds (L is a smooth low-dimensional surface) and principal graphs (e.g., L is a pluri-harmonic graph embedding) \([11, 7]\).

There exist multiple advantages of using quadratic potential \( u(x) \), because it leads to the most computationaly efficient algorithms usually based on the splitting schema, a variant of expectation-minimization approach \([7]\). For example, k-means algorithm solves the problem of finding the set of principal points and the standard iterative Singular Value Decomposition finds principal components. However, quadratic potential is known to be sensitive to outliers in the data set. Also, purely quadratic potentials can suffer from the curse of dimensionality, not being able to robustly discriminate “close” and “distant” point neighbours in a high-dimensional space \([12]\).

There exist several widely used ideas for increasing approximator’s robustness in presence of strong noise in data such as: (1) using medians instead of mean values, (2) substituting quadratic norm by L1 norm (e.g. \([13, 14]\), (3) outliers exclusion or fixed weighting or iterative reweighting during optimizing the data approximators (e.g. \([13, 16, 17]\), and (4) regularizing the PCA vectors by L1 norm \([18, 19, 20]\). In some works, it was suggested to utilize “trimming” averages, e.g. in the context of the k-means clustering or some generalizations of PCA \([14]\). In the context of regression, iterative reweighting is exploited to mimic the properties of L1 norm \([22]\). Several algorithms for constructing PCA with L1 norm have been suggested \([23, 24, 25]\) and systematically benchmarked \([26, 27]\). Some authors go even beyond linear metrics and suggests
that fractional norms (Lp metrics with p < 1) can be more appropriate in high-dimensional data approximation [12].

However, most of the suggested approaches exploiting properties of non-quadratic metrics either represent useful but still arbitrary heuristics or are not sufficiently scalable. The standard approach for minimizing L1-based norm consists in solving a linear programming task. Despite existence of many efficient linear programming optimizer implementations, by their nature these computations are much slower than the iterative methods used in the standard SVD algorithm or k-means.

In this paper, we provide implementations of the standard data approximators (mean point, k-means, principal components) using a PQSQ potential. In addition, we discuss exploiting similar approach in non-linear data approximation (i.e. principal manifolds and graphs) and regularized regression (i.e., lasso and elastic nets).

2. Piecewise quadratic potential of subquadratic growth (PQSQ)

2.1. Definition of the PQSQ potential

Let us split all non-negative numbers \( x \in R_{\geq 0} \) into \( p + 1 \) non-intersecting intervals \( R_0 = [0; r_1), R_1 = [r_1; r_2), ..., R_k = [r_k; r_{k+1}], ..., R_p = [r_p; \infty) \), for a set of thresholds \( r_1 < r_2 < ... < r_p \). For convenience, let us denote \( r_0 = 0, r_{p+1} = \infty \). Piecewise quadratic potential is a continuous monotonously growing function \( u(x) \) constructed from pieces of centered at zero parabolas \( y = b_k + a_kx^2 \), defined on intervals \( x \in [r_k, r_{k+1}] \), satisfying \( y(r_i) = f(r_i) \) (see Figure 1):

\[
u(x) = b_k + a_kx^2, \text{if } r_k \leq |x| < r_{k+1}, k = 0...p, \quad (2)\]

\[
a_k = \frac{f(r_k) - f(r_{k+1})}{r_k^2 - r_{k+1}^2}, \quad (3)
\]

\[
b_k = \frac{f(r_{k+1})r_k^2 - f(r_k)r_{k+1}^2}{r_k^2 - r_{k+1}^2} \quad (4)
\]

where \( f(x) \) is a majorating function, which is to be approximated (imitated) by \( u(x) \). For example, in the simplest case \( f(x) \) can be a linear function: \( f(x) = x \), in this case, \( \sum_k u(x^k) \) will approximate the L1-based error function.

Note that accordingly to (3,4), \( b_0 = 0, a_0 = 0, b_p = f(r_p) \). Therefore, the choice of \( r_p \) can naturally create a "trimmed" version of error potential \( u(x) \) such that some data points (outliers) do not have any contribution to the gradient of \( u(x) \), hence, will not affect the optimization procedure. However, this set of points can change during minimization of the potential.

The condition of subquadratic growth consists in the requirement \( a_{k+1} \leq a_k \) and \( b_{k+1} \geq b_k \). To guarantee this, the following simple condition on \( f(x) \) should be satisfied:

\[f' > 0, \quad f''x \leq f', \quad (5)\]

i.e., \( f(x) \) should grow not faster than any parabola \( ax^2 + cx, c > 0 \).

![Figure 1: Trimmed piecewise quadratic potential of sub-quadratic growth \( u(x) \) (solid blue line) defined for the majorating function \( f(x) \) (red dashed line) and several thresholds \( r_k \). Dotted lines show the parabolas which fragments are used to construct \( u(x) \). The last parabola is flat (\( a_p = 0 \)) which corresponds to trimmed potential.](image)

2.2. Basic approach for optimization

In order to use the PQSQ potential in an algorithm, a set of \( p \) interval thresholds \( r_k^s, s = 1...p \) for each coordinate \( k = 1...m \) should be provided. Matrices of \( a \) and \( b \) coefficients defined by (3) based on interval definitions: \( a_k^s, b_k^s, s = 0...p, k = 1...m \) are computed separately for each coordinate \( k \).

Minimization of PQSQ-based functional consists in several basic steps which can be combined in an algorithm:
1) For each coordinate \( k \), split all data point indices into non-overlapping sets \( \mathcal{R}_k^s \):

\[
\mathcal{R}_k^s = \{ i : r_s^k \leq |x_i^k - \beta_s^k| < r_{s+1}^k \}, \quad s = 0 \ldots p.
\]

where \( \beta \) is a matrix which depends on the nature of the algorithm.

2) Minimize PQSQ-based functional where each set of points \( \{ x \in \mathcal{R}_k^s \} \) contributes to the functional quadratically with coefficient \( a_s^k \). This is a quadratic optimization task.

3) Repeat (1)-(2) till convergence.

3. General theory of the piece-wise convex potentials as the cone of minorant functions

In order to deal in most general terms with the data approximation algorithms based on PQSQ potentials, let us consider a general case where a potential can be constructed from a set of functions \( \{ q_i(x) \} \) with only two requirements: 1) that each \( q_i(x) \) has a (local) minimum; 2) that the whole set of all possible \( q_i(x) \)'s forms a cone. In this case, instead of the operational definition \( \mathcal{M} \) it is convenient to define the potential \( u(x) \) as the minorant function for a set of functions as follows. For convenience, in this section, \( x \) will notify a vector \( \bar{x} \in \mathbb{R}^m \).

Let us consider a generating cone of functions \( Q \).

We remind that the definition of a cone implies that for any \( q(x) \in Q, p(x) \in Q \), we have \( a \alpha q(x) + b \beta p(x) \in Q \), where \( \alpha \geq 0, \beta \geq 0 \).

For any finite set of functions

\[
q_1(x) \in Q, q_2(x) \in Q, \ldots, q_s(x) \in Q,
\]

we define the minorant function (Figure 2):

\[
u_{q_1, q_2, \ldots, q_s}(x) = \min(q_1(x), q_2(x), \ldots, q_s(x)). (7)
\]

It is convenient to introduce a multiindex

\[
I_{q_1, q_2, \ldots, q_s}(x)
\]

indicating which particular function(s) \( q_i \) corresponds to the value of \( u(x) \), i.e.

\[
I_{q_1, q_2, \ldots, q_s}(x) = \{ i | u_{q_1, q_2, \ldots, q_s}(x) = q_i(x) \}. (8)
\]

For a cone \( Q \) let us define a set of all possible minorant functions \( \mathcal{M}(Q) \)

\[
\mathcal{M}(Q) = \{ u_{q_1, q_2, \ldots, q_s} | q_1 \in Q, q_2 \in Q, \]
\[
q_n \in Q, n = 1, 2, 3, \ldots \}. (9)
\]

Proposition 1. \( \mathcal{M}(Q) \) is a cone.

Proof For any two minorant functions

\[
u_{q_1, q_2, \ldots, q_s}, u_{q_1, q_2, \ldots, q_s} \in \mathcal{M}(Q)
\]

we have

\[
a \alpha u_{q_1, q_2, \ldots, q_s} + \beta u_{q_1, q_2, \ldots, q_s} = u_{(a \alpha q_1 + \beta q_s, \ldots, a \alpha q_s + \beta q_s)} \in \mathcal{M}(Q), (10)
\]

where \( \{ a \alpha q_1 + \beta q_s \} \) is a set of all possible linear combinations of functions from \( \{ q_1, q_2, \ldots, q_s \} \).

Proposition 2. Any restriction of \( \mathcal{M}(Q) \) onto a linear manifold \( L \) is a cone.

Proof Let us denote \( q(x)|_L \) a restriction of \( q(x) \) function onto \( L \), i.e. \( q(x)|_L \equiv \{ q(x)|x \in L \} \). \( q(x)|_L \) is a part of \( Q \). Set of all \( q(x)|_L \) forms a restriction \( Q|_L \) of \( Q \) onto \( L \). \( Q|_L \) is a cone, hence, \( \mathcal{M}(Q)|_L = \mathcal{M}(Q|_L) \) is a cone (Proposition 1).

Definition Splitting algorithm minimizing

\[
u_{q_1, q_2, \ldots, q_s}(x)
\]

is defined as Algorithm 1

Algorithm 1 Finding local minimum of a minorant function \( u_{q_1, q_2, \ldots, q_s}(x) \)

1: \textbf{procedure} MINIMIZING MINORANT FUNCTION
2: \quad initialize \( x \leftarrow x_0 \)
3: \quad repeat until stopping criterion has been met:
4: \quad \quad compute multiindex \( I_{q_1, q_2, \ldots, q_s}(x) \)
5: \quad \quad for all \( i \in I_{q_1, q_2, \ldots, q_s}(x) \)
6: \quad \quad \quad \quad \quad \textbf{select optimal} \( x_i \) :
7: \quad \quad \quad \quad \quad \quad \textbf{choose} \( x_{opt} \leftarrow \text{arg min}_x u(x) \)
8: \quad \quad \quad \quad \quad \quad x \leftarrow x_{opt} \)
9: \quad \quad \quad \quad \quad \textit{stopping criterion:} check if the multiindex \( I_{q_1, q_2, \ldots, q_s}(x) \) does not change compared to the previous iteration
10: \quad \quad \textbf{end for}
11: \quad \textbf{end repeat}

Theorem 3.1. Splitting algorithm (Algorithm 1) for minimizing \( u_{q_1, q_2, \ldots, q_s}(x) \) converges in a finite number of steps.
Proof Since the set of functions \{q_1, q_2, ..., q_n\} is finite then we only have to show that at each step the value of the function \(u_{q_1, q_2, ..., q_n}(x)\) can not increase. For any \(x\) and the value \(x' = \arg \min q_i(x)\) for \(i \in I_{q_1, q_2, ..., q_n}(x)\) we can have only two cases:

1. Either \(I_{q_1, q_2, ..., q_n}(x) = I_{q_1, q_2, ..., q_n}(x')\) (convergence, and in this case \(q_i(x') = q_i(x)\) for any \(i' \in I_{q_1, q_2, ..., q_n}(x')\);

2. Or \(u_{q_1, q_2, ..., q_n}(x') < u_{q_2, q_2, ..., q_n}(x)\) since, accordingly to the definition (10), \(q_i(x') < q_i(x)\), for any \(i' \in I_{q_1, q_2, ..., q_n}(x')\), \(i \in I_{q_1, q_2, ..., q_n}(x)\) (see Figure 2).

Note that in Algorithm 1 we do not specify exactly the way to find the local minimum of \(q_i(x)\). To be practical, the cone \(Q\) should contain only functions for which finding a local minimum is fast and explicit. Evident candidates for this role are positively defined quadratic functionals \(q(x) = q_0 + (q_1, x) + (x, Q_2x)\), where \(Q_2\) is a positively defined symmetric matrix. Any minorant function 7 constructed from positively defined quadratic functions will automatically provide subquadratic growth, since the minorant can not grow faster than any of the quadratic forms by which it is defined.

Operational definition of PQSQ given above (2), corresponds to a particular form of the quadratic functional, with \(Q_2\) being diagonal matrix. This choice corresponds to the coordinate-wise definition of data approximation error function 1 which is particularly simple to minimize. This circumstance is used in Algorithms 2,3

4. Commonly used data approximators with PQSQ potential

4.1. Mean value and k-means clustering in PQSQ approximation measure

Mean vector \(\hat{X}_k\) for a set of vectors \(X = \{x_i^k\}, i = 1...N, k = 1...m\) and an approximation error defined by potential \(f(x)\) can be defined as a point minimizing the mean error potential for all points in \(X\):

\[
\sum_k f(x_i^k - \hat{X}_k) \rightarrow \min . \tag{11}
\]

For Euclidean metrics \(L_2\) \((f(x) = x^2)\) it is the usual arithmetic mean.

For \(L_1\) metrics \((f(x) = |x|)\), (11) leads to the implicit equation \(#(x_i^k > \hat{X}_k) = #(x_i^k < \hat{X}_k)\), where \# stands for the number of points, which corresponds to the definition of median. This equation can not have a unique solution in case of even number of points or when some data point coordinates coincide: therefore, definition of median is usually accompanied by heuristics used for breaking ties, i.e. to deal with non-uniquely defined rankings. This situation reflects the general situation of existence of multiple local minima and possible non-uniqueness of global minimum of (11) (Figure 3).

For PQSQ approximation measure (2) it is difficult to write down an explicit formula for computing the mean value corresponding to the global minimum of (11). In order to find a point \(\hat{X}_{PQSQ}\) minimizing mean PQSQ potential, a simple iterative algorithm can be used:

The suggested algorithm converges to the local minimum which depends on the initial point approximation.

Based on the PQSQ approximation measure and the algorithm for computing the PQSQ mean value (Algorithm 2), one can construct the PQSQ-based k-means clustering procedure in the usual way, splitting estimation of cluster centroids given partitioning of the data points into \(k\) disjoint groups, and then re-calculating the partitioning using the PQSQ-based proximity measure.

4.2. Principal Component Analysis (PCA) in PQSQ metrics

Accordingly to the classical definition of the first principal component, it is a line best fit to the data set \(X\) \(\hat{\mathbf{e}}\). Let us define a line in the parametric form \(\mathbf{y} = \hat{V}u + \mathbf{\delta}\), where \(u \in \mathbb{R}^1\) is the parameter.
Algorithm 2 Computing PQSQ mean value
\begin{algorithm}
1: \textbf{procedure} PQSQ MEAN VALUE \\
2: \hspace{10pt} define intervals $r^k_s$, $s = 0...p$, $k = 1...m$ \\
3: \hspace{10pt} compute coefficients $a^k_s$ \\
4: \hspace{10pt} initialize $X_{P SQ}$ \\
5: \hspace{10pt} eg., by arithmetic mean \\
6: \hspace{10pt} repeat till convergence of $X_{P SQ}$: \\
7: \hspace{20pt} for each coordinate $k$ \\
8: \hspace{30pt} define sets of indices \\
9: \hspace{40pt} $\mathcal{R}_s^k = \{i : r^k_s \leq |x_k^i - X_{P SQ}^k| < r^k_{s+1}\}$, \hspace{10pt} $s = 0,...,p$ \\
10: \hspace{30pt} end for \\
11: \hspace{20pt} compute new approximation for $X_{P SQ}$: \\
12: \hspace{30pt} $X_{P SQ}^k \leftarrow \frac{\sum_{i \in \mathcal{R}_s^k} x_i^k}{\sum_{i \in \mathcal{R}_s^k} |x_i^k|}$ \\
13: \hspace{10pt} end for \\
14: \hspace{10pt} goto repeat till convergence
\end{algorithm}

Then the first principal component will be defined by vectors $\bar{V}, \bar{\delta}$ satisfying
\begin{equation}
\sum_i \sum_k u(x_k^i - V^k u_i - \delta^k) \rightarrow \min, \quad (12)
\end{equation}
where
\begin{equation}
u_i = \arg \min_s \sum_k u(x_k^i - V^k s - \delta^k). \quad (13)\end{equation}

The standard first principal component (PC1) corresponds to $u(x) = x^2$ when the vectors $\bar{V}, \bar{\delta}$ can be found by a simple iterative splitting algorithm for Singular Value Decomposition (SVD). If $X$ does not contain missing values then $\delta$ is the vector of arithmetic mean values. By contrast, computing $L1$-based principal components ($u(x) = |x|$) represents a much more challenging optimization problem. Several approximative algorithms for computing $L1$-norm PCA have been recently suggested and benchmarked. To our knowledge, there have not been a general efficient algorithm suggested for computing PCA in case of arbitrary approximation measure for some monotonous function $u(x)$.

Computing PCA based on PQSQ approximation error is only slightly more complicated than computing the standard $L2$ PCA by SVD. Here we provide a pseudo-code (Algorithm 3) of a simple iterative algorithm (similar to Algorithm 2) with guaranteed convergence (see Section 3).

Algorithm 3 Computing PQSQ PCA
\begin{algorithm}
1: \textbf{procedure} PQSQ FIRST PRINCIPAL COMPONENT \\
2: \hspace{10pt} define intervals $r^k_s$, $s = 0...p$, $k = 1...m$ \\
3: \hspace{10pt} compute coefficients $a^k_s$ \\
4: \hspace{10pt} $\bar{\delta} \leftarrow X_{P SQ}$ \\
5: \hspace{10pt} \text{initialize } \bar{V} \text{ : eg., by } L2\text{-based PC1} \\
6: \hspace{10pt} \text{initialize } \{u_i\} \text{ : eg., by} \\
7: \hspace{20pt} u_i = \frac{\sum_k V^k (x_k^i - \delta^k)}{\sum_k (|V^k|)^2} \\
8: \hspace{10pt} \text{repeat till convergence of } \bar{V} : \\
9: \hspace{20pt} \text{normalize } \bar{V} \leftarrow \frac{\bar{V}}{||\bar{V}||} \\
10: \hspace{20pt} \text{for each coordinate } k \\
11: \hspace{30pt} \text{define sets of indices} \\
12: \hspace{40pt} \mathcal{R}_s^k = \{i : r^k_s \leq |x_k^i - V^k u_i - \delta^k| < r^k_{s+1}\}, \quad s = 0...p \\
13: \hspace{30pt} \text{end for} \\
14: \hspace{30pt} \text{end for} \\
15: \hspace{20pt} \text{if all } a_{s+1} = 0 \text{ then } u_i \leftarrow 0 \text{ else} \\
16: \hspace{30pt} u_i' = \frac{\sum_k a_{s+1} V^k (x_k^i - \delta^k)}{\sum_k a_{s+1} (V^k)^2} \\
17: \hspace{30pt} \text{end for} \\
18: \hspace{20pt} \text{for each coordinate } k \\
19: \hspace{30pt} V^k = \frac{\sum_k a^k_s \sum_{i \in \mathcal{R}_s^k} (x_k^i - \delta^k) u_i}{\sum_k a^k_s \sum_{i \in \mathcal{R}_s^k} (u_i)^2} \\
20: \hspace{30pt} \text{end for} \\
21: \hspace{20pt} \text{end for} \\
22: \hspace{10pt} \text{goto repeat till convergence}
\end{algorithm}
ple, the “variance” function
abstract version of the
Theorem 3.1.
Hence,
M
the cone
minimum should be selected.
the deepest in PQSQ approximation error (1) min-
randomly or by data vectors
error to the linear subspace,
order to achieve the least possible approximation
estimate of
k
ways converge to a unique global minimum; the
principal components, the
Algorithm 3
to the dataset rotation. Moreover, unlike
non-orthogonal or even not invariant with respect
the data set, and the algorithm is applied to the
previously computed component are subtracted from
components follows the standard deflation ap-
concrete choice of PQSQ parameters (interval definitions).
4.3. Nonlinear methods: PQSQ-based Principal
Graphs and Manifolds
In a series of works, the authors of this article introduced a family of methods for constructing principal objects based on graph approximations (e.g., principal curves, principal manifolds, principal trees), which allows constructing explicit nonlinear data approximators (and, more generally, approximators with non-trivial topologies, suitable for approximating, e.g., datasets with branching or circular topology) [28, 29, 31, 11, 6, 7, 32]. The methodology is based on optimizing a piece-wise quadratic elastic energy functional (see short description below). A convenient graphical user interface was developed with implementation of some of these methods [33].
Let G be a simple undirected graph with set of vertices % and set of edges \( E \). For \( k \geq 2 \) a k-star in G is a subgraph with \( k + 1 \) vertices \( y_0, y_1, \ldots, y_k \in Y \) and \( k \) edges \( \{ (y_i, y_j) \mid i = 1, \ldots, k \} \subset E \). Suppose for each \( k \geq 2 \), a family \( S_k \) of k-stars in G has been selected. We call a graph G with selected families of k-stars \( S_k \) an elastic graph if, for all \( E^{(i)} \in E \) and \( S_k^{(j)} \subset S_k \), the correspondent elasticity moduli \( \lambda_i > 0 \) and \( \mu_{kj} > 0 \) are defined. Let \( E^{(i)}(0) \), \( E^{(i)}(1) \) be vertices of an edge \( E^{(i)} \) and \( S_k^{(j)}(0), \ldots, S_k^{(j)}(k) \) be vertices of a k-star \( S_k^{(j)} \) (among them, \( S_k^{(j)}(0) \) is the central vertex).
For any map \( \phi : Y \rightarrow R^m \) the energy of the graph is defined as
\[
U_\phi(G) := \sum_{E^{(i)}} \lambda_i \left\| \phi(E^{(i)}(0)) - \phi(E^{(i)}(1)) \right\|^2 + \sum_{S_k^{(j)}} \mu_{kj} \left\| \sum_{i=1}^{k} \phi(S_k^{(j)}(i)) - k \phi(S_k^{(j)}(0)) \right\|^2.
\]
For a given map \( \phi : Y \rightarrow R^m \) we divide the dataset \( D \) into node neighborhoods \( K^\nu, y \in Y \). The set \( K^\nu \) contains the data points for which the node \( \phi(y) \) is the closest one in \( \phi(Y) \). The energy of approximation is:
\[
U_\phi^A(G, D) = \sum_{y \in Y} \sum_{x \in K^\nu} w(x) \| x - \phi(y) \|^2,
\]
where \( w(x) \geq 0 \) are the point weights. Simple and fast algorithm for minimization of the energy
\[
U_\phi = U_\phi^A(G, D) + U_\phi(G)
\]
5. Numerical examples

5.1. Practical choices of parameters

The main parameters of PQSQ are (a) majorating function \( f(x) \) and (b) decomposition of each coordinate range into \( p + 1 \) non-overlapping intervals. Depending on these parameters, various approximation error properties can be exploited, including those providing robustness to outlier data points.

When defining the intervals \( r_j, j = 1 \ldots p \), it is desirable to achieve a small difference between \( f(\Delta x) \) and \( u(\Delta x) \) for expected argument values \( \Delta x \) (differences between an estimator and the data point), and choose the suitable value of the potential trimming threshold \( r_p \) in order to achieve the desired robustness properties. If no trimming is needed, then \( r_p \) should be made larger than the maximum expected difference between coordinate values (maximum \( \Delta x \)).

In our numerical experiments we used the following definition of intervals. For any data coordinate \( k \), we define a characteristic difference \( D^k \), for example

\[
D^k = \alpha_{\text{scale}}(\max_i(x^k_i) - \min_i(x^k_i)),
\]

where \( \alpha_{\text{scale}} \) is a scaling parameter, which can be put at 1 (in this case, the approximating potential will not be trimmed). In case of existence of outliers, for defining \( D^k \), instead of amplitude one can use other measures such as the median absolute deviation (MAD):

\[
D^k = \alpha_{\text{scale}} \cdot \text{median}_i(|x^k_i - \text{median}(\{x^k_i\})|);
\]

in this case, the scaling parameter should be made larger, i.e. \( \alpha_{\text{scale}} = 10 \), if no trimming is needed.

After defining \( D^k \) we use the following definition of intervals:

\[
r_j^k = D^k \frac{j^2}{p^2}, j = 0 \ldots p.
\]

More sophisticated approaches are also possible to apply such as, given the number of intervals \( p \) and the majorating function \( f(x) \), choose \( r_j, j = 1 \ldots p \) in order to minimize the integral difference

\[
\int_0^{r_p} (f(x) - u(x))^2 dx \to \min.
\]
We measured the ability of the first two principal component to separate clusters by computing the t-test between the two clusters projected in the 2D-space spanned by the first principal components of the global distribution (Figure 4D-E). As one can see, the average ability of the first principal components to separate clusters is significantly stronger in the case of PQSQ L1-based PCA which is able to robustly separate the clusters even in the presence of strong noise contamination (up to 80 noise points, i.e. 40% contamination).

5.4. Performance/stability trade-off benchmarking of L1-based PCA

In order to compare the computation time and the robustness of PQSQ-based PCA algorithm for the case $u(x) = |x|$ with existing R-based implementations of L1-based PCA methods (pcaL1 package), we follow the benchmark described in [26]. We compare performance of PQSQ-based PCA based on Algorithm 3 with several L1-based PCA algorithms: L1-PCA* [25], L1-PCA [23], PCA-PP [54], PCA-L1 [24]. As a reference point, we use the standard PCA algorithm based on quadratic norm and computed using the standard SVD iterations.

The idea of benchmarking is to generate a series of datasets of the same size ($N = 1000$ objects in $m = 10$ dimensions) such that the first 5 dimensions would be sampled from a uniform distribution $U(-10,10)$. Therefore, the first 5 dimensions represent “true manifold” sampled by points.

The values in the last 5 dimensions represent “noise+outlier” signal. The background noise is represented by Laplacian distribution of zero mean and 0.1 variance. The outlier signal is characterized by mean value $\mu$, dimension $p$ and frequency $\phi$. Then, for each data point with a probability $\phi$, in the first $p$ outlier dimensions a value is drawn from Laplace($\mu, 0.1$). The rest of the values is drawn from background noise distribution.

As in [26], we’ve generated 1300 test sets corresponding to $\phi = 0.1$, with 100 examples for each combination of $\mu = 1,5,10,25$ and $p = 1,2,3$.

For each test set 5 first principal components $\bar{V}_1, \ldots, \bar{V}_5$ of unit length were computed, with corresponding point projection distributions $U^1, \ldots, U^5$ and the mean vector $\bar{C}$. Therefore, for each initial data point $\vec{x}_i$, we have the “restored” data point

$$P(\vec{x}_i) = \sum_{k=1 \ldots 5} U_k^i \vec{V}_k + \bar{C}.$$ 

For computing the PQSQ-based PCA we used 5 intervals without trimming. Changing the number

principal variance direction of the contaminating distribution (Figure 3A-B). In higher dimensions, not only the first but also the first two principal components are not able to distinguish two clusters, which can hide an important data structure when applying the standard data visualization tools.

In the first test we study a switch of the first principal component from following the variance of the dense informative distribution (abscissa) to the sparse noise distribution (ordinate) as a function of the number of contaminating points, in $R^2$ (Figure 3A-C). We modeled two clusters as two 100-point samples from normal distribution centered in points $[-1; 0]$ and $[1; 0]$ with isotropic variance with the standard deviation 0.1. The sparse noise distribution was modeled as a $k$-point sample from the product of two Laplace distributions of zero means with the standard deviations 2 along abscissa and 4 along ordinate. The intervals for computing the PQSQ functional were defined by thresholds $R = \{0; 0.01; 0.1; 0.5; 1\}$ for each coordinate. Increasing the number of points in the contaminating distribution diminishes the average value of the abscissa coordinate of PC1, because the PC1 starts to be attracted by the contaminating distribution (Figure 3D). However, is it clear that on average PQSQ L1-based PCA is able to withstand much larger amplitude of the contaminating signal (very robust up to 20-30 points, i.e. 10-20% of strong noise contamination) compared to the standard L2-based PCA (which is robust to 2-3% of contamination).

In the second test we study the ability of the first two principal components to separate two clusters, in $R^{100}$ (Figure 4D-F). As in the first test, we modeled two clusters as two 100-point samples from normal distribution centered in points $[-1;0; \ldots;0]$ and $[1;0; \ldots;0]$ with isotropic variance with the standard deviation 0.1 in all 100 dimensions. The sparse noise distribution is modeled as a $k$-point sample from the product of 100 Laplace distributions of zero means with the standard deviations 1 along each coordinate besides the third coordinate (standard deviation of noise is 2) and the forth coordinate (standard deviation of noise is 4). Therefore, the first two principal component in the absence of noise are attracted by the dimensions 1 and 2, while in the presence of strong noise they are be attracted by dimensions 3 and 4, hiding the cluster structure of the dense part of the distribution. The definitions of the intervals were taken as in the first test. We measured the ability of the first two principal components to separate clusters by computing the t-test between the two clusters projected in the 2D-space spanned by the first principal components of the global distribution (Figure 4D-E). As one can see, the average ability of the first principal components to separate clusters is significantly stronger in the case of PQSQ L1-based PCA which is able to robustly separate the clusters even in the presence of strong noise contamination (up to 80 noise points, i.e. 40% contamination).
of intervals did not significantly varied the benchmarking results.

Two characteristics were measured: (1) computation time measured as a ratio to the computation of 5 first principal components using the standard L2-based PCA and (2) the sum of absolute values of the restored point coordinates in the “outlier” dimensions normalized on the number of points:

$$\epsilon = \frac{1}{N} \sum_{i=1}^{N} \sum_{k=6}^{10} |P^k(\vec{x}_i)|.$$  \hspace{1cm} (19)

Formally speaking, $\epsilon$ is $L1$-based distance from the point projection into the 5 principal components to the “true” subspace. In simple terms, larger values of $\epsilon$ correspond to the situation when the first 5 principal components do not represent well the first “true” dimensions, having significant loadings into the “outlier dimensions”. Only if the first 5 components do not have any non-zero loadings in the dimensions 6 . . . 10 then $\epsilon = 0$.

The results of the comparison, averaged over all 1300 test sets, are shown in Figure 5. As one can see, PQSQ-based computation of PCA outperforms by accuracy the existing heuristics such as PCA-L1 but remains computationally efficient being 100 times faster than L1-PCA giving almost the same accuracy and almost 500 times faster than the L1-PCA* algorithm which is, however, significantly gains in accuracy (mostly, due to being robust in the cases of strongest “outliers”). From Figure 5, one can see that PQSQ-based approach performs the best in terms of the accuracy in the family of fast iterative methods. The detailed tables of comparison for all combinations of parameters are provided in the table available on GitHub2. The scripts used to generate the datasets and compare the results can also be found there3.

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2http://goo.gl/sXBvqh
3https://github.com/auranic/PQSQ-DataApproximators
6. Conclusion

In this paper we develop a new machine learning framework (theory and application) allowing one to deal with arbitrary error potentials of not-faster than quadratic growth, imitated by piecewise quadratic function of sub-quadratic growth (PQSQ error potential).

We develop methods for constructing the standard data approximators (mean value, k-means clustering, principal components, principal graphs) for arbitrary non-quadratic approximation error with sub-quadratic growth by using a piecewise-quadratic error functional (PQSQ potential). These approximators can be computed by applying quasi-quadratic optimization procedures, which are organized as solutions of sequences of linear problems by standard and computationally efficient algorithms.

The suggested methodology have several advantages over existing ones:

(a) *Scalability:* the algorithms are computationally efficient and can be applied to large data sets containing millions of numerical values.

(b) *Flexibility:* the algorithms can be adapted to any type of data metrics with subquadratic growth, even if the metrics can not be expressed in explicit form. For example, the error potential can be chosen as adaptive metrics [35, 36].

(c) *Built-in (trimmed) robustness:* choice of intervals in PQSQ can be done in the way to achieve a trimmed version of the standard data approximators, when points distant from the approximator do not affect to the error minimization during the current optimization step.

(d) *Guaranteed convergence:* the suggested algorithms converge to local or global minimum just as the corresponding predecessor algorithms based on quadratic optimization and expectation/minimization-based splitting approach.

One of the application of the suggested methodology is approximating the popular in data mining $L_1$ metrics. We show by numerical simulations that PQSQ-based approximators perform as fast as the fast heuristical algorithms for computing $L_1$-based PCA but achieve better accuracy in a previously suggested benchmark test. PQSQ-based approximators are less accurate than the exact algorithms for optimizing $L_1$-based functions utilizing linear programming: however, they are several orders of magnitude faster. At the same time, PQSQ-based approximators can imitate a variety of sub-quadratic error potentials, including fractional ones.

In Table 1 we give a possible range of applications of PQSQ-based approximators. PQSQ potential can be applied in the task of regression, replacing the classical Least Squares or $L_1$-based Least Absolute Deviation methods. Moreover, PQSQ potential can be easily adapted to the problems of regularized regression with non-quadratic penalty onto the regression coefficients, such as lasso [1] or elastic net [2].

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Data approximation/Clustering/Manifold learning

| Method                      | Description                                                                 |
|-----------------------------|-----------------------------------------------------------------------------|
| Principal Component Analysis| Includes robust trimmed version of PCA, L1-based PCA, regularized PCA, and many other PCA modifications |
| Principal curves and manifolds| Provides possibility to use non-quadratic data approximation terms and trimmed robust version |
| Self-Organizing maps        | Same as above                                                               |
| Principal graphs/trees      | Same as above                                                               |
| K-means                     | Can include adaptive error potentials based on estimated error distributions inside clusters |

High-dimensional data mining

| Method                        | Description                                                                 |
|-------------------------------|-----------------------------------------------------------------------------|
| Use of fractional metrics     | Introducing fractional metrics in existing data-mining techniques can potentially deal with the curse of dimensionality, helping to better distinguish close from distant data points [12] |
| Regularized regression        | Application of PQSQ-based potentials should lead to speeding up the algorithm in case of large datasets |
| Elastic net                   | Same as above                                                               |

Table 1: List of methods which can use PQSQ-based error potentials

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