Multivariate Pade approximation using Quantifier Elimination

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Abstract

Pade approximation is a well-known technique and has a lot of applications in various fields of science and engineering. Given an analytic function, the technique approximates the function by a rational function in a such way that power series of the rational function agrees with the power series of the given function. When given function is univariate, the computation of Pade approximation is fairly simple. However, if given function is multivariate, the computation is rather complex. Besides, in the multivariate case, the rational function approximation often have poles (zeros of the denominator of the rational function) near the expansion point, which make applications of the Pade approximation difficult.

In this paper, we propose a multivariate Pade approximation that utilizes Quantifier Elimination to avoid poles near the expansion point. Quantifier Elimination is a new technique in Computer Algebra, and currently being investigated by many researchers. Given a mathematical formula with quantifiers such as $\forall, \exists$, Quantifier Elimination, in short, computes a quantifier free mathematical formula that is equivalent to the original mathematical formula. In our algorithms, we first set up free parameters in the multivariate Pade approximation, then we use the parameters and Quantifier Elimination to exclude poles near the expansion point. Some numerical examples are given to show effectiveness of our algorithms.

1 Introduction

Pade approximation is a well-known technique and has a lot of applications in various fields of science and engineering ([1],[2]). Given an analytic function, the technique approximates the function by a rational function in a such way that power series of the rational function agrees with the power series of the given function. The approximation is known to be the best approximation of a function by a rational function of given order.

When given function is univariate, the computation is Pade approximation is fairly simple, and a lot of software packages on programing language such as FORTRAN, MATLAB and

Mathematica are available. However, if given function is multivariate, the computation is rather complex. There are many ways to generalize univariate Pade approximation to multivariate one, and we need to decide what way to use ([3],[4]). Besides, in the multivariate case, the rational function approximation often have poles (zeros of the denominator of the rational function) near the expansion point, which make applications of the approximation difficult.

In this paper, we adopt Quantifier Elimination to exclude poles near the expansion point. Quantifier Elimination is a comparatively new technique and currently being studied by many researchers in various fields of science ([5]), although the research on Quantifier Elimination started in Computer Algebra.

Given a mathematical formula with quantifiers such as $\forall, \exists$, Quantifier Elimination, in short, computes a quantifier free mathematical formula that is equivalent to the original mathematical formula. This implies that we can treat a condition such that a given polynomial does not have zeros in the specified regions, which we utilize in our algorithms.

In our algorithms, we first set up free parameters in the multivariate Pade approximation, then we use the parameters and Quantifier Elimination to exclude poles near the expansion point. Some numerical examples are given to show effectiveness of out algorithms.

The paper is composed as follows; We first briefly explain Pade Approximation in Section 2, and show the problems in multivariate Pade approximation with numerical examples. Then, we show how to solve the problems, using Quantifier Elimination in Section 3. We give some numerical examples to show effectiveness of our algorithms. Lastly, we conclude in Section 4.

2 Pade Approximation

2.1 Univariate case

Given an analytic function $f(x)$, let

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k + \cdots \tag{1}$$

be its power series expansion. (m, n)th Pade approximation is a rational function in the form of

$$\frac{p_0 + p_1 + \cdots + p_m x^m}{1 + q_1 x + q_2 x^2 + \cdots + q_n x^n} \tag{2}$$

whose power series expansion agrees with (1) up to $(m+n)$th power of x. The above rational function is called "Pade approximant" in the rest of the paper. From (1) and (2), we see

$$\left(a_0 + a_1 x + a_2 x^2 + \cdots\right)\left(1 + q_1 x + q_2 x^2 + \cdots + q_n x^n\right) = p_0 + p_1 x + \cdots + p_m x^m. \tag{3}$$

Comparing coefficients of both sides of the above equation, we obtain

$$a_0 = p_0,\ a_1 + a_0 q_1 = p_1,\ \cdots,\ a_r + \sum_{j=1}^{r} a_{r-j} q_j = p_r. \tag{4}$$

Let us illustrate how to determine coefficients p_i, q_j in (1). We set $m = 1, n = 2$. This implies p_0, p_1, q_1, q_2 are unknowns and $p_i = 0\ (i \geq 2),\ q_j = 0\ (j \geq 3)$. Thus, from (4), we obtain

$$a_0 = p_0,\ a_1 + a_0 q_1 = p_1,\ a_2 + a_1 q_1 + a_0 q_2 = 0,\quad a_3 + a_2 q_1 + a_1 q_2 = 0. \tag{5}$$

Solving the above equation, we obtain

$$p_0 = a_0,\ p_1 = a_1 + \frac{a_0(a_1a_2 - a_0a_3)}{-a_1^2 + a0a_2},\ q_1 = \frac{a_0a_3 - a_1a_2}{a_1^2 - a_0a_2},\ q_2 = \frac{a_1a_3 - a_2^2}{a_1^2 - a_0a_2}. \tag{6}$$

Thus, we see

$$f(x) = a_0 + a_1x + a_2x^2 + \cdots \cong \frac{p_0 + p_1x}{1 + q_1x + q_2x^2}, \tag{7}$$

where p_0, p_1, q_1, q_2 are defined by (6). In this way, to compute (m, n)th Pade approximant, we need power series $a_0 + a_1x + a_2x^2 + \cdots$ of $f(x)$ up to $(m + n)$th power of x.

2.2 Multivariate case

Given an analytic function $g(x, y)$, let

$$a_{00} + a_{10}x + a_{01}y + a_{20}x^2 + a_{11}xy + a_{02}y^2 + \cdots + a_{k_1,k_2}x^{k_1}y^{k_2} + \cdots \tag{8}$$

be its power series expansion. We want a multivariate version of the univariate Pade approximant shown above. It is easy to come up with the following straightforward methods.

(a) Apply univariate Pade approximations recursively. First, apply univariate Pade approximations for variable x to $g(x, y)$ and compute a Pade approximant

$$\frac{p_0(y) + p_1(y)x + \cdots + p_m(y)x^m}{1 + q_1(y)x + q_2(y)x^2 + \cdots + q_n(y)x^n}.$$

Then, apply univariate Pade approximations for variable y to the coefficients $p_i(y), q_j(y)$ of x.

(b) Apply univariate Pade approximations for total degree. More concretely, apply univariate Pade approximations for variable t to $g(xt, yt)$ (variable t indicates total degree of variable x and y). Then let $t = 1$.

Although the above two methods seem to be natural, they have the following problem, when applied to real problems;

(i) The order of the Pade approximant tends to be high.

(ii) The Pade approximant often has poles near the expansion point.

Let us illustrate the problems by examples. Let $g(x, y)$ be

$$g(x, y) = (x^2 + xy + x - 2y^2 - y + 1)\cos(x - y), \tag{9}$$

whose power series expansion is given by

$$\begin{aligned} g(x,y) &= 1 - y - \frac{5}{2}y^2 + \cdots + \left(1 + 2y - \frac{3}{2}y^2 + \cdots\right)x + \left(\frac{1}{2} + \frac{3}{2}y + \frac{7}{4}y^2 + \cdots\right)x^2 + \cdots. \\ &= 1 + x - y + \frac{1}{2}x^2 + 2xy - \frac{5}{2}y^2 - \frac{1}{2}x^3 + \frac{3}{2}x^2y - \frac{3}{2}xy^2 + \frac{1}{2}y^3 + \cdots. \end{aligned} \tag{10}$$

Computing $(1,1)$th univariate Pade approximant of $g(x,y)$ for variable x, we obtain

$$\frac{1-y-\frac{5}{2}y^2+\left\{\frac{-4-24y-16y^2+4y^3-53y^4}{4(-2-4y+3y^2)}\right\}x}{1+\left\{\frac{2+6y+7y^2}{2(-2-4y+3y^2)}\right\}x} \tag{11}$$

For each coefficients of x in the above Pade approximant, we compute $(1,1)$th Pade for variable y and obtain

$$\frac{\frac{1-\frac{7}{2}y}{1-\frac{5}{2}y}+\left\{\frac{\frac{1}{2}+\frac{37}{16}y}{1+\frac{5}{8}y}\right\}x}{1+\left\{\frac{-\frac{1}{2}+y}{1-3y}\right\}x}=\frac{(1-3y)\left(-32-16x+92y-34xy+70y^2+185xy^2\right)}{(-2+5y)(8+5y)(2-x-6y+2xy)}. \tag{12}$$

As you can see, the above function has poles near the expansion point $(x,y)=(0,0)$ which makes it difficult to use as an approximation of the original function $g(x,y)$.

Let us try the other method (method (b)) on the same function $g(x,y)$. Since we have

$$g(xt,yt) \;=\; 1+(x-y)\,t+\left(\frac{1}{2}x^2+2xy-\frac{5}{2}y^2\right)t^2+\left(-\frac{1}{2}x^3+\frac{3}{2}x^2y-\frac{3}{2}xy^2+\frac{1}{2}y^3\right)t^3+\cdots,$$

computing $(1,2)$th univariate Pade approximant for variable t, we obtain

$$\frac{1+\left\{\frac{-x^2-10xy+11y^2}{x-7y}\right\}t}{1-\left\{\frac{2(x^2+xy-2y^2)}{x-7y}\right\}t+\left\{\frac{3(x-y)(x^2+2xy+9y^2)}{2(x-7y)}\right\}t^2}. \tag{13}$$

With $t=1$, we see that the above function can be simplified to

$$\frac{-2(-x+7y+x^2+10xy-11y^2)}{2x-14y-4x^2-4xy+8y^2+3x^3+3x^2y+21xy^2-27y^3}. \tag{14}$$

The expansion point $(x,y)=(0,0)$ is a zero of both of numerator and denominator of the above rational function, which also makes it difficult to use as an approximation of the original function $g(x,y)$.

As you can see, in these example, both methods compute the Pade approximants that have poles near the expansion point. To make a Pade approximant practical, we need to exclude poles near the expansion point. To solve the problem, we utilize Quantifier Elimination and propose a method to compute a multivariate Pade approximant that does not have poles near the expansion point.

3 Multivariate Pade approximation with Quantifier Elimination

3.1 Quantifier Elimination

First, we briefly explain Quantifier Elimination. Quantifier Elimination is a new technique in Computer Algebra. Given a mathematical formula with quantifiers $(\forall, \exists)$, Quantifier Elimination computes a quantifier free mathematical formula that is mathematically equivalent to the given mathematical formula.

Let us show you an example. Let $h(x) = ax^2 + bx + c$ and consider a mathematical formula $\forall x \in \mathbf{R},\ h(x) \neq 0$ (as you can see, the formula indicates the condition that $h(x) = 0$ does not have real roots). With Quantifier Elimination, an equivalent mathematical formula to the original formula is computed to be

$$(a = 0 \text{ and } b = 0 \text{ and } c \neq 0) \text{ or } \left(a \neq 0 \text{ and } 4ac - b^2 > 0\right). \tag{15}$$

3.2 Multivariate Pade approximant with free parameters

Let us review the process to compute univariate Pade approximants. We derived equations (4), comparing the coefficients in (3). Thus, let us consider multivariate version of (3).

$$\left(a_{00} + a_{10}x + a_{01}y + a_{20}x^2 + a_{11}xy + a_{02}y^2 + \cdots\right)\left(1 + q_{10}x + q_{01}y + \cdots + q_{n_1,n_2}x^{n_1}y^{n_2}\right) = p_{00} + p_{10}x + p_{01}y + \cdots + p_{m_1,m_2}x^{m_1}y^{m_2}. \tag{16}$$

To make explanation simple, let us set function $g(x, y)$ to $g(x, y)$ in (9) and consider the following problem;

$$\left(1 + x - y + \frac{1}{2}x^2 + 2xy - \frac{5}{2}y^2 + \cdots\right)(1 + q_{10}x + q_{01}y + q_{11}xy) = p_{00} + p_{10}x + p_{01}y \tag{17}$$

In the above equation, we have six unknowns $q_{10}, q_{01}, q_{11}, p_{00}, p_{10}, p_{01}$. Hence, looking coefficients of x, y, x^2, xy, y^2 and the constant term, we can determine these unknowns and obtain

$$q_{10} = -\frac{1}{2},\ q_{01} = -\frac{5}{2},\ q_{11} = 0,\ p_{00} = 1,\ p_{10} = \frac{1}{2},\ p_{01} = -\frac{7}{2}. \tag{18}$$

Thus, we obtain multivariate Pade approximant

$$1 + x - y + \frac{1}{2}x^2 + 2xy - \frac{5}{2}y^2 + \cdots \cong \frac{1 + \frac{1}{2}x - \frac{7}{2}y}{1 - \frac{1}{2}x - \frac{5}{2}y} = \frac{2 + x - 7y}{2 - x - 5y}. \tag{19}$$

The above Pade approximant has poles near the expansion point $(x, y) = (0, 0)$, concretely at $y = -\frac{1}{5}x + \frac{2}{5}$. To exclude poles near the expansion point, we set up free parameters in the Pade approximant. More concretely, we consider the following problem;

$$\left(1 + x - y + \frac{1}{2}x^2 + 2xy - \frac{5}{2}y^2 + \cdots\right)\left(1 + q_{10}x + q_{01}y + q_{20}x^2 + q_{11}xy + q_{02}y^2\right) = p_{00} + p_{10}x + p_{01}y. \tag{20}$$

Looking coefficients of x, y, x^2, xy, y^2 and the constant term, we obtain linear equations

$$p_{00} = 1,\ p_{01} - q_{01} = -1,\ p_{10} - q_{10} = 1,\ -q_{01} + q_{10} - q_{11} = 2,\ -q_{10} - q_{20} = \frac{1}{2},\ q_{01} - q_{02} = -\frac{5}{2}. \tag{21}$$

In the above equation, we have eight unknowns $q_{10}, q_{01}, q_{20}, q_{11}, q_{02}, p_{00}, p_{10}, p_{01}$. We let q_{20}, q_{02} be free parameters and determine six unknowns $q_{10}, q_{01}, q_{11}, p_{00}, p_{10}, p_{01}$. Solving (21) with respect to six unknowns, we obtain

$$q_{10} = -\frac{1}{2} - q_{20},\ q_{01} = -\frac{5}{2} + q_{02},\ q_{11} = -q_{20} - q_{02},\ p_{00} = 1,\ p_{10} = \frac{1}{2} - q_{20},\ p_{01} = -\frac{7}{2} + q_{02}. \tag{22}$$

Thus, we see

$$1 + x - y + \frac{1}{2}x^2 + 2xy - \frac{5}{2}y^2 + \cdots \simeq \frac{1 + \left(\frac{1}{2} - q_{20}\right)x + \left(-\frac{7}{2} + q_{02}\right)y}{1 + \left(-\frac{1}{2} - q_{20}\right)x + \left(-\frac{5}{2} + q_{02}\right)y + q_{20}x^2 + \left(-q_{20} - q_{02}\right)xy + q_{02}y^2}. \quad (23)$$

We can set any real numbers to free parameters q_{20}, q_{02}. For example, if we set $q_{20} = 0, q_{02} = \frac{7}{2}$, we obtain from the above equation

$$1 + x - y + \frac{1}{2}x^2 + 2xy - \frac{5}{2}y^2 + \cdots \simeq \frac{2 + x}{2 - x + 2y - 7xy + 7y^2}. \quad (24)$$

The above Pade approximant does not have any poles for the region

$$\{\ (x,\ y) \mid -1 < x < 1,\ -1 < y < 1\ \},$$

and can be useful as a Pade approximant. In this case, we are lucky enough to find such parameter values $q_{20} = 0, q_{02} = \frac{7}{2}$. However, such nice parameter values may not always be found by hand. Hence, we use Quantifier Elimination to find such values systematically.

3.3 Basic algorithm

Our basic algorithm computes a multivariate Pade approximant that does not have poles near the expansion points. More concretely, computed Pade approximant does not have any poles in the region

$$D(r) = \{\ (x,\ y) \mid x \in \mathbf{R},\ y \in \mathbf{R},\ -r < x < r,\ -r < y < r\ \}, \quad (25)$$

where r (> 0) is a given real number. The following are our **Basic algorithm** for computing a multivariate Pade approximant.

Basic algorithm

(i) Determine the form of Pade approximant (the form should have free parameters).

(ii) Derive linear equations looking at coefficients of (16). Then, compute the solution of the equation and determine Pade approximant $\frac{p(x,y)}{q(x,y)}$.

(iii) Determine real number r (> 0) and compute a quantifier free mathematical formula equivalent to

$$\forall (x, y) \in D(r),\ q(x, y) \neq 0 \quad (26)$$

by Quantifier Elimination. Then, determine free parameters in the Pade approximant so that the parameters satisfy the mathematical formula computed.

Let us show a numerical example of the above **Basic algorithm**. We set function $g(x, y)$ to $g(x, y)$ in (9) and compute a multivariate Pade approximant, following **Basic algorithm**.

Step (i)

We define the form of the Pade approximant to be

$$\frac{p_{00} + p_{10}x + p_{01}y}{1 + q_{10}x + q_{01}y + q_{20}x^2 + q_{11}xy + q_{02}y^2}, \tag{27}$$

where $q_{10}, q_{01}, q_{11}, p_{00}, p_{10}, p_{01}$ are unknowns and q_{20}, q_{02} are free parameters.

Step (ii)

Looking at coefficients of (16) (in this case, that is equal to (20)), we derive linear equations (21). Computing the solution of the equation, we obtain (22). Thus, computed Pade approximant is given by $\frac{p(x,y)}{q(x,y)}$ where $p(x,y), q(x,y)$ are

$$p(x,y) = 1 + \left(\frac{1}{2} - q_{20}\right)x + \left(-\frac{7}{2} + q_{02}\right)y, \tag{28}$$

$$q(x,y) = 1 + \left(-\frac{1}{2} - q_{20}\right)x + \left(-\frac{5}{2} + q_{02}\right)y + q_{20}x^2 + \left(-q_{20} - q_{02}\right)xy + q_{02}y^2. \tag{29}$$

Step (iii)

We let $r = 1$ and compute a quantifier free mathematical formula equivalent to

$$\forall (x,y) \in D(r), q(x,y) \neq 0 \tag{30}$$

by Quantifier Elimination (variable q_{20}, q_{02} are parameters). The result is shown in Fig. 1, where parameter region that satisfies the mathematical formula computed is shown by darker color. From the figure, we can, for example, choose $q_{20} = 0, q_{02} = 3.5$, which gives the same Pade approximant as the one in (24).

3.4 Applied algorithm

In our algorithms, variable r in (25) indicates the distance between the poles of the Pade approximant and the expansion point. In **Basic algorithm**, the value of variable r is determined by user in step (iii). However, it is possible to use variable r as parameters in Quantifier Elimination. More concretely, we skip the process to determine variable r and perform Quantifier Elimination on (26), leaving r as a parameter for Quantifier Elimination. Thus, we obtain the following **Applied algorithm**.

Applied algorithm

(i) Perform step (i) of **Basic algorithm**.

(ii) Perform step (ii) of **Basic algorithm**.

(iii) Compute a quantifier free mathematical formula equivalent to

$$\forall (x,y) \in D(r),\ q(x,y) \neq 0 \tag{31}$$

by Quantifier Elimination (note that variable r is used as a parameter). Then, determine free parameters in the Pade approximant so that the parameters satisfy the mathematical formula computed.

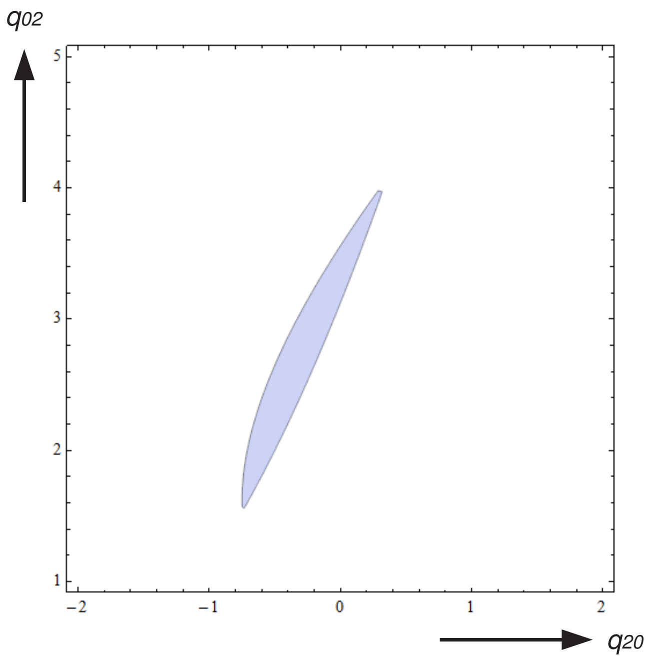

Figure 1: Parameter region satisfying (30)

As you can see, step (i) and step (ii) are the same as those in **Basic algorithm**. Let us illustrate how **Applied algorithm** works. We set function $g(x, y)$ to $g(x, y)$ in (9) and compute a multivariate Pade approximant, following **Applied algorithm**.

Step (i) and **Step (ii)**

We do the same as the numerical example of **Basic algorithm** in the previous subsection and obtain Pade approximant $\frac{p(x,y)}{q(x,y)}$, where $p(x, y), q(x, y)$ are given by (28) and (29).

Step (iii)

We compute a quantifier free mathematical formula equivalent to

$$\forall (x, y) \in D(r), q(x, y) \neq 0 \tag{32}$$

by Quantifier Elimination (variables r, q_{20}, q_{02} are parameters). The result is shown in Fig. 2, where parameter region that satisfies the mathematical formula computed is shown. In this case, we have three parameters r, q_{20}, q_{02} and the figure is three dimensional. As you can see, parameter regions for variable q_{20}, q_{02} becomes smaller as parameter r increases. We can maximize variable r, using the mathematical formula computed by Quantifier Elimination. To maximize variable r, we only have to see that at what value of r, parameter regions for variable q_{20}, q_{02} vanish. Looking at Fig. 2 and the mathematical formula computed by Quantifier Elimination closely, we see that the maximum of r is $r = 1.04$ when $q_{20} = -\frac{1}{2}, q_{02} = \frac{5}{2}$. This gives Pade approximant

$$1 + x - y + \frac{1}{2}x^2 + 2xy - \frac{5}{2}y^2 + \cdots \cong \frac{2(1 + x - y)}{2 - x^2 - 4xy + 5y^2}. \tag{33}$$

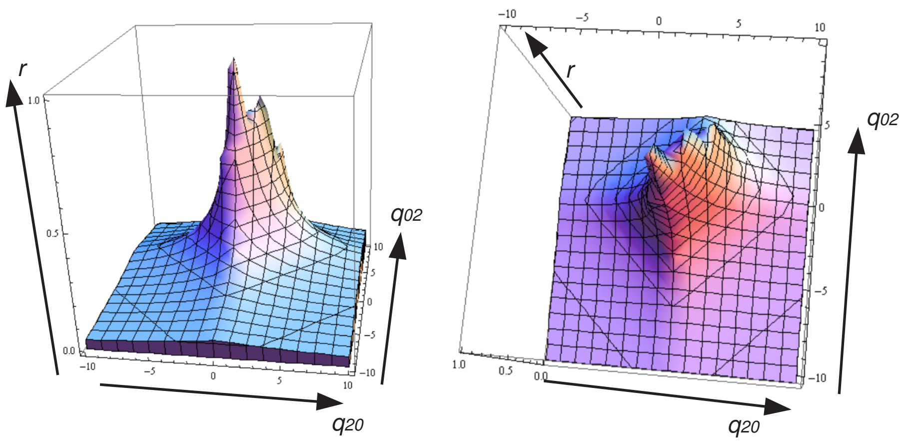

Figure 2: Parameter region satisfying (32)

4 Conclusion

Pade approximation is a well-known technique and has a variety of applications in various fields of science and engineering. Although the computation of a Pade approximant for a univariate function is fairly simple, it is rather complex for a multivariate one. Moreover, a multivariate Pade approximant often has poles near the expansion point, which make the application of the Pade approximant difficult. In this paper, we propose a method to compute a multivariate Pade approximant, utilizing Quantifier Elimination. Proposed algorithm **Basic algorithm** computes a Pade approximant that does not have any poles in the region $D(r) = \{ (x,\ y) \mid x \in \mathbf{R},\ y \in \mathbf{R},\ -r < x < r,\ -r < y < r \}$ for riven real number r. In **Applied algorithm**, variable r is leaved as undetermined and used as a parameters of Quantifier Elimination, which makes the relation between variable r and free parameters in Pade approximants clear. We showed some numerical examples to show effectiveness of the proposed algorithms.

The problem of our algorithms is its practicality. Although our algorithms is theoretically clear, the computation of our algorithm is heavy, since Quantifier Elimination is notorious for its heavy computation ([6]). Hence, our future tasks are (i) application of our algorithms to real problems, (ii) improvement of the efficiency of our algorithms.

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