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TOWARDS A RIGOROUS NUMERICAL STUDY OF THE KOT–SCHAFFER MODEL

SARAH DAY

Georgia Institute of Technology, Department of Mathematics, Atlanta, GA 30332–0190, USA. *E-mail:* sday@math.gatech.edu

ABSTRACT. Sensitive dependence on initial conditions, high or even infinite dimensional phase spaces, and other intrinsic properties of nonlinear dynamical systems present challenges to their study both analytically and numerically. However, the dynamical objects we wish to study are often low dimensional and possess more regularity than the typical elements in the natural phase space. Using these properties, in conjunction with topological tools such as the Conley index, we may overcome many of the initial difficulties to obtain existence results. We will discuss a rigorous numerical method based on these ideas as applied to the Kot–Schaffer model from ecology.

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1. INTRODUCTION

Dynamical systems may exhibit many beautiful and highly complicated behaviors which are often difficult to capture analytically. With recent advances in computing power, numerical analysis is a useful approach, either as an initial investigation or to study systems for which direct analysis is difficult or even impossible. However, numerical computations require a number of properties which some of the more interesting systems do not initially possess. In the very least, they require finite dimensional systems on discretized, compact domains. In addition, sensitive dependence, one of the defining properties of chaotic systems, leads errors to blow up in time. This makes straight forward simulations of the system problematic if not misleading. The subject of this work is to justify the reduction of a high dimensional dynamical system to one that is more computationally friendly yet still captures the essential features of the original system. This discussion is based on joint work with Konstantin Mischaikow, Oliver Junge, and Madjid Allili, to be presented in much greater detail in [1].

Two key observations give hope that a reduced system which captures the interesting dynamical properties exists. The first observation is that invariant sets often contain functions which are more regular than the typical functions of the natural phase space. This regularity, which has been shown by many, including [2], to be a

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property of a large number of interesting systems, allows for a restriction of the studied domain to a compact subset. Secondly, dynamical objects of interest are often low dimensional (e.g., fixed points, periodic orbits, homoclinic and heteroclinic orbits, horseshoes). An appropriate Galerkin projection of the full system onto a finite dimensional space should capture such low dimensional objects. This projection is a restriction to what are sometimes refered to as "determining modes". Again, Hale and others have shown that determining modes exist, at least abstractly, for a wide variety of systems (see [2]). As previously noted, these restrictions are essential if one wants to study a system numerically.

The final ingredient in this approach is a topological tool, the Conley index. This index is able to tolerate bounded errors in proving the existence of dynamical objects of various stability types. Performing the Galerkin projection and discretizing the studied domain, not to mention truncations introduced by the computer itself, all contribute to errors in the numerical study of the system. *Error is unavoidable and should be considered as an intrinsic element of the studied system.* For this reason, we actually study multi-valued systems which associate to each element of the domain an image which is a set of elements. This multi-valued system reflects the optimal knowledge of the projection of the full system, given that bounded errors are present. The Conley index is an algebraic topological invariant which can be computed for the multi-valued system. This index can detect the existence of the "coarse" dynamics which exists for any single-valued system contained within the multi-valued system. Finally, by verifying a few extra conditions, the index information may be lifted to the full, original system.

This approach has been used to study both continuous and discrete systems. It was first applied in the context of dissipative PDEs by Mischaikow and Zgliczyński in [5] to study the Kuramoto-Sivashinsky equation. More recently, we have used this approach to prove the existence of periodic orbits, connecting orbits, and horseshoes for the Kot–Schaffer map, an infinite dimensional, discrete system from ecology. For clarity, the following discussion will also refer to the Kot–Schaffer map. It is important to note, however, that the properties one needs to use this approach are satisfied by a wide class of systems. In particular, given an appropriate orthonormal basis (as a starting point for the Galerkin projection), the regularity assumption previously discussed, and that any nonlinearities are polynomial in nature, one may directly apply the following procedure. Each of these properties will be outlined in more detail in the following sections. For a more complete discussion, including a description of the computational implementation of the procedure, see [1].

2. THE MODEL

The general setting will be that of a discrete dynamical system given by $\Phi : X \to X$, where X is a Hilbert space. Further suppose X has an orthonormal basis with respect to which Φ exhibits some level of regularity, and any nonlinear terms are polynomial in nature. Though this description is vague, we will illustrate what is required in practice using the following example.

The Kot–Schaffer [3] model for plants describes the evolution of a population which has distinct growth and dispersal phases. It consists of a map $\Phi : L^2([-\pi,\pi]) \to L^2([-\pi,\pi])$ of the form

$$\Phi[a](y) := \frac{1}{2\pi}\int_{-\pi}^{\pi} b(x,y)f[a](x)dx, \tag{2.1}$$

with dispersal kernel $b(x,y) = b(x-y)$ and a polynomial growth function $f[a] = \sum_{p=0}^{d} c_p a^p$, $c_p \in L^2([-\pi,\pi])$.

Let the kernel $b(x,y)$ be given by $b(x,y) = \sum_{k=0}^{\infty} b_k\phi_k(x-y)$ where $b_k = 2^{-k}$ and $\phi_k(x) = \exp(-ikx)$ is the kth Fourier function. Then $\{\phi_k\}$ is an orthonormal basis for the space, and (b_k,ϕ_k) form eigenvalue/eigenfunction pairs for the linearized operator. Note that the decay of the eigenvalues should lead to contraction in the higher order modes. In addition, invariant sets will exhibit a similar decay property when expanded in this basis. This regularity, which will be stated more explicitly later, is determined by the regularity of the dispersal kernel b and the spatial heterogeneity of the coefficient functions c_p in the nonlinear term.

3. A NEW BASIS AND PROJECTION

Towards our goal of performing a Galerkin projection, we first expand the map in the new basis. Suppose $a = \sum_n a_n\phi_n$ and $c_p = \sum_n c_n^p\phi_n$ are the expansions of $a, c_p \in L^2([-\pi,\pi])$ respectively. Then, expansion of Φ corresponding to a monomial nonlinearity term c_pa^p yields the maps:

$$a_k \mapsto b_k \sum_{n_0,\ldots,n_{p-1}\in\mathbf{Z}} c_{n_0}^p a_{n_1}\ldots a_{n_{p-1}} a_{k-(n_0+\ldots+n_{p-1})}.$$

Though this expansion is given for the Kot–Schaffer map, it is important to note that terms of this form arise from expansions using appropriate bases of a wide variety of systems, both continuous and discrete, with polynomial nonlinearities. The first step in studying the system numerically is to truncate this possibly infinite system. In other words, make a Galerkin projection and consider only a finite number of the coefficients a_k as variables for the studied system. One can show that not only does this truncation make sense dynamically, but also that in practice, the truncated system can yield rigorous information about the original system. To do this we use the regularity of the system to restrict the studied domain to a series of coefficients

a_k with rapid decay. We then rigorously bound the truncated, or neglected, portion of the maps. As will be seen in Section 5, such bounds may be calculated for terms of the form

$$\sum_{n_0,\ldots,n_{p-1}\in\mathbf{Z}} c^p_{n_0} a_{n_1}\ldots a_{n_{p-1}} a_{k-(n_0+\ldots+n_{p-1})}$$

where the a_k exhibit either exponential or polynomial decay.

4. REGULARITY

In order to bound neglected terms, we must first restrict the domain to be studied numerically. This restriction is justified by the regularity of the map with respect to the basis, which induces a decay rule for elements of any invariant set. The following argument shows more explicitly what type of regularity is required for this procedure.

We restrict the domain to a set $Z = \prod_k \tilde{a}_k = W \times \prod_{k\geq M} \tilde{a}_k$ where $a_k \in \tilde{a}_k := [a_k^-, a_k^+]$ and for $k \geq M$, $0 \in \tilde{a}_k$ and $|\tilde{a}_k| = a_k^+ - a_k^-$ satisfies some decay rule. The justification of this restriction is given by the following lemma.

Lemma 4.1. *Any invariant set of the Kot–Schaffer map, Φ, is contained in a set Z of the form given above, where the decay in the higher modes reflects the decay of the eigenvalues, b_k, for the linear operator.*

Proof. Let $a \in L^2([-\pi,\pi])$ with corresponding Fourier expansion $\sum_k a_k\phi_k$. The projection of the image of a onto the kth mode is,

$$\begin{aligned}
<\Phi(a),\phi_k> &= \int_{-\pi}^{\pi} \Phi(a)(y)\phi_k(y)dy \\
&= \int_{-\pi}^{\pi} \frac{1}{2\pi}\int_{-\pi}^{\pi} b(x,y)f[a](x)\phi_k(y)dxdy \\
&= \frac{1}{2\pi}\sum_n b_n \int_{-\pi}^{\pi} \phi_n(x)f[a](x)\left(\int_{-\pi}^{\pi}\phi_n(y)\phi_k(y)dy\right)dx \\
&= b_k\int_{-\pi}^{\pi}\phi_k(x)f[a](x)dx \\
&= b_k <f[a],\phi_k> \\
&\leq \|f[a]\|b_k
\end{aligned}$$

where $\|f[a]\|$ does not depend on k.

In particular, any set which is invariant (forward and backward in time) must be contained in a set of the form of $Z = \prod_k \tilde{a}_k$, where for $k \geq M$, $|\tilde{a}_k| = a_k^+ - a_k^-$ is shrinking according to the contraction given by the eigenvalue b_k. □

In practice the domain intervals are determined by preliminary simulations with a decay rule reflecting the decay found in the eigenvalues for the linear operator.

5. PROJECTIONS AND ERROR BOUNDS

The next natural step is to make a Galerkin projection onto a finite number of modes. Again, simulations give a good guess as to how many of the first modes are required to capture the interesting dynamics. Rigorous verification of the results comes as a final step in the procedure. In our computations using the Kot–Schaffer map the first 5 modes were sufficient.

Now fix m and consider the projection onto the modes a_k with $|k| < m$. It is now necessary to bound the error from the neglected modes $|k| \geq m$. These bounds exploit the decay property of the new restricted domain $Z = \prod_k \tilde{a}_k$ given in the previous section. The eigenvalues given for the Kot–Schaffer model are 2^{-k} so we adopt a polynomial decay rule for the domain Z in this example. For additional error bound computations, including bounds corresponding to exponential decay, see [1].

Consider the more general case when the eigenvalues, b_k, for the linear operator exhibit polynomial decay. In other words, there exist constants $b > 1$ and $B > 0$ such that $|b_k| \leq \frac{B}{|k|^b}$ for all $k \in \mathbf{Z}\backslash\{\mathbf{0}\}$. Again, we assume that the sequence exhibits similar decay to that of the eigenvalues. That is, for some constants $A_s > 0$ and $s > 1$ initially given by simulations, $\tilde{a}_k = \frac{A_s}{|k|^s}[-1,1]$ for all $k > M$. Set $A = \max\{A_s, \max_{a_0 \in \tilde{a}_0} |a_0|, \max_{0<k<M, a_k \in \tilde{a}_k} |k|^s |a_k|\}$. Then $\tilde{a}_k \subseteq \frac{A}{|k|^s}[-1,1]$ for all $k \in \mathbf{Z}\backslash\{\mathbf{0}\}$ and $\tilde{a}_0 \subseteq A[-1,1]$.

Lemma 5.1. *Let* $\alpha = \frac{2}{s-1} + 2 + 3.5 \cdot 2^s$. *Then*

$$\sum_{n_1,\ldots,n_{p-1} \in \mathbf{Z}} \tilde{a}_{n_1} \ldots \tilde{a}_{n_{p-1}} \tilde{a}_{k-(n_1+\ldots+n_{p-1})} \subseteq \begin{cases} \frac{\alpha^{p-1} A^p}{|k|^s}[-1,1] & k \neq 0 \\ \alpha^{p-1} A^p [-1,1] & k = 0. \end{cases}$$

Proof. For $p = 1$ this inequality holds for all k. Now assume that

$$\sum_{n_1,\ldots,n_{p-2} \in \mathbf{Z}} \tilde{a}_{n_1} \ldots \tilde{a}_{n_{p-2}} \tilde{a}_{k-(n_1+\ldots+n_{p-2})} \subseteq \begin{cases} \frac{\alpha^{p-2} A^{p-1}}{|k|^s}[-1,1] & k \neq 0 \\ \alpha^{p-2} A^{p-1} [-1,1] & k = 0. \end{cases}$$

For $k = 0$,

$$\begin{aligned}
\sum_{n_1,\ldots,n_{p-1}} & \tilde{a}_{n_1} \ldots \tilde{a}_{n_{p-1}} \tilde{a}_{k-(n_1+\ldots+n_{p-1})} \\
& \subseteq \left(\sum_{n_1<0} \frac{A}{(-n_1)^s} \alpha^{p-2} A^{p-1} + A\alpha^{p-2} A^{p-1} \right. \\
& \qquad \left. + \sum_{n_1>0} \frac{A}{n_1^s} \alpha^{p-2} A^{p-1} \right) [-1,1] \\
& \subseteq \alpha^{p-2} A^p \left[2 \left(1 + \int_1^\infty t^{-s} dt \right) + 1 \right] [-1,1] \\
& = \alpha^{p-2} A^p \left[\frac{3s-2}{s-1} \right] [-1,1] \\
& \subset \alpha^{p-1} A^p [-1,1].
\end{aligned}$$

The following inequality is needed for the case $k > 0$.

$$\sum_{n=1}^{k-1} \frac{1}{n^s} \frac{1}{(k-n)^s} \leq \frac{3.5 \cdot 2^s}{k^s}.$$

First note that we may assume $k > 2$ since the sum is empty when $k = 1$ and the inequality holds for the single term when $k = 2$.

For $s = 2$,

$$\begin{aligned}
\sum_{n=1}^{k-1} \frac{1}{n^2} \frac{1}{(k-n)^2} & \leq \frac{2}{(k-1)^2} + \int_1^{k-1} \frac{1}{x^2(k-x)^2} dx \\
& \leq \frac{2}{(k-1)^2} + \frac{4}{k^3} \ln|k-1| + \frac{2(k-2)}{k^2(k-1)} \\
& \leq \frac{2}{(k-1)^2} + \frac{6}{k^2} \\
& < \frac{8}{k^2} + \frac{6}{k^2} \\
& = \frac{3.5 \cdot 2^2}{k^2}.
\end{aligned}$$

Here $\frac{2}{(k-1)^2} < \frac{8}{k^2}$ since $k > 2$.

Now assume that

$$\sum_{n=1}^{k-1} \frac{1}{n^{s-1}(k-n)^{s-1}} \leq \frac{3.5 \cdot 2^{s-1}}{k^{s-1}}$$

or, equivalently,

$$\sum_{n=1}^{k-1} \frac{k^{s-1}}{n^{s-1}(k-n)^{s-1}} \leq 3.5 \cdot 2^{s-1}.$$

Then

$$\begin{aligned}\sum_{n=1}^{k-1} \frac{k^s}{n^s(k-n)^s} &= \sum_{n=1}^{k-1} \left(\frac{k}{n(k-n)}\right) \frac{k^{s-1}}{n^{s-1}(k-n)^{s-1}} \\ &\leq \frac{k}{k-1} \sum_{n=1}^{k-1} \frac{k^{s-1}}{n^{s-1}(k-n)^{s-1}} \\ &\leq 2 \cdot 3.5 \cdot 2^{s-1} \\ &= 3.5 \cdot 2^s.\end{aligned}$$

Therefore,

$$\sum_{n=1}^{k-1} \frac{1}{n^s} \frac{1}{(k-n)^s} \leq \frac{3.5 \cdot 2^s}{k^s}$$

for all $s \geq 2$.

Now, for $k > 0$,

$$\begin{aligned}&\sum_{n_1,\ldots,n_{p-1}} \tilde{a}_{n_1} \ldots \tilde{a}_{n_{p-1}} \tilde{a}_{k-(n_1+\ldots+n_{p-1})} \\ &\subseteq \sum_{n_1} \tilde{a}_{n_1} | \frac{\alpha^{p-2} A^{p-1}}{|k-n_1|^s} [-1,1] \\ &\subseteq \left(\sum_{n_1<0} \frac{A}{(-n_1)^s} \frac{\alpha^{p-2}A^{p-1}}{(k-n_1)^s} + \frac{A\alpha^{p-2}A^{p-1}}{k^s} \right. \\ &\qquad \left. + \sum_{n_1=1}^{k-1} \frac{A}{n_1^s} \frac{\alpha^{p-2}A^{p-1}}{(k-n_1)^s} + \sum_{n_1>k} \frac{A}{n_1^s} \frac{\alpha^{p-2}A^{p-1}}{(n_1-k)^s} \right) [-1,1] \\ &\subseteq \alpha^{p-2} A^p \left[\frac{2}{k^s} \left(1 + \int_1^\infty t^{-s} dt \right) \right. \\ &\qquad \left. + \sum_{n_1=1}^{k-1} \frac{1}{n_1^s} \frac{1}{(k-n_1)^s} \right] [-1,1] \\ &\subseteq \alpha^{p-2} A^p \left[\frac{2}{k^s} \left(1 + \frac{1}{s-1} \right) + \frac{3.5 \cdot 2^s}{k^s} \right] [-1,1] \\ &\subseteq \frac{\alpha^{p-2} A^p}{k^s} \left[\frac{2}{s-1} + 2 + 3.5 \cdot 2^s \right] [-1,1] \\ &= \frac{\alpha^{p-1} A^p}{k^s} [-1,1].\end{aligned}$$

The case $k < 0$ may be reduced to the previous case via change of indices. □

We may extend this argument to the maps corresponding to ca^p provided that the expansion of the coefficient function also exhibits polynomial decay.

Corollary 5.2. *If there exists a constant C such that $c_n \in \tilde{c}_n := \frac{C}{|n|^s}[-1,1]$ for all n, then*

$$\sum_{n_0,n_1,\ldots,n_{p-1}\in\mathbf{Z}} \tilde{c}_{n_0}\tilde{a}_{n_1}\ldots\tilde{a}_{n_{p-1}}\tilde{a}_{k-(n_0+\ldots+n_{p-1})} \subseteq \begin{cases} \frac{\alpha^p A^p C}{|k|^s}[-1,1] & k \neq 0 \\ \alpha^p A^p C[-1,1] & k = 0. \end{cases}$$

These computations represent outer bounds for the image of the restricted domain Z and are used in a number of different ways. First, refinements of the computations yield even better error bounds for the truncations due to the Galerkin projection (see [1]). As previously mentioned, these error terms will be included in the multi-valued map to be studied numerically. Secondly, the error bounds can be used to control what is happening in the higher order modes. They allow us both to update our initial guess for the domain Z and to verify that the projection of the full map is contracting on the boundary of the set. This second property, shown for the Kot–Schaffer map in the following lemma, will allow us to apply Conley index theory.

Lemma 5.3. *Suppose the nonlinearity is $f(a) = \sum_{p=0}^{d} c_p a^p$ with the expansions of the coefficient functions satisfying the decay rules $c_n^p \in \tilde{c}_n^p := \frac{C_p}{|n|^s}[-1,1]$ for some constants C_p. Then for $k \geq M$, the projection of the image onto the kth coordinate direction exhibits more rapid decay:*

$$< [F_m(Z)], \phi_k > \subset \frac{A_{s+b}}{k^{s+b}}[-1,1]$$

where

$$A_{s+b} \quad = \quad B(C_0 + C_1 A\alpha + \ldots + C_d A^d \alpha^d).$$

Proof. For a fixed $k \geq M$, we have bounds for the projection onto the kth mode of the image of Z under the full map using the bounds for $|b_k|$ and the bounds for the sum given by Corollary 5.2.

$$\begin{aligned} < [F_m(Z)], \phi_k > &= b_k \sum_{p=0}^{d} \sum_{n_0,\ldots n_{p-1}} c_{n_0}^p \tilde{a}_{n_1} \ldots \tilde{a}_{k-(n_0+\ldots+n_{p-1}} \\ &\subseteq \frac{B}{k^b}\frac{1}{k^s}(C_0 + \alpha A C_1 + \ldots + \alpha^d A^d C_d)[-1,1] \\ &= \frac{A_{s+b}}{k^{(s+b)}}[-1,1] \end{aligned}$$

where A_{s+b} is as given in the statement of the lemma. □

By setting the new bounds to be the bounds on the image, we may obtain a faster decay rate while maintaining control of the dynamics on the boundary of the set. This control on the boundary is verification that isolation is preserved in the higher order modes. The property of isolation, which is essential to the Conley index, is defined and discussed in the following section.

6. CONLEY INDEX

The Conley index is an algebraic topological invariant which can detect the existence of coarse, or robust, dynamics. More importantly from a computational point of view, it is able to tolerate a priori bounded errors. Following is a very brief discussion of Conley index theory including some of the basic definitions. For a more detailed description, see [4].

Definition 6.1. A compact set $N \subset X$ is an *isolating neighborhood* for the map $f : X \to X$ if

$$Inv(N, f) \cap \partial N = \emptyset.$$

The isolating neighborhood is a basic building block for Conley index theory. The main idea is that we wish to understand something about the dynamics inside the neighborhood given information about the dynamics on the boundary. The index requires that no part of the associated invariant set $S = Inv(N, f)$ intersects the boundary of the set. If this property holds, we say that S is *isolated* or equivalently that N has the property of *isolation*. Note that isolation is a property which is robust with respect to perturbation.

Definition 6.2. A *multi-valued map*, $F : X \rightrightarrows X$, is a function from a set to its power set.

For our purposes, the multi-valued map is constructed by including the error bounds from Section 5 in the map given by considering only the first m modes as variables. This is the object which represents our optimal knowledge of the projection of the full map onto the first m modes. We call this projection of the full map a *continuous selector* for the constructed multi-valued map.

Definition 6.3. A *continuous selector* for F is a continuous, single-valued function $f : X \to X$ such that $f(x) \in F(x)$ for all $x \in X$.

If N is an isolating neighborhood for F then it is also an isolating neighborhood for any continuous selector f of F. Furthermore, the index information associated to F will hold for any continuous selector f of F. The index is defined in the remaining three definitions.

Definition 6.4. Let S be an isolated invariant set. A pair (N, L) of compact subsets of X is called an *index pair* for an isolated invariant set S if $L \subset N$ and the following three conditions are satisfied:

- $cl(N \backslash L)$ is an isolating neighborhood isolating S,
- $f(L) \cap N \subset L$ (positive invariance),
- $f(N \backslash L) \subset N$ (exit set).

Definition 6.5. The *index map* is the map $f_{N,L} : N/L \to N/L$ defined by

$$f_{N,L}([x]) = \begin{cases} f(x) & \text{if } f(x) \in N \backslash L \\ [L] & \text{otherwise.} \end{cases}$$

Definition 6.6. The *homological Conley index*, $Con_*(S)$, is defined to be the shift equivalence of $H_*(f_{N,L})$.

One may show that this index is well defined in that it does not depend on a particular choice of index pair, so long as the associated invariant set remains the same. The following *Ważewski Property* is one of the first and most basic results:

Theorem 6.7. *If the Conley index of $S = Inv(N, f)$ is nontrivial, then $S \neq \emptyset$.*

This index has a number of useful properties. First, it is an invariant of the associated invariant set $S = Inv(N, f)$. Secondly, it provides rigorous information about the existence and structure of S. For example, one can conclude the existence of periodic orbits, connecting orbits, and horseshoes (in the sense of symbolic dynamics) of various stability types. Efficient algorithms exist for computing index pairs for multi-valued maps as well as the index in low dimensions. Finally, the index can be lifted to higher dimensions, and in fact to the original infinite dimensional space, provided that certain conditions are satisfied. These conditions ensure that the key property of isolation is preserved in constructing the new neighborhood $\tilde{N} := N \times \tilde{a}_k$. Using continuity and compactness arguments the index information lifts to the original system.

7. ERROR REDUCTION

Clearly, the size of the error terms greatly affects the success of this method. If the errors are too large we will not achieve isolation and, therefore, cannot apply the index theory. On the other hand, to produce very small error bounds may prove too costly from a computational perspective. One of the objectives, then, is to decrease the errors just to the point where we may efficiently uncover interesting dynamics.

There are a few techniques for producing error reductions. The first is perhaps the most intuitive–increase the projection dimension. If we include more modes as variables we will decrease the amount of information being thrown away in the truncation. Fortunately, this may be done in an efficient manner which utilizes information previously computed for lower dimensions. Updating, or shrinking, the domain using the computations in Section 5 will also decrease the bound on the error term. Finally, refinements in the error bound computations themselves may adequately improve the bounds.

This method was applied to the Kot–Schaffer model to conclude the existence of periodic orbits, connecting orbits and horseshoes with errors reduced to the level of machine precision. For a more detailed discussion of the techniques and results, please see [1].

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