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# Adaptive space transformation: An invariant based method for predicting aerodynamic coefficients of hypersonic vehicles $\stackrel{\sim}{\sim}$



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# ABSTRACT

When developing a new hypersonic vehicle, thousands of wind tunnel tests to study its aerodynamic performance are needed. Due to limitations of experimental facilities and/or cost budget, only a part of flight parameters could be replicated. The point to predict might locate outside the convex hull of sample points. This makes it necessary but difficult to predict its aerodynamic coefficients under flight conditions so as to make the vehicle under control and be optimized. Approximation based methods including regression, nonlinear fit, artificial neural network, and support vector machine could predict well within the convex hull (interpolation). But the prediction performance will degenerate very fast as the new point gets away from the convex hull (extrapolation). In this paper, we suggest regarding the prediction not just a mathematical extrapolation, but a mathematics-assisted physical problem, and propose a supervised self-learning scheme, adaptive space transformation (AST), for the prediction. AST tries to automatically detect an underlying invariant relation with the known data under the supervision of physicists. Once the invariant is detected, it will be used for prediction. The result should be valid provided that the physical condition has not essentially changed. The study indicates that AST can predict the aerodynamic coefficient reliably, and is also a promising method for other extrapolation related predictions.

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# 1. Introduction

The prediction of aerodynamic coefficients is very important for designing a new hypersonic vehicle. Usually, thousands of wind tunnel tests are carried out to predict its aerodynamic force coefficients before it can really fly in the sky. A number of parameters including free-stream Mach number, total flow enthalpy, free-stream velocity, pressure altitude, free-stream Reynolds number, density ratio across shocks, test gas, and wall-to-total temperature ratio could affect the aerodynamic coefficients (Anderson (2006)). Due to the limitations of laboratory equipments and/or cost budget, it is very difficult, if not impossible, to duplicate all these flight conditions. In many wind tunnel experiments, only a part of them such as Mach number  $M_{\infty}$  and/or Reynolds number  $Re_{\infty}$  could be mimicked, where Mach number is the ratio of flow velocity and the local speed of sound, and

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http://dx.doi.org/10.1016/j.engappai.2015.09.001 0952-1976/© 2015 Elsevier Ltd. All rights reserved. Reynolds number reflects the ratio of inertia and viscous forces. Meanwhile, even for the mimicked parameters, the flight range could not be covered by wind tunnels. These make it very difficult to predict the flight behavior with ground test data. The prediction process is usually referred as ground to flight data correlation, also shorten as ground/flight correlation. During the design of a new hypersonic vehicle, it is an indispensable step.

A number of approximation based methods have been presented for the aerodynamic-coefficient prediction including least squares regression (Morelli and DeLoach, 2003), artificial neural network (Norgaard et al., 1997; Rajkumar and Bardina, 2002) and maximum likelihood method (Lee et al., 2009), and extrapolation (Peterson et al., 1980; Nicolì et al., 2006). We have also suggested an adaptive surrogate model (Luo et al., 2011) to improve the accuracy of approximation. In general, the prediction results of these methods are reliable within the convex hull of known data (interpolation). However, in many cases, the flight parameters could not be covered by wind tunnels. So the prediction needs to be done outside the convex hull (extrapolation). However, the above mentioned methods have poor performance on extrapolation, and their prediction results are not reliable.

Scaling parameter is an entirely different way of data correlation. A scaling parameter is a function of several aerodynamic parameters so

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that it can consider the total effect of these parameters. Several such scaling parameters (Macrossan, 2006), including Knudsen number (suggested by T. von Kármán), Tsien's parameter (Tsien, 1946), Cheng's rarefaction parameter (Cheng, 1961), and Bird's breakdown parameter (Bird, 1970) have already been proposed. However, these parameters are valid only for high-speed rarefied flow, and should not be used for data correlation in other cases. For example, to study the aerodynamic performance of near-space hypersonic vehicles, these parameters are no longer applicable because the flow around them is not a rarefied. Meanwhile, there is no such alternative scaling parameter available to describe the hypersonic near-space flight flow, and even worse, it is very difficult to get any of such scaling parameter. Usually, it requires strong expertise and experience to get a new scaling parameter.

In this work, we found the above mentioned scaling parameters share the common ideas, and they could be unified in the sense of space transformations. Based on this discovery, a new method, referred to as adaptive space transformation (AST), is proposed. The AST provides a self-learning scheme that can automatically generate new scaling parameters. It aims at detecting an invariant relation by analyzing all of the test data available under the supervision of physicists. Once the invariant relation is detected, it will be used for prediction. The prediction result should be reliable provided that its underlying physical nature remains unchanged (thus the invariant relation still holds). Comparisons and applications are also carried out to confirm the prediction capability of AST.

#### 2. Observation and discussion of existing scaling parameters

# 2.1. Observation

As above mentioned, various scaling parameters, including Knudsen number *Kn*, Tsien's parameter (Tsien, 1946), Cheng's rarefaction parameter (Cheng, 1961), and Bird's breakdown parameter (Bird, 1970) have been proposed to study the high-speed rarefied flow. Macrossan (2006) has analyzed their relationships and evaluated their performance on correlating drag on bodies in rarefied high-speed flow with



**Fig. 1.** Correlated results with existing scaling parameters and an ideal one. (a) (Macrossan, 2006, Fig. 1) Correlated data with Knudsen number: Kn, which is proportional to  $M_{\infty}/Re_{\infty}$ . (b) (Macrossan, 2006, Fig. 3) Correlated data with Tsien's parameter:  $M_{\infty}/\sqrt{Re_{\infty}}$ . (c) (Macrossan, 2006, Fig. 6) Correlated data with inverse Cheng's parameter:  $M^*M_{\infty}^2/Re_{\infty}$ . (d) Correlated curve (the red smooth curve) with an ideal scaling parameter  $s^* = f^*(M_{\infty}, Re_{\infty}, ...)$ . (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

three data-sets. He has found out that these scaling parameters are proportional to  $M_{\infty}/Re_{\infty}, M_{\infty}/\sqrt{Re_{\infty}}, M_{\infty}^2/Re_{\infty}$ , and  $C^*M_{\infty}^2/Re_{\infty}$ , respectively. Macrossan also concluded that Tsien's parameter is better than the Knudsen number *Kn* for the drag prediction, and Cheng's rarefaction parameter performs the best (see Fig. 1) on the prediction.

In fact, all of these scaling parameters transform the original 3dimensional dataset  $(M_{\infty}, Re_{\infty}, J) \subset \mathbb{R}^3$  of different Mach numbers into a 2-dimensional dataset  $(s, J) \subset \mathbb{R}^2$ , where the scaling parameter *s* is a function of Mach number and Reynolds number,  $s = f(M_{\infty}, Re_{\infty})$  (see Fig. 1). The correlation performance is closely related to the data distribution of the transformed dataset (s, J). Fig. 1 shows that the data distribution in Fig. 1(a) is more scattered than that in Fig. 1(b), and the data distribution in Fig. 1(c) is the most centralized among the three. Comparing these facts to the aforementioned conclusions of Macrossan, we get a scaling parameter that will have a better performance if the transformed data has a more centralized distribution. If, ideally, there exists an optimal correlation formula  $s^* = f^*(M_{\infty}, Re_{\infty})$  such that all transformed data tend to fit a smooth curve (shown in Fig. 1(d)), it will be a perfect scaling parameter.

#### 2.2. Discussion

Famous physicists such as von Kármán and Tsien prefer scaling parameters, rather than approximation based methods, why? What is the potential idea behind scaling parameters? Is it possible to get a better scaling parameter for the study of high-speed rarefied flow? Are these scaling parameters still valid for the study of near-space hypersonic vehicles, in which the free stream is no longer a rarefied flow? If not, how to get a suitable new one? These questions motivate us to develop a new correlation method. The answers are as follows.

(a) For the approximation based methods, the result is hard to interpret and the extrapolation capability is weak. It seems more natural to predict the aerodynamic coefficient J (such as lift coefficient  $C_L$ , drag coefficient  $C_D$ , lift-to-drag ratio  $C_L/C_D$ , pitch-moment coefficient  $C_{mz}$ , etc.) by constructing an approximate model like  $J = F(M_{\infty}, Re_{\infty}, ...)$ , where the approximate model could be created by interpolation. regression, nonlinear fit, artificial neural network, or support vector machine, with test data of wind tunnels. This does work in many applications. However, the result is still hard to interpret because there are several predictor variables involved such as Mach number  $M_{\infty}$ , Reynolds number  $Re_{\infty}$ , etc., and some of them might interfere each other. As a result, the landscape of the response could be a multimodal surface, and it is not easy to tell how these parameters affect the aerodynamic coefficient, even in 3-D space (illustrated in Fig. 2(a)). Scaling parameter can reduce a multi-parameter problem into a simpler one, and the result could be visualized in 2-D space (illustrated in Fig. 2(d)). This makes it easier to interpret and more convenient to use. Another fact about approximation based



**Fig. 2.** Detection of an invariant relation with respect to  $M_{\infty}$  by space transformations. (a) Original test data and their response surface. (b) Transformed data with an initial scaling parameter. (c) Transformed data with a better scaling parameter. (d) Transformed data with a best scaling parameter.

methods is that it is very risky to extrapolate directly with the approximate model. It is helpful to construct a response surface with test data to visually show the overall influence of these parameters on aerodynamic coefficients. But keep in mind that the response surface holds only within the range of test data (interpolation), and it could be very dangerous to use it for prediction outside of test range (extrapolation) for decision makers. Prediction by extrapolation is not reliable and might lead to damaging outcomes. This will be demonstrated in Section 4.1. For these reasons, many famous physicists including von Kármán and Tsien prefer using scaling parameter, rather than approximation based methods for the correlation of aerodynamic coefficient.

- (b) The idea behind scaling parameters is to detect an invariant relation. After the analysis of the above mentioned scaling parameters, we find that they share the common idea, invariant detection, which will be described in detail in Section 3, and thus they could be unified in the sense of space transformations.
- (c) Existing scaling parameters could be improved. As mentioned above, there are already several scaling parameters available, which could be formulated as  $M_{\infty}/Re_{\infty}, M_{\infty}/\sqrt{Re_{\infty}}, C^*M_{\infty}^2/Re_{\infty}$ , etc., to correlate test data of high speed rarefied flow, and M.N. Macrossan has shown that Cheng's rarefaction parameter  $(C^*M_{\infty}^2/Re_{\infty})$  performs the best among them. Note that these parameters were proposed before 1970s, and the formulas are obtained manually. At that time, optimization methods in function space such as genetic programming (Koza, 1992), grammatical evolution (O'Neill and Ryan, 2001), and parse-matrix evolution (Luo and Zhang, 2012) have not yet been proposed. Nowadays, the genetic programming and its variants are ready to use. This makes it possible to get a new better scaling parameter.
- (d) Existing scaling parameters is no longer valid for the aerodynamic-coefficient prediction of near-space hypersonic vehicles. In fact, the flow around the near-space hypersonic vehicles is a continuous flow, not a rarefied flow. Therefore, existing scaling parameters is no longer valid for the aerodynamic-coefficient prediction, and some new scaling parameters need to be derived. However, it is not easy to get any of such scaling parameter. Usually, it requires strong expertise and experience, as well as complicated theoretical analysis, sufficient experimental and computational data verification. This motivates us to design an automatic discovery method to search for optimal scaling parameters in function space. So that it can help the expert derive new scaling parameters more easily.

#### 3. Adaptive space transformation (AST)

## 3.1. Idea behind parameter correlation

It is a remarkable fact that the abscissa in Fig. 1 is neither the Mach number  $M_{\infty}$ , nor the Reynolds number  $Re_{\infty}$ , but a function of them (referred to as scaling parameter in the literature):  $s = M_{\infty}/Re_{\infty}$ ,  $s = M_{\infty}/\sqrt{Re_{\infty}}$ , or  $s = C^*M_{\infty}^2/Re_{\infty}$ , etc. In other words, Tsien et al. prefer considering the total effect of the involved parameters,  $M_{\infty}$  and  $Re_{\infty}$ . With the scaling parameter, the original 3-D data ( $M_{\infty}, Re_{\infty}, J$ ) are transformed into a 2-D space (s, J) (where  $s = f(M_{\infty}, Re_{\infty})$ ,  $J = C_D/C_{D_f}$ ). If the scaling parameter works well, the transformed data will tend to fit a smooth curve. Note that although these data are measured at different Mach numbers, range from 2.95 to 27, their transformed curves could almost overlap with each other. This means the proposed scaling parameter revealed an invariant relation among Mach number  $M_{\infty}$ , Reynolds number  $Re_{\infty}$ , and the drag coefficient J under these conditions.

Here, the invariant does not imply not varying, but the variations share the same path, just like the curves' overlap with each other. Invariant relation, if exists, is the most important feature of a system. In fact, invariant detection has been widely accepted in our daily cognition. For example, there might be many ways to describe an ellipse. But only if an invariant relation such as "The sum of the distances from any point  $P_i$  on a given ellipse to its two foci is a constant (see Fig. 3(a))" is detected, its essential property is grasped.

The invariant relation has a great recovery capability. For example, once the above invariant relation is detected, it can help recover the entire ellipse from a small part of the ellipse. That is, although only a part of an ellipse (e.g., the lower-left 1/4 part) is known, we can predict (recover) the rest of it (see Fig. 3(b)). The recover process is similar to data correlation, in which the objective is also to predict the unknown part by using the information of the known part.

Note that the kernel of the transformation (also known as scaling parameter) f must be determined carefully so that the transformed data (s, J) tend to fit a smooth curve. Unfortunately, it is not easy to get such a suitable scaling parameter in general cases. A trivial transformation, including the projection transform, does not work. For example, Fig. 2(b) shows the projection of a set of 3-D data with different Mach numbers into the 2-D space (s, J). The projected data are four separate curves, and still confusing. So better transformation kernels (i.e., scaling parameters) are needed. A better kernel  $f_b$  could bring these curves closer (Fig. 2(c)). Hopefully, there might be a best scaling parameter  $f^*$  in the function space, which could bring the curves together (Fig. 2(d)).

The four curves of different Mach numbers can overlap with each other. This means the scaling parameter  $s = f^*(M_{\infty}, Re_{\infty})$ 



Fig. 3. Variations and invariant of the ellipse. (a) Detection of an invariant relation. (b) Recovery of the unknown part by the invariant relation.

revealed an invariant relation about Mach number, represented by the overlapped curve. The variation of *J* is not explicitly related to  $M_{\infty}$ . So we can expect that for the data measured at a new Mach number  $M_{\text{new}}$ , its transformed curve J=J(s) (where  $s=f^*(M_{\text{new}}, Re_{\infty})$ ) could also overlap with the previous curves  $J=J(f^*(M_i, Re_{\infty})), i=1, 2, 3, 4$ . Thus, the scaling parameter  $s=f^*(M_{\infty}, Re_{\infty})$  can be used as a correlation parameter for prediction.

In summary, the potential idea behind the existing scaling parameters is that they use space transformations to find an invariant to describe the relation between the aerodynamic coefficient and flow parameters. In this sense, all the existing scaling parameters could be unified.

# 3.2. AST method

As discussed in the above sections, regarding the prediction as a merely mathematical extrapolation might get unreliable result. Scaling parameter makes prediction in a distinct way. It is essentially a physical based method, which uses the invariant of a system for prediction. However, all the existing scaling parameters are obtained manually, and it requires strong expertise and experience to get a working scaling parameter. Perhaps only experienced physicians are qualified for this mission. This limits the application scope of scaling parameters. A new method that can automatically detect the invariant of a system is desired.

With the development of computational intelligence, especially in genetic programming (GP), optimization in function space becomes feasible. This makes it possible to detect the kernel of space transformation (scaling parameter) automatically. Of course, keeping in mind that the optimization should be supervised by physicists. The physicists interact with GP only before and after the evolution process. For example, the parameter selection, nondimensionalization, and the interval choice should be considered aforehand, and the optimized result should also be chosen carefully. An unsupervised optimization is likely failed to detect an invariant. For example, the flight in Mach 3–7 could be considered as a system, but as the Mach number increases, new physical phenomena such as dissociation and ionization might arise and become non-ignorable gradually. In this case, pure mathematical optimization might result in misleading result.

Therefore, we suggest regarding the prediction as a mathematics-assisted physical problem, and propose an adaptive space transformation (AST) method for the prediction. AST is a supervised self-learning scheme. It tries to automatically detect an

underlying invariant of a system and give a new/better scaling parameter with the known data under the supervision of physicists. Once the invariant is detected, it will be used for prediction.

The optimization of scaling parameter (i.e., kernel of space transformation) in the function space could be driven by any genetic programming (GP) algorithm including the conventional genetic programming (Koza, 1992), grammatical evolution (O'Neill and Rvan, 2001), parse-matrix evolution (Luo and Zhang, 2012). etc. In this work, we use a special version of genetic programming, parse matrix evolution (PME; Luo and Zhang, 2012), since we know every detail of it, which can help ensure its global convergence. In PME, a chromosome is a parse-matrix with integer entries, and the mapping process from the chromosome to its analytical function is based on a mapping table containing terminals and operators. The evolutionary operators are adapted from traditional crossover and mutation. The crossover might be onepoint, two-point, or cut-and-splice in row, and the mutation is a kind of random mutation. The height of the parse-matrix can upper-bound the subtree-level of evolved expression so as to control the complexity of the resulted function.

Of course, the reader could choose any other GPs for the optimization process. Therefore, more detailed implementation and performance of GP itself is beyond the discussion scope of this paper, and we assume that the chosen GP is capable of getting a global optimal function in probability.

To describe a general AST method is difficult. As an illustrative example, suppose we need to detect the invariant about Mach number, an optimal scaling parameter  $f^*$  could be determined in the following steps.

- Divide the original data into different groups according to the Mach number: {(*M<sub>i</sub>*, *Re<sub>i,j</sub>*, *J<sub>i,j</sub>*)| *i* = 1, 2, ..., *N*; *j* = 1, 2, ..., *M<sub>i</sub>*}.
- (2) Construct characteristic curves in 2-D space (see Fig. 4(a)):  $J = \phi_i(s)$ , where  $s = f_k(M_i, Re_{i,j}), i = 1, 2, ..., N; j = 1, 2, ..., M_i$ .
- (3) Optimize and update the transformation kernel  $f_k$  by genetic programming such that the characteristic curves tend to overlap with each other (see Fig. 4(b)).
- (4) Repeat steps (2) and (3) until some stopping criteria are satisfied, and output the best transformation kernel *f*<sup>\*</sup> (as the optimal scaling parameter) and its corresponding characteristic curves.

In Step 2, a trivial kernel (e.g., the projection transform  $f(M_i, Re_{i,j}) = M_i$ ) could be used for the initialization of



Fig. 4. Initial and final state of AST. (a) Characteristic curves of a trivial scaling parameter. (b) Transformed curves with an optimal kernel.

characteristic curves. That is,  $f_0$  could be a random kernel if the user has little knowledge about it. However, a preset  $f_0$  is preferred for an experienced user since a good start might lead to a faster convergence.

The flowchart of AST could be briefly described in Fig. 5.



#### 3.3. Optimization models of AST method

The most important step in adaptive space transformation (AST) is the optimization of the kernel function  $f_k$  in Step (3), in which the objective is to drive the characteristic curves to overlap with each other. To this end, an optimization model that can measure the degree of overlapping is needed, and then the genetic programming could be applied to find an optimal scaling parameter  $f^*$  from the space of continuous functions  $C(\Omega)$ , where  $\Omega$  is a compact set in  $\mathbb{R}^m$ .

Suppose only one parameter *x* needs to correlate, a typical optimization model can be formulated as follows:

$$\min_{f \in C(\Omega)} G(f) = \sum_{i=2}^{N} \sum_{j=1}^{i-1} \int_{a}^{b} \|\phi_{i}[f(x_{i}, y)] - \phi_{j}[f(x_{j}, y)] \|ds/S_{\text{convhull}}$$
(1)

where the function  $z = \phi_i(s)$  describes a characteristic curve in  $\mathbb{R}^2$ , and the function s = f(x, y) is the transformation kernel to be optimized. The symbol  $S_{\text{convhull}}$  denotes the area of the convex hull of all transformed data { $(f(x_i, y_{i,j}), z_{i,j})|j = 1, 2, ..., m_i$ }. It is used only for nondimensionalization. The value of the objective function G(f)shows how close the characteristic curves are. Each characteristic curve is determined by a subgroup of the test data with  $x_i$  fixed: { $(x_i, y_{i,j}, z_{i,j})|j = 1, 2, ..., m_i$ }. The characteristic curve can be constructed by any of a robust approximation method such as fitting or regression.

When more parameters, i.e.,  $x_1, x_2, ..., x_m$ , need to correlate, a similar optimization model can be formulated in high dimensional space as follows.

Let the vector  $X = (x_1, x_2, ..., x_m), Y = (y_1, y_2, ..., y_n)$ , and  $S = (s_1, s_2, ..., s_p)$ , then

$$\min_{f \in \mathcal{C}(\Omega)} G(f) = \sum_{i=2}^{N} \sum_{j=1}^{i-1} \int_{\mathbb{S} \subset \mathbb{R}^p} \|\phi_i[f(X_i, Y)] - \phi_j[(X_j, Y)] \| dS/V_{\mathbb{S}}$$
(2)

where the function  $z = \phi_i(S)$  describes the characteristic hypersurface in  $\mathbb{R}^{p+1}$  with fixed  $X_i$  such that it fits its subgroup data  $\{(X_i, Y_{ij}, z_{ij}) | j = 1, 2, ..., m_i\}$ , and the function  $S = f(X, Y)(f : \mathbb{R}^{m+n} \mapsto \mathbb{R}^p)$  is the transformation kernel to be optimized. The symbol  $V_{\mathbb{S}}$  denotes the volume of the convex hull of all transformed data. The value of the objective function G(f) shows how close the characteristic hyper-surfaces are. Here the characteristic hyper-surfaces could also be constructed by any of a robust approximation method such as fitting or regression.

#### 3.4. Properties of kernel function

It is noteworthy that the optimal scaling parameter might be not unique. In addition, we have the following conclusion.

**Proposition 3.1.** Let the transformation kernel  $s = f^*(x, y)$  be an optimal scaling parameter. Then its nontrivial function  $F(f^*(x, y))$  is still an optimal one.

A typical example is as follows. If the scaling parameter  $f^*$  is perfect, i.e.,  $G(f^*) = 0$ , which means the characteristic curves is already overlapped as a single smooth curve (e.g., Fig. 6(b)). Therefore, under the nontrivial map of the composite function F(s) = F(f(x, y)), the transformed curve of the smooth curve should still be a smooth curve (see Fig. 6(c) and (d)).

Although the optimal scaling parameter is not unique, its capability of prediction is not affected. In fact, any one of the optimal scaling parameter can be used as the correlation parameter for prediction.

This is similar to the ellipse case mentioned above, where the invariant is also not unique. As an example, another invariant can be described as "the eccentricity of a given ellipse *e* is a constant". This invariant could also be used to predict the unknown part of the ellipse with a piece of it.

#### 3.5. Practical tricks and discussion

Note that there might be an offset between curves after the transformation, as can be seen from Figs. 2 and 6. In practical implementations, the offset must be restrained. The penalty function method (Mezura-Montes and Coello, 2011) has been used to suppress it in this work.

Another issue about AST method is that the complexity of the scaling parameter must be controlled. Otherwise, its performance will degenerate into that of nonlinear fit or regression. In this paper, the complexity is used as the second objective function, and the trade-off between the overlap degree of transformed curve and the complexity of kernel function is analyzed by multi-objective optimization method. Only the *knee* of Pareto front (Bechikh et al., 2011) is selected as the best scaling parameter.

For a given system, the invariant does not always exist. The proposed method is more suitable for those problems with invariant. However, in case the desired invariant does not exist, AST can help to get a best scaling parameter, which, in the worst case, is a fitting function.

## 4. Prediction results

Prediction capability, especially when the point to predict lies outside of the known range (extrapolation), is the most important feature of an correlation method. In this section, the prediction capability of adaptive space transformation (AST) is tested by comparing with two state-of-the-art approximate based methods, support vector machine (SVM) and artificial neural network (ANN), since both of the methods have been used for predicting the aerodynamic coefficients (Ravikiran and Ubaidulla, 2004; Norgaard et al., 1997; Rajkumar and Bardina, 2002). The proposed AST method is then applied to two real world problems. One is to improve the existing scaling parameters *Kn*, and the other is to



Fig. 6. A typical example with three perfect scaling parameters. (a) Projection of original data. (b) Transformed curves with a perfect scaling parameter. (c) Transformed curves with the square of the perfect scaling parameter. (d) Transformed curves with another function of scaling parameter.

detect a new scaling parameter for the drag prediction of a sharp cone at hypersonic speeds.

#### 4.1. Test of prediction capability

The toy problem,  $z = x^2 + y^2$ , is used to compare the prediction capability of AST with SVM and ANN. For all of the three methods, the learning set consists of 121 sample points, which are uniformly distributed in  $[-3, 3] \times [-3, 3]$ , while the set to predict is spread across the region  $[-6, 6] \times [-6, 6]$ . In this case, most of the points to predict (about 75%) lies out side of the known range. The predicted surfaces are shown in Fig. 7(a), (c) and (e). To show the performance of these methods more clearly, a test set of 625 points uniformly distributed in  $[-6, 6] \times [-6, 6]$  is taken to show the prediction deviation of each method (see Fig. 7(b), (d) and (f).

In this work, the genetic programming method used in AST is parse matrix evolution (PME), and the characteristic curves are constructed with an improved version of Kriging regression method, DACE (Lophaven et al., 2002). The SVM used in this work is a specialized version for regression, referred to as  $\epsilon$ -SVR in Chang and Lin (2011), with the kernel type of radial basis function (RBF). Another variant of SVM,  $\nu$ -SVR, is also tested on this problem. The parameters of SVR are set to their suggested default values. The ANN used in this work is a specialized version of the feed forward network for fitting an input-output relationship (de

Jesús and Hagan, 2007; Horn et al., 2009). The hidden layer size is set to 10. The sample data are divided into three parts for training, validation, and testing. The percentages are 70%, 15% and 15%, respectively.

Fig. 7 shows that all these methods work well to predict the value at the new point within the range the sampled region, but difficult to predict outside of the known range. The predicted value of  $\epsilon$ -SVR is far from its actual one outside the convex-hull (see Fig. 7(b)). The rescaled mean squared error  $1 - R^2$  is 0.079 for the test data within the convex-hull of samples (red in figure), and 2.061 for all the test data.  $\nu$ -SVR has a similar performance. The  $1-R^2$  is 0.0866 within the convex-hull, and 2.054 for all. ANN performs much better (see Fig. 7(d)). The  $1-R^2$  is 5.34 × 10<sup>-8</sup> within the convex-hull, and 0.0912 for all. However, if only an invariant is the detected, the proposed AST method works great on all valid regions (see Fig. 7(f)). The  $1-R^2$  is  $1.49 \times 10^{-8}$  within the convex-hull, and 2.56 ×  $10^{-8}$  for all.

### 4.2. Practical applications

Affected by random factors and measurement/computation errors, real-world data are much more complex than the above toy problem. This makes it more difficult to get a working scaling parameter. To test the capability of AST method, two real-world problems are considered. In problem one, the data are read from



**Fig. 7.** Comparison of extrapolation capability of SVR, ANN, and AST. (a) Predicted surface by e-SVR. (b) Prediction deviation of e-SVR. (c) Predicted surface by ANN. (d) Prediction deviation of ANN. (e) Predicted surface by AST. (f) Prediction deviation of AST. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

Fig. 1 in Macrossan (2006). Since there is already an existing scaling parameter, the Knudsen number Kn, the objective in this work is to find a better scaling parameter that could bring the transformed curves (of different Mach numbers, see Fig. 8) closer. From Fig. 8(b)–(d), we can see that the scaling parameter could be improved better and better by AST.

Although  $f_3$  is the best so far scaling parameter we could find, the transformed curves could not overlap each other. This means that the scaling parameter  $f_3$  is not a perfect one, and the combination of (*Kn*, *M*) is not suitable for constructing an scaling parameter. However, a better scaling parameter could be expected if more information of the data, e.g., Reynolds number, is available.



**Fig. 8.** Improvement of an existing scaling parameter by AST. (a) Correlated data with Kn. (b) Correlated data with  $s = f_1(Kn, M)$ . (c) Correlated data with  $s = f_2(Kn, M)$ . (d) Correlated data with  $s = f_3(Kn, M)$ .

The second problem is to find a scaling parameter for drag prediction of a sharp cone with 10° half-angle. The full length of the cone is 1.5 m. The scale of models ranges from 0.1° to 1.0°. The learning and test data are all obtained by computational fluid dynamics (CFD) simulation. For the test data, the Mach number of free stream ranges from 4 to 9, temperature from 50 K to 250 K, pressure from 560 Pa to 12 560 Pa, angle of attack (AoA) from 0° to 15°. However, the learning data has a much smaller range. All parameters are shrunk to their lower half part except the AoA. To get a reasonable result. 1024 cases are simulated, and 24 of outliers are removed. A part of them with smaller parameters are assigned to the learning set, and the others are used for testing the prediction capability of AST. All the data are aligned to 8 degree of AoA (this process is beyond the scope of this paper) for the invariant detection. Only non-dimensional parameters, Mach number and Reynolds number are considered to be correlated. Based on previous studies, the Reynolds number is transformed with a logarithmic function  $Log_{10}(\cdot)$ , and each component of the data is then linearly mapped to the interval [1, 2]. Or, more specifically, the minimum xmin and maximum values xmax of each parameter is normalized to [ymin, ymax] by the formula y=(ymax - ymin) \* (x - xmin) / (xmax - xmin) + ymin, where ymin = 1,and ymax=2. For example, the normalized Mach number  $M = (2-1)*(M_{\infty}-4)/(9-4) + 1 = (M_{\infty}-4)/5 + 1$ . Under the above conditions, Reynolds number  $Re_{\infty} \in [1.47E6, 3.69E9]$ . So we get

 $\log_{10}(Re_{\infty}) \in [6.17, 9.57]$ , and the normalized Reynolds number  $Re = (\log_{10}(Re_{\infty}) - 6.17)/3.4 + 1.$ 

Using the information from the 200 learning cases of smaller parameters, a new scaling parameter  $s = Re \cdot (1-M)$  is obtained by AST. It can transform the learning data into a smooth curve approximatively (see Fig. 9(a)). With this scaling parameter, the other 800 cases, most of them lies outside of the convex hull of the learning data, are predicted. The prediction results are compared with that of their corresponding CFD cases, the deviations are shown in Fig. 9(b). It shows that the prediction results agree well with CFD, no matter whether the case is inside (interpolation) the range of learning set or not (extrapolation). The rescaled mean squared error  $1 - R^2$  inside and outside of the convex-hull are 0.0018, and 0.0021, respectively.

Although AST works great on these problem, the extrapolation capability of AST should not be exaggerated. Keeping in mind that the extrapolated result is reliable only if the system has not essentially changed (so that the invariant still holds). For example, with the increase of flight speed, say  $M_{\infty} > 15$ , the real gas effect will become more and more important, and its influence on the coefficient of aerodynamic forces might be non-ignorable. In this case, the above scaling parameter might be inapplicable and should be improved. Here, whether the system has essentially changed or not should be decided by practical physicists. The decision process is beyond the scope of this paper.



Fig. 9. A best scaling parameter and its performance on cone-drag prediction. (a) A best scaling parameter for cone drag prediction. (b) Prediction deviation of AST.



**Fig. 10.** Prediction deviation of ANN (a) and *e*-SVR (b), inside and outside the convex-hull. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this paper.)

As a comparison, ANN and  $\epsilon$ -SVR are also applied to predict the drag coefficient  $C_A$  of the sharp cone (see Fig. 10). The study shows that both of the algorithms predict well inside the convex-hull of samples (red in figure). The rescaled mean squared error  $1 - R^2$  is 0.0075 and 0.0071, respectively. But the prediction performance degenerates greatly outside the convex-hull. The rescaled mean squared error  $1 - R^2$  is 0.1032 and 0.1457, respectively.

# 5. Conclusion

We found that the existing scaling parameters are essentially space transformations to detect invariant of the high-speed rarefied flow. Based on this discovery, a new method, referred to as adaptive space transformation (AST), is proposed for the prediction of aerodynamic coefficients. AST tries to detect an invariant relation of the system by analyzing the known data with genetic programming. Once the invariant relation is detected, it will be used for prediction. The prediction result should be reliable provided that the flow around the hypersonic vehicles has not essentially changed, i.e., no new physical phenomenon, such as dissociation or ionization, turns up and becomes non-ignorable. Under this assumption, the underlying physical nature will remain unchanged, and the invariant relation still holds. That is why the extrapolation results of AST are more reliable than that of approximation based methods. Practical results have confirmed its prediction capability.

The complexity of the transformation kernel (scaling parameter) is well controlled in AST. So the resulted formula is usually quite concise (e.g., the above result  $s = Re \cdot (1 - M)$ ). In addition, the transformed data could be visualized in a 2-D plane. So the result is easy to interpret and easy to use.

AST method can help improve existing scaling parameters, as well as derive a new one for new cases automatically. In this sense, existing scaling parameters could be regarded as typical solutions of AST method in the special case (for high-speed rarefied flow). AST provides a reliable method for predicting the aerodynamic coefficient of hypersonic vehicles.

Although AST is proposed under the background of predicting aerodynamic coefficients of hypersonic vehicles, it can be used for other data correlation problems, provided that the underlying invariant of the concerned system exists.

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