The Pade Approximant Based Network for Variational Problems

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ABSTRACT: In solving the variational problem, the key is to efficiently find the target function that minimizes or maximizes the specified functional. In this paper, by using the Pade approximant, we suggest a method for the variational problem. By comparing the method with those based on the radial basis function networks (RBF), the multilayer perception networks (MLP), and the Legendre polynomials, we show that the method searches the target function effectively and efficiently.

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1 Introduction

Many problems arising as variational problems, such as the principle of minimum action in theoretical physics and the optimal control problem in engineering. In solving the variational problem, the key is to efficiently find the target function that minimizes or maximizes the specified functional.

In using non-analytical methods to search for the target function, one faces two problems: firstly, to ensure that the target function is in the range of searching. Secondly, to ensure that the target function can be found under limited computing power and time. The first one is a problem of effectiveness and the second is a problem of efficiency.

The direct method of Ritz and Galerkin [1–3] tries to express the target function as linear combinations of basis functions and reduces the problem to that of solving equations of coefficients. However, the basis function is determined by the boundary condition, as a result, the target function might not be expressed by the basis function and thus be excluded in the range of searching.

One, to improve the method along this line, uses Walsh functions [4], orthogonal polynomials [5–8], and fourier series [9, 10] that are complete and orthogonal to express the target function and converts the boundary condition into a constraint of the coefficient. In that approach, it is the completeness of the basis function that ensures the effectiveness.

Recently, the multilayer perception networks (MLP) is used to solve the variational problem [11–13]. At this case, the functional becomes the loss function and the boundary condition usually becomes an extra term added to the loss function. The MLP is trained to learn the shape of the target function and meet the boundary condition simultaneously.
In that approach, it is the universal approximation property of the MLP [14–18] that
guarantees the effectiveness.

In a word, the completeness of the basis function or the universal approximation prop-
erty of the neural networks already solves the problem of effectiveness. Now the problem
of efficiency is to be considered. For example, in searching the target function with MLP,
the network might fall into the local minimum instead of the global minimum.

In this paper, by using the Pade approximant, we suggest a methods for the variational
problem. By comparing the method with those based on the radial basis function networks
(RBF), the multilayer perception networks (MLP), and the Legendre polynomials, we show
that the method searches the target function effectively and efficiently.

This paper is organized as following. In Sec. 2, we introduce the main method, where
the effective expression of the target function is constructed. In Sec. 3, we solve the
illustrative examples. Conclusions and outlooks are given in Sec. 4.

2 The main method

In this section, we show the detail of constructing an efficient expresion of the target function
based on the Pade approximant.

2.1 the Pade approximant: a brief review

The Pade approximant is a rational function of numerator degree \( m \) and denominator degree
\( n \) [19, 20],

\[
y_{pade}(x) = \frac{\sum_{j=1}^{m} w_j x^j + b_1}{\sum_{i=1}^{n} w'_i x^i + b_2} \tag{2.1}
\]

where \( w_j, w'_i, b_1, \) and \( b_2 \) are parameters. For the sake of convenience, we denote the
structure of the Pade approximant as Pade-[\( m/n \)].

Normally, the Pade-[\( m/n \)] ought to fit a power series through the orders \( 1, x, x^2, \ldots, x^{m+n} \)[19], that is

\[
\sum_{i=0}^{\infty} c_i x^i = \frac{\sum_{j=1}^{m} w_j x^j + b_1}{\sum_{i=1}^{n} w'_i x^i + b_2} + O(x^{m+n+1}) \tag{2.2}
\]

It is an highly efficient tool to approximate a complex real function with only countable
parameters and has wide applications in many problems [21–25]. Here, we use it as an
approximator for the target function.

2.2 The RBF, the MLP, and the Legendre Polynomial: brief reviews

In order to compare the method with those based on the radial basis function networks
(RBF), the multilayer perception networks (MLP), and the Legendre polynomials, we give
a brief review on the RBF, the MLP, and the Legendre Polynomial.

The MLP. The MLP or multilayer feed-forward networks is a typical feed-forward
neural network. It transforms an \( n \)-dimensional input \( x \) to a \( k \)-dimensional output \( y \) and
implements a class of mappings from \( \mathbb{R}^n \) to \( \mathbb{R}^k \) [14–18]. The building block of the MLP is
neurons where a linear and non-linear transforms are successively applied on the input. A collection of neurons forms a layer and a collection of layers gives a MLP. For example, for a one-layer MLP with the number of hidden node, the neuron in the layer, \( l \), the relation between the input \( x \) and the output \( y \) can be explicitly written as

\[
y_{\text{mlp}}(x) = \sum_{i=1}^{l} w'_i \sigma \left( \sum_{j=1}^{n} w_{ij} x_j + b_1 \right) + b_2, \tag{2.3}
\]

where \( y \) is a 1-dimensional output in this case, \( \sigma (x) \) is the non-linear map called the active function and is usually chosen to be \( \tanh(x) \) or \( \text{sigmoid}(x) = \frac{1}{1 + e^{-x}}. \tag{2.4} \)

\( w_{ij}, w'_i, b_1, \) and \( b_2 \) are parameters. By tuning the parameters, the MLP is capable of approximating a target function. For the sake of convenience, we denote the structure of the MLP as MLP-\([l, \sigma (x)]\). E.g., a two-layer MLP with 32 neurons in each layer and activate functions both \( \text{sigmoid}(x) \) is MPL-\([32, \text{sigmoid}], [32, \text{sigmoid}]\).

The RBF. Beyond the MLP, RBF or the radial basis function networks is another typical neural network. Similarly, it also transforms an \( n \)-dimensional input \( x \) to a \( k \)-dimensional output \( y \) and implements a class of mappings from \( \mathbb{R}^n \) to \( \mathbb{R}^k \) [26–28]. However, the structure of the RBF is different: the distance between the input and the center are transformed by a kernel function. The linear combination of the result of the kernel function gives the output \( y \). For example, for a RBF with \( l \) centers, the relation between the input \( x \) and the output \( y \) can be explicitly written as

\[
y_{\text{rbf}}(x) = \sum_{j=1}^{l} w_j \exp \left[ -\sum_{i=1}^{n} \frac{(x_i - c_{ji})^2}{2\sigma_j} \right] + b, \tag{2.5}
\]

where, the kernel function is the Gauss function in this case. The RBF is also a good approximator [26–28] and, at some cases, more efficient than the MLP. For the sake of convenience, we denote the structure of the RBF as RBF-\([l]\).

The Legendre polynomial. In real analysis, a real function can be expressed as a linear combination of basis such as complete polynomials [29]. The Legendre polynomial is complete and orthogonal. It satisfies the recurrent relations [30]

\[
P_{n+1}(x) = \frac{2n+1}{n+1} xP_n(x) - \frac{n}{n+1}P_{n-1}(x) \tag{2.6}
\]

for \( n = 1, 2, 3, \ldots \), where \( P_j(x) \) is Legendre polynomial of order \( j \), \( P_0(x) = 1 \), and \( P_1(x) = x \). In this work, we express the target function as

\[
y_{\text{legend}}(x) = \sum_{j=1}^{m} w_j P_j(x) + b \tag{2.7}
\]

with \( w_j \) and \( b \) being parameters. For the sake of convenience, we denote the structure as Leg-\( m \).
The power polynomial. For the reader, the power polynomial is a familiar tool to approximate a function. For example, the Taylor expansion, a textbook content, is based on it. Here, in order to show that the methods such as the MLP and the RBF are nothing mysterious but merely an approximator, we give the result based on the power polynomial. We express the target function as

\[ y_{\text{poly}}(x) = \sum_{j=1}^{m} w_j x^j + b, \quad (2.8) \]

where \( w_j \) and \( b \) are parameters. We show that the neural-network method differs from the power-polynomial method only in efficiency. For the sake of convenience, we denote the structure as Poly-\( m \).

2.3 The expression of the target function

In searching the target function that minimizes or maximizes the specified functional numerically, the parameter is tuned to shape the output function. However, the boundary condition might reduce the efficiency, because it becomes an extra constraint on the parameter, i.e., the parameter now is tuned not only to shape the function, but also to move the function to the fixed point. In this section, we suggest a expression for the target function which has the universal approximation property and satisfies the boundary condition automatically. With this approach, the boundary condition is no more an extra constraint on the parameter.

There are various kinds of boundary conditions in the variational problem. Here, without loss of generality, we focus on 1-dimensional problems with the fix-end boundary condition.

The boundary factor. We introduce the boundary factor,

\[ \text{bound}(x) = (x - x_a)^{m_a} (x_b - x)^{m_b}, \quad (2.9) \]

where \( m_a \) and \( m_b \) are parameters. \( x_a \) and \( x_b \) are boundaries of \( x \). We, for the sake of convenience, rewrite the output of Eqs. (2.1)-(2.8) as

\[ y_{\text{net}}(x) = \begin{cases} y_{\text{pade}}(x) \\ y_{\text{MLP}}(x) \\ y_{\text{RBF}}(x) \\ y_{\text{legendre}}(x) \\ y_{\text{poly}}(x) \end{cases}. \quad (2.10) \]

Multiplying the boundary factor, Eq. (2.9), to the output \( y_{\text{net}}(x) \) ensures that the output function passes through points \((x_a, 0)\) and \((x_b, 0)\).

The construction. In order to pass through the fix-end points \((x_a, y_a)\) and \((x_b, y_b)\), we add a function

\[ g(x) = x \ast \frac{y_b - y_a}{x_b - x_a} + \frac{x_b y_a - y_b x_a}{x_b - x_a} \quad (2.11) \]

to the output. Finally, the expression of the target function reads

\[ y_{\text{net}_\text{final}}(x) = y_{\text{net}}(x) \ast \text{bound}(x) + g(x). \quad (2.12) \]
Eq. (2.12) inherits the good approximate ability from the Pade approximant, the MLP and so on and passes through the fixed-end point simultaneously.

2.4 The loss function and the learn algorithm

The loss function. The specified functional now read

\[ J = \int_{x_a, y_a}^{x_b, y_b} dx F \left[ y_{\text{final}}(x), y'_{\text{final}}(x), \ldots \right], \tag{2.13} \]

where \( F \) is the specified function of \( y_{\text{final}}(x), y'_{\text{final}}(x) \), and so on. In order to conduct a numerical computation, Eq. (2.13) is approximated by a summation

\[ \text{loss} = \frac{(x_b - x_a)}{N} \sum_{i=1}^{N} F \left[ y_{\text{final}}(x_i), y'_{\text{final}}(x_i), \ldots \right], \tag{2.14} \]

where \( N \) is the number of sample points, \( x_i \) is sampled uniformly from \((x_a, x_b)\). Thus the variational problem converted into a optimization problem:

\[ \min_{w,b,m} \text{loss.} \tag{2.15} \]

The gradient descent method and the back-propagation algorithm. We use the gradient descent method to find the optimal parameter, e.g., the parameter is updated by the following equation

\[ w_{\text{new}} = w_{\text{old}} + l \frac{\partial \text{loss}}{\partial w} \bigg|_{w=w_{\text{old}}}, \tag{2.16} \]

where \( l \) is the learning rate. \( w_{\text{old}} \) and \( w_{\text{new}} \) are the old and new parameters after one step respectively. In Eq. (2.16), \( \frac{\partial \text{loss}}{\partial w} \) is calculated by the back-propagation algorithm

\[ \frac{\partial \text{loss}}{\partial w} = \frac{\partial \text{loss}}{\partial y_{\text{final}}} \frac{\partial y_{\text{final}}}{\partial w} + \frac{\partial \text{loss}}{\partial y'_{\text{final}}} \frac{\partial y'_{\text{final}}}{\partial w} + \ldots. \tag{2.17} \]

An implementation based on python and tensorflow is given in github. In the implementation, the back-propagation algorithm is automatically processed and the Adam algorithm, a developed gradient descent method is applied.

3 The illustrative example

In this section, we use the method to solve variational problems that are partly collected from the literatures [5–13]

1) The shortest path problem. The functional reads

\[ J = \int_{-1}^{1} \sqrt{1 + (y')^2} dx \tag{3.1} \]

with boundary condition

\[ y(-1) = 0 \text{ and } y(1) = 2. \tag{3.2} \]
Exact results are

\[ y_{exact}(x) = x + 1, \]
\[ J(y_{exact}) = 2\sqrt{2} \approx 2.8284. \] (3.3)

The \( y_{exact}(x) \) is a straight line at this case, however, it does not mean that the task is simple, because to find the target function without any pre-knowledge is much more difficult than to learn to express a known target function.

Numerical results are

| Structure     | number of parameters | \( J(y_{net, final}) \) | Relative error       |
|---------------|----------------------|-------------------------|----------------------|
| Pade-\([5/5]\) | 12                   | 2.8285                  | \(-3.5 \times 10^{-5}\) |
| RBF-\([8]\)   | 25                   | 2.8285                  | \(-3.5 \times 10^{-5}\) |
| MLP-\([8, \text{ sigmoid}]\) | 18                  | 2.8285                  | \(-3.5 \times 10^{-5}\) |
| Leg-10        | 11                   | 2.8274                  | \(-3.5 \times 10^{-4}\) |
| Poly-10       | 11                   | 2.8285                  | \(-3.5 \times 10^{-5}\) |

The efficiency of each method is shown in Fig. (1)

\[ \text{Figure 1. The loss versus the steps of different methods.} \]

From Fig. (1), one can see that the method based on the Pade approximant converges faster than those based on the RBF and the MLP. In the method based on Legendre polynomials and the power polynomials the initial value happens to be the target function.
2) *The minimum drag problem.* The functional reads

\[ J = \int_0^1 yy'^3 \, dx \]

with boundary condition

\[ y(0) = 0 \text{ and } y(1) = 1. \]  
(3.4)

Exact results are

\[ y_{exact}(x) = x^{3/4}, \]
\[ J(y_{exact}) = \frac{27}{64} \simeq 0.4219. \]  
(3.5)

Numerical results are

| Structure   | number of parameters | \( J(y_{net\_final}) \) | Relative error |
|-------------|----------------------|--------------------------|----------------|
| Pade-8/10   | 20                   | 0.4216                   | \( 7 \times 10^{-4} \) |
| RBF-[8]     | 25                   | 0.4217                   | \( 4.7 \times 10^{-4} \) |
| MLP,[[16, sigmoid]] | 34         | 0.4220                   | \( -2.3 \times 10^{-4} \) |
| Leg-15      | 16                   | 0.4218                   | \( 2.3 \times 10^{-4} \) |
| Poly-15     | 16                   | 0.4216                   | \( 7 \times 10^{-4} \) |

The efficiency of each methods are show in Fig. (2)

![Figure 2](image_url)  
Figure 2. The loss versus the step of different methods.
From Fig. (2), one can see the method based on the Pade approximant again converges faster. The method based on the power polynomials converges very slow at this time. Since we have shown that the method is capable to find the target function, in the later examples, we eliminate this method because it converges so slow.

3) A popular illustrative example. The functional reads

\[ J = \int_0^1 (y'^2 + xy') \, dx \]

with boundary condition

\[ y(0) = 0 \text{ and } y(1) = \frac{1}{4}. \]  

(3.6)

Exact results are

\[ y_{\text{exact}}(x) = \frac{1}{2} x \left(1 - \frac{1}{2} x\right), \]

\[ J(y_{\text{exact}}) = \frac{5}{3} \simeq 1.667 \]

Numerical results are

| Structure       | number of parameters | \( J (y_{\text{net, final}}) \) | Relative error |
|-----------------|----------------------|---------------------------------|----------------|
| Pade:8/10       | 20                   | 1.665                           | \( 1 \times 10^{-3} \) |
| RBF:[16]        | 49                   | 1.667                           | 0              |
| MLP:|[16, sigmoid]   | 34                   | 1.665                           | \( 1 \times 10^{-3} \) |
| Leg:15          | 16                   | 1.664                           | \( 2 \times 10^{-3} \) |

The efficiency of each methods are show in Fig. (3)
4) **Example 4.** The functional reads

\[
J = \int_{-\pi/2}^{\pi/2} \left[ y'^2 - 2y \cos \left( x + \frac{\pi}{2} \right) \right] \, dx
\]

with boundary condition

\[
y (\pi/2) = 0 \text{ and } y (-\pi/2) = 0.
\] (3.7)

Exact results are

\[
y_{exact}(x) = \cos \left( x + \frac{\pi}{2} \right) + \frac{2}{\pi} x,
\]

\[
J (y_{exact}) = \frac{4}{\pi} - \frac{\pi}{2} \approx -0.2976.
\] (3.8)

Numerical results are

| Structure     | number of parameters | \( J (y_{net\_final}) \) | Relative error |
|---------------|----------------------|-------------------------|----------------|
| Pade:4/5      | 11                   | -0.2969                 | \(-2 \times 10^{-3}\) |
| RBF:[16]      | 49                   | -0.2968                 | \(-3 \times 10^{-3}\) |
| MLP:[[16, sigmoid]] | 34                   | -0.2968                 | \(-3 \times 10^{-3}\) |
| Leg:15        | 16                   | -0.2965                 | \(-4 \times 10^{-3}\) |

The efficiency of each methods are show in Fig. (4)
5) Example 5. The functional reads

\[ J = \int_0^1 (y'^2 - y^2 - 2xy) \, dx \]

with boundary condition

\[ y(0) = 0 \quad \text{and} \quad y(1) = 0. \]  \hspace{1cm} (3.9)

Exact results are

\[ y_{\text{exact}}(x) = \frac{\sin x}{\sin 1 - x}, \]

\[ J(y_{\text{exact}}) = \cot 1 - \frac{2}{3} \approx -0.0246. \]  \hspace{1cm} (3.10)

Numerical results are

| Structure   | number of parameters | \( J(y_{\text{net \_ final}}) \) | Relative error |
|-------------|----------------------|-----------------|----------------|
| Pade:4/5   | 11                   | -0.0245         | -4 \times 10^{-3} |
| RBF:16     | 49                   | -0.0245         | -4 \times 10^{-3} |
| MLP:[16, sigmoid] | 34             | -0.0245         | -4 \times 10^{-3} |
| Leg:15     | 16                   | -0.0245         | -4 \times 10^{-3} |

The efficiency of each methods are show in Fig. (5)
4 Conclusions and outlooks

In solving the variational problem, the key is to efficiently find the target function that minimizes or maximizes the specified functional. Problems of effectiveness and efficiency are both important. In this paper, by using the Pade approximant, we suggest a method for the variational problem. In this approach, the fix-end boundary condition is satisfied simultaneously. By comparing the method with those based on the radial basis function networks (RBF), the multilayer perception networks (MLP), and the Legendre polynomials, we show that the method searches the target function effectively and efficiently.

The method shows that the Pade approximant can improve the efficiency of neural network. In solving a many-body system numerically in physics, the efficiency of the method is important, because the degree of freedom in such system is large. The method could be used in searching the wave function of a many-body system efficiently. Moreover, it could be used in other tasks, such as the task of classification and translation.

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