A FUNCTION FITTING METHOD

RAJESH DACHIRAJU

HYDERABAD, INDIA
E-mail address: rajesh.dachiraju@gmail.com

Abstract. In this article we describe a function fitting method that has potential applications to machine learning and prove relevant theorems. This function fitting method is a convex minimization problem and can be solved using a gradient descent algorithm. We also provide some analysis on the fitness of the function to the data. The function fitting problem is also shown to be a solution of a linear, weak PDE which contains some global terms. We describe a simple numerical solution using a gradient descent algorithm, that converges uniformly to the actual solution. As the minimization problem is also that of a quadratic form, there also exists a numerical method using linear algebra, instead of the gradient descent method.

1. Introduction

The problem of fitting a function to a given bunch of data, has been a very central problem in machine learning, as in most of the machine learning models, training involves in some way or the other, a need to fit a function to the training data, so that one can predict function values at test data points (data points that are not present in training samples). Some of the classic examples are Linear regression (fitting a straight line or a hyper plane to data), kernel based methods, and Neural networks with RMS loss function. The main problem with linear regression is that the solution is always in the space of hyper planes. The kernel methods [10] need a choice of kernel apriori, and the solution space is governed by the kernel picked. The neural networks solution space is the entire space of continuous functions [9],[1], while this is a huge advantage, the theoretical disadvantages are that the solution is not unique and the optimization is not a convex problem. In this article, we describe a function fitting method, which is a convex minimization problem with a unique solution and the solution space being the entire Sobolev space of continuous functions. We prove relevant theorems and describe numerical solutions that converge uniformly to the actual solution.

2. A FUNCTION FITTING PROBLEM

Let $p_i$, $i = 1, 2, 3, n$, are given interior points of $(0,1)^m$ and $a_i \in \mathbb{R}$, such that $\sum_{i=1}^{n} a_i = 0$. The $p_i$ and $a_i$ constitute the data, to which we need to fit a function.
There exist a class of well understood methods in machine learning, called kernel methods \cite{10}, whose primary drawback is the need to choose kernel apriori, and the function being fitted depends on the kernel chosen apriori. Later came methods that do not need a kernel specification, whose solution space is either the entire Hilbert space of smooth functions or the Sobolev space, like \cite{2}, \cite{5}, \cite{7}, \cite{6}, \cite{8}, \cite{3}, \cite{4} which pose this problem as an extension problem, which make apriori assumption that the function fits exactly on the given data, and involve extending it over entire domain, under some criteria like minimal norm. One major drawback of these methods, the algorithm needs access to all the training data \((p_i, a_i)\), not only at training time (one time work), but also during inference time (called query time), which is not an efficient way in machine learning, as the training data \((p_i, a_i)\) can be huge. In this article, we pose the function fitting problem as a purely minimization problem, which has a unique solution. We use a one time numerical method (training) that will compute the Nyquist sampled version of the solution function (uniformly spaced discrete samples), sampled at a certain frequency of our choice and store the samples. To predict the value at a point not in data (inference), we just need to pick the value at a discrete sample of the solution function, that is closest to the query data point and does not need access to the data \((p_i, a_i)\).

4. Definitions

Let \(M\) denote the set of all continuous functions, defined on \(\Omega = [0,1]^m\), that also meet the periodic boundary condition on the boundary \(\partial \Omega\). Let \(S = M \cap H^k(\Omega)\).

**Definition 4.1.** Define the \(k\)-gradient as
\[
\nabla^k f = \left( \frac{\partial^k f}{\partial x_1^k}, \frac{\partial^k f}{\partial x_2^k}, \ldots, \frac{\partial^k f}{\partial x_m^k} \right)
\]

**Definition 4.2.** Define \(k\)-Laplacian as
\[
\Delta^k f = \sum_{i=1}^{m} \frac{\partial^2 f}{\partial x_i^2}
\]

**Definition 4.3.** Define weak \(k\)-Laplacian as
\[
\Delta^k_W f = v \text{ such that } \int_{\Omega} \phi(x)v(x) \, d^m x = \int_{\Omega} \nabla^k \phi(x) \cdot \nabla^k f(x) \, d^m x \forall \phi \in C^\infty(\Omega) \cap M
\]

5. Minimization Problem

∀\(f \in S\), minimize the functional
\[
C(f) = \|f\|^2_{T^k(\Omega)} + \sum_{i=1}^{n} (f(p_i) - a_i)^2
\]

where
\[
\|f\|^2_{T^k(\Omega)} = \|f\|^2_{L^2(\Omega)} + \lambda \|\nabla^k f\|^2_{L^2(\Omega)}
\]

\(\lambda\) is a positive real constant.

**Theorem 5.1.** For this particular set \(S\), the norm \(\|\cdot\|_{T^k(\Omega)}\) is equivalent to the Sobolev norm \(\|\cdot\|_{H^k(\Omega)}\).
Proof. As the norms $\|\cdot\|_{T^k(\Omega)}$ for different $\lambda \in \mathbb{R}^+$ are equivalent, for this proof we consider only $\lambda = 1$. Let $l = (l_1, l_2, l_3, \ldots, l_m) \in Z^m$ and $\alpha$ a multi-index. Let $u$ be the Fourier series coefficients of $u \in S$

\begin{equation}
(5.3) \quad \|u\|_{H^k(\Omega)}^2 = \|u\|_{L^2(\Omega)}^2 + \sum_{|\alpha| = k} \|D^\alpha u\|_{L^2(\Omega)}^2.
\end{equation}

By plancherel formula

\begin{equation}
(5.4) \quad \sum_{|\alpha| = k} \|D^\alpha u\|_{L^2(\Omega)}^2 = \sum_{|\alpha| = k} \sum_{t \in Z^k} ((2\pi)^k l^\alpha)^2 |\hat{u}_t|^2 = \sum_{t \in Z^k} (|\hat{u}_t|^2 \sum_{|\alpha| = k} ((2\pi)^k l^\alpha)^2)
\end{equation}

By Arithmetic mean-Geometric mean inequality, it can be shown that

\begin{equation}
(5.5) \quad \sum_{|\alpha| = k} ((2\pi)^k l^\alpha)^2 \leq C_k \sum_{i = 1}^m (2\pi l_i)^{2k}
\end{equation}

$C_k$ depending only on $k$. So

\begin{equation}
(5.6) \quad \sum_{|\alpha| = k} \|D^\alpha u\|_{L^2(\Omega)}^2 \leq C_k \sum_{t \in Z^k} (|\hat{u}_t|^2 \sum_{i = 1}^m (2\pi l_i)^{2k}) = C_k \sum_{i = 1}^m (\sum_{t \in Z^k} (2\pi l_i)^{2k} |\hat{u}_t|^2)
\end{equation}

using equation 5.2 and applying Plancherel theorem in reverse

\begin{equation}
(5.7) \quad \|u\|_{L^2(\Omega)}^2 + \sum_{i = 1}^m (\sum_{t \in Z^k} (2\pi l_i)^{2k} |\hat{u}_t|^2) = \|u\|_{T^k(\Omega)}^2
\end{equation}

Therefore

\begin{equation}
(5.8) \quad \|u\|_{H^k(\Omega)} \leq D_k \|u\|_{T^k(\Omega)}
\end{equation}

$D_k$ a constant depending only on $k$. We can easily observe that $\|u\|_{H^k(\Omega)} \geq \|u\|_{T^k(\Omega)}$. Hence the norms are equivalent.

**Theorem 5.2.** Given that $k > \frac{m}{2}$, If $u \in H^k(\Omega)$, then

\begin{equation}
(5.9) \quad u \in L^\infty(\Omega)
\end{equation}

and

\begin{equation}
(5.10) \quad \|u\|_{L^\infty(\Omega)} \leq K \|u\|_{H^k(\Omega)}
\end{equation}

$K$ depending only on $k$ and $m$

**Proof.** Lets express $u$ in terms of its Fourier series coefficients $\hat{u}_l$, $l \in Z^m$, via the Fourier series expansion and then the trick is to multiply by 1 in disguise, with $\langle l \rangle := \sqrt{1 + |l|^2}$

\begin{equation}
(5.11) \quad u(x) = \sum_{l \in Z^m} \hat{u}_l e^{2\pi i l \cdot x} = \sum_{l \in Z^m} \hat{u}_l \langle l \rangle^{-k} e^{2\pi i l \cdot x}
\end{equation}

by Holder,

\begin{equation}
(5.12) \quad |u(x)| \leq \sum_{l \in Z^m} |\hat{u}_l\langle l \rangle^k| \langle l \rangle^{-k} \leq \sqrt{\sum_{l \in Z^m} |\hat{u}_l\langle l \rangle^k|^2} \sum_{l \in Z^m} |\langle l \rangle^{-k}|^2
\end{equation}

By Plancherel theorem, $\sqrt{\sum_{l \in Z^m} |\hat{u}_l\langle l \rangle^k|^2} = \|u\|_{H^k}$ $K = \sqrt{\sum_{l \in Z^m} |\langle l \rangle^{-k}|^2}$ is a constant depending only on $k, n$ and is finite as $k > m/2$. This completes the proof.
Theorem 5.3. Given that $k > \frac{m}{2}$, any sequence in $S$, that converges in the norm $\| \cdot \|_{T^k}$, also converges uniformly to a limit function in $S$.

Proof. Let $\{ f_n \} \to f$ under the norm $\| \cdot \|_{T^k}$, then $\| f_n - f \|_{T^k} \to 0$, so $\| f_n - f \|_{H^k} \to 0$, (as $\| \cdot \|_{T^k}$ is equivalent to $\| \cdot \|_{H^k}$ due to Theorem 5.1) and hence due to Theorem 5.2, $\| f_n - f \|_{L^\infty(\Omega)} \to 0$. So, as this sequence of continuous functions with periodic boundary conditions converges uniformly, the limit function $f$ is also a continuous function with periodic boundary conditions and so $f \in M$. It is evident that $f \in H^k(\Omega)$, so $f \in S$. □

Theorem 5.4. Given that $k > \frac{m}{2}$, the minimizer of the functional $C(f)$ over the set $S$ exists and is unique.

Proof. Let $\delta$ be the infimum of $C(f)$ over the set $S$. So there exists a sequence $\{ f_n \}, f_n \in S$ such that $C(f_n) \to \delta$. Since both terms of $C(f)$ are positive, due to first term, $\{ f_n \}$ is Cauchy under the norm $\| \cdot \|_{T^k}$. Due to theorem 5.3, $S$ is a closed linear subspace of the Hilbert space $H^k$, and with the inner product induced by restriction, is also a Hilbert space in its own right. Hence the sequence $\{ f_n \}$ converges to a limit function $g \in S$ under the norm $\| \cdot \|_{T^k}$. Again due to theorem 5.3, $\{ f_n \} \to g$ pointwise. So $f_n(p_i) \to g(p_i), i = 1, 2, .. N$. Already $\| f_n \|_{T^k} \to \| g \|_{T^k}$, so $C(g) = \delta$. Hence the infimum of $C(f)$ over set $S$ is attained in $S$. Uniqueness follows from the convexity of $C(f)$. □

So for the above given minimization problem, existence and uniqueness of the minimizer in $S$ is proven.

6. Euler-Lagrange Equation

We now derive the Euler-Lagrange equation of the minimization problem posed in earlier section, and show that it is a linear weak PDE with some global terms.

Minimize in $S$,

$$C(f) = \sum_{i=1}^{n} (f(p_i) - a_i)^2 + \| f \|_{L^2(\Omega)}^2 + \lambda \| \nabla f \|_{L^2(\Omega)}^2$$

Deriving the Euler Lagrange equation for the above problem, step by step for each term separately. For any $\phi \in C^\infty(\Omega) \cap M$

$$\frac{d}{ds}|_{s=0} f + s\phi = \frac{d}{ds}|_{s=0} \int_\Omega |f + s\phi|^2 = 2 \int_\Omega \phi f$$

where * can be justified by the dominated convergence theorem.

$$\frac{d}{ds}|_{s=0} \lambda \| \nabla f + s\phi \|_{L^2(\Omega)}^2 = \frac{d}{ds}|_{s=0} \int_\Omega \lambda |\nabla f + s\phi|^2 = 2 \lambda \int_\Omega \nabla f \cdot \nabla f$$

$$\frac{d}{ds}|_{s=0} \sum_{i=1}^{n} (f(p_i) + s\phi(p_i) - a_i)^2 = 2 \sum_{i=1}^{n} (f(p_i) - a_i) \phi(p_i)$$

and putting all terms together, we get the following PDE as the Euler-Lagrange equation for the minimization problem.
\( \lambda \int_{\Omega} \nabla^k \phi (x) \cdot \nabla^k f(x) \, d^m x + \sum_{i=1}^{n} (f(p_i) - a_i) \phi (p_i) = 0 \forall \phi \in C^\infty (\Omega) \cap M \)

using Definition 3, it can also be written as

\( \lambda \int_{\Omega} \phi (x) \Delta^k_{W} f(x) \, d^m x + \int_{\Omega} \phi (x) f(x) \, d^m x + \sum_{i=1}^{n} (f(p_i) - a_i) \phi (p_i) = 0 \forall \phi \in C^\infty (\Omega) \cap M \)

Strictly speaking this is not a pde, due to appearance of global terms like \( f(p_i) \). They are global because \( f(p_i) = \int_{\Omega} f(x) \delta (x - p_i) \).

7. Analysis of Fitness to data

In this section we describe how to control the fitness of the function on data points, by controlling the value of \( \lambda \). Let \( f_\lambda \) be the solution of the Euler Lagrange equation, i.e the minimizer of the minimization problem in 5.

**Theorem 7.1.** If \( f_\lambda \) is the minimizer of \( C(f) \), then

\[ \lim_{\lambda \to 0} f_\lambda (p_i) = a_i, \quad i = 1, 2, \ldots, n \]

and

\[ \lim_{\lambda \to 0} f_\lambda (x) = 0, \quad x \neq p_i, i = 1, 2, \ldots, n \]

**Proof.** Let \( B_r^i \) be balls of radius \( r \) around points \( p_i \), and let \( B^r = \bigcup_{i=1}^{n} B_r^i \)

Given any \( g \in S \), fixing \( g \), we can see that

\[ \lim_{\lambda \to 0} C(g) = \sum_{i=1}^{n} (g(p_i) - a_i)^2 + \| g \|^2_{L^2 (\Omega)} \]

Consider the function

\[ \theta_r = \sum_{i=1}^{n} \phi_i \]

where \( \phi_i \) is a bump function with support on the ball \( B_r^i \) and also \( \phi_i (p_i) = a_i \)

Therefore

\[ \lim_{\lambda \to 0} C(\theta_r) = \sum_{i=1}^{n} (\theta_r (p_i) - a_i)^2 + \| \theta_r \|^2_{L^2 (\Omega)} \]

For any given \( \lambda \), let \( f_\lambda \) denote the minimizer of the functional \( C(f) \). By definition of \( f_\lambda \), \( C(f_\lambda) \leq C(\theta_r) \),

\[ \lim_{\lambda \to 0} C(f_\lambda) \leq \lim_{\lambda \to 0} C(\theta_r) \forall r \]

there by

\[ \lim_{\lambda \to 0} C(f_\lambda) \leq \lim_{r \to 0} \lim_{\lambda \to 0} C(\theta_r) \]

(7.7)
using Equation 7.5, its easy to see that

\[
\lim_{\lambda \to 0} \lim_{r \to 0} C(\theta_r) = \lim_{r \to 0} \left\{ \sum_{i=1}^{n} (\theta_r(p_i) - a_i)^2 + \|\theta_r\|^2_{L^2(\Omega)} \right\} = 0
\]

So using Equations 7.7 and 7.8

\[
\lim_{\lambda \to 0} C(f_\lambda) = 0
\]

Hence each term of \( C(f_\lambda) \) should go to 0 as \( \lambda \to 0 \), which gives the following results

\[
\lim_{\lambda \to 0} \sum_{i=1}^{n} (f_\lambda(p_i) - a_i)^2 = 0
\]

\[
\lim_{\lambda \to 0} \|f_\lambda\|_{L^2(\Omega)} = 0
\]

and

\[
\lim_{\lambda \to 0} \lambda \|\nabla^k f_\lambda\|_{L^2(\Omega)} = 0
\]

As all terms in Equation 7.10 are positive,

\[
\lim_{\lambda \to 0} f_\lambda(p_i) = a_i
\]

which proves the first statement of the theorem.

To prove the undesirable effect, at first from Equation 7.10 and the fact that \( f_\lambda \) satisfies the Euler-Lagrange Equation 6.5,

\[
\lim_{\lambda \to 0} \lambda \int_\Omega \nabla^k \phi(x) \cdot \nabla^k f_\lambda(x) \, d^m x = - \lim_{\lambda \to 0} \int_\Omega \phi(x) f_\lambda(x) \, d^m x \forall \phi \in C^\infty(\Omega) \cap M
\]

By Cauchy-Schwartz inequality, there exists a positive real \( L \) such that

\[
\lambda \int_\Omega \nabla^k \phi(x) \cdot \nabla^k f_\lambda(x) \, d^m x \leq L \lambda \|\nabla^k f_\lambda\|_{L^2(\Omega)}\|\nabla^k \phi\|_{L^2(\Omega)}
\]

using Equations 7.10 and 7.12

\[
\lim_{\lambda \to 0} \lambda \int_\Omega \nabla^k \phi(x) \cdot \nabla^k f_\lambda(x) \, d^m x = 0
\]

Hence from Equations 7.14 and 7.16

\[
\lim_{\lambda \to 0} \int_\Omega \phi(x) f_\lambda(x) \, d^m x = 0 \forall \phi \in C^\infty(\Omega) \cap M
\]

This means that \( \lim_{\lambda \to 0} f_\lambda(x) = 0 \) almost everywhere. To complete the proof of second statement, it remains to be proved that \( \lim_{\lambda \to 0} f_\lambda(x) = 0 \) everywhere other than points \( p_i \), and we conjecture this. \(\square\)
7.1. Trade Off. Although the later statement of Theorem 7.1 seems undesirable effect, it is necessary to ensure smoothness in the vicinity of $\lambda = 0$, and this is ensured by the presence of the term $\|f\|_{L^2(\Omega)}$ in $C(f)$. So there is essentially a trade off between how good a fit we want on the data points, and how good a spread of the function over $\Omega$ (as opposed to concentrating only on data points), and this trade off can be controlled by appropriate choice of the parameter $\lambda$ for the minimization problem.

8. Numerical Solution

Instead of solving the PDE, we directly solve the minimization problem. The minimization problem is convex and hence can be solved using a simple gradient descent algorithm. As $S$ is an Hilbert space, the optimization can be directly applied on Fourier series coefficients (due to Plancheral theorem). Firstly we discretize the domain into uniformly spaced samples sampled at a frequency $\omega$ Hz, and also discretize the data so that the data points fall into one of these samples (If multiple data points fall into same discrete sample, the average of values at data points falling into that sample is taken as the data value of that sample). We then compute the Nyquist sampled version $f_\omega$ of the solution $f$. We do this by expressing $C(f_\omega)$ terms of the DFT (Discrete Fourier Transform) coefficients of $f_\omega$ via Plancheral theorem and minimize $C(f_\omega)$ by applying gradient descent algorithm on the DFT coefficients of $f_\omega$. In this way we numerically compute $f_\omega$, the sampled version of solution $f$ at a sampling frequency $\omega$. By choosing sufficiently high $\omega$ we can compute the sampled version of $f$ to desired accuracy and due to uniform convergence of Fourier series, the numerical solution converges uniformly to the actual solution $f$ as $\omega \to \infty$. Hence the method gives a numerical solution that converges uniformly to the actual solution.

9. Numerical solution using Linear Algebra

There is an alternate solution from Linear algebra, as when we express $C(f_\omega)$ of the minimization problem, in terms of the DFT coefficients of the discretely sampled function $f_\omega$ (it is easy due to Plancheral theorem), and taking derivatives with respect to each of the DFT coefficients and setting them to zero, we get a set of linear equations that are equal in number to the DFT coefficients. Hence this problem can be solved using Linear algebra. Further work need to be done to make this solution faster, using apriori properties of the involved matrices.

10. Storage and Retrieval

We store the discrete samples $f_\omega$ of the solution function $f$ in memory and when a query comes requesting the function value at some point $q_i$, we retrieve the value of $f_\omega$ at the discrete sample point that is nearest to the query point $q_i$. The retrieval time depends only on the sampling frequency $\omega$ and it is $O(\sum \omega_i)$. It is worth noting that the retrieval time does not depend on the data size, but only on sampling frequency $\omega$ and as accuracy increases as $\omega \to \infty$, the retrieval time scales with the desired accuracy rather than the data size.
11. SOME NOTES FROM NUMERICAL EXPERIMENTATION

Choice of $\lambda$ dictates how good a fit the solution function is to the data. If $\lambda$ is low, we get very good fit of data, but if it is too low, despite good fit, we may not like the solution as it would tend to concentrate on the data points. On the other hand if $\lambda$ is high, the function will spread well without concentrating on data points, but if its too high, it will not fit the data well. Good choice of $\lambda$ should be made, for the solution to be good for a given real world problem.

12. APPLICATIONS

This method can be used in Machine Learning, as in almost all problems in this field, there is a direct or indirect need for fitting a function to data. As the functions Machine Learning need not be periodic, this method can be used for non-periodic function, by even symmetric extension of both the domain and the data.

REFERENCES

5. Charles Fefferman and Bo'az Klartag, Fitting a $c^m$-smooth function to data I, Annals of mathematics (2009), 315–346.