

A FUNCTION FITTING METHOD

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1. A FUNCTION FITTING PROBLEM

Let \mathbf{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 \mathbf{p}_i and a_i constitute the data, to which we need to fit a function.

2. EARLIER WORK

Earlier works like [4],[6],[5],[7],[2],[3],[1] 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 data points (\mathbf{p}_i, a_i) , not only at one time work (usually called training), but every time when we need to compute the value of function at a point not in the data (called query time), which is not an efficient way in machine learning, as the data (\mathbf{p}_i, a_i) is 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 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, 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 (\mathbf{p}_i, a_i) .

3. 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 3.1. Define the k -gradient as

$$(3.1) \quad \nabla^k f = \left(\frac{\partial^k f}{\partial x_1^k}, \frac{\partial^k f}{\partial x_2^k}, \dots, \frac{\partial^k f}{\partial x_m^k} \right)$$

Definition 3.2. Define k -Laplacian as

$$(3.2) \quad \Delta^k f = \sum_{i=1}^m \frac{\partial^{2k} f}{\partial x_i^{2k}}$$

Definition 3.3. Define weak k -Laplacian as

$$(3.3) \quad \Delta_W^k f = v \text{ such that } \int_{\Omega} \phi(\mathbf{x}) v(\mathbf{x}) d^m \mathbf{x} = \int_{\Omega} \nabla^k \phi(\mathbf{x}) \cdot \nabla^k f(\mathbf{x}) d^m \mathbf{x} \forall \phi \in C^\infty(\Omega) \cap M$$

4. MINIMIZATION PROBLEM

$\forall f \in S$, minimize the functional

$$(4.1) \quad C(f) = \|f\|_{T^k(\Omega)}^2 + \sum_{i=1}^n (f(\mathbf{p}_i) - a_i)^2$$

where

$$(4.2) \quad \|f\|_{T^k(\Omega)}^2 = \|f\|_{L^2(\Omega)}^2 + \lambda \|\nabla^k f\|_{L^2(\Omega)}^2$$

λ is a positive real constant.

Theorem 4.1. *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 $\mathbf{l} = (l_1, l_2, l_3, \dots, l_m) \in \mathbb{Z}^m$ and α a multi-index. Let $u_{\mathbf{l}}$ be the Fourier series coefficients of $u \in S$

$$(4.3) \quad \|u\|_{H^k(\Omega)}^2 = \|u\|_{L^2(\Omega)}^2 + \sum_{|\alpha|=k} \|D^\alpha u\|_{L^2(\Omega)}^2.$$

By plancherel formula

$$(4.4) \quad \sum_{|\alpha|=k} \|D^\alpha u\|_{L^2(\Omega)}^2 = \sum_{|\alpha|=k} \sum_{\mathbf{l} \in \mathbb{Z}^k} ((2\pi)^k \mathbf{l}^\alpha)^2 |\hat{u}_{\mathbf{l}}|^2 = \sum_{\mathbf{l} \in \mathbb{Z}^k} (|\hat{u}_{\mathbf{l}}|^2 \sum_{|\alpha|=k} ((2\pi)^k \mathbf{l}^\alpha)^2)$$

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

$$(4.5) \quad \sum_{|\alpha|=k} ((2\pi)^k \mathbf{l}^\alpha)^2 \leq C_k \sum_{i=1}^m (2\pi l_i)^{2k}$$

C_k depending only on k . So

$$(4.6) \quad \sum_{|\alpha|=k} \|D^\alpha u\|_{L^2(\Omega)}^2 \leq C_k \sum_{\mathbf{l} \in \mathbb{Z}^k} (|\hat{u}_{\mathbf{l}}|^2 \sum_{i=1}^m (2\pi l_i)^{2k}) = C_k \sum_{i=1}^m \left(\sum_{\mathbf{l} \in \mathbb{Z}^k} (2\pi l_i)^{2k} |\hat{u}_{\mathbf{l}}|^2 \right)$$

using equation 4.2 and applying Plancherel theorem in reverse

$$(4.7) \quad \|u\|_{L^2(\Omega)}^2 + \sum_{i=1}^m \left(\sum_{\mathbf{l} \in \mathbb{Z}^k} (2\pi l_i)^{2k} \hat{u}_{\mathbf{l}}^2 \right) = \|u\|_{T^k(\Omega)}^2$$

Therefore

$$(4.8) \quad \|u\|_{H^k(\Omega)} \leq D_k \|u\|_{T^k(\Omega)}$$

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

Theorem 4.2. *Given that $k > \frac{m}{2}$, If $u \in H^k(\Omega)$, then*

$$(4.9) \quad u \in L^\infty(\Omega)$$

and

$$(4.10) \quad \|u\|_{L^\infty(\Omega)} \leq K \|u\|_{H^k(\Omega)}$$

K depending only on k and m

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

$$(4.11) \quad u(\mathbf{x}) = \sum_{\mathbf{l} \in \mathbb{Z}^m} \hat{u}_{\mathbf{l}} e^{2\pi i \mathbf{l} \cdot \mathbf{x}} = \sum_{\mathbf{l} \in \mathbb{Z}^m} \hat{u}_{\mathbf{l}} \langle \mathbf{l} \rangle^k \langle \mathbf{l} \rangle^{-k} e^{2\pi i \mathbf{l} \cdot \mathbf{x}}$$

by Holder,

$$(4.12) \quad |u(\mathbf{x})| \leq \sum_{\mathbf{l} \in \mathbb{Z}^m} |\hat{u}_{\mathbf{l}} \langle \mathbf{l} \rangle^k| \langle \mathbf{l} \rangle^{-k} \leq \sqrt{\sum_{\mathbf{l} \in \mathbb{Z}^m} |\hat{u}_{\mathbf{l}} \langle \mathbf{l} \rangle^k|^2} \sum_{\mathbf{l} \in \mathbb{Z}^m} |\langle \mathbf{l} \rangle^{-k}|^2$$

By Plancherel theorem, $\sqrt{\sum_{\mathbf{l} \in \mathbb{Z}^m} |\hat{u}_{\mathbf{l}} \langle \mathbf{l} \rangle^k|^2} = \|u\|_{H^k}$ $K = \sqrt{\sum_{\mathbf{l} \in \mathbb{Z}^m} |\langle \mathbf{l} \rangle^{-k}|^2}$ is a constant depending only on k, n and is finite as $k > m/2$. This completes the proof. \square

Theorem 4.3. *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 $\{f_n\} \rightarrow f$ under the norm $\|\cdot\|_{T^k}$, then $\|f_n - f\|_{T^k} \rightarrow 0$, so $\|f_n - f\|_{H^k} \rightarrow 0$, (as $\|\cdot\|_{T^k}$ is equivalent to $\|\cdot\|_{H^k}$ due to Theorem 4.1) and hence due to Theorem 4.2, $\|f_n - f\|_{L^\infty(\Omega)} \rightarrow 0$. 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 $f \in S$. \square

Theorem 4.4. *Given that $k > \frac{m}{2}$, the minimizer of the functional $C(f)$ over the set S exists and is unique.*

Proof. Let δ be the infimum of $C(f)$ over the set S and let it be attained at some $f_0 \in H^k(\Omega)$. As $C(f_0) = \delta$ is finite, this is a rational assumption. Since the point of infimum is unique (due to convexity of $C(f)$) and as $C(f)$ is a sum of two terms, both being atleast semi norms, if a sequence $\{f_n\}, f_n \in S$ such that $C(f_n)$ converges towards the infimum δ , then, due to second term of $C(f_n)$, $f_n(\mathbf{p}_i) \rightarrow f_0(\mathbf{p}_i)$, and due to first term of $C(f_n)$, $\|(f_n - f_0)\|_{T^k} \rightarrow 0$. As δ is an infimum, there exists a sequence $\{f_n\}, f_n \in S$, such that $C(f_n) \rightarrow \delta$. So $\|(f_n - f_0)\|_{T^k} \rightarrow 0$. Using Theorem 4.2, it can be seen that $\|f_n - f_0\|_{L^\infty(\Omega)} \leq K \|(f_n - f_0)\|_{T^k}$. Hence $\|f_n - f_0\|_{L^\infty(\Omega)} \rightarrow 0$. This implies f_0 is continuous and satisfies periodic boundary conditions. Hence $f_0 \in S$ and this proves the existence. Uniqueness follows from convexity of the functional $C(f)$ which is a semi-norm. \square

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

5. 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 ,

$$(5.1) \quad C(f) = \sum_{i=1}^n (f(\mathbf{p}_i) - a_i)^2 + \|f\|_{L^2(\Omega)}^2 + \lambda \|\nabla^k f\|_{L^2(\Omega)}^2$$

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

$$(5.2) \quad \frac{d}{ds}|_{s=0} \|f + s\phi\|_{L^2(\Omega)}^2 = \frac{d}{ds}|_{s=0} \int_{\Omega} |f + s\phi|^2 = 2 \int_{\Omega} \phi f$$

where $*$ can be justified by the dominated convergence theorem.

$$(5.3) \quad \frac{d}{ds}|_{s=0} \lambda \|\nabla^k(f + s\phi)\|_{L^2(\Omega)} = \frac{d}{ds}|_{s=0} \int_{\Omega} \lambda |\nabla^k f + s\nabla^k \phi|^2 = 2\lambda \int_{\Omega} \nabla^k \phi \cdot \nabla^k f$$

$$(5.4) \quad \frac{d}{ds}|_{s=0} \sum_{i=1}^n |f(\mathbf{p}_i) + s\phi(\mathbf{p}_i) - a_i|^2 = 2 \sum_{i=1}^n (f(\mathbf{p}_i) - a_i)\phi(\mathbf{p}_i)$$

and putting all terms together, we get the following PDE as the Euler-Lagrange equation for the minimization problem.

$$(5.5) \quad \lambda \int_{\Omega} \nabla^k \phi(\mathbf{x}) \cdot \nabla^k f(\mathbf{x}) d^m \mathbf{x} + \int_{\Omega} \phi(\mathbf{x}) f(\mathbf{x}) d^m \mathbf{x} + \sum_{i=1}^n (f(\mathbf{p}_i) - a_i)\phi(\mathbf{p}_i) = 0 \forall \phi \in C^\infty(\Omega) \cap M$$

using Definition 3, it can also be written as

$$(5.6) \quad \lambda \int_{\Omega} \phi(\mathbf{x}) \Delta_W^k f(\mathbf{x}) d^m \mathbf{x} + \int_{\Omega} \phi(\mathbf{x}) f(\mathbf{x}) d^m \mathbf{x} + \sum_{i=1}^n (f(\mathbf{p}_i) - a_i)\phi(\mathbf{p}_i) = 0 \forall \phi \in C^\infty(\Omega) \cap M$$

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

6. 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 λ . Let f_λ be the solution of the Euler Lagrange equation, i.e the minimizer of the minimization problem in 4.

Theorem 6.1. *If f_λ is the minimizer of $C(f)$, then (the desirable effect...)*

$$(6.1) \quad \lim_{\lambda \rightarrow 0} f_\lambda(\mathbf{p}_i) = a_i, i = 1, 2, \dots, n$$

and (the undesirable effect...)

$$(6.2) \quad \lim_{\lambda \rightarrow 0} f_\lambda(\mathbf{x}) = 0, \mathbf{x} \neq \mathbf{p}_i, i = 1, 2, \dots, n$$

Proof. Let B_i^r be balls of radius r around points \mathbf{p}_i , and let $B^r = \bigcup_{i=1}^n B_i^r$

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

$$(6.3) \quad \lim_{\lambda \rightarrow 0} C(g) = \sum_{i=1}^n (g(\mathbf{p}_i) - a_i)^2 + \|g\|_{L^2(\Omega)}^2$$

Consider the function

$$(6.4) \quad \theta_r = \sum_{i=1}^n \phi_i$$

where ϕ_i is a bump function with support on the ball B_i^r and also $\phi_i(\mathbf{p}_i) = a_i$. Therefore

$$(6.5) \quad \lim_{\lambda \rightarrow 0} C(\theta_r) = \sum_{i=1}^n (\theta_r(\mathbf{p}_i) - a_i)^2 + \|\theta_r\|_{L^2(\Omega)}^2$$

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

$$(6.6) \quad \lim_{\lambda \rightarrow 0} C(f_\lambda) \leq \lim_{\lambda \rightarrow 0} C(\theta_r) \forall r$$

there by

$$(6.7) \quad \lim_{\lambda \rightarrow 0} C(f_\lambda) \leq \lim_{r \rightarrow 0} \lim_{\lambda \rightarrow 0} C(\theta_r)$$

using Equation 6.5, its easy to see that

$$(6.8) \quad \lim_{r \rightarrow 0} C(\theta_r) = \lim_{r \rightarrow 0} \left\{ \sum_{i=1}^n (\theta_r(\mathbf{p}_i) - a_i)^2 + \|\theta_r\|_{L^2(\Omega)}^2 \right\} = 0$$

So using Equations 6.7 and 6.8

$$(6.9) \quad \lim_{\lambda \rightarrow 0} C(f_\lambda) = 0$$

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

$$(6.10) \quad \lim_{\lambda \rightarrow 0} \sum_{i=1}^n (f_\lambda(\mathbf{p}_i) - a_i)^2 = 0$$

$$(6.11) \quad \lim_{\lambda \rightarrow 0} \|f_\lambda\|_{L^2(\Omega)} = 0$$

and

$$(6.12) \quad \lim_{\lambda \rightarrow 0} \lambda \|\nabla^k f_\lambda\|_{L^2(\Omega)} = 0$$

As all terms in Equation 6.10 are positive,

$$(6.13) \quad \lim_{\lambda \rightarrow 0} f_\lambda(\mathbf{p}_i) = a_i$$

which proves the first statement(desirable effect) of the theorem.

To prove the undesirable effect, at first from equation 6.10 and the fact that f_λ satisfies the Euler-Lagrange Equation 5.5,

$$(6.14) \quad \lim_{\lambda \rightarrow 0} \lambda \int_{\Omega} \nabla^k \phi(\mathbf{x}) \cdot \nabla^k f_\lambda(\mathbf{x}) \, d^m \mathbf{x} = - \lim_{\lambda \rightarrow 0} \int_{\Omega} \phi(\mathbf{x}) f_\lambda(\mathbf{x}) \, d^m \mathbf{x} \forall \phi \in C^\infty(\Omega) \cap M$$

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

$$(6.15) \quad \lambda \int_{\Omega} \nabla^k \phi(\mathbf{x}) \cdot \nabla^k f_\lambda(\mathbf{x}) \, d^m \mathbf{x} \leq L \lambda \|\nabla^k f_\lambda\|_{L^2(\Omega)} \|\nabla^k \phi\|_{L^2(\Omega)}$$

using Equations 6.10 and 6.12

$$(6.16) \quad \lim_{\lambda \rightarrow 0} \lambda \int_{\Omega} \nabla^k \phi(\mathbf{x}) \cdot \nabla^k f_{\lambda}(\mathbf{x}) d^m \mathbf{x} = 0$$

Hence from Equations 6.14 and 6.16

$$(6.17) \quad \lim_{\lambda \rightarrow 0} \int_{\Omega} \phi(\mathbf{x}) f_{\lambda}(\mathbf{x}) d^m \mathbf{x} = 0 \forall \phi \in C^{\infty}(\Omega) \cap M$$

This means that $\lim_{\lambda \rightarrow 0} f_{\lambda}(x) = 0$ almost everywhere. It remains to be proved that $\lim_{\lambda \rightarrow 0} f_{\lambda}(\mathbf{x}) = 0$ everywhere other than points \mathbf{p}_i , and we conjecture this. \square

6.1. Trade Off. Although the later statement of Theorem 6.1 is referred as undesirable effect, it is necessary to ensure smoother solution 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 Ω (as opposed to concentrating only on data points), and this trade off can be controlled by appropriate choice of the parameter λ for the minimization problem.

7. 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 Plancherel theorem). Firstly we discretize the domain into uniformly spaced samples sampled at a frequency ω 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_{ω} of the solution f . We do this by expressing $C(f_{\omega})$ terms of the DFT (Discrete Fourier Transform) coefficients of f_{ω} via Plancherel theorem and minimize $C(f_{\omega})$ by applying gradient descent algorithm on the DFT coefficients of f_{ω} . In this way we numerically compute f_{ω} , the sampled version of solution f at a sampling frequency ω . By choosing sufficiently high ω 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 $\omega \rightarrow \infty$. Hence the method gives a numerical solution that converges uniformly to the actual solution.

8. 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_{ω} (it is easy due to Plancherel 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.

9. STORAGE AND RETRIEVAL

We store the discrete samples f_ω of the solution function f in memory and when a query comes requesting the function value at some point \mathbf{q}_i , we retrieve the value of f_ω at the discrete sample point that is nearest to the query point \mathbf{q}_i . The retrieval time depends only on the sampling frequency ω and it is $O(\sum_i \omega_i)$. It is worth noting that the retrieval time does not depend on the data size, but only on sampling frequency ω and as accuracy increases as $\omega \rightarrow \infty$, the retrieval time scales with the desired accuracy rather than the data size.

10. SOME NOTES FROM NUMERICAL EXPERIMENTATION

Choice of λ dictates how good a fit the solution function is to the data. If λ is low, we get very good fit of data, but if its 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 λ 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 λ should be made, for the solution to be good for a given real world problem.

11. 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.

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ABSTRACT. In this article we present a function fitting method, which 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.

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