CEE 598: Homework Assignment 1

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Problem 1

Part 1

Compute and plot the solution $\tilde{u}(x; \mathbf{a})$.

Given the information in the problem, we can write $\tilde{u}(x; \mathbf{a}) = g(x; \mathbf{a})(x)(x-1)$, where g will be given by function approximation. In particular, we are given that $g(x; \mathbf{a}) = a_1 + a_2 x$. To minimize the difference between the true function and the approximation over the given domain of $x \in [0, 1]$, we define the loss function as $\mathcal{L} = \int_0^1 R(x; \mathbf{a})^2 dx$. The optimal values of a_1, a_2 can then be found by solving,

$$(a_1^*, a_2^*) = \underset{a_1, a_2}{\arg\min}\, \mathcal{L}(a_1, a_2). \tag{1}$$

We will find the optimal parameters using the Galerkin projection method. We first apply first-order optimality conditions by solving the system of equations given by taking the partial differentials of the loss function with respect to the parameters and setting the result equal to 0, or,

$$\frac{\partial \mathcal{L}}{\partial a_i} = \frac{\partial}{\partial a_i} \int_0^1 R(x; \mathbf{a})^2 dx = \int_0^1 2R(x; \mathbf{a}) \frac{\partial R(x; \mathbf{a})}{\partial a_i} dx = 0, \ \ \forall i = 1, \ldots, N. \tag{2}$$

We now obtain the particular forms of the terms in this equation. The residual function for this problem is given as $R(x; \mathbf{a}) = \frac{d^2\tilde{u}}{dx^2} + \frac{d\tilde{u}}{dx} + x$. Given the assumed functional form of g, these terms are:

$$\tilde{u} = (a_1 + a_2 x)(x)(x-1) = a_1(x^2 - x) + a_2(x^3 - x^2) \tag{3}$$

$$\frac{d\tilde{u}}{dx} = a_1(2x-1) + a_2(3x^2 - 2x) \tag{4}$$

$$\frac{d^2\tilde{u}}{dx^2} = 2a_1 + a_2(6x - 2), \tag{5}$$

which gives

$$R = 2a_1 x + a_1 + 3a_2 x^2 + 4a_2 x - 2a_2 + x. \tag{6}$$

The partials with respect to R are then,

$$\frac{\partial R}{\partial a_1} = 2x + 1 \tag{7}$$
$$\frac{\partial R}{\partial a_2} = 3x^2 + 4x - 2, \tag{8}$$

which gives the system of equations

$$\frac{\partial \mathcal{L}}{\partial a_1} = 0 = \int_0^1 (2a_1x + a_1 + 3a_2x^2 + 4a_2x - 2a_2 + x)(2x + 1)dx \tag{9}$$
$$\frac{\partial \mathcal{L}}{\partial a_2} = 0 = \int_0^1 (2a_1x + a_1 + 3a_2x^2 + 4a_2x - 2a_2 + x)(3x^2 + 4x - 2)dx \tag{10}$$

Solving the integrals yields a system of equations,

$$\frac{\partial \mathcal{L}}{\partial a_1} = 0 = \frac{1}{6}(26a_1 + 19a_2 + 7) \tag{11}$$
$$\frac{\partial \mathcal{L}}{\partial a_2} = 0 = \frac{1}{60}(190a_1 + 308a_2 + 65) \tag{12}$$

which we solve using a system of equations-solver. This system of equations has solution $a_1 = -\frac{307}{1466}, a_2 = -\frac{60}{733}$. The function approximation is then given as

$$\tilde{u}(x; \mathbf{a}) = (-\frac{307}{1466} - \frac{60}{733}x)(x^2 - x), \tag{13}$$

and the resulting function approximation is shown in Figure 1.

Part 2

How to estimate the error in this solution if you do not know the true solution?

One could estimate the error of this solution by observing the magnitude of the residual function. Given two function approximations $\tilde{u}_1, \tilde{u}_2$, we say the approximation with the smaller residual better-approximates the true function, and therefore has a "better" error.

Part 3

Plot the residual $R(x)$ as a function of x.

See Figure 2.

Problem 2

Solve the same equation as in Part 1, but now assuming that one measurement of u is available: $u^* = 0.06377$ at the location $x^* = 0.5$.

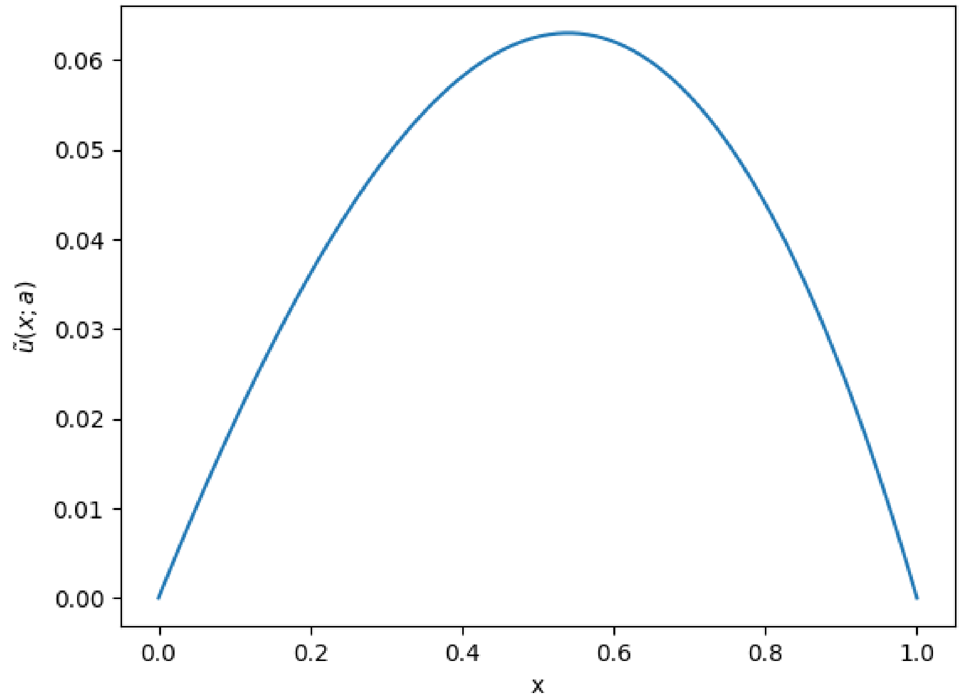

Figure 1: Problem 1, Part 1 - $\tilde{u}$ over the domain of [0, 1] with $a_1 = -\frac{307}{1466}, a_2 = -\frac{60}{733}$

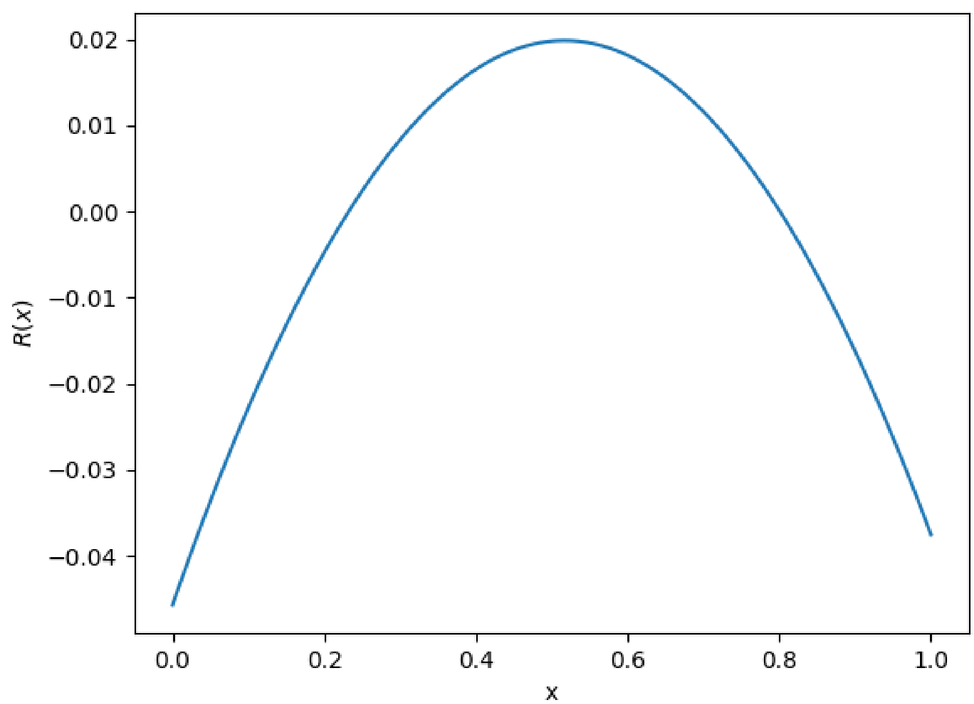

Figure 2: Problem 1, Part 3 - $R(x)$ over the domain of [0, 1] with $a_1 = -\frac{307}{1466}, a_2 = -\frac{60}{733}$

Part 1

Compute a_1, a_2 for $\lambda = 1, 100, 1000$.

We use the residual least-square method to account for the given measurement in the loss function. The modified loss function is given as,

$$\mathcal{L} = \int_0^1 R(x;\mathbf{a})^2 dx + \lambda[\tilde{u}(x^*;\mathbf{a}) - u^*]^2. \tag{14}$$

Using first-order optimality conditions, we get the system of equations,

$$\frac{\partial \mathcal{L}}{\partial a_i} = \int_0^1 2R(x;\mathbf{a})\frac{\partial R(x;\mathbf{a})}{\partial a_i}dx + 2\lambda[\tilde{u}(x^*;\mathbf{a}) - u^*]\frac{\partial \tilde{u}(x^*;\mathbf{a})}{\partial a_i} = 0, \ \ \forall i = 1, \ldots, N. \tag{15}$$

The partial derivatives are given as,

$$\frac{\partial \tilde{u}}{\partial a_1} = 1(x^2 - x) \tag{16}$$

$$\frac{\partial \tilde{u}}{\partial a_2} = x(x^2 - x), \tag{17}$$

which gives the system of equations,

$$\frac{\partial \mathcal{L}}{\partial a_1} = 0 = \frac{1}{6}(26a_1 + 19a_2 + 7) + \lambda[(a_1 + a_2 x)(x^2 - x) - u](x^2 - x)|_{x=x^*, u=u^*} \tag{18}$$

$$\frac{\partial \mathcal{L}}{\partial a_2} = 0 = \frac{1}{60}(190a_1 + 308a_2 + 65) + \lambda[(a_1 + a_2 x)(x^2 - x) - u](x^3 - x^2)|_{x=x^*, u=u^*}. \tag{19}$$

We use a system of equations-solver to solve for a_1, a_2 using the particular given values of x^*, u^*, λ. $\lambda = 1$ has solution $(a_1^*, a_2^*) \approx (-0.2095, -0.0818)$, $\lambda = 100$ has solution $(a_1^*, a_2^*) \approx (-0.2128, -0.0809)$, and $\lambda = 1000$ has solution $(a_1^*, a_2^*) \approx (-0.2146, -0.0804)$.

Part 2

Plot the solution $\tilde{u}(x;\mathbf{a})$ as a function of x for $\lambda = 1, 100, 1000$. On the same figure, plot the analytical solution $u(x) = -\frac{x^2}{2} + x + \frac{1}{2(1-e^{-1})}(e^{-x} - 1)$ and discuss the results.

As shown in Figure 3, a higher value of λ is associated with a function approximation that better-fits the given measurement. This makes sense, as an increased value of λ increases the amount of loss associated with a difference between the function approximation and the given measurement. The function approximation produced for the highest value of λ also closely matches the analytical solution, however this may not always be the case, especially for more-complex systems. This demonstrates the importance of checking multiple values of λ and comparing against a known analytical solution if one is available.

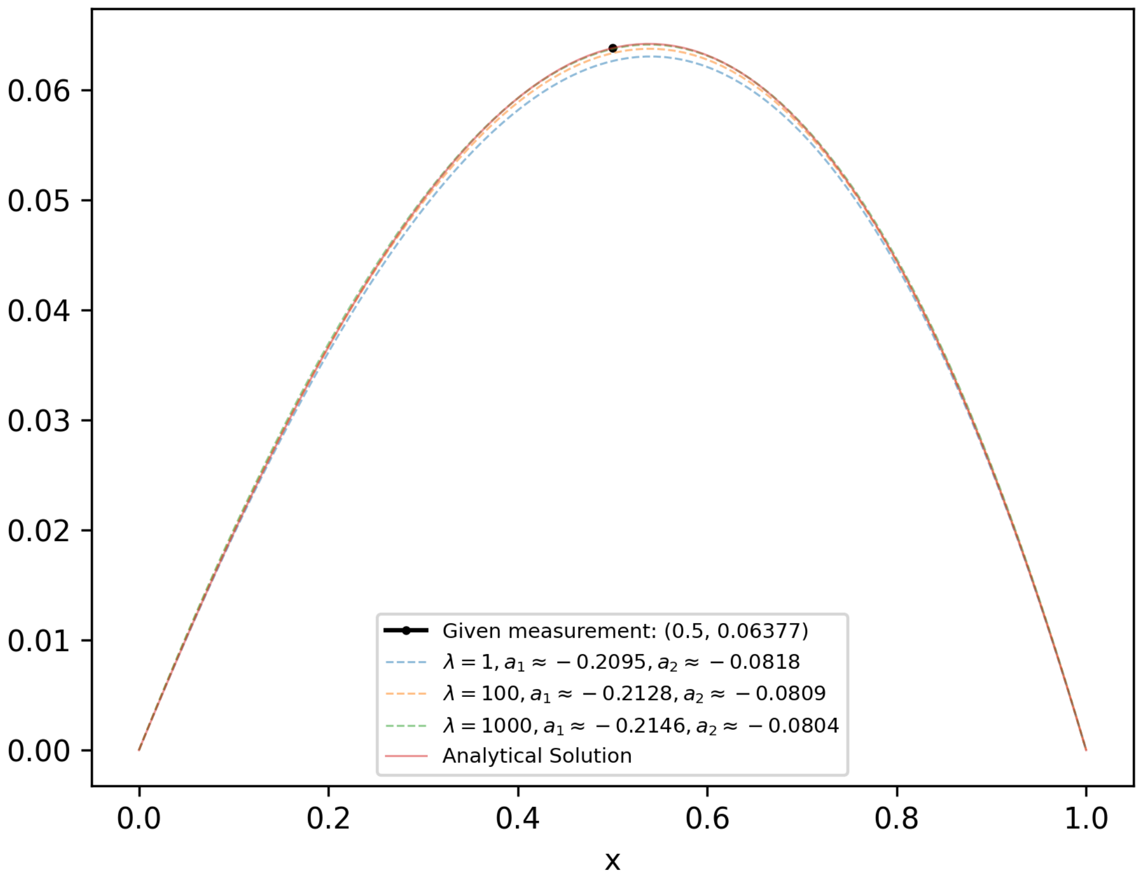

Figure 3: Problem 2, Part 2 - $\tilde{u}(x; \mathbf{a})$ as a function of x for $\lambda = 1, 100, 1000$

Part 3

Plot the residual $R(x; \mathbf{a})$ versus x for $\lambda = 0, 1, 100, 1000$.

As shown in Figure 4, higher values of λ demonstrate lower magnitudes of the residual as the approximate function approaches the given data measurement. However, higher values of λ have larger residuals further away from the given measurement compared to lower values of λ. An appropriate choice of λ would have to be determined by project requirements which would help determine an acceptable range for model accuracy at different values of x. For example, if a project requirement were "$|R(x)| < 0.05 \ \forall \ x \in [0, 1]$", we would not be able to use $\lambda = 1000$, but might instead choose $\lambda = 1$.

Beyond satisfying project requirements, choosing an extremely large value of λ is not always an effective approach, since the resulting model would likely overfit the given data points unless other regularization methods were also used. One form of regularization is choosing "simpler" models.[1] The residual function, which encodes knowledge of the system's behavior, then allows us to compare the residuals of different functional forms, which may help identify parsimonious, but effective function approximations.

References

[1] Nakkiran, P., Kaplun, G., Bansal, Y., Yang, T., Barak, B., and Sutskever, I. Deep double descent: Where bigger models and more data hurt. *Journal of Statistical Mechanics: Theory and Experiment 2021*, 12 (2021), 124003.

[1] "Simpler" is in quotes because effectively defining the complexity of machine learning systems is still an active area of research [1]. To effectively define complexity, we must not only consider simplicity of the model (number of parameters, functional form, etc.), but also data-dependent properties of the model such as bias and variance, and properties of the training procedure such as number of epochs. For example, $\tilde{g}(x) = a_1 \sin(a_2 x)$ only has two parameters and is composed of fairly simple functions, but the frequency parameter could be increased to interpolate an arbitrary set of data points by producing a high-variance, high-bias model.

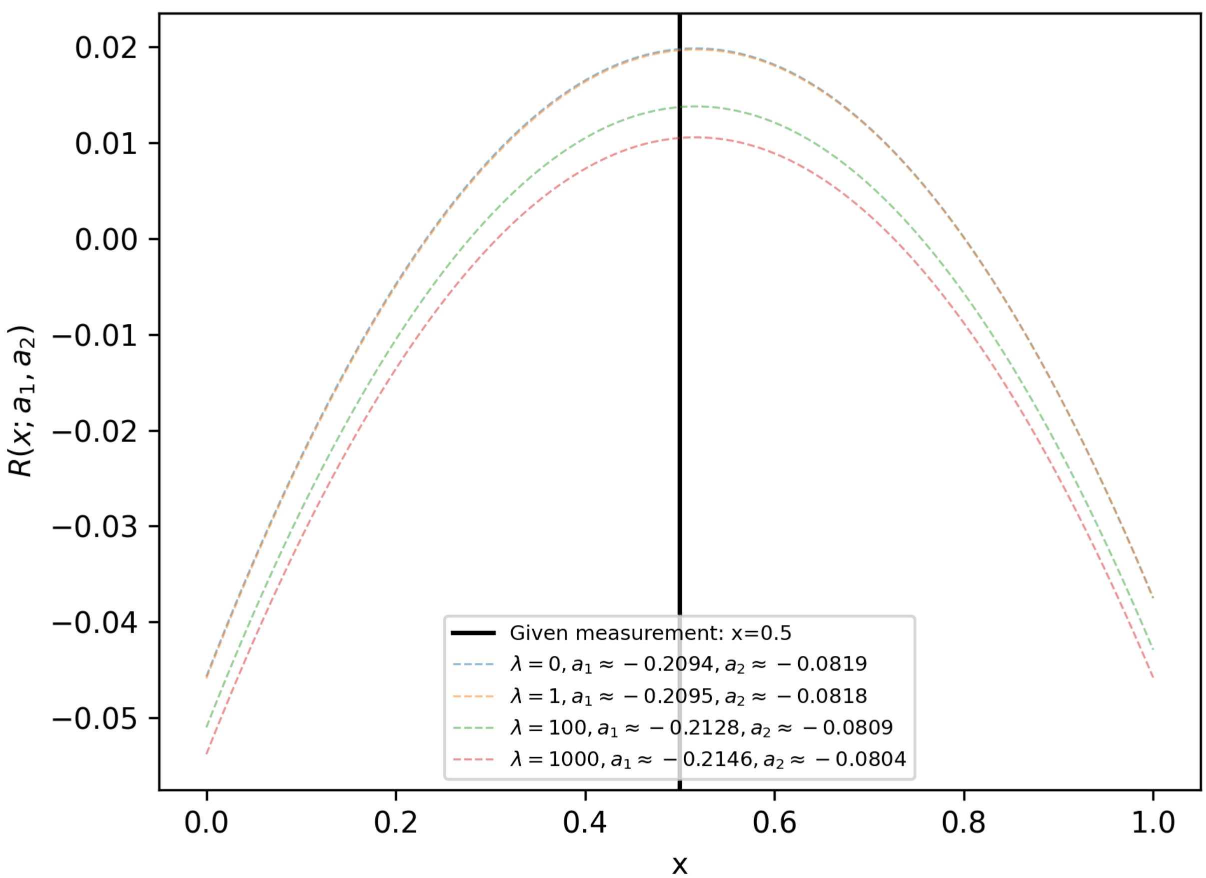

Figure 4: Problem 2, Part 3 - $R(x; \mathbf{a})$ versus x for $\lambda = 0, 1, 100, 1000$