Lecture 8: Least Squares
Overview

Today:

• Function approximation using *least squares* (instead of interpolation)
Goal: find a function $f_a(x)$, that approximates a given function, $f(x)$, accurately on $x \in [a, b]$

Last time:
(A) Write $f_a(x)$ as a linear combo of basis functions
(B) Solve for the $c_j$ using interpolation

This time:
(A) We will still express our $f_a(x)$ as a linear combination of basis functions in terms of unknown coefficients
(B) We will solve for the coefficients using a different approach than interpolation: least squares
The premise for least squares function approximation

(A) Pick a **subspace** that we want to approximate onto (e.g., $\mathcal{P}^n[a, b]$ or $\mathcal{T}^n[a, b]$)

(B) Pick a **basis** $\mathcal{B} = \{b_0(x), b_1(x), \ldots, b_n(x)\}$ for that subspace and express the approximate function, $f_a(x)$, as a linear combination of the basis functions in terms of unknown coefficients

$$f_a(x) = \sum_{j=0}^{n} c_j b_j(x) \quad (1)$$

(C) Need $n + 1$ equations to solve for the $n + 1$ unknown coefficients. Unlike in interpolation, we will develop these equations by trying to **minimize the overall error**. That is, we will look for an $f_a(x)$ that satisfies

$$\min_{f_a \in \mathcal{W}} | | f - f_a | |^2$$ \quad (2)

In words: seek an $f_a$ belonging to the desired subspace $\mathcal{W}$ such that the norm of the difference between $f$ and $f_a$ is the smallest possible.

Remember: the $| | \cdot | |$ symbol means “norm”, which is defined in terms of the inner product (review the error lecture if needed!)

Intuition: don’t explicitly require $f = f_a$ at any specific points. Just try to get an $f_a$ that is close to $f$ in a meaningful way.

OK, that may be a nice sentiment. But how do we construct $n + 1$ equations from that?
Constructing the $n+1$ equations in least squares approximation

**The key** to constructing the $n+1$ equations revolves around the following (non-obvious) fact:

The special $f_a$ that obeys the minimization criteria (2) satisfies

$$ (f - f_a, r) = 0 \text{ for any } r \in \mathcal{W} \quad (3) $$

i.e., the inner product between the error $e = f - f_a$ and any $r$ in the subspace $\mathcal{W}$ is zero

We will interpret the meaning of (3) later. But first, let’s identify why (3) is useful:

If (3) is true, then since each $b_i \in \mathcal{W}$ for $i = 0, \ldots, n$:

$$ (f - f_a, b_i) = 0, \quad i = 0, \ldots, n \quad (4) $$

Subbing equation (1) into (4) gives

$$ \left( f - \sum_{j=0}^{n} c_j b_j, b_i \right) = 0, \quad i = 0, \ldots, n $$

And with some rearranging:

$$ \sum_{j=0}^{n} c_j (b_j, b_i) = (f, b_i), \quad i = 0, \ldots, n \quad (5) $$
Breakout room activity

Turn equation (5) into a matrix system of equations $A\mathbf{c} = \mathbf{b}$, where $\mathbf{c}$ is the vector of unknown coefficients, $\mathbf{b}$ is a righthand side that involves known quantities, and $A$ is the appropriate matrix associated with the coefficient vector $\mathbf{c}$

**Answer.**

$$
\begin{bmatrix}
  (b_0, b_0) & (b_1, b_0) & \cdots & (b_{n-1}, b_0) & (b_n, b_0) \\
  (b_0, b_1) & (b_1, b_1) & \cdots & (b_{n-1}, b_1) & (b_n, b_1) \\
  \vdots & \vdots & \ddots & \vdots & \vdots \\
  (b_0, b_{n-1}) & (b_1, b_{n-1}) & \cdots & (b_{n-1}, b_{n-1}) & (b_n, b_{n-1}) \\
  (b_0, b_n) & (b_1, b_n) & \cdots & (b_{n-1}, b_n) & (b_n, b_n)
\end{bmatrix}
\begin{bmatrix}
  c_0 \\
  c_1 \\
  \vdots \\
  c_{n-1} \\
  c_n
\end{bmatrix}
=
\begin{bmatrix}
  (f, b_0) \\
  (f, b_1) \\
  \vdots \\
  (f, b_{n-1}) \\
  (f, b_n)
\end{bmatrix}
$$

(6)
Which inner product to use?

There are many good choices for an inner product. One option is the IP we considered in week 1, the function \((\cdot,\cdot)\) defined by

\[
(f,g) = \int_a^b f(x)g(x)dx \quad \text{for any } f, g \in \mathcal{V}
\]

So for this specific IP, the entry of the matrix in equation (6) involving \(b_2, b_3\) is

\[
(b_2,b_3) = \int_a^b b_2(x)b_3(x)dx
\]

OK great, so we now have what we need to approximate a function with least squares!

(A) Solve (6) for the unknown coefficients after filling in \(A\) and \(b\) using our chosen IP

(B) Now we have \(f_a(x)\) via equation (1)

But remember that this all assumed that (3) was true. Is it?! Yes, and let’s build some intuition for what it means!
Showing that equation (3) is true

We want to understand the statement that \((f - f_a, r) = 0\) for any \(r \in \mathcal{W}\).

The statement is most easily understood with finite-dimensional vectors. Let's say \(f \in \mathbb{R}^2\) is some vector that we want to approximate.

And let's say that we want to approximate this onto the subspace

\[ \mathcal{W} = \left\{ \alpha \begin{bmatrix} -1 \\ 1 \end{bmatrix} : \alpha \in \mathbb{R} \right\} \]

From linear algebra and/or geometry, you might recall that the \(f_a\) that best approximates \(f\) on \(\mathcal{W}\) satisfies \(f - f_a \perp \mathcal{W}\).

_Math appreciation break:_ by creating a framework for defining inner products and norms, we have a way for intuiting best approximation of functions using visualizable vectors!