10.34, Numerical Methods Applied to Chemical Engineering
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Lecture #10: Function Space.

Functional Approximation

(Variables are scalar in this example)

$f(x) \approx \sum_{n=0}^{N} c_n \phi_n(x) + \Delta(x)$ Figuring out $\Delta(x)$ is similar to solving whole problem

Increase N until function converges

$\{\varphi_n(x)\}$ favorite set of functions

$\{\underline{v}_n\}$ favorite set of vectors $\underline{w} \approx \sum_{n=0}^{N} c_n \underline{v}_n$ (length M) N<M

$\underline{v}_n \in \{\Re^m\}$

Basis: $\underline{e}_l = \sum_{n=0}^{N} d_{l,n} \underline{v}_n$ $\underline{w}^{approx} \approx \sum_{n=0}^{N} c_n \underline{v}_n = \sum_l a_l e_l = \sum_{l,n} a_l d_{l,n} \underline{v}_n$

$\underline{e}_l \cdot \underline{e}_j = \delta_{jl}$ ➔ orthonormal $\underline{c} = \underline{a}^T \underline{\underline{D}}$

We want to do the same with functions. How do you take dot product?

Define "$\varphi_n \cdot \varphi_m$" = $\int_{\text{interesting range of } x} dx\, g(x) \phi_n^*(x) \phi_m(x)$ "works": $\langle \varphi_m | \varphi_n \rangle = \delta_{mn}$

($g(x)$: weighting function)

g(x) = k x: 0 → 2π $\varphi_m = e^{imx} = \cos(mx) + i \cdot \sin(mx)$

$$\frac{e^{imx} + e^{-imx}}{2} = \cos(mx)$$

g(x) = 1 x: -1 → +1 Legendre polynomials

$g(x) = e^{-x^2}$ x: -∞ → +∞ Hermite polynomials

$g(x) = \dfrac{2}{\pi\sqrt{1-x^2}}$ x: -1 → +1 Chebyshev polynomials

1) We chose a basis $\{\varphi_n(x)\}$ and an inner product

orthonormal: $\langle \varphi_m | \varphi_n \rangle = \delta_{mn}$

2) We're trying to solve $\hat{O}f(x) = q(x)$ ($f(x)$: unknown; $q(x)$: given) ("In most problems, these are all vectors, but that looks too scary to start with")

Look for solutions: $f^{unknown}(x) \approx \sum c_n \phi_n(x)$

$$\underset{\substack{\text{favorite}\\\text{range}}}{\int_a^b} dx\, g(x)\phi_m^*(\lambda)\left[\hat{O}f(x)\right] = \int_a^b dx\, g(x)\phi_m^*(x)q(x)$$ solution will depend on a,b,$\underline{c}_n$,m.

$F(a,b,\underline{c}_n,m) = v(m,a,b)$

$F(\underline{c}_n,m) = v(m)$ Now solve for c_n.

If $\hat{O}$ is a linear operator:

$$\hat{O}f^{approx}(x) = \hat{O}\sum c_n \phi_n(x) = \sum c_n (\hat{O}\phi_n)$$

and if $\hat{O}\varphi_n = \lambda_n \varphi_n$ (i.e. φ_n is an eigenfunction of $\hat{O}$)

$$\hat{O}f^{approx}(x) = = \sum c_n \lambda_n \phi_n(x)$$

$$\int_a^b dx\, g(x)\phi_m^* \sum c_n \lambda_n \phi_n = \sum c_n \lambda_n \underbrace{\int_a^b dx\, g\phi_m^* \phi_n}$$ → $\langle\varphi_m|\varphi_n\rangle = \delta_{mn}$

$$\int_a^b dx\, g(x)\phi_m^* \hat{O}f^{approx} = \sum_{n=0}^{N} c_n \lambda_n \delta_{mn} = c_m \lambda_m$$

$$c_m \lambda_m = \int dx\, g(x)\phi_m^*(x)q(x) \equiv b_m$$

$$c_m = \frac{1}{\lambda_m}\int dx\, g(x)\phi_m^*(x)q(x)$$

$$\hat{O} = \left[k\frac{\partial^2}{\partial x^2} + h(x)\right]T(x)$$ Often this is the operator ($T(x)$ ← f(x))

sin, cos } are eigenfunctions (of $\frac{\partial^2}{\partial x^2}$)

Gives you a really messy equation:

Suppose $\hat{O} = \hat{O}_1 + h(x)$ {i.e. Schrodinger Equation}

Suppose $\hat{O}_1\varphi_n = \lambda_n \varphi$

$$\int_a^b dx\, g(x)\phi_m^*(x)\hat{O}f^{approx} = c_m\lambda_m + \underbrace{\int dx\, g(x)\phi_m^*(x)h(x)\sum c_n\phi_n(x)}_{\sum c_n \underbrace{\int dx\, g(x)\phi_m^*(x)h(x)\phi_n(x)}_{H_{mn}}}$$

$$c_m\lambda_m + \sum c_n H_{mn} = b_m$$

$(\underline{\underline{H}}+\underline{\underline{\Lambda}})\underline{c} = \underline{\underline{B}}$ m=1,…N   Linear Problem: $\underline{c} = (\underline{\underline{H}}+\underline{\underline{\Lambda}})\backslash\underline{b}$

$$\underline{\lambda}_m\underline{\underline{I}} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

Must evaluate integrals H_{mn}: difficult to evaluate, quantum mechanics requires 6-dimensional integrals. $\underline{\underline{H}}$ becomes a large matrix when n gets large.

Also have Boundary Conditions: $f(\underline{x} = 0) = f_0$

Adds another equation: $\sum c_n\phi_n(x=0) = f_0$

$$\underline{v}\cdot\underline{c} = f_0$$

How to solve? Can try to fit by least squares and just fit *all* the equations approximately. Can drop larger n terms to leave space for boundary conditions. Another way would be to not consider the boundary conditions and then craftily choose Φ_n so that they solve the boundary conditions.

To check if answer makes sense: write out the series and see if $\underline{c}_n$ converges

Evaluate Residuals

$\underline{R} = \hat{O}f - q$

max($\underline{R}$) < tol?

$||\underline{R}(x_i)||$ < tol?

we will evaluate this later