Numerical Analysis

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Gram–Schmidt orthogonalization procedure:

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Idea: Instead of

$$\{1, x, x^2, \dots, x^n\}$$

as a basis for Π_n , suppose we have a basis

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Gram–Schmidt orthogonalization procedure: the solution of the normal equations $A\alpha = \varphi$ for best least-squares polynomial approximation would be easy if A were diagonal.

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as a basis for Π_n , suppose we have a basis

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We shall choose the basis $\{\phi_0, \phi_1, \dots, \phi_n\}$ so as to ensure that the matrix A in the normal equations is diagonal.

With this choice of basis, we seek the polynomial of best approximation $p_n(x) = \sum_{k=0}^n \beta_k \phi_k(x)$. The normal equations then become

$$\int_{a}^{b} w(x) \left(f(x) - \sum_{k=0}^{n} \beta_{k} \phi_{k}(x) \right) \phi_{i}(x) \, \mathrm{d}x = 0, \quad i = 0, 1, \dots, n,$$

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or equivalently

$$\sum_{k=0}^{n} \left(\int_{a}^{b} w(x)\phi_{k}(x)\phi_{i}(x) \,\mathrm{d}x \right) \beta_{k} = \int_{a}^{b} w(x)f(x)\phi_{i}(x)\mathrm{d}x, \quad i = 0, 1, \dots, n,$$

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i.e.,

$$A\beta = \varphi, \tag{12.1}$$

where $eta=(eta_0,eta_1,\ldots,eta_n)^{\mathrm{T}}$, $arphi=(f_1,f_2,\ldots,f_n)^{\mathrm{T}}$ and now

$$a_{i,k} = \int_a^b w(x)\phi_k(x)\phi_i(x)\,\mathrm{d}x \qquad \text{and} \qquad f_i = \int_a^b w(x)f(x)\phi_i(x)\,\mathrm{d}x.$$

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So \boldsymbol{A} is diagonal if

$$\langle \phi_i, \phi_k \rangle = \int_a^b w(x)\phi_i(x)\phi_k(x) \,\mathrm{d}x \quad \begin{cases} = 0 & i \neq k \text{ and} \\ \neq 0 & i = k. \end{cases}$$

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We can create such a set of orthogonal polynomials

$$\{\phi_0,\phi_1,\ldots,\phi_n,\ldots\},\$$

with $\phi_i \in \Pi_i$ for each *i*, by the Gram–Schmidt procedure, which is based on the following lemma.

Lemma

Suppose that $\{\phi_0, \phi_1, \dots, \phi_k\}$, with $\phi_i \in \Pi_i$ for each i, are orthogonal with respect to the inner product $\langle f, g \rangle = \int_a^b w(x) f(x) g(x) \, \mathrm{d}x$. Then,

$$\phi_{k+1}(x) = x^{k+1} - \sum_{i=0}^{k} \lambda_i \phi_i(x)$$

satisfies

$$\langle \phi_{k+1}, \phi_j \rangle = \int_a^b w(x)\phi_{k+1}(x)\phi_j(x) \,\mathrm{d}x = 0, \qquad j = 0, 1, \dots, k,$$

when

$$\lambda_j = \frac{\langle x^{k+1}, \phi_j \rangle}{\langle \phi_j, \phi_j \rangle}, \qquad j = 0, 1, \dots, k.$$

Proof. For any j, $0 \le j \le k$,

$$\begin{aligned} \langle \phi_{k+1}, \phi_j \rangle &= \langle x^{k+1}, \phi_j \rangle - \sum_{i=0}^k \lambda_i \langle \phi_i, \phi_j \rangle \\ &= \langle x^{k+1}, \phi_j \rangle - \lambda_j \langle \phi_j, \phi_j \rangle \end{aligned}$$

by the orthogonality of ϕ_i and ϕ_j , $i \neq j$,

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$$= 0$$
 by definition of λ_j .

Notes:

- The Gram–Schmidt procedure does the above for k = 0, 1, ..., n successively.
- Ø φ_k is always of exact degree k, so {φ₀, φ₁,..., φ_ℓ} is a basis for Π_ℓ for every ℓ ≥ 0.
- **③** ϕ_k can be normalised/scaled to satisfy $\langle \phi_k, \phi_k \rangle = 1$ or to be monic.

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Examples:

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1. The inner product

$$\langle f,g \rangle = \int_{-1}^{1} f(x)g(x) \,\mathrm{d}x$$

has orthogonal polynomials called the Legendre polynomials,

$$\phi_0(x) \equiv 1, \ \phi_1(x) = x, \ \phi_2(x) = x^2 - \frac{1}{3}, \ \phi_3(x) = x^3 - \frac{3}{5}x, \dots$$

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2. The inner product

$$\langle f,g\rangle = \int_{-1}^{1} \frac{f(x)g(x)}{\sqrt{1-x^2}} \,\mathrm{d}x$$

gives orthogonal polynomials, which are the Chebyshev polynomials,

$$\phi_0(x) \equiv 1, \ \phi_1(x) = x, \ \phi_2(x) = 2x^2 - 1, \ \phi_3(x) = 4x^3 - 3x, \dots$$

3. The inner product

$$\langle f,g\rangle = \int_0^\infty \mathrm{e}^{-x} f(x)g(x)\,\mathrm{d}x$$

gives orthogonal polynomials, which are the Laguerre polynomials,

$$\phi_0(x) \equiv 1, \ \phi_1(x) = 1 - x, \ \phi_2(x) = 2 - 4x + x^2,$$

 $\phi_3(x) = 6 - 18x + 9x^2 - x^3, \dots$

Lemma

Suppose that $\{\phi_0, \phi_1, \dots, \phi_n, \dots\}$ are orthogonal polynomials for a given inner product $\langle \cdot, \cdot \rangle$. Then, $\langle \phi_k, q \rangle = 0$ whenever $q \in \Pi_{k-1}$.

Lemma

Suppose that $\{\phi_0, \phi_1, \dots, \phi_n, \dots\}$ are orthogonal polynomials for a given inner product $\langle \cdot, \cdot \rangle$. Then, $\langle \phi_k, q \rangle = 0$ whenever $q \in \Pi_{k-1}$.

Proof. This follows since if
$$q \in \Pi_{k-1}$$
, then $q(x) = \sum_{i=0}^{k-1} \sigma_i \phi_i(x)$ for some

 $\sigma_i \in \mathbb{R}, \ i=0,1,\ldots,k-1$, so

$$\langle \phi_k, q \rangle = \sum_{i=0}^{k-1} \sigma_i \langle \phi_k, \phi_i \rangle = 0.$$

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Remark: note from the above argument that if $q(x) = \sum_{i=0}^{k} \sigma_i \phi_i(x)$ is of exact degree k (so $\sigma_k \neq 0$), then $\langle \phi_k, q \rangle = \sigma_k \langle \phi_k, \phi_k \rangle \neq 0$.

Theorem

Suppose that $\{\phi_0, \phi_1, \ldots, \phi_n, \ldots\}$ is a set of orthogonal polynomials. Then, there exist sequences of real numbers $(\alpha_k)_{k=1}^{\infty}$, $(\beta_k)_{k=1}^{\infty}$, $(\gamma_k)_{k=1}^{\infty}$ such that a three-term recurrence relation of the form

$$\phi_{k+1}(x) = \alpha_k(x - \beta_k)\phi_k(x) - \gamma_k\phi_{k-1}(x), \qquad k = 1, 2, \dots,$$

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holds.

Proof. The polynomial $x\phi_k \in \Pi_{k+1}$, so there exist $\sigma_{k,0}, \sigma_{k,1}, \ldots, \sigma_{k,k+1}$ in $\mathbb R$ such that

$$x\phi_k(x) = \sum_{i=0}^{k+1} \sigma_{k,i}\phi_i(x)$$

as $\{\phi_0, \phi_1, \dots, \phi_{k+1}\}$ is a basis for Π_{k+1} .



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as $\{\phi_0, \phi_1, \dots, \phi_{k+1}\}$ is a basis for Π_{k+1} . Now take the inner product on both sides with ϕ_j , and note that $x\phi_j \in \Pi_{k-1}$ if $j \leq k-2$.

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$$\langle x\phi_k,\phi_j\rangle = \int_a^b w(x)x\phi_k(x)\phi_j(x)\,\mathrm{d}x = \int_a^b w(x)\phi_k(x)x\phi_j(x)\,\mathrm{d}x = \langle \phi_k,x\phi_j\rangle = 0$$

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by the above lemma for $j \leq k-2$.

Proof. The polynomial $x\phi_k \in \Pi_{k+1}$, so there exist $\sigma_{k,0}, \sigma_{k,1}, \ldots, \sigma_{k,k+1}$ in \mathbb{R} such that

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as $\{\phi_0, \phi_1, \dots, \phi_{k+1}\}$ is a basis for Π_{k+1} . Now take the inner product on both sides with ϕ_j , and note that $x\phi_j \in \Pi_{k-1}$ if $j \leq k-2$. Note that

$$\langle x\phi_k,\phi_j\rangle = \int_a^b w(x)x\phi_k(x)\phi_j(x)\,\mathrm{d}x = \int_a^b w(x)\phi_k(x)x\phi_j(x)\,\mathrm{d}x = \langle \phi_k,x\phi_j\rangle = 0$$

by the above lemma for $j \leq k-2$. In addition,

$$\left\langle \sum_{i=0}^{k+1} \sigma_{k,i} \phi_i, \phi_j \right\rangle = \sum_{i=0}^{k+1} \sigma_{k,i} \langle \phi_i, \phi_j \rangle = \sigma_{k,j} \langle \phi_j, \phi_j \rangle$$

by the linearity of $\langle \cdot, \cdot \rangle$ and orthogonality of ϕ_k and ϕ_j for $k \neq j$.

Hence $\sigma_{k,j} = 0$ for $j \leq k-2$, and so

$$x\phi_k(x) = \sigma_{k,k+1}\phi_{k+1}(x) + \sigma_{k,k}\phi_k(x) + \sigma_{k,k-1}\phi_{k-1}(x).$$

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$$x\phi_k(x) = \sigma_{k,k+1}\phi_{k+1}(x) + \sigma_{k,k}\phi_k(x) + \sigma_{k,k-1}\phi_{k-1}(x).$$

Taking the inner product with ϕ_{k+1} reveals that

$$\langle x\phi_k,\phi_{k+1}\rangle = \sigma_{k,k+1}\langle\phi_{k+1},\phi_{k+1}\rangle,$$

so $\sigma_{k,k+1} \neq 0$ by the above remark as $x\phi_k$ is of exact degree k+1.

Hence $\sigma_{k,j} = 0$ for $j \leq k-2$, and so

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so $\sigma_{k,k+1} \neq 0$ by the above remark as $x\phi_k$ is of exact degree k+1. Thus,

$$\phi_{k+1}(x) = \frac{1}{\sigma_{k,k+1}}(x - \sigma_{k,k})\phi_k(x) - \frac{\sigma_{k,k-1}}{\sigma_{k,k+1}}\phi_{k-1}(x),$$

which is of the given form, with

$$\alpha_k = \frac{1}{\sigma_{k,k+1}}, \qquad \beta_k = \sigma_{k,k}, \qquad \gamma_k = \frac{\sigma_{k,k-1}}{\sigma_{k,k+1}}, \qquad k = 1, 2, \dots \quad \Box$$

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Example. The inner product

$$\langle f,g \rangle = \int_{-\infty}^{\infty} e^{-x^2} f(x)g(x) \, \mathrm{d}x$$

has orthogonal polynomials called the Hermite polynomials,

$$\phi_0(x) \equiv 1, \ \phi_1(x) = 2x, \ \phi_{k+1}(x) = 2x\phi_k(x) - 2k\phi_{k-1}(x) \text{ for } k \ge 1.$$

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Matlab:

% cat hermite_polys.m

```
x=linspace(-2.2,2.2,200);
oldH=ones(1,200); plot(x,oldH), hold on
newH=2*x; plot(x,newH)
for n=1:2,...
    newnewH=2*x.*newH-2*n*oldH; plot(x,newnewH),...
    oldH=newH;newH=newnewH;
end
```

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```
% matlab
```

```
>> hermite_polys
```



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