Numerical Analysis

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Gram–Schmidt orthogonalization procedure:

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Idea: Instead of

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

as a basis for Π_n , suppose we have a basis

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

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

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With this choice of basis, we seek the polynomial of best approximation $p_n(x) = \sum_{n=1}^{n}$ $k=0$ $\beta_k\phi_k(x)$. The normal equations then become

$$
\int_a^b w(x) \left(f(x) - \sum_{k=0}^n \beta_k \phi_k(x) \right) \phi_i(x) dx = 0, \quad i = 0, 1, \dots, n,
$$

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$$

or equivalently

$$
\sum_{k=0}^n \left(\int_a^b w(x) \phi_k(x) \phi_i(x) dx \right) \beta_k = \int_a^b w(x) f(x) \phi_i(x) dx, \quad i = 0, 1, \dots, n,
$$

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$$

i.e.,

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

where $\beta=(\beta_0,\beta_1,\ldots,\beta_n)^{\rm T}$, $\varphi=(f_1,f_2,\ldots,f_n)^{\rm T}$ and now

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

So A is diagonal if

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

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.

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Lemma

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

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

satisfies

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

when

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

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

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

$$
= \langle x^{k+1}, \phi_j \rangle - \lambda_j \langle \phi_j, \phi_j \rangle
$$

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

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$$
= 0
$$
 by definition of λ_j .

Notes:

- **1** The Gram–Schmidt procedure does the above for $k = 0, 1, ..., n$ successively.
- $\bullet \phi_k$ is always of exact degree k, so $\{\phi_0, \phi_1, \ldots, \phi_\ell\}$ is a basis for Π_ℓ for every $\ell \geq 0$.
- $\bullet \phi_k$ 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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Examples:

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,

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

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$$

2. The inner product

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

gives orthogonal polynomials, which are the Chebyshev polynomials,

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

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3. The inner product

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

gives orthogonal polynomials, which are the Laguerre polynomials,

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

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

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Lemma

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

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Lemma

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

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

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

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 $\left\{ \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \end{array} \right.$

Remark: note from the above argument that if $q(x) = \sum_{i=1}^n \frac{1}{n_i}$ k $i=0$ $\sigma_i\phi_i(x)$ is of exact degree k (so $\sigma_k \neq 0$), then $\langle \phi_k, q \rangle = \sigma_k \langle \phi_k, \phi_k \rangle \neq 0.$

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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 R such that $k+1$

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

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

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 R such that

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

as $\{\phi_0, \phi_1, \ldots, \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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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 R such that

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as $\{\phi_0, \phi_1, \ldots, \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

$$
\langle x\phi_k, \phi_j \rangle = \int_a^b w(x)x\phi_k(x)\phi_j(x) \,dx = \int_a^b w(x)\phi_k(x)x\phi_j(x) \,dx = \langle \phi_k, x\phi_j \rangle = 0
$$

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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 R such that

$$
x\phi_k(x) = \sum_{i=0}^{k+1} \sigma_{k,i}\phi_i(x)
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as $\{\phi_0, \phi_1, \ldots, \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

$$
\langle x\phi_k, \phi_j \rangle = \int_a^b w(x)x\phi_k(x)\phi_j(x) \,dx = \int_a^b w(x)\phi_k(x)x\phi_j(x) \,dx = \langle \phi_k, x\phi_j \rangle = 0
$$

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

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

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

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

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

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

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

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

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

has orthogonal polynomials called the Hermite polynomials,

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

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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,\ldotsnewnewH=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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