# Some applications of Legendre and Hermite polynomials

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## 1. Gauss quadrature formula.

We discuss numerical evaluation of integrals. A *linear quadrature formula* approximates an integral of a function over an interval $(a, b)$ by a linear combination of values of this function at some points, which are called the *nodes*:

$$\int_a^b f(x)dx \approx \sum_{j=0}^{n} a_j f(x_j). \tag{1}$$

For example, a simple approximation is obtained if we take equally spaced nodes

$$x_j = a + j(b-a)/n,\ j = 0, \ldots, n,$$

and approximate $f$ on the $j$-th interval by $f(x_j)$. This corresponds to taking $a_j = (b-a)/n$ in (1).

The word "linear" means that for any two functions, if the integral of $f$ is approximated by $A$ and the integral of $g$ is approximated by $B$ then the integral of a linear combination $c_1 f + c_2 g$ is approximated by $c_1 A + c_2 B$, which is a very natural requirement.

The example given above can be improved (for example, by approximating the integral of $f$ on small intervals not by the areas of rectangles but by areas of trapezoids).

**Exercise.** What are the $a_k$ for the trapezoid formula?

So the question arises what is the "best" linear quadrature formula.

Of course one has to specify exactly what does one mean by the best. One formula may give better result for some functions, another for some other functions.

Since every continuous function on a closed interval can be uniformly approximated by polynomials, a very reasonable criterion is that the formula gives exact result for polynomials, up to certain degree. The following result is easy to prove:

**Theorem.** *Let an interval $[a, b]$ and $n+1$ nodes $a \leq x_0 < x_1 < \ldots < x_n \leq b$ be given. There exists a unique choice of $a_0, \ldots, a_n$ such that the formula (1) gives the exact result for all polynomials of degree at most $n$.*

*Proof.* The formula is exact for polynomials of degree at most $n$ if and only if it is exact for all monomials of degree at most $n$. So we want

$$\int_a^b x^k dx = \sum_{j=0}^n a_j x_j^k, \quad k = 0, \ldots, n. \tag{2}$$

The left hand side is

$$\frac{b^{k+1} - a^{k+1}}{k+1},$$

and we may consider (2) as a system of linear equations with respect to $a_j$. The determinant of this system is the familiar Vandermonde determinant from Linear algebra, and it is not equal to zero. Therefore the system has a unique solution which gives the required quadrature formula.

**Exercise.** Find an explicit solution $a_j$ of the system (2).

Hint. Consider the polynomials

$$e_k(x) = \frac{\prod_{j \neq k}(x - x_j)}{\prod_{j \neq k}(x_k - x_j)}.$$

These are polynomials of degree $n$ with the property $e_k(x_k) = 1$, and $e_k(x_j) = 0, \ j \neq k$. So for every polynomial $P$ of degree at most $n$ we have an *interpolation formula*

$$P(x) = \sum_{k=0}^n f(x_k) e_k(x).$$

Use this fact to find an explicit expression of $a_k$ in the linear quadrature formula which gives an exact answer for all polynomials of degree at most $n$.

Now the question is: can we do better than that? The answer is: we should do better, because we have not optimized the choice of the nodes yet; the Theorem above holds for *any* choice of the nodes. There must be some choices of the nodes, which will allow to write a quadrature formula which is exact for polynomials of higher degree. The remarkable solution was found by Gauss. Assume for simplicity that $[a, b] = [-1, 1]$; this does not restrict generality.

It turns out that the optimal choice of $x_k$ is the zeros of Legendre's polynomial of degree $n + 1$. (I wanted to put an exclamation sign (!) at the end of the previous sentence, but could not in fear that it might be confused with the factorial).

**Theorem** (Gauss). *Let $x_0, x_1, \ldots, x_n$ be the zeros of Legendre's polynomial $P_{n+1}$. Then here is a linear quadrature formula*

$$\int_{-1}^{1} f(x)dx \approx \sum_{k=0}^{n} a_k f(x_k) \tag{3}$$

*which is exact for all polynomials of degree at most $2n + 1$.*

*Proof.* Let $P$ be a polynomial of degree at most $2n + 1$. Divide it with remainder by the Legendre polynomials $P_{n+1}$:

$$P = QP_{n+1} + R, \quad \deg R \leq n. \tag{4}$$

It is easy to see that $\deg Q \leq n$, since the degrees are added when polynomials are multiplied. Then

$$\int_{-1}^{1} P(x)dx = \int_{-1}^{1} Q(x)P_{n+1}(x)dx + \int_{-1}^{1} R(x)dx.$$

The first integral is zero. Indeed, $P_{n+1}$ is orthogonal to all Legendre polynomials of smaller degrees, therefore it is orthogonal to all polynomials of degree at most $n$.

Now choose the zeros of $P_{n+1}$ as our nodes, and find for them the coefficients $a_j$ according to Theorem 1. Then we have

$$\int_{-1}^{1} P(x)dx = \int_{-1}^{1} R(x)dx = \sum_{k=0}^{n} a_k R(x_j)$$

since $\deg R \leq n$. But on the other hand, it is clear that $P(x_j) = R(x_j)$ which is seen by plugging $x_j$ to (4) and taking into account that $P_{n+1}(x_j) = 0$ by definition! So we obtain

$$\int_{-1}^{1} P(x)dx = \sum_{k=0}^{n} a_k P(x_k),$$

as advertised.

Gauss quadrature formula is actually used for evaluation of integrals by computers.

## 2. Application of Hermite polynomials: harmonic oscillator in quantum mechanics.

In classical mechanics, a harmonic oscillator, or linear pendulum is a system described by the differential equation

$$y'' + \omega^2 y = 0,$$

which models phenomena like small oscillations a load on a spring, small oscillations of a pendulum, or oscillations of current and voltage in a simple electric oscillator. A basis of solutions consists of $\cos(\omega t)$ and $\sin(\omega t)$.

Quantum-mechanical analog of this system is described by the eigenvalue problem for the differential equation

$$y''(x) + (E - x^2)y(x) = 0, \tag{5}$$

with boundary conditions

$$y \in L^2(-\infty, +\infty). \tag{6}$$

The problem is usual: to find all values of $E$ for which such a non-trivial solution exists. The physical meaning of eigenvalues $E_k$ is the energy levels, and eigenfunctions $y$ are the "wave functions" which describe the state of the system.

We will reduce (5) to Hermite's equation by a simple change of the variable $y = P(x)e^{-x^2/2}$:

$$y' = (P' - xP)e^{-x^2/2},$$

$$y'' = (P'' - xP' - P - xP' + x^2 P)e^{-x^2/2},$$

so $P$ satisfies

$$P'' - 2xP' + (E - 1)P = 0,$$

and in view of the boundary condition, for $y$, we see that $P \in L^2_w(-\infty, +\infty)$, where $w(x) = e^{-x^2}$. Indeed

$$\|P\|_w^2 = \int_{-\infty}^{\infty} |P(x)|^2 e^{-x^2} dx = \int_{-\infty}^{\infty} |y(x)|^2 dx.$$

So the boundary conditions for the Hermite equation are satisfied and we conclude that $E_n = 2n + 1$ for some $n = 0, 1, 2, \ldots$.

Equation (5) also arises in the separation of variables for the Laplace equaton in *parabolic* coordinates $(s, t)$ which are related to the rectangular coordinates $(x, y)$ in the plane by formulas

$$x = s^2 - t^2, \quad y = 2st.$$

The level lines $s = c$ and $t = c$ are parabolas with focus at the oprigin. For the details, see pp. 188–189 of the book.