

Integration with Gaussian quadratures

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August 29, 2021

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1 Introduction

2 Theoretical elements

Our goal is to numerically calculate the definite integral

$$I = \int_a^b f(x) dx \quad (1)$$

with f a well-behaved function (smooth and non-diverging) in the interval $[a, b]$. The **mean value theorem for integrals**¹ allows us to write the integral I as a sum of N terms

$$I = \sum_{i=1}^N \tilde{w}_i f(x_i) \quad x_i \in [a, b] \quad \forall i \quad (2)$$

where $\{x\}$ are the **integration nodes** and $\{\tilde{w}\}$ the **weights**. Solving the above equality would mean finding the exact values of $\{x\}$ and $\{\tilde{w}\}$, for *all* f . In theory, this could be possible, but then we'd have an analytical solution to the problem, thus no need for a numerical method.

Developing a numerical integration method consists in requiring that the equality holds exactly for *some* f and finding suitable values for the nodes and weights. For other functions, the sum will then be an *approximation* to the integral, so it's formally more correct to write: $I \simeq \sum_{i=1}^N \tilde{w}_i f(x_i)$. Note that we'll need $2N$ conditions to solve the $2N$ unknowns (N nodes and N weights).

As an example, let's analyze the popular trapezoid rule, in which we impose that $x_1 = a$, $x_N = b$ and that all nodes be equidistant. These N conditions for the nodes yield the familiar² $x_i = a + (i-1) \cdot h$, with $h = (b-a)/(N-1)$. On the other hand, we require the method to be *exact* for polynomials of degree zero *and* for polynomials of degree one, which translates to N additional conditions. These allow us to find the values for the weights: $\tilde{w}_1 = \tilde{w}_N = h/2$ and $\tilde{w}_i = h, i \in \{2, 3, \dots, N-1\}$.

¹ see appendix A

² Beware of the notation! N is the total number of nodes, not subintervals.

2.1 Gaussian quadratures

Before continuing we introduce a small change of notation³, $f = g \cdot v$. We're also slightly changing the equality between integral and sum⁴

$$\int_a^b g(x)v(x) dx \simeq \sum_{i=1}^N w_i g(x_i) . \quad (3)$$

Remember that our problem consists in solving $2N$ unknowns (N nodes and N weights), so we'll need $2N$ conditions. In Gaussian quadratures, we demand our solution to be *exact* for any polynomial T , with $0 \leq \deg(T) \leq 2N - 1$. *Habemus* our $2N$ conditions!

Let $\{\phi\}$ be an **orthogonal polynomial basis** of $L_v^2[a, b]$

$$\langle \phi_k | \phi_l \rangle = \int_a^b \phi_k(x) \phi_l(x) v(x) dx = A_k^2 \delta_{k,l} \quad (4)$$

with A_k^2 the normalization constant and $v(x)$ the weight function⁵. Additionally we demand that ϕ_k has k **simple roots** in $[a, b]$.

Now we take *any* polynomial of degree $N - 1$, R_{N-1} , which can be expanded (in the interval $[a, b]$) using the chosen orthogonal basis

$$R_{N-1}(x) = \sum_{k=0}^{N-1} \alpha_k \phi_k(x) , \quad (5)$$

and construct the function $g = \phi_N R_{N-1}$. Note that g is a polynomial of order $2N - 1$; if we calculate its integral, the equality in (3) will hold *exactly*

$$\int_a^b \phi_N(x) R_{N-1}(x) v(x) dx = \sum_{i=1}^N w_i \phi_N(x_i) R_{N-1}(x_i) . \quad (6)$$

Writing out the LHS, using (4) and (5)

$$\int_a^b \phi_N(x) R_{N-1}(x) v(x) dx = \sum_{k=0}^{N-1} \alpha_k \int_a^b \phi_N(x) \phi_k(x) v(x) dx = \sum_{k=0}^{N-1} \alpha_k A_k^2 \delta_{k,N} = 0 . \quad (7)$$

The RHS of (6) must also sum zero. In general, $R_{N-1}(x_i) \neq 0$ and, obviously, $w_i \neq 0$; thus: $\phi_N(x_i) = 0$.

First result: Our integration nodes will be the roots of the N -th degree polynomial of the $L_v^2[a, b]$ orthogonal basis $\{\phi\}$.

³ If f is well-behaved, there shouldn't be any problem in obtaining this decomposition.

⁴ You might be alarmed by the fact that we're messing with the mean value theorem, but we've only changed the weights (there's a map from the previously defined weights to these new ones).

⁵ Not to be confused with our weights $\{w\}$!

2.2 Lagrange interpolation

So far we've solved the N nodes $\{x_i\}$, using an $L_v^2[a, b]$ orthogonal polynomial basis $\{\phi\}$. We still have to find the value for the N weights $\{w_i\}$; to do so we use **Lagrange interpolation**.

Consider *any* function h and its Lagrange interpolator H_{N-1} , a polynomial of degree $N - 1$. In the interval $[a, b]$, we want them to coincide at N points, specifically the N roots of ϕ_N , $\{x_j\}$. We define H_{N-1} as

$$H_{N-1}(x) = \sum_{j=1}^N h(x_j) \frac{\phi_N(x)}{\phi'_N(x_j)(x - x_j)} \quad (8)$$

with ϕ'_N the derivative of ϕ_N . One might be worried about H_{N-1} diverging (we're apparently dividing by zero!). Remember that any polynomial can be written as a product of roots, particularly

$$\phi_N = c_N(x - x_1)(x - x_2) \cdots (x - x_N) \quad (9)$$

which makes it easy to check that for each term of the sum, the apparent zero in the denominator cancels out with a term in the numerator⁶. On the other hand, remember that ϕ_N has N simple roots, which implies⁷ $\phi'_N(x_j) \neq 0, \forall j$. Let's check if the two functions h and H_{N-1} coincide at the N roots⁸

$$H_{N-1}(x_k) = \lim_{x \rightarrow x_k} H_{N-1}(x) = \sum_{j=1}^N h(x_j) \lim_{x \rightarrow x_k} \frac{\phi_N(x)}{\phi'_N(x_j)(x - x_j)} = \sum_{j=1}^N h(x_j) \delta_{j,k} = h(x_k). \quad (10)$$

Now we particularize this expression for a polynomial of degree $2N - 1$, q_{2N-1} , whose Lagrange interpolator we denote Q_{N-1} . Remember that q_{2N-1} and Q_{N-1} coincide at N points, the roots of ϕ_N . We can write the difference $s = q_{2N-1} - Q_{N-1}$ (note that $\deg(s) = 2N - 1$) as

$$s(x) = q_{2N-1}(x) - Q_{N-1}(x) \quad (11)$$

$$= B(x - x_1)(x - x_2) \cdots (x - x_N)(x - \tilde{x}_1)(x - \tilde{x}_2) \cdots (x - \tilde{x}_{N-1}). \quad (12)$$

The first N roots of s coincide with those of ϕ_N , the remaining $N - 1$ roots isn't relevant. We define one last polynomial

$$r(x) = \frac{s(x)}{\phi_N(x)} = \frac{q_{2N-1}(x) - Q_{N-1}(x)}{\phi_N(x)} = B(x - \tilde{x}_1)(x - \tilde{x}_2) \cdots (x - \tilde{x}_{N-1}), \quad (13)$$

with $\deg(r) = N - 1$. Rearranging expression (13)

$$q_{2N-1} = Q_{N-1} + r\phi_N. \quad (14)$$

Finally we identify q_{2N-1} with the function g and, as we've done before, calculate its integral. Again, the equality in (3) will hold *exactly*

$$\int_a^b q_{2N-1}(x)v(x) dx = \sum_{i=1}^N w_i q_{2N-1}(x_i). \quad (15)$$

Using (14) we write out the LHS in (15)

$$\int_a^b q_{2N-1}(x)v(x) dx = \int_a^b Q_{N-1}(x)v(x) dx + \int_a^b r(x)\phi_N(x)v(x) dx \quad (16)$$

⁶ This also assures that $\deg(H_{N-1}) = N - 1$.

⁷ You might want to review your calculus notes ☺

⁸ The limit is not too difficult to calculate, try it! If you get stuck, see appendix B.

and substitute (8) in the first term

$$\int_a^b Q_{N-1}(x)v(x) dx = \int_a^b \sum_{j=1}^N q_{2N-1}(x_j) \frac{\phi_N(x)}{\phi'_N(x_j)(x-x_j)} v(x) dx. \quad (17)$$

Expanding r in the orthogonal basis $\{\phi\}$

$$r(x) = \sum_{k=0}^{N-1} \beta_k \phi_k(x) \quad (18)$$

and applying property (4) to the second term in (16)

$$\int_a^b r(x) \phi_N(x) v(x) dx = \sum_{k=0}^{N-1} \beta_k \int_a^b \phi_N(x) \phi_k(x) v(x) dx = \sum_{k=0}^{N-1} \beta_k A_k^2 \delta_{k,N} = 0. \quad (19)$$

Equating to the RHS in (15)

$$\sum_{j=1}^N q_{2N-1}(x_j) \int_a^b \frac{\phi_N(x)v(x)}{\phi'_N(x_j)(x-x_j)} dx = \sum_{i=1}^N w_i q_{2N-1}(x_i). \quad (20)$$

From this last expression we find the weights⁹, calculating N integrals, one for each root x_i .

Second result: We'll calculate our weights with the formula $w_i = \frac{1}{\phi'_N(x_i)} \int_a^b \frac{\phi_N(x)v(x)}{x-x_i} dx$.

2.3 Mathemagics

Virtually we've solved our problem of finding $\{x_i\}$ and $\{w_i\}$, but we've gone from calculating one single integral to calculating N integrals, one for each of the weights. This is rather counter-intuitive and time-consuming, specially if we choose a large value for N in order to obtain a *good* approximation.

We start solving this problem with something quite simple, adding and subtracting

$$\frac{1}{x-x_i} = \frac{1}{x-x_i} + \frac{1}{x-x_i} \left(\frac{x}{x_i} \right)^k - \frac{1}{x-x_i} \left(\frac{x}{x_i} \right)^k \quad (21)$$

$$= \frac{1}{x-x_i} \left[1 - \left(\frac{x}{x_i} \right)^k \right] + \frac{1}{x-x_i} \left(\frac{x}{x_i} \right)^k \quad (22)$$

$$= \frac{1}{x_i^k} \frac{x_i^k - x^k}{x-x_i} + \frac{1}{x_i^k} \frac{x^k}{x-x_i}. \quad (23)$$

Using equality (23) we calculate the integral

$$\int_a^b \frac{\phi_N(x)v(x)}{x-x_i} dx = \frac{1}{x_i^k} \int_a^b \phi_N(x)v(x) \frac{x_i^k - x^k}{x-x_i} dx + \frac{1}{x_i^k} \int_a^b \frac{x^k \phi_N(x)v(x)}{x-x_i} dx. \quad (24)$$

Note that the fraction $(x_i^k - x^k)/(x-x_i)$ in the first term is a polynomial of degree $k-1$ (both numerator and denominator share a common root, x_i). If $k \leq N$, this polynomial can be expanded in the interval $[a, b]$ as

$$\frac{x_i^k - x^k}{x-x_i} = \sum_{m=0}^{N-1} \gamma_m \phi_m(x).$$

⁹ Note that both i and j are dummy indices.

Applying property (4) in the first term of (24)

$$\frac{1}{x_i^k} \int_a^b \phi_N(x) v(x) \frac{x_i^k - x^k}{x - x_i} dx = \sum_{m=0}^{N-1} \frac{\gamma_m}{x_i^k} \int_a^b \phi_N(x) \phi_m(x) v(x) dx = \sum_{m=0}^{N-1} \frac{\gamma_m}{x_i^k} A_m^2 \delta_{m,N} = 0, \quad (25)$$

and (24) reduces to

$$\int_a^b \frac{\phi_N(x) v(x)}{x - x_i} dx = \frac{1}{x_i^k} \int_a^b \frac{x^k \phi_N(x) v(x)}{x - x_i} dx. \quad (26)$$

This “decomposition” is generalizable to any polynomial S with $\deg(S) \leq N$

$$\frac{1}{x - x_i} = \frac{1}{x - x_i} \left[1 - \frac{S(x)}{S(x_i)} \right] + \frac{1}{x - x_i} \frac{S(x)}{S(x_i)} \quad (27)$$

$$\int_a^b \frac{\phi_N(x) v(x)}{x - x_i} dx = \frac{1}{S(x_i)} \int_a^b \frac{S(x) \phi_N(x) v(x)}{x - x_i} dx. \quad (28)$$

In particular, we choose $S = \phi_{N-1}$ and rewrite the expression for our weights

$$w_i = \frac{1}{\phi'_N(x_i) \phi_{N-1}(x_i)} \int_a^b \frac{\phi_N(x) \phi_{N-1}(x) v(x)}{x - x_i} dx. \quad (29)$$

Remember from (9) that $\phi_N(x) = c_N(x - x_1)(x - x_2) \cdots (x - x_i) \cdots (x - x_N)$ and note that $\phi_N(x)/(x - x_i)$ is a polynomial of degree $N - 1$, which can be written as¹⁰

$$\frac{\phi_N(x)}{x - x_i} = c_N x^{N-1} + \sum_{k=0}^{N-2} C_k x^k = c_N x^{N-1} + \sum_{k=0}^{N-2} \epsilon_k \phi_k(x). \quad (30)$$

Substituting in the integral of (29) and applying property (4)

$$\int_a^b \frac{\phi_N(x) \phi_{N-1}(x) v(x)}{x - x_i} dx = c_N \int_a^b x^{N-1} \phi_{N-1}(x) v(x) dx + \sum_{k=0}^{N-2} \epsilon_k \int_a^b \phi_k(x) \phi_{N-1}(x) v(x) dx \quad (31)$$

$$= c_N \int_a^b x^{N-1} \phi_{N-1}(x) v(x) dx + \sum_{k=0}^{N-2} \epsilon_k A_k^2 \delta_{k,N-1} \quad (32)$$

$$= c_N \int_a^b x^{N-1} \phi_{N-1}(x) v(x) dx. \quad (33)$$

Finally, to get rid of the x^{N-1} in (33) we write

$$\phi_{N-1}(x) = c_{N-1} x^{N-1} + \sum_{k=0}^{N-2} D_k x^k = c_{N-1} x^{N-1} + \sum_{k=0}^{N-2} \zeta_k \phi_k \quad (34)$$

$$x^{N-1} = \frac{\phi_{N-1}(x)}{c_{N-1}} - \sum_{k=0}^{N-2} \frac{\zeta_k}{c_{N-1}} \phi_k. \quad (35)$$

Substituting in the integral of (33) and applying property (4)

$$c_N \int_a^b x^{N-1} \phi_{N-1}(x) v(x) dx = \frac{c_N}{c_{N-1}} \int_a^b \phi_{N-1}^2(x) v(x) dx - \sum_{k=0}^{N-2} \frac{c_N \zeta_k}{c_{N-1}} \int_a^b \phi_k(x) \phi_{N-1}(x) v(x) dx \quad (36)$$

$$= \frac{c_N}{c_{N-1}} A_{N-1}^2 - \sum_{k=0}^{N-2} \frac{c_N \zeta_k}{c_{N-1}} \delta_{k,N-1} \quad (37)$$

$$= \frac{c_N}{c_{N-1}} A_{N-1}^2. \quad (38)$$

¹⁰ Once again, we can expand the polynomial $\sum_{k=0}^{N-2} C_k x^k$ in the orthogonal basis $\{\phi\}$.

Tracing these results back to (29) we obtain a very compact expression for the weights

$$w_i = \frac{A_{N-1}^2}{\phi'_N(x_i)\phi_{N-1}(x_i)} \frac{c_N}{c_{N-1}}. \quad (39)$$

Conclusion: Choosing an $L^2_v[a, b]$ orthogonal polynomial basis $\{\phi\}$, our integration nodes will be the roots of ϕ_N , $\{x_i | \phi_N(x_i) = 0\}$, and we'll calculate the weights using the formula $w_i = \frac{A_{N-1}^2}{\phi'_N(x_i)\phi_{N-1}(x_i)} \frac{c_N}{c_{N-1}}$, with A^2 the normalization constant and c the coefficient of the largest monomial.

3 Gauss-Legendre quadrature

In the previous section we've derived the general form of Gaussian quadratures. Let's remember the relevant formulae

$$\int_a^b g(x)v(x) dx \simeq \sum_{i=1}^N w_i g(x_i) \quad (40)$$

$$x_i \rightarrow \phi_N(x_i) = 0 \quad (41)$$

$$w_i = \frac{A_{N-1}^2}{\phi'_N(x_i)\phi_{N-1}(x_i)} \frac{c_N}{c_{N-1}}. \quad (42)$$

Note that the only variability lies in the orthogonal polynomial basis $\{\phi\}$. The question that arises is: what basis do we use? The choice depends on the interval $[a, b]$.

If it's semi-infinite ($a = 0, b = \infty$), an appropriate basis are Laguerre polynomials; if the interval is infinite ($a = -\infty, b = \infty$), we'd use Hermite polynomials. If the interval is finite we can use Legendre polynomials or Chebyshev polynomials of the second kind. We choose the former since their weight function is $v(x) = 1$, as opposed to $v(x) = \sqrt{1-x^2}$ for the latter.

3.1 Interval shift

Legendre polynomials are defined in the interval $x \in [-1, 1]$, i.e. the conclusions of the previous section are valid *only* if $a = -1$ and $b = 1$. If we want to compute an integral with other bounds

$$I = \int_a^b f(y) dy \quad (43)$$

we have to perform a change of variables

$$y = \frac{b-a}{2}x + \frac{a+b}{2} \rightarrow dy = \frac{b-a}{2}dx \quad (44)$$

$$I = \frac{b-a}{2} \int_{-1}^1 f(x) dx. \quad (45)$$

3.2 Normalization constant

The normalization constant for Legendre polynomials is

$$A_n^2 = \int_{-1}^1 P_n^2(x) dx = \frac{2}{2n+1}, \quad (46)$$

and particularly of our interest

$$A_{N-1}^2 = \frac{2}{2(N-1)+1} = \frac{2}{2N-1}. \quad (47)$$

3.3 Rodrigues' formula

Legendre polynomials may be expressed using Rodrigues' formula

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} \left((x^2 - 1)^n \right), \quad (48)$$

which can be manipulated slightly

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^{2n} + O(x^{2n-1})) = \frac{1}{2^n n!} \left(\frac{(2n)!}{n!} x^n + O(x^{n-1}) \right). \quad (49)$$

From this expression we find

$$c_n = \frac{1}{2^n n!} \frac{(2n)!}{n!} = \frac{(2n)!}{2^n (n!)^2}, \quad (50)$$

and particularly

$$c_N = \frac{(2N)!}{2^N (N!)^2} \quad (51)$$

$$c_{N-1} = \frac{(2N-2)!}{2^{N-1} ((N-1)!)^2}. \quad (52)$$

Now we can compute the fraction

$$\frac{c_N}{c_{N-1}} = \frac{(2N)!}{2^N (N!)^2} \frac{2^{N-1} ((N-1)!)^2}{(2N-2)!} \quad (53)$$

$$= \frac{2N \cdot (2N-1) \cdot (2N-2)!}{2 \cdot 2^{N-1} \cdot N^2 \cdot ((N-1)!)^2} \frac{2^{N-1} ((N-1)!)^2}{(2N-2)!} \quad (54)$$

$$= \frac{2N \cdot (2N-1)}{2 \cdot N^2} \quad (55)$$

$$= \frac{2N-1}{N}. \quad (56)$$

3.4 Recurrence relations

There are a few interesting recurrence relations involving Legendre polynomials. Of particular interest are

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \quad (57)$$

and

$$(x^2 - 1)P'_n(x) = nxP_n(x) - nP_{n-1}(x). \quad (58)$$

We'll use the first in our algorithm and from the second

$$(x_i^2 - 1)P'_N(x_i) = Nx_iP_N(x_i) - NP_{N-1}(x_i) \rightarrow P'_N(x_i) = \frac{NP_{N-1}(x_i)}{1 - x_i^2}, \quad (59)$$

where we've used $P_N(x_i) = 0$.

Plugging (47), (56) and (59) into (42) we find

$$w_i = \frac{2}{N^2} \frac{1 - x_i^2}{P_{N-1}^2(x_i)}. \quad (60)$$

4 Computational algorithm

User input parameters:

- number of integration nodes, N
- integral bounds, a and b
- function, $f(y)$

The steps we have to implement are:

1. find the N roots of P_N , $\{x_i\}$
2. calculate the weights, $\{w_i\}$
3. perform the sum $\sum_{i=1}^N w_i f(x_i)$

To find the N roots of P_N we'll combine the secant and bisection methods. In order to do so, we'll need to narrow the interval where each root lies.

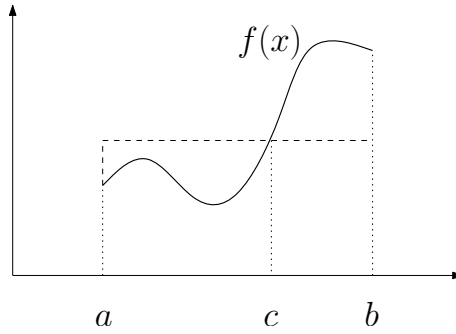
1. start with a step of $\Delta = 2/N$
2. sweep the interval $[-1, 1]$ with step Δ , $x_{j+1} = x_j + \Delta$
 - compare the sign of $P_N(x_j)$ and $P_N(x_{j+1})$
 - if there's a change of sign, record x_j and x_{j+1}
3. count the number of records, M
 - if $M < N$ repeat step 2 with $\Delta = \Delta/10$
 - if $M = N$ we're finished

Now that we've delimited the interval where each root lies we apply the enhanced secant method to find the integration nodes with a fixed precision, ϵ . This enhanced method consists simply in correcting the secant result, $x_{i+1} = x_i - f(x_i)(x_i - x_{i-1})/(f(x_i) - f(x_{i-1}))$, if it diverges from the interval, using the bisection result instead.

To compute the values of the Lagrange polynomials we'll need the recurrence relation (57) and the fact that $P_0 = 1$ and $P_1 = x$.

Remember that we'll have to remap the variable x into the variable y , using (44), in order to compute $f(x_i)$.

Appendix A



Given a well-behaved function f , there exists a value c , $a < c < b$, such that

$$\int_a^b f(x) dx = (b - a) \cdot f(c) . \quad (61)$$

Graphically this means that the area below the curve (between a and c) has the same value as the area above the curve (between c and b).

Appendix B

We want to show

$$\lim_{x \rightarrow x_k} \frac{\phi_N(x)}{\phi'_N(x_j)(x - x_j)} = \delta_{j,k} . \quad (62)$$

Rewriting (9)

$$\phi_N(x) = c_N(x - x_1)(x - x_2) \cdots (x - x_N) = c_N \prod_{i=1}^N (x - x_i) . \quad (63)$$

The denominator $x - x_j$ cancels with a term in the numerator, thus

$$\frac{\phi_N(x)}{x - x_j} = c_N \prod_{i \neq j}^N (x - x_i) . \quad (64)$$

Differentiating (63)

$$\begin{aligned} \phi'_N(x) &= c_N [(x - x_2)(x - x_3) \cdots (x - x_N) + (x - x_1)(x - x_3) \cdots (x - x_N) + \cdots \\ &\quad + (x - x_1)(x - x_2) \cdots (x - x_{N-1})] = c_N \sum_{m=1}^N \frac{\prod_{i=1}^N (x - x_i)}{x - x_m} = c_N \sum_{m=1}^N \prod_{i \neq m}^N (x - x_i) . \end{aligned} \quad (65)$$

Once again, the denominator $x - x_m$ cancels with a term in the numerator. Considering a specific value of $x = x_j$

$$\phi'_N(x_j) = c_N \sum_{m=1}^N \prod_{i \neq m}^N (x_j - x_i) . \quad (66)$$

Most of the summands in (66) include the term $i = j \rightarrow x_j - x_i = 0$. The only summand that survives is $i \neq j$, i.e. $m = j$ and

$$\phi'_N(x_j) = c_N \prod_{i \neq j} (x_j - x_i). \quad (67)$$

Substituting these expressions in the limit

$$\lim_{x \rightarrow x_k} \frac{\phi_N(x)}{\phi'_N(x_j)(x - x_j)} = \lim_{x \rightarrow x_k} \frac{c_N \prod_{i \neq j} (x - x_i)}{c_N \prod_{i \neq j} (x_j - x_i)} = \frac{\prod_{i \neq j} (x_k - x_i)}{\prod_{i \neq j} (x_j - x_i)}. \quad (68)$$

It's clear that in the case $k = j$ numerator and denominator are equal and the limit's value is 1. On the other hand, if $k \neq j$ there's a term in the numerator with $i = k \rightarrow x_k - x_i = 0$ and the limit's value is 0. Therefore

$$\lim_{x \rightarrow x_k} \frac{\phi_N(x)}{\phi'_N(x_j)(x - x_j)} = \delta_{j,k} \quad \text{Q.E.D.} \quad (69)$$