The inverse of the cumulative standard normal probability function.

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Abstract

Some properties of the inverse of the function $N(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} dt$ are studied. Its derivatives, integrals and asymptotic behavior are presented.

1 Introduction

It would be difficult to overestimate the importance of the standard normal (or Gauss) distribution. It finds widespread application in almost every scientific discipline, e.g., probability theory, the theory of errors, heat conduction, biology, economics, physics, neural networks [9], etc. It plays a fundamental role in the financial mathematics, being part of the Black-Scholes formula [2], and its inverse is used in computing the implied volatility of an option [8]. Yet, little is known about the properties of the inverse function, e.g., series expansions, asymptotic behavior, integral representations. The major work done has been in computing fast and accurate algorithms for numerical calculations [1].

Over the years a few articles have appeared with analytical studies of the closely related error function

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-t^2} dt$$

and its complement

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^2} dt .$$

Philip [10] introduced the notation “inverfc($x$)” to denote the inverse of the complementary error function. He gave the first terms in the power series for inverfc($x$), asymptotic formulas for small $x$ in terms of continued logarithms,

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and some expressions for the derivatives and integrals. Carlitz [3], studied the arithmetic properties of the coefficients in the power series of \( \text{inverfc}(x) \). Strecok [11] computed the first 200 terms in the series of \( \text{inverfc}(x) \), and some expansions in series of Chebyshev polynomials. Finally, Fettis [6] studied \( \text{inverfc}(x) \) for small \( x \), using an iterative sequence of logarithms.

The purpose of this paper is to present some new results on the derivatives, integrals, and asymptotics of the inverse of the cumulative standard normal probability function

\[
N(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} \, dt
\]

which we call \( S(x) \). In section 2 we derive an ODE satisfied by \( S(x) \), and solve it using a power series. We introduce a family of polynomials \( P_n \) related to the calculation of higher derivatives of \( S(x) \). In section 3 we study some properties of the \( P_n \), such as relations between coefficients, recurrences, and generating functions. We also derive a general formula for \( P_n \) using the idea of “nested derivatives”, and we compare the \( P_n \) with the Hermite polynomials \( H_n \).

In section 4 we extend the definition of the \( P_n \) to \( n < 0 \) and use them to calculate the integrals of \( S(x) \). We also compute the integrals of powers of \( S(x) \) on the interval \([0, 1]\). Section 5 is dedicated to asymptotics of \( S(x) \) for \( x \to 0, \ x \to 1 \) using the function Lambert W. With the help of those formulas we derive an approximation to \( S(x) \) valid in the interval \([0, 1]\) with error \( \varepsilon \), \( |\varepsilon| < 0.0023 \). Finally, appendix A contains the first 20 non-zero coefficients in the series of \( S(x) \), and the first 10 polynomials \( P_n \).

## 2 Derivatives

### Definition 1

Let \( S(x) \) denote the inverse of

\[
N(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} \, dt
\]

satisfying

\[
S \circ N(x) = N \circ S(x) = x \tag{1}
\]

In terms of the error function \( \text{erf}(x) \),

\[
N(x) = \frac{1}{2} \left[ \text{erf} \left( \frac{x}{\sqrt{2}} \right) + 1 \right]
\]

### Proposition 2

\( S(x) \) satisfies the IVP

\[
S'' = S(S')^2 \tag{2}
\]

\[
S \left( \frac{1}{2} \right) = 0, \ S' \left( \frac{1}{2} \right) = \sqrt{2\pi}
\]
Proof. Since \( N(0) = 1/2 \), in follows that \( S(1/2) = 0 \). From (2.1) we get
\[
S'[N(x)] = \frac{1}{N'(x)} = \sqrt{2\pi e^{s^2}} = \sqrt{2\pi e^{s^2/N(x)}}
\]
Substituting \( N(x) = y \) we have
\[
S'(y) = \sqrt{2\pi e^{s^2}}(\frac{1}{2}) = \sqrt{2\pi}
\]
Differentiating \( \ln[S'(y)] \), we get (2.2). 

Proposition 3
\[
S^{(n+2)}(x) = \sum_{i=0}^{n} \sum_{j=0}^{i} \binom{n}{i} \binom{i}{j} S^{(n-i)}(x)S^{(i-j+1)}(x)S^{(j+1)}(x), \quad n \geq 0.
\]

Proof. Taking the \( n \)th derivative of (2.2), and using Leibnitz’s Theorem, we have
\[
S^{(n+2)}(x) = \sum_{i=0}^{n} \sum_{j=0}^{i} \binom{n}{i} \binom{i}{j} S^{(n-i)}(S'S')^{(i)}
\]
\[
= \sum_{i=0}^{n} \sum_{j=0}^{i} \binom{n}{i} \binom{i}{j} S^{(n-i)}S^{(i-j+1)}S^{(j+1)}
\]

Corollary 4 If \( D_n = \frac{d^n}{dx^n} (\frac{1}{2}) \), then
\[
D_{2n} = 0, \quad n \geq 0.
\]

Putting \( D_n = (2\pi)^{\frac{n}{2}}C_n \), we can write
\[
S(x) = \sum_{n \geq 0} (2\pi)^{\frac{2n+1}{2}} \frac{C_{2n+1}}{(2n+1)!} (x - \frac{1}{2})^{2n+1}
\]
where
\[
C_1 = 1, \quad C_3 = 1, \quad C_5 = 7, \quad C_7 = 127, \ldots.
\]

Proposition 5
\[
S^{(n)} = P_{n-1}(S)(S')^n \quad n \geq 1
\]
where \( P_n(x) \) is a polynomial of degree \( n \) satisfying the recurrence
\[
P_0(x) = 1, \quad P_n(x) = P'_{n-1}(x) + nxP_{n-1}(x), \quad n \geq 1
\]
so that
\[
P_1(x) = x, \quad P_2(x) = 1 + 2x^2, \quad P_3(x) = 7x + 6x^3, \ldots.
\]
Proof. We use induction on \( n \). For \( n = 2 \) the result follows from (2.2). If we assume the result is true for \( n \) then

\[
S^{(n+1)} = [P_{n-1}(S)(S')^n]' \\
= P'_{n-1}(S)S'(S')^n + P_{n-1}(S)n(S')^{n-1}S'' \\
= P'_{n-1}(S)(S')^{n+1} + P_{n-1}(S)n(S')^{n-1}S(S')^2 \\
= [P'_{n-1}(S) + nSP_{n-1}(S)](S')^{n+1} \\
= P_n(S)(S')^{n+1}
\]

Since \( P_{n-1}(x) \) is a polynomial of degree \( n - 1 \) by hypothesis, is clear that

\[
P_n(x) = P'_{n-1}(x) + nxP_{n-1}(x)
\]

is a polynomial of degree \( n \). ■

Corollary 6

\[ C_n = P_{n-1}(0) \]

3 The polynomials \( P_n(x) \)

Lemma 7 If we write

\[
P_n(x) = \sum_{k=0}^{n} Q^n_k x^k
\]

we have

\[
Q^n_0 = Q^{n-1}_1 \\
Q^n_k = nQ^{n-1}_{k-1} + (k + 1)Q^n_{k+1} \quad k = 1, \ldots, n - 2 \\
Q^n_k = nQ^n_{k-1} \quad k = n - 1, n
\]  

Proof.

\[
\sum_{k=0}^{n} Q^n_k x^k = P_n \\
= \frac{d}{dx}P_{n-1} + nxP_{n-1} \\
= \sum_{k=0}^{n-1} Q^{n-1}_k x^{k-1} + \sum_{k=0}^{n-1} nQ^{n-1}_k x^{k+1} \\
= \sum_{k=0}^{n-2} Q^{n-1}_{k+1} (k + 1) x^k + \sum_{k=1}^{n} nQ^{n-1}_{k-1} x^k
\]

■
Corollary 8. In matrix form (3.1) reads \(A^{(n)}Q^{n-1} = Q^n\) where \(A^{(n)} \in \mathbb{R}^{(n+1) \times n}\) is given by

\[
A^{(n)} = \begin{cases} 
  i, & j = i + 1, \ i = 1, \ldots, n - 1 \\
  n, & j = i - 1, \ i = 2, \ldots, n + 1 \\
  0, & \text{otherwise}
\end{cases}
\]

In other words, \(A^{(n)}\) is a rectangular matrix with zeros in the diagonal, the numbers 1, 2, 3, \ldots, \(n - 1\) above it, the number \(n\) below it and zeros everywhere else.

\[
A^{(n)} = \begin{bmatrix} 
  0 & 1 & 0 & 0 & \cdots & 0 & 0 \\
  n & 0 & 2 & 0 & \cdots & 0 & 0 \\
  0 & n & 0 & 3 & \cdots & 0 & 0 \\
  \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
  0 & 0 & 0 & 0 & \cdots & 0 & n - 1 \\
  0 & 0 & 0 & 0 & \cdots & 0 & n \\
  0 & 0 & 0 & 0 & \cdots & 0 & n \\
\end{bmatrix}
\]

and

\[
Q^n = \begin{bmatrix} 
  Q_0^n \\
  Q_1^n \\
  Q_2^n \\
  \vdots \\
  Q_n^n \\
\end{bmatrix}
\]

With the help of these matrices, we have an expression for the coefficients of \(P_n(x)\)

\[
Q^n = \prod_{k=1}^{n} A^{(n-k+1)} = A^{(n)}A^{(n-1)}\ldots A^{(1)}
\]

Proposition 9. The polynomials \(P_n(x)\) satisfy the recurrence relation

\[
P_{n+1}(x) = \sum_{i=0}^{n} \sum_{j=0}^{i} \binom{n}{i} \binom{i}{j} P_{n-i-1}(x)P_{i-j}(x)P_j(x)
\]

Proof.

\[
P_{n+1}(S)(S')^{n+2}
= S^{(n+2)} = \sum_{i=0}^{n} \sum_{j=0}^{i} \binom{n}{i} \binom{i}{j} S^{(n-i)}S^{(i-j+1)}S^{(j+1)}
= \sum_{i=0}^{n} \sum_{j=0}^{i} \binom{n}{i} \binom{i}{j} P_{n-i-1}(S)(S')^{n-i}P_{i-j}(S)(S')^{i-j+1}P_j(S)(S')^{j+1}
= (S')^{n+2} \sum_{i=0}^{n} \sum_{j=0}^{i} \binom{n}{i} \binom{i}{j} P_{n-i-1}(S)P_{i-j}(S)P_j(S).
\]

\[
\square
\]
Proposition 10  The exponential generating function of the polynomials \( P_n(x) \) is
\[
e^{\frac{x}{2} S^2 [N(x) + tN'(x)] - \frac{x^2}{4}} = F(x, t) = \sum_{k \geq 0} P_k(x) \frac{t^k}{k!}
\]

Proof.  Since
\[
F(x, t) = \sum_{k \geq 0} P_k(x) \frac{t^k}{k!}
\]

\[
= 1 + \sum_{k \geq 1} \frac{d}{dx} P_{k-1}(x) \frac{t^k}{k!} + \sum_{k \geq 1} kxP_{k-1}(x) \frac{t^k}{k!}
\]

\[
= 1 + \sum_{k \geq 0} \frac{d}{dx} P_k(x) \frac{t^{k+1}}{(k+1)!} + \sum_{k \geq 0} xP_k(x) \frac{t^{k+1}}{(k+1)!}
\]

\[
= 1 + \int_0^t \frac{\partial}{\partial x} F(x, s) ds + xtF(x, t)
\]

it follows that \( F(x, t) \) satisfies the differential-integral equation
\[
1 + (xt - 1)F(x, t) + \frac{\partial}{\partial t} \int_0^t F(x, s) ds = 0 \tag{5}
\]

Differentiating (3.2) with respect to \( t \) we get
\[
xF(x, t) + (xt - 1) \frac{\partial}{\partial t} F(x, t) + \frac{\partial}{\partial x} F(x, t) = 0
\]

whose general solution is of the form
\[
F(x, t) = e^{-\frac{x^2}{4}} G \left( te^{-\frac{x^2}{4}} + \sqrt{2\pi} \left[ N(x) - \frac{1}{2} \right] \right)
\]

for some function \( G(z) \).
From (3.2) we know that \( F(x, 0) = 1 \), and hence
\[
G \left( \sqrt{2\pi} \left[ N(x) - \frac{1}{2} \right] \right) = e^{\frac{x^2}{2}},
\]

which implies that
\[
G(z) = e^{\frac{1}{2} S^2 (\sqrt{2\pi} z + \frac{1}{2})}.
\]

Therefore,
\[
F(x, t) = e^{\frac{1}{2} S^2 [N(x) + tN'(x)] - \frac{x^2}{4}}
\]
Definition 11 We define the “nested derivative” $\mathcal{D}^{(n)}$ by

$$\mathcal{D}^{(0)}[f](x) \equiv 1$$
$$\mathcal{D}^{(n)}[f](x) = \frac{d}{dx} \left\{ f(x) \times \mathcal{D}^{(n-1)}[f](x) \right\}, \quad n \geq 1$$

Example 12

1. $\mathcal{D}^{(n)}[e^{ax}] = n!a^ne^{ax}$

2. $\mathcal{D}^{(n)}[x] = 1$

3. $\mathcal{D}^{(n)}[x^2] = (n + 1)!x^n$

Proposition 13

$$P_n(x) = e^{-\frac{x^2}{2}} \mathcal{D}^{(n)} \left[ e^{\frac{x^2}{2}} \right]$$

Proof. We use induction on $n$. For $n = 0$ the result follows from the definition of $\mathcal{D}^{(n)}$. Assuming the result is true for $n - 1$

$$P_n(x) = P'_{n-1}(x) + nxP_{n-1}(x)$$
$$= \frac{d}{dx} \left[ e^{-\frac{(n-1)x^2}{2}} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}}) \right] + nxe^{-\frac{(n-1)x^2}{2}} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}})$$
$$= -(n-1)xe^{-\frac{(n-1)x^2}{2}} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}}) + e^{-\frac{(n-1)x^2}{2}} \frac{d}{dx} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}}) +$$
$$+ nxe^{-\frac{(n-1)x^2}{2}} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}})$$
$$= e^{-\frac{(n-1)x^2}{2}} \left[ xe^{-\frac{(n-1)x^2}{2}} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}}) + \frac{d}{dx} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}}) \right]$$
$$= e^{-\frac{(n-1)x^2}{2}} e^{-\frac{x^2}{2}} \frac{d}{dx} \left[ e^{\frac{x^2}{2}} \mathcal{D}^{(n-1)}(e^{\frac{x^2}{2}}) \right]$$
$$= e^{-\frac{x^2}{2}} \mathcal{D}^{(n)} \left[ e^{\frac{x^2}{2}} \right]$$

Summary 14 We conclude this section by comparing the properties of $P_n(x)$ with the well known formulas for the Hermite polynomials $H_n(x)$. Since the $H_n$ are deeply related with the function $N(x)$, we would expect to see some similarities between the $H_n$ and the $P_n$. 

7
\begin{align*}
\sum_{k \geq 0} P_k(x) t^k &= e^{x^2 t} H_n(x) = e^{-1/n} e^{x^2 t} d_{n+1} \left( e^{-x^2} \right) \\
\sum_{k \geq 0} H_k(x) t^k &= e^{2xt-t^2} \\
S^{(n)} = P_{n-1}(S)(S')^n &\quad \text{and the relation} \quad S^{(n)} = P_{n-1}(S)(S')^n
\end{align*}

4 Integrals of S(x)

Definition 15

\[ S^{(-n)}(x) = \int_0^x \cdots \int_0^{x_{n-1}} S(x_n) \, dx_n dx_{n-1} \cdots dx_1 \quad n \geq 1. \]

Lemma 16

\[ P_{n-1}(x) = e^{-x^2/2} \left[ P_{n-1}(0) + \int_0^x e^{x^2 t^2} P_n(t) \, dt \right] \]  

Proof. It follows immediately from solving the ODE for \( P_{n-1} \) in terms of \( P_n \).

Proposition 17 Using (4.1) to define \( P_n(x) \) for \( n < 0 \) yields

\begin{align*}
P_{-1}(x) &= x \\
P_{-2}(x) &= -1 \\
P_{-3}(x) &= -\sqrt{\pi} e^{x^2} N\left( \sqrt{x} \right) \\
\end{align*}

and the relation

\[ S^{(n)} = P_{n-1}(S)(S')^n \]

still holds.

Proof. For \( n = 0 \) we have

\begin{align*}
P_{-1}(x) &= P_{-1}(0) + x \\
S = S^{(0)} &= P_{-1}(S)
\end{align*}
so $P_{-1}(0) = 0$. For $n = -1$

$$P_{-2}(x) = e^{x^2/2} [P_{-2}(0) + 1] - 1$$

We can calculate $S^{(-1)}$ explicitly by

$$S^{(-1)}(x) = \int_0^x S(t) dt = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x S[N(z)] e^{-\frac{z^2}{2}} dz$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x z e^{-\frac{z^2}{2}} dz$$

$$= -\frac{1}{\sqrt{2\pi}} e^{\frac{2(x^2)}{2}} = -(S')^{-1}$$

Hence, $P_{-2}(0) = -1$.

Finally, for $n = -2$

$$P_{-3}(x) = e^{x^2} \left[ P_{-3}(0) - \sqrt{\pi} N(\sqrt{2}x) + \frac{\sqrt{\pi}}{2} \right]$$

A similar calculation as the one above, making a change of variables $t = N(z)$ in the integral of $S^{(-1)}(x)$ yields

$$S^{(-2)}(x) = -\frac{1}{2\sqrt{\pi}} N[\sqrt{2}S(x)]$$

and we conclude that $P_{-3}(0) = -\frac{\sqrt{\pi}}{2}$. □

Corollary 18

$$S \left[ -2\sqrt{\pi}S^{(-2)} \right] = \sqrt{2}S$$

Proposition 19

$$\int_0^1 S^n(x) dx = \begin{cases} \prod_{i=1}^k (2i + 1), & n = 2k, \quad k \geq 1 \\ 0, & n = 2k + 1, \quad k \geq 0 \end{cases}$$

Proof.

$$\int_0^1 S^n(x) dx = \int_{-\infty}^\infty z^n N'(z) dz$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty z^n e^{-\frac{z^2}{2}} dz$$

$$= \prod_{i=1}^k (2i + 1), \quad n = 2k, \quad k \geq 1$$

□
5 Asymptotics

Definition 20 We’ll denote by \( LW(x) \) the function Lambert W \[4\],
\[
LW(x)e^{LW(x)} = x
\] (8)

This function has the series representation \[5\]
\[
LW(x) = \sum_{n \geq 1} \frac{(-n)^{n-1}}{n!} x^n,
\]

the derivative
\[
\frac{d}{dx} LW = \frac{LW(x)}{x[1 + LW(x)]} \quad \text{if} \quad x \neq 0,
\]

and it has the asymptotic behavior
\[
LW(x) \sim \ln(x) - \ln[\ln(x)] \quad x \to \infty.
\]

Proposition 21
\[
S(x) \sim g_0(x) = -\sqrt{\frac{LW(1)}{2\pi x^2}}, \quad x \to 0
\]
\[
S(x) \sim g_1(x) = \sqrt{\frac{LW(1)}{2\pi (x-1)^2}}, \quad x \to 1
\]

Both functions \( g_0(x) \) and \( g_1(x) \) satisfy the ODE
\[
g'' = g(g')^2 \left[ 1 + \frac{2}{g^2(1 + g^2)} \right] \sim g(g')^2, \quad \text{for} \quad |g| \to \infty
\]

Proof.
\[
N(x) \sim \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \frac{1}{x}, \quad x \to -\infty
\]
\[
t \sim \frac{1}{\sqrt{2\pi}} e^{-\frac{\omega^2}{2}} \frac{1}{S(t)}, \quad t \to 0
\]
\[
S(t)e^{-\frac{\omega^2}{2}} \sim \frac{1}{\sqrt{2\pi t}}, \quad t \to 0
\]
\[
S^2(t)e^{S^2(t)} \sim \frac{1}{2\pi t^2}, \quad t \to 0
\]

Using the definition of \( LW(x) \) we have
\[
S^2(t) \sim LW(\frac{1}{2\pi t^2}), \quad t \to 0
\]
or
\[
S(t) \sim -\sqrt{LW(\frac{1}{2\pi t^2})}, \quad t \to 0
\]
The case \( x \to 1 \) is completely analogous. \[\blacksquare\]
Corollary 22 Combining the above expressions, we can get the approximation

\[ S(x) \simeq g_2(x) = (2x - 1) \sqrt{LW \left( \frac{1}{2\pi x^2 (x-1)} \right)} \]  

(9)

good through the interval \((0,1)\).
We can refine it even more by putting

\[ S(x) \simeq g_3(x) = Q(x) \sqrt{LW \left( \frac{1}{2\pi x^2 (x-1)} \right)} \]  

(10)

where \(Q(x)\) has been chosen such that

\[ Q(0) = -1, \ Q(1) = 0, \ Q(1/2) = 0, \ Q'(1/2) = \sqrt{2\pi}, \ Q''(1/2) = 0 \]

6 Appendix

The first 10 \(P_n(x)\) are

\[ P_0(x) = 1 \]
\[ P_1(x) = x \]
\[ P_2(x) = 1 + 2x^2 \]
\[ P_3(x) = 7x + 6x^3 \]
\[ P_4(x) = 7 + 46x^2 + 24x^4 \]
\[ P_5(x) = 127x + 326x^3 + 120x^5 \]
\[ P_6(x) = 127 + 1740x^2 + 2556x^4 + 720x^6 \]
\[ P_7(x) = 4369x + 22404x^3 + 22212x^5 + 5040x^7 \]
\[ P_8(x) = 4369 + 102164x^2 + 290292x^4 + 212976x^6 + 40320x^8 \]
\[ P_9(x) = 243649x + 208064x^3 + 389048x^5 + 2239344x^7 + 362880x^9 \]
\[ P_{10}(x) = 243649 + 8678422x^2 + 40258860x^4 + 54580248x^6 + \]
\[ + 25659360x^8 + 3628800x^{10} \]

The first few odd \(C_n\) are
\begin{tabular}{|c|c|}
\hline
\textbf{n} & \textbf{C}_n \\
\hline
1 & 1 \\
3 & 1 \\
5 & 7 \\
7 & 127 \\
9 & 4369 \\
11 & 243649 \\
13 & 20036983 \\
15 & 2280356863 \\
17 & 343141433761 \\
19 & 65967241200001 \\
21 & 15773461423793767 \\
23 & 4591227123230945407 \\
25 & 1598351733247609852849 \\
27 & 655782249799531714375489 \\
29 & 31316040486497385238669783 \\
31 & 172201685126573465512657343 \\
33 & 10802634947672041127839800617281 \\
35 & 76683701969726780307420968904733441 \\
37 & 61154674195324330125295778531172438727 \\
39 & 54441029530574028687402753580278549396607 \\
41 & 537898841016065502324949796685518122943569 \\
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\end{tabular}

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