1

Malliavin operators in the one-dimensional case

As anticipated in the Introduction, in order to develop the main tools for the normal approximations of the laws of random variables, we need to define and exploit a modicum of *Malliavin-type operators* – such as the *derivative*, *divergence* and *Ornstein–Uhlenbeck* operators. These objects act on random elements that are functionals of some Gaussian field, and will be fully described in Chapter 2. The aim of this chapter is to introduce the reader into the realm of Malliavin operators, by focusing on their one-dimensional counterparts. In particular, in what follows we are going to define derivative, divergence and Ornstein–Uhlenbeck operators acting on random variables of the type $F = f(N)$, where f is a deterministic function and $N \sim \mathscr{N}(0,1)$ has a standard Gaussian distribution. As we shall see below, one-dimensional Malliavin operators basically coincide with familiar objects of functional analysis. As such, one can describe their properties without any major technical difficulties. Many computations detailed below are further applied in Chapter 3, where we provide a thorough discussion of Stein's method for one-dimensional normal approximations.

For the rest of this chapter, every random object is defined on an appropriate probability space $(\Omega, \mathscr{F}, P)$. The symbols 'E' and 'Var' denote, respectively, the expectation and the variance associated with P.

1.1 Derivative operators

Let us consider the probability space $(\mathbb{R}, \mathscr{B}(\mathbb{R}), \gamma)$, where γ stands for the standard Gaussian probability measure, that is,

$$\gamma(A) = \frac{1}{\sqrt{2\pi}} \int_A e^{-x^2/2} dx,$$

for every Borel set A. A random variable N with distribution γ is called *standard Gaussian*; equivalently, we write $N \sim \mathscr{N}(0,1)$. We start with a simple (but crucial) statement.

Lemma 1.1.1 *Let $f : \mathbb{R} \to \mathbb{R}$ be an absolutely continuous function such that $f' \in L^1(\gamma)$. Then $x \mapsto xf(x) \in L^1(\gamma)$ and*

$$\int_{\mathbb{R}} xf(x) d\gamma(x) = \int_{\mathbb{R}} f'(x) d\gamma(x). \tag{1.1.1}$$

Proof Since $\int_{\mathbb{R}} |x| d\gamma(x) < \infty$, we can assume that $f(0) = 0$ without loss of generality. We first prove that the mapping $x \mapsto xf(x)$ is in $L^1(\gamma)$. Indeed,

$$\begin{aligned}
\int_{-\infty}^{\infty} |f(x)|\,|x| d\gamma(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left| \int_0^x f'(y) dy \right| |x| e^{-x^2/2} dx \\
&\le \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{0} \left(\int_x^0 |f'(y)| dy \right) (-x) e^{-x^2/2} dx \\
&\quad + \frac{1}{\sqrt{2\pi}} \int_0^{\infty} \left(\int_0^x |f'(y)| dy \right) x e^{-x^2/2} dx \\
&= \int_{-\infty}^{\infty} |f'(y)| d\gamma(y) < \infty,
\end{aligned}$$

where the last equality follows from a standard application of the Fubini theorem. To show relation (1.1.1), one can apply once again the Fubini theorem and infer that

$$\begin{aligned}
\int_{-\infty}^{\infty} f(x) x d\gamma(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{0} \left(\int_x^0 f'(y) dy \right) (-x) e^{-x^2/2} dx \\
&\quad + \frac{1}{\sqrt{2\pi}} \int_0^{\infty} \left(\int_0^x f'(y) dy \right) x e^{-x^2/2} dx = \int_{-\infty}^{\infty} f'(y) d\gamma(y).
\end{aligned}$$

□

Remark 1.1.2 Due to the fact that the assumptions in Lemma 1.1.1 are minimal, we proved relation (1.1.1) by using a Fubini argument instead of a (slightly more natural) integration by parts. Observe that one cannot remove the 'absolutely continuous' assumption on f. For instance, if $f = \mathbf{1}_{[0,\infty)}$, then $\int_{-\infty}^{\infty} xf(x) d\gamma(x) = \frac{1}{\sqrt{2\pi}}$, whereas $\int_{-\infty}^{\infty} f'(x) d\gamma(x) = 0$.

We record a useful consequence of Lemma 1.1.1, consisting in a characterization of the moments of γ, which we denote by

$$m_n(\gamma) = \int_{\mathbb{R}} x^n d\gamma(x), \quad n \ge 0. \tag{1.1.2}$$

Corollary 1.1.3 *The sequence $(m_n(\gamma))_{n \ge 0}$ satisfies the induction relation*

$$m_{n+1}(\gamma) = n \times m_{n-1}(\gamma), \quad n \ge 0. \tag{1.1.3}$$

In particular, one has $m_n(\gamma) = 0$ *if* n *is odd, and*

$$m_n(\gamma) = n!/(2^{n/2}(n/2)!) = (n-1)!! = 1 \cdot 3 \cdot 5 \cdot \ldots \cdot (n-1) \quad \textit{if } n \textit{ is even.}$$

Proof To obtain the induction relation (1.1.3), just apply (1.1.1) to the function $f(x) = x^n$, $n \geq 0$. The explicit value of $m_n(\gamma)$ is again computed by an induction argument. □

In what follows, we will denote by $\mathcal{S}$ the set of C^∞-functions $f : \mathbb{R} \to \mathbb{R}$ such that f and all its derivatives have at most polynomial growth. We call any element of $\mathcal{S}$ a *smooth* function.

Remark 1.1.4 The relevance of smooth functions is explained by the fact that the operators introduced below are all defined on domains that can be obtained as the closure of $\mathcal{S}$ with respect to an appropriate norm. We will see in the next chapter that an analogous role is played by the collection of the *smooth functionals* of a general Gaussian field. In the one-dimensional case, the reason for the success of this 'approximation procedure' is nested in the following statement.

Proposition 1.1.5 *The monomials* $\{x^n : n = 0, 1, 2, \ldots\}$ *generate a dense subspace of* $L^q(\gamma)$ *for every* $q \in [1, \infty)$. *In particular, for any* $q \in [1, \infty)$ *the space* $\mathcal{S}$ *is a dense subset of* $L^q(\gamma)$.

Proof Elementary Hahn–Banach theory (see Proposition E.1.3) implies that it is sufficient to show that, for every $\eta \in (1, \infty]$, if $g \in L^\eta(\gamma)$ is such that $\int_{\mathbb{R}} g(x)x^k d\gamma(x) = 0$ for every integer $k \geq 0$, then $g = 0$ almost everywhere. So, let $g \in L^\eta(\gamma)$ satisfy $\int_{\mathbb{R}} g(x)x^k d\gamma(x) = 0$ for every $k \geq 0$, and fix $t \in \mathbb{R}$. We have, for all $x \in \mathbb{R}$,

$$\left| g(x)e^{-\frac{x^2}{2}} \sum_{k=0}^{n} \frac{(itx)^k}{k!} \right| \leq |g(x)| e^{|tx| - \frac{x^2}{2}},$$

so that, by dominated convergence,[1] we have

$$\int_{\mathbb{R}} g(x)e^{itx} d\gamma(x) = \lim_{n\to\infty} \sum_{k=0}^{n} \frac{(it)^k}{k!} \int_{\mathbb{R}} g(x)x^k d\gamma(x) = 0.$$

[1] Indeed, by the Hölder inequality and by using the convention $\frac{\infty - 1}{\infty} = 1$ to deal with the case $\eta = \infty$, one has that

$$\int_{-\infty}^{\infty} |g(x)| e^{|tx| - \frac{x^2}{2}} dx = \sqrt{2\pi} \int_{-\infty}^{\infty} |g(x)| e^{|tx|} d\gamma(x) \leq \sqrt{2\pi} \|g\|_{L^\eta(\gamma)} \|e^{|t\cdot|}\|_{L^{(\eta-1)/\eta}(\gamma)} < \infty.$$

We have therefore proved that $\int_{\mathbb{R}} g(x)\exp(itx)d\gamma(x) = 0$ for every $t \in \mathbb{R}$, from which it follows immediately (by injectivity of the Fourier transform) that $g = 0$ almost everywhere. □

Fix $f \in \mathcal{S}$; for every $p = 1, 2, \ldots$, we write $f^{(p)}$ or, equivalently, $D^p f$ to indicate the pth derivative of f. Note that the mapping $f \mapsto D^p f$ is an operator from $\mathcal{S}$ into itself. We now prove that this operator is closable.

Lemma 1.1.6 *The operator* $D^p : \mathcal{S} \subset L^q(\gamma) \to L^q(\gamma)$ *is closable for every* $q \in [1, \infty)$ *and every integer* $p \geq 1$.

Proof We only consider the case $q > 1$; due to the duality $L^1(\gamma)/L^\infty(\gamma)$, the case $q = 1$ requires some specific argument and is left to the reader. Let (f_n) be a sequence of $\mathcal{S}$ such that: (i) f_n converges to zero in $L^q(\gamma)$; (ii) $f_n^{(p)}$ converge to some η in $L^q(\gamma)$. We have to prove that η is equal to zero. Let $g \in \mathcal{S}$, and define $\delta^p g \in \mathcal{S}$ iteratively by $\delta^r g = \delta^1 \delta^{r-1} g$, $r = 2, \ldots, p$, where $\delta^1 g(x) = \delta g(x) = xg(x) - g'(x)$ (note that this notation is consistent with the content of Section 1.2, where the operator δ will be fully characterized). We have, using Lemma 1.1.1 several times,

$$\begin{aligned}
\int_{\mathbb{R}} \eta(x)g(x)d\gamma(x) &= \lim_{n\to\infty} \int_{\mathbb{R}} f_n^{(p)}(x)g(x)d\gamma(x) \\
&= \lim_{n\to\infty} \int_{\mathbb{R}} f_n^{(p-1)}(x)\big(xg(x) - g'(x)\big)d\gamma(x) \\
&= \lim_{n\to\infty} \int_{\mathbb{R}} f_n^{(p-1)}(x)\delta g(x)d\gamma(x) \\
&= \ldots \\
&= \lim_{n\to\infty} \int_{\mathbb{R}} f_n(x)\delta^p g(x)d\gamma(x).
\end{aligned}$$

Hence, since $f_n \to 0$ in $L^q(\gamma)$ and $\delta^p g$ belongs to $\mathcal{S} \subset L^{\frac{q}{q-1}}(\gamma)$, we deduce, by applying the Hölder inequality, that $\int_{\mathbb{R}} \eta(x)g(x)d\gamma(x) = 0$. Since it is true for any $g \in \mathcal{S}$, we deduce from Proposition 1.1.5 that $\eta = 0$ almost everywhere, and the proof of the lemma is complete. □

Fix $q \in [1, \infty)$ and an integer $p \geq 1$. We set $\mathbb{D}^{p,q}$ to be the closure of $\mathcal{S}$ with respect to the norm

$$\|f\|_{\mathbb{D}^{p,q}} = \left(\int_{\mathbb{R}} |f(x)|^q d\gamma(x) + \int_{\mathbb{R}} |f'(x)|^q d\gamma(x) + \ldots + \int_{\mathbb{R}} |f^{(p)}(x)|^q d\gamma(x) \right)^{1/q}.$$

In other words, a function f is an element of $\mathbb{D}^{p,q}$ if and only if there exists a sequence $(f_n)_{n\geq 1} \subset \mathcal{S}$ such that (as $n \to \infty$): (i) f_n converges to f in $L^q(\gamma)$; and (ii) for every $j = 1, \ldots, p$, $f_n^{(j)}$ is a Cauchy sequence in $L^q(\gamma)$. For such an f, one defines

$$f^{(j)} = D^j f = \lim_{n\to\infty} D^j f_n = \lim_{n\to\infty} f_n^{(j)}, \tag{1.1.4}$$

where $j = 1, \ldots, p$, and the limit is in the sense of $L^q(\gamma)$. Observe that

$$\mathbb{D}^{p,q+\epsilon} \subset \mathbb{D}^{p+m,q}, \quad \forall m \geq 0, \forall \epsilon \geq 0. \tag{1.1.5}$$

We write $\mathbb{D}^{\infty,q} = \bigcap_{p\geq 1} \mathbb{D}^{p,q}$.

Remark 1.1.7 Equivalently, $\mathbb{D}^{p,q}$ is the Banach space of all functions in $L^q(\gamma)$ whose derivatives up to the order p in the sense of distributions also belong to $L^q(\gamma)$ – see, for example, Meyers and Serrin [78].

Definition 1.1.8 For $p = 1, 2, \ldots$, the mapping

$$D^p : \mathbb{D}^{p,q} \to L^q(\gamma) : f \mapsto D^p f, \tag{1.1.6}$$

as defined in (1.1.4), is called the pth **derivative operator** (associated with the $L^q(\gamma)$ norm). Note that, for every $q \neq q'$, the operators $D^p : \mathbb{D}^{p,q} \to L^q(\gamma)$ and $D^p : \mathbb{D}^{p,q'} \to L^{q'}(\gamma)$ coincide when acting on the intersection $\mathbb{D}^{p,q} \cap \mathbb{D}^{p,q'}$. When $p = 1$, we will often write D instead of D^1.

Since $L^2(\gamma)$ is a Hilbert space, the case $q = 2$ is very important,. In the next section, we characterize the adjoint of the operator $D^p : \mathbb{D}^{p,2} \to L^2(\gamma)$.

1.2 Divergences

Definition 1.2.1 We denote by $\mathrm{Dom}\,\delta^p$ the subset of $L^2(\gamma)$ composed of those functions g such that there exists $c > 0$ satisfying the property that, for all $f \in \mathcal{S}$ (or, equivalently, for all $f \in \mathbb{D}^{p,2}$),

$$\left| \int_{\mathbb{R}} f^{(p)}(x) g(x) d\gamma(x) \right| \leq c \sqrt{\int_{\mathbb{R}} f^2(x) d\gamma(x)}. \tag{1.2.1}$$

Fix $g \in \mathrm{Dom}\,\delta^p$. Since condition (1.2.1) holds, the linear operator $f \mapsto \int_{\mathbb{R}} f^{(p)}(x)g(x)d\gamma(x)$ is continuous from $\mathcal{S}$, equipped with the $L^2(\gamma)$-norm, into $\mathbb{R}$. Thus, we can extend this operator to a linear operator from $L^2(\gamma)$ into $\mathbb{R}$. By the Riesz representation theorem, there exists a unique element in $L^2(\gamma)$, denoted by $\delta^p g$, such that $\int_{\mathbb{R}} f^{(p)}(x)g(x)d\gamma(x) = \int_{\mathbb{R}} f(x)\delta^p g(x)d\gamma(x)$ for all $f \in \mathcal{S}$.

Definition 1.2.2 Fix an integer $p \geq 1$. The pth **divergence operator** δ^p is defined as follows. If $g \in \mathrm{Dom}\,\delta^p$, then $\delta^p g$ is the unique element of $L^2(\gamma)$ characterized by the following duality formula: for all $f \in \mathcal{S}$ (or, equivalently, for all $f \in \mathbb{D}^{p,2}$),

$$\int_{\mathbb{R}} f^{(p)}(x)g(x)d\gamma(x) = \int_{\mathbb{R}} f(x)\delta^p g(x)d\gamma(x). \tag{1.2.2}$$

When $p = 1$, we shall often write δ instead of δ^1.

Remark 1.2.3 Taking f to be equal to a constant in (1.2.2), we deduce that, for every $p \geq 1$ and every $g \in \mathrm{Dom}\,\delta^p$,

$$\int_{\mathbb{R}} \delta^p g(x) d\gamma(x) = 0. \tag{1.2.3}$$

Notice that the operator δ^p is closed (being the adjoint of D^p). Also,

$$\delta^p g = \delta(\delta^{p-1} g) = \delta^{p-1}(\delta g) \tag{1.2.4}$$

for every $g \in \mathrm{Dom}\,\delta^p$. In particular, the first equality in (1.2.4) implies that, if $g \in \mathrm{Dom}\,\delta^p$, then $\delta^{p-1} g \in \mathrm{Dom}\,\delta$, whereas from the second equality we infer that, if $g \in \mathrm{Dom}\,\delta^p$, then $\delta g \in \mathrm{Dom}\,\delta^{p-1}$.

Exercise 1.2.4 Prove the two equalities in (1.2.4).

For every $f, g \in \mathcal{S}$, we can write, by virtue of Lemma 1.1.1,

$$\int_{\mathbb{R}} f'(x)g(x)d\gamma(x) = \int_{\mathbb{R}} x f(x)g(x)d\gamma(x) - \int_{\mathbb{R}} f(x)g'(x)d\gamma(x). \tag{1.2.5}$$

Relation (1.2.5) implies that $\mathcal{S} \subset \mathrm{Dom}\,\delta$ and, for $g \in \mathcal{S}$, that $\delta g(x) = xg(x) - g'(x)$. By approximation, we deduce that $\mathbb{D}^{1,2} \subset \mathrm{Dom}\,\delta$, and also that the previous formula for δg continues to hold when $g \in \mathbb{D}^{1,2}$, that is, $\delta g = G - Dg$ for every $g \in \mathbb{D}^{1,2}$, where $G(x) = xg(x)$. More generally, we can prove that $\mathbb{D}^{p,2} \subset \mathrm{Dom}\,\delta^p$ for any $p \geq 1$.

1.3 Ornstein–Uhlenbeck operators

Definition 1.3.1 The **Ornstein–Uhlenbeck semigroup**, written $(P_t)_{t\geq 0}$, is defined as follows. For $f \in \mathcal{S}$ and $t \geq 0$,

$$P_t f(x) = \int_{\mathbb{R}} f(e^{-t}x + \sqrt{1 - e^{-2t}}y) d\gamma(y), \quad x \in \mathbb{R}. \tag{1.3.1}$$

The semigroup characterization is proved in Proposition 1.3.3. An explicit connection with Ornstein–Uhlenbeck stochastic processes is provided in Exercise 1.7.4.

Plainly, $P_0 f(x) = f(x)$. By using the fact that f is an element of $\mathcal{S}$ and by dominated convergence, it is immediate that $P_\infty f(x) := \lim_{t\to\infty} P_t f(x) = \int_{\mathbb{R}} f(y)d\gamma(y)$. On the other hand, by applying the Jensen inequality to the right-hand side of (1.3.1), we infer that, for every $q \in [1, \infty)$,

$$\int_{\mathbb{R}} |P_t f(x)|^q d\gamma(x) = \int_{\mathbb{R}} \left| \int_{\mathbb{R}} f(e^{-t}x + \sqrt{1-e^{-2t}}y)d\gamma(y) \right|^q d\gamma(x)$$
$$\leq \int_{\mathbb{R}^2} |f(e^{-t}x + \sqrt{1-e^{-2t}}y)|^q d\gamma(x)d\gamma(y)$$
$$= \int_{\mathbb{R}} |f(x)|^q d\gamma(x). \qquad (1.3.2)$$

The last equality in (1.3.2) follows from the well-known (and easily checked using the characteristic function) fact that, if N, N' are two independent standard Gaussian random variables, then $e^{-t}N + \sqrt{1-e^{-2t}}N'$ is also standard Gaussian.

The relations displayed in (1.3.2), together with Proposition 1.1.5, show that the expression on the right-hand side of (1.3.1) is indeed well defined for $f \in L^q(\gamma)$, $q \geq 1$. Moreover, a contraction property holds.

Proposition 1.3.2 *For every $t \geq 0$ and every $q \in [1, \infty)$, P_t extends to a linear contraction operator on $L^q(\gamma)$.*

As anticipated, the fundamental property of the class $(P_t)_{t\geq 0}$ is that it is a semigroup of operators.

Proposition 1.3.3 *For any $s, t \geq 0$, we have $P_t P_s = P_{t+s}$ on $L^1(\gamma)$.*

Proof For all $f \in L^1(\gamma)$, we can write

$$P_t P_s f(x) = \int_{\mathbb{R}^2} f(e^{-s-t}x + e^{-s}\sqrt{1-e^{-2t}}y + \sqrt{1-e^{-2s}}z)d\gamma(y)d\gamma(z)$$
$$= \int_{\mathbb{R}} f(e^{-s-t}x + \sqrt{1-e^{-2s-2t}}y)d\gamma(y) = P_{t+s}f(x),$$

where the second inequality follows from the easily verified fact that, if N, N' are two independent standard Gaussian random variables, then $e^{-s}\sqrt{1-e^{-2t}}N + \sqrt{1-e^{-2s}}N'$ and $\sqrt{1-e^{-2(s+t)}}N$ have the same law. □

The following result shows that P_t and D can be interchanged on $\mathbb{D}^{1,2}$.

Proposition 1.3.4 *Let $f \in \mathbb{D}^{1,2}$ and $t \geq 0$. Then $P_t f \in \mathbb{D}^{1,2}$ and $DP_t f = e^{-t}P_t Df$.*

Proof Suppose that $f \in \mathcal{S}$. Then, for any $x \in \mathbb{R}$,

$$DP_t f(x) = e^{-t}\int_{\mathbb{R}} f'(e^{-t}x + \sqrt{1-e^{-2t}}y)d\gamma(y) = e^{-t}P_t f'(x) = e^{-t}P_t Df(x).$$

The case of a general f follows from an approximation argument, as well as from the contraction property stated in Proposition 1.3.2. □

Now denote by $L = \frac{d}{dt}\big|_{t=0} P_t$ the infinitesimal generator of $(P_t)_{t\geq 0}$ on $L^2(\gamma)$, and by $\text{Dom}\, L$ its domain.

Remark 1.3.5 We recall that $\text{Dom}\, L$ is defined as the collection of those $f \in L^2(\gamma)$ such that the expression $\frac{P_h f - f}{h}$ converges in $L^2(\gamma)$, as h goes to zero.

On $\mathcal{S}$ one has that, for any $t \geq 0$,

$$\frac{d}{dt}P_t = \lim_{h\to 0}\frac{P_{t+h} - P_t}{h} = \lim_{h\to 0} P_t \frac{P_h - Id}{h} = P_t \lim_{h\to 0}\frac{P_h - Id}{h}$$
$$= P_t \frac{d}{dh}\bigg|_{h=0} P_h = P_t L,$$

and, similarly, $\frac{d}{dt}P_t = LP_t$. On the other hand, for $f \in \mathcal{S}$ and $x \in \mathbb{R}$, we can write, by differentiating with respect to t in (1.3.1) (note that the interchanging of differentiation and integration is justified by the fact that f is smooth),

$$\frac{d}{dt}P_t f(x) = -xe^{-t}\int_{\mathbb{R}} f'(e^{-t}x + \sqrt{1-e^{-2t}}y)d\gamma(y) + \frac{e^{-2t}}{\sqrt{1-e^{-2t}}}$$
$$\int_{\mathbb{R}} f'(e^{-t}x + \sqrt{1-e^{-2t}}y)yd\gamma(y)$$
$$= -xe^{-t}\int_{\mathbb{R}} f'(e^{-t}x + \sqrt{1-e^{-2t}}y)d\gamma(y) + e^{-2t}$$
$$\int_{\mathbb{R}} f''(e^{-t}x + \sqrt{1-e^{-2t}}y)d\gamma(y),$$

where we used Lemma 1.1.1 to get the last inequality. In particular, by specializing the previous calculations to $t = 0$ we infer that

$$Lf(x) = -xf'(x) + f''(x). \qquad (1.3.3)$$

This fact is reformulated in the next statement.

Proposition 1.3.6 *For any $f \in \mathcal{S}$, we have $Lf = -\delta Df$.*

The seemingly innocuous Proposition 1.3.6 is indeed quite powerful. As an illustration, we now use it in order to prove an important result about concentration of Gaussian random variables, known as *Poincaré inequality*.

Proposition 1.3.7 (Poincaré inequality) *Let $N \sim \mathcal{N}(0,1)$ and $f \in \mathbb{D}^{1,2}$. Then*

$$\mathrm{Var}[f(N)] \le E[f'^2(N)]. \tag{1.3.4}$$

Proof By an approximation argument, we may assume without loss of generality that $f \in \mathcal{S}$. Since we are now dealing with a function in $\mathcal{S}$, we can freely interchange derivatives and integrals, and write

$$\begin{aligned}
\mathrm{Var}[f(N)] &= E[f(N)(f(N)-E[f(N)])] = E[f(N)(P_0 f(N) - P_\infty f(N))] \\
&= -\int_0^\infty E[f(N)\frac{d}{dt}P_t f(N)]dt \\
&= \int_0^\infty E[f(N)\,\delta D P_t f(N)]dt \quad (\text{using } \tfrac{d}{dt}P_t = LP_t = -\delta D P_t) \\
&= \int_0^\infty E[f'(N)\,DP_t f(N)]dt \quad (\text{by the duality formula (1.2.2)}) \\
&= \int_0^\infty e^{-t} E[f'(N)\,P_t f'(N)]dt \quad (\text{by Proposition 1.3.4}) \\
&\le \int_0^\infty e^{-t}\sqrt{E[f'^2(N)]}\sqrt{E[(P_t f')^2(N)]}dt \quad (\text{by Cauchy–Schwarz}) \\
&\le E[f'^2(N)]\int_0^\infty e^{-t}dt \quad (\text{by Proposition 1.3.2}) \\
&= E[f'^2(N)],
\end{aligned}$$

yielding the desired conclusion. □

By using their definitions, one can immediately prove that δ and D enjoy the following 'Heisenberg commutativity relationship':

Proposition 1.3.8 *For every $f \in \mathcal{S}$, $(D\delta - \delta D)f = f$.*

Exercise 1.3.9 Combine Proposition 1.3.8 with an induction argument to prove that, for any integer $p \ge 2$,

$$(D\delta^p - \delta^p D)f = p\delta^{p-1}f \quad \text{for all } f \in \mathcal{S}. \tag{1.3.5}$$

See also Proposition 2.6.1.

In the subsequent sections, we present three applications of the theory developed above. In Section 1.4 we define and characterize an orthogonal basis of $L^2(\gamma)$, known as the class of *Hermite polynomials*. Section 1.5 deals with decompositions of variances. Section 1.6 provides some basic examples of normal approximations for the law of random variables of the type $F = f(N)$.

1.4 First application: Hermite polynomials

Definition 1.4.1 Let $p \ge 0$ be an integer. We define the pth **Hermite polynomial** as $H_0 = 1$ and $H_p = \delta^p 1$, $p \ge 1$. Here, 1 is a shorthand notation for the function that is identically one, which is of course an element of $\mathrm{Dom}\,\delta^p$ for every p. For instance, $H_1(x) = x$, $H_2(x) = x^2 - 1$, $H_3(x) = x^3 - 3x$, and so on. We shall also use the convention that $H_{-1}(x) = 0$.

The main properties of Hermite polynomials are gathered together in the next statement (which is one of the staples of the entire book):

Proposition 1.4.2 (i) *For any $p \ge 0$, we have $H_p' = pH_{p-1}$, $LH_p = -pH_p$ and $P_t H_p = e^{-pt}H_p$, $t \ge 0$.*

(ii) *For any $p \ge 0$, $H_{p+1}(x) = xH_p(x) - pH_{p-1}(x)$.*

(iii) *For any $p, q \ge 0$,*

$$\int_{\mathbb{R}} H_p(x)H_q(x)d\gamma(x) = \begin{cases} p! & \text{if } p = q \\ 0 & \text{otherwise.} \end{cases}$$

(iv) *The family $\left\{\frac{1}{\sqrt{p!}}H_p : p \ge 0\right\}$ is an orthonormal basis of $L^2(\gamma)$.*

(v) *If $f \in \mathbb{D}^{\infty,2}$ then $f = \sum_{p=0}^\infty \frac{1}{p!}\left(\int_{\mathbb{R}} f^{(p)}(x)d\gamma(x)\right)H_p$ in $L^2(\gamma)$.*

(vi) *For all $c \in \mathbb{R}$, we have $e^{cx-c^2/2} = \sum_{p=0}^\infty \frac{c^p}{p!}H_p(x)$ in $L^2(\gamma)$.*

(vii) *(Rodrigues's formula) For any $p \ge 1$, $H_p(x) = (-1)^p e^{x^2/2}\frac{d^p}{dx^p}e^{-x^2/2}$.*

(viii) *For every $p \ge 0$ and every real x, $H_p(-x) = (-1)^p H_p(x)$.*

Proof (i) By the definition of H_p, we have $H_p' = D\delta^p 1$. Hence, by applying the result of Exercise 1.3.9, we get $H_p' = p\delta^{p-1}1 + \delta^p D1 = pH_{p-1}$. We deduce that $LH_p = -\delta DH_p = -\delta H_p' = -p\delta H_{p-1} = -pH_p$. Fix $x \in \mathbb{R}$, and define $y_x : \mathbb{R}_+ \to \mathbb{R}$ by $y_x(t) = P_t H_p(x)$. We have $y_x(0) = P_0 H_p(x) = H_p(x)$ and, for $t > 0$,

$$y_x'(t) = \frac{d}{dt}\Big|_{t=0} P_t H_p(x) = P_t L H_p(x) = -pP_t H_p(x) = -py_x(t).$$

Hence $y_x(t) = e^{-pt}H_p(x)$, that is, $P_t H_p = e^{-pt}H_p$.

(ii) We can take $p \ge 1$. We have that $H_{p+1} = \delta^{p+1}1 = \delta\delta^p 1 = \delta H_p$. It follows that, by the definition of δ, $H_{p+1}(x) = xH_p(x) - H_p'(x)$. Since $H_p'(x) = pH_{p-1}(x)$ by part (i), we deduce the conclusion.

(iii) The case $p > q = 0$ is a direct consequence of (1.2.3). If $p \geq q \geq 1$, one can write

$$\begin{aligned}\int_{\mathbb{R}} H_p(x)H_q(x)d\gamma(x) &= \int_{\mathbb{R}} H_p(x)\delta^q 1(x)d\gamma(x)\\ &= \int_{\mathbb{R}} H_p'(x)\delta^{q-1}1(x)d\gamma(x) \quad \text{(by the duality formula (1.2.2))}\\ &= p\int_{\mathbb{R}} H_{p-1}(x)H_{q-1}(x)d\gamma(x) \quad \text{(by (i))}.\end{aligned}$$

Hence, the desired conclusion is proved by induction.

(iv) By the previous point, the family $\left\{\frac{1}{\sqrt{p!}}H_p : p \geq 0\right\}$ is orthonormal in $L^2(\gamma)$. On the other hand, it is simple to prove (e.g. by induction) that, for any $p \geq 0$, the polynomial H_p has degree p. Hence, the claim in this part is equivalent to saying that the monomials $\{x^p : p = 0, 1, 2, \ldots\}$ generate a dense subspace of $L^2(\gamma)$. The conclusion is now obtained by using Proposition 1.1.5 in the case $q = 2$.

(v) By part (iv), for any $f \in L^2(\gamma)$,

$$f = \sum_{p=0}^{\infty} \frac{1}{p!}\left(\int_{\mathbb{R}} f(x)H_p(x)d\gamma(x)\right) H_p.$$

If $f \in \mathbb{D}^{\infty,2}$ then, by applying (1.2.2) repeatedly, we can write

$$\int_{\mathbb{R}} f(x)H_p(x)d\gamma(x) = \int_{\mathbb{R}} f(x)\delta^p 1(x)d\gamma(x) = \int_{\mathbb{R}} f^{(p)}(x)d\gamma(x).$$

Hence, in this case, we also have

$$f = \sum_{p=0}^{\infty} \frac{1}{p!}\left(\int_{\mathbb{R}} f^{(p)}(x)d\gamma(x)\right) H_p,$$

as required.

(vi) If we choose $f(x) = e^{cx}$ in the previous identity for f, we get

$$e^{cx} = \sum_{p=0}^{\infty} \frac{c^p}{p!}\left(\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} e^{cx-x^2/2}dx\right) H_p(x) = e^{c^2/2}\sum_{p=0}^{\infty}\frac{c^p}{p!}H_p(x),$$

which is the desired formula.

(vii) We have

$$\begin{aligned} e^{cx-c^2/2} &= e^{x^2/2}e^{-(x-c)^2/2} = e^{x^2/2}\sum_{p=0}^{\infty}\frac{c^p}{p!} \times \frac{d^p}{dc^p}\bigg|_{c=0} e^{-(x-c)^2/2}\\ &= e^{x^2/2}\sum_{p=0}^{\infty}\frac{(-1)^p c^p}{p!}\frac{d^p}{dx^p}e^{-x^2/2}.\end{aligned}$$

By comparing with the formula in (vi), we deduce the conclusion.

(viii) Since $H_0(x) = 1$ and $H_1(x) = x$, the conclusion is trivially true for $p = 0, 1$. Using part (ii), we deduce the desired result by an induction argument. □

1.5 Second application: variance expansions

We will use the previous results in order to write two (infinite) series representations of the variance of $f(N)$, whenever $N \sim \mathscr{N}(0,1)$ and $f : \mathbb{R} \to \mathbb{R}$ is sufficiently regular.

Proposition 1.5.1 *Let $N \sim \mathscr{N}(0,1)$ and $f \in \mathbb{D}^{\infty,2}$. Then*

$$\mathrm{Var}[f(N)] = \sum_{n=1}^{\infty}\frac{1}{n!}E[f^{(n)}(N)]^2. \tag{1.5.1}$$

If, moreover, $E[f^{(n)}(N)^2]/n! \to 0$ as $n \to \infty$ and $f \in \mathcal{S}$, we also have

$$\mathrm{Var}[f(N)] = \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n!}E[f^{(n)}(N)^2]. \tag{1.5.2}$$

(The convergence of the infinite series in (1.5.1) and (1.5.2) is part of the conclusion.)

Proof The proof of (1.5.1) is easy: it suffices indeed to compute the $L^2(\gamma)$-norm on both sides of the formula appearing in part (v) of Proposition 1.4.2 – see also part (iv) therein.

For the proof of (1.5.2), let us consider the application

$$t \mapsto g(t) = E[(P_{\log(1/\sqrt{t})}f)^2(N)], \quad 0 < t \leq 1.$$

We have $g(1) = E[f^2(N)]$. Moreover, g can be extended to a continuous function on the interval $[0,1]$ by setting $g(0) = E[f(N)]^2$. In particular, $\mathrm{Var}[f(N)] = g(1) - g(0)$. For $t \in (0,1)$, let us compute $g'(t)$ (note that we can interchange derivatives and expectations, due to the assumptions on f):

$$
\begin{aligned}
g'(t) &= -\frac{1}{t}\, E[P_{\log(1/\sqrt{t})} f(N) \times L P_{\log(1/\sqrt{t})} f(N)] \\
&= \frac{1}{t}\, E[P_{\log(1/\sqrt{t})} f(N) \times \delta D P_{\log(1/\sqrt{t})} f(N)] \quad \text{(by Proposition 1.3.6)} \\
&= \frac{1}{t}\, E[(D P_{\log(1/\sqrt{t})} f)^2(N)] \quad \text{(by the duality formula (1.2.2))} \\
&= E[(P_{\log(1/\sqrt{t})} f')^2(N)] \quad \text{(by Proposition 1.3.4).}
\end{aligned}
$$

By induction, we easily infer that, for all $n \geq 1$ and $t \in (0, 1)$,

$$
g^{(n)}(t) = E[(P_{\log(1/\sqrt{t})} f^{(n)})^2(N)],
$$

and, in particular, $g^{(n)}$ can be extended to a continuous function on $[0, 1]$ by setting

$$
g^{(n)}(0) = E[f^{(n)}(N)]^2 \quad \text{and} \quad g^{(n)}(1) = E[f^{(n)}(N)^2].
$$

Taylor's formula yields, for any integer $m \geq 1$,

$$
\left| g(0) - g(1) + \sum_{n=1}^{m} \frac{(-1)^{n+1}}{n!} g^{(n)}(1) \right| = \frac{1}{m!} \int_0^1 g^{(m+1)}(t) t^m dt.
$$

By Proposition 1.3.2, we have that, for any $t \in (0, 1)$, $0 \leq g^{(m+1)}(t) \leq E[f^{(m+1)}(N)^2]$. Therefore,

$$
0 \leq \frac{1}{m!} \int_0^1 g^{(m+1)}(t) t^m dt \leq \frac{E[f^{(m+1)}(N)^2]}{(m+1)!} \to 0 \quad \text{as } m \to \infty,
$$

and the desired formula (1.5.2) follows. To finish, let us stress that we could recover (1.5.1) by using this time the expansion $g(1) = g(0) + \sum_{n=1}^{\infty} \frac{g^{(n)}(0)}{n!}$. (Such a series representation is valid because g is absolutely monotone; see, for example, Feller [38, p. 233].) □

1.6 Third application: second-order Poincaré inequalities

We will now take a first step towards the combination of Stein's method and Malliavin calculus. Let F and N denote two integrable random variables defined on the probability space $(\Omega, \mathscr{F}, P)$. The difference between the laws of F and N can be assessed by means of the so-called *Wasserstein distance*:

$$
d_W(F, N) = \sup_{h \in \mathrm{Lip}(1)} \left| E[h(F)] - E[h(N)] \right|.
$$

Here, $\mathrm{Lip}(K)$ stands for the set of functions $h : \mathbb{R} \to \mathbb{R}$ that are Lipschitz with constant $K > 0$, that is, satisfying $|h(x) - h(y)| \leq K|x - y|$ for all $x, y \in \mathbb{R}$.

When $N \sim \mathscr{N}(0, 1)$, there exists a remarkable result by Stein (which we will prove and discuss in full detail in Section 3.5) which states that

$$
d_W(F, N) \leq \sup_{\phi \in C^1 \cap \mathrm{Lip}(\sqrt{2/\pi})} \left| E[F\phi(F)] - E[\phi'(F)] \right|. \tag{1.6.1}
$$

In anticipation of the more general analysis that we will perform later on, we shall now study the case of F having the specific form $F = f(N)$, for $N \sim \mathscr{N}(0, 1)$ and $f : \mathbb{R} \to \mathbb{R}$ sufficiently regular. In particular, we shall prove a so-called *second-order Poincaré inequality*. The rationale linking Proposition 1.6.1 and the 'first-order' Poincaré inequality stated in Proposition 1.3.7 goes as follows. Formula (1.3.4) implies that a random variable of the type $f(N)$ is concentrated around its mean whenever f' is small, while inequality (1.6.2) roughly states that, whenever f'' is small compared to f', then $f(N)$ has approximately a Gaussian distribution.

Proposition 1.6.1 (Second-order Poincaré inequality) *Let $N \sim \mathscr{N}(0, 1)$ and $f \in \mathbb{D}^{2,4}$. Assume also that $E[f(N)] = 0$ and $E[f^2(N)] = 1$. Then*

$$
d_W(f(N), N) \leq \frac{3}{\sqrt{2\pi}} \left(E\left[f''^4(N) \right] \right)^{1/4} \left(E\left[f'^4(N) \right] \right)^{1/4}. \tag{1.6.2}
$$

Proof Assume first that $f \in \mathcal{S}$. By using the smoothness of f in order to interchange derivatives and integrals and by reasoning as in Proposition 1.3.7, we can write, for any C^1 function $\phi : \mathbb{R} \to \mathbb{R}$ with bounded derivative:

$$
\begin{aligned}
E[f(N)\phi(f(N))] &= E[(P_0 f(N) - P_\infty f(N))\phi(f(N))] \\
&= -\int_0^\infty E\left[\frac{d}{dt} P_t f(N) \phi(f(N)) \right] dt \\
&= \int_0^\infty E[\delta D P_t f(N) \phi(f(N))] dt \\
&= \int_0^\infty e^{-t} E[P_t f'(N) \phi'(f(N)) f'(N)] dt \\
&= E\left[\phi'(f(N)) f'(N) \int_0^\infty e^{-t} P_t f'(N) dt \right].
\end{aligned}
$$

In particular, for $\phi(x) = x$, we obtain

$$
1 = E[f^2(N)] = E\left[f'(N) \int_0^\infty e^{-t} P_t f'(N) dt \right].
$$

Therefore, for any $\phi \in C^1 \cap \mathrm{Lip}(\sqrt{2/\pi})$ and $f \in \mathcal{S}$,

$$\begin{aligned}
&\left|E[f(N)\phi(f(N))] - E[\phi'(f(N))]\right| \\
&= \left|E\left[\phi'(f(N))\left(f'(N)\int_0^\infty e^{-t}P_t f'(N)dt - 1\right)\right]\right| \\
&\leq \sqrt{\frac{2}{\pi}}\, E\left|f'(N)\int_0^\infty e^{-t}P_t f'(N)dt - 1\right| \\
&\leq \sqrt{\frac{2}{\pi}}\sqrt{\mathrm{Var}\left[f'(N)\int_0^\infty e^{-t}P_t f'(N)dt\right]}. \qquad (1.6.3)
\end{aligned}$$

To go further, we apply the Poincaré inequality (1.3.4) and then the triangle inequality to deduce that

$$\begin{aligned}
\sqrt{\mathrm{Var}\left[f'(N)\int_0^\infty e^{-t}P_t f'(N)dt\right]} &\leq \sqrt{E\left[\left(f'\int_0^\infty e^{-t}P_t f'dt\right)'^2(N)\right]} \\
&\leq \sqrt{E\left[f''^2(N)\left(\int_0^\infty e^{-t}P_t f'dt\right)^2(N)\right]} \\
&\quad + \sqrt{E\left[f'^2(N)\left(\int_0^\infty e^{-2t}P_t f''dt\right)^2(N)\right]}.
\end{aligned} \qquad (1.6.4)$$

Applying now the Cauchy–Schwarz inequality, Jensen inequality and the contraction property (see Proposition 1.3.2) for $p = 4$ yields

$$E\left[f''^2(N)\left(\int_0^\infty e^{-t}P_t f'dt\right)^2(N)\right] \leq \sqrt{E\left[f''^4(N)\right]}\sqrt{E\left[f'^4(N)\right]}.$$

Similarly,

$$E\left[f'^2(N)\left(\int_0^\infty e^{-2t}P_t f''dt\right)^2(N)\right] \leq \frac{1}{4}\sqrt{E\left[f''^4(N)\right]}\sqrt{E\left[f'^4(N)\right]}.$$

By exploiting these two inequalities in order to bound the right-hand side of (1.6.4) and by virtue of (1.6.3), we obtain that

$$\left|E[f(N)\phi(f(N))] - E[\phi'(f(N))]\right| \leq \frac{3}{\sqrt{2\pi}}\left(E\left[f''^4(N)\right]\right)^{1/4}\left(E\left[f'^4(N)\right]\right)^{1/4}, \qquad (1.6.5)$$

for any $\phi \in C^1 \cap \mathrm{Lip}(\sqrt{2/\pi})$ and $f \in \mathcal{S}$. By approximation, inequality (1.6.5) continues to hold when f is in $\mathbb{D}^{2,4}$. Finally, the desired inequality (1.6.2) follows by plugging (1.6.5) into Stein's bound (1.6.1). □

Note that Proposition 1.6.1 will be significantly generalized in Theorem 5.3.3; see also Exercise 5.3.4.

1.7 Exercises

1.7.1 Let $p, q \geq 1$ be two integers. Show the product formula for Hermite polynomials:

$$H_p H_q = \sum_{r=0}^{p\wedge q} r!\binom{p}{r}\binom{q}{r} H_{p+q-2r}.$$

(Hint: Use formula (v) of Proposition 1.4.2.)

1.7.2 Let $p \geq 1$ be an integer.

1. Show that $H_p(0) = 0$ if p is odd and $H_p(0) = \frac{(-1)^{p/2}}{2^{p/2}(p/2)!}$ if p is even.
   (Hint: Use Proposition 1.4.2(vi).)
2. Deduce that:

$$H_p(x) = \sum_{k=0}^{\lfloor p/2\rfloor} \frac{p!(-1)^k}{k!(p-2k)!2^k}x^{p-2k}.$$

(Hint: Use $H_p' = pH_{p-1}$ and proceed by induction.)

1.7.3 Let $f \in \mathcal{S}$ and $x \in \mathbb{R}$. Show that

$$\int_0^\infty e^{-2t}P_t f''(x)dt - x\int_0^\infty e^{-t}P_t f'(x)dt = f(x) - \int_{\mathbb{R}} f(y)d\gamma(y).$$

(Hint: Use $\frac{d}{dt}P_t = LP_t = \ldots$)

1.7.4 **(Ornstein–Uhlenbeck processes)** Let $B = (B_t)_{t\geq 0}$ be a Brownian motion. Consider the linear stochastic differential equation

$$dX_t^x = \sqrt{2}dB_t - X_t^x dt, \quad t \geq 0, \quad X_0^x = x \in \mathbb{R}. \qquad (1.7.1)$$

The solution of (1.7.1) is called an **Ornstein–Uhlenbeck** stochastic process.

1. For any $x \in \mathbb{R}$, show that the solution to (1.7.1) is given by

$$X_t^x = e^{-t}x + \sqrt{2}\int_0^t e^{-(t-s)}dB_s, \quad t \geq 0.$$

2. If $f \in \mathcal{S}$ and $x \in \mathbb{R}$, show that $P_t f(x) = E[f(X_t^x)]$.

1.7.5 Let $N \sim \mathcal{N}(0,1)$ and $f \in \mathcal{S}$. If $\frac{1}{2^n n!}E[f^{(n)}(N)^2] \to 0$ as $n \to \infty$, show that

$$\mathrm{Var}[f(N)] = \sum_{n=1}^{\infty} \frac{1}{2^n n!}\left(E[f^{(n)}(N)]^2 + (-1)^{n+1}E[f^{(n)}(N)^2]\right).$$

(Hint: Expand $g(1/2)$ around 0 and 1, with g the function introduced in the proof of Proposition 1.5.1.)

1.7.6 Let $f, g \in \mathbb{D}^{1,2}$, and let $N, \widetilde{N} \sim \mathcal{N}(0,1)$ be jointly Gaussian, with covariance ρ.

1. Prove that $\mathrm{Cov}[f(N), g(\widetilde{N})] = E\left[f(N)\left(P_{\ln(1/\rho)}g(N) - P_\infty g(N)\right)\right]$. (Hint: Use the fact that $(N, \widetilde{N})$ and $(N, \rho N + \sqrt{1-\rho^2}\hat{N})$ have the same law whenever $N, \hat{N} \sim \mathcal{N}(0,1)$ are independent and $\rho = \mathrm{Cov}[N, \widetilde{N}]$.)
2. Deduce that $\left|\mathrm{Cov}[f(N), g(\widetilde{N})]\right| \leq |\mathrm{Cov}[N, \widetilde{N}]|\sqrt{E[f'^2(N)]}\sqrt{E[g'^2(N)]}$.

1.7.7 For $\varepsilon > 0$, let $p_\varepsilon(x) = \frac{1}{\sqrt{2\pi\varepsilon}}e^{-\frac{x^2}{2\varepsilon}}$ be the heat kernel with variance ε.

1. Show that $\int_{\mathbb{R}} p_\varepsilon(x-u)d\gamma(x) = p_{1+\varepsilon}(u)$ for all $u \in \mathbb{R}$.
2. For any $n \geq 0$ and $u \in \mathbb{R}$, show that $p_\varepsilon^{(n)}(u) = (-1)^n \varepsilon^{-n/2} p_\varepsilon(u) H_n(u/\sqrt{\varepsilon})$. (Hint: Use formula (vi) of Proposition 1.4.2.)
3. Deduce, for any $n \geq 0$ and $u \in \mathbb{R}$, that
$$\int_{\mathbb{R}} p_\varepsilon^{(n)}(x-u)d\gamma(x) = (1+\varepsilon)^{-n/2} p_{1+\varepsilon}(u) H_n(u/\sqrt{1+\varepsilon}).$$
4. Finally, prove the following identity in $L^2(\gamma)$:
$$p_\varepsilon = \frac{1}{\sqrt{2\pi(1+\varepsilon)}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2n)!2^n(1+\varepsilon)^n} H_{2n}.$$
(Hint: Use Proposition 1.4.2(v).)

1.8 Bibliographic comments

Sections 1.1–1.4 are strongly inspired by the first chapter in Malliavin's monograph [70]. The Poincaré inequality (1.3.4) was first proved by Nash in [80], and then rediscovered by Chernoff in [24] (both proofs use Hermite

polynomials). A general, infinite-dimensional version of Poincaré inequality is proved by Houdré and Pérez-Abreu in [51]. The variance expansions presented in Section 1.5 are one-dimensional versions of the results proved by Houdré and Kagan [50]. An excellent reference for Stein's method is [22], by Chen, Goldstein and Shao. The reader is also referred to Stein's original paper [135] and monograph [136] – see Chapter 3 for more details. The concept of a second-order Poincaré inequality such as (1.6.2) first appeared in Chatterjee [20], in connection with normal fluctuations of eigenvalues of Gausssian-subordinated random matrices. Infinite-dimensional second-order Poincaré inequalities are proved in Nourdin *et al.* [93], building on the findings by Nourdin and Peccati [88]. In particular, [88] was the first reference to point out an explicit connection between Stein's method and Malliavin calculus.