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Mark M. Meerschaert, Alla Sikorskii

STOCHASTIC MODELS FOR FRACTIONAL CALCULUS

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Mark M. Meerschaert
Alla Sikorskii

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Preface

This book is based on a series of lecture notes for a graduate course in the Department of Statistics and Probability at Michigan State University. The goal is to prepare graduate students for research in the area of fractional calculus, anomalous diffusion, and heavy tails. The book covers basic limit theorems for random variables and random vectors with heavy tails. This includes regular variation, triangular arrays, infinitely divisible laws, random walks, and stochastic process convergence in the Skorokhod topology. The basic ideas of fractional calculus and anomalous diffusion are introduced in the context of probability theory. Each section of the book provides material roughly equivalent to one lecture. Most sections conclude with some additional details, intended for individual reading, and to make the book relatively self-contained.

Heavy tails are applied in finance, insurance, physics, geophysics, cell biology, ecology, medicine, and computer engineering. A random variable has heavy tails if $P(|X| > x) \approx Cx^{-\alpha}$ for some $\alpha > 0$. If $\alpha < 2$, then the second moment of X is undefined, so the usual central limit theorem does not apply. A heavy-tailed version of the central limit theorem leads to a stable distribution. Random walks with heavy tails converge to a stable Lévy motion, similar to Brownian motion. The densities of Brownian motion solve the diffusion equation, which provides a powerful link between differential equations and stochastic processes. Densities of a stable Lévy motion solve a fractional diffusion equation like

$$\frac{\partial}{\partial t}p(x,t) = c\frac{\partial^\alpha}{\partial x^\alpha}p(x,t)$$

using a fractional derivative of order α. Fractional derivatives are limits of fractional difference quotients, using the same fractional difference operator that appears in time series models of long range dependence.

Vector models with heavy tails are useful in many applications, since physical space is not one dimensional. A heavy tailed version of the central limit theorem for random vectors leads to an operator stable limit distribution, which can have a combination of normal and stable components. Vector random walks with heavy tails converge to an operator stable Lévy motion. Probability densities of this random walk limit solve a vector fractional diffusion equation like

$$\frac{\partial}{\partial t}p(x,y,t) = c_1\frac{\partial^\alpha}{\partial x^\alpha}p(x,y,t) + c_2\frac{\partial^\beta}{\partial y^\beta}p(x,y,t)$$

with a different fractional derivative in each coordinate.

Many interesting research problems in this area remain open. This book will guide the motivated reader to understand the essential background needed to read and understand current research papers, and to gain the insights and techniques needed to begin making their own contributions to this rapidly growing field.

East Lansing, November 2011 Mark M. Meerschaert, Alla Sikorskii

Acknowledgments

The material in this book relies on results from many hundreds of research papers, by a large number of talented authors. These works come from mathematics, physics, statistics, and many related areas of science and engineering. Although we did attempt to highlight connections with the existing literature, it seems inevitable that we should leave out some important contributors, for which we can only beg their forgiveness.

The book in its present form owes a great deal to those students and colleagues who reviewed portions of the book for accuracy and content. A special thanks goes to Farzad Sabzikar, Michigan State University, for reading and re-reading the entire manuscript. We would also like to thank Philippe Barbe from the French Centre National de la Recherche Scientifique (CNRS), Enrico Scalas from the Italian Università del Piemonte Orientale, Hans-Peter Scheffler from the German Universität Siegen, and Peter Straka from Michigan State University, for many helpful suggestions. Any remaining errors are the sole responsibility of the authors.

Finally, the authors would like to thank their spouses and families. Your love, support, and patience makes everything possible.

Contents

Chapter 1

Introduction

Fractional calculus is a rapidly growing field of research, at the interface between probability, differential equations, and mathematical physics. Fractional calculus is used to model anomalous diffusion, in which a cloud of particles spreads in a different manner than traditional diffusion. This book develops the basic theory of fractional calculus and anomalous diffusion, from the point of view of probability.

Traditional diffusion represents the long-time limit of a random walk, where finite variance jumps occur at regularly spaced intervals. Eventually, after each particle makes a series of random steps, a histogram of particle locations follows a bell-shaped normal density. The central limit theorem of probability ensures that this same bell-shaped curve will eventually emerge from any random walk with finite variance jumps, so that this diffusion model can be considered universal. The random walk limit is a Brownian motion, whose probability densities solve the diffusion equation. This link between differential equations and probability is a powerful tool. For example, a method called particle tracking computes approximate solutions of differential equations, by simulating the underlying stochastic process.

However, anomalous diffusion is often observed in real data. The "particles" might be pollutants in ground water, stock prices, sound waves, proteins crossing a cell boundary, or animals invading a new ecosystem. The anomalous diffusion can manifest in asymmetric densities, heavy tails, sharp peaks, and/or different spreading rates. The square root scaling in the central limit theorem implies that the width of a particle histogram should spread like the square root of the elapsed time. Both anomalous super-diffusion (a faster spreading rate) and sub-diffusion have been observed in real applications. In this book, we will develop models for both, based on fractional calculus.

The traditional diffusion equation relates the first time derivative of particle concentration to the second derivative in space. The fractional diffusion equation replaces the space and/or time derivatives with their fractional analogues. We will see that fractional derivatives are related to heavy tailed random walks. Fractional derivatives in space model super-diffusion, related to long power-law particle jumps. Fractional derivatives in time model sub-diffusion, related to long power-law waiting times between particle jumps. Fractional derivatives were invented by Leibnitz soon after their more familiar integer-order cousins, but they have become popular in practical applications only in the past few decades. In this book, we will see how fractional calculus and anomalous diffusion can be understood at a deep and intuitive level, using ideas from probability.

The first chapter of this book presents the basic ideas of fractional calculus and anomalous diffusion in the simplest setting. All of the material introduced here will be developed further in later chapters.

1.1 The traditional diffusion model

The traditional model for diffusion combines elements of probability, differential equations, and physics. A random walk provides the basic physical model of particle motion. The central limit theorem gives convergence to a Brownian motion, whose probability densities solve the diffusion equation. We start with a sequence of independent and identically distributed (iid) random variables $Y, Y_1, Y_2, Y_3, \ldots$ that represent the jumps of a randomly selected particle. The *random walk*

$$S_n = Y_1 + \cdots + Y_n$$

gives the location of that particle after n jumps. Next we recall the well-known *central limit theorem*, which shows that the probability distribution of S_n converges to a normal limit. Here we sketch the argument in the simplest case, using Fourier transforms. Details are provided at the end of this section to make the argument rigorous. A complete proof of the central limit theorem will be given in Theorem 3.36 using different methods. Then in Theorem 4.5, we will use regular variation to show that the same normal limit governs a somewhat broader class of random walks.

Let $F(x) = \mathbb{P}[Y \le x]$ denote the cumulative distribution function (cdf) of the jumps, and assume that the probability density function (pdf) $f(x) = F'(x)$ exists. Then we have

$$P[a \le Y \le b] = \int_a^b f(x)\,dx = F(b) - F(a)$$

for any real numbers $a < b$. The moments of this distribution are given by

$$\mu_p = \mathbb{E}\left[Y^p\right] = \int x^p f(x)\,dx$$

where the integral is taken over the domain of the function f.

The *Fourier transform* (FT) of the pdf is

$$\hat{f}(k) = \mathbb{E}\left[e^{-ikY}\right] = \int e^{-ikx} f(x)\,dx.$$

The FT is closely related to the *characteristic function* $\mathbb{E}\left[e^{ikY}\right] = \hat{f}(-k)$. If the first two moments exist, a Taylor series expansion $e^z = 1 + z + z^2/2! + \cdots$ leads to

$$\hat{f}(k) = \int \left(1 - ikx + \frac{1}{2!}(-ikx)^2 + \cdots\right) f(x)\,dx = 1 - ik\mu_1 - \tfrac{1}{2}k^2\mu_2 + o(k^2) \quad (1.1)$$

since $\int f(x)\,dx = 1$. Here $o(k^2)$ denotes a function that tends to zero faster than k^2 as $k \to 0$. A formal proof of (1.1) is included in the details at the end of this section.

Suppose $\mu_1 = 0$ and $\mu_2 = 2$, i.e., the jumps have mean zero and variance 2. Then we have

$$\hat{f}(k) = 1 - k^2 + o(k^2)$$

as $k \to 0$. The sum $S_n = Y_1 + \cdots + Y_n$ has FT

$$\begin{aligned}\mathbb{E}\left[e^{-ikS_n}\right] &= \mathbb{E}\left[e^{-ik(Y_1+\cdots+Y_n)}\right]\\ &= \mathbb{E}\left[e^{-ikY_1}\right]\cdots\mathbb{E}\left[e^{-ikY_n}\right]\\ &= \mathbb{E}\left[e^{-ikY}\right]^n = \hat{f}(k)^n\end{aligned}$$

and so the normalized sum $n^{-1/2}S_n$ has FT

$$\begin{aligned}\mathbb{E}\left[e^{-ik(n^{-1/2}S_n)}\right] &= \mathbb{E}\left[e^{-i(n^{-1/2}k)S_n}\right] = \hat{f}(n^{-1/2}k)^n\\ &= \left(1 - \frac{k^2}{n} + o(n^{-1})\right)^n \to e^{-k^2}\end{aligned} \quad (1.2)$$

using the general fact that $(1 + (r/n) + o(n^{-1}))^n \to e^r$ as $n \to \infty$ for any $r \in \mathbb{R}$ (see details). The limit

$$e^{-k^2} = \mathbb{E}\left[e^{-ikZ}\right] = \int e^{-ikx}\frac{1}{\sqrt{4\pi}}e^{-x^2/4}\,dx$$

using the standard formula from FT tables [190, p. 524]. Then the continuity theorem for FT (see details) yields the traditional central limit theorem (CLT):

$$n^{-1/2}S_n = \frac{Y_1 + \cdots + Y_n}{\sqrt{n}} \Rightarrow Z \quad (1.3)$$

where $\Rightarrow$ indicates convergence in distribution. The limit Z in (1.3) is normal with mean zero and variance 2.

An easy extension of this argument gives convergence of the rescaled random walk:

$$S_{[ct]} = Y_1 + \cdots + Y_{[ct]}$$

gives the particle location at time $t > 0$ at any time scale $c > 0$. Increasing the time scale c makes time go faster, e.g., multiply c by 60 to change from minutes to hours. The long-time limit of the rescaled random walk is a Brownian motion: As $c \to \infty$ we have

$$\mathbb{E}\left[e^{-ik\,c^{-1/2}S_{[ct]}}\right] = \left(1 - \frac{k^2}{c} + o(c^{-1})\right)^{[ct]} = \left[\left(1 - \frac{k^2}{c} + o(c^{-1})\right)^c\right]^{\frac{[ct]}{c}} \to e^{-tk^2} \quad (1.4)$$

where the limit

$$e^{-tk^2} = \hat{p}(k,t) = \int e^{-ikx} p(x,t)\, dx$$

is the FT of a normal density

$$p(x,t) = \frac{1}{\sqrt{4\pi t}}\, e^{-x^2/(4t)}$$

with mean zero and variance $2t$. Then the continuity theorem for FT implies that

$$c^{-1/2} S_{[ct]} \Rightarrow Z_t$$

where the Brownian motion Z_t is normal with mean zero and variance $2t$.

Clearly the FT $\hat{p}(k,t) = e^{-tk^2}$ solves a differential equation

$$\frac{d\hat{p}}{dt} = -k^2 \hat{p} = (ik)^2 \hat{p}. \tag{1.5}$$

If f' exists and if f, f' are integrable, then the FT of $f'(x)$ is $(ik)\hat{f}(k)$ (see details). Using this fact, we can invert the FT on both sides of (1.5) to get (see details)

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2}. \tag{1.6}$$

This shows that the pdf of Z_t solves the diffusion equation (1.6). The diffusion equation models the spreading of a cloud of particles. The random walk S_n gives the location of a randomly selected particle, and the long-time limit density $p(x,t)$ gives the relative concentration of particles at location x at time $t > 0$.

More generally, suppose that $\mu_1 = \mathbb{E}[Y_n] = 0$ and $\mu_2 = \mathbb{E}[Y_n^2] = \sigma^2 > 0$. Then

$$\hat{f}(k) = 1 - \tfrac{1}{2}\sigma^2 k^2 + o(k^2)$$

leads to

$$\mathbb{E}[e^{-ik\, n^{-1/2} S_n}] = \left(1 - \frac{\sigma^2 k^2}{2n} + o(n^{-1})\right)^n \to \exp(-\tfrac{1}{2}\sigma^2 k^2)$$

and

$$\mathbb{E}[e^{-ik\, c^{-1/2} S_{[ct]}}] = \left(1 - \frac{\sigma^2 k^2}{2c} + o(c^{-1})\right)^{[ct]} \to \exp(-\tfrac{1}{2}t\sigma^2 k^2) = \hat{p}(k,t). \tag{1.7}$$

This FT inverts to a normal density

$$p(x,t) = \frac{1}{\sqrt{2\pi\sigma^2 t}} e^{-x^2/(2\sigma^2 t)}$$

with mean zero and variance $\sigma^2 t$. The FT solves

$$\frac{d\hat{p}}{dt} = -\frac{\sigma^2}{2} k^2 \hat{p} = \frac{\sigma^2}{2} (ik)^2 \hat{p}$$

which inverts to

$$\frac{\partial p}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2 p}{\partial x^2}. \tag{1.8}$$

This form of the diffusion equation shows the relation between the *dispersivity* $D = \sigma^2/2$ and the particle jump variance. Apply the continuity theorem for FT to (1.7) to get random walk convergence:

$$c^{-1/2}S_{[ct]} \Rightarrow Z_t$$

where Z_t is a Brownian motion, normal with mean zero and variance $\sigma^2 t$.

In many applications, it is useful to add a drift: $vt + Z_t$ has FT

$$\mathbb{E}[e^{-ik(vt+Z_t)}] = e^{-ikvt-\frac{1}{2}t\sigma^2k^2} = \hat{p}(k,t),$$

which solves

$$\frac{d\hat{p}}{dt} = \left(-ikv + \frac{\sigma^2}{2}(ik)^2\right)\hat{p}.$$

Invert the FT to obtain the diffusion equation with drift:

$$\frac{\partial p}{\partial t} = -v\frac{\partial p}{\partial x} + \frac{\sigma^2}{2}\frac{\partial^2 p}{\partial x^2}. \tag{1.9}$$

This represents the long-time limit of a random walk whose jumps have a non-zero mean $v = \mu_1$ (see details). Figure 1.1 shows a typical concentration profile, a normal pdf

$$p(x,t) = \frac{1}{\sqrt{2\pi\sigma^2 t}}e^{-(x-vt)^2/(2\sigma^2 t)} \tag{1.10}$$

that solves the diffusion equation with drift (1.9). Figure 1.2 shows how the solution evolves in time. Since $vt + Z_t$ has mean vt, the center of mass is proportional to the time variable. Since $vt + Z_t$ has variance $\sigma^2 t$, the standard deviation is $\sigma\sqrt{t}$, so the particle plume spreads proportional to the square root of time. Setting $x = vt$ in (1.10) shows that the peak concentration falls like the square root of time. The simple R codes used to produce the plots in Figures 1.1 and 1.2 will be presented and discussed in Examples 5.1 and 5.2, respectively.

Details

The FT $\hat{f}(k) = \int e^{-ikx}f(x)\,dx$ is defined for integrable functions f, since $|e^{-ikx}| = 1$. Hence the pdf of any random variable X has a FT. In fact, the FT $\hat{f}(k) = \mathbb{E}[e^{-ikX}]$ exists for all $k \in \mathbb{R}$, for any random variable X, whether or not it has a density. The next two results justify the FT expansion (1.1).

Proposition 1.1. *If $\mu_p = \mathbb{E}[|Y|^p]$ exists, then*

$$\mu_p = (-i)^p\hat{f}^{(p)}(0) = (-i)^p\frac{d^p}{dk^p}\mathbb{E}\left[e^{-ikX}\right]_{k=0} \tag{1.11}$$

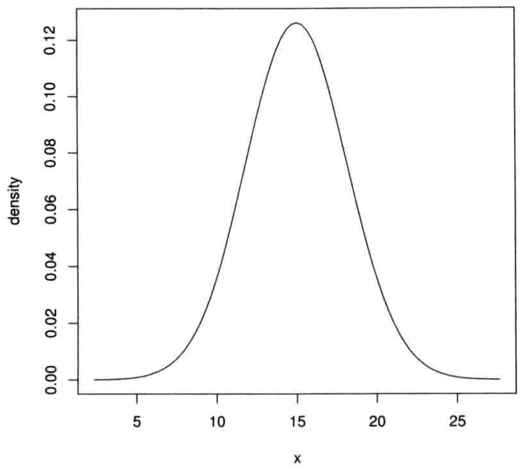

Figure 1.1. Solution to diffusion equation (1.9) at time $t = 5.0$ with velocity $v = 3.0$ and variance $\sigma^2 = 2.0$.

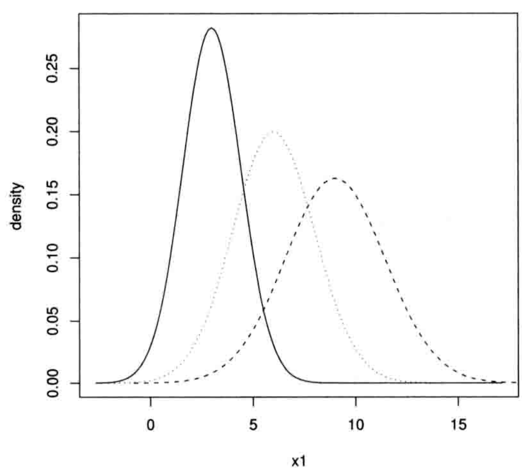

Figure 1.2. Solution to diffusion equation (1.9) at times $t_1 = 1.0$ (solid line), $t_2 = 2.0$ (dotted line), and $t_3 = 3.0$ (dashed line). The velocity $v = 3.0$ and variance $\sigma^2 = 2.0$.

Proof. The first derivative of the FT is

$$\begin{aligned}\hat{f}^{(1)}(k) &= \lim_{h\to 0} \frac{\hat{f}(k+h) - \hat{f}(k)}{h} \\ &= \lim_{h\to 0} h^{-1}\left(\mathbb{E}\left[e^{-i(k+h)X}\right] - \mathbb{E}\left[e^{-ikX}\right]\right) = \lim_{h\to 0} \mathbb{E}[g_h(X)]\end{aligned}$$

where $g_h(x) = h^{-1}(e^{-i(k+h)x} - e^{-ikx}) = h^{-1}(e^{-ihx} - 1)e^{-ikx}$ is the difference quotient for the differentiable function $k \mapsto e^{-ikx}$, so that $g_h(x) \to g(x) = -ixe^{-ikx}$ as $h \to 0$. From the geometric interpretation of e^{iy} as a vector in complex plane, it follows that $|e^{iy} - 1| \le |y|$ for all $y \in \mathbb{R}$. Then

$$|g_h(x)| = \left|\frac{e^{-ihx} - 1}{h}\right| \cdot |e^{-ikx}| \le |x|$$

for all $h \in \mathbb{R}$ and all $x \in \mathbb{R}$. The *Dominated Convergence Theorem* states that if $g_h(x) \to g(x)$ for all $x \in \mathbb{R}$ and if $|g_h(x)| \le r(x)$ for all h and all $x \in \mathbb{R}$, and if $\mathbb{E}[r(X)]$ is finite, then $\mathbb{E}[g_h(X)] \to \mathbb{E}[g(X)]$ and these expectations exist (e.g., see Durrett [59, Theorem 1.6.7, p. 29]). Since $\mathbb{E}[|X|]$ exists, the dominated convergence theorem with $r(x) = |x|$ implies that

$$\hat{f}^{(1)}(k) = \lim_{h\to 0} \mathbb{E}[g_h(X)] = \mathbb{E}[g(X)] = \mathbb{E}\left[(-iX)\, e^{-ikX}\right].$$

Set $k = 0$ to arrive at (1.11) in the case $p = 1$. The case $p > 1$ is similar, using the fact that $g_h(x) = h^{-p}(e^{-ihx} - 1)^p e^{-ikx}$ is the pth order difference quotient for $k \mapsto e^{-ikx}$. Alternatively, the proof for the case $p > 1$ can be completed using an induction argument. □

Proposition 1.2. *If $\mu_p = \mathbb{E}[|Y|^p]$ exists, then the FT of Y is*

$$\hat{f}(k) = \sum_{j=1}^{p} \frac{(-ik)^j}{j!}\mu_j + o(k^p) \tag{1.12}$$

as $k \to 0$.

Proof. If the FT $\hat{f}(k)$ is p times differentiable, then the Taylor expansion

$$\hat{f}(k) = \sum_{j=1}^{p} \frac{k^j}{j!} \hat{f}^{(p)}(0) + o(k^p)$$

is valid for all $k \in \mathbb{R}$. Apply Proposition 1.1 to arrive at (1.12). □

In equation (1.2) we used the fact that

$$\left(1 + \frac{r}{n} + o(1/n)\right)^n \to e^r \quad \text{as } n \to \infty. \tag{1.13}$$

To verify this, write $o(1/n) = \varepsilon_n/n$ where $\varepsilon_n \to 0$ as $n \to \infty$. Note that $|r + \varepsilon_n| < 1$ for n sufficiently large, and then use the fact that $\ln(1+z) = z + O(z^2)$ as $z \to 0$. This notation means that for some $\delta > 0$ we have

$$\left| \frac{\ln(1+z) - z}{z^2} \right| < C$$

for some constant $C > 0$, for all $|z| < \delta$. Then we can write

$$\ln\left[\left(1 + \frac{r+\varepsilon_n}{n}\right)^n\right] = n \ln\left[1 + \frac{r+\varepsilon_n}{n}\right]$$
$$= n\left[\frac{r+\varepsilon_n}{n} + O\left(\frac{1}{n^2}\right)\right] = r + \varepsilon_n + O\left(\frac{1}{n}\right) \to r.$$

Then apply the continuous function $\exp(z)$ to both sides to conclude that (1.13) holds.

In (1.3) we use the idea of weak convergence. Suppose that X_n is a sequence of random variables with cdf $F_n(x) = \mathbb{P}[X_n \le x]$, and X is a random variable with cdf $F(x) = \mathbb{P}[X \le x]$. We write $X_n \Rightarrow X$ if $F_n(x) \to F(x)$ for all $x \in \mathbb{R}$ such that F is continuous at x. This is equivalent to the condition that $\mathbb{E}[h(X_n)] \to \mathbb{E}[h(X)]$ for all bounded, continuous functions $h : \mathbb{R} \to \mathbb{R}$. See for example Billingsley [36].

In (1.3) we use the continuity theorem for the Fourier transform. Let $\hat{f}_n(k) = \mathbb{E}[e^{-ikX_n}]$ and $\hat{f}(k) = \mathbb{E}[e^{-ikX}]$. The Lévy Continuity Theorem [135, Theorem 1.3.6] implies that $X_n \Rightarrow X$ if and only if $\hat{f}_n(k) \to \hat{f}(k)$. More precisely, we have:

Theorem 1.3 (Lévy Continuity Theorem). *If X_n, X are random variables on $\mathbb{R}$, then $X_n \Rightarrow X$ implies that $\hat{f}_n(k) \to \hat{f}(k)$ for each $k \in \mathbb{R}$, uniformly on compact subsets. Conversely, if X_n is a sequence of random variables such that $\hat{f}_n(k) \to \hat{f}(k)$ for each $k \in \mathbb{R}$, and the limit $\hat{f}(k)$ is continuous at $k = 0$, then $\hat{f}(k)$ is the FT of some random variable X, and $X_n \Rightarrow X$.*

In (1.6) we used the fact that the FT of $f'(x)$ is $(ik)\hat{f}(k)$. If $f'(x)$ exists and is integrable, the limits

$$\lim_{x\to\infty} f(x) = f(0) + \lim_{x\to\infty} \int_0^x f'(u)du \quad \text{and} \quad \lim_{x\to-\infty} f(x) = f(0) - \lim_{x\to-\infty} \int_x^0 f'(u)du$$

exist. If f is integrable, then these limits must equal zero. Then we can integrate by parts to get

$$\int_{-\infty}^{\infty} e^{-ikx} f'(x)\,dx = \left[e^{-ikx} f(x)\right]_{x=-\infty}^{\infty} + \int_{-\infty}^{\infty} ike^{-ikx} f(x)\,dx = 0 + (ik)\hat{f}(k). \quad (1.14)$$

Applying this fact to the function f' shows that, if f'' is also integrable, then its FT equals $(ik)^2\hat{f}(k)$, and so

$$(ik)^2\hat{p}(k,t) = \int e^{-ikx} \frac{\partial^2}{\partial x^2} p(x,t)\,dx. \quad (1.15)$$

To arrive at (1.6), we inverted the FT (1.5). This can be justified using the following theorem.