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Some explicit expressions for the probability distribution of force magnitude

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Abstract. Recently, empirical investigations have suggested that the components of contact forces follow the exponential distribution. However, explicit expressions for the probability distribution of the corresponding force magnitude have not been known and only approximations have been used in the literature. In this note, for the first time, I provide explicit expressions for the probability distribution of the force magnitude. Both two-dimensional and three-dimensional cases are considered.

Keywords. Contact forces; exponential distribution; force component; force magnitude; Maple.

1. Introduction

The probability distribution of contact force magnitudes is of special interest in materials sciences. Until now, there have been various approaches: some of them purely empirical and others based on mathematical theory, (Sandstrom & Tucker 1993), Brockbank *et al* (1997), Radjai *et al* (1999), Schollmann (1999), Erikson *et al* (2002), Kruyt & Rothenburg (2002), Radeke *et al* (2002), Bagi (2003), Edwards *et al* (2003), Kruyt (2003), Vargas *et al* (2003), Goddard (2004), Metzger (2004), Radeke *et al* (2004), Chan & Ngan (2005), Nicot & Darve (2005), Tighe *et al* (2005), Youngquist *et al* (2005), Chan & Ngan (2006), Liu (2006), Ostojic *et al* (2006), and Snoeijer *et al* (2006). The theoretical approaches were pioneered by Kruyt & Rothenburg (2002) and Bagi (2003). The idea is to derive distributions that are related to the maximum entropy principle.

Suppose F_i denotes the absolute value of the ith force component corresponding to a global coordinate system for an assembly of particles. Then, in two- and three-dimensions, the force magnitude, say F, can be expressed as

$$F = \sqrt{F_1^2 + F_2^2} \tag{1}$$

and

$$F = \sqrt{F_1^2 + F_2^2 + F_3^2}, \tag{2}$$

respectively. The most popular theoretical model for (1) and (2) is the one suggested by Bagi (2003). It was suggested that the F_i be modelled by the exponential distribution specified by the probability density function (pdf):

$$g_i(F_i) = \lambda_i \exp(-\lambda_i F_i) \tag{3}$$

for $i = 1, 2, \ldots$. Bagi (2003) provided empirical and theoretical arguments for the model given by (3). Statistical analyses of simulated data have shown a good agreement with the exponential prediction in case of frictionless particles and a good agreement in case of particles with relatively small fraction. Theoretically, the exponential distribution in (3) is the distribution of maximum entropy in the set of all distributions of positive random variables with mean $1/\lambda_i$ (Cover & Thomas 1991).

The model given by (3) has been followed up by more recent papers, Goddard (2004), Metzger (2004) and Radeke *et al* (2004). The most generalized form of (3) suggested by Radeke *et al* (2004) has the joint post distribution force (pdf) given by

$$P(F_1, F_2, F_3) = \frac{\theta_1\theta_2\theta_3}{(1-\theta)^2} S_3\left(\frac{\rho\theta_1\theta_2\theta_3 F_1 F_2 F_3}{(1-\rho)^2}\right) \exp\left\{-\frac{\theta_1 F_1 + \theta_2 F_2 + \theta_3 F_3}{1-\rho}\right\}, \tag{4}$$

where $S_3(z) = \sum_{i=0}^{\infty} z^i/(i!)^3$, see Section 4 of Radeke *et al* (2004). This model arose because many simulations showed that the force components F_i in (1) and (2) are more or less correlated. Thus, these correlations must be considered.

It appears, however, that explicit expressions for the pdfs of the force magnitudes, (1) and (2), have not been known. This has led to some approximations. For example, gamma distributions have been used to approximate the pdfs of (1) and (2). In this note, I would like to show that the need for this can be avoided. I derive explicit expressions for the pdfs of F under the models given by (3) and (4), see §2 and 3. Some computer programs for their implementation are given in §4.

2. Force magnitude PDFs for (3)

First, consider (1) with the F_i, $i = 1, 2$ having the distribution given by (3). Transform $F_1 = r\cos\theta$ and $F_2 = r\sin\theta$. Then $r = \sqrt{F_1^2 + F_2^2} = F$ and its pdf can be obtained as

$$\begin{aligned}
P(r) &= r\lambda_1\lambda_2 \int_0^{\pi/2} \exp\{-\lambda_1 r\cos\theta - \lambda_2 r\sin\theta\} d\theta \\
&= r\lambda_1\lambda_2 \int_0^{\pi/2} \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} (\lambda_1\cos\theta + \lambda_2\sin\theta)^k d\theta \\
&= r\lambda_1\lambda_2 \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} \int_0^{\pi/2} (\lambda_1\cos\theta + \lambda_2\sin\theta)^k d\theta
\end{aligned}$$

$$= r\lambda_1\lambda_2 \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} \sum_{l=0}^{k} \binom{k}{l} \lambda_1^l \lambda_2^{k-l} \int_0^{\pi/2} \cos^l\theta \sin^{k-l}\theta d\theta$$

$$= \frac{r\lambda_1\lambda_2}{2} \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} \sum_{l=0}^{k} \binom{k}{l} \lambda_1^l \lambda_2^{k-l} B\left(\frac{l+1}{2}, \frac{k-l+1}{2}\right), \quad (5)$$

for $0 < r < \infty$, where the last step follows by equation (2·5·12·26) in Prudnikov *et al* (1986) and $B(a, b)$ denotes the beta function defined by

$$B(a, b) = \int_0^1 t^{a-1}(1-t)^{b-1} dt.$$

In the particular case $\lambda_1 = \lambda_2 = \lambda$, (5) reduces to the simpler form

$$P(r) = \frac{r\lambda^2}{2} \sum_{k=0}^{\infty} \frac{(-\lambda r)^k}{k!} \sum_{l=0}^{k} \binom{k}{l} B\left(\frac{l+1}{2}, \frac{k-l+1}{2}\right)$$

for $0 < r < \infty$. Using the relation

$$\begin{aligned} &\exp\{-\lambda_1 r\cos\theta - \lambda_2 r \sin\theta\} \\ &\quad = \{1-[1-\exp(-\lambda_1 r)]\}^{\cos\theta}\{1-[1-\exp(-\lambda_2 r)]\}^{\sin\theta} \\ &\quad = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}(-1)^{k+l}\binom{\cos\theta}{k}\binom{\sin\theta}{l}[1-\exp(-\lambda_1 r)]^k[1-\exp(-\lambda_2 r)]^l, \end{aligned}$$

one can obtain the asymptotic expansion

$$P(r) = r\lambda_1\lambda_2 \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}(-1)^{k+l} A_1(k,l)[1-\exp(-\lambda_1 r)]^k[1-\exp(-\lambda_2 r)]^l, \quad (6)$$

where

$$A_1(k,l) = \int_0^{\pi/2} \binom{\cos\theta}{k}\binom{\sin\theta}{l} d\theta.$$

Note that the leading term in (6) is $(\pi/2)\lambda_1\lambda_2 r$. Figure 1 shows the variation of (5) versus r for $\lambda_1 = \lambda_2 = 1, 2, 3, 4$. The Maple procedure `pdf1(r, lambda1, lambda2)` in §4 was used to compute (5).

Now, consider (2) with the F_i, $i = 1, 2, 3$ having the distribution given by (3). Transform $F_1 = r\sin\phi\cos\theta$, $F_2 = r\sin\phi\sin\theta$ and $F_3 = r\cos\phi$. Then $r = \sqrt{F_1^2 + F_2^2 + F_3^2} = F$ and its pdf can be obtained as

$$\begin{aligned} P(r) &= r\lambda_1\lambda_2\lambda_3 \int_0^{\pi/2}\int_0^{\pi/2} \exp\{-\lambda_1 r\sin\phi\cos\theta - \lambda_2 r\sin\phi\sin\theta - \lambda_3 r\cos\phi\} d\theta d\phi \\ &= r\lambda_1\lambda_2\lambda_3 \int_0^{\pi/2}\int_0^{\pi/2} \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} (\lambda_1 r\sin\phi\cos\theta + \lambda_2 r\sin\phi\sin\theta + \lambda_3 r\cos\phi)^k d\theta d\phi \end{aligned}$$

$$= r\lambda_1\lambda_2\lambda_3 \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} \int_0^{\pi/2} \int_0^{\pi/2} (\lambda_1 \sin\phi \cos\theta + \lambda_2 \sin\phi \sin\theta + \lambda_3 \cos\phi)^k d\theta d\phi$$

$$= r\lambda_1\lambda_2\lambda_3 \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} \sum_{0\leq l+m\leq k} \frac{k!}{l!m!(k-l-m)!} \lambda_1^l \lambda_2^m \lambda_3^{k-l-m}$$

$$\times \int_0^{\pi/2} \int_0^{\pi/2} (\sin\phi)^{l+m} (\cos\phi)^{k-l-m} (\sin\theta)^m (\cos\theta)^l d\theta d\phi$$

$$= \frac{r\lambda_1\lambda_2\lambda_3}{4} \sum_{k=0}^{\infty} \frac{(-r)^k}{k!} \sum_{0\leq l+m\leq k} \frac{k!}{l!m!(k-l-m)!} \lambda_1^l \lambda_2^m \lambda_3^{k-l-m}$$

$$\times B\left(\frac{m+1}{2}, \frac{l+1}{2}\right) B\left(\frac{l+m+1}{2}, \frac{k-l-m+1}{2}\right) \quad (7)$$

for $0 < r < \infty$, where the last step follows by equation (2·5·12·26) in Prudnikov *et al* (1986). In the particular case $\lambda_1 = \lambda_2 = \lambda_3 = \lambda$, (7) reduces to the simpler form

$$P(r) = \frac{r\lambda^3}{4} \sum_{k=0}^{\infty} \frac{(-\lambda r)^k}{k!} \sum_{0\leq l+m\leq k} \frac{k!}{l!m!(k-l-m)!}$$

$$\times B\left(\frac{m+1}{2}, \frac{l+1}{2}\right) B\left(\frac{l+m+1}{2}, \frac{k-l-m+1}{2}\right)$$

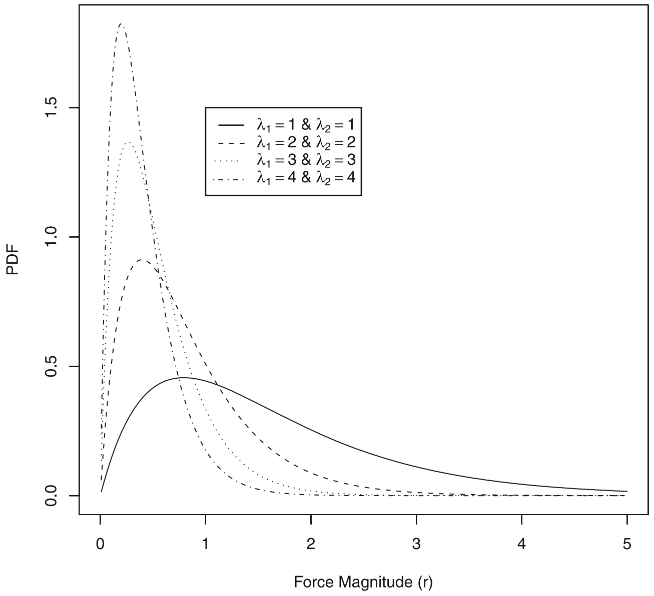

Figure 1. Plots of the pdf (5) for $\lambda_1 = \lambda_2 = 1, 2, 3, 4$.

for $0 < r < \infty$. Using the relation

$$\begin{aligned}
&\exp\{-\lambda_1 r \sin\phi\cos\theta - \lambda_2 r \sin\phi \sin\theta - \lambda_3 r\cos\phi\} \\
&\quad = \{1 - [1 - \exp(-\lambda_1 r)]\}^{\sin\phi\cos\theta}\{1 - [1 - \exp(-\lambda_2 r)]\}^{\sin\phi\sin\theta} \\
&\qquad \times \{1 - [1 - \exp(-\lambda_3 r)]\}^{\cos\phi} \\
&\quad = \sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}(-1)^{k+l+m}\binom{\sin\phi\cos\theta}{k}\binom{\sin\phi\sin\theta}{l}\binom{\cos\phi}{m} \\
&\qquad \times [1 - \exp(-\lambda_1 r)]^k[1 - \exp(-\lambda_2 r)]^l[1 - \exp(-\lambda_3 r)]^m,
\end{aligned}$$

one can obtain the asymptotic expansion

$$\begin{aligned}
P(r) = r\lambda_1\lambda_2\lambda_3 &\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}(-1)^{k+l+m}A_2(k,l,m) \\
&\times [1 - \exp(-\lambda_1 r)]^k[1 - \exp(-\lambda_2 r)]^l[1 - \exp(-\lambda_3 r)]^m, \qquad (8)
\end{aligned}$$

where

$$A_2(k,l,m) = \int_0^{\pi/2}\int_0^{\pi/2}\binom{\sin\phi\cos\theta}{k}\binom{\sin\phi\sin\theta}{l}\binom{\cos\phi}{m}\,d\theta d\phi.$$

Note that the leading term in (8) is $(\pi/2)^2\lambda_1\lambda_2\lambda_3 r$. Figure 2 shows the variation of (7) versus r for $\lambda_1 = \lambda_2 = \lambda_3 = 1, 2, 3, 4$. The Maple procedure pdf2(r, lambda1, lambda2, lambda3) in §4 was used to compute (7).

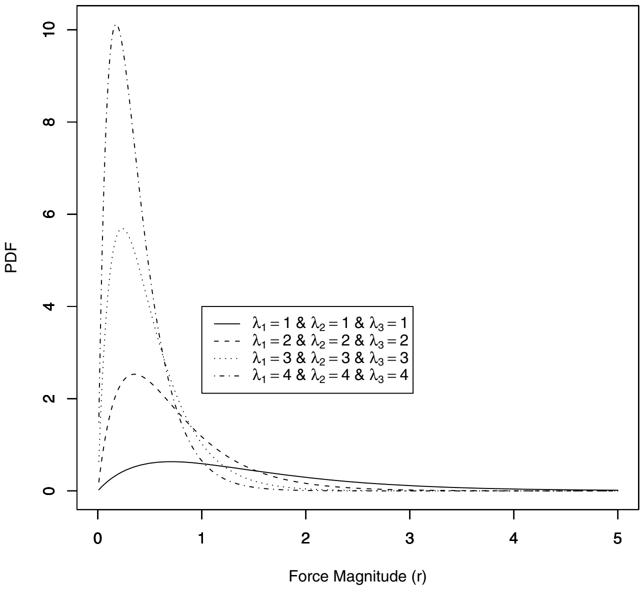

Figure 2. Plots of the pdf (7) for $\lambda_1 = \lambda_2 = \lambda_3 = 1, 2, 3, 4$.

3. Force magnitude PDF for (4)

Here, I consider (2) with the F_i, $i = 1, 2, 3$ having the distribution given by (4). Transform $F_1 = r\sin\phi\cos\theta$, $F_2 = r\sin\phi\sin\theta$ and $F_3 = r\cos\phi$. Then $r = \sqrt{F_1^2 + F_2^2 + F_3^2} = F$ and its pdf can be obtained as

$$
\begin{aligned}
P(r) = {} & \frac{r\theta_1\theta_2\theta_3}{(1-\rho)^2} \int_0^{\pi/2}\int_0^{\pi/2} S_3\left(\frac{\rho\theta_1\theta_2\theta_3 r^3 \sin^2\phi\cos\phi\sin\theta\cos\theta}{(1-\rho)^2}\right) \\
& \times \exp\left\{-r\frac{\theta_1\sin\phi\cos\theta + \theta_2\sin\phi\sin\theta + \theta_3\cos\phi}{1-\rho}\right\} d\theta d\phi \\
= {} & \frac{r\theta_1\theta_2\theta_3}{(1-\rho)^2}\sum_{i=0}^{\infty}\frac{\rho^i\theta_1^i\theta_2^i\theta_3^i r^{3i}}{(i!)^3(1-\rho)^{2i}}\int_0^{\pi/2}\int_0^{\pi/2}\sin^{2i}\phi\cos^i\phi\sin^i\theta\cos^i\theta \\
& \times \exp\left\{-r\frac{\theta_1\sin\phi\cos\theta + \theta_2\sin\phi\sin\theta + \theta_3\cos\phi}{1-\rho}\right\} d\theta d\phi \\
= {} & \frac{r\theta_1\theta_2\theta_3}{(1-\rho)^2}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\frac{\rho^i\theta_1^i\theta_2^i\theta_3^i r^{3i+j}(-1)^j}{j!(i!)^3(1-\rho)^{2i+j}}\int_0^{\pi/2}\int_0^{\pi/2}\sin^{2i}\phi\cos^i\phi\sin^i\theta\cos^i\theta \\
& \times (\theta_1\sin\phi\cos\theta + \theta_2\sin\phi\sin\theta + \theta_3\cos\phi)^j d\theta d\phi \\
= {} & \frac{r\theta_1\theta_2\theta_3}{(1-\rho)^2}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\frac{\rho^i\theta_1^i\theta_2^i\theta_3^i r^{3i+j}(-1)^j}{j!(i!)^3(1-\rho)^{2i+j}}\sum_{0\le k+l\le j}\frac{j!\theta_1^k\theta_2^l\theta_3^{j-k-l}}{k!l!(j-k-l)!} \\
& \times \int_0^{\pi/2}\int_0^{\pi/2}\sin^{2i+k+l}\phi\cos^{i+j-k-l}\phi\sin^{i+l}\theta\cos^{i+k}\theta d\theta d\phi \\
= {} & \frac{r\theta_1\theta_2\theta_3}{(1-\rho)^2}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\frac{(\rho\theta_1\theta_2\theta_3)^i r^{3i+j}(-1)^j}{j!(i!)^3(1-\rho)^{2i+j}}\sum_{0\le k+l\le j}\frac{j!\theta_1^k\theta_2^l\theta_3^{j-k-l}}{k!l!(j-k-l)!} \\
& \times B\left(\frac{l+i+1}{2}, \frac{k+i+1}{2}\right) B\left(\frac{k+l+2i+1}{2}, \frac{j-k-l+i+1}{2}\right) \qquad (9)
\end{aligned}
$$

for $0 < r < \infty$. In the particular case $\theta_1 = \theta_2 = \theta_3 = \theta$, (9) reduces to the simpler form

$$
\begin{aligned}
P(r) = {} & \frac{r\theta^3}{(1-\rho)^2}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\frac{(\rho\theta^3)^i r^{3i+j}(-\theta)^j}{j!(i!)^3(1-\rho)^{2i+j}}\sum_{0\le k+l\le j}\frac{j!}{k!l!(j-k-l)!} \\
& \times B\left(\frac{l+i+1}{2}, \frac{k+i+1}{2}\right) B\left(\frac{k+l+2i+1}{2}, \frac{j-k-l+i+1}{2}\right)
\end{aligned}
$$

for $0 < r < \infty$. Using the relation

$$\begin{aligned}
&\exp\left\{-r\frac{\theta_1 \sin\phi\cos\theta + \theta_2 \sin\phi\sin\theta + \theta_3\cos\phi}{1-\rho}\right\} \\
&= \left\{1-\left[1-\exp\left(-\frac{\theta_1 r}{1-\rho}\right)\right]\right\}^{\sin\phi\cos\theta}\left\{1-\left[1-\exp\left(-\frac{\theta_2 r}{1-\rho}\right)\right]\right\}^{\sin\phi\sin\theta} \\
&\quad\times\left\{1-\left[1-\exp\left(-\frac{\theta_3 r}{1-\rho}\right)\right]\right\}^{\cos\phi} \\
&= \sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}(-1)^{j+k+l}\binom{\sin\phi\cos\theta}{j}\binom{\sin\phi\sin\theta}{k}\binom{\cos\phi}{l} \\
&\quad\times\left[1-\exp\left(-\frac{\theta_1 r}{1-\rho}\right)\right]^{j}\left[1-\exp\left(-\frac{\theta_2 r}{1-\rho}\right)\right]^{k} \\
&\quad\times\left[1-\exp\left(-\frac{\theta_3 r}{1-\rho}\right)\right]^{l},
\end{aligned}$$

one can obtain the asymptotic expansion

$$\begin{aligned}
P(r) = {} & \frac{r\theta_1\theta_2\theta_3}{(1-\rho)^2}\sum_{i=0}^{\infty}\frac{\rho^i\theta_1^i\theta_2^i\theta_3^i r^{3i}}{(i!)^3(1-\rho)^{2i}}\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\sum_{l=0}^{\infty}(-1)^{j+k+l}A_3(i,j,k,l) \\
&\times\left[1-\exp\left(-\frac{\theta_1 r}{1-\rho}\right)\right]^{j}\left[1-\exp\left(-\frac{\theta_2 r}{1-\rho}\right)\right]^{k}\left[1-\exp\left(-\frac{\theta_3 r}{1-\rho}\right)\right]^{l},
\end{aligned} \tag{10}$$

where

$$\begin{aligned}
&A_3(i,j,k,l) \\
&= \int_0^{\pi/2}\int_0^{\pi/2}\sin^{2i}\phi\cos^i\phi\sin^i\theta\cos^i\theta\binom{\sin\phi\cos\theta}{j}\binom{\sin\phi\sin\theta}{k}\binom{\cos\phi}{l}d\theta d\phi.
\end{aligned}$$

Note that the leading term in (10) is $r\theta_1\theta_2\theta_3(1-\rho)^{-2}\sum_{i=0}^{\infty}\rho^i\theta_1^i\theta_2^i\theta_3^i r^{3i}(i!)^{-3}(1-\rho)^{-2i}A_3(i,0,0,0)$. Figure 3 shows the variation of (9) versus r for $\theta_1 = \theta_2 = \theta_3 = 1$ and $\rho = -0{\cdot}5, 0, 0{\cdot}5, 0{\cdot}8$. The Maple procedure `pdf3(r, rho, theta1, theta2, theta3)` in §4 was used to compute (9).

4. Computer programs

Note that the expressions in (5), (7) and (9) are infinite sums of elementary functions. These infinite sums can be easily computed in most computer packages. The following procedures show how it can be done using Maple. The procedures `pdf1(r, lambda1, lambda2)`, `pdf2(r, lambda1, lambda2, lambda3)` and `pdf3(r, rho, theta1, theta2, theta3)` will return the values of (5), (7) and (9), respectively.

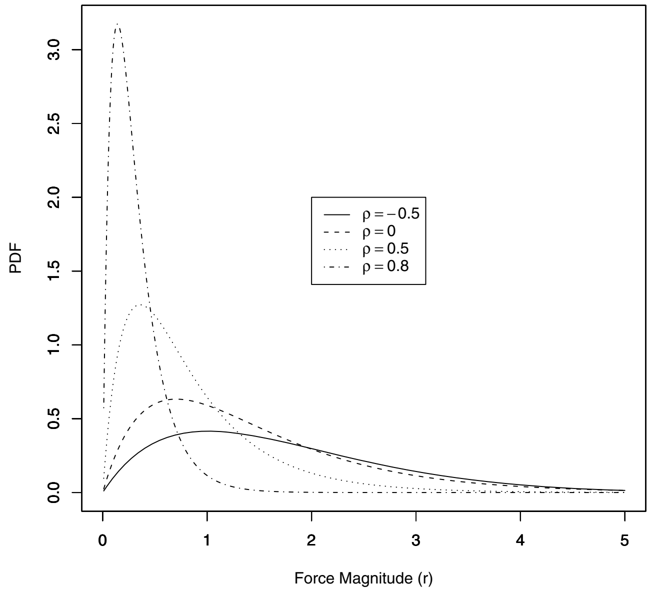

Figure 3. Plots of the pdf (9) for $\theta_1 = \theta_2 = \theta_3 = 1$ and $\rho = -0{\cdot}5, 0, 0{\cdot}5, 0{\cdot}8$.

```
pdf1:=proc(r,lambda1,lambda2)
local f,t,k,l;
f:=(-r)**k*(1/factorial(k))*binomial(k,l)*lambda1**l*lambda2
   **(k-l);
f:=f*Beta((l+1)/2,(k-l+1)/2);
t:=sum(sum(f,l=0..k),k=0..infinity);
t:=evalf(0.5*r*lambda1*lambda2*t);
end proc;
```

```
pdf2:=proc(r,lambda1,lambda2,lambda3)
local f,t,k,l,m;
f:=(-r)**k*(1/factorial(k))*multinomial(k,l,m);
f:=f*lambda1**l*lambda2**m*lambda3**(k-l-m);
f:=f*Beta((m+1)/2,(l+1)/2)*Beta((l+m+1)/2,(k-l-m+1)/2);
t:=sum(sum(sum(f,m=0..(k-l)),l=0..k),k=0..infinity);
t:=evalf(0.25*r*lambda1*lambda2*lambda3*t);
end proc;
```

```
pdf3:=proc(r,rho,theta1,theta2,theta3)
local f,t,i,j,k,l;
f:=r**(3*i+j+1)*(-1)**j/(factorial(j)*factorial(i)**3);
f:=f*rho**i*theta1**(i+k)*theta2**(i+l)*theta3**(i+j-k-l);
f:=f*multinomial(j,k,l)*Beta((l+i+1)/2,(k+i+1)/2);
f:=f*Beta((k+l+2*i+1)/2,(j-k-l+i+1)/2)/(1-rho)**(2*i+j);
t:=sum(sum(sum(sum(f,l=0..(j-k)),k=0..j),j=0..infinity),
   i=0..infinity);
t:=evalf(theta1*theta2*theta3*t/(1-rho)**2);
end proc;
```

The electronic version of the above programs can be obtained from the author.

5. Conclusions

We have derived explicit expressions for the probability distribution of the force magnitude when the components of contact forces follow the exponential distribution. We have considered both two-dimensional and three-dimensional cases.

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