University of Bern
Institute of Mathematical Statistics and Actuarial Science
Technical Report 71

On an Auxiliary Function for Log-Density Estimation

Madeleine L. Cule and Lutz Dümbgen

(University of Cambridge and University of Bern)

July 2008, minor revisions in January 2016

Abstract

In this note we provide explicit expressions and expansions for a special function J which appears in nonparametric estimation of log-densities. This function returns the integral of a log-linear function on a simplex of arbitrary dimension. In particular it is used in the R-package *LogCondDEAD* by Cule et al. (2007).

Contents

1 Introduction

Suppose one wants to estimate a probability density f on a certain compact region $C \subset \mathbb{R}^d$, based on an empirical distribution $\hat{P}$ of a sample from f. One possibility is to embed C into a union

$$S = \bigcup_{j=1}^{m} S_j$$

of simplices $S_j \subset \mathbb{R}^d$ with pairwise disjoint interior. By a simplex in $\mathbb{R}^d$ we mean the convex hull of $d + 1$ points. Then we consider the family $\mathcal{G} = \mathcal{G}(S_1, \ldots, S_m)$ of all continuous functions $\psi : S \to \mathbb{R}$ which are linear on each simplex S_j. Now

$$\hat{\psi} := \arg\max_{\psi \in \mathcal{G}} \left(\int_S \psi \, d\hat{P} - \int_S \exp(\psi(x)) \, dx \right) \tag{1}$$

defines a maximum likelihood estimator $\hat{f} := \exp(\hat{\psi})$ of a probability density on S, based on $\hat{P}$. For existence and uniqueness of this estimator see, for instance, Cule et al. (2008).

To compute $\hat{\psi}$ explicitly, note that $\psi \in \mathcal{G}$ is uniquely determined by its values at the corners (extremal points) of all simplices S_j, and $\int \psi \, d\hat{P}$ is a linear function of these values. The second integral in (1) may be represented as follows: Let S_j be the convex hull of $\boldsymbol{x}_{0j}, \boldsymbol{x}_{1j}, \ldots, \boldsymbol{x}_{dj} \in \mathbb{R}^d$, and set $y_{ij} := \psi(\boldsymbol{x}_{ij})$. Then

$$\int_S \exp(\psi(x)) \, dx = \sum_{i=1}^{m} \int_{S_i} \exp(\psi(x)) \, dx = \sum_{i=1}^{m} D_j \cdot J(y_{0j}, y_{1j}, \ldots, y_{dj}),$$

where

$$D_j := \det\big[\boldsymbol{x}_{1j} - \boldsymbol{x}_{0j}, \boldsymbol{x}_{2j} - \boldsymbol{x}_{0j}, \ldots, \boldsymbol{x}_{dj} - \boldsymbol{x}_{0j}\big],$$

while $J(\cdot)$ is an auxiliary function defined and analyzed subsequently.

2 The special function $J(\cdot)$

2.1 Definition of $J(\cdot)$

For $d \in \mathbb{N}$ let

$$\mathcal{T}_d := \Big\{\boldsymbol{u} \in (0,1)^d : \sum_{i=1}^{d} u_i < 1\Big\}.$$

Then for $y_0, y_1, \ldots, y_d \in \mathbb{R}$ we define

$$J(y_0, y_1, \ldots, y_d) := \int_{\mathcal{T}_d} \exp\Big((1 - u_+)y_0 + \sum_{i=1}^{d} u_i y_i\Big) d\boldsymbol{u}$$

with $u_+ := \sum_{i=1}^{d} u_i$.

Standard considerations in connection with beta- and gamma-distributions as described in Section 6 reveal the following alternative representation:

$$J(y_0, y_1, \ldots, y_d) := \frac{1}{d!} \mathbb{E} \exp\Big(\sum_{i=0}^{d} B_i y_i\Big)$$

with $B_i = B_{d,i} := E_i / \sum_{s=0}^{d} E_s$ and stochastically independent, standard exponential random variables $E_0, E_1, \ldots, E_d$. This representation shows clearly that $J(\cdot)$ is symmetric in its arguments.

An often useful identity is

$$J(y_0, y_1, \ldots, y_d) = \exp(y_*) J(y_0 - y_*, y_1 - y_*, \ldots, y_d - y_*) \quad \text{for any } y_* \in \mathbb{R}. \quad (2)$$

2.2 A first recursion formula

For $d = 1$ one can compute $J(y_0, y_1)$ explicitly:

$$J(y_0, y_1) = \int_0^1 \exp\big((1-u)y_0 + uy_1\big) du = \begin{cases} \dfrac{\exp(y_1) - \exp(y_0)}{y_1 - y_0} & \text{if } y_0 \neq y_1, \\ \exp(y_0) & \text{if } y_0 = y_1. \end{cases}$$

For $d \geq 2$ one may use the following recursion formula:

$$J(y_0, y_1, \ldots, y_d) = \begin{cases} \dfrac{J(y_1, y_2, \ldots, y_d) - J(y_0, y_2, \ldots, y_d)}{y_1 - y_0} & \text{if } y_0 \neq y_1, \\ \dfrac{\partial}{\partial y_1} J(y_1, y_2, \ldots, y_d) & \text{if } y_0 = y_1. \end{cases} \quad (3)$$

3

Since $J(y_0, y_1, \ldots, y_d)$ is continuous in $y_0, y_1, \ldots, y_d$, it suffices to verify (3) in case of $y_0 \neq y_1$. We may identify $\mathcal{T}_d$ with the set $\{(v, \boldsymbol{u}) : \boldsymbol{u} \in \mathcal{T}_{d-1}, v \in (0, 1 - u_+)\}$. Then it follows from Fubini's theorem that

$$
\begin{aligned}
&J(y_0, y_1, \ldots, y_d) \\
&= \int_{\mathcal{T}_{d-1}} \int_0^{1-u_+} \exp\Big((1 - u_+ - v)y_0 + vy_1 + \sum_{i=2}^d u_{i-1}y_i\Big) \, dv \, d\boldsymbol{u} \\
&= \int_{\mathcal{T}_{d-1}} \Big(\frac{\exp\big((1 - u_+ - v)y_0 + vy_1 + \sum_{i=2}^d u_{i-1}y_i\big)}{y_1 - y_0}\Big)\Big|_{v=0}^{1-u_+} d\boldsymbol{u} \\
&= \int_{\mathcal{T}_{d-1}} \frac{\exp\big((1 - u_+)y_1 + \sum_{i=2}^d u_{i-1}y_i\big) - \exp\big((1 - u_+)y_0 + \sum_{i=2}^d u_{i-1}y_i\big)}{y_1 - y_0} \, d\boldsymbol{u} \\
&= \frac{J(y_1, y_2, \ldots, y_d) - J(y_0, y_2, \ldots, y_d)}{y_1 - y_0}.
\end{aligned}
$$

2.3 Another recursion formula

It is well-known that for any integer $0 \leq j < d$,

$$
\Big(\frac{E_i}{\sum_{s=0}^j E_s}\Big)_{i=0}^j, \quad B := \frac{\sum_{i=0}^j E_i}{\sum_{s=0}^d E_s}, \quad \Big(\frac{E_i}{\sum_{s=j+1}^d E_s}\Big)_{i=j+1}^d
$$

are stochastically independent with $B \sim \text{Beta}(j + 1, d - j)$; see also Section 6. Hence we end up with the following recursive identity:

$$
\begin{aligned}
&J(y_0, y_1, \ldots, y_d) \\
&= \frac{j!(d - j - 1)!}{d!} \mathbb{E}\big(J(By_0, \ldots, By_j)J((1 - B)y_{j+1}, \ldots, (1 - B)y_d)\big) \\
&= \int_0^1 u^j (1 - u)^{d-j-1} J(uy_0, \ldots, uy_j) J((1 - u)y_{j+1}, \ldots, (1 - u)y_d) \, du
\end{aligned}
$$

with

$$
J(r) := \exp(r).
$$

Here we used the well-known identity

$$
\int (1 - u)^\ell u^m \, du = \frac{\ell! m!}{(\ell + m + 1)!} \quad \text{for integers } \ell, m \geq 0. \tag{4}
$$

Plugging in $j = d - 1$ into the previous recursive equation leads to

$$
J(y_0, y_1, \ldots, y_d) = \int_0^1 u^{d-1} J(uy_0, \ldots, uy_{d-1}) \exp((1 - u)y_d) \, du. \tag{5}
$$

4

3 An expansion for $J(\cdot)$

With $\bar{y} := (d+1)^{-1} \sum_{i=0}^{d} y_i$ and $z_i := y_i - \bar{y}$ one may write

$$J(y_0, y_1, \ldots, y_d) \;=\; \exp(\bar{y}) J(z_0, z_1, \ldots, z_d)$$

by virtue of (2). Note that $z_+ := \sum_{i=0}^{d} z_i = 0$. As $\boldsymbol{z} := (z_i)_{i=0}^{d} \to \boldsymbol{0}$,

$$
\begin{aligned}
&d!\, J(z_0, z_1, \ldots, z_d) \\
&= \; 1 + \sum_{i=0}^{d} \mathbb{E}(B_i) z_i + \frac{1}{2} \sum_{i,j=0}^{d} \mathbb{E}(B_i B_j) z_i z_j + \frac{1}{6} \sum_{i,j,k=0}^{d} \mathbb{E}(B_i B_j B_k) z_i z_j z_k + O(\|\boldsymbol{z}\|^4).
\end{aligned}
$$

It follows from Lemma 6.1 that

$$\mathbb{E}\left(\prod_{i=0}^{d} B_i^{k_i}\right) \;=\; \prod_{i=0}^{d} k_i! \Big/ [d + k_+]_{k_+} \quad \text{for integers } k_0, k_1, \ldots, k_d \geq 0.$$

In particular,

$$\mathbb{E}(B_0) \;=\; \frac{1}{d+1},$$

$$\mathbb{E}(B_0^2) \;=\; \frac{2}{[d+2]_2}, \qquad \mathbb{E}(B_0 B_1) \;=\; \frac{1}{[d+2]_2},$$

$$\mathbb{E}(B_0^3) \;=\; \frac{6}{[d+3]_3}, \qquad \mathbb{E}(B_0^2 B_1) \;=\; \frac{2}{[d+3]_3}, \qquad \mathbb{E}(B_0 B_1 B_2) \;=\; \frac{1}{[d+3]_3}.$$

Consequently, $\sum_{i=0}^{d} \mathbb{E}(B_i) z_i = \mathbb{E}(B_0) z_+ = 0$,

$$
\begin{aligned}
[d+2]_2 \sum_{i,j=0}^{d} \mathbb{E}(B_i B_j) z_i z_j \;&=\; \sum_{i,j=0}^{d} \left(1_{[i=j]} \cdot 2 + 1_{[i \neq j]}\right) z_i z_j \\
&=\; \sum_{i,j=0}^{d} \left(1_{[i=j]} + 1\right) z_i z_j \\
&=\; \sum_{i=0}^{d} z_i^2 + z_+^2 \\
&=\; \sum_{i=0}^{d} z_i^2,
\end{aligned}
$$

and

$$[d+3]_3 \sum_{i,j,k=0}^{d} \mathbb{E}(B_i B_j B_k) z_i z_j z_k$$

$$= \sum_{i,j,k=0}^{d} \left(1_{[i=j=k]} \cdot 6 + 1_{[\#\{i,j,k\}=2]} \cdot 2 + 1_{[\#\{i,j,k\}=3]}\right) z_i z_j z_k$$

$$= \sum_{i,j,k=0}^{d} \left(1_{[i=j=k]} \cdot 5 + 1_{[\#\{i,j,k\}=2]} + 1\right) z_i z_j z_k$$

$$= 5 \sum_{i=0}^{d} z_i^3 + 3 \sum_{s,t=0}^{d} 1_{[s \neq t]} z_s^2 z_t + z_+^3$$

$$= 5 \sum_{i=0}^{d} z_i^3 + 3 \sum_{s=0}^{d} z_s^2 z_+ - 3 \sum_{s=0}^{d} z_s^3 + z_+^3$$

$$= 2 \sum_{i=0}^{d} z_i^3.$$

Consequently,

$$J(y_0, y_1, \ldots, y_d) = \exp(\bar{y}) \left(\frac{1}{d!} + \frac{1}{2(d+2)!} \sum_{i=0}^{d} z_i^2 + \frac{1}{3(d+3)!} \sum_{i=0}^{d} z_i^3 + O(\|z\|^4) \right). \quad (6)$$

4 A recursive implementation of $J(\cdot)$ and its partial derivatives

By means of (3) and the Taylor expansion (6) one can implement the function $J(\cdot)$ in a recursive fashion. In what follows we use the abbreviation

$$y_{a:b} = \begin{cases} (y_a, \ldots, y_b) & \text{if } a \leq b \\ () & \text{if } a > b \end{cases}$$

To compute $J(y_{0:d})$ we assume without loss of generality that $y_0 \leq y_1 \leq \cdots \leq y_d$. It follows from (3) and symmetry of $J(\cdot)$ that

$$J(y_{0:d}) = \frac{J(y_{1:d}) - J(y_{0:d-1})}{y_d - y_0}$$

if $y_0 \neq y_d$. This formula is okay numerically if $y_d - y_0$ is not too small. Otherwise one should use (6). This leads to the the pseudo code in Table 1.

To avoid messy formulae, one can express partial derivatives of $J(\cdot)$ in terms of higher order versions of $J(\cdot)$ by means of the recursion (3). For instance,

$$\frac{\partial J(y_{0:d})}{\partial y_0} = \lim_{\epsilon \to 0} \frac{J(y_0 + \epsilon, \, y_{1:d}) - J(y_0, \, y_{1:d})}{\epsilon}$$

$$= \lim_{\epsilon \to 0} J(y_0, y_0 + \epsilon, \, y_{1:d})$$

$$= J(y_0, y_0, y_{1:d}).$$

6

$$
\begin{array}{|l|}
\hline
\textbf{Algorithm } J \leftarrow \mathbf{J}(y, d, \epsilon) \\
\textbf{if } y_d - y_0 < \epsilon \textbf{ then} \\
\qquad \bar{y} \leftarrow \sum_{i=0}^{d} y_i/(d+1) \\
\qquad z_2 \leftarrow \sum_{i=0}^{d} (y_i - \bar{y})^2/2 \\
\qquad z_3 \leftarrow \sum_{i=0}^{d} (y_i - \bar{y})^3/3 \\
\qquad J \leftarrow \exp(\bar{y})\big(1/d! + z_2/(d+2)! + z_3/(d+3)!\big) \\
\textbf{else} \\
\qquad J \leftarrow \big(\mathbf{J}(y_{1:d}, d-1, \epsilon) - \mathbf{J}(y_{0:d-1}, d-1, \epsilon)\big)/(y_d - y_0) \\
\textbf{end if.} \\
\hline
\end{array}
$$

Table 1: Pseudo-code for $J(y)$ with ordered input vector y.

Similarly,

$$
\begin{aligned}
\frac{\partial^2 J(y_{0:d})}{\partial y_0^2}
&= \lim_{\epsilon \to 0}\Big(\frac{J(y_0 + \epsilon,\, y_{1:d}) - J(y_0,\, y_{1:d})}{\epsilon} - \frac{J(y_0,\, y_{1:d}) - J(y_0 - \epsilon,\, y_{1:d})}{\epsilon}\Big)/\epsilon \\
&= 2 \lim_{\epsilon \to 0} \frac{J(y_0, y_0 + \epsilon,\, y_{1:d}) - J(y_0, y_0 - \epsilon,\, y_{1:d})}{2\epsilon} \\
&= 2 \lim_{\epsilon \to 0} J(y_0, y_0 - \epsilon, y_0 + \epsilon,\, y_{1:d}) \\
&= 2\, J(y_0, y_0, y_0,\, y_{1:d}),
\end{aligned}
$$

while

$$
\begin{aligned}
\frac{\partial^2 J(y_{0:d})}{\partial y_0 \partial y_1}
&= \lim_{\epsilon \to 0}\Big(\frac{J(y_0 + \epsilon, y_1 + \epsilon,\, y_{2:d}) - J(y_0, y_1 + \epsilon,\, y_{2:d})}{\epsilon} \\
&\qquad\qquad - \frac{J(y_0 + \epsilon, y_1,\, y_{2:d}) - J(y_0, y_1,\, y_{2:d})}{\epsilon}\Big)/\epsilon \\
&= \lim_{\epsilon \to 0} \frac{J(y_0, y_0 + \epsilon, y_1 + \epsilon,\, y_{2:d}) - J(y_0, y_0 + \epsilon, y_1,\, y_{2:d})}{\epsilon} \\
&= \lim_{\epsilon \to 0} J(y_0, y_0 + \epsilon, y_1, y_1 + \epsilon,\, y_{2:d}) \\
&= J(y_0, y_0, y_1, y_1,\, y_{2:d}).
\end{aligned}
$$

5 The special cases $d = 1$ and $d = 2$

For small dimension d it may be worthwhile to work with non-recursive implementations of the function $J(\cdot)$. Here we collect and extend some results of Dümbgen et al. (2007).

5.1 General considerations about a bivariate function

In view of (3) we consider an arbitrary function $f : \mathbb{R} \to \mathbb{R}$ which is infinitely often differentiable. Then

$$
h(r, s) := \begin{cases} \dfrac{f(s) - f(r)}{s - r} & \text{if } s \neq r \\[2ex] f'(r) & \text{if } s = r \end{cases}
$$

defines a smooth and symmetric function $h : \mathbb{R}^2 \to \mathbb{R}$ such that

$$h(r, s) \;=\; f'(r) + \frac{f''(r)}{2}(s - r) + O\big((s - r)^2\big) \quad \text{as } s \to r.$$

Its first partial derivatives of order one and two are given by

$$\frac{\partial h(r, s)}{\partial r} \;=\; \begin{cases} \dfrac{f(s) - f(r) - f'(r)(s - r)}{(s - r)^2} & \text{if } s \neq r, \\[3mm] \dfrac{f''(r)}{2} + \dfrac{f'''(r)}{6}(s - r) + O\big((s - r)^2\big) & \text{as } s \to r, \end{cases}$$

$$\frac{\partial^2 h(r, s)}{\partial r^2} \;=\; \begin{cases} \dfrac{2\big(f(s) - f(r) - f'(r)(s - r)\big) - (s - r)^2 f''(r)}{(s - r)^3} & \text{if } s \neq r, \\[3mm] \dfrac{f'''(r)}{3} + \dfrac{f''''(r)}{12}(s - r) + O\big((s - r)^2\big) & \text{as } s \to r, \end{cases}$$

$$\frac{\partial^2 h(r, s)}{\partial r \partial s} \;=\; \begin{cases} \dfrac{(s - r)\big(f'(r) + f'(s)\big) - 2\big(f(s) - f(r)\big)}{(s - r)^3} & \text{if } s \neq r, \\[3mm] \dfrac{f'''(r)}{6} + \dfrac{f''''(r)}{12}(s - r) + O\big((s - r)^2\big) & \text{as } s \to r. \end{cases}$$

The other partial derivatives of order one and two follow via symmetry considerations.

5.2 More details for the case $d = 1$

Recall that

$$J(r, s) \;=\; \int_0^1 \exp\big((1 - u)r + us\big) \, du \;=\; \begin{cases} \dfrac{\exp(s) - \exp(r)}{s - r} & \text{if } r \neq s, \\[3mm] \exp(r) & \text{if } r = s. \end{cases}$$

This is just the function introduced by Dümbgen, Hüsler and Rufibach (2007). Let us recall some properties and formulae for the corresponding partial derivatives

$$J_{a,b}(r, s) \;:=\; \frac{\partial^{a+b}}{\partial r^a \partial s^b} \, J(r, s) \;=\; \int_0^1 (1 - u)^a u^b \exp((1 - u)r + us) \, du.$$

Note first that

$$J_{a,b}(r, s) \;=\; J_{b,a}(s, r) \;=\; \exp(r) J_{a,b}(0, s - r).$$

Thus it suffices to derive formulae for $(r, s) = (0, y)$ and $b \le a$. It follows from (4) that

$$\begin{aligned} J_{a,0}(0, y) &\;=\; \int_0^1 (1 - u)^a \sum_{k=0}^\infty \frac{u^k}{k!} y^k \, du \\ &\;=\; \sum_{k=0}^\infty \frac{1}{k!} \int_0^1 (1 - u)^a u^k \, du \cdot y^k \\ &\;=\; \sum_{k=0}^\infty \frac{a!}{(k + a + 1)!} y^k \\ &\;=\; \frac{a!}{y^{a+1}} \Big(\exp(y) - \sum_{\ell=0}^a \frac{y^\ell}{\ell!} \Big). \end{aligned}$$

8

In particular,

$$J_{1,0}(0,y) = \frac{\exp(y) - 1 - y}{y^2}$$

$$= \frac{1}{2} + \frac{y}{6} + \frac{y^2}{24} + \frac{y^3}{120} + O(y^4) \quad (y \to 0),$$

$$J_{2,0}(0,y) = \frac{2(\exp(y) - 1 - y - y^2/2)}{y^3}$$

$$= \frac{1}{3} + \frac{y}{12} + \frac{y^2}{60} + \frac{y^3}{360} + O(y^4) \quad (y \to 0),$$

$$J_{3,0}(0,y) = \frac{6(\exp(y) - 1 - y - y^2/2 - y^3/6)}{y^4}$$

$$= \frac{1}{4} + \frac{y}{20} + \frac{y^2}{120} + \frac{y^3}{840} + O(y^4) \quad (y \to 0),$$

$$J_{4,0}(0,y) = \frac{24(\exp(y) - 1 - y - y^2/2 - y^3/6 - y^4/24)}{y^5}$$

$$= \frac{1}{5} + \frac{y}{30} + \frac{y^2}{210} + \frac{y^3}{1680} + O(y^4) \quad (y \to 0).$$

Another general observation is that

$$J_{a,b}(r,s) = \int_0^1 (1-u)^a (1 - (1-u))^b \exp((1-u)r + us) \, du$$

$$= \sum_{i=0}^{b} \binom{b}{i} (-1)^i J_{a+i,0}(r,s).$$

In particular,

$$J_{a,1}(r,s) = J_{a,0}(r,s) - J_{a+1,0}(r,s),$$

$$J_{a,2}(r,s) = J_{a,0}(r,s) - 2J_{a+1,0}(r,s) + J_{a+2,0}(r,s).$$

On the other hand,

$$J_{a,b}(0,y) = \sum_{k=0}^{\infty} \frac{y^k}{k!} \int_0^1 (1-u)^a u^{k+b} \, du$$

$$= \sum_{k=0}^{\infty} \frac{a![k+b]_b}{(k+a+b+1)!} y^k$$

with $[r]_0 := 1$ and $[r]_m := \prod_{i=0}^{m-1}(r-i)$ for integers $m > 0$. In particular,

$$J_{1,1}(0,y) = \frac{\exp(y)(y-2) + 2 + y}{y^3}$$

$$= \frac{1}{6} + \frac{y}{12} + \frac{y^2}{40} + \frac{y^3}{180} + O(y^4) \quad (y \to 0).$$

5.3 The case $d = 2$

Our recursion formula (3) yields

$$
J(r, s, t) = \begin{cases} \dfrac{J(s,t) - J(r,t)}{s - r} & \text{if } r \neq s, \\ J_{10}(r, t) & \text{if } r = s. \end{cases}
$$

Because of J's symmetry we may rewrite this in terms of the order statistics $y_{(0)} \leq y_{(1)} \leq y_{(2)}$ of $(y_i)_{i=0}^2$ as

$$
J(r, s, t) = \begin{cases} \dfrac{J(y_{(1)}, y_{(2)}) - J(y_{(0)}, y_{(1)})}{y_{(2)} - y_{(0)}} & \text{if } y_{(0)} < y_{(2)}, \\ \dfrac{\exp(y_{(0)})}{2} & \text{if } y_{(0)} = y_{(2)}. \end{cases}
$$

For fixed third argument t, this function $J(r, s, t)$ corresponds to $h(r, s)$ in Section 5.1 with $f(x) := J(x, t)$. Thus

$$
\frac{\partial J(r, s, t)}{\partial r} = \begin{cases} \dfrac{J(s,t) - J(r,t) - J_{1,0}(r,t)(s-r)}{(s-r)^2} & \text{if } r \neq s, \\ \dfrac{J_{2,0}(r,t)}{2} + \dfrac{J_{3,0}(r,t)(s-r)}{6} + O\big((s-r)^2\big) & \text{as } s \to r. \end{cases}
$$

Moreover,

$$
\frac{\partial^2 J(r, s, t)}{\partial r^2} = \begin{cases} \dfrac{2\big(J(s,t) - J(r,t) - J_{1,0}(r,t)(s-r)\big) - (s-r)^2 J_{2,0}}{(s-r)^3} & \text{if } r \neq s, \\ \dfrac{J_{3,0}(r,t)}{3} + \dfrac{J_{4,0}(r,t)(s-r)}{12} + O\big((s-r)^2\big) & \text{as } s \to r, \end{cases}
$$

$$
\frac{\partial^2 J(r, s, t)}{\partial r \partial s} = \begin{cases} \dfrac{\big(J_{1,0}(r,t) + J_{1,0}(s,t)\big)(s-r) - 2\big(J(s,t) - J(r,t)\big)}{(s-r)^3} & \text{if } r \neq s, \\ \dfrac{J_{3,0}(r,t)}{6} + \dfrac{J_{4,0}(r,t)(s-r)}{12} + O\big((s-r)^2\big) & \text{as } s \to r. \end{cases}
$$

6 Gamma and multivariate beta (Dirichlet) distributions

Let $G_0, G_1, \ldots, G_m$ be stochastically independent random variables with $G_i \sim \mathrm{Gamma}(a_i)$ for certain parameters $a_i > 0$. That means, for any Borel set $A \subset (0, \infty)$,

$$
\mathbb{P}(G_i \in A) = \int_A \Gamma(a_i)^{-1} y^{a_i - 1} \exp(-y) \, dy.
$$

Now we define $a_+ := \sum_{i=0}^m a_i$, $G_+ := \sum_{i=0}^m G_i$ and

$$
\tilde{\boldsymbol{B}} := (G_i/G_+)_{i=0}^m, \quad \boldsymbol{B} := (G_i/G_+)_{i=1}^m.
$$

Note that $\tilde{\boldsymbol{B}}$ is contained in the unit simplex in $\mathbb{R}^{m+1}$, while $\boldsymbol{B}$ is contained in the open set $\mathcal{T}_m = \big\{ \boldsymbol{u} \in (0,1)^m : u_+ < 1 \big\}$ with $u_+ := \sum_{i=1}^m u_i$. We also define $u_0 := 1 - u_+$ for any $\boldsymbol{u} \in \mathcal{T}_m$.

Lemma 6.1. *The random vector $\boldsymbol{B}$ and the random variable G_+ are stochastically independent. Moreover,*

$$G_+ \; \sim \; \mathrm{Gamma}(a_+)$$

while $\boldsymbol{B}$ is distributed according to the Lebesgue density

$$f(\boldsymbol{u}) \; := \; \frac{\Gamma(a_+)}{\prod_{i=0}^{m} \Gamma(a_i)} \prod_{i=0}^{m} u_i^{a_i - 1}$$

on $\mathcal{T}_m$. For arbitrary numbers $k_0, k_1, \ldots, k_m \geq 0$ and $k_+ := \sum_{i=0}^{m} k_i$,

$$\mathbb{E}\Big(\prod_{i=0}^{m} B_i^{k_i}\Big) \; = \; \frac{\Gamma(a_+)}{\Gamma(a_+ + k_+)} \prod_{i=0}^{m} \frac{\Gamma(a_i + k_i)}{\Gamma(a_i)}.$$

As a by-product of this lemma we obtain the following formula:

Corollary 6.2. *For arbitrary numbers $a_0, a_1, \ldots, a_m > 0$,*

$$\int_{\mathcal{T}_m} \prod_{i=0}^{m} u_i^{a_i - 1} \, d\boldsymbol{u} \; = \; \Gamma(a_+)^{-1} \prod_{i=0}^{m} \Gamma(a_i).$$

Proof of Lemma 6.1. Note that $\boldsymbol{G} = (G_i)_{i=0}^{m}$ my be written as $\Xi(G_+, \boldsymbol{B})$ with the bijective mapping $\Xi : (0, \infty) \times \mathcal{T}_m \to (0, \infty)^{m+1}$,

$$\Xi(s, \boldsymbol{u}) \; := \; (s u_i)_{i=0}^{m}.$$

Note also that

$$\det D\Xi(s, \boldsymbol{u}) \; = \; \det \begin{pmatrix} u_0 & -s & -s & \cdots & -s \\ u_1 & s & 0 & \cdots & 0 \\ u_2 & 0 & s & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & 0 \\ u_m & 0 & \cdots & 0 & s \end{pmatrix} = \det \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ u_1 & s & 0 & \cdots & 0 \\ u_2 & 0 & s & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & 0 \\ u_m & 0 & \cdots & 0 & s \end{pmatrix} = s^m.$$

Thus the distribution of $(G_+, \boldsymbol{B})$ has a Lebesgue density h on $(0, \infty) \times \mathcal{T}_m$ which is given by

$$\begin{aligned}
h(s, \boldsymbol{u}) \; &= \; \prod_{i=0}^{m} \big(\Gamma(a_i)^{-1} \Xi(s, \boldsymbol{u})_i^{a_i - 1} \exp(-\Xi(s, \boldsymbol{u})_i)\big) \cdot \big|\det D\Xi(s, \boldsymbol{u})\big| \\
&= \; \prod_{i=0}^{m} \big(\Gamma(a_i)^{-1} (s u_i)^{a_i - 1} \exp(-s u_i)\big) \cdot s^m \\
&= \; s^{a_+ - 1} \exp(-s) \prod_{i=0}^{m} \big(\Gamma(a_i)^{-1} u_i^{a_i - 1}\big) \\
&= \; \Gamma(a_+)^{-1} s^{a_+ - 1} \exp(-s) \cdot f(\boldsymbol{u}).
\end{aligned}$$

Since this is the density of $\mathrm{Gamma}(a_+)$ at s times $f(\boldsymbol{u})$, we see that G_+ and $\boldsymbol{B}$ are stochastically independent, where G_+ has distribution $\mathrm{Gamma}(a_+)$, and that f is indeed a probability density on $\mathcal{T}_m$ describing the distribution of $\boldsymbol{B}$.

The fact that f integrates to one over $\mathcal{T}_m$ entails Corollary 6.2. But then we can conclude that

$$\mathbb{E}\Big(\prod_{i=0}^{m} B_i^{k(i)}\Big) \;=\; \int_{\mathcal{T}_m} \prod_{i=0}^{m} u_i^{a_i+k_i-1}\, d\boldsymbol{u} \Big/ \int_{\mathcal{T}_m} \prod_{i=0}^{m} u_i^{a_i-1}\, d\boldsymbol{u}$$

$$=\; \frac{\Gamma(a_+)}{\Gamma(a_+ + k_+)} \prod_{i=0}^{m} \frac{\Gamma(a_i + k_i)}{\Gamma(a_i)}.$$

$\square$

References

[1] M.L. CULE, R.B. GRAMACY, and R.J. SAMWORTH (2007). LogConcDEAD, An R package for log-concave density estimation in arbitrary dimensions. Available from `http://cran.r-project.org/`.

[2] M.L. CULE, R.J. SAMWORTH and M.I. STEWART (2008). Maximum likelihood estimation of a multidimensional log-concave density. Preprint.

[3] L. DÜMBGEN, A. HÜSLER and K. RUFIBACH (2007). Active set and EM algorithms for log-concave densities based on complete and censored data. Technical report 61, IMSV, University of Bern (arXiv:0707.4643).