DERIVATIVES OF PROBABILITY AND INTEGRAL FUNCTIONS: General Theory and Examples

Probability functions *probability function* are commonly used for the analysis of models with uncertainties or variabilities in parameters. For instance, in risk and reliability analysis, performance functions, characterizing the operation of systems, are formulated as probabilities of successful or unsuccessful accomplishment of their missions (core damage probability of a nuclear power plant, probability of successful landing of an aircraft, probability of profitable transactions in a stock market, or percentiles of the risks in public risk assessments). Sensitivity analysis of such performance functions involves evaluating of their derivatives with respect to the parameters. Also, the derivatives of the probability function can be used to solve stochastic optimization *stochastic optimization* problems [1].

A probability function can be formally presented as an expectation of a discontinuous indicator function of a set, or as an integral over a domain - depending upon parameters. Nevertheless, differentiability conditions of the probability function do not follow from similar conditions of the expectations of continuous (smooth or convex) functions.

The derivative of the probability function has many equivalent representations. It can be represented as an integral over the surface, an integral over the volume, or a sum of integrals over the volume and over the surface. Also, it can be calculated using weak derivatives of the probability measures or conditional expectations.

The first general result on the differentiability of the probability function was obtained by Raik [8]. He represented the gradient of the probability function with one constraint in the form of the surface integral. Uryasev [10] extended Raik's formula for probability functions with many constraints. Kibzun and Tretyakov [3] extended it to the piece-wise smooth constraint and probability density function. Special cases of probability function with normal and gamma distributions were investigated by Prékopa [6]. Pflug [5] represented the gradient of probability function in the form of an expectation using weak probability measures.

Uryasev [9] expressed the gradient of the probability function as a volume integral. Also, using a change of variables, Marti [4] derived the probability function gradient in the form of the volume integral.

A general analytical formula for the derivative of probability functions *derivative of probability function gradient of probability function* with many constraints was obtained by Uryasev [10]; it calculates the gradient as an integral over the surface, an integral over the volume, or the sum of integrals over the surface and the volume. Special cases of this formula correspond to the Raik formula [8], the Uryasev formula [9], and the change–of–variables approach [4].

The gradient of the quantile function was obtained by Kibzun et al. [2].

Notations and Definitions.

Let an integral over the volume *integral over the volume*

$$F(x) = \int_{f(x,y) \le 0} p(x,y)\, dy \qquad (1)$$

is defined on the Euclidean space $\mathbb{R}^n$, where $f: \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^k$ and $p: \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ are some functions. The inequality $f(x,y) \le 0$ in the integral is a system of inequalities

$$f_i(x,y) \le 0\,, \quad i = 1, \dots, k\,.$$

Both the kernel function $p(x,y)$ and the function $f(x,y)$ defining the integration set depend upon the parameter x. For example, let

$$F(x) = P\{f(x,\zeta(\omega)) \le 0\} \qquad (2)$$

be a *probability function*, where $\zeta(\omega)$ is a random vector in $\mathbb{R}^m$. The random vector $\zeta(\omega)$ is assumed to have a probability density $p(x,y)$

probability function
stochastic optimization
derivative of probability function
gradient of probability function
integral over the volume

that depends on a parameter $x \in \mathbb{R}^n$. The probability function can be represented as an expectation of an indicator function *expectation of indicator function*, which equals one on the integration set, and equals zero outside of it. For example, let

$$F(x) = \mathbb{E}\big[I_{\{f(x,\boldsymbol{\zeta}) \le 0\}}\, g(x,\boldsymbol{\zeta})\big]$$

$$= \int\limits_{f(x,y) \le 0} g(x,y)\, \rho(x,y)\; dy$$

$$= \int\limits_{f(x,y) \le 0} p(x,y)\; dy\,, \tag{3}$$

where $I_{\{\}}$ is an indicator function, and random vector $\boldsymbol{\zeta}$ in $\mathbb{R}^m$ has a probability density $\rho(x,y)$ that depends on a parameter $x \in \mathbb{R}$.

Integral Over the Surface Formula.

The following formula calculates the gradient of an integral (1) over the set given by nonlinear inequalities as sum of integral over the volume plus integral over the surface of the integration set. We call this *the integral over the surface formula* because if density $p(x,y)$ does not depend upon x the gradient of the integral (1) equals an integral over the surface. This formula for the case of one inequality was obtained by Raik [8] and generalized for the case with many inequalities by Uryasev [10].

Let us denote by $\mu(x)$ the integration set

$$\mu(x) = \{\, y \in \mathbb{R}^m \,:\, f(x,y) \le 0 \,\}$$

$$\stackrel{def}{=} \{\, y \in \mathbb{R}^m \,:\, f_l(x,y) \le 0\,,\ 1 \le l \le k \,\}$$

and by $\partial\mu(x)$ the surface of this set $\mu(x)$. Also, let us denote by $\partial_i\mu(x)$ a part of the surface which corresponds to the function $f_i(x,y)$, i.e.,

$$\partial_i\mu(x) = \mu(x) \bigcap \{\, y \in \mathbb{R}^m \,:\, f_i(x,y) = 0 \,\}\,.$$

If the constraint functions are differentiable and the following integral exist, then gradient of integral (1) equals

$$\nabla_x F(x) = \int\limits_{\mu(x)} \nabla_x p(x,y)\; dy$$

$$- \sum_{i=1}^{k} \int\limits_{\partial_i\mu(x)} \frac{p(x,y)}{||\nabla_y f_i(x,y)||} \nabla_x f_i(x,y)\; dS\,. \tag{4}$$

A potential disadvantage of this formula is that in multidimensional case it is difficult to calculate the integral over the nonlinear surface. Most well known numerical techniques, such as Monte-Carlo algorithms, are applicable to volume integrals. Nevertheless, this formula can be quite useful in various special cases, such as the linear case.

Example 1. Linear Case: Integral Over the Surface Formula [10] .

Let $A(\omega)$, be a random $l \times n$ matrix with the joint density $p(A)$. Suppose that $x \in \mathbb{R}^n$ and $x_j \ne 0$, $j = 1, \ldots, n$. Let us define

$$F(x) = P\{\, A(\omega)x \le b\,,\ A(\omega) \ge 0 \,\}\,, \tag{5}$$

$$b = (b_1, \ldots, b_l) \in \mathbb{R}^l\,, \quad x \in \mathbb{R}^n\,,$$

i.e. $F(x)$ is the probability that the linear constraints $A(\omega)x \le b$, $A(\omega) \ge 0$ are satisfied. The constraint, $A(\omega) \ge 0$, means that all elements $a_{ij}(\omega)$ of the matrix $A(\omega)$ are non-negativity. Let us denote by A_i and A^i the i-th row and column of the matrix A

$$A = \begin{pmatrix} A_1 \\ \vdots \\ A_l \end{pmatrix} = \left(A^1, \cdots, A^n\right)\,,$$

then

$$f(x,A) = \begin{pmatrix} f_1(x,A) \\ \vdots \\ f_k(x,A) \end{pmatrix} = \begin{pmatrix} A_1 x - b_1 \\ \vdots \\ A_l x - b_l \\ -A^1 \\ \vdots \\ -A^n \end{pmatrix},$$

$$k = l + l \times n\,.$$

The function $F(x)$ equals

$$F(x) = \int\limits_{f(x,A) \le 0} p(A)\; dA\,. \tag{6}$$

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expectation of indicator function

We use formula (4) to calculate the gradient $\nabla_x F(x)$ as an integral over the surface. The function $p(A)$ does not depend upon x and $\nabla_x p(A) = 0$. Formula (4) implies that $\nabla_x F(x)$ equals

$$- \sum_{i=1}^{k} \int\limits_{\partial_i \mu(x)} \frac{p(A)}{||\nabla_A f_i(x,A)||} \nabla_x f_i(x,A) \; dS \, .$$

Since $\nabla_x f_i(x,A) = 0$ for $i = l+1, \dots, k$, then $\nabla_x F(x)$ equals

$$- \sum_{i=1}^{l} \int\limits_{\partial_i \mu(x)} \frac{p(A)}{||\nabla_A f_i(x,A)||} \nabla_x f_i(x,A) \; dS \; =$$

$$- \sum_{i=1}^{l} \int\limits_{\partial_i \mu(x)} \frac{p(A)}{||x||} A_i^T \; dS \; =$$

$$- \, ||x||^{-1} \sum_{i=1}^{l} \int\limits_{\substack{Ax \le b \, , \, A \ge 0 \\ A_i x = b_i}} p(A) \, A_i^T \; dS \, .$$

Integral Over the Volume Formula. This section presents gradient of the function (1) in the form of volume integral. Let us introduce the following shorthand notations

$$f_{1l}(x,y) = \begin{pmatrix} f_1(x,y) \\ \vdots \\ f_l(x,y) \end{pmatrix} \, , \quad f(x,y) = f_{1k}(x,y) \, ,$$

$$\nabla_y f(x,y) = \begin{pmatrix} \frac{\partial f_1(x,y)}{\partial y_1} \, , & \dots & , \frac{\partial f_k(x,y)}{\partial y_1} \\ & \vdots & \\ \frac{\partial f_1(x,y)}{\partial y_m} \, , & \dots & , \frac{\partial f_k(x,y)}{\partial y_m} \end{pmatrix} \, .$$

Divergence for the $n \times m$ matrix H consisting of the elements h_{ji} is denoted by

$$div_y \, H = \begin{pmatrix} \sum_{i=1}^{m} \frac{\partial h_{1i}}{\partial y_i} \\ \vdots \\ \sum_{i=1}^{m} \frac{\partial h_{ni}}{\partial y_i} \end{pmatrix} \, .$$

Following [10], derivative of the function (1) is represented as an integral over the volume

$$\nabla_x F(x) = \int\limits_{\mu(x)} \nabla_x p(x,y) \, dy$$

$$+ \int\limits_{\mu(x)} div_y \big(p(x,y) H(x,y) \big) \, dy \, , \qquad (7)$$

where a matrix function $H \; : \; \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^{n \times m}$ satisfies the equation

$$H(x,y) \, \nabla_y f(x,y) \; + \; \nabla_x f(x,y) \; = \; 0 \, . \qquad (8)$$

The last system of equations may have many solutions, therefore formula (7) provides a number of equivalent expressions for the gradient. The following section gives analytical solutions of this system of equations. In some cases, this system does not have any solution, and formula (7) is not valid. The following section deals with such cases and provides a general formula where system of equations can be solved only for some of the functions defining the integration set.

Example 2. Linear Case: Integral Over the Volume Formula [10].

With formula (7), the gradient of probability function (5) with linear constrains considered in the *Example 1* can be represented as the integral over the volume. It can be shown that equation (8) does not have a solution in this case. Nevertheless, we can slightly modify the constraints, such that integration set is not changed and equation (8) has a solution. In the vector function $f(x,A)$ we multiply column A^i on x^i if x^i is positive or multiply it on $-x^i$ if x^i is negative. Therefore, we have the following constraint function

$$f(x,A) = \begin{pmatrix} A_1 x - b_1 \\ \vdots \\ A_l x - b_l \\ -(+) x_1 A^1 \\ \vdots \\ -(+) x_n A^n \end{pmatrix} \, , \qquad (9)$$

where $-(+)$ means that we take an appropriate sign. It can be directly checked that, the matrix $H_l^*(x,A)$

$$H^*(x,A) \; = \; \big(h^1(x,A_1), \dots, h^l(x,A_l) \big) \, ,$$

$$h^i(x,A_i) \; = \; - \begin{pmatrix} a_{i1} x_1^{-1} & & 0 \\ & \ddots & \\ 0 & & a_{in} x_n^{-1} \end{pmatrix}$$

is a solution of system (8)). As it will be shown in the next section, this analytical solution follows from the fact that change of the variables $Y^i = x_i A^i \; i = 1, \ldots, n$ eliminates variables x^i, $i = 1, \ldots, n$ from the constraints (9).

Since $\nabla_x p(A) = 0$ and $div_A\big(p(A) H^*(x,A)\big)$ equals

$$-\begin{pmatrix} x_1^{-1}\Big(l\, p(A) + \sum_{i=1}^{l} a_{i1}\frac{\partial}{\partial a_{i1}} p(A)\Big) \\ \vdots \\ x_n^{-1}\Big(l\, p(A) + \sum_{i=1}^{l} a_{in}\frac{\partial}{\partial a_{in}} p(A)\Big) \end{pmatrix}$$

formula (7) implies that $\frac{\partial F(x)}{\partial x_j}$ equals

$$-x_j^{-1}\int\limits_{\substack{Ax \le b \\ A \ge 0}} \left(l\, p(A) + \sum_{i=1}^{l} a_{ij}\frac{\partial}{\partial a_{ij}} p(A)\right) dA\,.$$

General Formula. Further, we give a general formula [9, 10] for the differentiation of integral (1). A gradient of the integral is represented as a sum of integrals taken over a volume and over a surface. This formula is useful when system of equations (8) does not have a solution. We split the set of constraints $K \stackrel{def}{=} \{1, \ldots, k\}$ into two subsets K_1 and K_2. Without loss of generality we suppose that

$$K_1 = \{1, \ldots, l\}\,, \quad K_2 = \{l+1, \ldots, k\}\,.$$

The derivative of integral (1) can be represented as the sum of the volume and surface integrals

$$\nabla_x F(x) = \int\limits_{\mu(x)} \nabla_x p(x,y)\, dy$$

$$+ \int\limits_{\mu(x)} div_y\big(p(x,y) H_l(x,y)\big)\, dy$$

$$- \sum_{i=l+1}^{k} \int\limits_{\partial_i \mu(x)} \frac{p(x,y)}{||\nabla_y f_i(x,y)||}\Big[\nabla_x f_i(x,y)$$

$$+ H_l(x,y)\,\nabla_y f_i(x,y)\Big]\, dS\,, \qquad (10)$$

where the matrix $H_l : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^{n\times m}$ satisfies the equation

$$H_l(x,y)\,\nabla_y f_{1l}(x,y) + \nabla_x f_{1l}(x,y) = 0\,. \qquad (11)$$

The last equation can have a lot of solutions and we can choose an arbitrary one, differentiable with respect to the variable y.

The general formula contains as a special cases the integral over the surface formula (4) and integral over the volume formula (7). When the set K_1 is empty, the matrix H_l is absent and the general formula is reduced to the integral over the surface. Also, when the set K_2 is empty we have integral over the volume formula (7). Except these extreme cases, the general formula provides number of intermediate expressions for the gradient in the form of the sum of an integral over the surface and an integral over the volume. Thus, we have a number of equivalent representations of the gradient corresponding to the various sets K_1 and K_2 and solutions of equation (11).

Equation (11) (and equation (8) which is a partial case of equation (11)) can be solved explicitly. Usually, this equation has many solutions. The matrix

$$-\nabla_x f_{1l}(x,y)\big(\nabla_y^T f_{1l}(x,y)$$

$$\times \nabla_y f_{1l}(x,y)\big)^{-1}\nabla_y^T f_{1l}(x,y) \qquad (12)$$

is a solution of equation (11). Also, in many cases there is another way to solve equation (11) using change of variables. Suppose that there is a change of variables

$$y = \gamma(x,z)$$

which eliminates vector x from the function $f(x,y)$ defining integration set, i.e., function $f(x,\gamma(x,z))$ does not depend upon the variable x. Denote by $\gamma^{-1}(x,y)$ the inverse function, defined by the equation

$$\gamma^{-1}\big(x, \gamma(x,z)\big) = z\,.$$

Let us show that the following matrix

$$H(x,y) = \nabla_x \gamma(x,z)|_{z=\gamma^{-1}(x,y)} \qquad (13)$$

is a solution of (11). Indeed, the gradient of the function $\gamma(x, y(x,z))$ with respect to x equals zero, therefore

$$0 = \nabla_x f_{1l}(x,\gamma(x,z))$$

$$= \nabla_x \gamma(x,z) \nabla_y f_{1l}(x,y)|_{y=\gamma(x,z)}$$

$$+\nabla_x f_{1l}(x,y)|_{y=\gamma(x,z)},$$

and function $\nabla_x \gamma(x,z)|_{z=\gamma^{-1}(x,y)}$ is a solution of equation (11).

Formula (7) with matrix (13) gives the derivative formulas which can be obtained with change of variables in the integration set [4].

Example 3. While investigating the operational strategies for inspected components (see [7]) the following integral was considered

$$F(x) = \int\limits_{\substack{b(y)\le x\,,\\ y_i\ge\theta\,,\ i=1,\dots,m}} p(y)\,dy\,, \qquad (14)$$

where $x\in \mathbb{R}^1, y\in \mathbb{R}^m, p:\ \mathbb{R}^m\to \mathbb{R}^1$, $\theta>0$, $b(y)=\sum_{i=1}^m y_i^\alpha$. In this case

$$f(x,y) = \begin{pmatrix} b(y)-x \\ \theta-y_1 \\ \vdots \\ \theta-y_m \end{pmatrix},$$

and

$$F(x) = \int\limits_{f(x,y)\le 0} p(y)\,dy \;=\; \int\limits_{\mu(x)} p(y)\,dy\,.$$

Let us consider that $l=1$, i.e. $K_1=\{1\}$ and $K_2=\{2,\dots,m+1\}$. The gradient $\nabla_x F(x)$ equals

$$\int\limits_{\mu(x)} \big[\,\nabla_x p(y) \;+\; div_y\big(p(y)H_1(x,y)\big)\big]\,dy \;-$$

$$-\sum_{i=2}^{m+1}\int\limits_{\partial_i\mu(x)} \frac{p(y)}{||\nabla_y f_i(x,y)||}\big[\,\nabla_x f_i(x,y)$$

$$+H_1(x,y)\,\nabla_y f_i(x,y)\big]\;dS\,, \qquad (15)$$

Where the matrix $H_1(x,y)$ satisfies equation (11). In view of

$$\nabla_y f_1(x,y) = \alpha\begin{pmatrix} y_1^{\alpha-1} \\ \vdots \\ y_m^{\alpha-1}\end{pmatrix},\ \nabla_x f_1(x,y) = -1.$$

a solution $H_1^*(x,y)$ of equation (11) equals

$$H_1^*(x,y) \;=\; h(y) \;\stackrel{def}{=}\; \big(h_1(y_1),\dots,h_m(y_m)\big)$$

$$=\; \frac{1}{\alpha m}\left(y_1^{1-\alpha},\dots,y_m^{1-\alpha}\right)\,. \qquad (16)$$

Let us denote

$$(\theta_i \mid y) \;=\; (y_1,\dots,y_{i-1},\theta,y_{i+1},\dots,y_m)\,,$$

$$y^{-i} \;=\; (y_1,\dots,y_{i-1},y_{i+1},\dots,y_m)\,,$$

$$b(\theta_i \mid y) \;=\; \theta^\alpha + \sum_{\substack{j=1\\ j\ne i}}^m y_j^\alpha\,.$$

We denote by $y^{-i}\ge\theta$ the set of inequalities

$$y_j\ge\theta\,,\quad j=1,\dots,i-1,i+1,\dots,m\,.$$

The sets $\partial_i\mu(x)$, $i=2,\dots,m+1$ have a simple structure

$$\partial_i\mu(x) \;=\; \mu(x)\bigcap\{\,y\in \mathbb{R}^m\;:\;y_i=\theta\,\}$$

$$=\;\{y^{-i}\in \mathbb{R}^{m-1}\;:\;b(\theta_i|y)\le x\,,\ y^{-i}\ge 0\,\}\,.$$

For $i=2,\dots,m+1$, we have

$$\big(\nabla_y f_i(y)\big)_j = 0,\ j=1,\dots,m,\ j\ne i-1, \quad (17)$$

$$\big(\nabla_y f_i(y)\big)_{i-1} = -1\,,\ ||\nabla_y f_i(y)|| = 1. \qquad (18)$$

The function $p(y)$ and the functions $f_i(y)$, $i=2,\dots,m+1$ do not depend on x , consequently

$$\nabla_x p(y) = 0\,, \qquad (19)$$

$$\nabla_x f_i(y) = 0\,,\quad i=2,\dots,m+1\,. \qquad (20)$$

Equations (15) - (20) imply

$$\nabla_x F(x) \;=\; \int\limits_{\mu(x)} div_y\big(p(y)h(y)\big)\,dy$$

$$-\sum_{i=2}^{m+1}\int\limits_{\partial_i\mu(x)} \frac{p(y)}{||\nabla_y f_i(y)||}\,h(y)\nabla_y f_i(y)\,dS$$

$$=\int\limits_{\mu(x)} div_y\big(p(y)h(y)\big)\,dy$$

$$+\sum_{i=2}^{m+1} h_{i-1}(\theta)\int\limits_{\partial_i\mu(x)} p(y)\,dS$$

$$=\int\limits_{\substack{b(y)\le x\,,\\ y_i\ge\theta\,,\ i=1,\dots,m}} div_y\big(p(y)h(y)\big)\,dy$$

$$+ \sum_{i=1}^{m} \frac{\theta^{1-\alpha}}{\alpha m} \int\limits_{\substack{b(\theta_i|y)\le x\,, \\ y^{-i}\ge\theta}} p(\theta_i \mid y)\; dy^{-i}\ .$$

Since

$$div_y\big(p(y)h(y)\big)$$

$$= \; h(y)\nabla_y p(y) \; + \; p(y) div_y h(y)$$

$$= \; \frac{1}{\alpha m}\sum_{i=1}^{m} \frac{\partial p(y)}{\partial y_i} y_i^{1-\alpha} \; + \; p(y)\frac{1-\alpha}{\alpha m}\sum_{i=1}^{m} y_i^{-\alpha}\ ,$$

we, finally, obtain that the gradient $\nabla_x F(x)$ equals

$$\int\limits_{\substack{b(y)\le x\,, \\ y_i\ge\theta,\, i=1,\dots,m}} \sum_{i=1}^{m} \frac{y_i^{-\alpha}}{\alpha m}\Big[y_i \frac{\partial p(y)}{\partial y_i} + (1-\alpha)p(y)\Big] dy$$

$$+ \frac{\theta^{1-\alpha}}{\alpha m} \sum_{i=1}^{m} \int\limits_{\substack{b(\theta_i|y)\le x\,, \\ y^{-i}\ge\theta}} p(\theta_i \mid y)\; dy^{-i}\ .$$

The formula for $\nabla_x F(x)$ is valid for an arbitrary sufficiently smooth function $p(y)$.

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