New insight into partial differentiation with non-independent variables

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Summary
We use to work with models defined through a function and some equations connecting the input variables such as a given function subject to some constraints involving input variables. For such models, it is interesting to better determine the partial derivatives with respect to each input variable that comply with the constrained equations. As the equations connecting the input variables introduce some dependency structures among input variables, and the theory of probability allows for better characterizing the dependencies among variables, In this abstract, we propose new partial derivatives for functions with non-independent variables by making use of the formal definition of independence or dependence such as the cumulative distribution function (CDF). The proposed new partial derivatives are based on the classical gradient and the CDF. Such derivatives are uniquely defined and do not require any additional assumption. Our approach can be extended for determining cross-partial derivatives as well.

Main results

In this section, we include the distribution of inputs to derive the partial derivatives. It is to be noted that each initial input X_j lies in a given domain $\Omega_j \subseteq \mathbb{R}$ with $j = 1, \ldots, d$, and we assume that we are able to attribute to X_j a distribution. It is common to attribute a normal distribution with a higher variance when we do have much information about the variable, which comes down to make use of uniform distribution for a bounded domain Ω_j.

Therefore, the input variables $\mathbf{X} = (X_1, \ldots, X_d)$ have a given distribution F, and we are interested in a function given by $f(\mathbf{X})$ and $h(\mathbf{X}) = 0$. In what follows, we assume that $F = \prod_{j=1}^{d} F_j$ with F_j the CDF of X_j, which means that the initial input variables are independent. The equation $h(\mathbf{X}) = 0$ introduces some dependencies, and this yields to new dependent variables $\mathbf{X}^c \sim F^c$. It is worth noting that the inputs $\mathbf{X}^c$ must satisfies $h(\mathbf{X}^c) = 0$ and we have

$$Y = \left\{ \begin{array}{l} f(\mathbf{X}) \\ \text{s.t.} \quad h(\mathbf{X}) = 0 \end{array} \right. \stackrel{d}{=} f(\mathbf{X}^c),$$

provided that F^c is known.

Formally, $\mathbf{X}^c \stackrel{d}{=} \{\mathbf{X} \sim F \, : h(\mathbf{X}) = 0\}$, and we are able to find the distribution of $\mathbf{X}^c$. Indeed, some analytic derivation of F^c can be found in [1]. For complex function h, a copula-based approach is suitable to fit a distribution to simulated data. Based on F^c or the estimated distribution $\widehat{F^c}$, the multivariate conditional quantile transform (see [2,3,4]) implies a regression representation of $\mathbf{X}^c$ (see [5,6]), which also implies a dependency function of $\mathbf{X}^c$ given by ([1,7])

$$\mathbf{X}^c_{\sim j} = r_j \left(X^c_j, \mathbf{U} \right) \, ,$$

where X_j is independent of $\mathbf{U}$; $f_j : \mathbb{R}^d \to \mathbb{R}^{d-1}$ and $\left(X^c_j, \mathbf{X}^c_{\sim j} \right) \stackrel{d}{=} \left(X^c_j, r_j \left(X^c_j, \mathbf{U} \right) \right) \sim F^c$.

Now we have all the elements in hand to provide the partial derivatives (see Theorem 1). To that end, we use

$$\nabla_j f := \left[f'_{x_j}, f'_{x_{w_1}}, \ldots, f'_{x_{w_{d-1}}} \right]^T \; ; \quad J^c_j := \left[1, \frac{\partial r_{w_1,j}}{\partial x_j}, \ldots, \frac{\partial r_{w_{d-1},j}}{\partial x_j} \right]^T \, ,$$

for the gradient and the partial derivatives of each component of r_j w.r.t. x_j, respectively. Moreover, we use $J^c_j(\ell)$ the ℓ^{th} component of J^c_j and

$$J^c_{w_k} := \left[\frac{1}{J^c_j(k+1)}, \frac{J^c_j(2)}{J^c_j(k+1)}, \ldots, \frac{J^c_j(d)}{J^c_j(k+1)} \right]^T ; \; \forall \, k \in \{1, \ldots d-1\} \, .$$

Theorem 1. If the functions f and r_j are differentiable w.r.t. their inputs, then we have

$$\frac{\partial f}{\partial x_j} \left(\mathbf{x} \right) = \nabla_j f(\mathbf{x})^T J^c_j \left(x_j, \mathbf{u} \right) \quad \text{or} \quad \frac{\partial f}{\partial x_j} \left(\mathbf{x} \right) = \nabla_j f(\mathbf{x})^T J^c_j \left(x_j, r_j^{-1}(\mathbf{x}_{\sim j}) \right) \; ; \tag{1}$$

$$\frac{\partial f}{\partial x_{w_k}} \left(\mathbf{x} \right) = \nabla_j f(\mathbf{x})^T J^c_{w_k} \left(x_j, r_j^{-1}(\mathbf{x}_{\sim j}) \right) \; \forall \, k \in \{1, \ldots d-1\} \, . \tag{2}$$

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