Lemma 1. Functional Delta Method (univariate). *Suppose $\mathcal{P}_n$ is the empirical distribution of a random sample $X_1, \ldots, X_n$ from a distribution P, and ϕ is a function that maps the distribution of interest into some space. Define the Gateaus derivative*

$$\phi_P'(\delta_x - P) = \frac{d}{dt}\big|_{t=0} \phi((1-t)P + t\delta_x) = IF_{\phi,P}(x),$$

which is also the Influence Function, and $\gamma^2 = \int IF_{\phi,P}(x)^2 dP$. If integration and differentiation can be exchanged, then

$$\int \phi_P'(\delta_x - P) dP = 0.$$

Further, if $\sqrt{n}R_n \xrightarrow{P} 0$, where

$$R_n = \phi(\mathcal{P}_n) - \phi(P) - \frac{1}{n}\sum_i \phi_P'(\delta_{x_i} - P),$$

then from the Central Limit Theory that

$$\sqrt{n}(\phi(\mathcal{P}_n) - \phi(P)) \xrightarrow{d} N(0, \gamma^2).$$

Lemma 2. Functional Delta Method (multivariate). *Suppose $\mathcal{P}_n$ is the empirical distribution of a random sample $X_1, \ldots, X_n$ from a distribution P, and $\boldsymbol{\phi} : \mathcal{R}^d \to \mathcal{R}^k$. Define the Gateaus derivative*

$$\boldsymbol{\phi}_P'(\delta_x - P) = \frac{d}{dt}\big|_{t=0} \boldsymbol{\phi}((1-t)P + t\delta_x) = IF_{\boldsymbol{\phi},P}(x),$$

which is also the Influence Function, and $[\mathbf{V}_0]_{i,j} = \int \langle [IF_{\boldsymbol{\phi},P}(x)]_i, [IF_{\boldsymbol{\phi},P}(x)]_j \rangle dP$. If integration and differentiation can be exchanged, then

$$\int \boldsymbol{\phi}_P'(\delta_x - P) dP = 0.$$

Further, if $\sqrt{n}\mathbf{R}_n \xrightarrow{P} 0$, where

$$\mathbf{R}_n = \boldsymbol{\phi}(\mathcal{P}_n) - \boldsymbol{\phi}(P) - \frac{1}{n}\sum_i \boldsymbol{\phi}_P'(\delta_{x_i} - P),$$

then from the Central Limit Theory that

$$\sqrt{n}(\boldsymbol{\phi}(\mathcal{P}_n) - \boldsymbol{\phi}(P)) \xrightarrow{d} MVN(0, \mathbf{V}_0).$$

Theorem 1. Asymptotic Distribution of Variable Importance (univariate). *Suppose $y_i = f_0(x_i) + \epsilon_i$, $\epsilon_i \sim N(0, \sigma^2)$, $i = 1, \ldots, n$. Denote $D_p : f \to \frac{\partial}{\partial x_p} f$ the differentiation operator, $H_p = D_p^\top D_p$ the inner product of D_p, define*

$$\psi_p(f) = \|D_p(f)\|_n^2 = \frac{1}{n} \langle D_p f, D_p f \rangle = \frac{1}{n} f^\top H_p f. \tag{1}$$

If the following conditions are satisfied:

i) $\text{rank}(H_p) = o_p(\sqrt{n})$;

ii) $\lambda_{max}(H_p) = O_p(1)$;

iii) $\hat{f}_n$ is an unbiased estimator of f_0.

Then

$$\sqrt{n}(\psi_p(\hat{f}_n) - \psi_p(f_0)) \overset{d}{\to} N(0, 4\sigma^2 \|H_p f_0\|_n^2).$$

Proof. From the definition in (1), we have

$$\psi_p'(f) = \frac{\partial}{\partial f} \psi_p(f) = \frac{2}{n} H_p f.$$

Define a mean function $m : F \to E(F)$, where F is the distribution. Then in our case, $f_0 = E(F) = m(F)$. According to **Lemma 1**, we have

$$\psi_p(f_0) = \psi_p(E(F)) = \psi_p(m(F)) = \phi(F),$$

i.e., $\phi(\cdot) = \psi_p(m(\cdot))$. Therefore,

$$
\begin{aligned}
\phi_F'(\delta_y - F) &= \psi_p'(m(\delta_y - F)) \\
&= \frac{d}{dt}|_{t=0} \psi_p(m((1-t)F + t\delta_y)) \\
&= \frac{d}{dt}|_{t=0} \psi_p((1-t)f_0 + ty) \\
&= \frac{d}{dt}|_{t=0} \frac{1}{n}[(1-t)f_0 + ty]^\top H_p[(1-t)f_0 + ty] \\
&= \frac{2}{n}(y - f_0)^\top H_p f_0 \\
&= IF_{\phi,F}(y).
\end{aligned}
$$

On the other hand,

$$
\begin{aligned}
\gamma^2 &= \int IF_{\phi,F}(y)^2 dF \\
&= 4 \int \frac{1}{n} \cdot f_0^\top H_p(y - f_0)(y - f_0)^\top H_p f_0 \cdot \frac{1}{n} dF \\
&= 4\sigma^2 \|H_p f_0\|_n^2.
\end{aligned}
$$

Moreover, we have

$$\int \phi_F'(\delta_y - F) dF = \frac{2}{n} \int (y - f_0)^\top H_p f_0 dF = 0,$$

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and

$$\sqrt{n}R_n = \sqrt{n}[\phi(\mathcal{F}_n) - \phi(F) - \frac{1}{n}\sum_i \phi'_F(\delta_{y_i} - F)]$$

$$= \sqrt{n}[\psi_p(\hat{f}_n) - \psi_p(f_0) - \frac{1}{n}\cdot\frac{2}{n}\sum_i (y_i - f_{0,i})^\top [H_p f_0]_i]$$

$$= \sqrt{n}[\frac{1}{n}\cdot(\hat{f}_n^\top H_p \hat{f}_n - f_0^\top H_p f_0) - \frac{1}{n}\cdot\frac{2}{n}(y - f_0)^\top H_p f_0]$$

$$= \frac{1}{\sqrt{n}}[\hat{f}_n^\top H_p \hat{f}_n - \hat{f}_n^\top H_p f_0 + \hat{f}_n^\top H_p f_0 - f_0^\top H_p f_0 - \frac{2}{n}(y - f_0)^\top H_p f_0]$$

$$= \frac{1}{\sqrt{n}}[(\hat{f}_n - f_0)^\top H_p(\hat{f}_n + f_0) - \frac{2}{n}(y - f_0)^\top H_p f_0]$$

$$= \frac{1}{\sqrt{n}}[(\hat{f}_n - f_0)^\top H_p(\hat{f}_n - f_0) + 2(\hat{f}_n - f_0)^\top H_p f_0 - \frac{2}{n}(y - f_0)^\top H_p f_0]$$

$$= \frac{1}{\sqrt{n}}[\hat{e}_n^\top H_p \hat{e}_n + 2\hat{e}_n^\top H_p f_0 - \frac{2}{n}(y - f_0)^\top H_p f_0] \tag{2}$$

$$= \frac{1}{\sqrt{n}}o_p(\sqrt{n}) \tag{3}$$

$$= o_p(1) \xrightarrow{P} 0,$$

where $\hat{e}_n = \hat{f}_n - f_0$. We can prove the result from (2) to (3) as following: Denote $k = \text{rank}(H_p)$, then the eigendecomposition of H_p is $H_p = U_p \Lambda U_p^\top$, with $U_p = [u_1, \dots, u_k]$ a $n \times k$ orthogonal matrix and Λ a $k \times k$ diagonal matrix with elements $\{\lambda_i\}_{i=1}^k$ being the eigenvalues of H_p, then define

$$v = U_p^\top \hat{e}_n = \begin{bmatrix} u_1^\top \hat{e}_n \\ \vdots \\ u_k^\top \hat{e}_n \end{bmatrix}.$$

Therefore,

$$\hat{e}_n^\top H_p \hat{e}_n = v^\top \Lambda v = \sum_{i=1}^k \lambda_i v_i^2$$

$$\leqslant \lambda_{max}(H_p) \sum_{i=1}^k v_i^2$$

$$= \lambda_{max}(H_p) \sum_{i=1}^k u_i^\top \hat{\Sigma}_n u_i$$

$$\leqslant \lambda_{max}(H_p) \sum_{i=1}^k \lambda_{max}(\hat{\Sigma}_n)$$

$$= k \cdot \lambda_{max}(H_p) \cdot \lambda_{max}(\hat{\Sigma}_n)$$

$$= o_p(\sqrt{n}) \cdot O_p(1) \cdot O_p(1)$$

$$= o_p(\sqrt{n}),$$

where $\hat{e}_n \sim N(0, \hat{\Sigma}_n)$, $\lambda_{max}(H_p)$ is the largest eigenvalue of H_p and $\lambda_{max}(\hat{\Sigma}_n)$ the largest eigenvalue of $\hat{\Sigma}_n$.

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On the other hand, $2\hat{e}_n^\top H_p f_0 = o_p(\sqrt{n})$ because $\hat{f}_n$ is a consistent estimator of f_0. Moreover, since $y_i - f_{0,i} = O_p(1)$, we know $\frac{2}{n}(y - f_0)^\top H_p f_0 = o_p(\sqrt{n})$. So,

$$\hat{e}_n^\top H_p \hat{e}_n + 2\hat{e}_n^\top H_p f_0 - \frac{2}{n}(y - f_0)^\top H_p f_0 = o_p(\sqrt{n}) \tag{4}$$

Therefore, by **Lemma 1**, we have

$$\sqrt{n}(\psi_p(\hat{f}_n) - \psi_p(f_0)) \xrightarrow{d} N(0, 4\sigma^2 \|H_p f_0\|_n^2).$$

$\square$

Theorem 2. Asymptotic Distribution of Variable Importance (multivariate). *Suppose $y_i = f_0(x_i) + \epsilon_i$, $\epsilon_i \sim N(0, \sigma^2)$, $x_i \in \mathcal{R}^P$, $i = 1, \ldots, n$. Denote $\psi = [\psi_1, \ldots, \psi_P]$ for ψ_p as defined in (1). If the following conditions are satisfied:*

i) $\mathrm{rank}(H_p) = o_p(\sqrt{n}), p = 1, \ldots, P$;

ii) $\lambda_{max}(H_p) = O_p(1), p = 1, \ldots, P$;

iii) $\hat{f}_n$ is an unbiased estimator of f_0.

Then $\psi(\hat{f}_n)$ asymptotically converges toward a multivariate normal distribution surrounding $\psi(f_0)$, i.e.,

$$\sqrt{n}(\psi(\hat{f}_n) - \psi(f_0)) \xrightarrow{d} MVN(\mathbf{0}, \mathbf{V}_0),$$

where $\mathbf{V}_0$ is a $P \times P$ matrix such that $[\mathbf{V}_0]_{p1,p2} = 4\sigma^2 \langle H_{p1} f_0, H_{p2} f_0 \rangle_n$.

Proof. Define a mean function $m : F \to E(F)$, where F is the distribution. Then in our case, $f_0 = E(F) = m(F)$. According to **Lemma 2**, we have

$$[\psi(f_0)]_p = \psi_p(E(F)) = \psi_p(m(F)) = [\phi(F)]_p,$$

i.e., $\phi(\cdot) = \psi(m(\cdot))$ and $[\phi(\cdot)]_p = \psi_p(m(\cdot))$, where $\phi : \mathcal{R} \to \mathcal{R}^P$. Therefore,

$$\begin{aligned}
[\phi_F'(\delta_y - F)]_p &= \psi_p'(m(\delta_y - F)) \\
&= \frac{d}{dt}\Big|_{t=0} \psi_p(m((1-t)F + t\delta_y)) \\
&= \frac{d}{dt}\Big|_{t=0} \psi_p((1-t)f_0 + ty) \\
&= \frac{d}{dt}\Big|_{t=0} \frac{1}{n}[(1-t)f_0 + ty]^\top H_p [(1-t)f_0 + ty] \\
&= \frac{2}{n}(y - f_0)^\top H_p f_0 \\
&= [IF_{\phi,F}(y)]_p.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
[\mathbf{V}_0]_{p1,p2} &= \int \langle [IF_{\phi,F}(y)]_{p1}, [IF_{\phi,F}(y)]_{p2} \rangle dF \\
&= 4 \int \frac{1}{n} \cdot f_0^\top H_{p1}(y - f_0)(y - f_0)^\top H_{p2} f_0 \cdot \frac{1}{n} dF \\
&= 4\sigma^2 \langle H_{p1} f_0, H_{p2} f_0 \rangle_n.
\end{aligned}$$

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Moreover, we have

$$[\int \boldsymbol{\phi}_F'(\delta_y - F)dF]_p = \frac{2}{n}\int (y - f_0)^\top H_p f_0 dF = 0,$$

and

$$[\sqrt{n}\mathbf{R}_n]_p = \sqrt{n}[[\boldsymbol{\phi}(\mathcal{F}_n)]_p - [\boldsymbol{\phi}(F)]_p - \frac{1}{n}\sum_i [\boldsymbol{\phi}_F'(\delta_{y_i} - F)]_p]$$

$$= \frac{1}{\sqrt{n}}[\hat{f}_n^\top H_p \hat{f}_n - f_0^\top H_p f_0 - \frac{2}{n}(y - f_0)^\top H_p f_0]$$

$$= \frac{1}{\sqrt{n}}[(\hat{f}_n - f_0)^\top H_p(\hat{f}_n - f_0) + 2(\hat{f}_n - f_0)^\top H_p f_0 - \frac{2}{n}(y - f_0)^\top H_p f_0]$$

$$= \frac{1}{\sqrt{n}}[\hat{\epsilon}_n^\top H_p \hat{\epsilon}_n + 2\hat{\epsilon}_n^\top H_p f_0 - \frac{2}{n}(y - f_0)^\top H_p f_0] \tag{5}$$

$$= \frac{1}{\sqrt{n}}o_p(\sqrt{n}) \tag{6}$$

$$= o_p(1) \overset{P}{\to} 0,$$

where $\hat{\epsilon}_n = \hat{f}_n - f_0$ and the reason from (5) to (6) is because of (4). Therefore, by **Lemma 2**, we have

$$\sqrt{n}(\boldsymbol{\psi}(\hat{f}_n) - \boldsymbol{\psi}(f_0)) \overset{d}{\to} MVN(\mathbf{0}, \mathbf{V}_0),$$

where $\mathbf{V}_0$ is a $P \times P$ matrix such that $[\mathbf{V}_0]_{p1,p2} = 4\sigma^2 \langle H_{p1}f_0, H_{p2}f_0\rangle_n$. $\qquad\square$