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ON FUNCTIONALS OF A DENSITY

E. NADARAYA AND G. SOKHADZE

Abstract. A probability density functional (nonlinear and unbounded, generally speaking) is considered. The consistency and asymptotic normality conditions are established for the plug-in-estimator. A convergence order estimator is obtained.

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1. INTRODUCTION

Problems of probability density estimation are the subject of investigation of many scientists. Interesting results were obtained for various classes of functionals. Both the bounded functional estimators ([1-5]) and the unbounded have been studied (in particular, Fisher information and Shannon entropy integral functional [6-8]).

In [9], L. Goldstein and K. Messer analyzed the general probability density functional and the regression function functionals. General estimation results were obtained. An attempt of a general approach was also made in [10] for the Gasser–Müller regression function.

The present paper deals with the case, where the functional is of a general form. In particular, it may be nonlinear, or unbounded. In this case a class of functionals is identified for which a plug-in-estimator is valid and the consistency and asymptotic normality of the estimator is shown.

Let X be a random variable with an unknown distribution density f(x). Let X_1, X_2, \ldots, X_n be a sample of independent copies of X. Further, let \mathfrak{M} be a functional defined on a subspace $\mathcal{L} \subset L_2(R)$ having a second order derivative. Assume that $f \in \mathcal{L}$ and hence we believe that $\mathfrak{M}f$ exists. Our aim is to study the problem of consistence of the estimator $\mathfrak{M}f$ with the help of a plug-in-estimator, $\mathfrak{M}\widehat{f}_n$, where \widehat{f}_n is an estimator of f.

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In order to estimate f and its derivatives we use the Rosenblatt–Parzen probability density kernel estimators (see [11–13]) having the form

$$\widehat{f}_{n}^{(j)}(x) = \frac{1}{nh_{n}^{j+1}} \sum_{i=1}^{n} K^{(j)}\left(\frac{x-X_{i}}{h_{n}}\right), \quad j = 0, 1, \dots, m,$$
(1)

where h_n a sequence of vanishing positive numbers, K(x) is a function with density properties.

The stated problem considers the case including both bounded functional estimators (integral or other type), information and entropy functional.

2. NOTATION AND CONDITIONS

Here we introduce the notation and some conditions that will be needed in the sequel. Let X be a random variable with a probability distribution density f(x). Suppose that the following conditions hold:

(f1) f(x) has continuous derivatives of the *m*-th order inclusively and for a $C_f > 0$, we have

$$\sup_{x \in \mathbb{R}} |f^{(i)}(x)| \le C_f < \infty, \ i = 0, 1, \dots, m;$$

(f2) a strictly increasing continuous function H(x), exists such that

$$\sup_{|y| \le x} \frac{1}{f(y)} \le H(x).$$
⁽²⁾

Consider a real-valued function $K(x) \ge 0$ and assume that the following conditions are satisfied:

- (k1) the support of the function K(x) is compact;
- (k2) $\int_{-\infty}^{\infty} K(x) dx = 1;$

(k3) K(x) has continuous derivatives up to the *m*-th order inclusively. In particular, these conditions imply that for $C_K > 0$, we have

$$|K^{(i)}(x)| \le C_K < \infty, \ i = 0, 1, \dots, m.$$

For the sequences h_n we assume the condition

(h) $h_n, n = 1, 2, ...,$ is a sequence of positive monotonically vanishing numbers, such that

$$h_n \ge \frac{c \log n}{n}$$
 for $c > 0$.

It is known (see [14]) that under the conditions (f1), (f2), (k1)–(k3) and (h), we have

$$\sup_{x \in \mathbb{R}} \left| \widehat{f}_n(x) - E\widehat{f}_n(x) \right| = O\left(\frac{\sqrt{|\log h_n| \vee \log \log n}}{\sqrt{nh_n}}\right)$$
(3)

with probability 1.

For the functional \mathfrak{M} we assume the following. Let $W_m = W_m(R)$ be a Sobolev space of functions from $L_2(R)$ with continuous derivatives up to the *m*-th order, inclusively, with the norm

$$||g||_m = \sqrt{\sum_{j=0}^m \int_{-\infty}^\infty |g^{(j)}(x)|^2 dx}.$$

In the space W_m we have a scalar product

$$(g_1, g_2)_m = \sum_{j=0}^m \int_{-\infty}^\infty g_1^{(j)}(x) g_2^{(j)}(x) \, dx.$$

We consider the functional \mathfrak{M} having the following properties:

- $(\mathfrak{M1})$ the functional \mathfrak{M} is defined on the subspace $\mathcal{L} \subset W_m$;
- $(\mathfrak{M2})$ there exists a $\mathfrak{M}f$;
- (**M3**) there exists functionals \mathfrak{M}_k , $k = 0, 1, \ldots$, and a sequence $s_k \to \infty$, such that
 - (i) the domain of definition of the functional \mathfrak{M}_k is $\mathcal{L}_k = W_m([-s_k; s_k])$ for every $k = 1, 2, \ldots, \mathcal{L}_k$ and is canonically viewed as a subspace of \mathcal{L} ;
 - (ii) $\widehat{f}_n \in \mathcal{L}_k$ for every $k = 1, 2, \ldots$;
 - (iii) for any $g \in \mathcal{L}$, $\mathfrak{M}_k g \to \mathfrak{M} g$ as $k \to \infty$;
 - (iv) the functional \mathfrak{M}_k is smooth in the sense that there exists a derivative up to the second order, inclusively: \mathfrak{M}'_k is a linear functional on \mathcal{L}_k and \mathfrak{M}''_k is a bilinear functional on \mathcal{L}_k which satisfy the following inequalities

$$\|\mathfrak{M}_{k}^{(i)}g\|_{m} \leq C \cdot s_{k}^{\alpha} \cdot \|g\|^{\beta} \cdot \|g\|_{km}^{2}, \ g \in \mathcal{L}_{k}, \ \alpha \geq 0, \ \beta \leq 0, \ i = 1, 2,$$

where ||g|| denotes a uniform norm of the element g, and $||g||_{km}$ is a norm in \mathcal{L}_k .

Denote $f_n(x) = E \widehat{f}_n(x)$. We have the equality

$$f_n(x) = E \widehat{f_n}(x) =$$

$$= \frac{1}{nh_n} \sum_{i=1-\infty}^n \int_{-\infty}^\infty K\left(\frac{x-t}{h_n}\right) f(t) dt = \int_{-\infty}^\infty K(u) f(x-uh_n) du.$$

This implies that $f_n(x) \to f(x)$ converges almost everywhere $x \in R$. It also implies the convergence of

$$|\mathfrak{M}f - \mathfrak{M}f_n| \longrightarrow 0 \text{ a.s. as } n \to \infty.$$
 (4)

It should be noted here that

$$\mathfrak{M}f - \mathfrak{M}_n \widehat{f}_n | \le |\mathfrak{M}f - \mathfrak{M}_n f_n| + |\mathfrak{M}_n \widehat{f}_n - \mathfrak{M}_n f_n|.$$
(5)

Further, for a sufficiently large s_n , we have

$$\mathfrak{M}f - \mathfrak{M}_n f_n | \le |\mathfrak{M}f - \mathfrak{M}_n f| + |\mathfrak{M}_n f - \mathfrak{M}_n f_n|.$$
(6)

It follows from the condition (**M3**), (iii) that $|\mathfrak{M}f - \mathfrak{M}_n f| \to 0$ as $s_n \to \infty$. The same condition together with (4) imply that $|\mathfrak{M}_n f - \mathfrak{M}_n f_n| \to 0$ as $s_n \to \infty$. Thus in representation (5) the main point is to estimate the second summand in the right-hand side.

3. Remainder Estimation

Consider the difference $\mathfrak{M}_n \widehat{f}_n - \mathfrak{M}_n f_n$ and with the help of the condition ($\mathfrak{M3}$) (iv) write it as follows:

$$\mathfrak{M}_n f_n - \mathfrak{M}_n f_n = S_n(h_n) + R_n, \tag{7}$$

where $S_n(h_n)$ is the result how the derivative of the functional (here a linear functional) \mathfrak{M}_n acts on $\hat{f}_n - f_n$. In (7),

$$R_n = O\left(\left\|\mathfrak{M}_n''(\widehat{f}_n - f_n)\right\|_{nm}\right).$$
(8)

Estimate R_n . It follows from (3) that under the condition

$$\frac{\log\log n}{nh_n^{2m+1}} \longrightarrow 0, \quad n \to \infty,$$

we have

$$-C_f \le \widehat{f}_n(x) \le C_f.$$

Therefore we may assume that $f_n \in \mathcal{L}_n$ and apply the condition ($\mathfrak{M3}$), (iv). Hence

$$|R_n| \le C s_n^{\alpha} ||f||^{\beta} ||\widehat{f}_n - f_n||_{nm}^2.$$
(9)

Expression (9) according to conditions (f1), (f2) results in

$$|R_n| \le C s_n^{\alpha} H(s_n)^{\beta} \|\widehat{f}_n - f_n\|_{nm}^2.$$

Denote

$$s_n^{\alpha} H(s_n)^{\beta} := d(s_n), \quad \|\widehat{f}_n - f_n\|_m^2 := r(n).$$

We have

$$|R_n| \le Cd(s_n)r(n). \tag{10}$$

Here d(x) is a strictly increasing function. In order to estimate r(n), we apply a technique used for a similar problem in [5].

Let

$$Y_i = Y_i(x) = \frac{1}{n} \left\{ \frac{1}{h_n} K\left(\frac{x - X_i}{h_n}\right) - f_n(x) \right\}.$$

Then

$$\sum_{i=1}^{n} Y_i(x) = \frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{1}{h_n} K\left(\frac{x - X_i}{h_n}\right) - f_n(x) \right\} = \widehat{f_n}(x) - f_n(x).$$

Therefore,

$$r_n(m) = \left\| \sum_{i=1}^n Y_i(x) \right\|_m^2.$$
 (11)

Estimate the function

$$g_i = g_i(x) = \frac{1}{nh_n} K\left(\frac{x - X_i}{h_n}\right)$$

through the norm $\|\cdot\|_m$ for every i = 1, ..., n. We have

$$\begin{split} \|g_i\|_m^2 &= \sum_{j=0}^m \frac{1}{n^2} \int_{-\infty}^\infty \left(\frac{1}{h_n^{j+1}} \, K^{(j)} \left(\frac{x - X_i}{h_n} \right) \right)^2 dx = \\ &= \frac{1}{n^2} \sum_{j=0}^m \frac{1}{h_n^{2j+1}} \int_{-\infty}^\infty \left(K^{(j)} \left(\frac{x - X_i}{h_n} \right) \right)^2 d \, \frac{x - X_i}{h_n} \le \\ &\le \frac{1}{n^2 h_n^{2m+1}} \sum_{j=0}^m \int_{-\infty}^\infty \left(K^{(j)}(u) \right)^2 du. \end{split}$$

Hence

$$\|g_i\|_m \le \frac{1}{nh_n^{m+\frac{1}{2}}} \|K\|_m \stackrel{def}{=} A_n.$$
(12)

By virtue of (k3) and (k4), $||K||_m$ is finite. From (12), we have

$$||Y_i||_m \le ||g_i||_m + E||g_i||_m \le 2A_n.$$
(13)

In order to estimate r(n), we apply McDiarmid's inequality, which will be stated here for convenience.

McDiarmid's inequality. Let $L(y_1, \ldots, y_k)$ be a real function such that for each $i = 1, \ldots, m$ and some c_i , the supremum in y_1, \ldots, y_k, y , of the difference

$$\left| L(y_1, \ldots, y_{i-1}, y_i, y_{i+1}, \ldots, y_k) - L(y_1, \ldots, y_{i-1}, y, y_{i+1}, \ldots, y_k) \right| \le c_i.$$

Then if Y_1, \ldots, Y_k are independent random variables taking values in the domain of the function $L(y_1, \ldots, y_k)$, then for every t > 0,

$$P\left\{ \left| L(Y_1, \dots, Y_k) - EL(Y_1, \dots, Y_k) \right| \ge t \right\} \le 2e^{-\frac{2t^2}{\sum_{i=1}^{k} c_i^2}}.$$

We apply McDiarmid's inequality to the expression

$$L(Y_1,\ldots,Y_n) = \left\|\sum_{i=1}^n Y_i\right\|_m$$

and $c_i = 4A_n$, for i = 1, ..., n. For any t > 0, taking into consideration (13), we have

$$P\left\{\left\|\sum_{i=1}^{n} Y_{i}\right\|_{m} - E\left\|\sum_{i=1}^{n} Y_{i}\right\|_{m}\right| \ge t\right\} \le 2e^{-\frac{t^{2}nh_{n}^{2m+1}}{2\|K\|_{m}^{2}}}.$$
(14)

Substituting

$$t = \frac{2\|K\|_m \sqrt{\log n}}{\sqrt{nh_n^{2m+1}}}$$

in (14) and applying the Borel–Cantelli lemma, we have

$$\left\|\sum_{i=1}^{n} Y_{i}\right\|_{m} = E\left\|\sum_{i=1}^{n} Y_{i}\right\|_{m} + O\left(\frac{\sqrt{\log n}}{\sqrt{nh_{n}^{2m+1}}}\right)$$
(15)

with probability 1. Estimate now $\|\sum_{i=1}^{n} Y_i\|_m^2$. Towards this end, we use Jensen's inequality

$$\begin{split} \left(E \left\|\sum_{i=1}^{n} Y_{i}\right\|_{m}\right)^{2} &\leq E \left\|\sum_{i=1}^{n} Y_{i}\right\|_{m}^{2} = \sum_{i=1}^{n} \sum_{j=0}^{m} \int_{-\infty}^{\infty} (Y_{i}^{(j)}(x))^{2} dx \leq \\ &\leq \frac{1}{n^{2}} \sum_{i=1}^{n} \sum_{j=0}^{m} \int_{-\infty}^{\infty} E \left\{\frac{1}{h_{n}^{j+1}} K^{(j)} \left(\frac{x - X_{i}}{h_{n}}\right) - f_{n}^{(j)}(x)\right\}^{2} dx \leq \\ &\leq \frac{1}{n^{2}} \sum_{i=1}^{n} \sum_{j=0}^{m} \left\{\int_{-\infty}^{\infty} E \left(\frac{1}{h_{n}^{j+1}} K^{(j)} \left(\frac{x - X_{i}}{h_{n}}\right)\right)^{2} dx\right\}^{2} \leq \\ &\leq \frac{1}{n^{2} h_{n}^{2m+2}} \sum_{i=1}^{n} \sum_{j=0}^{m} \left\{\int_{-\infty}^{\infty} E \left(K^{(j)} \left(\frac{x - X_{i}}{h_{n}}\right)\right)^{2} dx\right\} = \\ &= \frac{1}{n^{2} h_{n}^{2m+2}} \sum_{i=1}^{n} \sum_{j=0}^{m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (K^{(j)})^{2} \left(\frac{x - y}{h_{n}}\right) f(y) dy dx \leq \\ &\leq \frac{C_{f}}{n h_{n}^{2m+1}} \|K\|_{m}^{2}. \end{split}$$
(16)

From (11), (15) and (16) it follows that almost everywhere we have

$$r(n) = O\left(\frac{\log n}{nh_n^{2m+1}}\right).$$

Then the following theorem is true.

Theorem 1. If the conditions (f1), (f2), (k1)–(k3), (h) and (M1)–(M3) are satisfied, then in representation (14) for the remainder we have

$$R_n = O\left(\frac{d(s_n)\log n}{nh_n^{2m+1}}\right).$$
(17)

4. Consistency

Let $\varepsilon > 0$ be a fixed number. Choose a sequence h_n such that

$$\frac{\log n}{nh_n^{2m+1}} \longrightarrow 0 \text{ as } n \to \infty.$$
(18)

We select s_n as a solution of the equation

$$\frac{\log n}{nh_n^{2m+1}} = \frac{\varepsilon}{d(s_n)},\tag{19}$$

where

$$d(x) = x^{\alpha} H^{\beta}(x).$$

The function y = d(x) for x > 0 is continuous, strictly increasing and taking all values in the interval $(0; \infty)$. Therefore equation (19) has a solution with respect to s_n . Besides, $s_n \to \infty$, as $n \to \infty$. Consequently,

 $|R_n| < \varepsilon$ for a sufficiently large n.

Now we estimate the main summand $S_n(h_n)$ in the equality

$$\mathfrak{M}_n \widehat{f}_n - \mathfrak{M}_n f_n = S_n(h_n) + R_n.$$

Let

$$\overline{K}_{in}(x) := K\left(\frac{x - X_i}{h_n}\right) \text{ and } Z_i(h_n) := \frac{1}{h_n} \mathfrak{M}'_n \overline{K}_{in}.$$

Then $S_n(h_n)$ can be represented as a sum of independent random variables

$$S_n(h_n) = \frac{1}{n} \sum_{i=1}^n \{ Z_i(h_n) - E Z_i(h_n) \}.$$

Let [-k, k] be the smallest interval containing the support of K(x) (such an interval exists, what follows from (k1). Note that for a sufficiently large n, we have $s_n > k$, and therefore $Z_i(h_n) = 0$ for $s_n > k$. Taking this into consideration together with the condition (M3), (iv), we write

$$|Z_i(h_n)| \le C \mathbb{k}^{\alpha} H^{\beta}(\mathbb{k}) \left\| \frac{1}{h_n} K\left(\frac{\cdot - X_i}{h_n}\right) \right\|_m^2.$$
⁽²⁰⁾

Hence

$$|Z_i(h_n)| \le N \mathbb{k}^{\alpha} H^{\beta}(\mathbb{k}) \sum_{j=0}^m \frac{1}{h_n^{j+1}} \int_{-\mathbb{k}}^{\mathbb{k}} K^{(j)}\left(\frac{x-X_i}{h_n}\right) dx \le B h_n^{-m}$$

for a sufficiently large n and some B.

Apply Hoeffding's inequality.

Hoeffding's inequality. Let X_1, \ldots, X_n be independent random variables. Assume that the X_i are almost surely bounded

$$P\{a_i \le X_i \le b_i\} = 1.$$

Then

$$P\left\{ \left| \frac{1}{n} \sum_{i=1}^{n} X_i - \frac{1}{n} \sum_{i=1}^{n} EX_i \right| \ge t \right\} \le 2 \exp\left\{ -\frac{2n^2 t^2}{\sum_{i=1}^{n} (b_i - a_i)^2} \right\}$$

This inequality results in

$$P\{|S_n(h_n)| > t\} \le 2\exp\left\{-\frac{nt^2h_n^{2m}}{2B^2}\right\}.$$

Take

$$t = \frac{2B\sqrt{\log n}}{\sqrt{n}h_n^m}$$

We have

$$P\left\{|S_n(h_n)| > \frac{2B\sqrt{\log n}}{\sqrt{n}h_n^m}\right\} \le 2\exp\left\{-2\log n\right\}.$$

By virtue of the Borel–Cantelli lemma, we have

$$S_n(h_n) = O\left(\sqrt{\frac{\log n}{nh_n^{2m}}}\right)$$

with probability 1.

Note that the condition

$$\frac{\log n}{nh_n^{2m+1}} \longrightarrow 0 \ \text{ as } \ n \to \infty$$

leads to the convergence of

$$\frac{\log n}{nh_n^{2m}} \longrightarrow 0 \text{ as } n \to \infty.$$

Therefore $S_n(h_n) \to 0$, as $n \to \infty$.

Consequently, the following theorem is true.

Theorem 2. Let the conditions (f1), (f2), (k1)–(k3), (h) and (M1)–(M3) be satisfied. As the equivalence of positive numbers h_n monotonically vanishes, therefore

$$\frac{\log n}{nh_n^{2m+1}} \longrightarrow 0 \quad as \quad n \to \infty.$$

If for every n, s_n there is a solution of equation (19), we have

$$I(\widehat{f}_n, s_n) - I(f) \longrightarrow 0$$

with probability 1.

5. Central Limit Theorem

Remember the following representation:

$$\mathfrak{M}_n \widehat{f}_n - \mathfrak{M}_n f_n = \mathfrak{M}'_n (f_n) (\widehat{f}_n - f_n) + R_n.$$
(21)

 \mathbf{If}

$$Z_i(h_n) = \frac{1}{h_n} \mathfrak{M}'_n \overline{K}_{in},$$

then $S_n(h_n)=\mathfrak{M}'_n(f_n)(\widehat{f_n}-f_n)$ can be represented as a sum of independent random variables

$$S_n(h_n) = \frac{1}{n} \sum_{i=1}^n \{ Z_i(h_n) - E Z_i(h_n) \}.$$
 (22)

Find the moments of $Z_i(h_n)$.

We have

$$EZ_i(h_n) = \int_{-\infty}^{\infty} \mathfrak{M}'_n(f_n(\cdot)) \frac{1}{h_n} K\Big(\frac{\cdot - y}{h_n}\Big) f(y) \, dy =$$
$$= \int_{-\infty}^{\infty} \mathfrak{M}'_n(f_n(y + \cdot h_n)) K(\cdot) f(y) \, dy.$$

As $n \to \infty$, $h_n \downarrow 0$. Therefore

$$EZ_i(h_n) \longrightarrow E\mathfrak{M}'(f(X))K.$$

Now let $0 \leq j, v \leq n$. Consider the value

$$\mu_{j,v}(y) = EZ_j(h_n)Z_v(h_n) =$$

$$= \int_{-\infty}^{\infty} \mathfrak{M}'_n(f_n(\cdot)) \frac{1}{h_n} K\Big(\frac{\cdot - y}{h_n}\Big) \mathfrak{M}'_n(f_n(\cdot)) \frac{1}{h_n} K\Big(\frac{\cdot - y}{h_n}\Big) f(y) \, dy =$$

$$= \int_{-\infty}^{\infty} \mathfrak{M}'_n(f_n(y + \cdot h_n)) K(\cdot) \mathfrak{M}'_n(f_n(y + \cdot h_n)) K(\cdot) f(y) \, dy$$

which for $n \to \infty$ yields

$$EZ_i^2(h_n) \longrightarrow E[\mathfrak{M}'(f(X))K]^2.$$

Absolutely similarly, we can show that for $n \to \infty$, we have

$$EZ_i^4(h_n) \longrightarrow E\big[\mathfrak{M}'(f(X))K\big]^4.$$

After calculations we can see that under the defined conditions for $n \to \infty$, $h_n \to 0$, we obtain

$$n\operatorname{Var}(S_n(h_n)) = \operatorname{Var}(Z_i(h_n)) \longrightarrow \operatorname{Var}\left(\mathfrak{M}'(f(X))K\right) \stackrel{def}{=} \sigma^2(f) < \infty$$

and

$$EZ_i^4(h_n) \longrightarrow E[\mathfrak{M}'(f(X))K]^4 < \infty.$$

By Lyapunov's central limit theorem, we obtain the following result.

Theorem 3. Let the conditions (f1), (f2), (k1)–(k3), (h), (M1)–(M3) be satisfied and the sequence of positive numbers h_n monotonically vanish, so that

$$\frac{\log n}{nh_n^{2m+1}} \longrightarrow 0 \quad as \quad n \to \infty$$

for every n, s_n , there is a solution of equation (19). Then

$$\sqrt{n}\left\{I\mathfrak{M}_n\widehat{f}_n-\mathfrak{M}_nf_n\right\} \stackrel{d}{\longrightarrow} N(0,\sigma^2(f)).$$

6. Example

Consider the functional

$$\mathfrak{M}g = \int_{-\infty}^{\infty} \varphi(x, g(x), g'(x), \dots, g^{(n)}(x)) \, dx.$$

In this case, instead of the functional $\mathfrak{M}_k, \ k = 0, 1, \ldots$, we have integral functionals

$$\mathfrak{M}_k g = \int_{-s_k}^{s_k} \varphi \big(x, g(x), g'(x), \dots, g^{(n)}(x) \big) \, dx.$$

Under the appropriate condition imposed on the function φ , we can obtain all results of [15], in particular, the estimators for Fisher's information functional and Shannon entropies.

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Authors' addresses:

E. Nadaraya

I. Javakhishvili Tbilisi State University

2 University St. Tbilisi 0186, Georgia

E-mail: elizbar.nadaraya@tsu.ge

G. Sokhadze

I. Vekua Institute of Applied Mathematics of

I. Javakhishvili Tbilisi State University

2 University St. Tbilisi 0186, Georgia

E-mail: grigol.sokhadze@tsu.ge