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SOME STOCHASTIC PROPERTIES
OF THE BEST DETERMINED TERMS METHOD

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Some stochastic properties of the best determined terms method (BDT) are derived and some criteria based on the concept of the measure of information are given for an approximate determination of the normal solution to the Fredholm integral equation of the first kind.

1.

The system considered assumes after discretization the form

$$(1.1) \quad Kx = y + \varepsilon,$$

where $x \in R^n$ (the norm in R^n is the Euclidean norm $\|x\|_n^2 = \sum_{k=1}^n |x_k|^2$, $x = (x_1, \dots, x_n)^T$) $y, \varepsilon \in R^m$ and ε is a random vector with normal distribution and given covariance matrix $D(\varepsilon)$ ($D(\varepsilon) = E\{[\varepsilon - E(\varepsilon)][\varepsilon - E(\varepsilon)]^T\}$). In particular $E(\varepsilon) = 0$, where $E(\varepsilon)$ is the expected value of ε . By K we denote a linear mapping of R^n to R^m . The problem is to find a suitable approximation to the normal solution x_0 of

$$(1.2) \quad Kx = y.$$

By the normal solution we mean a vector fulfilling the following conditions:

- (i) $Kx_0 = y$,
- (ii) $\|x_0\|_n$ is minimal among all vectors fulfilling (1.2). The existence of such a solution is assumed.

It is well known that $D(\varepsilon)$ can be decomposed into a product $D(\varepsilon) = T^T T$, where T^T is a lower triangular matrix. Multiplying (1.1) by $(T^T)^{-1}$ one obtains

$$(1.3) \quad \hat{K}x = \hat{y} + \hat{\varepsilon},$$

where $\hat{K} = (T^T)^{-1} K$, $\hat{y} + \hat{\varepsilon} = (T^T)^{-1} (y + \varepsilon)$. Consequently, the system (1.1) is reduced to (1.3) and, in addition, $D(\hat{\varepsilon}) = I$.

It is well known [1, p. 5] that the matrix K can be decomposed as follows (singular value decomposition—SVD):

$$\hat{K} = U^T D V,$$

where U and V is $m \times m$ and $n \times n$ unitary matrix respectively, and the $m \times n$ matrix $D = (d_{jk})$ is such that $d_{jk} = 0$ if $j \neq k$ and $d_{jj} = \sigma_j \geq 0$, $j = 1, \dots, r = \min(m, n)$. Without loss of generality we may assume that $\sigma_1 \geq \dots \geq \sigma_r$. The system (1.3) can be further simplified if we let $u = Vx$ and $\varphi + \delta\varphi = U(\hat{y} + \hat{\varepsilon})$. We thus obtain

$$(1.4) \quad Du = \varphi + \delta\varphi.$$

2.

In this section some basic stochastic properties of the solution of the first kind of the system (1.1) and thus (1.4), the definition of which is given below, will be presented. Some limit properties of this solution are shown in [5].

If τ is a random variable with normal distribution then we say that $\tau \in N(E, D)$, where $E(\tau) = E$ is the expected value of τ and $E[\tau - E(\tau)]^2 = D$ its dispersion.

Let us choose $\Delta \geq 0$ such that $\|\delta\varphi\|_m^2 \leq \Delta$ with a certain probability. We also assume that $\delta\varphi_j \in N(0, 1)$, where $(\delta\varphi_1, \dots, \delta\varphi_m)^T = \delta\varphi$ and the components $\delta\varphi_j$, $j = 1, \dots, m$ are uncorrelated. Then (see [8, p. 85]) $\sum_{j=1}^m (\delta\varphi_j)^2$ is a random variable with the χ^2 -distribution, consequently

$$(2.1) \quad E\left[\sum_{j=1}^m (\delta\varphi_j)^2\right] = m.$$

It follows that $\Delta = m$.

Remark. If the matrix $D(\varepsilon)$ is diagonal with diagonal elements $(D(\varepsilon))_{jj} = \sigma^2$, $j = 1, \dots, m$, we have

$$E\left[\sum_{j=1}^m (\delta\varphi_j)^2\right] = E\left[\sum_{j=1}^m (\varepsilon_j)^2\right] \sigma^2 = m\sigma^2.$$

We further define the vectors (see e.g. in [2], [4])

$$(2.2) \quad u^k = \sum_{j=1}^k \sigma_j^+ (\varphi_j + \delta\varphi_j) e_j,$$

$k = 1, \dots, r$, where e_j is the unit vector with all its components zero except for the j^{th} component which is one. We use the notation $\sigma_j^+ = \sigma_j^{-1}$ if $\sigma_j > 0$ and $\sigma_j^+ = 0$ if $\sigma_j = 0$.

Definition 2.1. A vector $u^{k(\Delta)}$ is called a solution of the first kind to (1.4), if it fulfils

- (i) $\|Du^{k(\Delta)} - (\varphi + \delta\varphi)\|_m^2 \leq \Delta$,
- (ii) if u^k fulfils (i) with $k \neq k(\Delta)$, then $k > k(\Delta)$.

Theorem 2.1. The covariance matrix $D(u^{k(\Delta)})$ fulfils

$$D(u^{k(\Delta)}) = D^{k(\Delta)}[D^{k(\Delta)}]^T,$$

where $D^{k(\Delta)} = (d_{jk}^{k(\Delta)})$ and $d_{jk}^{k(\Delta)} = 0$ if $j \neq k$ and $j = k > k(\Delta)$ and $d_{jj}^{k(\Delta)} = \sigma_j^+$ for $j = 1, \dots, k(\Delta)$.

Proof. We easily verify that

$$u^{k(\Delta)} = D^{k(\Delta)}(\varphi + \delta\varphi).$$

Hence,

$$\begin{aligned} D(u^{k(\Delta)}) &= D^{k(\Delta)} E\{[u^{k(\Delta)} - E(u^{k(\Delta)})][u^{k(\Delta)} - E(u^{k(\Delta)})]^T\} [D^{k(\Delta)}]^T = \\ &= D^{k(\Delta)}[D^{k(\Delta)}]^T. \end{aligned}$$

This completes the proof.

The importance of Theorem 2.1 is emphasized by the fact which is its simple consequence, namely, that $(\sigma_j^+)^2$ is exactly the dispersion of the j^{th} component of $u^{k(\Delta)}$.

Theorem 2.2. The solution of the first kind to the system (1.4) is an unbiased estimate of the normal solution u_0 of

$$(2.3) \quad Du = \varphi,$$

if and only if $\varphi_{k(\Delta)+1} = \dots = \varphi_m = 0$.

Remark. By the assumption of Theorem 2.2, $E(u^{k(\Delta)}) = u_0$.

Proof. If $\varphi_{k(\Delta)+1} = \dots = \varphi_m = 0$ then $u^{k(\Delta)} = D^{k(\Delta)}(\varphi + \delta\varphi)$. This implies that

$$E[u^{k(\Delta)}] = u_0.$$

Since the converse assertion is obvious, the proof is complete.

The previous result has some rather important consequences. One usually has $k(\Delta)$ small – see e.g. in [3], where some problems of spectrophotometric diagnostics of planetary nebulae are studied, the author shows that $k(\Delta) \approx 7$. In this case the vector $u^{k(\Delta)}$ is not an unbiased estimate of the normal solution u_0 . This is a serious disadvantage of using solutions, of the first kind as approximations to the normal solution u_0 .

The following theorem describes a rather important extremal property of the covariance matrix of the solution of the first kind.

Theorem 2.3. Let \tilde{u} be an arbitrary unbiased estimate (i.e. $\tilde{u} = C(\varphi + \delta\varphi)$), where C is an, $n \times m$ matrix, $\varphi \in R^m$ an arbitrary vector and $E(D\tilde{u}) = \varphi$ of u_0 . Then the covariance matrix of the solution of the first kind of (1.4) fulfils

$$D(u^{k(A)}) \leq D(\tilde{u}).$$

Proof. By hypothesis, $\tilde{u} = C(\varphi + \delta\varphi)$ with some $n \times m$ matrix C . The unbiasedness of \tilde{u} implies that $CD\varphi = \varphi$. We then simply deduce that $CD = I^s$, where $\sigma_s > 0$ and $\sigma_{s+1} = \dots = \sigma_r = 0$, the matrix I^s being of the type $n \times n$ and

$$(2.5) \quad \begin{aligned} (I^s)_{jk} &= 0 \quad \text{if } j \neq k \quad \text{and } j = k = s + 1, \dots, n \\ (I^s)_{jj} &= 1 \quad \text{if } j = 1, \dots, s. \end{aligned}$$

It is an easy matter to verify the validity of

$$(2.6) \quad CC^T = D^+(D^+)^T + (C - D^+)(C - D^+)^T,$$

where D^+ denotes the generalized inverse to D , i.e. [6, p. 1], by virtue of the relation $D^+ = (D^T D)^+ D^T$. The required assertion of Theorem 2.3 then follows from (2.6). The proof is complete.

3.

We now consider some problems concerning the best approximations of the normal solution of the system (1.1).

Let $\{u^1, \dots, u^r\}$ be a set of vectors defined by (2.2). Our task is to present a decision criterion according to which one would find an index k such that

$$(3.1) \quad \|u^k - u_0\|_n = \min \{\|u^j - u_0\|_n : j = 1, \dots, r\},$$

where u_0 is the normal solution to (2.4). This problem is rather complicated because u^k is a random vector. A further complication is that the vector φ is not known as a rule. We are going to study some properties of the best approximation (best with respect to a given set $\{u^1, \dots, u^r\}$). We find it natural to use nondeterministic approach

Theorem 3.1. The vector u^k is the best approximation with respect to $\{u^1, \dots, u^r\}$ if and only if

$$\begin{aligned} \text{(i)} \quad & 2 \sum_{i=j+1}^k (\sigma_i^+)^2 (\varphi_i + \delta\varphi_i) \delta\varphi_i \leq \sum_{i=j+1}^k (\sigma_i^+)^2 (\varphi_i + \delta\varphi_i)^2 \quad \text{for } j = 1, \dots, k-1, \\ \text{(ii)} \quad & 2 \sum_{i=k+1}^j (\sigma_i^+)^2 (\varphi_i + \delta\varphi_i) \delta\varphi_i \geq \sum_{i=k+1}^j (\sigma_i^+)^2 (\varphi_i + \delta\varphi_i)^2 \quad \text{for } j = k+1, \dots, r. \end{aligned}$$

Proof. By definition, u^k is the best approximation if and only if

$$\|u^k - u_0\|_n^2 \leq \|u^j - u_0\|_n^2$$

for $j = 1, \dots, r$.

Hence,

$$(3.2) \quad \sum_{i=1}^k (\sigma_i^+ \delta \varphi_i)^2 + \sum_{i=k+1}^r (\sigma_i^+ \varphi_i)^2 \leq \sum_{i=1}^j (\sigma_i^+ \delta \varphi_i)^2 + \sum_{i=j+1}^r (\sigma_i^+ \varphi_i)^2.$$

In the case $j = 1, \dots, k-1$, (3.2) is equivalent to

$$\sum_{i=j+1}^k (\delta \varphi_i \sigma_i^+)^2 \leq \sum_{i=j+1}^k (\sigma_i^+ \varphi_i)^2.$$

It follows that

$$2 \sum_{i=j+1}^k (\sigma_i^+)^2 (\varphi_i + \delta \varphi_i) \delta \varphi_i \leq \sum_{i=j+1}^k (\sigma_i^+)^2 (\varphi_i + \delta \varphi_i)^2.$$

The case $j = k+1, \dots, r$ can be considered in the same way. This completes the proof.

A vector u^k satisfies the condition (3.1) if and only if the vectors φ and $\delta \varphi$ satisfy the conditions (i) and (ii). We write $\varphi^* = \varphi + \delta \varphi$, where φ^* is a known vector and we define random variables w_j^k , $j \in \{1, \dots, r\} \setminus \{k\}$ and $k = 2, \dots, r-1$ as follows:

$$w_j^k = \sum_{i=j+1}^k \varphi_i^* (\sigma_i^+)^2 \delta \varphi_i \quad \text{for } j = 1, \dots, k-1$$

and

$$w_j^k = \sum_{i=k+1}^j \varphi_i^* (\sigma_i^+)^2 \delta \varphi_i \quad \text{for } j = k+1, \dots, r.$$

We further define for $k = 2, \dots, r-1$ the quantities

$$h_j^k = \frac{1}{2} \sum_{i=j+1}^k (\varphi_i^* \sigma_i^+)^2 \quad \text{for } j = 1, \dots, k-1$$

and

$$h_j^k = \frac{1}{2} \sum_{i=k+1}^j (\varphi_i^* \sigma_i^+)^2 \quad \text{for } j = k+1, \dots, r.$$

Definition 3.1. Let, for $j = 2, \dots, r-1$,

$$(3.3) \quad P_j = P(w_j^j \leq h_1^j, \dots, w_{j-1}^j \leq h_{j-1}^j, w_{j+1}^j \geq h_{j+1}^j, \dots, w_r^j \geq h_r^j),$$

where P is the probability measure derived from the probability density corresponding to the random vector $w^j = (w_1^j, \dots, w_{j-1}^j, w_{j+1}^j, \dots, w_r^j)^T \in R^{r-1}$.

We say that u^k is a solution of (1.4) if

$$P_k = \max \{P_j : j = 2, \dots, r-1\}.$$

We now evaluate these probabilities. We use the same simple method shown e.g. [8, p. 43]. The definition of w^k for $k = 2, \dots, r - 1$ allows us to write

$$(3.4) \quad \varphi_j^*(\sigma_j^+)^2 \delta\varphi_j = w_{j-1}^k - w_j^k \quad \text{for } j = 2, \dots, k - 1$$

and

$$\varphi_j^*(\sigma_j^+)^2 \delta\varphi_j = w_j^k - w_{j-1}^k \quad \text{for } j = k + 2, \dots, r$$

and

$$\varphi_k^*(\sigma_k^+)^2 \delta\varphi_k = w_{k-1}^k, \quad \varphi_{k+1}^*(\sigma_{k+1}^+)^2 \delta\varphi_{k+1} = w_{k+1}^k.$$

We always have in mind that $\delta\varphi_j \in N(0, 1)$, $j = 1, \dots, m$.

Let us consider the case when

$$\varphi_j^*(\sigma_j^+)^2 = 0$$

for some $j = 1, \dots, r$. Let $j \leq k = 1$ (if $j \geq k + 1$ the considerations are just the same). We have $w_j^k = w_{j-1}^k - \dots = w_{\hat{j}}^k$, where $\hat{j} \in \{1, \dots, j - 1\}$ is the last index smaller than j such that $\varphi_{\hat{j}+1}^* \sigma_{\hat{j}+1}^+ = 0$. There is a possibility to choose a subset $p(1), \dots, p(c)$ of $\{1, \dots, r\}$, where $c \leq r$, such that $\varphi_j^*(\sigma_j^+)^2 \neq 0$ for $j = p(1), \dots, p(c)$ and $p(1) \leq p(2) \leq \dots \leq p(c)$. Let $p(l)$ be an index such that $w_{p(l)}^k = w_{k-1}^k$. The conditions (i) and (ii) in Theorem 3.1 can be expressed as follows:

$$(i') \quad w_j^k \leq h_j^k \quad \text{for } j = p(1), \dots, p(l),$$

$$(ii') \quad w_j^k \geq h_j^k \quad \text{for } j = p(l + 2), \dots, p(c).$$

It follows that

$$P_k = \int_{\Omega(k)} g_k(t_1, \dots, t_{c-1}) dt_1, \dots, dt_{c-1},$$

where

$$\Omega(k) = (-\infty, h_{p(1)}) \times \dots \times (-\infty, h_{p(l)}) \times (h_{p(l+2)}, +\infty) \times \dots \times (h_{p(c)}, +\infty)$$

and $g_k(t_1, \dots, t_{c-1})$ is the probability density of the vector $(w_{p(1)}^k, \dots, w_{p(l)}^k, w_{p(l+2)}^k, \dots, w_{p(c)}^k)^T$.

According to [8, p. 44]

$$g_k(t_1, \dots, t_{c-1}) = (\det S_k)^{1/2} f(t^T S_k t).$$

Here $f(t_1, \dots, t_{c-1})$ is the probability density of the random vector $(\delta\varphi_1, \dots, \delta\varphi_{c-1})^T$, $t = (t_1, \dots, t_{c-1})^T \in R_{c-1}$ and S_k is a matrix $(c - 1) \times (c - 1)$:

$$S_k = \left(\begin{array}{c|c} A_k & 0 \\ \hline 0 & B_k \end{array} \right)$$

with square diagonal blocks A_k and B_k the dimensions of which equal l and $c - l - 1$ respectively.

Explicitly,

$$A_k = \begin{pmatrix} \alpha_2, & -\alpha_2, & 0, & \dots\dots\dots \\ -\alpha_2, & \alpha_2 + \alpha_3, & -\alpha_3, & 0 \dots\dots\dots \\ 0, & -\alpha_3, & \alpha_3 + \alpha_4, & -\alpha_4, & 0 \dots\dots\dots \\ \dots\dots\dots \\ 0, & \dots\dots\dots 0, & -\alpha_{l-1}, & \alpha_{l-1} + \alpha_l \end{pmatrix},$$

$$B_k = \begin{pmatrix} \alpha_{l+1} + \alpha_{l+2}, & -\alpha_{l+2}, & 0, & \dots\dots\dots \\ -\alpha_{l+1}, & \alpha_{l+2} + \alpha_{l+3}, & -\alpha_{l+3}, & 0, & \dots\dots\dots \\ \dots\dots\dots \\ \dots\dots\dots 0, & -\alpha_{c-1}, & \alpha_c \end{pmatrix}$$

where $\alpha_j = [\varphi_{p(j)}^*(\sigma_{p(j)}^+)^2]^{-2}$ for $j = 2, \dots, c$.
 We easily verify that

$$\det A_k = \left(\prod_{j=p(2)}^{p(l)} \varphi_j^*(\sigma_j^+)^2 \right)^{-2},$$

$$\det B_k = \left(\prod_{j=p(l+1)}^{p(c)} \varphi_j^*(\sigma_j^+)^2 \right)^{-2}.$$

Consequently,

$$(3.6) \quad g_k(t_1, \dots, t_{c+1}) = \frac{1}{(2\pi)^{l/2}} \left[\prod_{j=2}^c \varphi_{p(j)}^*(\sigma_{p(j)}^+)^2 \right]^{-1} \exp\left(-\frac{t^T S_k t}{2}\right).$$

Since the matrix S_k is symmetric and, by hypothesis, regular there is a lower triangular matrix L such that $S_k = L^T L$. Let us substitute $\hat{t} = Lt$ into (3.6); we obtain

$$(3.7) \quad \hat{g}_k(\hat{t}_1, \dots, \hat{t}_{c-1}) = \text{const} \exp\left(-\frac{\hat{t}^T \hat{t}}{2}\right)$$

where const is independent of k .

Let H_k be the set defined as follows:

$$H_k = \{ \hat{t} \in R^{c-1} : -\Delta \leq \hat{t}_1 \leq h_{p(1)}^k, \dots, -\Delta \leq \hat{t}_l \leq h_{p(l)}^k, h_{p(l+1)}^k \leq \hat{t}_{l+1} \leq \Delta, \dots, h_{p(c)}^k \leq \hat{t}_{c-1} \leq \Delta \},$$

where $\Delta' > 0$ is given.

Further, let

$$\hat{P}_k = \int_{L(H_k)} \hat{g}_k(\hat{t}_1, \dots, \hat{t}_{c-1}) d\hat{t}_1, \dots, d\hat{t}_{c-1}.$$

Definition 3.2. We say that u^k is the solution of the second kind of the system (1.4) if $\hat{P}_k = \max \{ \hat{P}_j : j = 2, \dots, r - 1 \}$.

Remark. If $\Delta > 0$ is large, then $\hat{P}_k \approx P_k$. Hence the solution of the second kind is correctly defined.

Practical results using this criterion can be found in [3].

4.

In this section we characterize the BDT method using the concept of measure of information. It is shown in [7] that this approach offers certain advantages for determining a suitable decision criterion. In this paper we use the concept of measure of information to establish new decision criterion. First we modify the BDT method slightly. The advantages of the modification will be clear later.

For the sake of simplicity we consider a simplified system

$$(4.1) \quad Kx = y + \varepsilon,$$

in which $x \in R^n$, $y, \varepsilon \in R^n$ and K maps R^n to R^n . The requirements concerning the random vector on the right hand side are same as for the general case considered in the previous section. We see that all the above consideration remains valid for the special case $m = n$. In particular, (4.1) is equivalent to $\hat{K}x = \hat{y} + \hat{\varepsilon}$, with $\hat{K} = (T^T)^{-1}K$ etc.

Using the same notation as in (2.5) we define $I_{k+1} = I - I^k$, where I is the $n \times n$ unit matrix. We correspondingly define the vectors

$$x^k(\eta) = V^T(D^n + \eta I_{k+1}) U(\hat{y} + \hat{\varepsilon}), \quad k = 1, \dots, n,$$

where $\eta > 0$ and D^k is from Theorem 2.1.

It follows that

$$\|x^k(\eta) - x^k\| \leq \eta \|\hat{y} + \hat{\varepsilon}\|.$$

By choosing η appropriately, x^k can be approximated by $x^k(\eta)$ with an arbitrarily small error. We also easily determine the covariance matrix

$$D(x^k(\eta)) = V^T[D^k(D^k)^T + \eta^2 I_{k+1}] V.$$

Let

$$f(t_1, \dots, t_n) = \frac{1}{\sqrt{2\pi}} \{\det [D(x^k(\eta))]\}^{-1/2} \exp \left\{ -\frac{1}{2} (t - \mu)^T D(x^k(\eta)) (t - \mu) \right\}$$

where the components of the vector $x^k(\eta)$ belong to $N(\mu, D(x^k(\eta)))$, where $\mu = V^T(D^k + \eta I_{k+1}) U \hat{y}$ and $t = (t_1, \dots, t_n)^T$.

Definition 4.1. *The quantity*

$$(4.2) \quad J(x^k(\eta)) = \int f(t) \log f(t) dt_1, \dots, dt_n$$

is called the measure of information with respect to the vector $x^k(\eta)$.

After the substitution $\hat{t} = (T^T(\eta))^{-1} V(t - \mu)$, where $D(x^k(\eta)) = T^T(\eta) T(\eta)$ with a lower triangular matrix $T^T(\eta)$, into (4.2) we obtain

$$J(x^k(\eta)) = c_1(n) - c_2(n) \log \sigma_1^+, \dots, \sigma_k^+ \eta^{n-k}$$

for $k = 1, \dots, n$. In this formula the numbers $c_1(n)$ and $c_2(n)$ are independent of \hat{K} and $\hat{y} + \hat{\varepsilon}$. We further have

$$\det Dx^k(\eta) = (\sigma_1^+, \dots, \sigma_k^+ \eta^{n-k})^2.$$

If

$$(4.3) \quad 0 < \eta \ll \sigma_1^+ \leq \dots \leq \sigma_s^+, \quad s \in \{1, \dots, n\},$$

we deduce that $J(x^k(\eta))$ is non-increasing as a function of k . The rate of a possible decrease gives us tools for determining a suitable decision criterion.

We first determine components of the measure of information with respect to the direction v_k , where $V = (v_1 | \dots | v_n)$. Let us denote

$$J(k) = J(x^k(\eta)) - J(x^{k-1}(\varphi)) \quad \text{for } k = 2, \dots, n$$

and

$$J(1) = a(n, \eta) + (\log \eta \sigma_1) c_2(n),$$

where $a(n, \eta) = c_2(n) - c_2(n) \log \eta$. It follows from (4.3) that $J(k) \geq J(k+1)$ and we see that the measure of information with respect to the direction is a non-increasing function of k . This is in a good accordance with the intuition.

Decision criterion.

We say that the vector x^k in an α -approximation to the normal solution of (4.1) if $J(k) - J(k+1) \geq \alpha$ and the relation $J(s) - J(s+1) \geq \alpha$ implies that $s \geq k$.

This criterion has been tested on some inverse problems of spectroscopic diagnostics of planetary nebulae. The results will be published elsewhere.

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Souhrn

NĚKTERÉ STOCHASTICKÉ VLASTNOSTI METODY
NEJLÉPE URČENÝCH TERMŮ

JÍŘÍ NEUBERG

Jsou studovány některé stochastické vlastnosti metody nejlépe určených termů a některá kritéria založená na konceptu míry informace pro určení aproximace normálního řešení Fredholmových integrálních rovnic prvního druhu.

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