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Grid refinement in multiscale dynamic optimization*

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Abstract

In the present work we explore an adaptive discretization scheme for dynamic optimization problems applied to input and state estimation. The proposed method is embedded into a solution methodology where the dynamic optimization problem is approximated by a hierarchy of successively refined finite dimensional problems. Information on the solution of the coarser approximations is used to construct a fully adaptive, problem dependent discretization where the finite dimensional spaces are spanned by biorthogonal wavelets arising from B-splines. We demonstrate exemplarily that the proposed strategy is capable to identify accurate discretization meshes which are more economical than uniform meshes with respect to the ratio of approximation quality vs. number of used trial functions.

Keywords: dynamic optimization, large scale systems, direct method, adaptive mesh refinement, input estimation, state estimation, simultaneous approach, wavelets

1 Introduction

The numerical solution of dynamic optimization problems is typically quite challenging for large–scale applications. The challenge becomes even more severe when real–time applications are envisaged, since the response time where a valid solution has to be prompted is fixed. In on–line applications usually the numerical cost and the associated solution time is conservatively estimated and the optimization problem is solved with well developed numerical methods (e.g. Tanartkit and Biegler, 1997, and Bock *et al.*, 1999). The numerical effort is determined to a large extent by the complexity of the finite dimensional approximation. In fact, the computational effort grows at least superlinearly with an increasing number of decision variables. Problem adapted discretization of the control vector might be considered if one is interested in lowering the computational burden associated to a specified accuracy while at the same time the robustness of the solution algorithm is improved. In particular a discretization which is too coarse on a uniform grid or which locally resolves the profiles in the wrong location on a nonuniform grid cannot meet prespecified accuracy requirements. On the other hand, a discretization which is too fine often leads to inappropriately high computational cost and might cause robustness problems in addition. However, it is not trivial to generate a problem adapted mesh a

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priori. There have been only few attempts to incorporate adaptivity into the discretization scheme with the objective of automatically determining an appropriate mesh (e.g. Waldraff, 1996; Tanartkit and Biegler, 1997; Betts and Huffman, 1998; and Binder *et al.*,1998).

In this contribution, we want to address adaptive discretization strategies for input and state estimation problems which are formulated as dynamic optimization problems. The optimization problem is approximated by a nonlinear program (NLP) where states and inputs are discretized *simultaneously.* We suggest a systematic framework which automatically generates sequences of nonuniform grids with an increasing degree of resolution. The method is started from a coarse grid ($\ell = 0$) with few decision variables which can be solved efficiently and robustly. In every following refinement cycle ($\ell := \ell + 1$) the discretization mesh is improved in order to meet local accuracy requirements. In particular the optimization problem is formulated in a weak sense and discretized using a Wavelet–Galerkin approach. Biorthogonal wavelets arising from B-splines are employed to span the test and trial functions. The aim of this paper is to explore potential reuse of the current solution for an adaptive refinement. Improvements on the approximation of the measurements are established employing thresholding techniques. Error analysis techniques based on one–step methods are used to monitor the discretization error of the model equations whereas unknown input functions in the estimation problem are refined based on *gradient* information of potential trial functions. The suggested refinement procedure leads to problem adapted approximations with local resolution to guarantee prespecified local error bounds.

2 Problem formulation

We consider estimation problems formulated as a dynamic otpimization problem given by

$$\min_{\boldsymbol{x}_0, \boldsymbol{w}} \int_{t_0}^{t_f} f_0(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{w}, \boldsymbol{z}) \, d\tau \tag{P1}$$

under the restrictions

$$\begin{aligned}
\dot{\boldsymbol{x}} &= \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{w}, t), \quad t \in [t_0, t_f] \quad , && (1)\\
\boldsymbol{y} &= \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{w}, t), \quad t \in [t_0, t_f] \quad , && (2)\\
\boldsymbol{0} &\geq \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{w}, t), \quad t \in [t_0, t_f] \quad , && (3)\\
\boldsymbol{0} &= \boldsymbol{x}(t_0) - \boldsymbol{x}_0 \quad . && (4)
\end{aligned}$$

$\boldsymbol{x}(t), \boldsymbol{x}_0 \in \mathbb{R}^{n_x}$ denote the state and initial condition. $\boldsymbol{y}(t) \in \mathbb{R}^{n_y}$ are the model outputs and $\boldsymbol{u}(t) \in \mathbb{R}^{n_u}$ are the inputs which are assumed to be measureable and therefore *known.* $\boldsymbol{w}(t) \in \mathbb{R}^{n_w}$ is an *unknown* time variant input function which might reflect disturbances in the process or uncertainty in the process model. $\boldsymbol{z}(t) \in \mathbb{R}^{n_z}$ is a reference or measurement function and *known.* $\boldsymbol{u}$ and $\boldsymbol{z}$ are interpolated functions based upon possibly denoised measurement samples $\boldsymbol{z}(t_i), \boldsymbol{u}(t_i)$. $\boldsymbol{f}$and $\boldsymbol{c}$ denote the process model of appropiate dimensions. Mixed constraints are denoted by $\boldsymbol{g}$. f_0 specifies the cost functional where t_0, t_f denote the initial and final times.

A multiscale formulation of the process model which permits model representation of various resolutions is obtained by a weak formulation of equations (1)–(4):

$$\begin{aligned}
\langle \dot{\boldsymbol{x}} - \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{w}, t), \boldsymbol{\zeta}_x \rangle &= \mathbf{0} \ \forall\, \boldsymbol{\zeta}_x \in (L_2(I))^{n_x} && (5)\\
\langle \boldsymbol{y} - \boldsymbol{c}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{w}, t), \boldsymbol{\zeta}_y \rangle &= \mathbf{0} \ \forall\, \boldsymbol{\zeta}_y \in (L_2(I))^{n_y} && (6)\\
\langle \boldsymbol{g}(\boldsymbol{x}, \boldsymbol{w}, t), \boldsymbol{\nu} \rangle &\le \mathbf{0} \ \forall\, \boldsymbol{\nu} \in (L_2^+(I))^{n_g} && (7)\\
\langle \boldsymbol{x} - \boldsymbol{x}_0, \delta(t - t_0) \rangle &= \mathbf{0} \quad . && (8)
\end{aligned}$$

Here δ denotes the dirac function and $I := [t_0, t_f]$. For convenience we gather $\boldsymbol{\Upsilon} := (\boldsymbol{x}^T, \boldsymbol{y}^T, \boldsymbol{u}^T, \boldsymbol{w}^T, \boldsymbol{z}^T)^T \in \boldsymbol{\Upsilon}$ and $\boldsymbol{\zeta} := (\boldsymbol{\zeta}_x^T, \boldsymbol{\zeta}_y^T, \nu^T) \in M$ where $\boldsymbol{\Upsilon}$ and $\boldsymbol{\mathcal{M}}$ refer to appropiately chosen functions spaces. We choose appropriate finite dimensional *wavelet* spaces $\boldsymbol{\Upsilon}_\Lambda$ and $\boldsymbol{\mathcal{M}}_\Lambda$ as subsets of $\boldsymbol{\Upsilon}$ and $\boldsymbol{\mathcal{M}}$. Wavelets $\psi_{j,k}$, are specialized functions of local support which enable an efficient approximation of an arbitrary function f, e.g. $f \approx \sum_{k \in \mathcal{I}_{j_0}} d_{j_0-1,k} \varphi_{j_0,k} + \sum_{j=j_0}^{J} \sum_{k \in \mathcal{J}_j} d_{j,k} \psi_{j,k}$ where $\mathcal{I}_{j0}, \mathcal{J}_j$ denote appropiate index sets. Wavelets are constructed such that the Euclidean norm of the wavelet coefficients $d_{j,k}$ is always proportional to the L_2 norm of f (see e.g Dahmen, 1997 for a survey). Thus discarding small coefficients $d_{j,k}$ will cause only small changes in approximate representations of f. Moreover, in regions where f is smooth the values $|d_{j,k}|$ will be quite small. Therefore functions that exhibit strong variations only locally, can be approximated very accurately by linear combinations of only relatively few wavelets corresponding to the *significant* coefficients $d_{j,k}$. Denoting the set of the corresponding indices (j,k) by Λ, the sparse basis $\Psi_\Lambda := \{\psi_{j,k} : (j,k) \in \Lambda\}$ is expected to lead to a particularly *adapted* approximation to f.

In particular we discretize (P1) using hat wavelets $\psi_{j,k}$ to approximate $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$ and Haar wavelets $\psi_{j,k}^H$ for $\boldsymbol{u}, \boldsymbol{w}$, e. g. $\boldsymbol{x} \approx \boldsymbol{x}_\Lambda := \boldsymbol{d}_x^T \boldsymbol{\Psi}_{\Lambda_x}$, $\boldsymbol{y} \approx \boldsymbol{y}_\Lambda := \boldsymbol{d}_y^T \boldsymbol{\Psi}_{\Lambda_y}$, $\boldsymbol{z} \approx \boldsymbol{z}_\Lambda := \boldsymbol{d}_z^T \boldsymbol{\Psi}_{\Lambda_z}$, $\boldsymbol{u} \approx \boldsymbol{u}_\Lambda := \boldsymbol{d}_u^T \boldsymbol{\Psi}_{\Lambda_u}^H$ $\boldsymbol{w} \approx \boldsymbol{w}_\Lambda := \boldsymbol{d}_w^T \boldsymbol{\Psi}_{\Lambda_w}^H$. The state and output equations (5),(6) are tested by appropriately chosen dual wavelets (see Binder *et al.*, 1998 for further details on the discretization). Since the trial functions employed are *piecewise constant* ($\psi_{j,k}^H$) or *piecewise linear* ($\psi_{j,k}$) it is sufficient to evaluate the inequalities (7) *pointwise* on a possibly *nonuniform mesh* $\triangle_\Lambda := \{t_i \in I\}$ which captures the finite number of knots in the approximation. The optimization problem in discretized form is now given by

$$\min \Theta_\Lambda(\boldsymbol{d}_x, \boldsymbol{d}_y, \boldsymbol{d}_w, \boldsymbol{d}_z) \qquad \text{(P2)}$$

under the restrictions

$$\begin{aligned}
\boldsymbol{f}_\Lambda(\boldsymbol{d}_x, \boldsymbol{d}_u, \boldsymbol{d}_w, t) &= \boldsymbol{u} \quad ,\\
\boldsymbol{c}_\Lambda(\boldsymbol{d}_x, \boldsymbol{d}_y, \boldsymbol{d}_u, \boldsymbol{d}_w, t) &= \mathbf{0} \quad ,\\
\boldsymbol{g}_\Lambda(\boldsymbol{d}_x, \boldsymbol{d}_w, t_i) &\le \mathbf{0}, \quad \forall\, t_i \in \triangle_\Lambda, \quad ,\\
\boldsymbol{e}_\Lambda(\boldsymbol{d}_x, \boldsymbol{x}_0) &= \mathbf{0} \quad ,
\end{aligned}$$

where $\boldsymbol{f}_\Lambda, \boldsymbol{c}_\Lambda, \boldsymbol{g}_\Lambda$ are the finite dimensional model equations resulting from (5), (6) and (7) after projection. $\boldsymbol{e}_\Lambda := \boldsymbol{d}_x^T \boldsymbol{\Psi}_\Lambda(t_0)$ approximates (4) and $\Theta_\Lambda := \int f_0(\boldsymbol{x}_\Lambda, \boldsymbol{y}_\Lambda, \boldsymbol{z}_\Lambda) d\tau$ is the discretized cost functional of problem P1.

3 Adaptive Algorithm

Refinement of known quantities: $\boldsymbol{z}, \boldsymbol{u}$ are measurement functions, which have been obtained by interpolation of the possibly non–uniform discrete measurements. We limit ourselves to the treatment of $\boldsymbol{z}$ since refinement of $\boldsymbol{u}$ is obtained in a similar way in every refinement step ℓ. We are interested in compressed approximations $z^{\ell}_{\Lambda_i}$ satisfying

$$\frac{\| z_i - z^{\ell}_{\Lambda_i} \|_{L_2}}{\| z_i \|_{L_2}} \leq \varepsilon'_{\ell} \quad, i = 1, \dots, n_z \quad , \tag{9}$$

with given tolerance ε'_{ℓ}. Let $\boldsymbol{d}^J_{z_i}$ be the coefficient vector of the expansion $z_i = \boldsymbol{d}^{J\,T}_{z_i} \boldsymbol{\Psi}_{\Lambda^J_i}$ where $\boldsymbol{\Psi}_{\Lambda^J_i}$ is sufficiently rich to capture all measurement samples. On account of the norm equivalences (Dahmen, 1997) we simply have to neglect the elements of $\boldsymbol{d}^J_{z_i}$ which are smaller than a threshold ε which uniquely depends on ε'_{ℓ}. The remaining entries are the *significant* coefficients and their indices form the index set $\Lambda^{\ell}_{z_i}$. Typically the number of significant wavelet coefficients is far less than the number of discrete measurement samples. During the refinement sequence the approximation quality is increased $\varepsilon'_{\ell+1} \leq \varepsilon'_{\ell}$. Thus the approximation from step ℓ to $\ell + 1$ is refined adding trial functions with indices $\Gamma^{\ell}_{z_i} := \Lambda^{\ell+1}_{z_i} \cap \Lambda^{\ell}_{z_i}$. Hence, $\Gamma^{\ell}_{z_i}$ is called refinement set of step ℓ.

Refinement of states $\boldsymbol{x}$ and outputs $\boldsymbol{y}$: Although the discretization structure allows individual non–uniform meshes for the components of $\boldsymbol{x}$ and $\boldsymbol{y}$ we restrict ourselves to the simpler case where a common mesh is used to discretize all x_i, y_i. The refinement is based on an error analysis of $\boldsymbol{x}^{\ell}_{\Lambda}$ only since errors in $\boldsymbol{y}_{\Lambda}$ are directly linked to errors in $\boldsymbol{x}_{\Lambda}$. Error analysis either involves local error estimation or residual evaluation. The latter is computationally inexpensive and gives usually a qualitatively good grasp on the error behavior. However, sharp error estimates are difficult to obtain. Therefore the refinement is based on local error estimation where $\boldsymbol{x}^{*\ell}_{\Lambda}$ is compared to *locally* refined solutions keeping $\boldsymbol{x}^{*\ell}_0$, $\boldsymbol{u}^{\ell}_{\Lambda}$ and $\boldsymbol{w}^{*,\ell}_{\Lambda}$ at their current optimal values. In particular error tests are performed at the midpoints of the current mesh associated to Λ^{ℓ}_x. The error tests require the solution of equation systems of size n_x for each midpoint. At first glance this seems to be a substantial numerical effort. But one has to realize that the local solutions are computed by solving a sequence of decoupled equation systems of relatively small size. This is obviously much cheaper than resolving the complete refined optimization problem. The local error estimates are then checked if they satisfy error bounds which depend uniquely on the approximation quality of $\boldsymbol{z}^{\ell}_{\Lambda}, \boldsymbol{u}^{\ell}_{\Lambda}, \boldsymbol{w}^{\ell}_{\Lambda}$. Regions where the error bounds are violated are locally refined with appropriate trial functions whose indices are collected in the refinement set Γ^{ℓ}_x.

Refinement of unknown inputs $\boldsymbol{w}$: The central idea for an improved approximation of $\boldsymbol{w}$ is to evaluate gradients of the Lagrange functional $\mathcal{L}_{\Lambda} := \Theta_{\Lambda} + \boldsymbol{\lambda}^T_{\Lambda} \boldsymbol{f}_{\Lambda} + \boldsymbol{\mu}^T_{\Lambda} \boldsymbol{c}_{\Lambda} + \boldsymbol{\nu}^T_{\Lambda} \boldsymbol{g}_{\Lambda} + \boldsymbol{\eta}^T_{\Lambda} \boldsymbol{e}_{\Lambda}$ of problem P2, where $\boldsymbol{\lambda}_{\Lambda}, \boldsymbol{\mu}_{\Lambda}, \boldsymbol{\nu}_{\Lambda}, \boldsymbol{\eta}_{\Lambda}$ are the associated Lagrange multipliers, with respect to *potentially new* trial functions collected in the set $\Pi^{\ell}_{w_i}$ and encoded by their expansion coefficients $\boldsymbol{d}^{\ell}_{w_i,\Pi_i}$. Large gradients are taken as an indication to identify parameterization functions of large impact. In particular, the current $w^{\ell}_{\Lambda_i}$ is expanded by *zero*, i. e. $w^{\ell}_{\Lambda_i} = \boldsymbol{d}^{\ell\,T}_{w_i} \boldsymbol{\Psi}_{\Lambda_{w_i}} + \boldsymbol{d}^{\ell\,T}_{w_i,\Pi_i} \boldsymbol{\Psi}_{\Pi_{w_i}}$ with $\boldsymbol{d}^{\ell}_{w_i,\Pi_i} = \boldsymbol{0}$. Local neighbors of the trial functions in $\Lambda^{\ell}_{w_i}$ are excellent *candidates* for for $\Pi^{\ell}_{w_i}$ where we require $\Pi^{\ell}_{w_i} \cap \Lambda^{\ell}_{w_i} = 0$. Once the gradients

$$\boldsymbol{r}^{\ell}_i := \frac{\partial \mathcal{L}_{\Lambda}}{\partial \boldsymbol{d}^{\ell}_{w_i,\Pi_i}} |_{\xi = \xi^{*\ell}_{\Lambda}}, \quad i = 1, \dots, n_w$$

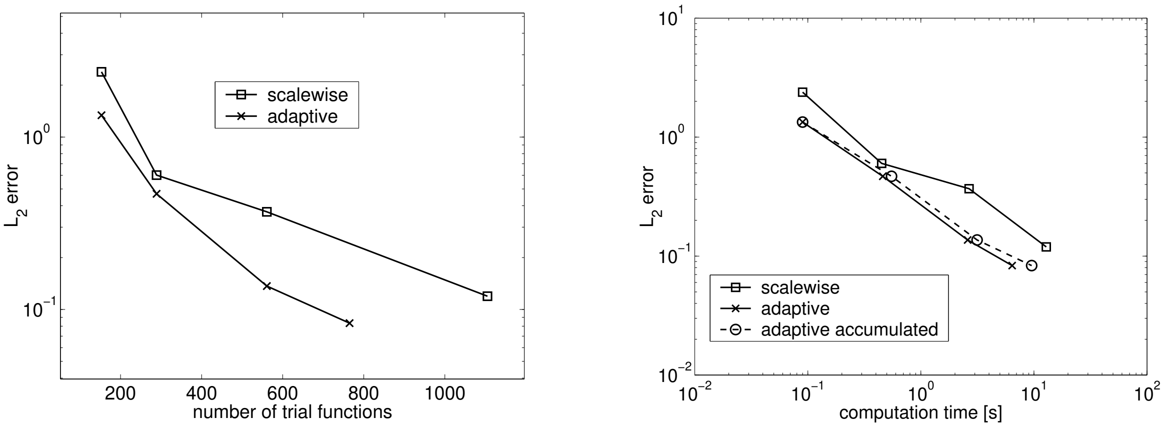

Figure 1: Comparison of scale wise vs. adaptive refinement

are computed at the current optimal solution $\xi_\Lambda^{*\ell} := \{\boldsymbol{x}_\Lambda^{*\ell}, \boldsymbol{y}_\Lambda^{*\ell}, \boldsymbol{\lambda}_\Lambda^{*\ell}, \boldsymbol{u}_\Lambda^{*\ell}, \boldsymbol{\nu}_\Lambda^{*\ell}, \boldsymbol{\eta}_\Lambda^{*\ell}\}$ we collect the trial functions associated to the larger absolute gradients in the $\Gamma_{w_i}^\ell$ while the smaller ones are neglected. The directional gradients can be inexpensively evaluated using the adjoint formula (Fletcher, 1987) taking the already computed Lagrange multipliers $\boldsymbol{\lambda}_\Lambda^{*\ell}, \boldsymbol{\mu}_\Lambda^{*\ell}, \boldsymbol{\nu}_\Lambda^{*\ell}$ associated to the optimal solution $\xi_\Lambda^{*\ell}$ into account. In areas where inequality restrictions are active large gradients might be obtained. Here, refinement might not increase the approximation quality since the active inequalities already bound the solution. However, simple heuristics can be applied which exclude refinement in these areas by analyzing the active inequalities.

Eliminating trial functions: The discretization structure of the approximations for $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{w}$ might change during the cycles of refinement such that we are interested in the elimination of currently unnecessary trial functions in $\boldsymbol{x}_\Lambda^\ell, \boldsymbol{y}_\Lambda^\ell, \boldsymbol{w}_\Lambda^\ell$. Similar to the previous section, the compression is based on the norm equivalences and the vectors $\boldsymbol{d}_x^\ell, \boldsymbol{d}_y^\ell, \boldsymbol{d}_w^\ell$ and are searched for their significant coefficients which are collected in $\tilde{\Lambda}_x^\ell \subseteq \Lambda_x^\ell$, $\tilde{\Lambda}_y^\ell \subseteq \Lambda_y^\ell$, $\tilde{\Lambda}_w^\ell \subseteq \Lambda_w^\ell$.

Final algorithm: The refinement algorithm proceeds as follows:

(1) Solve problem P2 at Λ^ℓ.
(2) Refine $\boldsymbol{z}, \boldsymbol{u}$ by thresholding $\to \Gamma_z^\ell, \Gamma_u^\ell$.
(3) Estimate discretization error of $\boldsymbol{x}_\Lambda^\ell, \boldsymbol{y}_\Lambda^\ell$ and locally refine areas with large errors $\to \Gamma_x^\ell, \Gamma_y^\ell$.
(4) Perform gradient tests of potential refinement functions for $\boldsymbol{w} \to \Gamma_w$. Check error and gradient tolerances and terminate refinement if satisfied.
(5) Compress current approximations $\boldsymbol{x}_\Lambda^\ell$, $\boldsymbol{y}_\Lambda^\ell$, $\boldsymbol{w}_\Lambda^\ell$ by thresholding $\to \tilde{\Lambda}_x^\ell, \tilde{\Lambda}_y^\ell, \tilde{\Lambda}_w^\ell$ and define $\tilde{\Lambda}_z^\ell := \Lambda_z^\ell$, $\tilde{\Lambda}_u^\ell := \Lambda_u^\ell$.
(6) Construct a new approximation $\Lambda^{\ell+1} := \tilde{\Lambda}^\ell \cup \Gamma^\ell$ taking interdependencies into account.
(7) $\ell := \ell + 1$, go to 1.

Potential savings are illustrated in Figure 1 where a comparison of the outlined adaptive algorithm with respect to uniform (scalewise) discretization is shown. The figure is based on a linear estimation problem generated from nonlinear model equations of an ethylene glycol process. In the adaptive case we start with a non–uniform mesh which has been computed by analysis of the measurement functions as outlined. Adaptive refinement uses less trial functions to obtain similar approximation quality compared to the scalewise approach. The CPU times of the QP solver needed to execute the refinement steps are shown as well. Since the computation time is strongly coupled to the number of trial functions adaptive discretization is more economical, even if one considers the accumulated times. Note, that here, although in principle possible, the computation does not employ a warm start using the previous solution $\xi_\Lambda^{*\ell-1}$.

4 Conclusions

We presented a framework which steadily refines the discretization of a dynamic optimization problem starting from an initial coarse grid and suggested a methodology which reuses the current solutions to generate improved discretization meshes. The suggested procedure leads to economic and nonuniform grids on which the optimization problem might be evaluated at less computational expense then on a uniform mesh of comparable accuracy. The approach explores differences in the time-frequency behavior of the solution. Local areas containing low frequencies are parameterized with large step sizes while on the high frequency areas the step size is chosen to be rather fine. Reductions in numerical expense should not be expected if the optimal solution does not reveal local differences in frequency content. The framework is not restricted to estimation problems, it can be applied to other more general dynamic optimization problems including nonlinear model predictive control (MPC) or nonlinear moving horizon estimation (RHE).

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