Felipe Souza Lima

Enhancement and versatility in self-optimizing control through surrogate models

Campina Grande, Paraíba, Brasil

Março, 2020

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Enhancement and versatility in self-optimizing control through surrogate models

Dissertação apresentada ao Programa de Pós-Graduação em Engenharia Química da Universidade Federal de Campina Grande, como requisito parcial para obtenção do grau de Mestre. Área de concentração: Engenharia Química.

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Supervisor: Dr. Antônio Carlos Brandão de Araújo

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For those who doubt themselves. Just embrace it.

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1 Os nomes dos integrantes do primeiro projeto abnTeX foram extraídos de `http://codigolivre.org.br/projects/abntex/`
2 `http://www.cpai.unb.br/`
3 `http://groups.google.com/group/latex-br`
4 `http://groups.google.com/group/abntex2` e `http://www.abntex.net.br/`

“To love the journey is to accept no such end.
I have found, through painful experience, that the most important step a person can take is always the next one.
(Dalinar Kholin, Oathbringer.)

Resumo

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Abstract

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Keywords: latex. abntex. text editoration.

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List of abbreviations and acronyms

CV	Controlled Variable
NLP	Non Linear Problem
RTO	Real Time Optimization
SOC	Self-Optimizing Control

List of symbols

Chapter 2

c	Controlled variable
d	Process disturbances
F	Optimal measurement sensitivity matrix with respect to the disturbances
G^y	Gain matrix with respect to the measurements
G^y_d	Gain matrix with respect to the disturbances
H	Linear combination matrix
J	Process objective function
J_{opt}	Optimal value of J
J_{ud}	Hessian of cost function with respect to the disturbance variables $\left(\frac{\partial^2 J}{\partial u \partial d}\right)$
J_{uu}	Hessian of cost function with respect to the manipulated variables $\left(\frac{\partial^2 J}{\partial^2 u}\right)$
L	Loss
n	Implementation error
$n^{y'}$	Implementation error with respect to the measurements
u	Manipulated variable
u_0	Process degrees of freedom
W_d	Diagonal magnitude matrix of disturbances
W_n	Diagonal magnitude matrix of measurement errors
x	Process states
y	Measurements
z	Loss variable

Chapter 3

$\hat{y}$	Metamodel (approximation) of y
$\mathcal{F}, f(x)$	Polynomial regression function
σ_l^2	Process variance

θ	*Kriging* hyperparameter of variable activity
ε	Residuals or random noise
p	*Kriging* hyperparameter of correlation smoothness
x	Input of a process, or sample
y	Function that calculates the output of a process
z	Stochastic departure function

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1 Introduction

This dissertation is about an assembly of several methodologies into a software tool, called *Metacontrol*, which enables a fast implementation of the Self-Optimizing Control (SOC) technique. This assembly consist of three major methodologies: *Kriging* metamodels, optimization through infill criteria and SOC. The dissertation is organized as follows:

Chapter 2 gives a brief summary of the key concepts involving SOC methodology and the main the reason why this research and software tool development was needed.

Chapter 3 presents a discussion of *Kriging* metamodels and its reasoning.

Chapter 4 introduces the process of constrained nonlinear optimization using *Kriging* metamodels. This process is also known as infill criteria.

Chapter 5 demonstrates how the assembly of the methodologies shown in chapters 2, 3 and 4 are combined to form the core concept behind *Metacontrol*.

Chapter 6 is dedicated to case-studies using *Metacontrol*. In addition, there is a brief discussion on good practices involving the use of the software tool.

The *Metacontrol* software is publicly available at `https://github.com/feslima/metacontrol`. There, the reader can find instructions on how to install the open-source tool. Also, for each technique discussed in chapters 2, 3 and 4, there is an open-source Python package as result. Their links are found in their respective chapters.

2 The Self-Optimizing Control overview

Every industrial process is under limitations ranging from design/safety (e.g. temperature or pressure which an equipment can operate, etc.), environmental (e.g. pollutant emissions), to quality specifications (e.g. product purity), and economic viability. More often than not, these constraints are applied all at once and can be conflicting. Therefore, it is mandatory to operate such processes optimally (or, at least, close to its optimal point) in order to attain maximum profits or keep expenses at minimum while still obeying these specifications.

One way to achieve this is through the application of plantwide control methodologies. In particular, Self-Optimizing Control (MORARI; STEPHANOPOULOS, 1980; SKOGESTAD, 2000; ALSTAD; SKOGESTAD; HORI, 2009) is a practical way to design a control structure of a process following a criterion (for instance: economic, environmental, performance) considering a constant set-point policy (ALVES et al., 2018). The SOC methodology is advantageous in this scenario because there is no need to reoptimize the process every time that a disturbance occurs.

However, the review presented here contains merely the paramount elements needed to understand the main concepts and expressions that translate the ideas behind the method. The author recommends them if the reader needs a more detailed explanation (SKOGESTAD, 2000; HALVORSEN et al., 2003; HORI; SKOGESTAD; ALSTAD, 2005; HORI; SKOGESTAD, 2007; ALSTAD; SKOGESTAD; HORI, 2009; ALVES et al., 2018; KARIWALA; CAO; JANARDHANAN, 2008; KARIWALA; CAO, 2009; UMAR et al., 2012).

The main concept of Self-optimizing control consists in the pursue of a control structure that is based on a constant setpoint policy, leading to near-optimal operation. From Skogestad (2004):

> "Self-optimizing control is when one can achieve an acceptable loss with constant setpoint values for the controlled variables without the need to reoptimize when disturbances occur."

It is assumed the process objective function, assumed scalar, is influenced by its steady-state operation. Therefore, the optimization problem described in Equation 2.1 is formed, with u_0 being the degrees of freedom available, x and d representing the states and the disturbances of the system, respectively.

$$\begin{aligned} \underset{u_0}{\text{minimize}} \quad & J_0\left(x, u_0, d\right) \\ \text{subject to} \quad & g_1\left(x, u_0, d\right) = 0 \\ & g_2\left(x, u_0, d\right) \leq 0 \end{aligned} \tag{2.1}$$

Regarding the disturbances, these can be: change in feed conditions, prices of the products and raw materials, specifications (constraints) and/or changes in the model. Using NLP solvers, the objective function can be optimized considering the expected disturbances and implementation errors.

Since the whole technology considers near-optimal operation, as a result of keeping constant setpoints (differently from RTO, for instance), there will always exist a (positive) loss, given by Equation 2.2

$$L = J_0(d, n) - J_{opt}(d) \tag{2.2}$$

Metacontrol focus on the first four steps of the Self-Optimizing Control technology, named by Skogestad (2000) as “top-down” analysis. In these steps, the variable selection seeking the usage of the steady-state degrees of freedom is the main problem to be addressed with the systematic procedure proposed. It is possible to search for a Self-Optimizing Control structure basically using two methods:

1. Manually testing each CV candidate, reoptimizing the process for different disturbances’ scenarios, and choosing the strucutre that yields the lowest (worst-case or average-case) loss;

2. Using local methods based on second-order Taylor series expansion of the objective function, that are capable of easily and quickly “pre-screening” the most promising CV candidates.

The manual nature of method 1 and the possibility of creating an automated framework using method 2 motivated the creation of *Metacontrol* itself. Applying, comprehensively, the second method in a software was also a key motivation for this work. Therefore, it is logical that the usage of the linear methods will be discussed in this section, since they are the ones implemented within *Metacontrol*.

A linear model with respect to the plant measurements can be represented as Equation 2.3

$$\Delta y = G^y \Delta u + G_d^y \Delta d \tag{2.3}$$

With

$$\begin{aligned} \Delta y &= y - y^* \\ \Delta u &= u - u^* \\ \Delta d &= d - d^* \end{aligned} \tag{2.4}$$

G^y and G_d^y are the gain matrices with respect to the measurements and disturbances, respectively. Regarding the CVs, linearization will give Equation 2.5

$$\Delta c = H \Delta y = G \Delta u + G_d \Delta d \tag{2.5}$$

With

$$\begin{aligned} G &= H G^y \\ G_d &= H G_d^y \end{aligned} \tag{2.6}$$

Linearizing the loss function results in Equation 2.7:

$$\begin{aligned} L = J(u,d) - J_{opt}(d) &= \frac{1}{2} \|z\|_2^2 \\ z = J_{uu}^{\frac{1}{2}} \left(u - u_{opt}\right) &= J_{uu}^{\frac{1}{2}} G^{-1} \left(c - c_{opt}\right) \end{aligned} \tag{2.7}$$

Later, Halvorsen et al. (2003) developing the exact local method, showed that the loss function can be rewritten as in Equation 2.8

$$z = J_{uu}^{\frac{1}{2}} \left[\left(J_{uu}^{-1} J_{ud} - G^{-1} G_d \right) \Delta d + G^{-1} n \right] \tag{2.8}$$

With J_{ud} and J_{uu} corresponding to the hessian with respect to the disturbances and manipulated variables $\left(\frac{\partial^2 J}{\partial u \partial d}\right)$ and with respect to the manipulated variables $\left(\frac{\partial^2 J}{\partial^2 u}\right)$, respectively. If one assumes that W_d is a (diagonal) magnitude matrix that considers the disturbances and W_n^y the magnitude matrix that takes into account the measurement error, and considering that both are 2-norm-bounded (Halvorsen et al. (2003) and Alstad, Skogestad, and Hori (2009) contains a discussion and justification for using 2-norm), Equations 2.9 to 2.11 can be defined to scale the system:

$$d - d^* = W_d d' \tag{2.9}$$

$$n = HW_n^y n^{y'} = W_n n^{y'} \tag{2.10}$$

$$\left\| \begin{pmatrix} d' \\ n^{y'} \end{pmatrix} \right\|_2 \leq 1 \tag{2.11}$$

The loss function from Equation 2.7 can be also written in a more appropriate way considering the definition of (ALSTAD; SKOGESTAD; HORI, 2009) of the uncertainty variables regarding the contribution of the disturbances and measurement error on the incurred loss, Equation 2.12 and considering the scaled system from Equations 2.9 to 2.11

$$M \triangleq [M_d \quad M_n^y] \tag{2.12}$$

where

$$\begin{aligned} M_d &= -J_{uu}^{1/2} \left(HG^y\right)^{-1} HFW_d \\ M_{n^y} &= -J_{uu}^{1/2} \left(HG^y\right)^{-1} HW_{n^v} \end{aligned} \tag{2.13}$$

with F corresponding to the optimal measurement sensitivity matrix with respect to the disturbances.

Finally, if one uses all the definitions described so far, the worst-case loss for the effect of the disturbances and measurement error is given by Equation 2.14

$$L_{worst-case} = \max_{\left\| \begin{pmatrix} d' \\ n^{y'} \end{pmatrix} \right\|_2 \leq 1} = \frac{\bar{\sigma}(M)^2}{2} \tag{2.14}$$

Equation 2.14 shows that in order to minimize the worst-case loss, it is necessary to minimize $\bar{\sigma}(M)$, Equation 2.15:

$$H = \arg\min_{H} \bar{\sigma}(M) \tag{2.15}$$

This optimization problem was initially solved using a numerical search, as proposed by Halvorsen et al. (2003). Fortunately, Alstad, Skogestad, and Hori (2009) derived an explicit solution that gives the optimal linear combination of measurements coefficient matrix (H) that minimize the worst-case loss that exists due to the effect of the disturbances and measurement errors, in Equation 2.16

$$H^T = \left(\tilde{F}\tilde{F}^T\right)^{-1} G^y \left(G^{yT}\left(\tilde{F}\tilde{F}^T\right)^{-1} G^y\right)^{-1} J_{uu}^{1/2} \tag{2.16}$$

where

$$\tilde{F} = [FW_d W_n^y] \tag{2.17}$$

Assuming that $\tilde{F}\tilde{F}^T$ is full rank.

Equation 2.16 has three interesting properties proved by Alstad, Skogestad, and Hori (2009):

1. It applies to any number of measurements (n_y).
2. The solution for H was proved to minimize not only the worst-case, but also the average-case loss. Therefore, if one uses Equation 2.16 seeking the determination of a control strucutre that minimizes the loss at the worst-case scenario, he is also minimizing the loss for the average-case scenario. This was called as a "super-optimality" by Alstad, Skogestad, and Hori (2009).
3. The solution proposed minimizes the *combined* effect of the disturbances and the measurement errors, simultaneously.

Therefore, the usage of the explicit solution will give both the minimized worst and average case losses using a single evaluation, and will also consider the combined effect of the disturbances and measurement errors of the problem. Therefore, this solution it is the default one used in *Metacontrol*.

Another way of solving the optimization problem from Equation 2.15 is to use the Extended nullspace method (ALSTAD; SKOGESTAD; HORI, 2009). Differently from Equation 2.16, this solution does not consider the combined effect of the disturbances and measurement errors simultaneously. Instead, the problem is solved in two steps. The first regards "disturbance rejection": The loss is minimized with respect to disturbances. If there are remaining degrees of freedom, then the effect of the measurement errors can be minimized. The extended nullspace, differently from the exact local method, is not an optimal solution, instead being considered sub-optimal. (ALSTAD; SKOGESTAD, 2007; ALSTAD; SKOGESTAD; HORI, 2009). However, the authors of Alves et al. (2018) also translated the mathematical formulations of the extended nullspace method into Python, and it is intended to be implemented within *Metacontrol* GUI in future releases merely as a secondary feature, giving its sub-optimality. The solution using the extended nullspace method is depicted in Equation 2.18:

$$H = M_n^{-1}\tilde{J}\left(W_{n^y}^{-1}\tilde{G}^y\right)^{\dagger}W_{n^y}^{-1} \tag{2.18}$$

Since Equation 2.16 also minimizes the worst-case loss, its evaluation was also considered inside *Metacontrol*: the user can inspect the expected average-case loss for each control structure that can exist in the combinatorial problem. The expression for the average-case loss is a result of the work of Kariwala, Cao, and Janardhanan (2008) and is described in Equation 2.19:

$$L_{\text{average}} = \frac{1}{6\left(n_y + n_d\right)}\left\| J_{uu}^{\frac{1}{2}}\left(HG^y\right)^{-1}H\widetilde{F}\right\|_F^2 \tag{2.19}$$

Lastly, it was necessary to implement within *Metacontrol* a branch-and-bound algorithm capable of quickly searching the best control structures for each possible subset of a given process, using the incurred loss as metric. This was considered by the authors of Alves et al. (2018) as an obligatory feature, since when *Metacontrol* is being used, it was understood that the main idea was to, in a comprehensive software, the user operating it should be capable of inspecting the most promising control structures, and discarding the unnecessary evaluation of the unpromising structures (i.e.: With a high incurred loss - both average of worst-case scenario) to save time and effort. It is important to remember that there is an evident combinatorial problem that grows in an explosive fashion, as the number of the unconstrained degrees of freedom of the reduced space problem and the number of available measurements both increases. Without a search method that is capable of quickly discarding undesired solutions, the usability of *Metacontrol* would be seriously compromised. Luckily, there are several implementations of branch-and-bound algorithms tailored for Self-Optimizing Control studies purposes, such as in Cao and Saha (2005), Cao and Kariwala (2008) and Kariwala and Cao (2009).

From the aforementioned works, Kariwala and Cao (2009) it is of particular interest: the monotonic criterion implemented consists of the exact local method from Halvorsen et al. (2003) and derived explicitly by Alstad, Skogestad, and Hori (2009), which is used as the default methodology to pre-screen the most promising self-optimizing CV candidates in *Metacontrol*. Therefore, the usage of the proposed branch-and-bound algorithm by Kariwala and Cao (2009) it is not only convenient, making the software more effective, but also keeps the “calculation engine” from *Metacontrol* using the same criterion. It would not make any sense, for instance, using a branch-and-bound algorithm that outputs the index of the most promising CVs using the maximum singular value rule from Skogestad and Postlethwaite (2007) and use the CV index sequence from this algorithm to evaluate the worst-case loss. Fundamentally speaking, the orders of “best” control structures would not be the same, simply because the search method would be using an different criterion from the linear method implemented to evaluate the H matrix.

The Branch-and-Bound algorithm developed by Kariwala and Cao (2009) that was originally implemented in MATLAB® by them was translated to Python by the main author of Alves et al. (2018). The same is true for equations of Exact Local and Extended Nullspace methods described by Alstad, Skogestad, and Hori (2009). Those Python routines were packaged under the name of *pySOC* (Python-based Self-Optimizing Control), and can be found in `https://github.com/feslima/pySOC`, with the code being freely available for inspection, revision and suggestions.

3 *Kriging* reasoning

Metamodels are a way to represent the world in simpler terms. Think of them as a photograph, they do not capture the moment as whole but can represent it good enough. In this analogy, the moment is a complex process that it is too cumbersome to explain it completely in mathematical terms, and metamodels, as photographs, may serve the purpose of capturing the core trends of this process without being too unwieldy and not losing too much information.

There is a family of metamodeling methodologies, ranging from a simple linear regression to complex neural networks. However, this chapter will be dedicated to discuss *Kriging* surrogates.

The simplest form to represent a real world process (y) through a metamodel ($\hat{y}$) and its error (ε) is done through Equation 3.1.

$$y(x) = \hat{y}(x) + \varepsilon \tag{3.1}$$

The error ε is associated with the unmodeled effects of the inputs x and random noise (i.e. it cannot be explained in detail but cannot be ignored as well.). When using the *Kriging* methodology as metamodel, this error is assumed to be a probabilistic function of x, or in other words, this error is assumed to be *not* independent and identically distributed. The specific probabilistic function is represented by a Gaussian distribution with mean zero and variance σ^2.

$$\varepsilon = \varepsilon(x) \sim \mathcal{N}(0, \sigma^2) \tag{3.2}$$

As from Søren Nymand Lophaven, Hans Bruun Nielsen, and Jacob Søndergaard (2002), a *Kriging* metamodel is comprised of two parts: a polynomial regression $\mathcal{F}$ and departure function z of stochastic nature, as can be seen in Equation 3.3.

$$\hat{y}_l(x) = \mathcal{F}\left(\beta_{:,l}, x\right) + z_l(x), \quad l = 1, \ldots, q \tag{3.3}$$

The regression model, considered as a linear combination of t functions ($f_j : \mathbb{R}^n \to \mathbb{R}$), as defined in Equation 3.4.

$$\mathcal{F}\left(\beta_{:,l}, x\right) \equiv f(x)^T \beta_{:,l} \tag{3.4}$$

The most common choices for $f(x)$ are polynomials with orders ranging from zero (constant) to two (quadratic). It is assumed that z has mean zero, and the covariance between to given points, arbitrarily named w and x for instance, is defined by Equation 3.5:

$$\mathrm{Cov}\left[z_l(w), z_l(x)\right] = \sigma_l^2 \mathcal{R}\left(\theta_l, w, x\right), \quad l = 1, \ldots, q \tag{3.5}$$

With σ_l^2 being the process variance for the *lth* response component, and $\mathcal{R}(\theta, w, x)$ defined as the correlation model. In *Metacontrol*, the correlation model used is described in Equation 3.6.

$$\mathcal{R}\left(\theta_l, w, x\right) = \exp\left(-\sum_{i=1}^{m} \theta_l \left(w - x_i\right)^p\right), \quad \left(\theta_l \geq 0, p_l \in [0, 2]\right) \tag{3.6}$$

Two important concepts must be addressed at this point: The first regards the meaning of the hyperparameter θ, being interpreted as the "activity" of variable x, meaning that, a low value of θ indicates that the points are highly correlated (ALVES et al., 2018). In addition, the value of θ also indicates how fast the correlation goes to zero as the process moves in the *lth* direction, as discussed by Caballero and Grossmann (2008). The second concept regards the parameter p in Equation 3.6, that represents the "smoothness" of the correlation. As its value reduces, the rate of the initial correlation drops as the distance between w and x_i increases. When $p \approx 0$, there is a discontinuity between $Y(w)$ and $Y\left(x_i\right)$ (FORRESTER; SOBESTER; KEANE, 2008) and there is no immediate correlation between the given points.

The hyperparameters θ are degrees of freedom available for optimization purposes, seeking the improvement of the metamodel fitness. In Søren Nymand Lophaven, Hans Bruun Nielsen, and Jacob Søndergaard (2002), the optimal set of hyperparameters θ^* corresponds to the maximum likelihood estimation. Assuming a Gaussian process (LOPHAVEN, S.; NIELSEN, H.; SØNDERGAARD, Jacob, 2002), the optimal values of the hyperparameters solves Equation 3.9:

$$\min_{\theta} \left\{\psi(\theta) \equiv |R|^{\frac{1}{m}} \sigma^2\right\} \tag{3.7}$$

Where $|R|$ is the determinant of the correlation matrix. The internal optimizer used in *DACE* corresponds to a modified version of the *Hooke & Jeeves* method, as showed by S. N. Lophaven, H. B. Nielsen, and J. Søndergaard (2002).

As stated before, high-order data obtainment it is an obligatory step in the proposed methodology implemented in *Metacontrol*. Fortunately, Søren Nymand Lophaven, Hans Bruun Nielsen, and Jacob Søndergaard (2002) also derived expressions for Jacobian evaluation of a *Kriging* prediction (for full demonstration, consult Søren Nymand Lophaven, Hans Bruun Nielsen, and Jacob Søndergaard (2002)), given in Equation 3.8:

$$\hat{y}'(x) = J_f(x)^T \beta^* + J_r(x)^T \gamma^* \tag{3.8}$$

The expression for Hessian evaluation was derived by Alves et al. (2018) (full demonstration in appendix A of their work), and it is depicted in Equation 3.9:

$$\hat{y}''(x) = H_f(x) \beta^* + H_r(x) \gamma^* \tag{3.9}$$

Equations 3.8 and 3.9, differently from numeric/automatic differentiation, are not approximations and, instead, are analytical expressions derived by Søren Nymand Lophaven, Hans Bruun Nielsen, and Jacob Søndergaard (2002) and Alves et al. (2018). Therefore, it is expected a reduced error when one is using these expressions, if compared to techniques based in numerical approximation, considering that the *Kriging* metamodel used is precise enough.

For the design of experiments part, it was decided to implement the Latin Hypercube Sampling (LHS) because it allows to better sample the optimization domain without introducing ill-conditioning in the spatial correlation matrix calculated by the *Kriging* builder.

Lastly, both the LHS function and *Kriging* model builder/predictor were implemented as a separated package in Python under the name of *pydace* (from *Python toolbox for Design and Analysis of Experiments*). This package is a partial code translation from the MATLAB® toolbox implemented by Søren Nymand Lophaven, Hans Bruun Nielsen, and Jacob Søndergaard (2002) named *DACE* to the Python programming language. The link to the open-source code is `https://github.com/feslima/pydace`. There the reader can find a brief documentation on how to install and example of usage.

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Appendix

APPENDIX A – Quisque libero justo

Quisque facilisis auctor sapien. Pellentesque gravida hendrerit lectus. Mauris rutrum sodales sapien. Fusce hendrerit sem vel lorem. Integer pellentesque massa vel augue. Integer elit tortor, feugiat quis, sagittis et, ornare non, lacus. Vestibulum posuere pellentesque eros. Quisque venenatis ipsum dictum nulla. Aliquam quis quam non metus eleifend interdum. Nam eget sapien ac mauris malesuada adipiscing. Etiam eleifend neque sed quam. Nulla facilisi. Proin a ligula. Sed id dui eu nibh egestas tincidunt. Suspendisse arcu.

APPENDIX B – Nullam elementum urna vel imperdiet sodales elit ipsum pharetra ligula ac pretium ante justo a nulla curabitur tristique arcu eu metus

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Annex

ANNEX A – Morbi ultrices rutrum lorem.

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ANNEX B – Cras non urna sed feugiat cum sociis natoque penatibus et magnis dis parturient montes nascetur ridiculus mus

Sed consequat tellus et tortor. Ut tempor laoreet quam. Nullam id wisi a libero tristique semper. Nullam nisl massa, rutrum ut, egestas semper, mollis id, leo. Nulla ac massa eu risus blandit mattis. Mauris ut nunc. In hac habitasse platea dictumst. Aliquam eget tortor. Quisque dapibus pede in erat. Nunc enim. In dui nulla, commodo at, consectetuer nec, malesuada nec, elit. Aliquam ornare tellus eu urna. Sed nec metus. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas.

ANNEX C – Fusce facilisis lacinia dui

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