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KRIGING APPROXIMATION IN CEMENT PASTE EXPERIMENTAL PERFORMANCE

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Summary: *This contribution presents experiences and difficulties encountered during interpolation of experimental results by Kriging/DACE metamodel. Particularly, several combinations of regression and correlation parts have been tested and optimized in order to ensure monotonicity of the response. Even though a certain progress is reported in the current paper, the selection of the proper model still remains a challenging task.*

1. Introduction

Cement paste is a fundamental scale from which concrete inherits majority of its properties. Experimental results show considerable scatter in the elastic response of cement paste samples, however, virtual testing in a computer allows testing the influence of input parameters on resulting macroscopic response (Šmilauer, 2006). Last year, a combination of CEMHYD3D model with homogenization processes was employed as a basis for an optimization (Šmilauer et al., 2008), where the Young modulus and heat of hydration appear as objective functions. Question arises, whether results from the optimization of the virtual model can be trusted. Our proposed solution is based on a so-called robust optimization (Beyer and Sendhoff, 2007) where some selected distance to existing experimental results is employed as the robustness measure. Hence, our goal is to create the closest approximation to available experimental data and to provide estimation of the quality of that approximation.

In this contribution, we demonstrate that actually popular Kriging/DACE (acronym for Design and Analysis of Computer Experiments (Sacks et al., 1989)) approximation is far away from the surface that is expected to describe physical process underneath. Therefore, nonlinear optimization of the maximum monotonicity is presented. Overall, dozen of combinations of regression and correlation parts have been tested. Unfortunately, the importance of a proper regression part is more crucial than presented in the optimization literature (Jones, 2001). The authors have found a regression part that almost ideally describes the physical problem, however, the strict monotonicity has not been preserved.

2. Kriging metamodel

Since the response in terms of mixture parameters is non-linear, the Kriging/DACE (Jones, 2001) approximation in the space of hydration heat of available real measurements seems as

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natural choice. Generally, Kriging predictor is composed of a regression and interpolation part that constitutes the nonlinear surface among available data (Lophaven,, 2002):

$$\hat{y} = \boldsymbol{f}(\boldsymbol{x})^T \boldsymbol{\beta}^* + \boldsymbol{r}(\boldsymbol{x})^T \boldsymbol{\gamma}^* \ , \tag{1}$$

where ***f(x)*** is an a-priori selected set of basis functions creating the response surface and ***r(x)*** is the correlation term between an unsampled point $\boldsymbol{x}$ and known points $\boldsymbol{s}_i$, $i=1,...,m$: ***r(x)*** = $[R(\boldsymbol{\theta}; \boldsymbol{s}_1; \boldsymbol{x}) \ ... \ R(\boldsymbol{\theta}; \boldsymbol{s}_m; \boldsymbol{x})]^T$, where R is a-priori selected correlation function with unknown coefficients $\boldsymbol{\theta}$, see later. The regression part is solved by a generalized least squares solution

$$\boldsymbol{\beta}^* = (\mathbf{F}^T \mathbf{R}^{-1} \mathbf{F})^{-1} \mathbf{F}^T \mathbf{R}^{-1} \mathbf{Y} \ , \tag{2}$$

where $\mathbf{F}$ is a matrix containing ***f(x)*** evaluated at known sites $\boldsymbol{s}_i$, $\mathbf{R}$ stems for correlation among $\boldsymbol{s}_i$ using again the correlation function R and $\mathbf{Y}$ are known values of y_i at $\boldsymbol{s}_i$. The Kriging part then interpolates the residual leading to the system of linear equations

$$\mathbf{R}\boldsymbol{\gamma}^* = \mathbf{Y} - \mathbf{F}\boldsymbol{\beta}^* \ . \tag{3}$$

The use of such metamodel for optimization purposes is less demanding on the regression part since an interpolation is dominant and hence, the constant regression part usually suffices. Then, the correlation function is traditionally selected to obtain a positive-definite system of equations, mainly restricted to the form

$$\mathrm{R}(\boldsymbol{\theta}, \boldsymbol{w}, \boldsymbol{x}) = \prod_{j=1}^{n} \boldsymbol{R}_j(\boldsymbol{\theta}, w_j - w_i) \ . \tag{4}$$

In our case, a free Matlab toolbox DACE (Lophaven,, 2002) is utilized providing seven correlation functions, where five of them are presented in this work:

Name	$R(\boldsymbol{\theta}; d_j)$, $d_j = w_j - w_i$
EXP	$\exp(-\theta_j \lvert d_j \rvert)$
GAUSS	$\exp(-\theta_j d_j^2)$
LIN	$\max\{0, 1-\theta_j \lvert d_j \rvert\}$
SPHERICAL	$1-1.5\xi_j+0.5\xi_j^3, \quad \xi_j = \min\{1, \theta_j \lvert d_j \rvert\}$
SPLINE	$1-15\xi_j+30\xi_j^3$, for $0 \le \xi_j \le 0.2$
	$1.25(1-\xi_j)^3$, for $0.2 \le \xi_j \le 1$
	0 , for $\xi_j > 1$, $\xi_j = \theta_j \lvert d_j \rvert$

Tab. 1: Correlation functions

Note that at this point we still do not know the tuning/shape parameters $\boldsymbol{\theta}$. Their functionality is twofold: they express the anisotropy among dimensions and also determine the shape of the metamodel in the vicinity of given samples. Traditionally, these parameters are found a-posteriori by minimizing an expected mean squared error (MSE), which leads to the constrained nonlinear optimization problem. See e.g. (Jones, 2001) for discussion how to efficiently solve this problem without re-calculation of $\boldsymbol{\beta}^*$ and $\boldsymbol{\gamma}^*$ for this new $\boldsymbol{\theta}$.

Designation	C3S	C2S	C3A	C4AF	Gypsum	w/c	Fineness	Hydration heat (time in h, heat in J/g of cement)		
	Mass %	Mass %	Mass %	Mass %	Vol %	-	m2/kg			
Aalborg white	0,6660	0,2380	0,0340	0,0040	0,0360	0,400	390	24	48	168 [h]
								170,3	234	327 [J/g]
Principallo	0,554	0,184	0,082	0,091	0,051	0,375	530	9,42	80,24	400,00 [h]
								63,388	323,247	377,466 [J/g]
BAM Fontana	0,492	0,243	0,090	0,076	0,0652	0,300	380	10,01	144,03	310,69 [h]
								159,2624	295,6692	322,3247 [J/g]
Hua	0,688	0,075	0,081	0,092	0,04	0,420	400	24,00	168,00	600,00 [h]
								233,4	317,25	339,8 [J/g]
Robeyst	0,634	0,084	0,074	0,100	0,05	0,500	390	14,66	45,79	140,99 [h]
								94,07	238,623	348,757 [J/g]
Smolik_Litos	0,612	0,126	0,070	0,100	0,05	0,500	306	10,01	19,19	261,78 [h]
								59,9159	329,2083	466,1589 [J/g]
Tamtsia early	0,465	0,246	0,104	0,083	0,05	0,500	340	18,00	24,00	102,00 [h]
								279,4076	307,3484	447,0522 [J/g]

Tab. 2: Experimental results of hydration heat

3. Fitting of experimental data

Particular application is shown on experimental data see Tab. 2, obtained from seven sources, consecutively from top: Data measured at CTU by TAMAir isothermal calorimeter, from (Principallo et al., 2003), data from private communication and determined from evaporable water content and assumed potential hydration heat 480 J/g, from (Hua et al., 1995), (Robeyst et al., 2007), data measured at CTU by TAMAir isothermal calorimeter and finally, from (Tamtsia et al., 2004) assuming potential heat 500 J/g. In Tab.2 cement chemical composition, gypsum content, w/c and fineness are presented along with measurements of hydration heat at three different times recalculated for the same reference temperature of 20°C.

First, almost linear dependency within the input data caused by volume unity and hence the resulting ill-conditioning is solved by Principal Component Analysis (PCA) by transforming inputs into the space of principal directions and removing the direction with the smallest eigenvalue. Therefore, our approximation is a real function (hydration heat) of seven inputs – time plus seven original inputs transformed with PCA to the six dimensions. Next, several combinations of regression and correlation functions have been tested, see Fig. 1 and 2. Horizontal axes are for time and vertical axes for hydration heat. Note that zero point [0 h, 0 J/g] has been added to enforce a physically reasonable start of the heat-time relationship.

There are two main requirements on the approximation. We need an interpolation of experimental data to precisely describe the behavior in the vicinity of existing experiments and oppositely, the best possible description of the trend in extrapolation. This is of great importance since there is low number of available data and the range of parameters covered is usually also small. The deficiency of created metamodels for extrapolation purposes is clearly visible from Fig. 1 and 2. Whenever the metamodel is far away from given data, the prediction is approaching the mean trend. This means that in distant extrapolation we would obtain a flat surface in the case of a constant regression term and a linear surface in a linear case.

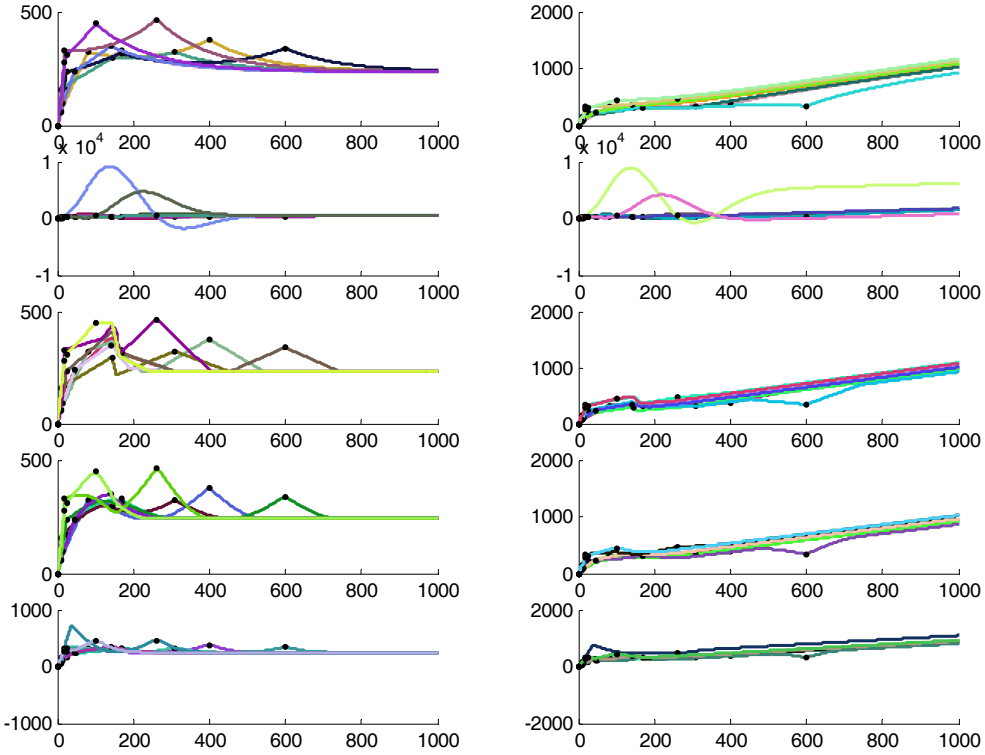

Fig. 1: Cuts of approximations for **not optimized weights** θ: Constant regression term (left column), linear regression term (right column) and (from top) five correlation functions.

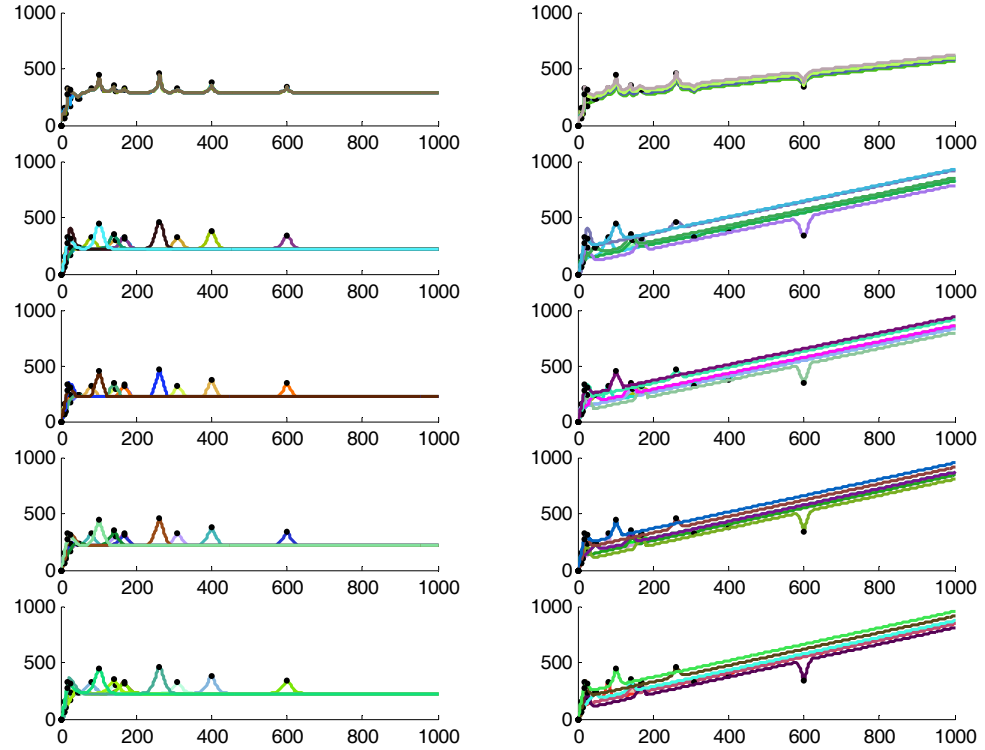

Fig. 2: Cuts of approximations for **optimized weights** θ **for minimal MSE**: Constant regression term (left column), linear regression term (right column) and (from top) five correlation functions.

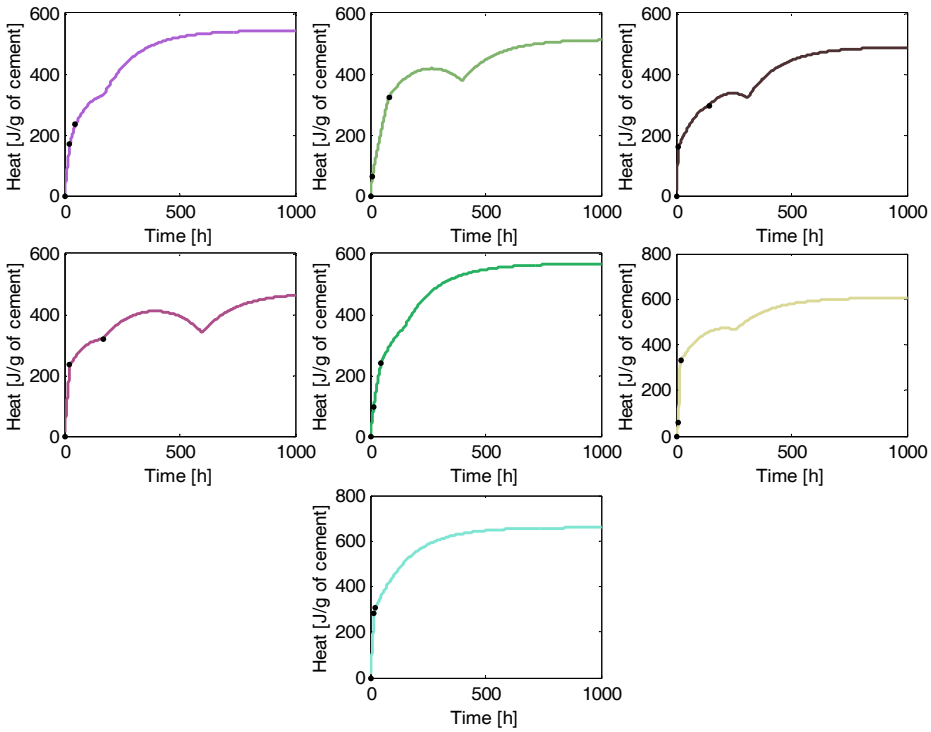

Fig. 3: Cut of approximation through experiments using exponential correlation function, linear term of composition and exponential regression term in time for **not optimized weights** θ.

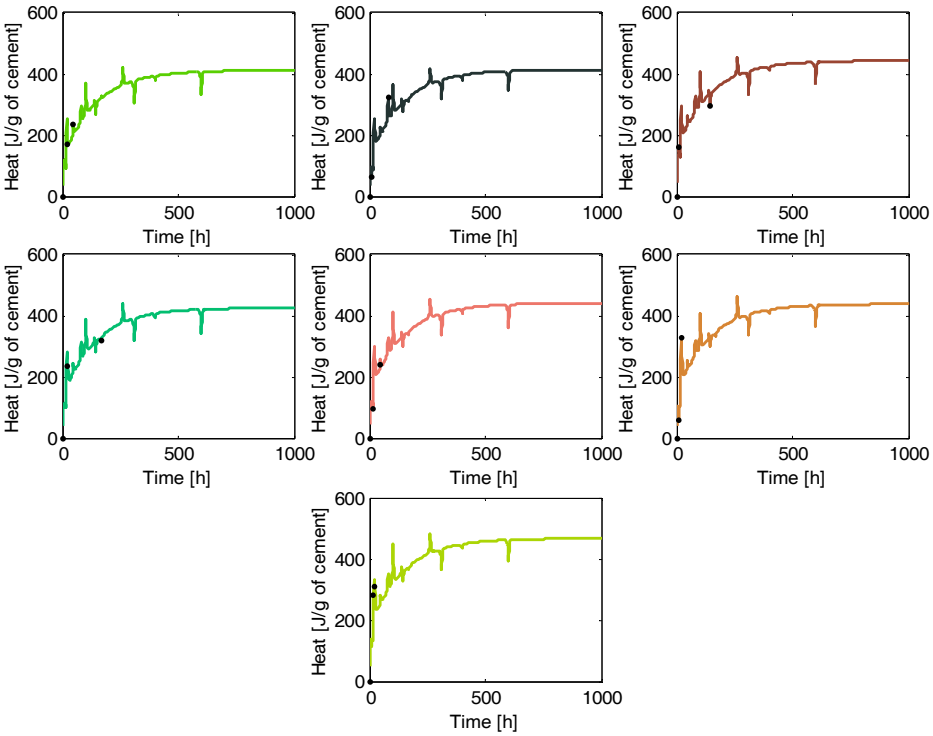

Fig. 4: Cut of approximation through experiments using exponential correlation function, linear term of composition and exponential regression term in time for **optimized weights θ for minimal MSE**.

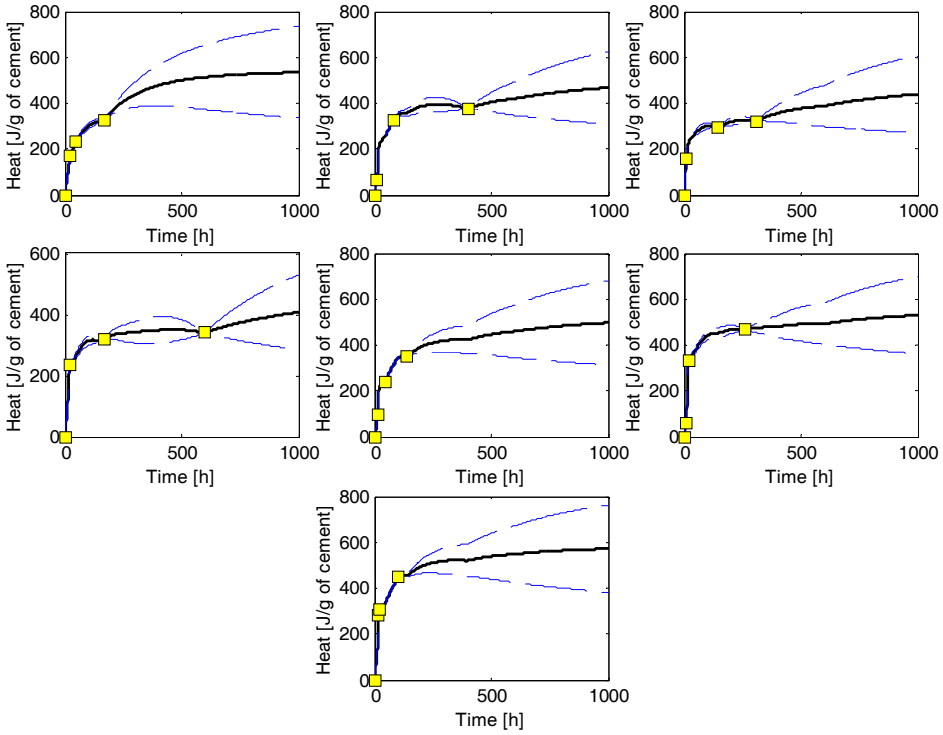

Fig. 5: Cut of approximation through experiments with expected mean (black continuous line) and MSE bounds (blue dashed lines) for **optimized weights θ for maximal monotonicity**.

We have tried a dozen of combinations of regression descriptions and correlation functions and finally, a combination of an exponential correlation function, a linear regression of mixture parameters and an exponential regression term $(1\text{-}e^{-T})$ for time T gives reasonable regression output, see Fig. 3. In Fig. 4, the result for optimized weights θ with respect to the minimal MSE is presented. Since the curve of hydration heat history should be (from physical principles) monotonous, the traditional MSE minimization is replaced by minimization of a negative (numerical) derivative of a resulting curve in the time direction. As an optimization algorithm, the Quasi-Newton line-search method available in Matlab Optimization toolbox was used. The optimization algorithm ran 6.5 minutes on AMD Turion MT-37 notebook processor with more than 700 evaluations of the metamodel. The resulting curves are presented in Fig. 5. The approximation that almost ideally describes the physical problem has been found, however, the strict monotonicity has not been preserved, see again Fig. 5.

4. Conclusion

The main advantage of the proposed methodology is that except expected mean Kriging prediction also offers an expected mean squared error (MSE) which serves as a good proxy for the distance from the available experimental data, i.e. MSE is zero at given points and is monotonously growing with the distance from the nearest known values, see again Fig. 5. Oppositely, main disadvantage is the exhausting search for proper model functions.

Finally, the search for the best closed-form approximation is still a black magic and is a part of know-how of every experienced curve fitter. Note that Genetic Programming can be used to solve this task using a burden of computational power, see e.g. (Streeter, 2001) for more details.

5. Acknowledgement

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