

HIGH DIMENSIONAL MODEL REPRESENTATION

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Abstrakt: In practical applications of the control theory, there is lack of approximation techniques applicable to intractable dynamic-programming equations describing the optimality controller. In the paper, we consider use of the technique coming from chemistry and called high dimensional model representation (HDMR). Its main advantages are finite order of expansion and rapid convergence for “well-defined” systems. The system model is “well-defined” if higher-order variable correlations are weak, permitting the model to be captured by the first few low-order terms of expansion. In fact, this is the only assumption for a meaningful application of HDMR. Provided it is satisfied, HDMR could play a role similar to neural networks. However it has clear mathematical background, which increases chance for success and offers novel opportunities for applications and theoretical research.

Use of the HDMR expansion to Bellman function – a solution of the the dynamic programming – is tempting. It separates original high dimensional input–output mapping into sum of low-order (possibly non-linear) mappings acting on orthogonal subspaces. The presented example indicates the way how the HDMR can be tailored to the control design and serves for inspection whether the basic HDMR assumption is applicable.

Keywords: nonlinear function approximation, HDMR, integral equations

1. INTRODUCTION

The key question in many scientific problems is to find the map between sets of high dimensional input and output system variables. That is the place where so called “curse of dimensionality” arises. Full space analysis without any a priori assumption has an exponentially growing computational complexity. Thus, some smart approximation is necessary.

High dimensional model representations (HDMR) (Rabitz and Alis, 1999) is a set of general approximative tools stimulated by applications in chemistry. In its background there stands the simple observation: only low-order correlations amongst the input variables have a significant impact upon the outputs. Such a presumption permits expressing single multidimensional mapping as a sum of many low dimensional mappings. The general form of the resulting expansion is:

$$f(x_1, x_2, \dots, x_n) \equiv f(x) \equiv f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{i=1}^n \sum_{j=1}^{i-1} f_{ij}(x_i, x_j) + \dots + f_{12..n}(x_1, x_2, \dots, x_n)$$

Here f_0 denotes effect of zero-order correlations, i.e., it is a constant value over the domain of $f(x)$; $f_1(x_1)$ describes an independent effect of x_1 ; $f_{12}(x_1, x_2)$ represents the joint effect of variables x_1 and x_2 and so on. Considering full n th order expansion we get only different, but still exact representation of the original mapping. Experience shows that even a low order HDMR expansion provides often a sufficient description of $f(x)$ in real problems. This motivates the usage of the second order expansion throughout this paper:

$$f(x) \approx \tilde{f}(x) \equiv f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{i=1}^n \sum_{j=1}^{i-1} f_{ij}(x_i, x_j)$$

Such a function approximation (representation) provides two main advantages. The first is data reduction. The exponentially growing amount of function values is represented via polynomially growing tables holding each function component (term in the general expansion). This property helps us to cope with high dimensional problems of real world. The second advantage is reduction of computational complexity. As we see below, HDMR is generated by a family of (linear) projections $P_{ijk\dots}$. Consequently, it allows splitting of any linear problem into easier low-dimensional subproblems.

Both these properties are promising in the context of control theory, where we face huge data spaces and unmanageable computational requirements. Unfortunately, the basic optimality condition arising from dynamic programming is highly non-linear. It is the well-known Bellman equation (Bellman, 1967), roughly written in this form:

$$V_t(d(t-1)) = \min_{a_t} \{E[z(y_t, a_t) + V_{t+1}(d(t)) | a_t, d(t-1)]\}, \quad d_t \equiv (y_t, a_t), \quad d(t) \equiv (d_1, \dots, d_t),$$

where $E[\cdot|\cdot]$ denotes conditional expectation. The strategy generating actions a_t satisfying this relation for all t minimizes the expectation of the overall loss $Z(y_T, a_T, \dots, y_1, a_1) \equiv \sum_{t=1}^T z(y_t, a_t)$. Its non-linearity is caused by the operator of minimization, which strongly reduces the possibility of using the HDMR.

That is why we formulate our problem in terms of fully probabilistic control design (Kárný *et al.*, 2005). Its optimality condition is also non-linear, but it allows us to make linear approximations easily. Resulting equations are linear integral equations for upper and lower bound of the exact solution. Then HDMR projectors are well-fitting not only for memory savings: important synergies arise also from the problem simplification.

Illustrative example is included at the end of this paper.

2. MATHEMATICAL BACKGROUND OF HDMR

The HDMR expansions are based on exploiting the correlated effect of the input variables. Let us assume that our input-output mapping is represented by a real scalar function $f(x) \equiv f(x_1, x_2, \dots, x_n)$ defined on the unit hypercube $K^n = [0, 1]^n$. On the same domain, we consider non-negative weight function $w(x)$ and define inner product of functions f and g as follows:

$$\langle f, g \rangle \equiv \int_{K^n} f(x)g(x)w(x)dx$$

Let X be vector space of functions with finite norm $\|\cdot\|$ inducted by this product and $f \in X$.

For convenience, we introduce a slightly generalized form of the inner product:

$$\langle f, g \rangle_M \equiv \int_{K^{n-|M|}} f(x_1, \dots, x_n) g(x_1, \dots, x_n) w(x_1, \dots, x_n) \prod_{i \notin M} dx_i$$

It returns $|M|$ -dimensional scalar function of all x_i for indices $i \in M \subseteq \{1..n\}$. Using $0 \equiv \emptyset$, we get $\langle f, g \rangle \equiv \langle f, g \rangle_0$.

Our aim is to find decomposition components f_0 , $f_i(x_i)$ and $f_{ij}(x_i, x_j)$ minimizing the approximation error $\|f(x) - \hat{f}(x)\|$. Its components are generated by projector operators defined in the following manner:

$$\begin{aligned} P_0[f] &\equiv f_0 = \frac{\langle f, 1 \rangle_0}{\langle 1, 1 \rangle_0} \\ P_i[f] &\equiv f_i(x_i) = \frac{\langle f, 1 \rangle_i}{\langle 1, 1 \rangle_i} - f_0 \\ P_{ij}[f] &\equiv f_{ij}(x_i, x_j) = \frac{\langle f, 1 \rangle_{i,j}}{\langle 1, 1 \rangle_{i,j}} - f_i(x_i) - f_j(x_j) - f_0 \end{aligned}$$

Construction of higher order HDMM decompositions is a simple generalization of this procedure.

The subsequent property of zero order component f_0 is crucial. For any real constant h it holds:

$$\langle f(x) - f_0, h \rangle = 0$$

It easily implies $\|f(x) - f_0 - h\|^2 = \langle f(x) - f_0 - h, f(x) - f_0 - h \rangle = \langle f(x) - f_0, f(x) - f_0 \rangle - 2\langle f(x) - f_0, h \rangle + \langle h, h \rangle = \|f(x) - f_0\|^2 + \|h\|^2 \geq \|f(x) - f_0\|^2$. In other words, f_0 is the best constant approximation of the original function $f(x)$. Similar identities are fulfilled also by higher order components and their meaning is analogous. Each HDMM component is the best approximation of $f_r(x)$ in the relevant class of functions with the same domain (here $f_r(x)$ denotes residuum of $f(x)$ after subtraction of all lower order HDMM components).

There is one important class of HDMM decompositions which is very comfortable to use. It is the case of separable weight function $w(x) \equiv \prod_{i=1}^n w_i(x_i)$. Then, all HDMM projectors are mutually orthogonal and the function space X could be written as a direct sum of their ranges.

We can reconsider our weight function and moreover require its normalization, $w(x)$ becomes probability density distribution over K^n whenever $\langle 1, 1 \rangle = \int_{K^n} w(x) dx = 1$. Now our well-known term $\frac{\langle f, 1 \rangle_i}{\langle 1, 1 \rangle_i}$ corresponds to the mean value of $f(x)$ over the conditional probability $w(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n \mid x_i)$. Reinterpretation of other terms is similar.

3. FULLY PROBABILISTIC DESIGN

This control design is based on two connected ideas. The first is to express loss function fully in probabilistic terms, i.e., to define desired probability densities of user actions a_t and observable output values y_t . Both are called ideal probability density function or briefly ideal pdf.

Next we search for the nearest admissible randomized strategy which is again some pdf. On that account we need to measure the distance of two pdfs. So called Kullback-Leibler divergence (Kullback and Leibler, 1951) is widely used in this context.

Let f, g be a pair of pdfs acting on a common set. Then, the Kullback-Leibler divergence $\mathcal{D}(f||g)$ is defined by the formula

$$\mathcal{D}(f||g) \equiv \int f(x) \ln \left(\frac{f(x)}{g(x)} \right) dx$$

Basic properties of KL divergence are the following ones:

1. $\mathcal{D}(f||g) \geq 0$
2. $\mathcal{D}(f||g) = 0$ iff $f = g$ (a.e.)
3. $\mathcal{D}(f||g) = \infty$ iff on a set of a positive dominating measure $f > 0$ and $g = 0$
4. $\mathcal{D}(f||g) \neq \mathcal{D}(g||f)$

The joint pdf $f(y_t, a_t, \dots, y_1, a_1)$ is fully describing all observable values for any $t \in \{1..T\}$ where T is horizon of optimization. We assume that this pdf can be factorized by a repetitive use of the well-known chain rule:

$$f(y_t, a_t, \dots, y_1, a_1) = \prod_{t=1}^T f(y_t|a_t, d(t-1)) f(a_t|d(t-1))$$

Where the first factors $\{f(y_t|a_t, d(t-1))\}_t$ describe possible reactions of the system on the decision a_t under the experience $d(t-1) \equiv (y_{t-1}, a_{t-1}, \dots, y_1, a_1)$. These pdfs form so called outer model of the system. Similarly, the pdfs $\{f(a_t|d(t-1))\}_t$ represent an outer model of the randomized decision strategy to be chosen. Next we factorize the desired ideal pdf consisting of "ideal system" pdf and "ideal input" pdf:

$${}^I f(y_t, a_t, d(t-1)) = \prod_{t=1}^T {}^I f(y_t|a_t, d(t-1)) {}^I f(a_t|d(t-1))$$

Now, the fully probabilistic design can be formulated. The optimal admissible, possibly randomized, decision strategy is defined as a minimizer of $\mathcal{D}(f || {}^I f)$. In (Kárný *et al.*, 2005; Kárný and Guy, 2006) we can found explicit formula for optimal strategy:

$$f(a_t|d(t-1)) = {}^I f(a_t|d(t-1)) \frac{\exp[-\omega_\gamma(a_t, d(t-1))]}{\gamma(d(t-1))},$$

where $\gamma(d(T)) \equiv 1$ and $\gamma(d(t-1))$ is just pdf normalization factor:

$$\gamma(d(t-1)) \equiv \int \exp[-\omega_\gamma(a_t, d(t-1))] {}^I f(a_t|d(t-1)) da_t$$

Function $\omega_\gamma(a_t, d(t-1))$ is determined by the following integral equation:

$$\omega_\gamma(a_t, d(t-1)) = \omega(a_t, d(t-1)) - \int f(y_t|a_t, d(t-1)) \log(\gamma(y_t, a_t, d(t-1))) dy_t \quad (1)$$

where $\omega(a_t, d(t-1))$ is known function defined this way:

$$\omega(a_t, d(t-1)) \equiv \int f(y_t|a_t, d(t-1)) \log \left(\frac{f(y_t|a_t, d(t-1))}{{}^I f(y_t|a_t, d(t-1))} \right) dy_t$$

We try to approximate equation (1) using second order HDMR projections. Optimal strategy $f(a_t|d(t-1))$ then arise from the knowledge of ω_γ easily.

4. APPROXIMATION OF BASIC FPD EQUATION

We must firstly linearize equation (1) to apply HDMR projectors efficiently. The use of the well-known Jensen inequality is promising. For convex function \exp , probabilistic measure $\mu(x)$ and any integrable function $h(x)$ it reads:

$$\int \exp[h(x)]d\mu(x) \geq \exp \left[\int h(x)d\mu(x) \right] \quad (2)$$

4.1 Upper bound of ω_γ

There are two possible applications of the Jensen inequality. The first give us lower bound for $\log(\gamma(d(t)))$:

$$\log \left[\int \exp[-\omega_\gamma(a_{t+1}, d(t))] {}^L f(a_{t+1}|d(t)) da_{t+1} \right] \geq - \int \omega_\gamma(a_{t+1}, d(t)) {}^L f(a_{t+1}|d(t)) da_{t+1}$$

and so the original exact equation (1) transform this way:

$$\omega_\gamma(a_t, d(t-1)) \leq \omega(a_t, d(t-1)) + \int \omega_\gamma(a_{t+1}, d(t)) {}^L f(a_{t+1}|d(t)) f(y_t|a_t, d(t-1)) da_{t+1} dy_t$$

This is the right time to redefine ω_γ as we need to fix its domain. We postulate the existence of sufficient statistic σ and define $\hat{\omega}_\gamma(\sigma(a_{t+1}, d(t))) = \omega_\gamma(a_{t+1}, d(t))$ where for all $t \in \{1..T\}$ and all possible actions a_{t+1} and realizations $d(t)$ it holds $v = \sigma(a_{t+1}, d(t)) \in V$. Than V is the domain of $\hat{\omega}_\gamma$. As the statistic is sufficient, all other functions dependant on a_{t+1} or $d(t)$ can be represented by functions of $v \in V$, e.g. $f(y_t|a_t, d(t-1)) = \hat{f}(y_t|\sigma(a_t, d(t-1))) \equiv \hat{f}(y_t|v)$. Now we rewrite the last inequality in more comfortable notation (omitting sign '^^'):

$$\omega_\gamma(u) \leq \omega(u) + \int k(u, v) \omega_\gamma(v) dv, \quad u = \sigma(a_t, d(t-1))$$

The probability densities ${}^L f(a_{t+1}|y_t, u)$ and $f(y_t|u)$ are hidden in the kernel function $k(u, v)$. It must also describe the dynamics of controlled system, i.e., $k(u, v)$ is nonzero only for compatible pairs of $u = \sigma(a_t, d(t-1))$ and $v = \sigma(a_{t+1}, d(t))$. The construction of such kernel function can be quite complicated, but it is always feasible. Considering only the equality part of above formula we conclude:

$$\bar{\omega}_\gamma(u) = \omega(u) + \int k(u, v) \bar{\omega}_\gamma(v) dv \quad (3)$$

It is a linear integral equation for $\bar{\omega}_\gamma$ and its solution fulfills $\bar{\omega}_\gamma \geq \omega_\gamma$. On the finite control horizon there is not any problem with the existence and uniqueness of solution (it could be analytically derived from boundary condition similarly to backward evaluation of the original equation (1)).

4.2 Lower bound of ω_γ

Multiplying equation (1) by -1 and applying exponential function on both sides we get:

$$\exp(-\omega_\gamma(a_t, d(t-1))) = \exp(-\omega(a_t, d(t-1))) \exp \left[\int \log(\gamma(y_t, a_t, d(t-1))) f(y_t|a_t, d(t-1)) dy_t \right]$$

The result is arranged for straight application of the Jensen inequality (2). After the introduction of the same sufficient statistics as in previous case and using identical kernel function $k(u, v)$ we get the following equation:

$$\exp(-\omega_\gamma(u)) \leq \exp(-\omega(u)) \int k(u, v) \exp(-\omega_\gamma(v)) dv$$

Rewriting it using definitions $\Omega_\gamma \equiv \exp(-\omega_\gamma)$ and $K(u, v) \equiv \exp(-\omega(u)) k(u, v)$ we obtain:

$$\Omega_\gamma(u) \leq \int K(u, v) \Omega_\gamma(v) dv$$

Now considering again only the equality part we get upper bound for $\Omega_\gamma(u)$:

$$\bar{\Omega}_\gamma(u) = \int K(u, v) \bar{\Omega}_\gamma(v) dv \quad (4)$$

It is again linear integral equation and in fact its solution gives us the lower bound of ω_γ :

$$\underline{\omega}_\gamma \equiv -\log(\bar{\Omega}_\gamma) \leq -\log(\Omega_\gamma) \equiv \omega_\gamma$$

Now we try to find numerical approximation of solution of both integral equations (3) and (4) which are formally almost equal.

5. HDMR BASED SOLVING OF LINEAR INTEGRAL EQUATIONS

Here we consider general integral equation of the second kind for unknown real scalar function $\phi(x)$ defined for all $x \in X$, $\dim(X) = n$, $X = \prod_{j=1}^n X_j$, and $f(x), \kappa(x, y)$ are also real scalar functions $\text{dom}(f) = X, \text{dom}(\kappa) = X \times X$:

$$\phi(x) = f(x) + \int_X \kappa(x, y) \phi(y) dy \quad (5)$$

The classical technique of successive approximation is well developed for integral equations of this kind. Even though we do not use it, mainly for colossal memory demands of our data. We try HDMR based approximation. The idea is straightforward: split this equation through HDMR projections and solve it separately on each component. Firstly we must decompose the data, still up to the second order.

$$\phi(x) \approx \tilde{\phi}(x) \equiv \phi_0 + \sum_{i=1}^n \phi_i(x_i) + \sum_{i=1}^n \sum_{j=1}^{i-1} \phi_{ij}(x_i, x_j)$$

$$f(x) \approx \tilde{f}(x) \equiv f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{i=1}^n \sum_{j=1}^{i-1} f_{ij}(x_i, x_j)$$

The function $\kappa(x, y)$ is decomposed only in the first variable, i.e. for all $y \in X$ we decompose $\kappa_y(x) \equiv \kappa(x, y)$ and then for each component we return to the expanded notation:

$$\kappa(x, y) \approx \tilde{\kappa}(x, y) \equiv \kappa_0(y) + \sum_{i=1}^n \kappa_i(x_i, y) + \sum_{i=1}^n \sum_{j=1}^{i-1} \kappa_{ij}(x_i, x_j, y)$$

Now introduce set Λ_n which contains all possible indexes of HDMR projectors up to second order, $I_n = \{1..n\}$:

$$\Lambda_n = \binom{I_n}{0} \cup \binom{I_n}{1} \cup \binom{I_n}{2}$$

Then for each $\lambda, \nu \in \Lambda_n$ we define ensuing marginalization of each kernel function component:

$$M_\nu^\lambda(y_\lambda) \equiv \int \kappa_\nu(x_\nu, y) \prod_{i \notin \lambda} dy_i,$$

where y_λ is usable shortcut with following meaning: $f(y_{\{i,j\}})$ stands for $f(y_i, y_j)$ and $f(y_{\{0\}}) \equiv f(\emptyset)$ denotes real constant. Other cases are similar. One more particular example will help to understand this notation properly:

$$M_1^{2,4}(y_2, y_4) \equiv M_{\{1\}}^{\{2,4\}}(y_{\{2,4\}}) = \int \kappa_1(x_1, y_1, \dots, y_n) \prod_{i \notin \{2,4\}} dy_i$$

Substituting $\tilde{\phi}(x)$, $\tilde{f}(x)$ and $\tilde{\kappa}(x, y)$ into the original integral equation (5) we get system of linear equations indexed by $\lambda \in \Lambda_n$:

$$\phi_\lambda(x_\lambda) = f_\lambda(x_\lambda) + \phi_0 M_\lambda^0(x_\lambda) + \sum_{i=1}^n \int_{X_i} \left[\phi_i(y_i) M_\lambda^i(x_\lambda, y_i) + \sum_{j=1}^{i-1} \int_{X_j} \phi_{ij}(y_i, y_j) M_\lambda^{ij}(x_\lambda, y_i, y_j) dy_j \right] dy_i$$

Where the dimension of each equation correspond to the size of $x_\lambda \in \Lambda_n$. For $\lambda = \{0\}$ it reduces to just one equation. For $\lambda = \{i\}$ is x_λ vector corresponding to the sample points in subspace X_i and this equation can be rewritten into classical matrix notation. For λ consisting of two elements is situation more complicated but the key observation is still valid: for each unknown scalar variable on the left side we have exactly one linear algebraic equation. Thus we have complete system of linear equations and we can determine all $\phi_\lambda(x_\lambda)$. In other words we determine the HDMR approximation of $\phi(x)$ which is the exact solution of general integral equation (5).

6. ILLUSTRATIVE EXAMPLE

In last section we developed HDMR based technique for solution of linear integral equations to solve equations (3) and (4) for exact solution bounds $\bar{\omega}_\gamma(u)$ and $\underline{\omega}_\gamma(u)$. Here we show one example of proposed method.

Our problem is one of the simplest control problems, the problem of Unknown coin tossing. We play hazard game with (two-sided) coin. Only one side is the winning one as usual in such games. What is more, this coin is unfair and we do not know the pay-off probability of any side. We do not even know if the result of tossing depends somehow on the coin starting orientation. Our only, but crucial knowledge is that the pay-off probabilities are fixed, i.e. we still play with the same coin. The very last note to the rules: we are lazy players, as usual, and therefore we prefer not to turn coin between subsequent game turns. If the coin fall on tail, for instance, we will let it be and toss again - if the expected gain of coin turning is low.

Using previous notation have $T > 0$ as a number of game turns, $y_t, a_t \in \{0, 1\}$ for all $t \in \{1..T\}$ where y_t represent observed value (side of coin) and a_t our action (selected coin side

before tossing). As the coin is still the same, we can easily define sufficient statistics. For any combination of $k, l \in \{0, 1\}$ let $n_{k/l}^t \equiv \sum_{i=1}^t \delta_{y_i, k} \delta_{a_i, l}$, then

$$\sigma(a_t, y_{t-1}, a_{t-1}, \dots, y_1, a_1) = (a_t, n_{0/0}^t, n_{0/1}^t, n_{1/0}^t, n_{1/1}^t)$$

It implies form of solution domain $V = \{0, 1\} \times \{0..T\}^4$ with one important constraint: for any $k, l \in \{0, 1\}$ we see $n_{k/l}^0 \equiv 0$, than in each game turn must occur exactly one of these four possibilities, therefore $n_{0/0}^t + n_{0/1}^t + n_{1/0}^t + n_{1/1}^t = t \leq T$. This is our motivation for usage of general non-separable weight in HDMR decomposition. It will be the characteristic function of set realizing this constraint.

By the technique of Bayesian estimation (Kárný *et al.*, 2005) we get the pdf of system model:

$$f(y_t|v) \equiv f(y_t|a_t, d(t-1)) = \frac{n_{y_t/a_t}^t + 1}{n_{0/a_t}^t + n_{1/a_t}^t + 2}$$

Now we must express our aims in terms of ideal pdfs. Both are defined over two point discrete set, therefore each of them is characterized by one scalar constant. Ideal system model express our aim of achieving just one, winning side of coin (let us say it is the side "0"). This pdf is parameterized by $\epsilon \in (0, 1)$:

$${}^I f(y_t | a_t, d(t-1)) \equiv {}^I f(y_t) = \epsilon \delta_{y_t, 1} + (1 - \epsilon) \delta_{y_t, 0}$$

Our ϵ is small but nonzero, as support of ${}^I f$ must coincide with set of observable values. Ideal user input express our "laziness" which is parameterized by $\tau \in (-1, 1)$:

$${}^I f(a_t | d(t-1)) \equiv {}^I f(a_t | y_{t-1}) = \frac{1 - \tau}{2} + \tau \delta_{a_t, y_{t-1}}$$

For $\tau \geq 0$ it penalize coin turning, $\tau = 0$ means we are coin-turning indifferent and $\tau \leq 0$ express even our positive fixation on coin-turning.

Take look at equations (3) and (4) we now miss only the formula for kernel function $k(u, v)$. It could be written this way: for $u \equiv (\bar{a}, \bar{n}_{0/0}, \bar{n}_{0/1}, \bar{n}_{1/0}, \bar{n}_{1/1})$ and $v \equiv (a, n_{0/0}, n_{0/1}, n_{1/0}, n_{1/1})$

$$k(u, v) = \sum_{y \in \{0,1\}} \prod_{i,j \in \{0,1\}} \delta_{\bar{n}_{ij}, n_{ij} + \delta_{y,i}} \delta_{a,j} {}^I f(a | y) f(y | u)$$

The rest of work consist mainly from kernel function marginalization and composition of following linear system, which could be easily solved as common problem of numerical mathematics.

7. CONCLUSIONS

We made just few experiments with values $T = 10$, $\epsilon = 0.1$ and $\tau = 0.5$. The choice of such a low horizon is determined by need of the exact solution to compare with. Lower and upper bounds of ω_γ seem to be rather good, their maximal difference is only about 30%. Other results are strange for a first sight, optimal strategy tends to give worse results than its approximation. Now we can not conclude anything more as this idea is fresh and needs more examination.

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