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A multi-objective optimization concept for risk-based early-warning monitoring networks in well catchments

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Abstract

Groundwater wells are often protected by restricted land use within wellhead protection zones. Unfortunately, one cannot restrict land use in the entire catchment (especially in urban areas), and there is uncertainty in wellhead delineation. Thus, nearly all well catchments have an entire inventory of risk sources. Each of these risk sources may fail at any time, release contamination and affect the well earlier or later. In fact, most catchments are equipped with some form of monitoring network. Such networks, however, often grow historically, follow various purposes that changed over time, and thus are often suboptimal (if not even inadequate) for rigorous risk control. In this work, we propose a concept to plan monitoring networks through multi-objective optimization. The different objectives are minimal costs, maximal probability to detect all possible contaminants once they entered the aquifer, and earliest possible detection. Also, risk sources that are classified as severe versus medium or tolerable should be treated with different priorities. Therefore, we propose to treat detection probability and early-warning time as separate objectives for each risk class. The concept will allow catchment managers to obtain optimal monitoring networks for risk control, and to gain insight into the costs of certainty, the costs of early warning, and the costs of covering top risks versus the luxury situation of controlling even minor risks.

Keywords: Optimal monitoring, detection probability, early-warning time, multi-objective optimization, uncertainty, risk

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1. Motivation and state of the art in catchment monitoring

Groundwater wells are often protected by restricted land use within wellhead protection zones [1], but this does not remove all risks due to two reasons. First, one cannot restrict land use in the entire catchment (especially in urban areas). Second, there is no absolute certainty in knowing the catchment of the well [2]. Thus, nearly all well catchments have an entire inventory of hazardous activities or places [3], called risk sources in the following. Each risk source may fail at any time, release contaminants and affect the produced water quality earlier or later. This issue triggered research for (probabilistic) aquifer/well vulnerability or risk analysis [4,5,6,7,8]. While such works help to evaluate the risk sources to which the production well is exposed, it is not yet helpful in controlling them.

In order to track the quality of groundwater prior to pumping, most well catchments are equipped with monitoring networks. Unfortunately, such networks usually grow historically, following various purposes over time (e.g., monitoring groundwater levels or risks that ceased to exist). Therefore, they are suboptimal, if not even inadequate, for rigorous and cost-efficient risk control. The prioritization according to risk perception is done implicit (because monitoring wells are often added to monitor the risk sources currently perceived as most severe), but seldom done in a coordinated fashion.

Overall, an increase in safety and cost efficiency could be achieved by formal, risk-prioritized optimization of monitoring networks. In this context, one must acknowledge that the goals of monitoring are manifold; they include maximal detection probability, the earliest possible detection (resulting in a maximal time available to install counter measures), and least costs for the network installation and operation. Hence, concepts of multi-objective optimization [9] seem adequate.

There is ample literature on groundwater monitoring [10]. However, such studies focus on monitoring a known, existing large-scale quality problem or a single plume. They do not account for the fact that there are multiple known risk sources which need to be monitored for potential future contaminant release. Alternatively, there is research on detection sensor networks in the signal processing literature [11], but without existing applications in well catchments.

Also, early warning systems are often found in the context of natural hazards (such as tsunami or earthquake warning systems, e.g., [12]), but their only appearance in contaminant hydrogeology is the study by Yenigül et al. [13] for landfill monitoring. These authors account for early warning through a cost penalty for the more difficult remediation of longer plumes after later detection.

Next, it is well known in the field of long-term groundwater quality monitoring that the monitoring objectives are diverse and may even change over time. Examples for competing monitoring objectives are to estimate total contaminant fluxes, to estimate spatial maps of concentrations, to identify the outline of a plume, and so forth [14]. Therefore, multi-objective optimization has found many applications in that area. Yet, in the context of risk control for well catchments, no such ideas can be found to date. Finally, there are indeed many studies on vulnerability and risk quantification, but their output has never been used to find a risk-prioritized monitoring network design.

2. Goals, suggested approach and expected benefits

Our overall motivation is to provide risk control in well catchments through optimal monitoring. We wish to detect with maximum probability all possible future contaminations that might affect the well’s water quality. Second, we wish to provide maximal early warning time for installing counter actions. Third, we seek minimal costs for installing and operating the monitoring network. Finally, we want to acknowledge that contaminations can emanate from more or less severe risk sources.

Our suggested approach is to categorize all known risk sources (e.g., high, medium, tolerable risk sources), and then define detection and early warning as separate objectives for each of these risk
categories. Only the objective of minimum costs cannot be separated in a meaningful manner, because individual monitoring wells might serve to simultaneously monitor several risk sources from different categories. Technically, we propose to combine models for flow and transport, Monte-Carlo methods to account for uncertainty, qualitative risk analysis and multi-objective approaches (detection, early warning and cost efficiency) for an overall optimization of monitoring networks in well catchments. It follows from the above state of the art, that this proposed combination is novel in many aspects.

Why use multi-objective optimization? We see the following two advantages:

1. The considered objectives are competitive and mutually exclusive. The actual trade-off and best compromise between these goals cannot be predicted in advance. Instead, they depend on the hydro(geo)logy of the catchment, the risk inventory, pre-existing monitoring wells, legal boundary conditions, health standards, the willingness to pay for monitoring, and on the speed at which counter actions can be installed. With multi-objective optimization, the actual preferences of the decision maker between these competing objectives do not have to be known a priori. Instead, they can evolve while viewing the multi-objective results [9]: The solution of a multi-objective optimization problem is not a unique optimum, because multiple competing objectives do not infer a unique ranking. Instead, solutions are ranked according to their domination. A solution is said to be dominant over a second solution, if it is better in at least one objective, and equal in all others. The multi-objective solution is the so-called Pareto front, i.e., the set of dominant solutions. The final decision is found by discussion and then choosing from the Pareto-optimal solutions.

2. Risk perception is a difficult matter. In specific, the aversion against risk is subjective, and may depend on the involved persons, legal boundary conditions, availability of funds to treat risk, and on corporate philosophies concerning safety standards [15]. Thus, if risk perception is ambiguous, then risk prioritization for monitoring is not an easy task. Our idea is to define different objectives for the different risk categories. The approach of multi-objective optimization will then disclose the trade-off between covering (certain and early detection) only severe risks or also medium and tolerable risks versus the additional costs, and so deliver substantial decision support.

Why use qualitative risk categorization? The existing alternatives are only to not quantify risk at all, or to perform qualitative risk assessment. The former will not help for risk-based prioritization of the monitoring. The latter is certainly the scientifically soundest option, minimally subjective [16], and might even achieve a risk-based weighting of all risk sources as prioritization scheme. When admitting realistic conditions, however, quantitative risk assessment is practically not achievable. In fact, for each risk source within the catchment, a lot of data would have to be known. Examples are the complete list and masses of stored or handled contaminants, the probability distribution of possible contaminant release masses and durations in case of failure, the failure frequency, and so forth [17]. For realistically-sized catchments in urban regions, this is immensely infeasible. Depending on national laws, such data will even be protected and impossible to collect.

3. The proposed concept and methods in detail

3.1. Multi-objective optimization formulation

The multi-objective optimization problem sketched in Section 2 can be formulated as:

$$d_{opt} = \arg \min_{d \in D} \left[ f_{\text{detect}} \cdot f_{\text{warn}} \cdot f_{\text{cost}} \right], \quad (1)$$
where \( \mathbf{d}_{\text{opt}} \) is the optimal choice for the decision variables \( \mathbf{d} \) that define the monitoring system (e.g., monitoring well positions, filtering depth and window), \( \mathbf{D} \) is the space of allowable designs (containing spatial restrictions for installing monitoring wells, maximum admissible costs and so forth), and \( f_{\text{detect}}, f_{\text{warn}}, f_{\text{cost}} \) are the three competing objectives. Each objective is formulated as a minimization problem, i.e., the minimal probability of not detecting any emitted plume, the minimal lost time between contaminant spill and detection, and minimal costs for installation and operation.

After discretizing the well catchment into a fine grid of candidate positions for monitoring wells, the decision vector \( \mathbf{d} \) resembles a spatial grid of Boolean yes/no decisions, possibly augmented by additional values for screening intervals or for sampling frequency. Other parameterization options are available as well. The choice made here results in a discrete optimization problem. Regardless of that choice, the resulting optimization problem is multi-objective, non-linear and high-dimensional. Available options include the NSGA-II, \( \varepsilon \)-NSGA-II, AMALGAM, or Borg algorithms, as reviewed by Reed et al. [18].

\[ \mathbf{d}_{\text{opt}} = \arg \min_{\mathbf{d} \in \mathbf{D}} \left[ f_{\text{detect}}^{\text{(red)}}, f_{\text{warn}}^{\text{(red)}}, f_{\text{detect}}^{\text{(yellow)}}, f_{\text{warn}}^{\text{(yellow)}}, f_{\text{detect}}^{\text{(green)}}, f_{\text{warn}}^{\text{(green)}}, f_{\text{cost}} \right]. \] (2)

3.2. Extending the multi-objective optimization for risk categories and model uncertainty

The objective functions \( f_{\text{detect}} \) and \( f_{\text{warn}} \) require some form of flow and transport models, which will be subject to uncertainty (see Section 3.3). Accounting for this uncertainty will make the optimized monitoring networks robust against model/parameter errors. Thus, we replace the affected objectives in Eq. (1) by their expected values, denoted by \( \langle f_{\text{detect}} \rangle \) and \( \langle f_{\text{warn}} \rangle \). The expected value is a risk-neutral approach to optimization under uncertainty [19]. Other choices will be mentioned in Section 3.3.

In Eq. (1), the optimization does not yet prioritize according to the risk posed by the risk sources. Following the idea of qualitative risk assessment (Section 2), we categorize the risk inventory into high-risk, medium risk and tolerable risk sources [16]. Such a risk ranking can be visualized with the colors of traffic lights, i.e., as red, yellow and green risk sources. These categories might be found with quantitative or semi-qualitative risk assessment methods, if desired. The minimal requirement, however, is merely that the classification reflects the risk perception and prioritization preferences of the involved stakeholders, in the sense that “red” risk sources should be covered with first priority, “yellow” ones later, and “green” ones only if their monitoring involves little or no additional costs. The risk ranking may even be influenced on purpose to reflect public risk perception, the corporate philosophy of the water supplier, or any other aspect that is relevant to yield a well-justifiable and transparent result.

In combination, we denote the detection probability and early warning time for each risk category as separate objective functions, and obtain a total of seven objectives (detection and early warning for each of the three risk categories, and the overall costs). With this step, we harvest the benefits of multi-objective optimization for the risk prioritization as discussed already in Section 2. Also, we harvest the advantages of robust optimization when using expected values of the objective functions as discussed in the same section. More details will be provided in Section 3.3. Finally, we obtain:

\[ \mathbf{d}_{\text{opt}} = \arg \min_{\mathbf{d} \in \mathbf{D}} \left[ f_{\text{detect}}^{\text{(red)}}, f_{\text{warn}}^{\text{(red)}}, f_{\text{detect}}^{\text{(yellow)}}, f_{\text{warn}}^{\text{(yellow)}}, f_{\text{detect}}^{\text{(green)}}, f_{\text{warn}}^{\text{(green)}}, f_{\text{cost}} \right]. \] (2)

3.3. Model-based formulation for the individual objective functions

We start with a flow and transport model to predict the transport of possible contaminant spills from risk sources to the well. Numerically, we recommend particle-tracking random walk algorithms due to their ease of implementation and their absence of numerical dispersion [20]. For each risk source, we
obtain maps of detectability (with concentration values above a given detection limit \( c_{\text{detect}} \)) and of early-warning time (time between detectability and first arrival of the contamination at the well). For the sake of computational efficiency, we propose to assume conservative tracer transport, which is actually a worst-case scenario for risk classification, and hence seems justified in the current context.

The resulting maps are subject to uncertainty due to the imperfection of models, parameter uncertainty, and due to changing hydrological drivers of the catchment. To cover the latter, one can work with a few hydrological scenarios (e.g., wet, medium or dry seasonal conditions; high, medium or low pumping rates at the well). If one wishes to represent parameter or conceptual uncertainty, then calibration-constrained Monte-Carlo simulations [21] or Bayesian model averaging [22] can be applied. In any case, one obtains a set of possible maps for each risk source that serve to represent uncertainty.

3.4. Formulating the individual objective functions

Monte-Carlo or scenario analysis with \( k=1\ldots n_k \) realizations of flow and transport from all \( i=1\ldots n_i \) risk sources via all \( j=1\ldots n_j \) potential monitoring well locations to the well yields the following data:

\[
\delta_{ijk} = \begin{cases} 
1 &: \text{failure of risk source } i \text{ at location } x_i \text{ exceeds detectable concentration } c_{i,\text{detect}} \\
0 &: \text{no detectable concentration} 
\end{cases}
\]

(3)

If \( \delta_{ijk}=1 \), we can also obtain the time \( \tau_{ijk,\text{detect}} \) between failure of risk source \( i \) and first arrival of a detectable concentration at monitoring candidate \( j \), as well as a time \( \tau_{ik,\text{well}} \) for first arrival of a critical concentration \( c_{i,\text{crit}} \) from risk source \( i \) at the production well in realization \( k \). Their difference yields the respective maximum achievable early warning time \( \tau_{ijk,\text{max}} \):

\[
\tau_{ijk,\text{max}} = \begin{cases} 
\max(\tau_{ik,\text{well}},\tau_{ijk,\text{detect}}) &: \text{maximum achievable early warning time (if } \delta_{ijk}=1) \\
0 &: \text{no early warning (if no detection, } \delta_{ijk}=0) 
\end{cases}
\]

(4)

However, the time intervals \( t_{\text{sampling}} \) between sampling rounds will reduce the actual early warning time by \( t_{\text{sampling}} \) multiplies with a random number \( u \) that is uniform on [0,1]. For the cost, one can write:

\[
b_i = b_{\text{install}}(x_i) + b_{\text{sample}} \left( \frac{\Delta t_{\text{budget}}}{\Delta t_{\text{sampling}}} \right)
\]

(5)

(or any more complex formulation), where the fraction after the required budget per sampling round \( b_{\text{sample}} \) resembles the number of sampling rounds per budget period \( \Delta t_{\text{budget}} \) that is relevant for the cost calculation. Based on these data, for each given monitoring network suggestion \( d \) (which fixes the choice of monitoring locations \( j \)), we obtain \( n_i \times n_k \) numbers \( \delta_{ik}^{(d)} \) and \( \tau_{ik}^{(d)} \) that express the performance of \( d \) to detect and provide early warning for each risk source \( i \) in realization \( k \), along with costs \( b_i^{(d)} \).

The remaining step is to combine these numbers into single numbers for the individual objective functions, where several options are perceivable: One might optimize the performance on average over
uncertainty by averaging over the realizations $k=1…n_k$ and over the random number $u$. Alternatively, one might optimize the guaranteed worst-case performance (using the minimum over the realizations including the random number $u$), or optimize for performances that can be guaranteed with a suitable probability (using percentiles). In fact, any statistical position parameter could be chosen.

With this choice done, one aggregated the $n_i \times n_k$ numbers $\delta_{ik}^{(d)}$ and $\tau_{ik}^{(d)}$ to only $n_i$ numbers $\delta_i^{(d)}$ and $\tau_i^{(d)}$. The resulting numbers reflect the performance of $d$ for each risk source $i$. These can be broken down into three smaller groups for each risk category (red, yellow, green). Finally, one has to choose how to rate the overall performance of a monitoring network across several risk sources within the same risk category. Again, the decision maker may choose any suitable statistical position parameter.

4. Illustration and discussion

Fig. 1 is a graphical illustration of how the optimization results may look like. For the sake of easy visualization, the figure shows only the three objectives considered in Eq. (1). Each sphere is one possible network design, located in the axes according to its goal attainment levels. The theoretical optimum (blue) is idealistic: fully certain and early detection cannot come at zero costs. The red spheres mark the Pareto front: none of them is dominated by any other sphere (recall Section 2 for the definition). All other suggestions are black, and equipped with transparency to visualize their domination rank (from black to invisible for increasing rank).

The green sphere illustrates a historically grown network. It has neither been optimized in a formal manner, nor under these objectives, and is therefore far below Pareto optimal. For example, by following the vertical green line, one could find a solution that has the same detection capability and costs, but can achieve a better early warning time. Minimum-cost transition strategies from a pre-existing network to an optimal one can be optimized as well by assigning no installation costs to positions with pre-existing wells. This will magnetically attract reasonable monitoring positions from the vicinity, and lead to new suggestions with small changes over the past network.

![Fig. 1. Illustration of multi-objective optimization results for monitoring networks.](image)

Next, we illustrate what locations of monitoring wells are optimal in the multi-objective sense. Fig. 2a shows a map of all locations where contaminant spills at a single risk source (red circle) are detectable without considering uncertainty. The map is shaded according to the early warning time from early
(green) to late (red). Thus, a good monitoring well is close to the risk source (crossed circle). In Fig. 2b, three risk sources from the same risk category (here: “red”) are monitored at the same costs (still using only one monitoring well). The optimal detection probability is achieved at locations where the involved flow/transport model predicts that the individual plumes will overlap. Such overlap can occur due to transverse dispersion, or if the plumes travel at different depth levels, yet are all visible in a fully filtered monitoring well. Within that overlap area, the optimum is again dictated through early warning.

However, the early warning level is now lower than in Fig. 2a. This clarifies the competing character of safe, cheap detection and early warning. To revert to the better early warning time from Fig. 2a, Fig 2c spends two monitoring wells, achieving a maximum early warning at increased costs.

In Fig. 2d, we start considering uncertainty. Even for a single risk source, there are several plausible transport paths, and thus the choice made in Fig. 2a is not robust under uncertainty. Instead, robust optimal monitoring wells reside where the possible plumes from a single risk source coincide with maximum probability. Thus, monitoring wells in the following will only appear in regions where predicted plumes are wide (because this correlates with maximum overlap probability). In fact, Fig. 2e moves one of the monitoring wells in Fig. 2c to a more robust position, at the price of later warning.

In Figs. 2f and 2g, we consider a second risk category (here: “yellow”). In Fig 2f, this is achieved at large additional costs, since no performance losses for “red” are accepted. However, at relatively small concessions in “red”, “yellow” can be covered at no additional costs. A possible least-cost option would actually be to use only the one monitoring well marked red in Fig. 2g, since it offers 100% detection probability for “red”, 50% for “yellow”, achieves a reasonable early warning time, and minimizes costs.

5. Conclusion and Outlook

In an ongoing project, we are applying this concept to obtain optimal monitoring networks. We work with simple synthetic catchments (rectangular domains and hypothetically inserted risk sources) in order to validate the method and its implementation. This is followed by application to a real test case, where

![Fig. 2. Illustration of effects that coordinate the position of Pareto-optimal monitoring wells: (a) single well for single risk source; (b)&(c) one or two wells for three risk sources (all from category “red”); (d) influence of uncertainty; (e) reaction to uncertainty; (f) including a second risk category (“yellow”) at large additional costs; (g) including yellow risk category at constant costs.](image-url)
we feature a German well catchment in collaboration with a German water supply company. While the
current study only provides the concept and discusses its properties, results from the synthetic test cases
(not shown here) and first attempts on the real application case make us confident that our proposed
concept is a highly promising and powerful framework to provide cost-efficient, safe and robust early-
warning mechanisms for risk control in drinking water well catchments.

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